



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:15 AM UTC

PDB ID : 6XOB / pdb_00006xob
EMDB ID : EMD-22277
Title : CryoEM structure of Eastern Equine Encephalitis (EEEV) VLP with Fab EEEV-143.
Authors : Binshtein, E.; Crowe, J.E.
Deposited on : 2020-07-06
Resolution : 8.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

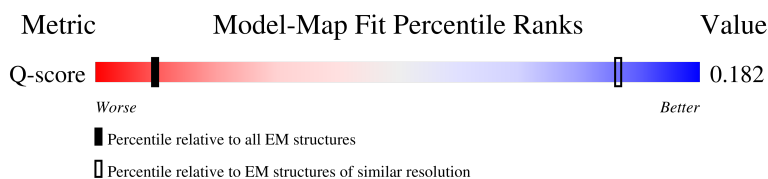
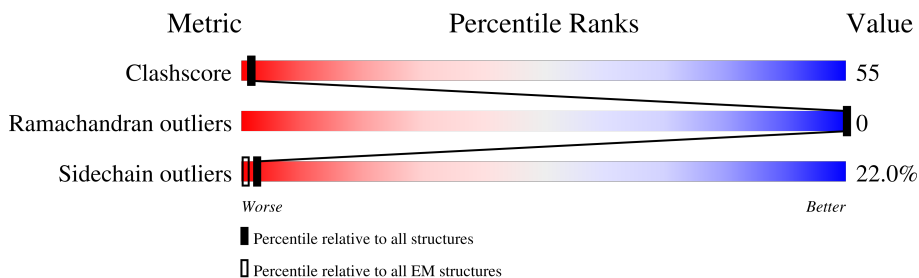
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.50 Å.

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



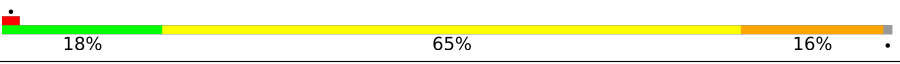
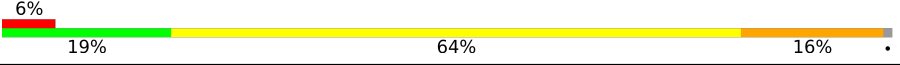
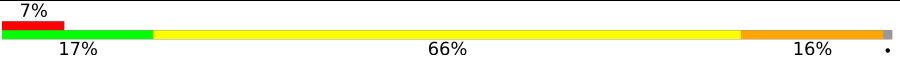
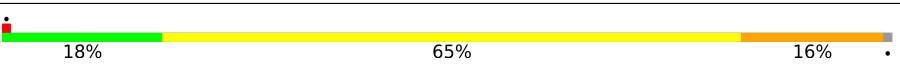
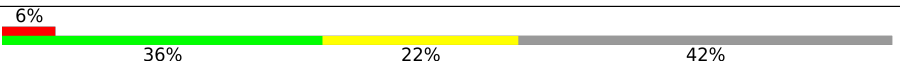
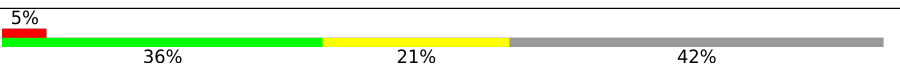
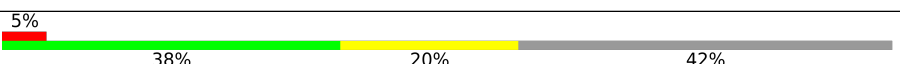
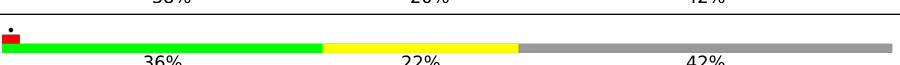
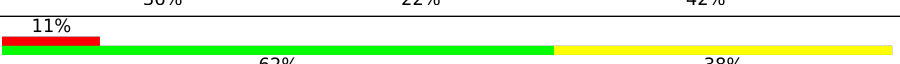
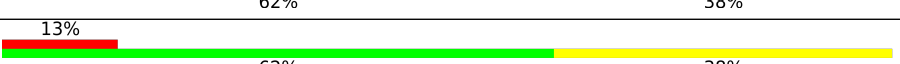
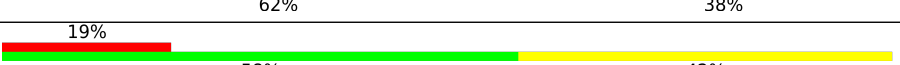
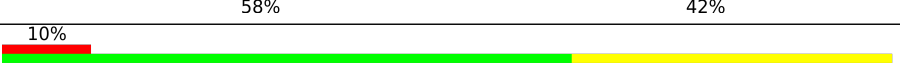
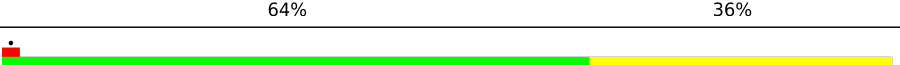
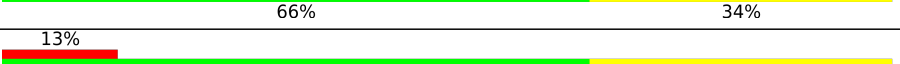
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	328 (8.00 - 9.00)

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

Mol	Chain	Length	Quality of chain
1	A	441	
1	D	441	
1	G	441	
1	J	441	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	420	
2	E	420	
2	H	420	
2	K	420	
3	C	261	
3	F	261	
3	I	261	
3	L	261	
4	M	214	
4	O	214	
4	Q	214	
4	S	214	
5	N	213	
5	P	213	
5	R	213	
5	T	213	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 37540 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 Togavirin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	433	Total	C	N	O	S	0	0
			3306	2111	549	626	20		
1	D	433	Total	C	N	O	S	0	0
			3306	2111	549	626	20		
1	G	433	Total	C	N	O	S	0	0
			3306	2111	549	626	20		
1	J	433	Total	C	N	O	S	0	0
			3306	2111	549	626	20		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	TYR	TRP	conflict	UNP Q88678
D	89	TYR	TRP	conflict	UNP Q88678
G	89	TYR	TRP	conflict	UNP Q88678
J	89	TYR	TRP	conflict	UNP Q88678

- Molecule 2 is a protein called Togavirin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	414	Total	C	N	O	S	0	0
			3238	2049	585	580	24		
2	E	414	Total	C	N	O	S	0	0
			3238	2049	585	580	24		
2	H	414	Total	C	N	O	S	0	0
			3238	2049	585	580	24		
2	K	414	Total	C	N	O	S	0	0
			3238	2049	585	580	24		

- Molecule 3 is a protein called Togavirin.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	151	Total	C	N	O	0	0
			736	434	151	151		
3	F	151	Total	C	N	O	0	0
			736	434	151	151		
3	I	151	Total	C	N	O	0	0
			736	434	151	151		
3	L	151	Total	C	N	O	0	0
			736	434	151	151		

- Molecule 4 is a protein called EEEV-143 Fab heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	M	214	Total	C	N	O	0	0
			1051	623	214	214		
4	O	214	Total	C	N	O	0	0
			1051	623	214	214		
4	Q	214	Total	C	N	O	0	0
			1051	623	214	214		
4	S	214	Total	C	N	O	0	0
			1051	623	214	214		

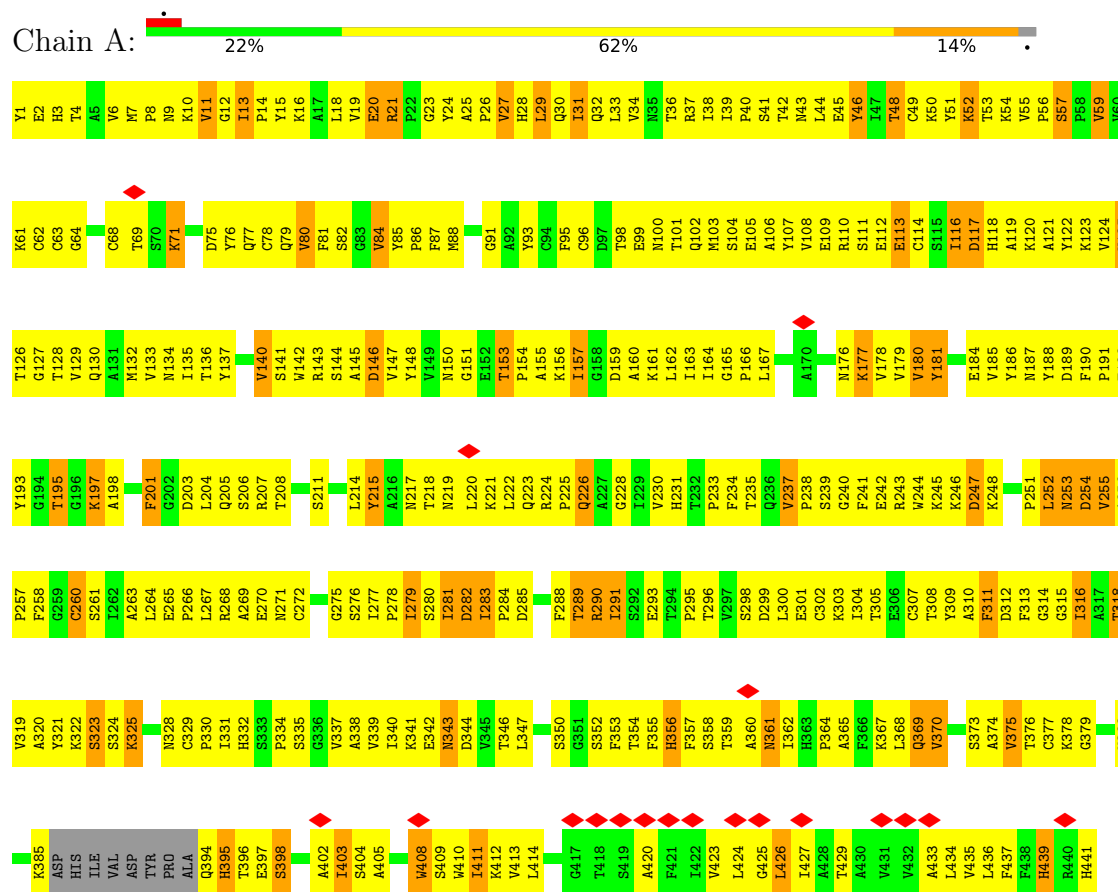
- Molecule 5 is a protein called EEEV-143 Fab light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	N	213	Total	C	N	O	0	0
			1054	628	213	213		
5	P	213	Total	C	N	O	0	0
			1054	628	213	213		
5	R	213	Total	C	N	O	0	0
			1054	628	213	213		
5	T	213	Total	C	N	O	0	0
			1054	628	213	213		

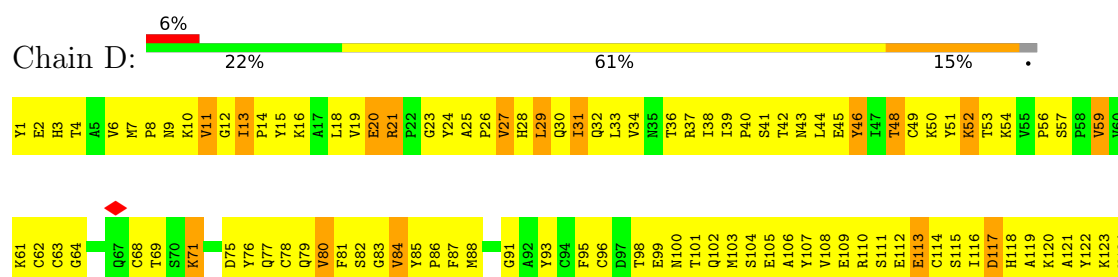
3 Residue-property plots

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

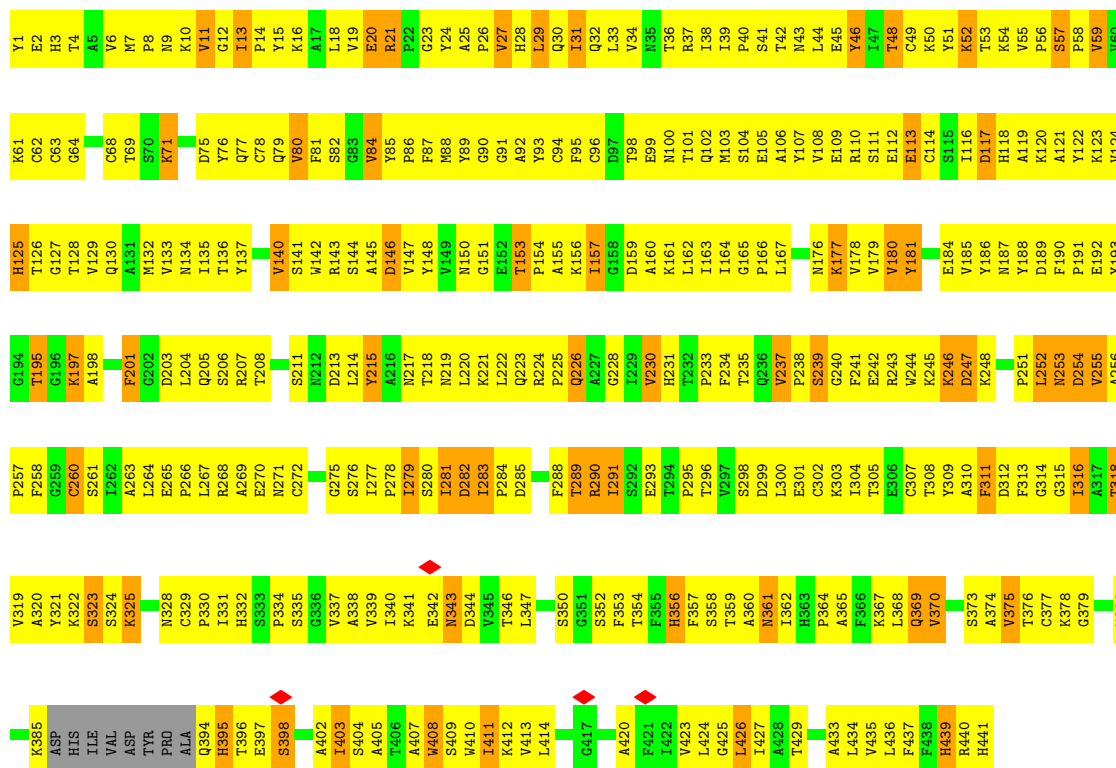
• Molecule 1: Togavirin



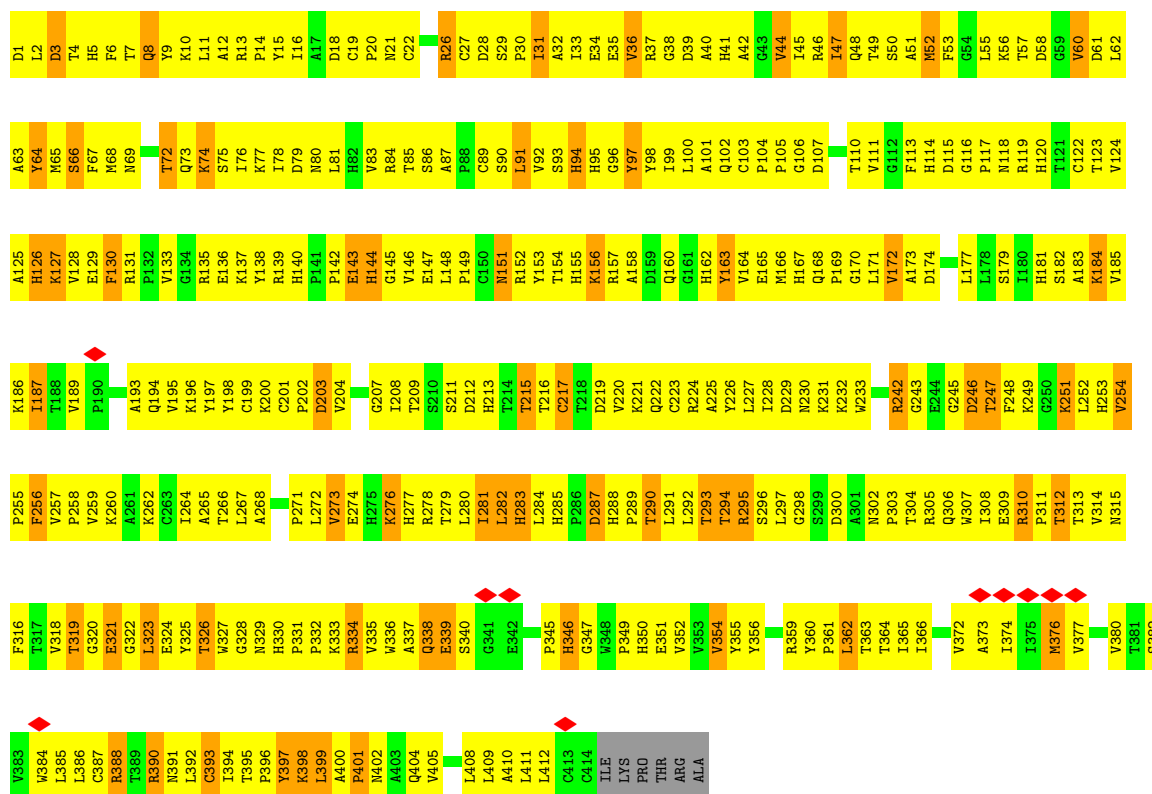
• Molecule 1: Togavirin



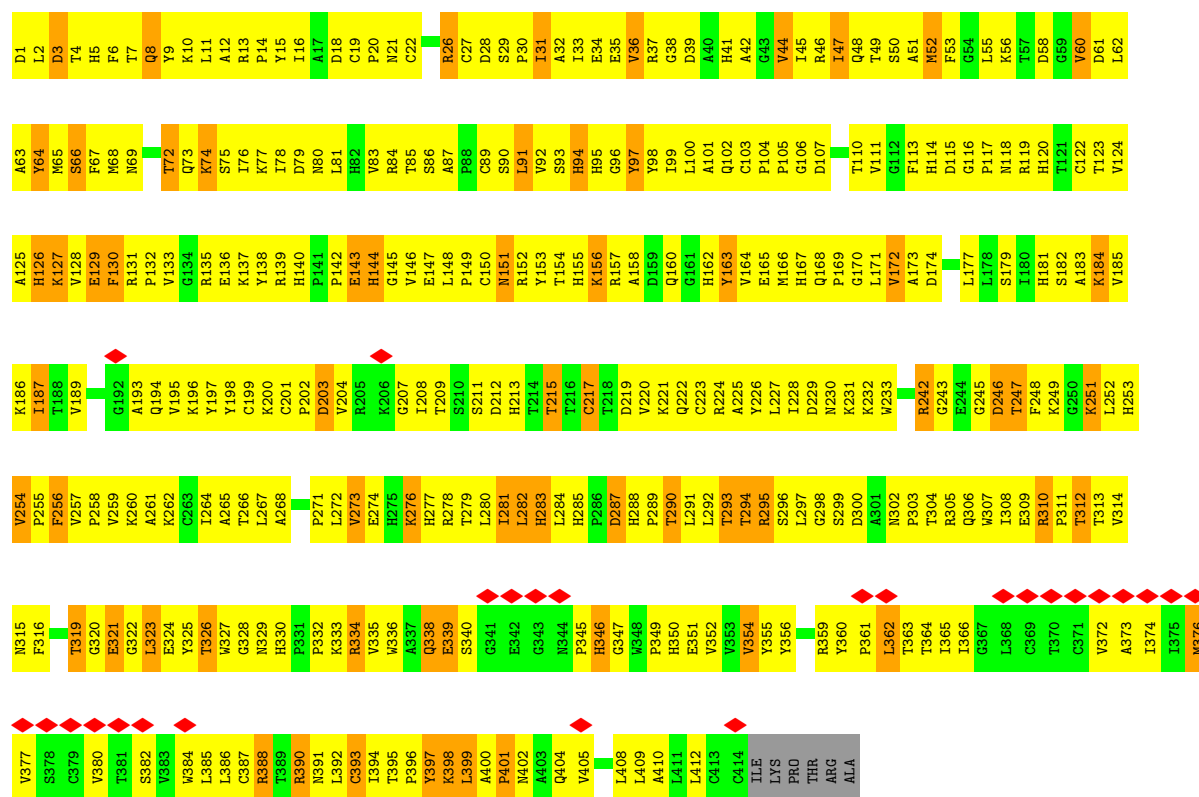




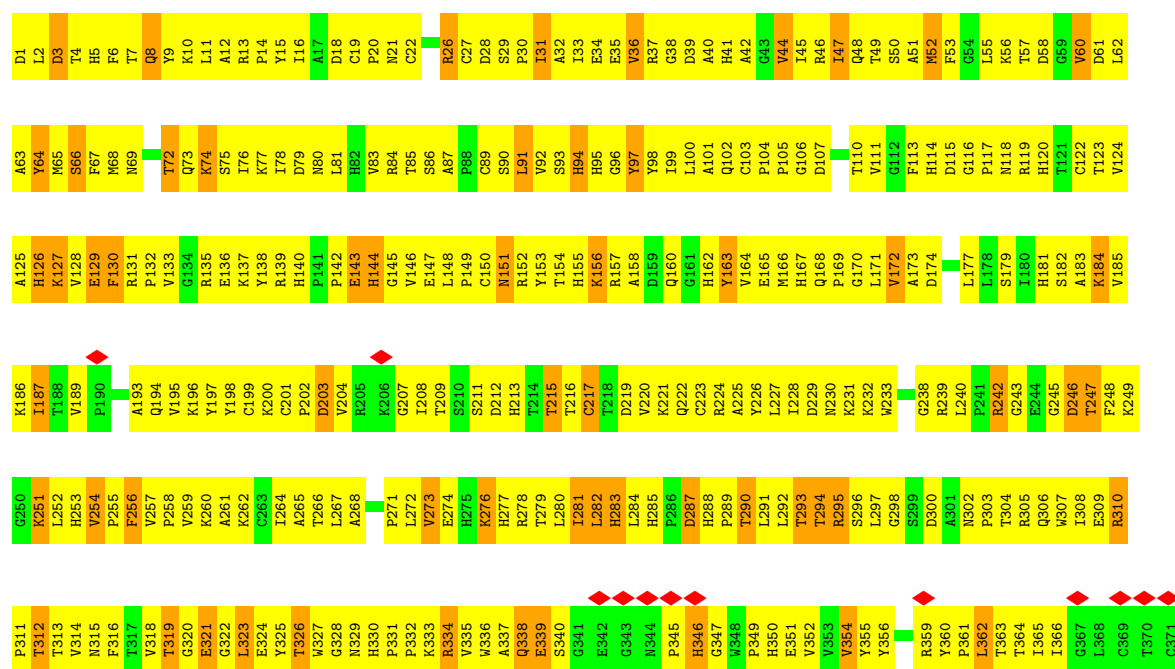
• Molecule 2: Togavirin

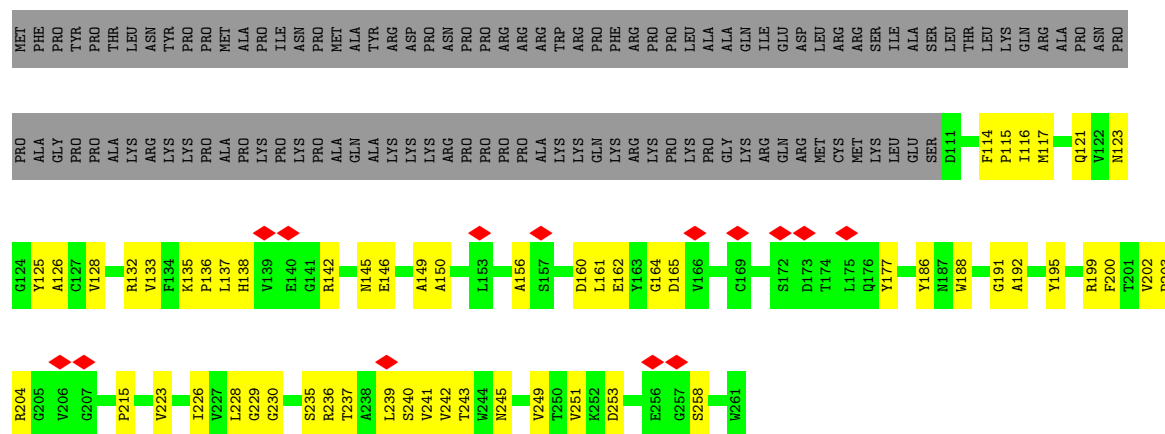


• Molecule 2: Togavirin

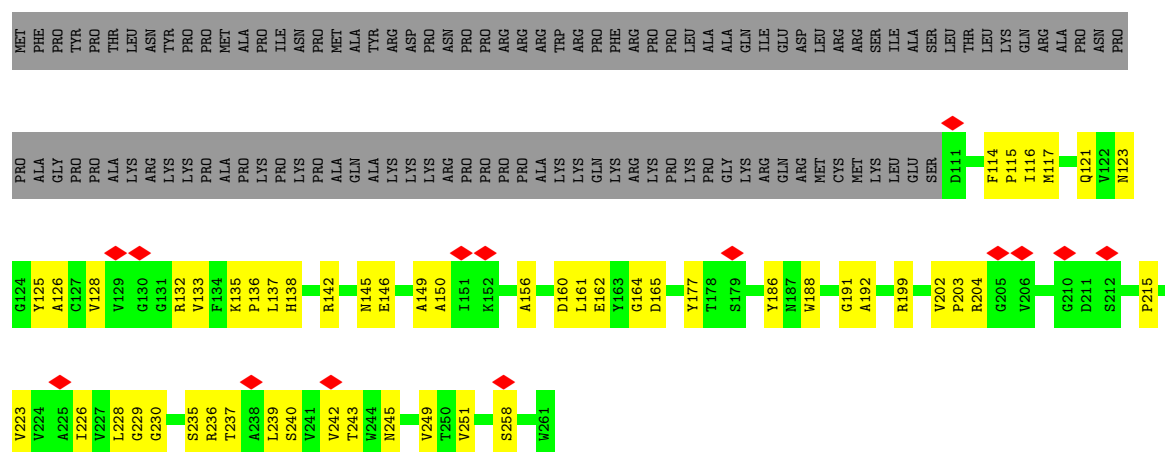


• Molecule 2: Togavirin

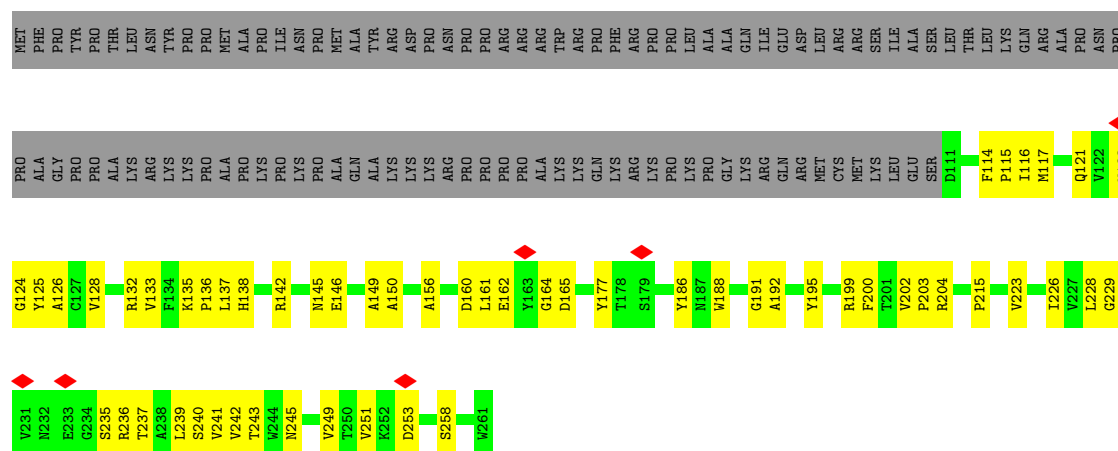




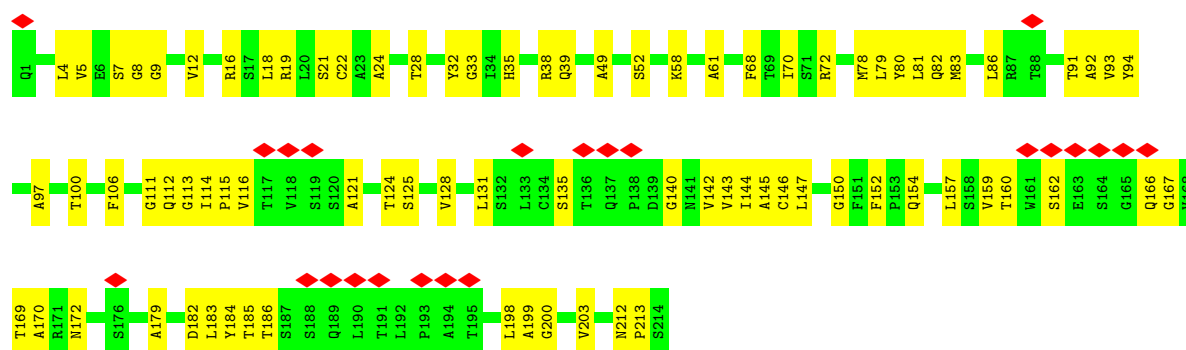
• Molecule 3: Togavirin



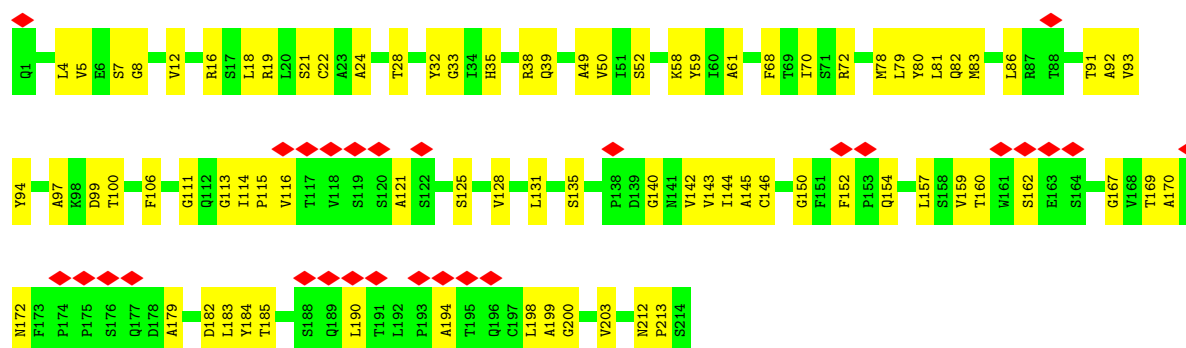
• Molecule 3: Togavirin



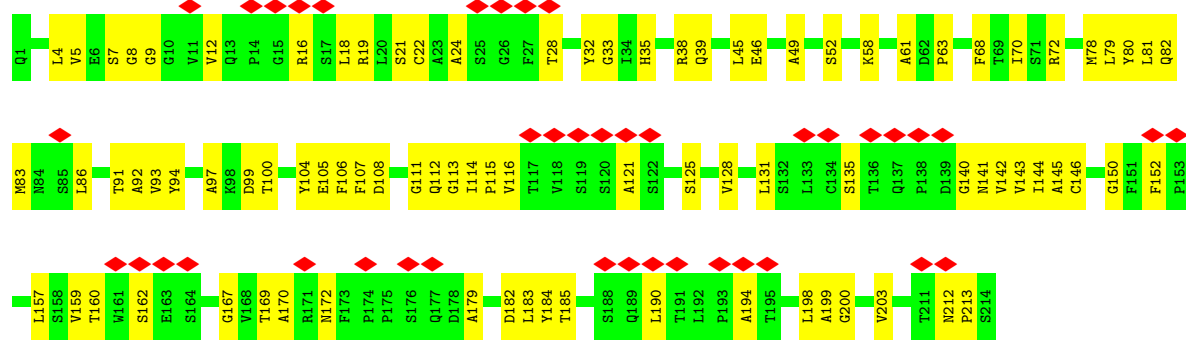
• Molecule 4: EEEV-143 Fab heavy chain



• Molecule 4: EEEV-143 Fab heavy chain

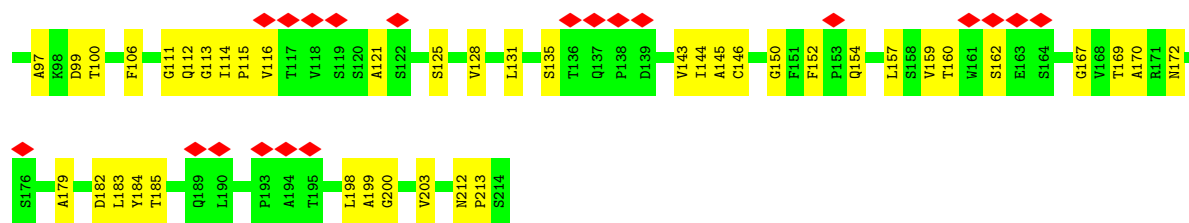


• Molecule 4: EEEV-143 Fab heavy chain

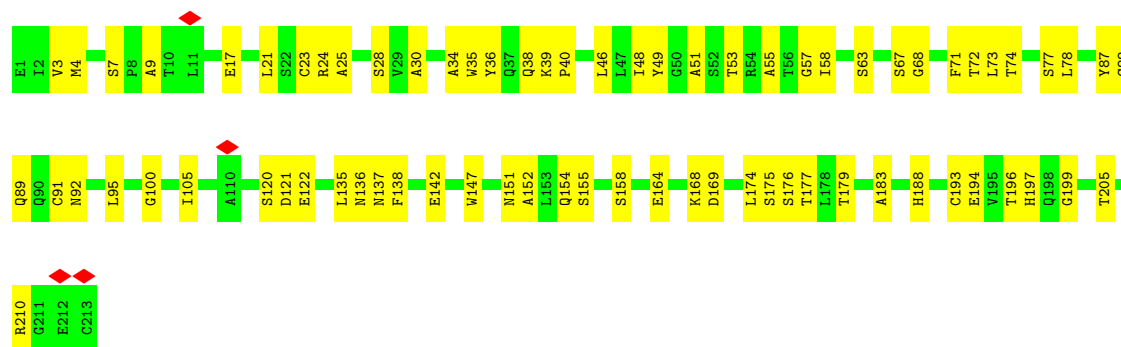


• Molecule 4: EEEV-143 Fab heavy chain

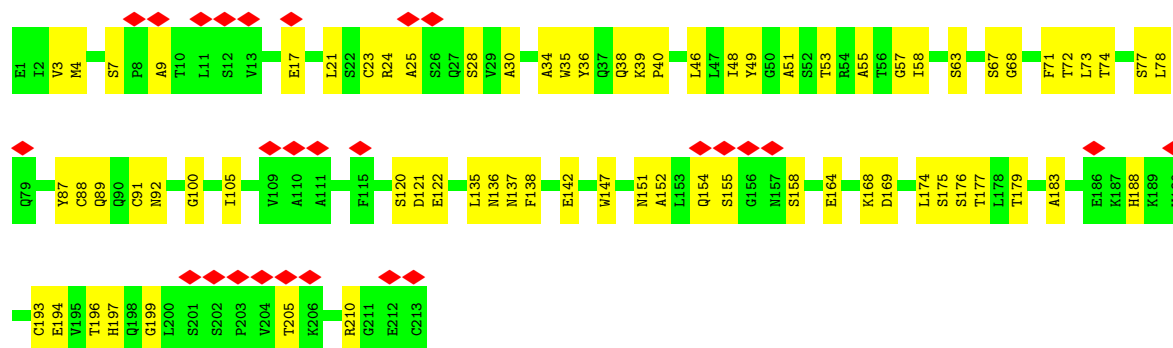




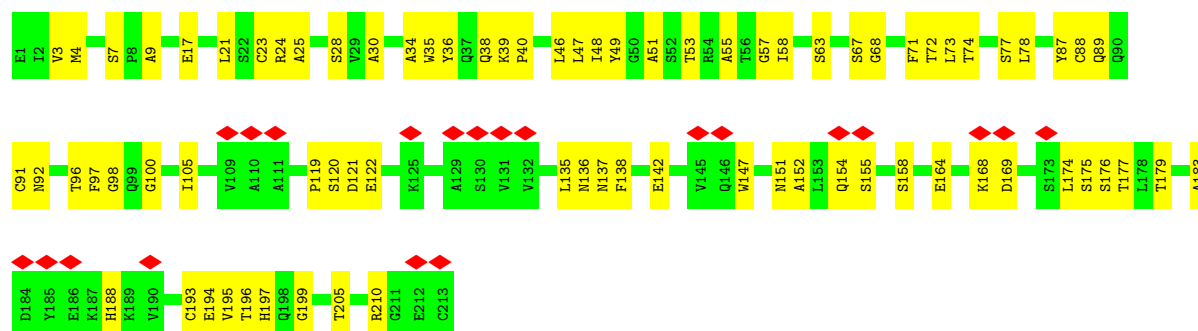
• Molecule 5: EEEV-143 Fab light chain



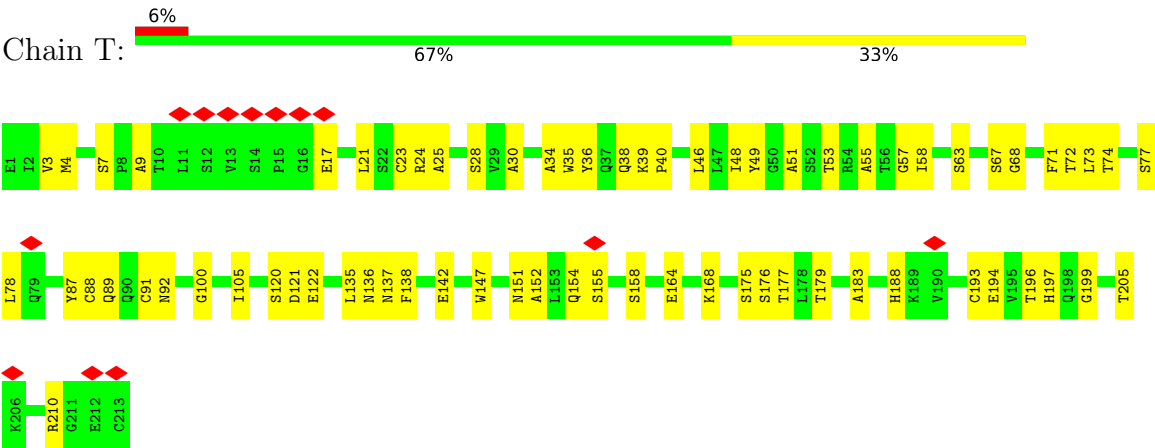
• Molecule 5: EEEV-143 Fab light chain



• Molecule 5: EEEV-143 Fab light chain



● Molecule 5: EEfV-143 Fab light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1300	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.201	Depositor
Minimum map value	-0.119	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	932.484, 932.484, 932.484	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.2202, 2.2202, 2.2202	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.22	0/3395	0.49	0/4630
1	D	0.22	0/3395	0.49	0/4630
1	G	0.22	0/3395	0.49	0/4630
1	J	0.22	0/3395	0.49	0/4630
2	B	0.21	0/3332	0.48	0/4547
2	E	0.21	0/3332	0.48	0/4547
2	H	0.21	0/3332	0.48	0/4547
2	K	0.21	0/3332	0.48	0/4547
3	C	0.18	0/735	0.48	0/1016
3	F	0.18	0/735	0.48	0/1016
3	I	0.18	0/735	0.48	0/1016
3	L	0.18	0/735	0.48	0/1016
4	M	0.20	0/1050	0.53	0/1457
4	O	0.20	0/1050	0.53	0/1457
4	Q	0.20	0/1050	0.53	0/1457
4	S	0.20	0/1050	0.53	0/1457
5	N	0.20	0/1054	0.52	0/1467
5	P	0.20	0/1054	0.52	0/1467
5	R	0.19	0/1054	0.51	0/1467
5	T	0.20	0/1054	0.52	0/1467
All	All	0.21	0/38264	0.49	0/52468

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3306	0	3226	408	0
1	D	3306	0	3226	409	0
1	G	3306	0	3226	423	0
1	J	3306	0	3226	432	0
2	B	3238	0	3188	397	0
2	E	3238	0	3188	395	0
2	H	3238	0	3188	414	0
2	K	3238	0	3188	424	0
3	C	736	0	332	38	0
3	F	736	0	332	37	0
3	I	736	0	332	35	0
3	L	736	0	332	38	0
4	M	1051	0	474	52	0
4	O	1051	0	474	50	0
4	Q	1051	0	474	64	0
4	S	1051	0	474	47	0
5	N	1054	0	488	44	0
5	P	1054	0	488	43	0
5	R	1054	0	488	58	0
5	T	1054	0	488	41	0
All	All	37540	0	30832	3764	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 55.

All (3764) 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:J:94:CYS:HA	2:K:226:TYR:HE1	1.12	1.06
1:J:94:CYS:HA	2:K:226:TYR:CE1	1.96	0.99
1:A:313:PHE:HA	1:A:358:SER:HB2	1.48	0.95
5:T:39:LYS:HA	5:T:88:CYS:HA	1.50	0.94
1:D:313:PHE:HA	1:D:358:SER:HB2	1.48	0.94
5:P:39:LYS:HA	5:P:88:CYS:HA	1.50	0.93
1:G:313:PHE:HA	1:G:358:SER:HB2	1.48	0.93
5:R:39:LYS:HA	5:R:88:CYS:HA	1.50	0.93
1:J:313:PHE:HA	1:J:358:SER:HB2	1.48	0.92
5:N:39:LYS:HA	5:N:88:CYS:HA	1.50	0.92
4:Q:46:GLU:HA	5:R:98:GLY:HA3	1.51	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:120:SER:HA	5:P:137:ASN:HA	1.53	0.91
1:D:253:ASN:O	2:E:295:ARG:NH2	2.04	0.90
5:R:120:SER:HA	5:R:137:ASN:HA	1.54	0.90
5:T:120:SER:HA	5:T:137:ASN:HA	1.53	0.90
2:H:152:ARG:HH22	2:H:155:HIS:HB3	1.37	0.89
5:R:4:MET:HA	5:R:24:ARG:HA	1.54	0.89
2:E:152:ARG:HH22	2:E:155:HIS:HB3	1.37	0.88
2:B:152:ARG:HH22	2:B:155:HIS:HB3	1.37	0.88
1:J:88:MET:HE1	2:K:172:VAL:HG23	1.53	0.88
5:N:4:MET:HA	5:N:24:ARG:HA	1.54	0.88
2:E:199:CYS:HB3	2:E:217:CYS:HB2	1.56	0.88
2:K:152:ARG:HH22	2:K:155:HIS:HB3	1.37	0.88
5:T:4:MET:HA	5:T:24:ARG:HA	1.54	0.88
5:P:4:MET:HA	5:P:24:ARG:HA	1.54	0.87
2:B:310:ARG:NH2	2:B:311:PRO:O	2.07	0.87
2:E:310:ARG:NH2	2:E:311:PRO:O	2.07	0.87
2:H:310:ARG:NH2	2:H:311:PRO:O	2.07	0.87
2:K:310:ARG:NH2	2:K:311:PRO:O	2.07	0.87
2:K:199:CYS:HB3	2:K:217:CYS:HB2	1.56	0.87
1:G:89:TYR:CZ	2:H:16:ILE:HD11	2.09	0.86
5:N:120:SER:HA	5:N:137:ASN:HA	1.53	0.86
2:B:199:CYS:HB3	2:B:217:CYS:HB2	1.56	0.86
2:H:199:CYS:HB3	2:H:217:CYS:HB2	1.56	0.85
4:Q:106:PHE:HA	5:R:48:ILE:CB	2.06	0.84
2:H:13:ARG:HH22	2:H:68:MET:HG3	1.42	0.84
2:B:166:MET:HE2	2:B:252:LEU:HD21	1.59	0.84
1:G:302:CYS:HA	1:G:319:VAL:HA	1.60	0.84
2:K:166:MET:HE2	2:K:252:LEU:HD21	1.59	0.84
3:L:132:ARG:HA	3:L:165:ASP:H	1.43	0.84
2:B:13:ARG:HH22	2:B:68:MET:HG3	1.42	0.84
3:I:132:ARG:HA	3:I:165:ASP:H	1.43	0.84
2:K:13:ARG:HH22	2:K:68:MET:HG3	1.42	0.84
2:H:166:MET:HE2	2:H:252:LEU:HD21	1.59	0.83
3:C:132:ARG:HA	3:C:165:ASP:H	1.43	0.83
1:A:253:ASN:O	2:B:295:ARG:NH2	2.12	0.83
1:A:302:CYS:HA	1:A:319:VAL:HA	1.60	0.83
2:B:168:GLN:HA	2:B:233:TRP:HD1	1.44	0.82
1:D:302:CYS:HA	1:D:319:VAL:HA	1.60	0.82
2:E:166:MET:HE2	2:E:252:LEU:HD21	1.59	0.82
3:F:132:ARG:HA	3:F:165:ASP:H	1.43	0.82
2:K:168:GLN:HA	2:K:233:TRP:HD1	1.44	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:302:CYS:HA	1:J:319:VAL:HA	1.60	0.82
1:D:322:LYS:HA	1:D:350:SER:HA	1.62	0.81
2:E:168:GLN:HA	2:E:233:TRP:HD1	1.44	0.81
2:E:13:ARG:HH22	2:E:68:MET:HG3	1.42	0.81
2:H:168:GLN:HA	2:H:233:TRP:HD1	1.44	0.81
1:J:322:LYS:HA	1:J:350:SER:HA	1.62	0.81
1:G:322:LYS:HA	1:G:350:SER:HA	1.62	0.81
3:L:137:LEU:H	3:L:161:LEU:HA	1.46	0.81
2:B:285:HIS:HA	2:B:311:PRO:HA	1.63	0.81
2:H:285:HIS:HA	2:H:311:PRO:HA	1.63	0.81
2:K:285:HIS:HA	2:K:311:PRO:HA	1.63	0.81
1:A:322:LYS:HA	1:A:350:SER:HA	1.62	0.81
2:E:184:LYS:NZ	2:E:185:VAL:O	2.15	0.80
4:O:167:GLY:HA2	4:O:185:THR:HA	1.63	0.80
1:A:120:LYS:HB3	1:A:122:TYR:HE2	1.46	0.80
1:G:120:LYS:HB3	1:G:122:TYR:HE2	1.46	0.80
4:S:167:GLY:HA2	4:S:185:THR:HA	1.63	0.80
2:B:184:LYS:NZ	2:B:185:VAL:O	2.15	0.80
1:J:59:VAL:HA	2:K:242:ARG:HB2	1.63	0.80
1:J:120:LYS:HB3	1:J:122:TYR:HE2	1.46	0.80
4:Q:167:GLY:HA2	4:Q:185:THR:HA	1.63	0.80
3:C:137:LEU:H	3:C:161:LEU:HA	1.46	0.80
2:K:184:LYS:NZ	2:K:185:VAL:O	2.15	0.80
2:K:145:GLY:HA3	2:K:266:THR:HA	1.63	0.80
1:J:405:ALA:HB1	2:K:346:HIS:CE1	2.16	0.79
2:B:145:GLY:HA3	2:B:266:THR:HA	1.63	0.79
2:B:8:GLN:HA	2:B:252:LEU:HD13	1.65	0.79
2:E:145:GLY:HA3	2:E:266:THR:HA	1.63	0.79
2:H:184:LYS:NZ	2:H:185:VAL:O	2.15	0.79
2:K:8:GLN:HA	2:K:252:LEU:HD13	1.64	0.79
1:G:15:TYR:HB3	1:G:31:ILE:HG22	1.65	0.79
4:M:167:GLY:HA2	4:M:185:THR:HA	1.63	0.79
3:F:137:LEU:H	3:F:161:LEU:HA	1.46	0.79
2:H:145:GLY:HA3	2:H:266:THR:HA	1.63	0.79
1:J:187:ASN:H	1:J:252:LEU:HD21	1.47	0.79
1:J:256:ALA:O	2:K:295:ARG:NE	2.15	0.79
1:G:82:SER:HA	1:G:100:ASN:HA	1.65	0.79
1:D:15:TYR:HB3	1:D:31:ILE:HG22	1.65	0.79
1:D:187:ASN:H	1:D:252:LEU:HD21	1.47	0.79
2:E:285:HIS:HA	2:E:311:PRO:HA	1.63	0.79
1:A:187:ASN:H	1:A:252:LEU:HD21	1.47	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:THR:HA	1:A:354:THR:HA	1.65	0.78
1:J:15:TYR:HB3	1:J:31:ILE:HG22	1.65	0.78
4:S:125:SER:HA	4:S:146:CYS:HA	1.65	0.78
1:J:88:MET:SD	2:K:173:ALA:N	2.55	0.78
4:O:125:SER:HA	4:O:146:CYS:HA	1.65	0.78
2:E:219:ASP:HB2	2:E:221:LYS:HE2	1.66	0.78
1:G:254:ASP:N	1:G:254:ASP:OD1	2.17	0.78
2:B:219:ASP:HB2	2:B:221:LYS:HE2	1.66	0.78
1:G:187:ASN:H	1:G:252:LEU:HD21	1.47	0.78
3:I:137:LEU:H	3:I:161:LEU:HA	1.46	0.78
1:J:82:SER:HA	1:J:100:ASN:HA	1.65	0.78
1:A:82:SER:HA	1:A:100:ASN:HA	1.65	0.78
1:D:318:THR:HA	1:D:354:THR:HA	1.65	0.78
2:E:8:GLN:HA	2:E:252:LEU:HD13	1.64	0.78
4:M:121:ALA:HB3	4:M:150:GLY:H	1.47	0.78
4:Q:121:ALA:HB3	4:Q:150:GLY:H	1.47	0.78
1:A:254:ASP:N	1:A:254:ASP:OD1	2.17	0.78
2:K:219:ASP:HB2	2:K:221:LYS:HE2	1.66	0.78
5:T:152:ALA:HA	5:T:158:SER:H	1.49	0.78
1:J:407:ALA:HB2	2:K:346:HIS:HB3	1.65	0.78
1:J:254:ASP:N	1:J:254:ASP:OD1	2.17	0.77
1:D:120:LYS:HB3	1:D:122:TYR:HE2	1.46	0.77
1:D:30:GLN:HE22	1:D:32:GLN:HB2	1.50	0.77
1:D:82:SER:HA	1:D:100:ASN:HA	1.65	0.77
2:H:8:GLN:HA	2:H:252:LEU:HD13	1.64	0.77
4:O:121:ALA:HB3	4:O:150:GLY:H	1.47	0.77
1:A:367:LYS:HZ1	1:A:374:ALA:HB1	1.50	0.77
1:A:30:GLN:HE22	1:A:32:GLN:HB2	1.50	0.77
4:M:125:SER:HA	4:M:146:CYS:HA	1.65	0.77
2:H:219:ASP:HB2	2:H:221:LYS:HE2	1.66	0.77
1:J:30:GLN:HE22	1:J:32:GLN:HB2	1.50	0.77
4:Q:125:SER:HA	4:Q:146:CYS:HA	1.65	0.77
2:K:310:ARG:HH21	2:K:312:THR:HG23	1.51	0.77
1:D:52:LYS:HD3	1:D:111:SER:HA	1.67	0.76
3:L:202:VAL:O	3:L:237:THR:N	2.18	0.76
1:J:52:LYS:HD3	1:J:111:SER:HA	1.67	0.76
1:A:15:TYR:HB3	1:A:31:ILE:HG22	1.65	0.76
1:G:369:GLN:HA	1:G:374:ALA:HA	1.68	0.76
2:K:169:PRO:HG2	2:K:230:ASN:HA	1.68	0.76
5:R:152:ALA:HA	5:R:158:SER:H	1.49	0.76
2:E:169:PRO:HG2	2:E:230:ASN:HA	1.68	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:30:GLN:HE22	1:G:32:GLN:HB2	1.50	0.76
1:J:318:THR:HA	1:J:354:THR:HA	1.65	0.76
1:A:52:LYS:HD3	1:A:111:SER:HA	1.67	0.76
2:B:169:PRO:HG2	2:B:230:ASN:HA	1.68	0.76
1:G:318:THR:HA	1:G:354:THR:HA	1.65	0.76
1:J:426:LEU:HG	2:K:386:LEU:HG	1.65	0.76
1:D:369:GLN:HA	1:D:374:ALA:HA	1.68	0.76
5:N:152:ALA:HA	5:N:158:SER:H	1.49	0.76
2:B:310:ARG:HH21	2:B:312:THR:HG23	1.50	0.76
2:E:283:HIS:HA	2:E:313:THR:HA	1.68	0.76
5:P:152:ALA:HA	5:P:158:SER:H	1.49	0.76
4:S:70:ILE:HA	4:S:81:LEU:HA	1.67	0.76
4:S:121:ALA:HB3	4:S:150:GLY:H	1.47	0.76
2:H:8:GLN:NE2	2:H:253:HIS:O	2.19	0.76
2:H:283:HIS:HA	2:H:313:THR:HA	1.68	0.76
3:C:202:VAL:O	3:C:237:THR:N	2.18	0.76
1:G:52:LYS:HD3	1:G:111:SER:HA	1.67	0.76
2:E:8:GLN:NE2	2:E:253:HIS:O	2.19	0.75
4:O:145:ALA:HA	4:O:182:ASP:HA	1.69	0.75
1:A:238:PRO:HB2	1:A:243:ARG:HE	1.51	0.75
4:M:70:ILE:HA	4:M:81:LEU:HA	1.67	0.75
4:M:145:ALA:HA	4:M:182:ASP:HA	1.69	0.75
1:A:161:LYS:HB3	1:A:282:ASP:HB3	1.69	0.75
2:B:8:GLN:NE2	2:B:253:HIS:O	2.19	0.75
1:D:161:LYS:HB3	1:D:282:ASP:HB3	1.69	0.75
2:H:146:VAL:N	2:H:265:ALA:O	2.18	0.75
4:Q:107:PHE:CB	5:R:47:LEU:HA	2.16	0.75
2:E:310:ARG:HH21	2:E:312:THR:HG23	1.50	0.75
2:K:8:GLN:NE2	2:K:253:HIS:O	2.19	0.75
2:K:146:VAL:N	2:K:265:ALA:O	2.18	0.75
4:Q:70:ILE:HA	4:Q:81:LEU:HA	1.67	0.75
1:G:361:ASN:HA	1:G:403:ILE:HA	1.69	0.75
1:J:238:PRO:HB2	1:J:243:ARG:HE	1.51	0.75
2:K:283:HIS:HA	2:K:313:THR:HA	1.68	0.75
2:B:283:HIS:HA	2:B:313:THR:HA	1.68	0.75
1:J:161:LYS:HB3	1:J:282:ASP:HB3	1.69	0.75
2:E:146:VAL:N	2:E:265:ALA:O	2.18	0.74
1:G:161:LYS:HB3	1:G:282:ASP:HB3	1.69	0.74
1:D:254:ASP:N	1:D:254:ASP:OD1	2.17	0.74
1:D:311:PHE:O	1:D:395:HIS:NE2	2.20	0.74
3:I:202:VAL:O	3:I:237:THR:N	2.18	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:PHE:O	1:A:395:HIS:NE2	2.20	0.74
3:F:202:VAL:O	3:F:237:THR:N	2.18	0.74
1:G:238:PRO:HB2	1:G:243:ARG:HE	1.51	0.74
1:A:313:PHE:O	1:A:356:HIS:ND1	2.21	0.74
2:B:146:VAL:N	2:B:265:ALA:O	2.18	0.74
2:H:169:PRO:HG2	2:H:230:ASN:HA	1.68	0.74
1:J:361:ASN:HA	1:J:403:ILE:HA	1.69	0.74
1:J:369:GLN:HA	1:J:374:ALA:HA	1.68	0.74
4:O:70:ILE:HA	4:O:81:LEU:HA	1.67	0.74
1:G:37:ARG:HH12	1:G:132:MET:HB2	1.52	0.74
1:J:311:PHE:O	1:J:395:HIS:NE2	2.21	0.74
2:H:310:ARG:HH21	2:H:312:THR:HG23	1.51	0.74
1:J:313:PHE:O	1:J:356:HIS:ND1	2.21	0.74
1:G:311:PHE:O	1:G:395:HIS:NE2	2.20	0.74
5:R:49:TYR:O	5:R:57:GLY:N	2.21	0.74
1:A:369:GLN:HA	1:A:374:ALA:HA	1.68	0.74
1:J:37:ARG:HH12	1:J:132:MET:HB2	1.52	0.73
2:K:13:ARG:HB3	2:K:232:LYS:HB2	1.70	0.73
1:A:154:PRO:HG3	1:D:195:THR:HB	1.69	0.73
1:G:341:LYS:NZ	1:G:342:GLU:OE2	2.20	0.73
2:B:95:HIS:HB2	2:B:157:ARG:HE	1.53	0.73
2:E:394:ILE:O	2:E:398:LYS:NZ	2.21	0.73
1:G:155:ALA:O	1:G:162:LEU:N	2.22	0.73
1:G:313:PHE:O	1:G:356:HIS:ND1	2.21	0.73
1:A:54:LYS:HG3	1:A:107:TYR:HB3	1.70	0.73
1:D:361:ASN:HA	1:D:403:ILE:HA	1.69	0.73
4:Q:145:ALA:HA	4:Q:182:ASP:HA	1.68	0.73
5:T:183:ALA:HB3	5:T:188:HIS:H	1.54	0.73
2:B:42:ALA:O	2:B:102:GLN:NE2	2.21	0.73
1:D:155:ALA:O	1:D:162:LEU:N	2.22	0.73
1:D:238:PRO:HB2	1:D:243:ARG:HE	1.51	0.73
2:H:42:ALA:O	2:H:102:GLN:NE2	2.21	0.73
2:K:173:ALA:HA	2:K:226:TYR:HA	1.71	0.73
5:P:183:ALA:HB3	5:P:188:HIS:H	1.54	0.73
5:R:183:ALA:HB3	5:R:188:HIS:H	1.54	0.73
5:P:49:TYR:O	5:P:57:GLY:N	2.21	0.73
1:A:25:ALA:HB3	1:A:289:THR:HG23	1.71	0.73
2:H:13:ARG:HB3	2:H:232:LYS:HB2	1.70	0.73
1:J:54:LYS:HG3	1:J:107:TYR:HB3	1.70	0.73
4:S:145:ALA:HA	4:S:182:ASP:HA	1.69	0.73
1:A:155:ALA:O	1:A:162:LEU:N	2.22	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:341:LYS:NZ	1:J:342:GLU:OE2	2.20	0.73
1:J:394:GLN:HB2	2:K:336:TRP:CE2	2.23	0.73
2:K:42:ALA:O	2:K:102:GLN:NE2	2.21	0.73
1:A:361:ASN:HA	1:A:403:ILE:HA	1.69	0.72
2:H:394:ILE:O	2:H:398:LYS:NZ	2.21	0.72
1:J:155:ALA:O	1:J:162:LEU:N	2.22	0.72
2:E:13:ARG:HB3	2:E:232:LYS:HB2	1.70	0.72
2:E:173:ALA:HA	2:E:226:TYR:HA	1.71	0.72
2:E:292:LEU:HB2	2:E:327:TRP:HB2	1.71	0.72
5:N:49:TYR:O	5:N:57:GLY:N	2.21	0.72
1:D:192:GLU:O	1:D:205:GLN:NE2	2.22	0.72
1:D:364:PRO:HG2	1:D:379:GLY:HA3	1.72	0.72
1:J:192:GLU:O	1:J:205:GLN:NE2	2.22	0.72
2:K:392:LEU:O	2:K:395:THR:OG1	2.08	0.72
4:Q:169:THR:HA	4:Q:183:LEU:HA	1.72	0.72
1:A:364:PRO:HG2	1:A:379:GLY:HA3	1.72	0.72
1:G:364:PRO:HG2	1:G:379:GLY:HA3	1.72	0.72
2:H:173:ALA:HA	2:H:226:TYR:HA	1.71	0.72
1:A:192:GLU:O	1:A:205:GLN:NE2	2.22	0.72
2:B:292:LEU:HB2	2:B:327:TRP:HB2	1.71	0.72
2:B:13:ARG:HB3	2:B:232:LYS:HB2	1.70	0.72
2:K:95:HIS:HB2	2:K:157:ARG:HE	1.53	0.72
5:T:49:TYR:O	5:T:57:GLY:N	2.21	0.72
1:A:113:GLU:O	1:A:117:ASP:N	2.17	0.72
2:B:394:ILE:O	2:B:398:LYS:NZ	2.21	0.72
1:D:37:ARG:HH12	1:D:132:MET:HB2	1.52	0.72
1:D:54:LYS:HG3	1:D:107:TYR:HB3	1.70	0.72
1:D:319:VAL:HG22	1:D:353:PHE:H	1.54	0.72
2:E:196:LYS:HB3	2:E:226:TYR:HB2	1.72	0.72
1:A:226:GLN:H	1:A:231:HIS:HE1	1.38	0.72
2:E:95:HIS:HB2	2:E:157:ARG:HE	1.53	0.72
2:K:196:LYS:HB3	2:K:226:TYR:HB2	1.72	0.72
1:D:341:LYS:NZ	1:D:342:GLU:OE2	2.20	0.71
4:M:49:ALA:HA	4:M:61:ALA:H	1.55	0.71
1:J:25:ALA:HB3	1:J:289:THR:HG23	1.71	0.71
2:K:292:LEU:HB2	2:K:327:TRP:HB2	1.71	0.71
1:A:37:ARG:HH12	1:A:132:MET:HB2	1.52	0.71
1:A:341:LYS:NZ	1:A:342:GLU:OE2	2.20	0.71
2:E:42:ALA:O	2:E:102:GLN:NE2	2.21	0.71
2:H:196:LYS:HB3	2:H:226:TYR:HB2	1.72	0.71
5:N:183:ALA:HB3	5:N:188:HIS:H	1.54	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:25:ALA:HB3	1:G:289:THR:HG23	1.71	0.71
1:G:54:LYS:HG3	1:G:107:TYR:HB3	1.70	0.71
1:G:192:GLU:O	1:G:205:GLN:NE2	2.22	0.71
2:H:107:ASP:O	2:H:126:HIS:N	2.19	0.71
1:J:82:SER:O	1:J:224:ARG:NH2	2.24	0.71
5:T:17:GLU:HA	5:T:78:LEU:HA	1.73	0.71
1:D:25:ALA:HB3	1:D:289:THR:HG23	1.71	0.71
1:D:436:LEU:O	1:D:439:HIS:ND1	2.22	0.71
1:G:226:GLN:H	1:G:231:HIS:HE1	1.38	0.71
2:K:46:ARG:HH12	2:K:254:VAL:HG23	1.56	0.71
4:O:72:ARG:HA	4:O:79:LEU:HA	1.73	0.71
1:G:82:SER:O	1:G:224:ARG:NH2	2.24	0.71
2:H:95:HIS:HB2	2:H:157:ARG:HE	1.53	0.71
4:O:49:ALA:HA	4:O:61:ALA:H	1.55	0.71
5:R:23:CYS:HA	5:R:72:THR:HA	1.73	0.71
1:D:82:SER:O	1:D:224:ARG:NH2	2.24	0.70
5:P:23:CYS:HA	5:P:72:THR:HA	1.73	0.70
4:Q:49:ALA:HA	4:Q:61:ALA:H	1.55	0.70
2:B:196:LYS:HB3	2:B:226:TYR:HB2	1.72	0.70
2:B:392:LEU:O	2:B:395:THR:OG1	2.08	0.70
1:D:313:PHE:O	1:D:356:HIS:ND1	2.21	0.70
2:E:392:LEU:O	2:E:395:THR:OG1	2.08	0.70
2:H:268:ALA:HB2	2:H:328:GLY:HA3	1.74	0.70
2:H:292:LEU:HB2	2:H:327:TRP:HB2	1.71	0.70
4:O:199:ALA:N	4:O:212:ASN:O	2.24	0.70
2:B:135:ARG:NH2	2:B:326:THR:O	2.25	0.70
3:F:128:VAL:HA	3:F:133:VAL:HA	1.73	0.70
1:J:364:PRO:HG2	1:J:379:GLY:HA3	1.72	0.70
2:K:13:ARG:NH1	2:K:14:PRO:O	2.25	0.70
2:K:290:THR:HG1	2:K:327:TRP:CD1	2.08	0.70
5:N:17:GLU:HA	5:N:78:LEU:HA	1.73	0.70
2:B:297:LEU:HD11	2:B:334:ARG:HB3	1.73	0.70
3:F:146:GLU:HA	3:F:149:ALA:HB3	1.74	0.70
1:A:82:SER:O	1:A:224:ARG:NH2	2.24	0.70
1:A:319:VAL:HG22	1:A:353:PHE:H	1.54	0.70
2:B:173:ALA:HA	2:B:226:TYR:HA	1.71	0.70
2:E:46:ARG:HH12	2:E:254:VAL:HG23	1.56	0.70
1:J:319:VAL:HG22	1:J:353:PHE:H	1.54	0.70
2:K:268:ALA:HB2	2:K:328:GLY:HA3	1.74	0.70
4:M:169:THR:HA	4:M:183:LEU:HA	1.72	0.70
4:O:169:THR:HA	4:O:183:LEU:HA	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:169:THR:HA	4:S:183:LEU:HA	1.72	0.70
2:H:392:LEU:O	2:H:395:THR:OG1	2.08	0.70
4:S:49:ALA:HA	4:S:61:ALA:H	1.55	0.70
2:B:46:ARG:HH12	2:B:254:VAL:HG23	1.56	0.70
1:G:253:ASN:O	2:H:295:ARG:NH2	2.24	0.70
1:G:253:ASN:OD1	1:G:253:ASN:N	2.25	0.70
5:T:23:CYS:HA	5:T:72:THR:HA	1.74	0.70
3:C:128:VAL:HA	3:C:133:VAL:HA	1.73	0.70
2:E:13:ARG:NH1	2:E:14:PRO:O	2.25	0.70
3:I:128:VAL:HA	3:I:133:VAL:HA	1.73	0.70
1:J:253:ASN:OD1	1:J:253:ASN:N	2.25	0.70
4:M:199:ALA:N	4:M:212:ASN:O	2.24	0.70
1:D:340:ILE:HG22	1:D:342:GLU:H	1.56	0.69
1:G:340:ILE:HG22	1:G:342:GLU:H	1.56	0.69
2:H:13:ARG:NH1	2:H:14:PRO:O	2.25	0.69
4:S:199:ALA:N	4:S:212:ASN:O	2.24	0.69
1:A:340:ILE:HG22	1:A:342:GLU:H	1.56	0.69
2:E:135:ARG:NH2	2:E:326:THR:O	2.25	0.69
1:G:244:TRP:O	1:G:247:ASP:N	2.25	0.69
1:G:319:VAL:HG22	1:G:353:PHE:H	1.54	0.69
1:G:367:LYS:HZ1	1:G:374:ALA:HB1	1.57	0.69
2:H:46:ARG:HH12	2:H:254:VAL:HG23	1.56	0.69
1:J:437:PHE:CZ	2:K:396:PRO:HG3	2.26	0.69
2:K:135:ARG:NH2	2:K:326:THR:O	2.25	0.69
2:K:297:LEU:HD11	2:K:334:ARG:HB3	1.73	0.69
3:L:146:GLU:HA	3:L:149:ALA:HB3	1.74	0.69
4:Q:199:ALA:N	4:Q:212:ASN:O	2.25	0.69
1:A:244:TRP:O	1:A:247:ASP:N	2.25	0.69
2:B:13:ARG:NH1	2:B:14:PRO:O	2.25	0.69
2:B:290:THR:HG1	2:B:327:TRP:CD1	2.11	0.69
2:E:107:ASP:O	2:E:126:HIS:N	2.19	0.69
2:H:152:ARG:HH12	2:H:155:HIS:H	1.40	0.69
1:J:332:HIS:H	1:J:369:GLN:HE21	1.41	0.69
5:P:17:GLU:HA	5:P:78:LEU:HA	1.73	0.69
2:E:297:LEU:HD11	2:E:334:ARG:HB3	1.73	0.69
1:J:226:GLN:H	1:J:231:HIS:HE1	1.38	0.69
4:M:72:ARG:HA	4:M:79:LEU:HA	1.73	0.69
1:D:2:GLU:HA	1:D:282:ASP:HA	1.75	0.69
2:E:242:ARG:NH1	2:E:243:GLY:O	2.26	0.69
1:J:114:CYS:O	1:J:118:HIS:ND1	2.25	0.69
2:K:394:ILE:O	2:K:398:LYS:NZ	2.21	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:17:GLU:HA	5:R:78:LEU:HA	1.73	0.69
4:S:72:ARG:HA	4:S:79:LEU:HA	1.73	0.69
1:A:114:CYS:O	1:A:118:HIS:ND1	2.25	0.69
2:B:152:ARG:HH12	2:B:155:HIS:H	1.41	0.69
2:B:268:ALA:HB2	2:B:328:GLY:HA3	1.74	0.69
2:E:268:ALA:HB2	2:E:328:GLY:HA3	1.74	0.69
1:G:312:ASP:O	1:G:314:GLY:N	2.25	0.69
2:H:135:ARG:NH2	2:H:326:THR:O	2.25	0.69
2:H:297:LEU:HD11	2:H:334:ARG:HB3	1.73	0.69
1:J:367:LYS:HZ1	1:J:374:ALA:HB1	1.57	0.69
2:K:152:ARG:HH12	2:K:155:HIS:H	1.41	0.69
3:L:128:VAL:HA	3:L:133:VAL:HA	1.73	0.69
5:N:51:ALA:N	5:N:55:ALA:O	2.26	0.69
4:Q:72:ARG:HA	4:Q:79:LEU:HA	1.73	0.69
1:A:7:MET:O	1:A:277:ILE:N	2.25	0.69
1:A:335:SER:OG	1:A:367:LYS:O	2.11	0.69
1:D:86:PRO:HA	1:D:228:GLY:HA2	1.75	0.69
1:G:114:CYS:O	1:G:118:HIS:ND1	2.25	0.69
3:C:145:ASN:O	3:C:149:ALA:N	2.24	0.69
1:D:244:TRP:O	1:D:247:ASP:N	2.25	0.69
2:H:242:ARG:NH1	2:H:243:GLY:O	2.26	0.69
1:J:163:ILE:HB	1:J:280:SER:HB3	1.75	0.69
2:K:163:TYR:HB2	2:K:251:LYS:HB3	1.75	0.69
1:D:114:CYS:O	1:D:118:HIS:ND1	2.25	0.68
1:D:226:GLN:H	1:D:231:HIS:HE1	1.38	0.68
1:G:163:ILE:HB	1:G:280:SER:HB3	1.75	0.68
3:I:146:GLU:HA	3:I:149:ALA:HB3	1.74	0.68
1:J:340:ILE:HG22	1:J:342:GLU:H	1.56	0.68
3:C:146:GLU:HA	3:C:149:ALA:HB3	1.74	0.68
5:P:51:ALA:N	5:P:55:ALA:O	2.26	0.68
1:A:312:ASP:O	1:A:314:GLY:N	2.25	0.68
2:B:172:VAL:HG13	2:B:227:LEU:HB3	1.76	0.68
1:D:10:LYS:HE3	1:D:15:TYR:HB2	1.76	0.68
1:D:113:GLU:O	1:D:117:ASP:N	2.17	0.68
1:J:298:SER:OG	1:J:322:LYS:O	2.11	0.68
4:S:35:HIS:N	4:S:97:ALA:O	2.27	0.68
5:T:51:ALA:N	5:T:55:ALA:O	2.26	0.68
1:D:335:SER:OG	1:D:367:LYS:O	2.11	0.68
1:G:8:PRO:HA	1:G:276:SER:HA	1.75	0.68
1:J:244:TRP:O	1:J:247:ASP:N	2.25	0.68
1:J:312:ASP:O	1:J:314:GLY:N	2.25	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:67:PHE:N	2:K:74:LYS:O	2.27	0.68
2:K:242:ARG:NH1	2:K:243:GLY:O	2.26	0.68
5:N:23:CYS:HA	5:N:72:THR:HA	1.74	0.68
1:A:86:PRO:HA	1:A:228:GLY:HA2	1.75	0.68
2:B:242:ARG:NH1	2:B:243:GLY:O	2.26	0.68
1:D:312:ASP:O	1:D:314:GLY:N	2.25	0.68
1:D:332:HIS:H	1:D:369:GLN:HE21	1.41	0.68
2:E:276:LYS:O	2:E:276:LYS:NZ	2.26	0.68
2:E:290:THR:HG1	2:E:327:TRP:CD1	2.12	0.68
2:K:168:GLN:HA	2:K:233:TRP:CD1	2.29	0.68
1:A:11:VAL:HG11	1:A:271:ASN:HB3	1.76	0.68
1:G:10:LYS:HE3	1:G:15:TYR:HB2	1.76	0.68
1:G:230:VAL:O	2:H:239:ARG:NE	2.26	0.68
2:H:10:LYS:HG3	2:H:11:LEU:HG	1.76	0.68
1:J:8:PRO:HA	1:J:276:SER:HA	1.76	0.68
1:J:436:LEU:O	1:J:439:HIS:ND1	2.22	0.68
5:R:51:ALA:N	5:R:55:ALA:O	2.26	0.68
2:E:163:TYR:HB2	2:E:251:LYS:HB3	1.76	0.68
1:G:335:SER:OG	1:G:367:LYS:O	2.11	0.68
1:J:113:GLU:O	1:J:117:ASP:N	2.17	0.68
1:J:335:SER:OG	1:J:367:LYS:O	2.11	0.68
2:K:46:ARG:HB3	2:K:100:LEU:HD13	1.75	0.68
4:Q:28:THR:O	4:Q:32:TYR:N	2.27	0.68
1:A:163:ILE:HB	1:A:280:SER:HB3	1.75	0.68
2:B:67:PHE:N	2:B:74:LYS:O	2.27	0.68
1:G:2:GLU:HA	1:G:282:ASP:HA	1.75	0.68
1:G:436:LEU:O	1:G:439:HIS:ND1	2.22	0.68
1:J:2:GLU:HA	1:J:282:ASP:HA	1.75	0.68
1:J:295:PRO:HA	1:J:325:LYS:HZ3	1.57	0.68
1:D:163:ILE:HB	1:D:280:SER:HB3	1.75	0.68
2:E:168:GLN:HA	2:E:233:TRP:CD1	2.29	0.68
2:K:51:ALA:HB1	2:K:67:PHE:HA	1.75	0.68
2:B:46:ARG:HD3	2:B:153:TYR:CG	2.29	0.68
2:B:51:ALA:HB1	2:B:67:PHE:HA	1.75	0.68
1:D:7:MET:O	1:D:277:ILE:N	2.25	0.68
2:E:46:ARG:HD3	2:E:153:TYR:CG	2.29	0.68
2:E:152:ARG:HH12	2:E:155:HIS:H	1.41	0.68
2:H:67:PHE:N	2:H:74:LYS:O	2.27	0.68
1:J:59:VAL:HA	2:K:242:ARG:CB	2.24	0.68
2:K:48:GLN:HB2	2:K:98:TYR:HA	1.75	0.68
4:M:28:THR:O	4:M:32:TYR:N	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:GLN:HB2	2:B:98:TYR:HA	1.75	0.67
2:E:67:PHE:N	2:E:74:LYS:O	2.27	0.67
2:E:151:ASN:HA	2:E:260:LYS:HA	1.76	0.67
2:H:46:ARG:HD3	2:H:153:TYR:CG	2.29	0.67
2:H:51:ALA:HB1	2:H:67:PHE:HA	1.75	0.67
1:J:10:LYS:HE3	1:J:15:TYR:HB2	1.76	0.67
1:A:2:GLU:HA	1:A:282:ASP:HA	1.75	0.67
4:O:160:THR:N	4:O:198:LEU:O	2.22	0.67
5:R:193:CYS:HA	5:R:210:ARG:HA	1.76	0.67
5:N:193:CYS:HA	5:N:210:ARG:HA	1.76	0.67
4:O:28:THR:O	4:O:32:TYR:N	2.27	0.67
1:A:332:HIS:H	1:A:369:GLN:HE21	1.41	0.67
1:D:11:VAL:HG11	1:D:271:ASN:HB3	1.76	0.67
1:D:298:SER:OG	1:D:322:LYS:O	2.11	0.67
2:E:51:ALA:HB1	2:E:67:PHE:HA	1.75	0.67
2:H:46:ARG:HB3	2:H:100:LEU:HD13	1.76	0.67
2:H:168:GLN:HA	2:H:233:TRP:CD1	2.29	0.67
1:J:86:PRO:HA	1:J:228:GLY:HA2	1.75	0.67
1:A:298:SER:OG	1:A:322:LYS:O	2.11	0.67
2:H:48:GLN:HB2	2:H:98:TYR:HA	1.75	0.67
5:P:38:GLN:HA	5:P:49:TYR:H	1.60	0.67
4:M:160:THR:N	4:M:198:LEU:O	2.22	0.67
4:Q:63:PRO:CB	5:R:98:GLY:H	2.06	0.67
5:T:193:CYS:HA	5:T:210:ARG:HA	1.76	0.67
2:E:46:ARG:HB3	2:E:100:LEU:HD13	1.75	0.67
2:E:139:ARG:NH2	2:K:107:ASP:OD2	2.28	0.67
1:G:6:VAL:HA	1:G:278:PRO:HA	1.77	0.67
1:G:11:VAL:HG11	1:G:271:ASN:HB3	1.76	0.67
1:G:48:THR:O	1:G:119:ALA:N	2.28	0.67
1:G:113:GLU:O	1:G:117:ASP:N	2.17	0.67
1:G:332:HIS:H	1:G:369:GLN:HE21	1.41	0.67
1:J:7:MET:O	1:J:277:ILE:N	2.25	0.67
2:K:46:ARG:HD3	2:K:153:TYR:CG	2.29	0.67
1:J:337:VAL:O	1:J:398:SER:OG	2.12	0.67
2:K:172:VAL:HG13	2:K:227:LEU:HB3	1.76	0.67
5:N:38:GLN:HA	5:N:49:TYR:H	1.60	0.67
4:Q:35:HIS:N	4:Q:97:ALA:O	2.27	0.67
1:A:6:VAL:HA	1:A:278:PRO:HA	1.77	0.67
2:B:163:TYR:HB2	2:B:251:LYS:HB3	1.75	0.67
1:G:337:VAL:O	1:G:398:SER:OG	2.12	0.67
3:I:245:ASN:N	3:I:249:VAL:O	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:35:HIS:N	4:O:97:ALA:O	2.27	0.67
1:A:8:PRO:HA	1:A:276:SER:HA	1.75	0.67
2:B:10:LYS:HG3	2:B:11:LEU:HG	1.76	0.67
1:D:253:ASN:OD1	1:D:253:ASN:N	2.25	0.67
2:H:163:TYR:HB2	2:H:251:LYS:HB3	1.75	0.67
3:L:245:ASN:N	3:L:249:VAL:O	2.28	0.67
5:P:193:CYS:HA	5:P:210:ARG:HA	1.76	0.67
2:B:168:GLN:HA	2:B:233:TRP:CD1	2.29	0.66
2:E:10:LYS:HG3	2:E:11:LEU:HG	1.76	0.66
1:G:134:ASN:HA	1:G:144:SER:HA	1.77	0.66
1:J:48:THR:O	1:J:119:ALA:N	2.28	0.66
2:K:277:HIS:HB3	2:K:340:SER:HB3	1.77	0.66
2:E:172:VAL:HG13	2:E:227:LEU:HB3	1.76	0.66
1:J:11:VAL:HG11	1:J:271:ASN:HB3	1.76	0.66
4:M:35:HIS:N	4:M:97:ALA:O	2.27	0.66
2:B:151:ASN:HA	2:B:260:LYS:HA	1.76	0.66
1:D:367:LYS:HZ1	1:D:374:ALA:HB1	1.60	0.66
2:E:48:GLN:HB2	2:E:98:TYR:HA	1.74	0.66
2:H:172:VAL:HG13	2:H:227:LEU:HB3	1.76	0.66
5:R:38:GLN:HA	5:R:49:TYR:H	1.60	0.66
2:B:172:VAL:O	2:B:227:LEU:N	2.29	0.66
1:D:337:VAL:O	1:D:398:SER:OG	2.12	0.66
1:G:298:SER:OG	1:G:322:LYS:O	2.11	0.66
2:H:292:LEU:H	2:H:306:GLN:NE2	1.93	0.66
2:K:10:LYS:HG3	2:K:11:LEU:HG	1.76	0.66
5:T:38:GLN:HA	5:T:49:TYR:H	1.60	0.66
1:G:96:CYS:HA	2:H:224:ARG:HH21	1.61	0.66
2:K:151:ASN:HA	2:K:260:LYS:HA	1.76	0.66
2:K:292:LEU:H	2:K:306:GLN:NE2	1.93	0.66
1:D:8:PRO:HA	1:D:276:SER:HA	1.76	0.66
1:D:48:THR:O	1:D:119:ALA:N	2.28	0.66
1:D:134:ASN:HA	1:D:144:SER:HA	1.77	0.66
2:E:292:LEU:H	2:E:306:GLN:NE2	1.93	0.66
2:H:26:ARG:NH2	2:H:28:ASP:OD2	2.29	0.66
1:A:337:VAL:O	1:A:398:SER:OG	2.12	0.66
1:G:64:GLY:O	1:G:101:THR:OG1	2.12	0.66
1:G:86:PRO:HA	1:G:228:GLY:HA2	1.75	0.66
4:Q:160:THR:N	4:Q:198:LEU:O	2.22	0.66
4:S:28:THR:O	4:S:32:TYR:N	2.27	0.66
5:T:36:TYR:HA	5:T:53:THR:H	1.60	0.66
1:D:37:ARG:HA	1:D:268:ARG:HG3	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:GLU:OE1	1:D:242:GLU:N	2.29	0.66
3:F:245:ASN:N	3:F:249:VAL:O	2.28	0.66
2:H:84:ARG:HA	2:H:89:CYS:H	1.61	0.66
5:R:36:TYR:HA	5:R:53:THR:H	1.60	0.66
2:B:46:ARG:HB3	2:B:100:LEU:HD13	1.76	0.66
2:B:292:LEU:H	2:B:306:GLN:NE2	1.93	0.66
1:D:6:VAL:HA	1:D:278:PRO:HA	1.77	0.66
2:E:84:ARG:HA	2:E:89:CYS:H	1.61	0.66
1:G:231:HIS:HB3	2:H:239:ARG:HH21	1.61	0.66
2:H:172:VAL:O	2:H:227:LEU:N	2.29	0.66
1:J:37:ARG:HA	1:J:268:ARG:HG3	1.78	0.66
2:K:276:LYS:O	2:K:276:LYS:NZ	2.26	0.66
5:N:36:TYR:HA	5:N:53:THR:H	1.60	0.66
1:G:7:MET:O	1:G:277:ILE:N	2.25	0.66
1:J:394:GLN:HB2	2:K:336:TRP:CD2	2.31	0.66
1:A:10:LYS:HE3	1:A:15:TYR:HB2	1.76	0.65
1:A:79:GLN:NE2	1:A:80:VAL:O	2.30	0.65
2:B:277:HIS:HB3	2:B:340:SER:HB3	1.77	0.65
1:G:121:ALA:HA	1:G:179:VAL:HG12	1.79	0.65
1:J:40:PRO:HG3	1:J:267:LEU:HD23	1.78	0.65
1:A:289:THR:OG1	1:A:290:ARG:N	2.30	0.65
2:E:26:ARG:NH2	2:E:28:ASP:OD2	2.29	0.65
2:E:30:PRO:HG2	2:E:67:PHE:HD2	1.61	0.65
1:J:134:ASN:HA	1:J:144:SER:HA	1.77	0.65
2:K:21:ASN:OD1	2:K:26:ARG:N	2.29	0.65
2:B:26:ARG:NH2	2:B:28:ASP:OD2	2.29	0.65
2:H:151:ASN:HA	2:H:260:LYS:HA	1.76	0.65
2:H:277:HIS:HB3	2:H:340:SER:HB3	1.77	0.65
1:J:6:VAL:HA	1:J:278:PRO:HA	1.77	0.65
1:J:289:THR:OG1	1:J:290:ARG:N	2.30	0.65
4:Q:19:ARG:HA	4:Q:82:GLN:HA	1.79	0.65
1:J:37:ARG:O	1:J:130:GLN:N	2.23	0.65
2:B:107:ASP:O	2:B:126:HIS:N	2.19	0.65
2:B:272:LEU:N	2:B:283:HIS:O	2.18	0.65
3:C:245:ASN:N	3:C:249:VAL:O	2.28	0.65
1:D:79:GLN:NE2	1:D:80:VAL:O	2.30	0.65
2:E:47:ILE:O	2:E:99:ILE:N	2.25	0.65
1:G:79:GLN:NE2	1:G:80:VAL:O	2.30	0.65
1:J:79:GLN:NE2	1:J:80:VAL:O	2.30	0.65
1:J:121:ALA:HA	1:J:179:VAL:HG12	1.79	0.65
4:S:19:ARG:HA	4:S:82:GLN:HA	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:ASN:OD1	2:B:26:ARG:N	2.29	0.65
2:B:30:PRO:HG2	2:B:67:PHE:HD2	1.61	0.65
2:E:172:VAL:O	2:E:227:LEU:N	2.29	0.65
2:H:30:PRO:HG2	2:H:67:PHE:HD2	1.61	0.65
1:J:242:GLU:OE1	1:J:242:GLU:N	2.29	0.65
2:K:84:ARG:HA	2:K:89:CYS:H	1.61	0.65
1:A:121:ALA:HA	1:A:179:VAL:HG12	1.79	0.65
2:E:21:ASN:OD1	2:E:26:ARG:N	2.29	0.65
2:E:185:VAL:HG12	2:E:220:VAL:HG12	1.79	0.65
2:E:277:HIS:HB3	2:E:340:SER:HB3	1.77	0.65
2:H:185:VAL:HG12	2:H:220:VAL:HG12	1.79	0.65
1:A:37:ARG:HA	1:A:268:ARG:HG3	1.78	0.65
1:A:436:LEU:O	1:A:439:HIS:ND1	2.22	0.65
1:D:289:THR:OG1	1:D:290:ARG:N	2.30	0.65
2:K:172:VAL:O	2:K:227:LEU:N	2.29	0.65
2:K:278:ARG:NH1	2:K:340:SER:OG	2.30	0.65
4:M:19:ARG:HA	4:M:82:GLN:HA	1.79	0.65
2:B:106:GLY:O	2:B:128:VAL:N	2.26	0.65
2:B:278:ARG:NH1	2:B:340:SER:OG	2.30	0.65
3:F:145:ASN:O	3:F:149:ALA:N	2.24	0.65
5:P:36:TYR:HA	5:P:53:THR:H	1.60	0.65
1:A:40:PRO:HG3	1:A:267:LEU:HD23	1.78	0.64
1:A:48:THR:O	1:A:119:ALA:N	2.28	0.64
1:A:253:ASN:OD1	1:A:253:ASN:N	2.25	0.64
2:B:84:ARG:HA	2:B:89:CYS:H	1.61	0.64
1:D:64:GLY:O	1:D:101:THR:OG1	2.12	0.64
2:H:19:CYS:N	2:H:27:CYS:O	2.30	0.64
2:H:47:ILE:O	2:H:99:ILE:N	2.25	0.64
2:K:26:ARG:NH2	2:K:28:ASP:OD2	2.29	0.64
1:A:134:ASN:HA	1:A:144:SER:HA	1.77	0.64
1:D:40:PRO:HG3	1:D:267:LEU:HD23	1.78	0.64
1:D:192:GLU:HB3	1:D:195:THR:HG23	1.80	0.64
2:E:9:TYR:OH	2:E:53:PHE:O	2.16	0.64
5:R:164:GLU:HA	5:R:179:THR:HA	1.80	0.64
1:A:64:GLY:O	1:A:101:THR:OG1	2.12	0.64
1:G:58:PRO:HD3	2:H:238:GLY:HA2	1.79	0.64
2:H:9:TYR:OH	2:H:53:PHE:O	2.16	0.64
2:H:21:ASN:OD1	2:H:26:ARG:N	2.29	0.64
2:K:247:THR:OG1	2:K:248:PHE:N	2.29	0.64
2:B:360:TYR:O	2:B:364:THR:OG1	2.11	0.64
2:E:19:CYS:N	2:E:27:CYS:O	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41:HIS:ND1	2:E:151:ASN:OD1	2.22	0.64
1:G:289:THR:OG1	1:G:290:ARG:N	2.30	0.64
2:H:278:ARG:NH1	2:H:340:SER:OG	2.30	0.64
2:B:197:TYR:OH	2:B:212:ASP:OD2	2.16	0.64
2:B:247:THR:OG1	2:B:248:PHE:N	2.29	0.64
1:J:123:LYS:HG3	1:J:125:HIS:CD2	2.33	0.64
1:A:303:LYS:NZ	1:A:304:ILE:O	2.30	0.64
1:D:38:ILE:HG13	1:D:129:VAL:HG13	1.79	0.64
2:E:278:ARG:NH1	2:E:340:SER:OG	2.30	0.64
1:G:242:GLU:OE1	1:G:242:GLU:N	2.29	0.64
1:G:310:ALA:O	1:G:358:SER:OG	2.16	0.64
1:J:32:GLN:O	1:J:134:ASN:N	2.31	0.64
5:P:164:GLU:HA	5:P:179:THR:HA	1.80	0.64
4:S:160:THR:N	4:S:198:LEU:O	2.22	0.64
5:T:164:GLU:HA	5:T:179:THR:HA	1.80	0.64
1:A:38:ILE:HG13	1:A:129:VAL:HG13	1.79	0.64
1:A:339:VAL:N	1:A:358:SER:O	2.25	0.64
3:C:203:PRO:HA	3:C:236:ARG:HA	1.80	0.64
1:G:40:PRO:HG3	1:G:267:LEU:HD23	1.78	0.64
1:G:192:GLU:HB3	1:G:195:THR:HG23	1.80	0.64
2:K:185:VAL:HG12	2:K:220:VAL:HG12	1.79	0.64
1:A:123:LYS:HG3	1:A:125:HIS:CD2	2.33	0.64
2:B:185:VAL:HG12	2:B:220:VAL:HG12	1.79	0.64
2:H:360:TYR:O	2:H:364:THR:OG1	2.11	0.64
1:J:57:SER:HB3	2:K:242:ARG:HA	1.80	0.64
1:J:242:GLU:O	1:J:246:LYS:NZ	2.28	0.64
1:A:310:ALA:O	1:A:358:SER:OG	2.16	0.64
2:B:19:CYS:N	2:B:27:CYS:O	2.30	0.64
1:D:75:ASP:OD2	1:D:219:ASN:N	2.31	0.64
1:G:38:ILE:HG13	1:G:129:VAL:HG13	1.79	0.64
3:I:203:PRO:HA	3:I:236:ARG:HA	1.80	0.64
2:K:19:CYS:N	2:K:27:CYS:O	2.30	0.64
1:D:123:LYS:HG3	1:D:125:HIS:CD2	2.33	0.64
1:G:37:ARG:HA	1:G:268:ARG:HG3	1.78	0.64
3:L:203:PRO:HA	3:L:236:ARG:HA	1.80	0.64
2:B:47:ILE:O	2:B:99:ILE:N	2.25	0.63
2:H:135:ARG:NH2	2:H:291:LEU:O	2.26	0.63
2:E:45:ILE:HG22	2:E:47:ILE:HG23	1.81	0.63
1:J:75:ASP:OD2	1:J:219:ASN:N	2.31	0.63
2:K:45:ILE:HG22	2:K:47:ILE:HG23	1.81	0.63
2:K:272:LEU:N	2:K:283:HIS:O	2.18	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:292:LEU:HD21	2:K:294:THR:HG23	1.80	0.63
4:O:19:ARG:HA	4:O:82:GLN:HA	1.79	0.63
1:A:192:GLU:HB3	1:A:195:THR:HG23	1.80	0.63
1:D:121:ALA:HA	1:D:179:VAL:HG12	1.78	0.63
1:G:123:LYS:HG3	1:G:125:HIS:CD2	2.33	0.63
2:K:30:PRO:HG2	2:K:67:PHE:HD2	1.61	0.63
2:K:107:ASP:O	2:K:126:HIS:N	2.19	0.63
1:G:18:LEU:HA	1:G:28:HIS:HA	1.81	0.63
2:H:45:ILE:HG22	2:H:47:ILE:HG23	1.81	0.63
2:H:292:LEU:HD21	2:H:294:THR:HG23	1.80	0.63
1:J:192:GLU:HB3	1:J:195:THR:HG23	1.80	0.63
2:K:135:ARG:NH2	2:K:291:LEU:O	2.26	0.63
3:L:204:ARG:N	3:L:235:SER:O	2.30	0.63
1:D:111:SER:OG	1:D:113:GLU:OE1	2.16	0.63
3:I:204:ARG:N	3:I:235:SER:O	2.30	0.63
1:J:310:ALA:O	1:J:358:SER:OG	2.16	0.63
2:K:9:TYR:OH	2:K:53:PHE:O	2.16	0.63
2:K:197:TYR:OH	2:K:212:ASP:OD2	2.16	0.63
4:Q:143:VAL:HA	4:Q:184:TYR:HA	1.81	0.63
2:E:135:ARG:NH2	2:E:291:LEU:O	2.26	0.63
2:H:106:GLY:O	2:H:128:VAL:N	2.26	0.63
5:N:164:GLU:HA	5:N:179:THR:HA	1.80	0.63
1:A:39:ILE:O	1:A:128:THR:N	2.28	0.63
1:A:41:SER:O	1:A:125:HIS:ND1	2.31	0.63
1:D:32:GLN:O	1:D:134:ASN:N	2.31	0.63
4:O:143:VAL:HA	4:O:184:TYR:HA	1.81	0.63
1:A:75:ASP:OD2	1:A:219:ASN:N	2.31	0.62
1:D:303:LYS:NZ	1:D:304:ILE:O	2.30	0.62
2:H:282:LEU:O	2:H:314:VAL:N	2.32	0.62
1:J:38:ILE:HG13	1:J:129:VAL:HG13	1.79	0.62
4:S:143:VAL:HA	4:S:184:TYR:HA	1.81	0.62
2:E:292:LEU:HD21	2:E:294:THR:HG23	1.80	0.62
2:H:402:ASN:O	2:H:404:GLN:NE2	2.32	0.62
1:J:41:SER:O	1:J:125:HIS:ND1	2.31	0.62
1:J:49:CYS:HB3	1:J:118:HIS:HA	1.81	0.62
1:J:64:GLY:O	1:J:101:THR:OG1	2.12	0.62
2:K:324:GLU:HA	2:K:334:ARG:HG3	1.81	0.62
1:A:18:LEU:HA	1:A:28:HIS:HA	1.81	0.62
2:B:9:TYR:OH	2:B:53:PHE:O	2.16	0.62
1:D:318:THR:OG1	1:D:319:VAL:N	2.32	0.62
3:F:203:PRO:HA	3:F:236:ARG:HA	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:TYR:O	1:G:283:ILE:N	2.19	0.62
2:H:189:VAL:HG11	2:H:209:THR:HA	1.81	0.62
2:B:292:LEU:HD21	2:B:294:THR:HG23	1.80	0.62
2:B:402:ASN:O	2:B:404:GLN:NE2	2.32	0.62
1:D:1:TYR:O	1:D:283:ILE:N	2.19	0.62
1:D:37:ARG:O	1:D:130:GLN:N	2.23	0.62
1:D:49:CYS:HB3	1:D:118:HIS:HA	1.81	0.62
1:D:310:ALA:O	1:D:358:SER:OG	2.16	0.62
1:J:221:LYS:O	1:J:235:THR:N	2.30	0.62
1:A:46:TYR:HA	1:A:207:ARG:O	2.00	0.62
1:A:207:ARG:NE	1:A:215:TYR:OH	2.33	0.62
1:D:46:TYR:HA	1:D:207:ARG:O	2.00	0.62
1:D:207:ARG:NE	1:D:215:TYR:OH	2.33	0.62
1:D:221:LYS:O	1:D:235:THR:N	2.31	0.62
1:G:41:SER:O	1:G:125:HIS:ND1	2.31	0.62
1:G:318:THR:OG1	1:G:319:VAL:N	2.32	0.62
2:H:267:LEU:HA	2:H:329:ASN:HB2	1.82	0.62
2:H:276:LYS:O	2:H:276:LYS:NZ	2.26	0.62
1:J:1:TYR:O	1:J:283:ILE:N	2.19	0.62
1:J:46:TYR:HA	1:J:207:ARG:O	2.00	0.62
1:A:242:GLU:OE1	1:A:242:GLU:N	2.29	0.62
2:B:282:LEU:O	2:B:314:VAL:N	2.32	0.62
2:E:402:ASN:O	2:E:404:GLN:NE2	2.32	0.62
3:I:145:ASN:O	3:I:149:ALA:N	2.24	0.62
1:J:59:VAL:HG23	1:J:101:THR:HG22	1.82	0.62
1:A:1:TYR:O	1:A:283:ILE:N	2.19	0.62
2:B:276:LYS:O	2:B:276:LYS:NZ	2.26	0.62
1:D:39:ILE:O	1:D:128:THR:N	2.28	0.62
1:D:41:SER:O	1:D:125:HIS:ND1	2.32	0.62
2:E:247:THR:OG1	2:E:248:PHE:N	2.29	0.62
1:G:49:CYS:HB3	1:G:118:HIS:HA	1.81	0.62
2:K:189:VAL:HG11	2:K:209:THR:HA	1.81	0.62
2:B:324:GLU:HA	2:B:334:ARG:HG3	1.81	0.62
2:E:267:LEU:HA	2:E:329:ASN:HB2	1.82	0.62
1:G:207:ARG:NE	1:G:215:TYR:OH	2.33	0.62
1:J:318:THR:OG1	1:J:319:VAL:N	2.32	0.62
1:A:159:ASP:HB3	1:A:284:PRO:HD3	1.82	0.62
1:D:300:LEU:HD13	1:D:375:VAL:HG22	1.82	0.62
1:G:303:LYS:NZ	1:G:304:ILE:O	2.30	0.62
1:A:318:THR:OG1	1:A:319:VAL:N	2.32	0.62
1:A:341:LYS:N	1:A:356:HIS:O	2.31	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:LEU:HA	2:B:329:ASN:HB2	1.82	0.62
1:G:39:ILE:O	1:G:128:THR:N	2.28	0.62
1:J:303:LYS:NZ	1:J:304:ILE:O	2.30	0.62
1:J:341:LYS:N	1:J:356:HIS:O	2.31	0.62
1:D:59:VAL:HG23	1:D:101:THR:HG22	1.82	0.61
2:E:272:LEU:N	2:E:283:HIS:O	2.18	0.61
2:H:247:THR:OG1	2:H:248:PHE:N	2.29	0.61
1:A:111:SER:OG	1:A:113:GLU:OE1	2.16	0.61
2:B:45:ILE:HG22	2:B:47:ILE:HG23	1.81	0.61
1:D:18:LEU:HA	1:D:28:HIS:HA	1.81	0.61
2:E:189:VAL:HG11	2:E:209:THR:HA	1.81	0.61
1:G:59:VAL:HG23	1:G:101:THR:HG22	1.82	0.61
1:G:137:TYR:H	1:G:140:VAL:HG12	1.65	0.61
1:J:159:ASP:HB3	1:J:284:PRO:HD3	1.82	0.61
2:K:402:ASN:O	2:K:404:GLN:NE2	2.32	0.61
2:B:56:LYS:N	2:B:60:VAL:O	2.26	0.61
2:E:324:GLU:HA	2:E:334:ARG:HG3	1.81	0.61
3:I:230:GLY:HA2	3:I:258:SER:HA	1.82	0.61
1:J:137:TYR:H	1:J:140:VAL:HG12	1.65	0.61
4:S:49:ALA:HA	4:S:61:ALA:N	2.15	0.61
1:A:59:VAL:HG23	1:A:101:THR:HG22	1.82	0.61
1:G:159:ASP:HB3	1:G:284:PRO:HD3	1.82	0.61
4:M:143:VAL:HA	4:M:184:TYR:HA	1.81	0.61
1:A:193:TYR:HB3	1:A:207:ARG:HH12	1.65	0.61
1:G:75:ASP:OD2	1:G:219:ASN:N	2.31	0.61
1:J:122:TYR:O	1:J:177:LYS:NZ	2.29	0.61
1:A:49:CYS:HB3	1:A:118:HIS:HA	1.81	0.61
1:G:341:LYS:N	1:G:356:HIS:O	2.31	0.61
1:J:18:LEU:HA	1:J:28:HIS:HA	1.81	0.61
1:J:193:TYR:HB3	1:J:207:ARG:HH12	1.65	0.61
2:K:62:LEU:HD22	2:K:94:HIS:CE1	2.35	0.61
2:K:267:LEU:HA	2:K:329:ASN:HB2	1.82	0.61
1:A:137:TYR:H	1:A:140:VAL:HG12	1.65	0.61
1:A:295:PRO:HA	1:A:325:LYS:HZ3	1.66	0.61
2:E:106:GLY:O	2:E:128:VAL:N	2.26	0.61
1:J:207:ARG:NE	1:J:215:TYR:OH	2.33	0.61
2:K:84:ARG:HG2	2:K:85:THR:O	2.01	0.61
2:K:297:LEU:HG	2:K:323:LEU:HA	1.83	0.61
2:K:388:ARG:HA	2:K:391:ASN:HD21	1.66	0.61
4:M:49:ALA:HA	4:M:61:ALA:N	2.15	0.61
5:T:168:LYS:O	5:T:176:SER:N	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ARG:NE	2:B:39:ASP:OD2	2.34	0.61
2:B:62:LEU:HD22	2:B:94:HIS:CE1	2.35	0.61
3:C:230:GLY:HA2	3:C:258:SER:HA	1.83	0.61
1:D:341:LYS:N	1:D:356:HIS:O	2.31	0.61
2:E:282:LEU:O	2:E:314:VAL:N	2.32	0.61
3:F:135:LYS:O	3:F:162:GLU:N	2.34	0.61
1:G:193:TYR:HB3	1:G:207:ARG:HH12	1.65	0.61
1:J:48:THR:HA	1:J:204:LEU:HB3	1.83	0.61
2:K:56:LYS:N	2:K:60:VAL:O	2.26	0.61
2:B:114:HIS:HA	2:B:119:ARG:NE	2.16	0.61
3:C:204:ARG:N	3:C:235:SER:O	2.30	0.61
1:D:218:THR:O	1:D:237:VAL:N	2.34	0.61
2:H:197:TYR:OH	2:H:212:ASP:OD2	2.16	0.61
2:K:110:THR:HA	2:K:123:THR:HG22	1.83	0.61
1:A:48:THR:HA	1:A:204:LEU:HB3	1.83	0.61
1:A:122:TYR:O	1:A:177:LYS:NZ	2.29	0.61
2:B:189:VAL:HG11	2:B:209:THR:HA	1.81	0.61
2:B:388:ARG:HA	2:B:391:ASN:HD21	1.66	0.61
1:D:339:VAL:N	1:D:358:SER:O	2.25	0.61
2:K:282:LEU:O	2:K:314:VAL:N	2.32	0.61
5:P:40:PRO:HA	5:P:46:LEU:HA	1.83	0.61
5:R:168:LYS:O	5:R:176:SER:N	2.34	0.61
1:D:137:TYR:H	1:D:140:VAL:HG12	1.65	0.60
2:E:84:ARG:HG2	2:E:85:THR:O	2.01	0.60
2:E:147:GLU:HA	2:E:264:ILE:HA	1.83	0.60
3:F:230:GLY:HA2	3:F:258:SER:HA	1.83	0.60
1:G:32:GLN:O	1:G:134:ASN:N	2.31	0.60
1:G:221:LYS:O	1:G:235:THR:N	2.30	0.60
2:H:324:GLU:HA	2:H:334:ARG:HG3	1.81	0.60
3:I:135:LYS:O	3:I:162:GLU:N	2.34	0.60
2:K:106:GLY:O	2:K:128:VAL:N	2.26	0.60
2:E:62:LEU:HD22	2:E:94:HIS:CE1	2.35	0.60
1:J:18:LEU:H	1:J:332:HIS:CD2	2.19	0.60
3:C:135:LYS:O	3:C:162:GLU:N	2.34	0.60
2:E:114:HIS:HA	2:E:119:ARG:NE	2.16	0.60
1:G:46:TYR:HA	1:G:207:ARG:O	2.00	0.60
1:G:122:TYR:O	1:G:177:LYS:NZ	2.29	0.60
2:H:41:HIS:ND1	2:H:151:ASN:OD1	2.22	0.60
2:H:147:GLU:HA	2:H:264:ILE:HA	1.83	0.60
4:Q:49:ALA:HA	4:Q:61:ALA:N	2.15	0.60
1:A:324:SER:OG	1:A:325:LYS:NZ	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ASP:HB3	1:D:284:PRO:HD3	1.82	0.60
2:E:156:LYS:NZ	2:E:255:PRO:O	2.34	0.60
2:E:220:VAL:H	2:E:221:LYS:HZ3	1.47	0.60
1:G:324:SER:OG	1:G:325:LYS:NZ	2.35	0.60
2:H:187:ILE:O	2:H:211:SER:OG	2.17	0.60
2:K:114:HIS:HA	2:K:119:ARG:NE	2.16	0.60
5:N:168:LYS:O	5:N:176:SER:N	2.34	0.60
2:E:110:THR:HA	2:E:123:THR:HG22	1.83	0.60
2:H:62:LEU:HD22	2:H:94:HIS:CE1	2.35	0.60
2:H:84:ARG:HG2	2:H:85:THR:O	2.01	0.60
2:H:110:THR:HA	2:H:123:THR:HG22	1.83	0.60
2:K:220:VAL:H	2:K:221:LYS:HZ3	1.46	0.60
5:N:40:PRO:HA	5:N:46:LEU:HA	1.83	0.60
5:T:40:PRO:HA	5:T:46:LEU:HA	1.83	0.60
1:A:32:GLN:O	1:A:134:ASN:N	2.31	0.60
2:B:297:LEU:HG	2:B:323:LEU:HA	1.83	0.60
2:E:297:LEU:HG	2:E:323:LEU:HA	1.83	0.60
2:H:114:HIS:HA	2:H:119:ARG:NE	2.16	0.60
2:K:125:ALA:O	2:K:126:HIS:ND1	2.35	0.60
4:O:49:ALA:HA	4:O:61:ALA:N	2.15	0.60
5:P:168:LYS:O	5:P:176:SER:N	2.34	0.60
1:A:18:LEU:H	1:A:332:HIS:CD2	2.20	0.60
2:B:80:ASN:HB3	2:B:114:HIS:HB2	1.84	0.60
2:B:84:ARG:HG2	2:B:85:THR:O	2.01	0.60
1:D:193:TYR:HB3	1:D:207:ARG:HH12	1.65	0.60
1:D:324:SER:OG	1:D:325:LYS:NZ	2.35	0.60
2:E:125:ALA:O	2:E:126:HIS:ND1	2.35	0.60
2:E:197:TYR:OH	2:E:212:ASP:OD2	2.16	0.60
1:G:124:VAL:O	1:G:176:ASN:ND2	2.31	0.60
3:L:230:GLY:HA2	3:L:258:SER:HA	1.83	0.60
2:B:147:GLU:HA	2:B:264:ILE:HA	1.83	0.60
2:B:331:PRO:O	2:B:333:LYS:NZ	2.30	0.60
2:H:9:TYR:CE2	2:H:55:LEU:HB2	2.37	0.60
3:L:135:LYS:O	3:L:162:GLU:N	2.34	0.60
1:D:18:LEU:H	1:D:332:HIS:CD2	2.19	0.60
1:G:18:LEU:H	1:G:332:HIS:CD2	2.20	0.60
1:G:218:THR:O	1:G:237:VAL:N	2.34	0.60
1:J:218:THR:O	1:J:237:VAL:N	2.34	0.60
1:J:324:SER:OG	1:J:325:LYS:NZ	2.35	0.60
2:K:37:ARG:NE	2:K:39:ASP:OD2	2.34	0.60
3:L:145:ASN:O	3:L:149:ALA:N	2.24	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:128:VAL:N	4:M:143:VAL:O	2.35	0.60
5:R:40:PRO:HA	5:R:46:LEU:HA	1.83	0.60
1:A:37:ARG:O	1:A:130:GLN:N	2.22	0.60
1:A:218:THR:O	1:A:237:VAL:N	2.34	0.60
1:D:48:THR:HA	1:D:204:LEU:HB3	1.83	0.60
2:H:125:ALA:O	2:H:126:HIS:ND1	2.35	0.60
3:L:133:VAL:H	3:L:164:GLY:HA3	1.66	0.60
4:S:128:VAL:N	4:S:143:VAL:O	2.35	0.60
1:A:300:LEU:HD13	1:A:375:VAL:HG22	1.82	0.59
2:B:9:TYR:CE2	2:B:55:LEU:HB2	2.37	0.59
1:G:300:LEU:HD13	1:G:375:VAL:HG22	1.82	0.59
2:E:80:ASN:O	2:E:114:HIS:N	2.28	0.59
2:H:297:LEU:HG	2:H:323:LEU:HA	1.83	0.59
2:B:41:HIS:ND1	2:B:151:ASN:OD1	2.22	0.59
2:B:80:ASN:O	2:B:114:HIS:N	2.29	0.59
1:D:340:ILE:HD13	1:D:357:PHE:HB3	1.84	0.59
3:F:133:VAL:H	3:F:164:GLY:HA3	1.66	0.59
1:J:132:MET:HA	1:J:146:ASP:HA	1.84	0.59
4:O:128:VAL:N	4:O:143:VAL:O	2.35	0.59
5:P:137:ASN:O	5:P:179:THR:N	2.35	0.59
1:A:132:MET:HA	1:A:146:ASP:HA	1.84	0.59
2:B:135:ARG:NH2	2:B:291:LEU:O	2.26	0.59
1:D:132:MET:HA	1:D:146:ASP:HA	1.84	0.59
2:E:83:VAL:HG11	2:E:91:LEU:HD13	1.84	0.59
2:E:388:ARG:HA	2:E:391:ASN:HD21	1.66	0.59
1:J:319:VAL:HG23	1:J:352:SER:HA	1.85	0.59
1:A:46:TYR:HB2	1:A:207:ARG:HA	1.85	0.59
3:C:133:VAL:H	3:C:164:GLY:HA3	1.66	0.59
1:D:46:TYR:HB2	1:D:207:ARG:HA	1.85	0.59
2:E:9:TYR:CE2	2:E:55:LEU:HB2	2.37	0.59
1:G:29:LEU:HA	1:G:137:TYR:HA	1.84	0.59
1:J:300:LEU:HD13	1:J:375:VAL:HG22	1.82	0.59
1:G:37:ARG:NH1	1:G:132:MET:HB2	2.18	0.59
1:G:179:VAL:N	1:G:186:TYR:O	2.32	0.59
2:H:156:LYS:NZ	2:H:255:PRO:O	2.34	0.59
1:J:29:LEU:HA	1:J:137:TYR:HA	1.84	0.59
1:J:40:PRO:HA	1:J:127:GLY:HA3	1.85	0.59
3:L:243:THR:O	3:L:251:VAL:N	2.36	0.59
1:A:52:LYS:N	1:A:109:GLU:O	2.32	0.59
1:A:340:ILE:HD13	1:A:357:PHE:HB3	1.85	0.59
2:B:110:THR:HA	2:B:123:THR:HG22	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:LYS:HD3	5:N:95:LEU:CB	2.33	0.59
2:B:220:VAL:HG22	2:B:221:LYS:HZ3	1.67	0.59
1:D:205:GLN:HB3	1:D:215:TYR:CD2	2.38	0.59
2:E:80:ASN:HB3	2:E:114:HIS:HB2	1.84	0.59
1:G:40:PRO:HA	1:G:127:GLY:HA3	1.85	0.59
2:H:83:VAL:HG11	2:H:91:LEU:HD13	1.85	0.59
2:K:147:GLU:HA	2:K:264:ILE:HA	1.83	0.59
5:N:137:ASN:O	5:N:179:THR:N	2.36	0.59
1:A:40:PRO:HA	1:A:127:GLY:HA3	1.85	0.59
1:D:12:GLY:O	1:D:32:GLN:NE2	2.24	0.59
1:D:29:LEU:HA	1:D:137:TYR:HA	1.84	0.59
1:D:141:SER:H	1:D:143:ARG:NH2	2.00	0.59
2:H:388:ARG:HA	2:H:391:ASN:HD21	1.66	0.59
3:I:243:THR:O	3:I:251:VAL:N	2.36	0.59
2:K:80:ASN:O	2:K:114:HIS:N	2.28	0.59
2:K:80:ASN:HB3	2:K:114:HIS:HB2	1.84	0.59
2:K:95:HIS:HD1	2:K:98:TYR:HD1	1.50	0.59
1:A:190:PHE:CE2	1:A:192:GLU:HA	2.38	0.59
1:A:205:GLN:HB3	1:A:215:TYR:CD2	2.38	0.59
3:F:243:THR:O	3:F:251:VAL:N	2.36	0.59
5:T:137:ASN:O	5:T:179:THR:N	2.36	0.59
1:A:141:SER:H	1:A:143:ARG:NH2	2.00	0.59
2:E:95:HIS:HD1	2:E:98:TYR:HD1	1.50	0.59
1:G:141:SER:H	1:G:143:ARG:NH2	2.00	0.59
1:G:319:VAL:HG23	1:G:352:SER:HA	1.85	0.59
2:H:80:ASN:HB3	2:H:114:HIS:HB2	1.84	0.59
4:Q:128:VAL:N	4:Q:143:VAL:O	2.35	0.59
1:A:319:VAL:HG23	1:A:352:SER:HA	1.85	0.58
2:B:93:SER:OG	2:B:94:HIS:N	2.36	0.58
2:B:125:ALA:O	2:B:126:HIS:ND1	2.35	0.58
3:C:243:THR:O	3:C:251:VAL:N	2.36	0.58
1:D:122:TYR:O	1:D:177:LYS:NZ	2.29	0.58
2:E:39:ASP:O	2:E:131:ARG:NH2	2.36	0.58
3:F:204:ARG:N	3:F:235:SER:O	2.30	0.58
1:G:16:LYS:HD2	1:G:343:ASN:HB2	1.86	0.58
2:H:56:LYS:N	2:H:60:VAL:O	2.26	0.58
1:J:16:LYS:HD2	1:J:343:ASN:HB2	1.85	0.58
1:J:205:GLN:HB3	1:J:215:TYR:CD2	2.38	0.58
2:K:9:TYR:CE2	2:K:55:LEU:HB2	2.37	0.58
1:A:37:ARG:N	1:A:130:GLN:O	2.30	0.58
1:A:179:VAL:N	1:A:186:TYR:O	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:37:ARG:NE	2:E:39:ASP:OD2	2.34	0.58
1:G:238:PRO:O	1:G:243:ARG:NH2	2.36	0.58
2:H:39:ASP:O	2:H:131:ARG:NH2	2.36	0.58
2:H:292:LEU:HA	2:H:326:THR:O	2.03	0.58
1:J:238:PRO:O	1:J:243:ARG:NH2	2.36	0.58
1:J:359:THR:OG1	1:J:361:ASN:OD1	2.22	0.58
5:R:137:ASN:O	5:R:179:THR:N	2.35	0.58
1:D:238:PRO:O	1:D:243:ARG:NH2	2.36	0.58
1:G:37:ARG:HE	1:G:130:GLN:HG3	1.68	0.58
1:G:48:THR:HA	1:G:204:LEU:HB3	1.83	0.58
1:G:132:MET:HA	1:G:146:ASP:HA	1.84	0.58
3:I:133:VAL:H	3:I:164:GLY:HA3	1.66	0.58
1:A:238:PRO:O	1:A:243:ARG:NH2	2.36	0.58
1:D:10:LYS:HB2	1:D:13:ILE:HG22	1.86	0.58
1:D:16:LYS:HD2	1:D:343:ASN:HB2	1.86	0.58
1:G:205:GLN:HB3	1:G:215:TYR:CD2	2.38	0.58
2:H:221:LYS:O	2:H:224:ARG:NH1	2.36	0.58
1:J:190:PHE:CE2	1:J:192:GLU:HA	2.38	0.58
1:J:254:ASP:O	2:K:295:ARG:NH1	2.36	0.58
2:K:39:ASP:O	2:K:131:ARG:NH2	2.36	0.58
4:O:33:GLY:H	4:O:100:THR:HA	1.69	0.58
1:A:10:LYS:HB2	1:A:13:ILE:HG22	1.86	0.58
1:A:16:LYS:HD2	1:A:343:ASN:HB2	1.86	0.58
1:A:394:GLN:HB2	2:B:336:TRP:CD2	2.38	0.58
2:B:185:VAL:HG23	2:B:213:HIS:HB2	1.85	0.58
1:G:190:PHE:CE2	1:G:192:GLU:HA	2.38	0.58
2:K:47:ILE:O	2:K:99:ILE:N	2.25	0.58
2:K:292:LEU:HA	2:K:326:THR:O	2.03	0.58
1:D:311:PHE:CD2	1:D:394:GLN:HB3	2.39	0.58
2:E:116:GLY:H	2:E:119:ARG:HH21	1.52	0.58
2:E:196:LYS:O	2:E:226:TYR:N	2.37	0.58
2:E:221:LYS:O	2:E:224:ARG:NH1	2.36	0.58
1:J:37:ARG:HE	1:J:130:GLN:HG3	1.68	0.58
4:M:33:GLY:H	4:M:100:THR:HA	1.69	0.58
1:D:135:ILE:HD11	1:D:137:TYR:HB3	1.86	0.58
1:D:190:PHE:CE2	1:D:192:GLU:HA	2.38	0.58
2:E:47:ILE:HG12	2:E:99:ILE:HB	1.86	0.58
2:E:93:SER:OG	2:E:94:HIS:N	2.37	0.58
2:E:271:PRO:HB3	2:E:284:LEU:HB2	1.85	0.58
1:G:10:LYS:HB2	1:G:13:ILE:HG22	1.86	0.58
1:G:311:PHE:CD2	1:G:394:GLN:HB3	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:95:HIS:HD1	2:H:98:TYR:HD1	1.50	0.58
1:J:311:PHE:CD2	1:J:394:GLN:HB3	2.39	0.58
2:K:93:SER:OG	2:K:94:HIS:N	2.37	0.58
2:B:39:ASP:O	2:B:131:ARG:NH2	2.36	0.58
2:B:156:LYS:NZ	2:B:255:PRO:O	2.34	0.58
1:D:71:LYS:NZ	1:D:106:ALA:O	2.37	0.58
1:D:319:VAL:HG23	1:D:352:SER:HA	1.85	0.58
2:E:185:VAL:HG23	2:E:213:HIS:HB2	1.85	0.58
2:E:292:LEU:HA	2:E:326:THR:O	2.03	0.58
1:G:111:SER:OG	1:G:113:GLU:OE1	2.16	0.58
2:H:37:ARG:NE	2:H:39:ASP:OD2	2.34	0.58
2:H:47:ILE:HG12	2:H:99:ILE:HB	1.86	0.58
1:J:52:LYS:NZ	1:J:110:ARG:O	2.31	0.58
1:J:340:ILE:HD13	1:J:357:PHE:HB3	1.85	0.58
2:K:271:PRO:HB3	2:K:284:LEU:HB2	1.85	0.58
4:S:33:GLY:H	4:S:100:THR:HA	1.68	0.58
1:A:37:ARG:HE	1:A:130:GLN:HG3	1.68	0.58
2:B:83:VAL:HG11	2:B:91:LEU:HD13	1.84	0.58
1:D:37:ARG:HE	1:D:130:GLN:HG3	1.68	0.58
2:E:360:TYR:O	2:E:364:THR:OG1	2.12	0.58
1:G:340:ILE:HD13	1:G:357:PHE:HB3	1.85	0.58
1:J:58:PRO:O	2:K:242:ARG:HB2	2.04	0.58
1:J:71:LYS:NZ	1:J:106:ALA:O	2.37	0.58
1:J:141:SER:H	1:J:143:ARG:NH2	2.00	0.58
2:K:156:LYS:NZ	2:K:255:PRO:O	2.34	0.58
2:K:196:LYS:O	2:K:226:TYR:N	2.37	0.58
2:B:95:HIS:HD1	2:B:98:TYR:HD1	1.50	0.58
2:B:221:LYS:O	2:B:224:ARG:NH1	2.36	0.58
1:D:40:PRO:HA	1:D:127:GLY:HA3	1.85	0.58
1:D:88:MET:HG3	1:D:91:GLY:HA3	1.86	0.58
1:G:71:LYS:NZ	1:G:106:ALA:O	2.37	0.58
2:H:164:VAL:O	2:H:252:LEU:N	2.35	0.58
1:J:37:ARG:NH1	1:J:132:MET:HB2	2.18	0.58
1:J:135:ILE:HD11	1:J:137:TYR:HB3	1.86	0.58
2:K:8:GLN:NE2	2:K:98:TYR:OH	2.37	0.58
2:B:292:LEU:HA	2:B:326:THR:O	2.03	0.57
1:D:157:ILE:HG23	1:D:160:ALA:HB3	1.86	0.57
1:G:37:ARG:HB2	1:G:130:GLN:HG3	1.86	0.57
1:G:102:GLN:NE2	1:G:104:SER:OG	2.34	0.57
2:H:272:LEU:N	2:H:283:HIS:O	2.18	0.57
1:J:179:VAL:N	1:J:186:TYR:O	2.32	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:83:VAL:HG11	2:K:91:LEU:HD13	1.84	0.57
1:A:29:LEU:HA	1:A:137:TYR:HA	1.84	0.57
1:A:157:ILE:HG23	1:A:160:ALA:HB3	1.86	0.57
2:B:11:LEU:HB3	2:B:233:TRP:CE3	2.39	0.57
1:G:88:MET:HG3	1:G:91:GLY:HA3	1.86	0.57
1:A:167:LEU:HD11	1:A:275:GLY:HA3	1.87	0.57
2:B:8:GLN:NE2	2:B:98:TYR:OH	2.37	0.57
2:E:326:THR:OG1	2:E:330:HIS:O	2.17	0.57
2:K:11:LEU:HB3	2:K:233:TRP:CE3	2.39	0.57
2:K:47:ILE:HG12	2:K:99:ILE:HB	1.86	0.57
2:K:152:ARG:N	2:K:259:VAL:O	2.37	0.57
2:B:222:GLN:NE2	2:B:222:GLN:O	2.38	0.57
2:B:271:PRO:HB3	2:B:284:LEU:HB2	1.85	0.57
2:E:8:GLN:NE2	2:E:98:TYR:OH	2.37	0.57
2:E:187:ILE:O	2:E:211:SER:OG	2.17	0.57
2:E:222:GLN:NE2	2:E:222:GLN:O	2.38	0.57
2:H:138:TYR:HA	2:H:288:HIS:CD2	2.40	0.57
2:H:179:SER:O	2:H:186:LYS:N	2.38	0.57
2:K:41:HIS:ND1	2:K:151:ASN:OD1	2.22	0.57
2:B:47:ILE:HG12	2:B:99:ILE:HB	1.86	0.57
1:D:263:ALA:HB3	1:D:268:ARG:HB3	1.87	0.57
2:E:1:ASP:OD2	2:E:4:THR:N	2.32	0.57
2:H:184:LYS:HZ1	2:H:213:HIS:HB2	1.70	0.57
2:K:319:THR:HG23	2:K:321:GLU:HG2	1.86	0.57
4:Q:33:GLY:H	4:Q:100:THR:HA	1.69	0.57
1:A:37:ARG:NH1	1:A:132:MET:HB2	2.18	0.57
1:A:71:LYS:NZ	1:A:106:ALA:O	2.37	0.57
2:H:11:LEU:HB3	2:H:233:TRP:CE3	2.39	0.57
1:J:39:ILE:O	1:J:128:THR:N	2.28	0.57
1:J:88:MET:HG3	1:J:91:GLY:HA3	1.86	0.57
1:J:328:ASN:HA	1:J:347:LEU:H	1.70	0.57
2:K:185:VAL:HG23	2:K:213:HIS:HB2	1.85	0.57
5:N:68:GLY:HA2	5:N:73:LEU:HA	1.87	0.57
1:D:48:THR:HG22	1:D:119:ALA:HB2	1.86	0.57
1:D:328:ASN:HA	1:D:347:LEU:H	1.70	0.57
2:H:93:SER:OG	2:H:94:HIS:N	2.37	0.57
2:H:220:VAL:H	2:H:221:LYS:HZ3	1.51	0.57
1:A:37:ARG:HB2	1:A:130:GLN:HG3	1.86	0.57
1:A:135:ILE:HG23	1:A:143:ARG:HB2	1.87	0.57
1:A:178:VAL:HA	1:A:187:ASN:HA	1.87	0.57
1:A:370:VAL:O	1:A:373:SER:OG	2.17	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:GLN:OE1	2:B:253:HIS:ND1	2.38	0.57
2:B:138:TYR:HA	2:B:288:HIS:CD2	2.40	0.57
1:G:37:ARG:O	1:G:130:GLN:N	2.23	0.57
1:G:46:TYR:HB2	1:G:207:ARG:HA	1.85	0.57
1:G:135:ILE:HG23	1:G:143:ARG:HB2	1.87	0.57
1:G:157:ILE:HG23	1:G:160:ALA:HB3	1.86	0.57
1:J:46:TYR:HB2	1:J:207:ARG:HA	1.85	0.57
1:J:157:ILE:HG23	1:J:160:ALA:HB3	1.86	0.57
2:K:138:TYR:HA	2:K:288:HIS:CD2	2.40	0.57
1:A:88:MET:HG3	1:A:91:GLY:HA3	1.86	0.57
1:A:223:GLN:HB2	1:A:233:PRO:HB2	1.87	0.57
1:A:263:ALA:HB3	1:A:268:ARG:HB3	1.87	0.57
1:A:293:GLU:N	1:A:293:GLU:OE1	2.38	0.57
1:A:311:PHE:CD2	1:A:394:GLN:HB3	2.39	0.57
1:D:226:GLN:H	1:D:231:HIS:CE1	2.22	0.57
1:D:289:THR:OG1	1:D:293:GLU:OE2	2.23	0.57
1:D:359:THR:OG1	1:D:361:ASN:OD1	2.22	0.57
1:G:141:SER:H	1:G:143:ARG:HH21	1.53	0.57
1:G:223:GLN:HB2	1:G:233:PRO:HB2	1.87	0.57
1:G:299:ASP:HB2	1:G:322:LYS:H	1.70	0.57
2:H:8:GLN:NE2	2:H:98:TYR:OH	2.37	0.57
2:H:185:VAL:HG23	2:H:213:HIS:HB2	1.85	0.57
2:H:229:ASP:OD1	2:H:230:ASN:N	2.38	0.57
1:J:102:GLN:NE2	1:J:104:SER:OG	2.34	0.57
1:J:163:ILE:N	1:J:280:SER:O	2.36	0.57
1:J:263:ALA:HB3	1:J:268:ARG:HB3	1.87	0.57
2:K:116:GLY:H	2:K:119:ARG:HH21	1.52	0.57
4:Q:170:ALA:HB3	4:Q:182:ASP:H	1.70	0.57
4:S:170:ALA:HB3	4:S:182:ASP:H	1.70	0.57
1:A:141:SER:H	1:A:143:ARG:HH21	1.53	0.57
2:B:196:LYS:O	2:B:226:TYR:N	2.37	0.57
2:B:323:LEU:O	2:B:334:ARG:HA	2.05	0.57
1:D:37:ARG:HB2	1:D:130:GLN:HG3	1.86	0.57
2:E:8:GLN:OE1	2:E:253:HIS:ND1	2.38	0.57
2:E:323:LEU:O	2:E:334:ARG:HA	2.05	0.57
2:H:194:GLN:NE2	2:H:207:GLY:O	2.38	0.57
2:K:47:ILE:N	2:K:99:ILE:O	2.27	0.57
5:T:68:GLY:HA2	5:T:73:LEU:HA	1.87	0.57
1:A:135:ILE:HD11	1:A:137:TYR:HB3	1.86	0.56
1:A:163:ILE:N	1:A:280:SER:O	2.36	0.56
1:A:221:LYS:O	1:A:235:THR:N	2.30	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:ALA:HA	1:D:359:THR:HB	1.87	0.56
1:G:135:ILE:HD11	1:G:137:TYR:HB3	1.86	0.56
1:G:178:VAL:HA	1:G:187:ASN:HA	1.87	0.56
1:G:328:ASN:HA	1:G:347:LEU:H	1.70	0.56
2:H:281:ILE:HA	2:H:315:ASN:HA	1.87	0.56
2:H:319:THR:HG23	2:H:321:GLU:HG2	1.87	0.56
1:J:111:SER:OG	1:J:113:GLU:OE1	2.16	0.56
2:K:45:ILE:N	2:K:101:ALA:O	2.25	0.56
2:K:229:ASP:OD1	2:K:230:ASN:N	2.38	0.56
2:B:18:ASP:HB2	2:B:26:ARG:HD2	1.88	0.56
2:B:229:ASP:OD1	2:B:230:ASN:N	2.38	0.56
1:D:223:GLN:HB2	1:D:233:PRO:HB2	1.87	0.56
2:E:179:SER:O	2:E:186:LYS:N	2.38	0.56
2:E:194:GLN:NE2	2:E:207:GLY:O	2.38	0.56
1:G:130:GLN:CB	1:G:148:TYR:HA	2.35	0.56
1:G:167:LEU:HD11	1:G:275:GLY:HA3	1.87	0.56
2:H:323:LEU:O	2:H:334:ARG:HA	2.05	0.56
1:J:135:ILE:HG23	1:J:143:ARG:HB2	1.87	0.56
1:J:230:VAL:O	2:K:239:ARG:HA	2.05	0.56
1:J:361:ASN:ND2	1:J:364:PRO:HB3	2.20	0.56
1:A:322:LYS:HD3	1:A:323:SER:N	2.21	0.56
1:A:361:ASN:ND2	1:A:364:PRO:HB3	2.20	0.56
2:B:89:CYS:HA	2:B:104:PRO:HD2	1.88	0.56
2:B:224:ARG:HB3	2:B:226:TYR:CE2	2.40	0.56
1:D:293:GLU:N	1:D:293:GLU:OE1	2.38	0.56
1:D:408:TRP:N	1:D:408:TRP:CD1	2.74	0.56
2:E:56:LYS:N	2:E:60:VAL:O	2.26	0.56
2:E:89:CYS:HA	2:E:104:PRO:HD2	1.88	0.56
2:E:138:TYR:HA	2:E:288:HIS:CD2	2.40	0.56
2:E:224:ARG:HB3	2:E:226:TYR:CE2	2.40	0.56
2:E:229:ASP:OD1	2:E:230:ASN:N	2.38	0.56
2:E:322:GLY:HA2	2:E:335:VAL:C	2.30	0.56
1:G:52:LYS:N	1:G:109:GLU:O	2.32	0.56
2:H:8:GLN:OE1	2:H:253:HIS:ND1	2.38	0.56
2:H:196:LYS:O	2:H:226:TYR:N	2.37	0.56
2:H:222:GLN:NE2	2:H:222:GLN:O	2.38	0.56
1:J:141:SER:H	1:J:143:ARG:HH21	1.53	0.56
2:K:1:ASP:OD2	2:K:4:THR:N	2.32	0.56
2:K:194:GLN:NE2	2:K:207:GLY:O	2.38	0.56
2:K:224:ARG:HB3	2:K:226:TYR:CE2	2.40	0.56
2:K:281:ILE:HA	2:K:315:ASN:HA	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:170:ALA:HB3	4:M:182:ASP:H	1.70	0.56
5:R:68:GLY:HA2	5:R:73:LEU:HA	1.87	0.56
5:R:121:ASP:O	5:R:136:ASN:N	2.37	0.56
1:A:48:THR:HG22	1:A:119:ALA:HB2	1.86	0.56
1:A:289:THR:OG1	1:A:293:GLU:OE2	2.23	0.56
1:A:299:ASP:HB2	1:A:322:LYS:H	1.70	0.56
2:E:11:LEU:HB3	2:E:233:TRP:CE3	2.39	0.56
1:G:359:THR:OG1	1:G:361:ASN:OD1	2.21	0.56
2:H:94:HIS:HA	2:H:100:LEU:H	1.71	0.56
2:H:271:PRO:HB3	2:H:284:LEU:HB2	1.85	0.56
2:H:322:GLY:HA2	2:H:335:VAL:C	2.30	0.56
1:J:37:ARG:HB2	1:J:130:GLN:HG3	1.86	0.56
1:J:42:THR:OG1	1:J:43:ASN:N	2.38	0.56
1:J:48:THR:HG22	1:J:119:ALA:HB2	1.86	0.56
2:K:179:SER:O	2:K:186:LYS:N	2.38	0.56
2:B:179:SER:O	2:B:186:LYS:N	2.38	0.56
1:D:361:ASN:ND2	1:D:364:PRO:HB3	2.20	0.56
3:F:117:MET:HA	3:F:121:GLN:O	2.06	0.56
1:J:38:ILE:HG23	1:J:129:VAL:HG22	1.88	0.56
1:J:130:GLN:CB	1:J:148:TYR:HA	2.35	0.56
2:K:221:LYS:O	2:K:224:ARG:NH1	2.36	0.56
2:K:322:GLY:HA2	2:K:335:VAL:C	2.30	0.56
3:L:117:MET:HA	3:L:121:GLN:O	2.06	0.56
1:D:42:THR:OG1	1:D:43:ASN:N	2.38	0.56
1:D:141:SER:H	1:D:143:ARG:HH21	1.53	0.56
1:G:293:GLU:OE1	1:G:293:GLU:N	2.38	0.56
1:G:385:LYS:NZ	2:H:339:GLU:O	2.20	0.56
2:H:152:ARG:N	2:H:259:VAL:O	2.37	0.56
1:J:37:ARG:N	1:J:130:GLN:O	2.30	0.56
1:J:178:VAL:HA	1:J:187:ASN:HA	1.87	0.56
1:J:338:ALA:HA	1:J:359:THR:HB	1.87	0.56
2:K:184:LYS:HZ1	2:K:213:HIS:HB2	1.71	0.56
2:K:323:LEU:O	2:K:334:ARG:HA	2.05	0.56
1:A:123:LYS:HD2	1:A:176:ASN:HB3	1.88	0.56
2:B:12:ALA:O	2:B:232:LYS:NZ	2.31	0.56
2:B:152:ARG:N	2:B:259:VAL:O	2.37	0.56
1:D:178:VAL:HA	1:D:187:ASN:HA	1.87	0.56
2:E:18:ASP:HB2	2:E:26:ARG:HD2	1.88	0.56
1:G:361:ASN:ND2	1:G:364:PRO:HB3	2.20	0.56
1:J:87:PHE:HB2	1:J:93:TYR:CZ	2.41	0.56
1:J:223:GLN:HB2	1:J:233:PRO:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:164:VAL:O	2:K:252:LEU:N	2.35	0.56
1:A:130:GLN:CB	1:A:148:TYR:HA	2.35	0.56
2:B:194:GLN:NE2	2:B:207:GLY:O	2.38	0.56
2:B:319:THR:HG23	2:B:321:GLU:HG2	1.87	0.56
1:D:87:PHE:HB2	1:D:93:TYR:CZ	2.41	0.56
1:D:123:LYS:HD2	1:D:176:ASN:HB3	1.88	0.56
1:D:136:THR:HG23	1:D:141:SER:HA	1.88	0.56
2:E:94:HIS:HA	2:E:100:LEU:H	1.71	0.56
1:G:87:PHE:HB2	1:G:93:TYR:CZ	2.41	0.56
2:H:22:CYS:SG	2:H:123:THR:OG1	2.64	0.56
2:H:116:GLY:H	2:H:119:ARG:HH21	1.52	0.56
1:J:407:ALA:CB	2:K:346:HIS:HB3	2.34	0.56
2:K:360:TYR:O	2:K:364:THR:OG1	2.11	0.56
5:P:154:GLN:N	5:P:193:CYS:O	2.29	0.56
1:A:328:ASN:HA	1:A:347:LEU:H	1.70	0.56
2:B:116:GLY:H	2:B:119:ARG:HH21	1.52	0.56
1:D:167:LEU:HD11	1:D:275:GLY:HA3	1.87	0.56
1:D:322:LYS:HD3	1:D:323:SER:N	2.21	0.56
2:E:47:ILE:N	2:E:99:ILE:O	2.27	0.56
1:G:338:ALA:HA	1:G:359:THR:HB	1.87	0.56
1:J:10:LYS:HB2	1:J:13:ILE:HG22	1.86	0.56
1:J:52:LYS:N	1:J:109:GLU:O	2.32	0.56
1:J:226:GLN:H	1:J:231:HIS:CE1	2.22	0.56
1:J:289:THR:OG1	1:J:293:GLU:OE2	2.23	0.56
2:K:146:VAL:O	2:K:265:ALA:N	2.39	0.56
5:P:68:GLY:HA2	5:P:73:LEU:HA	1.87	0.56
1:A:12:GLY:O	1:A:32:GLN:NE2	2.24	0.56
1:D:299:ASP:HB2	1:D:322:LYS:H	1.70	0.56
1:D:334:PRO:HD2	1:D:368:LEU:HB2	1.88	0.56
2:E:281:ILE:HA	2:E:315:ASN:HA	1.87	0.56
2:E:319:THR:HG23	2:E:321:GLU:HG2	1.86	0.56
3:F:228:LEU:N	3:F:240:SER:O	2.33	0.56
1:G:34:VAL:N	1:G:132:MET:O	2.29	0.56
1:G:38:ILE:HG23	1:G:129:VAL:HG22	1.88	0.56
1:G:263:ALA:HB3	1:G:268:ARG:HB3	1.87	0.56
1:G:289:THR:OG1	1:G:293:GLU:OE2	2.23	0.56
1:J:136:THR:HG23	1:J:141:SER:HA	1.88	0.56
1:A:195:THR:O	1:A:205:GLN:NE2	2.40	0.55
1:D:135:ILE:HG23	1:D:143:ARG:HB2	1.87	0.55
1:D:258:PHE:HB2	1:D:272:CYS:SG	2.46	0.55
2:E:45:ILE:N	2:E:101:ALA:O	2.25	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:224:ARG:HB3	2:H:226:TYR:CE2	2.40	0.55
3:I:229:GLY:O	3:I:240:SER:N	2.25	0.55
1:J:92:ALA:HB3	2:K:226:TYR:CE2	2.41	0.55
1:J:293:GLU:OE1	1:J:293:GLU:N	2.38	0.55
1:J:370:VAL:O	1:J:373:SER:OG	2.17	0.55
2:K:326:THR:OG1	2:K:330:HIS:O	2.17	0.55
4:O:170:ALA:HB3	4:O:182:ASP:H	1.70	0.55
1:A:37:ARG:NH2	1:A:146:ASP:OD2	2.40	0.55
2:B:322:GLY:HA2	2:B:335:VAL:C	2.30	0.55
1:G:12:GLY:O	1:G:32:GLN:NE2	2.24	0.55
2:H:80:ASN:O	2:H:114:HIS:N	2.29	0.55
2:H:290:THR:HG1	2:H:327:TRP:CD1	2.24	0.55
3:I:116:ILE:O	3:I:123:ASN:N	2.40	0.55
1:J:258:PHE:HB2	1:J:272:CYS:SG	2.46	0.55
4:O:52:SER:H	4:O:58:LYS:HA	1.71	0.55
1:A:38:ILE:HG23	1:A:129:VAL:HG22	1.88	0.55
1:A:87:PHE:HB2	1:A:93:TYR:CZ	2.41	0.55
1:G:48:THR:HG22	1:G:119:ALA:HB2	1.86	0.55
2:H:197:TYR:HA	2:H:224:ARG:O	2.06	0.55
1:J:123:LYS:HD2	1:J:176:ASN:HB3	1.88	0.55
1:J:339:VAL:N	1:J:358:SER:O	2.25	0.55
2:K:351:GLU:O	2:K:354:VAL:HG22	2.07	0.55
3:L:117:MET:N	3:L:142:ARG:O	2.29	0.55
1:A:136:THR:HG23	1:A:141:SER:HA	1.88	0.55
1:D:4:THR:OG1	1:D:279:ILE:O	2.20	0.55
1:D:37:ARG:NH1	1:D:132:MET:HB2	2.18	0.55
1:D:130:GLN:CB	1:D:148:TYR:HA	2.35	0.55
2:H:184:LYS:HD2	2:H:215:THR:HG23	1.89	0.55
1:J:195:THR:O	1:J:205:GLN:NE2	2.40	0.55
2:B:22:CYS:HG	2:B:123:THR:HG1	1.48	0.55
1:D:38:ILE:HG23	1:D:129:VAL:HG22	1.88	0.55
2:E:184:LYS:HD2	2:E:215:THR:HG23	1.89	0.55
1:G:408:TRP:N	1:G:408:TRP:CD1	2.74	0.55
2:H:146:VAL:O	2:H:265:ALA:N	2.39	0.55
3:L:116:ILE:O	3:L:123:ASN:N	2.40	0.55
5:P:121:ASP:O	5:P:136:ASN:N	2.37	0.55
1:A:226:GLN:H	1:A:231:HIS:CE1	2.22	0.55
2:B:326:THR:OG1	2:B:330:HIS:O	2.17	0.55
2:B:351:GLU:O	2:B:354:VAL:HG22	2.07	0.55
2:E:351:GLU:O	2:E:354:VAL:HG22	2.07	0.55
3:F:116:ILE:O	3:F:123:ASN:N	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:258:PHE:HB2	1:G:272:CYS:SG	2.46	0.55
1:G:322:LYS:HD3	1:G:323:SER:N	2.21	0.55
2:H:89:CYS:HA	2:H:104:PRO:HD2	1.88	0.55
1:A:42:THR:OG1	1:A:43:ASN:N	2.38	0.55
1:A:258:PHE:HB2	1:A:272:CYS:SG	2.46	0.55
1:D:37:ARG:NH2	1:D:146:ASP:OD2	2.40	0.55
1:D:124:VAL:O	1:D:176:ASN:ND2	2.31	0.55
1:G:42:THR:OG1	1:G:43:ASN:N	2.38	0.55
2:H:18:ASP:HB2	2:H:26:ARG:HD2	1.88	0.55
2:H:130:PHE:HZ	2:H:133:VAL:HG13	1.72	0.55
5:P:9:ALA:HA	5:P:105:ILE:N	2.22	0.55
5:R:154:GLN:N	5:R:193:CYS:O	2.29	0.55
1:A:408:TRP:N	1:A:408:TRP:CD1	2.74	0.55
1:D:370:VAL:O	1:D:373:SER:OG	2.17	0.55
1:G:195:THR:O	1:G:205:GLN:NE2	2.40	0.55
1:G:339:VAL:N	1:G:358:SER:O	2.25	0.55
2:H:12:ALA:O	2:H:232:LYS:NZ	2.31	0.55
2:H:68:MET:HA	2:H:73:GLN:HA	1.89	0.55
1:J:167:LEU:HD11	1:J:275:GLY:HA3	1.87	0.55
1:J:230:VAL:HG21	2:K:241:PRO:N	2.22	0.55
1:J:322:LYS:HD3	1:J:323:SER:N	2.21	0.55
2:K:94:HIS:HA	2:K:100:LEU:H	1.71	0.55
2:K:184:LYS:HD2	2:K:215:THR:HG23	1.89	0.55
4:M:52:SER:H	4:M:58:LYS:HA	1.71	0.55
2:B:36:VAL:HA	2:B:47:ILE:HG22	1.88	0.55
1:D:37:ARG:N	1:D:130:GLN:O	2.30	0.55
2:E:197:TYR:HA	2:E:224:ARG:O	2.06	0.55
1:G:37:ARG:NH2	1:G:146:ASP:OD2	2.40	0.55
1:G:93:TYR:HB3	1:G:95:PHE:CE1	2.42	0.55
3:I:117:MET:N	3:I:142:ARG:O	2.29	0.55
1:J:33:LEU:HA	1:J:133:VAL:HA	1.89	0.55
1:J:396:THR:OG1	1:J:397:GLU:N	2.40	0.55
2:K:18:ASP:HB2	2:K:26:ARG:HD2	1.88	0.55
2:K:68:MET:HA	2:K:73:GLN:HA	1.89	0.55
5:R:142:GLU:N	5:R:175:SER:O	2.26	0.55
4:S:170:ALA:O	4:S:172:ASN:N	2.40	0.55
1:A:359:THR:OG1	1:A:361:ASN:OD1	2.21	0.55
2:B:197:TYR:HA	2:B:224:ARG:O	2.06	0.55
2:B:281:ILE:HA	2:B:315:ASN:HA	1.87	0.55
1:D:134:ASN:HD21	1:D:142:TRP:HB3	1.72	0.55
1:J:299:ASP:HB2	1:J:322:LYS:H	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:89:CYS:HA	2:K:104:PRO:HD2	1.88	0.55
1:A:4:THR:OG1	1:A:279:ILE:O	2.20	0.54
1:A:334:PRO:HD2	1:A:368:LEU:HB2	1.88	0.54
1:A:434:LEU:HA	1:A:437:PHE:CD2	2.42	0.54
1:D:81:PHE:HB2	1:D:102:GLN:HB3	1.90	0.54
1:D:93:TYR:HB3	1:D:95:PHE:CE1	2.42	0.54
1:D:195:THR:O	1:D:205:GLN:NE2	2.40	0.54
2:E:152:ARG:N	2:E:259:VAL:O	2.37	0.54
1:G:7:MET:N	1:G:277:ILE:O	2.40	0.54
1:G:96:CYS:SG	2:H:222:GLN:NE2	2.71	0.54
2:H:196:LYS:HD2	2:H:226:TYR:HB2	1.90	0.54
2:H:393:CYS:O	2:H:396:PRO:HD2	2.07	0.54
3:I:228:LEU:N	3:I:240:SER:O	2.33	0.54
1:J:37:ARG:NH2	1:J:146:ASP:OD2	2.40	0.54
1:J:163:ILE:O	1:J:280:SER:N	2.35	0.54
2:K:197:TYR:HA	2:K:224:ARG:O	2.06	0.54
2:K:246:ASP:OD1	2:K:246:ASP:N	2.31	0.54
5:R:9:ALA:HA	5:R:105:ILE:N	2.22	0.54
1:A:338:ALA:HA	1:A:359:THR:HB	1.87	0.54
2:B:20:PRO:HA	2:B:26:ARG:HA	1.89	0.54
2:B:47:ILE:N	2:B:99:ILE:O	2.27	0.54
1:D:179:VAL:N	1:D:186:TYR:O	2.32	0.54
1:G:163:ILE:N	1:G:280:SER:O	2.36	0.54
1:J:408:TRP:N	1:J:408:TRP:CD1	2.74	0.54
2:K:196:LYS:HD2	2:K:226:TYR:HB2	1.89	0.54
4:M:157:LEU:N	4:M:200:GLY:O	2.40	0.54
3:C:156:ALA:O	3:C:160:ASP:N	2.40	0.54
2:E:20:PRO:HA	2:E:26:ARG:HA	1.89	0.54
1:G:134:ASN:HD21	1:G:142:TRP:HB3	1.72	0.54
2:H:45:ILE:N	2:H:101:ALA:O	2.25	0.54
1:J:15:TYR:N	1:J:31:ILE:O	2.41	0.54
2:K:36:VAL:HA	2:K:47:ILE:HG22	1.88	0.54
4:O:198:LEU:HA	4:O:213:PRO:HA	1.89	0.54
1:A:81:PHE:HB2	1:A:102:GLN:HB3	1.89	0.54
1:A:408:TRP:CD1	1:A:408:TRP:H	2.26	0.54
2:B:11:LEU:O	2:B:233:TRP:N	2.41	0.54
2:B:68:MET:HA	2:B:73:GLN:HA	1.89	0.54
2:B:130:PHE:HZ	2:B:133:VAL:HG13	1.72	0.54
3:C:116:ILE:O	3:C:123:ASN:N	2.40	0.54
1:D:33:LEU:HA	1:D:133:VAL:HA	1.89	0.54
1:G:123:LYS:HD2	1:G:176:ASN:HB3	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:226:GLN:H	1:G:231:HIS:CE1	2.22	0.54
2:H:20:PRO:HA	2:H:26:ARG:HA	1.89	0.54
4:S:157:LEU:N	4:S:200:GLY:O	2.40	0.54
4:S:198:LEU:HA	4:S:213:PRO:HA	1.89	0.54
5:T:154:GLN:N	5:T:193:CYS:O	2.29	0.54
1:A:396:THR:OG1	1:A:397:GLU:N	2.40	0.54
2:B:146:VAL:O	2:B:265:ALA:N	2.39	0.54
2:E:36:VAL:HA	2:E:47:ILE:HG22	1.89	0.54
1:G:136:THR:HG23	1:G:141:SER:HA	1.88	0.54
3:I:117:MET:HA	3:I:121:GLN:O	2.06	0.54
4:M:4:LEU:HA	4:M:24:ALA:HA	1.89	0.54
5:N:9:ALA:HA	5:N:105:ILE:N	2.22	0.54
4:Q:157:LEU:N	4:Q:200:GLY:O	2.40	0.54
4:Q:198:LEU:HA	4:Q:213:PRO:HA	1.89	0.54
1:A:134:ASN:HD21	1:A:142:TRP:HB3	1.72	0.54
2:E:130:PHE:HZ	2:E:133:VAL:HG13	1.72	0.54
2:E:393:CYS:O	2:E:396:PRO:HD2	2.07	0.54
1:G:334:PRO:HD2	1:G:368:LEU:HB2	1.88	0.54
1:G:408:TRP:CD1	1:G:408:TRP:H	2.26	0.54
2:H:177:LEU:HD22	2:H:195:VAL:HG11	1.90	0.54
2:K:11:LEU:O	2:K:233:TRP:N	2.41	0.54
5:N:154:GLN:N	5:N:193:CYS:O	2.29	0.54
1:A:93:TYR:HB3	1:A:95:PHE:CE1	2.42	0.54
1:A:361:ASN:HD22	1:A:364:PRO:HB3	1.73	0.54
1:D:163:ILE:N	1:D:280:SER:O	2.36	0.54
1:G:434:LEU:HA	1:G:437:PHE:CD2	2.42	0.54
2:H:36:VAL:HA	2:H:47:ILE:HG22	1.88	0.54
1:J:93:TYR:HB3	1:J:95:PHE:CE1	2.42	0.54
4:Q:4:LEU:HA	4:Q:24:ALA:HA	1.89	0.54
4:S:4:LEU:HA	4:S:24:ALA:HA	1.89	0.54
1:D:63:CYS:SG	1:D:64:GLY:N	2.81	0.54
2:E:177:LEU:HD22	2:E:195:VAL:HG11	1.90	0.54
2:H:1:ASP:OD2	2:H:4:THR:N	2.32	0.54
2:H:349:PRO:HA	2:H:352:VAL:HG22	1.90	0.54
1:J:231:HIS:HA	2:K:238:GLY:O	2.07	0.54
1:J:334:PRO:HD2	1:J:368:LEU:HB2	1.88	0.54
2:K:130:PHE:HZ	2:K:133:VAL:HG13	1.72	0.54
4:O:157:LEU:N	4:O:200:GLY:O	2.40	0.54
4:S:16:ARG:O	4:S:86:LEU:N	2.41	0.54
4:S:52:SER:H	4:S:58:LYS:HA	1.71	0.54
5:T:121:ASP:O	5:T:136:ASN:N	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:142:GLU:N	5:T:175:SER:O	2.26	0.54
1:A:102:GLN:NE2	1:A:104:SER:OG	2.34	0.54
3:C:114:PHE:N	3:C:126:ALA:O	2.41	0.54
2:E:22:CYS:HG	2:E:123:THR:HG1	1.55	0.54
2:K:393:CYS:O	2:K:396:PRO:HD2	2.08	0.54
5:N:142:GLU:N	5:N:175:SER:O	2.26	0.54
5:T:9:ALA:HA	5:T:105:ILE:N	2.22	0.54
2:B:94:HIS:HA	2:B:100:LEU:H	1.71	0.54
2:B:164:VAL:O	2:B:252:LEU:N	2.35	0.54
3:C:117:MET:HA	3:C:121:GLN:O	2.06	0.54
1:D:367:LYS:NZ	1:D:374:ALA:HB1	2.22	0.54
1:G:396:THR:OG1	1:G:397:GLU:N	2.40	0.54
3:I:114:PHE:N	3:I:126:ALA:O	2.41	0.54
3:I:156:ALA:O	3:I:160:ASP:N	2.40	0.54
1:J:12:GLY:O	1:J:32:GLN:NE2	2.24	0.54
1:J:367:LYS:NZ	1:J:374:ALA:HB1	2.22	0.54
4:O:21:SER:HA	4:O:80:TYR:HA	1.90	0.54
1:A:63:CYS:SG	1:A:64:GLY:N	2.81	0.53
1:A:426:LEU:O	1:A:429:THR:OG1	2.19	0.53
1:D:242:GLU:O	1:D:246:LYS:NZ	2.28	0.53
2:E:11:LEU:O	2:E:233:TRP:N	2.41	0.53
3:F:156:ALA:O	3:F:160:ASP:N	2.40	0.53
1:G:33:LEU:HA	1:G:133:VAL:HA	1.89	0.53
1:G:81:PHE:HB2	1:G:102:GLN:HB3	1.90	0.53
2:H:351:GLU:O	2:H:354:VAL:HG22	2.07	0.53
1:J:61:LYS:HG3	1:J:101:THR:HG21	1.90	0.53
2:K:168:GLN:CD	2:K:233:TRP:HE1	2.16	0.53
4:M:198:LEU:HA	4:M:213:PRO:HA	1.89	0.53
4:O:4:LEU:HA	4:O:24:ALA:HA	1.89	0.53
4:Q:52:SER:H	4:Q:58:LYS:HA	1.71	0.53
1:A:258:PHE:HA	2:B:297:LEU:O	2.09	0.53
2:B:289:PRO:HB2	2:B:307:TRP:HB3	1.90	0.53
1:D:258:PHE:CE1	2:E:299:SER:HA	2.43	0.53
1:G:15:TYR:N	1:G:31:ILE:O	2.41	0.53
1:G:367:LYS:NZ	1:G:374:ALA:HB1	2.22	0.53
1:J:134:ASN:HD21	1:J:142:TRP:HB3	1.72	0.53
3:L:228:LEU:N	3:L:240:SER:O	2.33	0.53
5:P:142:GLU:N	5:P:175:SER:O	2.26	0.53
1:A:15:TYR:N	1:A:31:ILE:O	2.41	0.53
2:B:196:LYS:HD2	2:B:226:TYR:HB2	1.89	0.53
1:D:61:LYS:HG3	1:D:101:THR:HG21	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:CYS:SG	1:D:96:CYS:N	2.81	0.53
1:D:206:SER:OG	1:D:211:SER:O	2.24	0.53
2:E:350:HIS:O	2:E:354:VAL:HG13	2.09	0.53
1:G:362:ILE:O	1:G:382:LYS:N	2.42	0.53
1:J:63:CYS:SG	1:J:64:GLY:N	2.81	0.53
1:J:124:VAL:O	1:J:176:ASN:ND2	2.31	0.53
1:J:408:TRP:CD1	1:J:408:TRP:H	2.26	0.53
2:K:20:PRO:HA	2:K:26:ARG:HA	1.89	0.53
2:K:177:LEU:HD22	2:K:195:VAL:HG11	1.90	0.53
2:K:289:PRO:HB2	2:K:307:TRP:HB3	1.91	0.53
4:M:16:ARG:O	4:M:86:LEU:N	2.41	0.53
4:Q:21:SER:HA	4:Q:80:TYR:HA	1.90	0.53
1:A:33:LEU:HA	1:A:133:VAL:HA	1.89	0.53
1:A:61:LYS:HG3	1:A:101:THR:HG21	1.91	0.53
2:B:393:CYS:O	2:B:396:PRO:HD2	2.08	0.53
1:D:21:ARG:NH1	1:D:285:ASP:OD1	2.28	0.53
2:H:47:ILE:N	2:H:99:ILE:O	2.27	0.53
2:H:350:HIS:O	2:H:354:VAL:HG13	2.09	0.53
1:J:91:GLY:HA2	2:K:173:ALA:O	2.07	0.53
2:K:8:GLN:OE1	2:K:253:HIS:ND1	2.38	0.53
4:S:21:SER:HA	4:S:80:TYR:HA	1.90	0.53
1:A:362:ILE:O	1:A:382:LYS:N	2.42	0.53
2:B:65:MET:O	2:B:75:SER:HA	2.09	0.53
2:B:273:VAL:HA	2:B:281:ILE:O	2.09	0.53
3:C:228:LEU:N	3:C:240:SER:O	2.33	0.53
1:D:15:TYR:N	1:D:31:ILE:O	2.41	0.53
1:D:396:THR:OG1	1:D:397:GLU:N	2.40	0.53
1:D:434:LEU:HD13	1:D:437:PHE:HD2	1.74	0.53
2:E:146:VAL:O	2:E:265:ALA:N	2.39	0.53
2:E:199:CYS:H	2:E:203:ASP:CG	2.17	0.53
3:F:117:MET:N	3:F:142:ARG:O	2.29	0.53
2:H:168:GLN:CD	2:H:233:TRP:HE1	2.16	0.53
1:J:49:CYS:H	1:J:204:LEU:HB3	1.73	0.53
1:J:81:PHE:HB2	1:J:102:GLN:HB3	1.90	0.53
1:A:7:MET:N	1:A:277:ILE:O	2.40	0.53
1:A:75:ASP:O	1:A:77:GLN:NE2	2.42	0.53
1:A:365:ALA:HA	1:A:378:LYS:HB2	1.91	0.53
1:A:434:LEU:HD13	1:A:437:PHE:HD2	1.74	0.53
1:D:49:CYS:H	1:D:204:LEU:HB3	1.73	0.53
1:D:156:LYS:NZ	1:D:282:ASP:OD2	2.42	0.53
1:D:362:ILE:O	1:D:382:LYS:N	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:LEU:HA	1:D:437:PHE:CD2	2.43	0.53
1:G:75:ASP:O	1:G:77:GLN:NE2	2.42	0.53
1:G:420:ALA:O	1:G:424:LEU:HG	2.09	0.53
2:H:7:THR:HG22	2:H:252:LEU:HD22	1.91	0.53
2:K:95:HIS:HA	2:K:157:ARG:HH21	1.74	0.53
2:B:95:HIS:HA	2:B:157:ARG:HH21	1.74	0.53
2:B:177:LEU:HD22	2:B:195:VAL:HG11	1.90	0.53
2:B:349:PRO:HA	2:B:352:VAL:HG22	1.90	0.53
1:D:34:VAL:N	1:D:132:MET:O	2.29	0.53
1:D:52:LYS:N	1:D:109:GLU:O	2.32	0.53
1:D:75:ASP:O	1:D:77:GLN:NE2	2.42	0.53
1:D:307:CYS:HB2	1:D:357:PHE:HE2	1.74	0.53
2:E:168:GLN:CD	2:E:233:TRP:HE1	2.16	0.53
1:G:63:CYS:SG	1:G:64:GLY:N	2.81	0.53
1:G:156:LYS:NZ	1:G:282:ASP:OD2	2.42	0.53
1:G:361:ASN:HD22	1:G:364:PRO:HB3	1.73	0.53
1:J:403:ILE:H	1:J:403:ILE:HD13	1.74	0.53
1:J:434:LEU:HA	1:J:437:PHE:CD2	2.42	0.53
2:K:349:PRO:HA	2:K:352:VAL:HG22	1.90	0.53
2:B:114:HIS:HA	2:B:119:ARG:HE	1.74	0.53
1:D:365:ALA:HA	1:D:378:LYS:HB2	1.91	0.53
1:D:403:ILE:HD13	1:D:403:ILE:H	1.74	0.53
2:E:273:VAL:HA	2:E:281:ILE:O	2.09	0.53
2:E:290:THR:O	2:E:307:TRP:HA	2.09	0.53
2:E:349:PRO:HA	2:E:352:VAL:HG22	1.90	0.53
1:G:21:ARG:NH1	1:G:285:ASP:OD1	2.28	0.53
2:H:11:LEU:O	2:H:233:TRP:N	2.41	0.53
2:K:12:ALA:O	2:K:232:LYS:NZ	2.31	0.53
1:A:57:SER:HB3	2:B:242:ARG:HA	1.89	0.53
1:A:156:LYS:NZ	1:A:282:ASP:OD2	2.42	0.53
2:B:168:GLN:CD	2:B:233:TRP:HE1	2.16	0.53
2:B:184:LYS:HD2	2:B:215:THR:HG23	1.89	0.53
2:B:290:THR:O	2:B:307:TRP:HA	2.09	0.53
1:D:420:ALA:O	1:D:424:LEU:HG	2.09	0.53
1:J:87:PHE:HA	1:J:93:TYR:HA	1.91	0.53
2:K:7:THR:HG22	2:K:252:LEU:HD22	1.91	0.53
3:L:114:PHE:N	3:L:126:ALA:O	2.42	0.53
4:O:170:ALA:O	4:O:172:ASN:N	2.39	0.53
2:B:45:ILE:N	2:B:101:ALA:O	2.25	0.53
2:B:350:HIS:O	2:B:354:VAL:HG13	2.09	0.53
2:E:289:PRO:HB2	2:E:307:TRP:HB3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:114:PHE:N	3:F:126:ALA:O	2.41	0.53
1:G:61:LYS:HG3	1:G:101:THR:HG21	1.90	0.53
1:G:370:VAL:O	1:G:373:SER:OG	2.18	0.53
2:H:183:ALA:HB2	5:R:96:THR:CB	2.39	0.53
2:H:229:ASP:OD1	2:H:231:LYS:NZ	2.42	0.53
2:H:332:PRO:O	2:H:334:ARG:NH1	2.42	0.53
1:J:75:ASP:O	1:J:77:GLN:NE2	2.42	0.53
1:J:151:GLY:HA3	1:J:166:PRO:HD3	1.91	0.53
1:J:420:ALA:O	1:J:424:LEU:HG	2.09	0.53
2:K:331:PRO:O	2:K:333:LYS:NZ	2.30	0.53
3:L:156:ALA:O	3:L:160:ASP:N	2.40	0.53
1:A:191:PRO:HB2	1:A:193:TYR:CE2	2.45	0.52
1:A:339:VAL:O	1:A:357:PHE:HA	2.10	0.52
1:D:191:PRO:HB2	1:D:193:TYR:CE2	2.44	0.52
2:E:65:MET:O	2:E:75:SER:HA	2.09	0.52
2:E:68:MET:HA	2:E:73:GLN:HA	1.89	0.52
2:E:196:LYS:HD2	2:E:226:TYR:HB2	1.89	0.52
2:K:65:MET:O	2:K:75:SER:HA	2.09	0.52
2:K:187:ILE:O	2:K:211:SER:OG	2.17	0.52
2:K:290:THR:O	2:K:307:TRP:HA	2.09	0.52
2:K:350:HIS:O	2:K:354:VAL:HG13	2.09	0.52
2:K:356:TYR:HA	2:K:359:ARG:HD3	1.91	0.52
1:D:220:LEU:O	1:D:221:LYS:NZ	2.38	0.52
1:D:408:TRP:CD1	1:D:408:TRP:H	2.26	0.52
2:E:332:PRO:O	2:E:334:ARG:NH1	2.42	0.52
2:E:356:TYR:HA	2:E:359:ARG:HD3	1.91	0.52
4:M:21:SER:HA	4:M:80:TYR:HA	1.90	0.52
4:S:131:LEU:O	4:S:135:SER:N	2.42	0.52
5:T:197:HIS:HA	5:T:205:THR:H	1.75	0.52
1:A:403:ILE:HD13	1:A:403:ILE:H	1.74	0.52
1:A:420:ALA:O	1:A:424:LEU:HG	2.09	0.52
1:D:261:SER:O	1:D:270:GLU:N	2.42	0.52
2:E:7:THR:HG22	2:E:252:LEU:HD22	1.91	0.52
2:E:95:HIS:HA	2:E:157:ARG:HH21	1.74	0.52
2:E:164:VAL:O	2:E:252:LEU:N	2.35	0.52
2:H:293:THR:HA	2:H:304:THR:O	2.10	0.52
1:J:156:LYS:NZ	1:J:282:ASP:OD2	2.42	0.52
2:K:199:CYS:N	2:K:203:ASP:OD2	2.38	0.52
1:A:9:ASN:N	1:A:275:GLY:O	2.30	0.52
1:A:151:GLY:HA3	1:A:166:PRO:HD3	1.91	0.52
3:C:226:ILE:O	3:C:242:VAL:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:PHE:HA	1:D:93:TYR:HA	1.91	0.52
2:E:79:ASP:OD1	2:E:79:ASP:N	2.42	0.52
2:E:114:HIS:HA	2:E:119:ARG:HE	1.74	0.52
1:G:191:PRO:HB2	1:G:193:TYR:CE2	2.44	0.52
1:J:265:GLU:H	1:J:265:GLU:CD	2.17	0.52
2:K:293:THR:HA	2:K:304:THR:O	2.10	0.52
2:K:332:PRO:O	2:K:334:ARG:NH1	2.42	0.52
5:R:197:HIS:HA	5:R:205:THR:H	1.74	0.52
1:A:307:CYS:HB2	1:A:357:PHE:HE2	1.74	0.52
2:E:118:ASN:CG	2:E:120:HIS:H	2.17	0.52
1:G:34:VAL:HB	1:G:132:MET:HG2	1.92	0.52
1:G:307:CYS:HB2	1:G:357:PHE:HE2	1.74	0.52
2:H:95:HIS:CB	2:H:157:ARG:HE	2.22	0.52
2:H:95:HIS:HA	2:H:157:ARG:HH21	1.74	0.52
2:H:166:MET:SD	2:H:252:LEU:HD11	2.50	0.52
1:J:62:CYS:SG	1:J:96:CYS:N	2.81	0.52
1:J:362:ILE:O	1:J:382:LYS:N	2.42	0.52
1:J:365:ALA:HA	1:J:378:LYS:HB2	1.91	0.52
4:O:16:ARG:O	4:O:86:LEU:N	2.41	0.52
4:Q:16:ARG:O	4:Q:86:LEU:N	2.41	0.52
4:Q:131:LEU:O	4:Q:135:SER:N	2.42	0.52
1:A:34:VAL:N	1:A:132:MET:O	2.28	0.52
1:A:49:CYS:H	1:A:204:LEU:HB3	1.73	0.52
2:B:7:THR:HG22	2:B:252:LEU:HD22	1.91	0.52
1:D:361:ASN:HD22	1:D:364:PRO:HB3	1.73	0.52
1:G:265:GLU:H	1:G:265:GLU:CD	2.17	0.52
2:H:65:MET:O	2:H:75:SER:HA	2.09	0.52
2:H:273:VAL:HA	2:H:281:ILE:O	2.09	0.52
2:K:95:HIS:CB	2:K:157:ARG:HE	2.22	0.52
1:A:265:GLU:H	1:A:265:GLU:CD	2.17	0.52
2:B:199:CYS:H	2:B:203:ASP:CG	2.17	0.52
1:G:37:ARG:HH21	1:G:130:GLN:CD	2.18	0.52
1:G:137:TYR:O	1:G:140:VAL:N	2.34	0.52
1:G:163:ILE:O	1:G:280:SER:N	2.35	0.52
1:G:365:ALA:HA	1:G:378:LYS:HB2	1.91	0.52
1:J:34:VAL:HB	1:J:132:MET:HG2	1.92	0.52
1:J:328:ASN:OD1	1:J:329:CYS:N	2.43	0.52
1:J:339:VAL:O	1:J:357:PHE:HA	2.10	0.52
1:J:361:ASN:HD22	1:J:364:PRO:HB3	1.73	0.52
2:K:170:GLY:HA3	2:K:243:GLY:CA	2.40	0.52
4:M:170:ALA:O	4:M:172:ASN:N	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:VAL:HB	1:A:132:MET:HG2	1.92	0.52
2:B:194:GLN:OE1	2:B:209:THR:N	2.43	0.52
2:B:356:TYR:HA	2:B:359:ARG:HD3	1.91	0.52
1:D:52:LYS:NZ	1:D:110:ARG:O	2.31	0.52
2:E:280:LEU:N	2:E:316:PHE:O	2.39	0.52
2:E:293:THR:HA	2:E:304:THR:O	2.09	0.52
1:G:403:ILE:HD13	1:G:403:ILE:H	1.74	0.52
2:H:290:THR:O	2:H:307:TRP:HA	2.09	0.52
4:M:131:LEU:O	4:M:135:SER:N	2.42	0.52
5:N:197:HIS:HA	5:N:205:THR:H	1.75	0.52
1:A:37:ARG:HH21	1:A:130:GLN:CD	2.18	0.52
1:A:256:ALA:O	2:B:295:ARG:NE	2.26	0.52
1:A:309:TYR:HD1	1:A:382:LYS:HB2	1.75	0.52
2:B:46:ARG:HD2	2:B:256:PHE:HB2	1.92	0.52
2:E:395:THR:O	2:E:398:LYS:HG2	2.10	0.52
1:G:151:GLY:HA3	1:G:166:PRO:HD3	1.91	0.52
1:G:339:VAL:O	1:G:357:PHE:HA	2.10	0.52
2:H:114:HIS:HA	2:H:119:ARG:HE	1.74	0.52
2:H:289:PRO:HB2	2:H:307:TRP:HB3	1.91	0.52
1:J:7:MET:N	1:J:277:ILE:O	2.40	0.52
1:J:90:GLY:O	2:K:174:ASP:HA	2.10	0.52
1:J:307:CYS:HB2	1:J:357:PHE:HE2	1.74	0.52
2:K:46:ARG:HD2	2:K:256:PHE:HB2	1.92	0.52
2:K:118:ASN:CG	2:K:120:HIS:H	2.17	0.52
2:K:169:PRO:HD3	2:K:233:TRP:HA	1.92	0.52
1:A:240:GLY:HA2	1:A:243:ARG:HG3	1.92	0.52
1:D:193:TYR:HB3	1:D:207:ARG:HH22	1.75	0.52
1:D:339:VAL:O	1:D:357:PHE:HA	2.10	0.52
2:E:3:ASP:OD1	2:E:3:ASP:N	2.43	0.52
2:E:12:ALA:O	2:E:232:LYS:NZ	2.31	0.52
2:E:46:ARG:HD2	2:E:256:PHE:HB2	1.92	0.52
1:G:128:THR:OG1	1:G:129:VAL:N	2.43	0.52
1:G:434:LEU:HD13	1:G:437:PHE:HD2	1.74	0.52
2:H:46:ARG:HD2	2:H:256:PHE:HB2	1.92	0.52
2:H:118:ASN:CG	2:H:120:HIS:H	2.17	0.52
2:H:199:CYS:N	2:H:203:ASP:OD2	2.38	0.52
1:J:191:PRO:HB2	1:J:193:TYR:CE2	2.44	0.52
1:J:240:GLY:HA2	1:J:243:ARG:HG3	1.92	0.52
5:P:197:HIS:HA	5:P:205:THR:H	1.74	0.52
1:A:30:GLN:NE2	1:A:32:GLN:HB2	2.23	0.51
1:A:367:LYS:NZ	1:A:374:ALA:HB1	2.22	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:ASN:CG	2:B:120:HIS:H	2.17	0.51
2:B:166:MET:SD	2:B:252:LEU:HD11	2.50	0.51
2:B:306:GLN:HG2	2:B:327:TRP:HZ3	1.75	0.51
3:C:115:PRO:HA	3:C:125:TYR:HA	1.92	0.51
1:D:24:TYR:HD2	1:D:288:PHE:CG	2.28	0.51
1:D:265:GLU:H	1:D:265:GLU:CD	2.17	0.51
1:D:309:TYR:HD1	1:D:382:LYS:HB2	1.75	0.51
2:E:194:GLN:OE1	2:E:209:THR:N	2.43	0.51
1:G:16:LYS:HE3	1:G:28:HIS:HB2	1.92	0.51
1:G:266:PRO:HG2	1:G:268:ARG:HB3	1.93	0.51
2:H:194:GLN:OE1	2:H:209:THR:N	2.43	0.51
1:J:91:GLY:HA2	2:K:173:ALA:C	2.35	0.51
1:J:309:TYR:HD1	1:J:382:LYS:HB2	1.75	0.51
1:J:436:LEU:HA	1:J:439:HIS:HB3	1.92	0.51
2:K:114:HIS:HA	2:K:119:ARG:HE	1.74	0.51
2:K:273:VAL:HA	2:K:281:ILE:O	2.09	0.51
2:K:395:THR:O	2:K:398:LYS:HG2	2.10	0.51
4:O:131:LEU:O	4:O:135:SER:N	2.42	0.51
2:B:293:THR:HA	2:B:304:THR:O	2.10	0.51
1:D:305:THR:HB	1:D:316:ILE:O	2.11	0.51
1:D:436:LEU:HA	1:D:439:HIS:HB3	1.92	0.51
2:E:118:ASN:OD1	2:E:119:ARG:N	2.44	0.51
1:G:18:LEU:HD12	1:G:27:VAL:C	2.36	0.51
1:G:49:CYS:H	1:G:204:LEU:HB3	1.73	0.51
1:G:87:PHE:HA	1:G:93:TYR:HA	1.91	0.51
1:G:206:SER:OG	1:G:211:SER:O	2.25	0.51
1:G:240:GLY:HA2	1:G:243:ARG:HG3	1.92	0.51
2:H:3:ASP:OD1	2:H:3:ASP:N	2.43	0.51
2:H:118:ASN:OD1	2:H:119:ARG:N	2.44	0.51
2:H:199:CYS:H	2:H:203:ASP:CG	2.17	0.51
2:H:395:THR:O	2:H:398:LYS:HG2	2.10	0.51
1:J:37:ARG:HH21	1:J:130:GLN:CD	2.18	0.51
1:J:434:LEU:HD13	1:J:437:PHE:HD2	1.74	0.51
1:A:195:THR:HG22	1:D:152:GLU:OE2	2.10	0.51
2:B:199:CYS:N	2:B:203:ASP:OD2	2.39	0.51
1:D:328:ASN:OD1	1:D:329:CYS:N	2.43	0.51
1:D:409:SER:HA	1:D:412:LYS:HG2	1.93	0.51
2:K:185:VAL:HG11	2:K:223:CYS:SG	2.50	0.51
3:L:226:ILE:O	3:L:242:VAL:N	2.42	0.51
1:A:409:SER:HA	1:A:412:LYS:HG2	1.93	0.51
2:B:395:THR:O	2:B:398:LYS:HG2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:ARG:HH12	1:D:146:ASP:HB2	1.76	0.51
1:D:37:ARG:HH21	1:D:130:GLN:CD	2.18	0.51
1:D:39:ILE:N	1:D:128:THR:O	2.43	0.51
2:E:160:GLN:NE2	2:E:253:HIS:HB3	2.25	0.51
2:E:166:MET:SD	2:E:252:LEU:HD11	2.50	0.51
2:E:185:VAL:HG11	2:E:223:CYS:SG	2.50	0.51
1:G:9:ASN:N	1:G:275:GLY:O	2.30	0.51
2:H:170:GLY:HA3	2:H:243:GLY:CA	2.40	0.51
3:I:226:ILE:O	3:I:242:VAL:N	2.42	0.51
1:J:11:VAL:HG13	1:J:33:LEU:HD22	1.92	0.51
1:J:24:TYR:HD2	1:J:288:PHE:CG	2.28	0.51
1:J:39:ILE:N	1:J:128:THR:O	2.44	0.51
1:J:266:PRO:HG2	1:J:268:ARG:HB3	1.92	0.51
2:K:166:MET:SD	2:K:252:LEU:HD11	2.50	0.51
2:K:194:GLN:OE1	2:K:209:THR:N	2.43	0.51
2:K:310:ARG:CZ	2:K:310:ARG:HB2	2.40	0.51
4:Q:108:ASP:O	5:R:46:LEU:O	2.28	0.51
1:A:193:TYR:HB3	1:A:207:ARG:HH22	1.75	0.51
2:E:170:GLY:HA3	2:E:243:GLY:CA	2.40	0.51
2:H:160:GLN:NE2	2:H:253:HIS:HB3	2.26	0.51
2:H:185:VAL:HG11	2:H:223:CYS:SG	2.50	0.51
3:I:115:PRO:HA	3:I:125:TYR:HA	1.92	0.51
2:K:7:THR:O	2:K:10:LYS:NZ	2.42	0.51
1:A:328:ASN:OD1	1:A:329:CYS:N	2.43	0.51
1:A:405:ALA:HB1	2:B:346:HIS:CE1	2.46	0.51
2:B:185:VAL:HG11	2:B:223:CYS:SG	2.50	0.51
1:D:233:PRO:HB3	2:H:144:HIS:CD2	2.46	0.51
2:E:255:PRO:HG2	2:E:256:PHE:CE2	2.46	0.51
1:G:24:TYR:HD2	1:G:288:PHE:CG	2.28	0.51
1:G:125:HIS:CD2	1:G:125:HIS:N	2.79	0.51
1:G:193:TYR:HB3	1:G:207:ARG:HH22	1.75	0.51
1:G:309:TYR:HD1	1:G:382:LYS:HB2	1.75	0.51
2:H:356:TYR:HA	2:H:359:ARG:HD3	1.91	0.51
4:O:68:PHE:HA	4:O:83:MET:HA	1.93	0.51
1:A:265:GLU:CD	1:A:266:PRO:HD3	2.36	0.51
2:B:255:PRO:HG2	2:B:256:PHE:CE2	2.46	0.51
2:B:332:PRO:O	2:B:334:ARG:NH1	2.42	0.51
3:C:117:MET:N	3:C:142:ARG:O	2.29	0.51
1:D:16:LYS:HE3	1:D:28:HIS:HB2	1.93	0.51
1:G:328:ASN:OD1	1:G:329:CYS:N	2.43	0.51
1:J:59:VAL:HA	2:K:242:ARG:CG	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:305:THR:HB	1:J:316:ILE:O	2.10	0.51
1:J:409:SER:HA	1:J:412:LYS:HG2	1.93	0.51
2:K:160:GLN:NE2	2:K:253:HIS:HB3	2.26	0.51
2:K:199:CYS:H	2:K:203:ASP:CG	2.17	0.51
1:A:16:LYS:HE3	1:A:28:HIS:HB2	1.93	0.51
2:B:272:LEU:HD22	2:B:283:HIS:CD2	2.46	0.51
1:D:30:GLN:NE2	1:D:32:GLN:HB2	2.23	0.51
1:G:37:ARG:HH12	1:G:146:ASP:HB2	1.76	0.51
1:J:18:LEU:HD12	1:J:27:VAL:C	2.36	0.51
1:J:92:ALA:H	2:K:173:ALA:CB	2.24	0.51
2:K:229:ASP:OD1	2:K:231:LYS:NZ	2.42	0.51
3:L:115:PRO:HA	3:L:125:TYR:HA	1.92	0.51
1:A:23:GLY:O	1:A:290:ARG:NH1	2.44	0.51
1:A:87:PHE:HA	1:A:93:TYR:HA	1.91	0.51
2:B:310:ARG:HB2	2:B:310:ARG:CZ	2.40	0.51
2:E:7:THR:O	2:E:10:LYS:NZ	2.42	0.51
2:E:36:VAL:HG21	2:E:126:HIS:HD2	1.76	0.51
2:E:272:LEU:HD22	2:E:283:HIS:CD2	2.46	0.51
1:G:265:GLU:CD	1:G:266:PRO:HD3	2.36	0.51
1:G:305:THR:HB	1:G:316:ILE:O	2.11	0.51
2:H:143:GLU:OE1	2:H:144:HIS:ND1	2.44	0.51
2:H:169:PRO:HD3	2:H:233:TRP:HA	1.92	0.51
1:J:193:TYR:HB3	1:J:207:ARG:HH22	1.75	0.51
1:J:319:VAL:N	1:J:353:PHE:O	2.44	0.51
2:K:255:PRO:HG2	2:K:256:PHE:CE2	2.46	0.51
5:N:89:GLN:O	5:N:91:CYS:N	2.44	0.51
5:P:89:GLN:O	5:P:91:CYS:N	2.44	0.51
4:Q:170:ALA:O	4:Q:172:ASN:N	2.39	0.51
1:A:124:VAL:O	1:A:176:ASN:ND2	2.31	0.51
2:B:3:ASP:OD1	2:B:3:ASP:N	2.43	0.51
2:B:95:HIS:CB	2:B:157:ARG:HE	2.22	0.51
2:B:170:GLY:HA3	2:B:243:GLY:CA	2.40	0.51
2:B:267:LEU:HD12	2:B:329:ASN:HB2	1.93	0.51
1:D:151:GLY:HA3	1:D:166:PRO:HD3	1.91	0.51
1:D:163:ILE:O	1:D:280:SER:N	2.35	0.51
3:F:115:PRO:HA	3:F:125:TYR:HA	1.92	0.51
2:H:306:GLN:HG2	2:H:327:TRP:HZ3	1.75	0.51
1:J:16:LYS:HE3	1:J:28:HIS:HB2	1.92	0.51
1:J:261:SER:O	1:J:270:GLU:N	2.42	0.51
1:A:21:ARG:NH1	1:A:285:ASP:OD1	2.28	0.50
1:A:254:ASP:O	2:B:295:ARG:NH1	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:VAL:N	1:A:353:PHE:O	2.44	0.50
1:D:34:VAL:HB	1:D:132:MET:HG2	1.92	0.50
1:D:102:GLN:NE2	1:D:104:SER:OG	2.34	0.50
1:D:240:GLY:HA2	1:D:243:ARG:HG3	1.92	0.50
1:D:265:GLU:CD	1:D:266:PRO:HD3	2.36	0.50
1:D:266:PRO:HG2	1:D:268:ARG:HB3	1.92	0.50
2:H:291:LEU:HD12	2:H:307:TRP:NE1	2.27	0.50
1:J:59:VAL:CA	2:K:242:ARG:HB2	2.37	0.50
1:J:128:THR:OG1	1:J:129:VAL:N	2.43	0.50
2:K:19:CYS:O	2:K:27:CYS:N	2.45	0.50
2:K:44:VAL:HA	2:K:102:GLN:HA	1.93	0.50
2:K:46:ARG:HA	2:K:100:LEU:HA	1.93	0.50
2:K:118:ASN:OD1	2:K:119:ARG:N	2.44	0.50
5:N:121:ASP:O	5:N:136:ASN:N	2.37	0.50
4:Q:61:ALA:HA	5:R:96:THR:O	2.11	0.50
5:R:89:GLN:O	5:R:91:CYS:N	2.44	0.50
1:A:38:ILE:HB	1:A:269:ALA:HB3	1.93	0.50
1:A:305:THR:HB	1:A:316:ILE:O	2.11	0.50
1:A:436:LEU:HA	1:A:439:HIS:HB3	1.92	0.50
2:B:160:GLN:NE2	2:B:253:HIS:HB3	2.26	0.50
1:D:18:LEU:HD12	1:D:27:VAL:C	2.36	0.50
1:G:37:ARG:N	1:G:130:GLN:O	2.30	0.50
2:H:7:THR:O	2:H:10:LYS:NZ	2.42	0.50
2:H:63:ALA:O	2:H:77:LYS:HD3	2.11	0.50
2:H:79:ASP:N	2:H:79:ASP:OD1	2.42	0.50
2:H:294:THR:O	2:H:303:PRO:HA	2.12	0.50
2:H:335:VAL:HG12	2:H:336:TRP:O	2.12	0.50
2:K:3:ASP:N	2:K:3:ASP:OD1	2.43	0.50
2:K:143:GLU:OE1	2:K:144:HIS:ND1	2.44	0.50
2:K:272:LEU:HD22	2:K:283:HIS:CD2	2.46	0.50
2:K:294:THR:O	2:K:303:PRO:HA	2.12	0.50
5:T:89:GLN:O	5:T:91:CYS:N	2.44	0.50
2:B:1:ASP:OD2	2:B:4:THR:N	2.32	0.50
2:B:44:VAL:HA	2:B:102:GLN:HA	1.93	0.50
2:B:220:VAL:H	2:B:221:LYS:HZ1	1.60	0.50
2:B:335:VAL:HG12	2:B:336:TRP:O	2.12	0.50
1:D:31:ILE:HG13	1:D:133:VAL:HG21	1.93	0.50
1:D:128:THR:OG1	1:D:129:VAL:N	2.43	0.50
2:E:44:VAL:HA	2:E:102:GLN:HA	1.93	0.50
1:G:31:ILE:HG13	1:G:133:VAL:HG21	1.93	0.50
4:Q:61:ALA:HB1	5:R:97:PHE:HA	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:THR:OG1	1:A:129:VAL:N	2.43	0.50
1:A:206:SER:OG	1:A:211:SER:O	2.24	0.50
2:B:118:ASN:OD1	2:B:119:ARG:N	2.44	0.50
2:B:287:ASP:O	2:B:288:HIS:ND1	2.45	0.50
1:D:7:MET:N	1:D:277:ILE:O	2.40	0.50
1:D:11:VAL:HG13	1:D:33:LEU:HD22	1.93	0.50
1:D:405:ALA:HB3	1:D:408:TRP:NE1	2.27	0.50
2:E:291:LEU:HD12	2:E:307:TRP:NE1	2.27	0.50
1:G:220:LEU:O	1:G:221:LYS:NZ	2.38	0.50
2:H:255:PRO:HG2	2:H:256:PHE:CE2	2.46	0.50
1:J:206:SER:OG	1:J:211:SER:O	2.25	0.50
5:T:92:ASN:N	5:T:100:GLY:HA2	2.27	0.50
1:A:31:ILE:HG13	1:A:133:VAL:HG21	1.93	0.50
2:B:143:GLU:OE1	2:B:144:HIS:ND1	2.44	0.50
1:D:23:GLY:O	1:D:290:ARG:NH1	2.44	0.50
2:E:19:CYS:O	2:E:27:CYS:N	2.45	0.50
2:E:63:ALA:O	2:E:77:LYS:HD3	2.11	0.50
2:E:94:HIS:HA	2:E:99:ILE:HA	1.94	0.50
2:E:169:PRO:HD3	2:E:233:TRP:HA	1.92	0.50
1:G:62:CYS:SG	1:G:96:CYS:N	2.81	0.50
2:H:36:VAL:HG21	2:H:126:HIS:HD2	1.76	0.50
2:H:272:LEU:HD22	2:H:283:HIS:CD2	2.46	0.50
1:J:23:GLY:O	1:J:290:ARG:NH1	2.44	0.50
1:J:37:ARG:HH12	1:J:146:ASP:HB2	1.76	0.50
2:K:306:GLN:HG2	2:K:327:TRP:HZ3	1.76	0.50
4:M:68:PHE:HA	4:M:83:MET:HA	1.93	0.50
1:A:37:ARG:HH12	1:A:146:ASP:HB2	1.76	0.50
2:B:46:ARG:HA	2:B:100:LEU:HA	1.93	0.50
2:B:291:LEU:HD12	2:B:307:TRP:NE1	2.27	0.50
2:B:294:THR:O	2:B:303:PRO:HA	2.12	0.50
2:B:390:ARG:O	2:B:394:ILE:HG12	2.12	0.50
2:E:184:LYS:HZ1	2:E:213:HIS:HB2	1.77	0.50
2:E:187:ILE:HD12	2:E:208:ILE:HD11	1.94	0.50
2:E:294:THR:O	2:E:303:PRO:HA	2.12	0.50
2:E:360:TYR:HB2	2:E:364:THR:H	1.77	0.50
1:G:11:VAL:HG13	1:G:33:LEU:HD22	1.92	0.50
1:G:38:ILE:HB	1:G:269:ALA:HB3	1.94	0.50
1:G:261:SER:O	1:G:270:GLU:N	2.42	0.50
1:G:409:SER:HA	1:G:412:LYS:HG2	1.92	0.50
2:H:287:ASP:O	2:H:288:HIS:ND1	2.45	0.50
1:J:34:VAL:N	1:J:132:MET:O	2.29	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:265:GLU:CD	1:J:266:PRO:HD3	2.36	0.50
2:K:36:VAL:HG21	2:K:126:HIS:HD2	1.76	0.50
2:K:74:LYS:HE2	2:K:75:SER:H	1.77	0.50
4:Q:114:ILE:O	4:Q:116:VAL:N	2.43	0.50
1:A:11:VAL:HG13	1:A:33:LEU:HD22	1.92	0.50
1:A:24:TYR:HD2	1:A:288:PHE:CG	2.28	0.50
1:A:53:THR:HG22	1:A:108:VAL:HG22	1.94	0.50
2:B:169:PRO:HD3	2:B:233:TRP:HA	1.92	0.50
2:E:267:LEU:HD12	2:E:329:ASN:HB2	1.93	0.50
2:E:306:GLN:HG2	2:E:327:TRP:HZ3	1.76	0.50
2:E:310:ARG:CZ	2:E:310:ARG:HB2	2.40	0.50
1:G:21:ARG:HG2	1:G:24:TYR:CG	2.47	0.50
1:G:192:GLU:HB2	1:G:197:LYS:HE2	1.93	0.50
2:H:384:TRP:HE3	2:H:385:LEU:HD22	1.77	0.50
1:J:44:LEU:HA	1:J:122:TYR:HA	1.94	0.50
2:K:63:ALA:O	2:K:77:LYS:HD3	2.11	0.50
4:Q:68:PHE:HA	4:Q:83:MET:HA	1.93	0.50
1:A:21:ARG:HG2	1:A:24:TYR:CG	2.47	0.50
1:A:193:TYR:HB3	1:A:207:ARG:NH1	2.27	0.50
2:B:63:ALA:O	2:B:77:LYS:HD3	2.11	0.50
3:C:229:GLY:O	3:C:240:SER:N	2.25	0.50
1:D:125:HIS:CD2	1:D:125:HIS:N	2.79	0.50
2:E:143:GLU:OE1	2:E:144:HIS:ND1	2.44	0.50
2:E:384:TRP:HE3	2:E:385:LEU:HD22	1.77	0.50
3:F:229:GLY:O	3:F:240:SER:N	2.25	0.50
2:H:360:TYR:HB2	2:H:364:THR:H	1.77	0.50
1:J:81:PHE:HD2	1:J:102:GLN:HG3	1.77	0.50
1:J:204:LEU:HA	1:J:214:LEU:HD21	1.94	0.50
1:J:405:ALA:HB3	1:J:408:TRP:NE1	2.27	0.50
2:K:287:ASP:O	2:K:288:HIS:ND1	2.45	0.50
5:R:3:VAL:O	5:R:25:ALA:N	2.45	0.50
1:A:62:CYS:SG	1:A:96:CYS:N	2.81	0.50
1:A:266:PRO:HG2	1:A:268:ARG:HB3	1.92	0.50
2:B:79:ASP:OD1	2:B:79:ASP:N	2.42	0.50
1:D:53:THR:HG22	1:D:108:VAL:HG22	1.94	0.50
1:D:206:SER:OG	1:D:211:SER:OG	2.30	0.50
1:D:302:CYS:HB3	1:D:319:VAL:HG12	1.94	0.50
2:E:146:VAL:C	2:E:264:ILE:HG13	2.37	0.50
2:E:287:ASP:O	2:E:288:HIS:ND1	2.45	0.50
2:E:291:LEU:HG	2:E:306:GLN:H	1.77	0.50
1:G:426:LEU:O	1:G:429:THR:OG1	2.19	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:187:ILE:HD12	2:H:208:ILE:HD11	1.94	0.50
1:J:31:ILE:HG13	1:J:133:VAL:HG21	1.93	0.50
2:K:11:LEU:HB2	2:K:166:MET:SD	2.52	0.50
4:M:22:CYS:O	4:M:79:LEU:N	2.45	0.50
5:N:3:VAL:O	5:N:25:ALA:N	2.45	0.50
1:A:18:LEU:HD12	1:A:27:VAL:C	2.36	0.49
2:B:11:LEU:HB2	2:B:166:MET:SD	2.52	0.49
1:G:39:ILE:N	1:G:128:THR:O	2.43	0.49
1:G:43:ASN:OD1	1:G:125:HIS:NE2	2.44	0.49
3:I:146:GLU:O	3:I:150:ALA:N	2.45	0.49
2:K:291:LEU:HD12	2:K:307:TRP:NE1	2.27	0.49
4:S:68:PHE:HA	4:S:83:MET:HA	1.93	0.49
2:B:45:ILE:HD12	2:B:102:GLN:HA	1.94	0.49
2:B:146:VAL:C	2:B:264:ILE:HG13	2.37	0.49
2:E:198:TYR:HD1	2:E:202:PRO:HA	1.77	0.49
1:G:58:PRO:HD2	2:H:240:LEU:O	2.12	0.49
1:G:436:LEU:HA	1:G:439:HIS:HB3	1.92	0.49
2:H:315:ASN:OD1	2:H:316:PHE:N	2.46	0.49
2:K:94:HIS:HA	2:K:99:ILE:HA	1.94	0.49
2:K:335:VAL:HG12	2:K:336:TRP:O	2.12	0.49
4:M:12:VAL:O	4:M:115:PRO:HA	2.12	0.49
4:O:12:VAL:O	4:O:115:PRO:HA	2.12	0.49
4:O:22:CYS:O	4:O:79:LEU:N	2.45	0.49
4:O:114:ILE:O	4:O:116:VAL:N	2.43	0.49
1:A:295:PRO:HB3	1:A:325:LYS:HG2	1.95	0.49
1:D:193:TYR:HB3	1:D:207:ARG:NH1	2.27	0.49
2:E:181:HIS:O	2:E:182:SER:OG	2.29	0.49
2:H:11:LEU:HB2	2:H:166:MET:SD	2.52	0.49
2:H:46:ARG:HA	2:H:100:LEU:HA	1.93	0.49
2:H:291:LEU:HG	2:H:306:GLN:H	1.77	0.49
1:A:39:ILE:N	1:A:128:THR:O	2.43	0.49
1:A:43:ASN:OD1	1:A:125:HIS:NE2	2.44	0.49
1:A:44:LEU:HA	1:A:122:TYR:HA	1.94	0.49
1:A:118:HIS:H	1:A:120:LYS:NZ	2.10	0.49
2:E:41:HIS:O	2:E:131:ARG:HB2	2.13	0.49
2:E:335:VAL:HG12	2:E:336:TRP:O	2.12	0.49
1:G:204:LEU:HA	1:G:214:LEU:HD21	1.94	0.49
1:G:295:PRO:HB3	1:G:325:LYS:HG2	1.95	0.49
2:H:74:LYS:HE2	2:H:75:SER:H	1.77	0.49
2:H:146:VAL:C	2:H:264:ILE:HG13	2.37	0.49
1:J:4:THR:OG1	1:J:279:ILE:O	2.20	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:118:HIS:H	1:J:120:LYS:NZ	2.10	0.49
1:J:426:LEU:O	1:J:429:THR:OG1	2.19	0.49
2:K:92:VAL:H	2:K:101:ALA:HA	1.78	0.49
2:K:146:VAL:C	2:K:264:ILE:HG13	2.37	0.49
2:K:384:TRP:HE3	2:K:385:LEU:HD22	1.77	0.49
1:A:133:VAL:N	1:A:145:ALA:O	2.31	0.49
1:A:302:CYS:HB3	1:A:319:VAL:HG12	1.95	0.49
2:B:36:VAL:HG21	2:B:126:HIS:HD2	1.76	0.49
2:B:41:HIS:O	2:B:131:ARG:HB2	2.13	0.49
1:D:20:GLU:HB3	1:D:26:PRO:HG3	1.95	0.49
2:E:199:CYS:N	2:E:203:ASP:OD2	2.38	0.49
2:E:315:ASN:OD1	2:E:316:PHE:N	2.46	0.49
1:G:118:HIS:H	1:G:120:LYS:HZ2	1.61	0.49
1:G:405:ALA:HB3	1:G:408:TRP:NE1	2.27	0.49
2:H:92:VAL:H	2:H:101:ALA:HA	1.78	0.49
2:K:267:LEU:HD12	2:K:329:ASN:HB2	1.93	0.49
4:Q:104:TYR:O	5:R:34:ALA:HB1	2.11	0.49
4:Q:131:LEU:HA	5:R:120:SER:O	2.12	0.49
5:R:92:ASN:N	5:R:100:GLY:HA2	2.27	0.49
4:S:18:LEU:O	4:S:83:MET:N	2.45	0.49
1:A:237:VAL:HG13	1:A:238:PRO:O	2.13	0.49
1:A:405:ALA:HB3	1:A:408:TRP:NE1	2.27	0.49
2:B:187:ILE:HD12	2:B:208:ILE:HD11	1.94	0.49
1:D:192:GLU:HB2	1:D:197:LYS:HE2	1.93	0.49
1:D:295:PRO:HB3	1:D:325:LYS:HG2	1.95	0.49
2:E:11:LEU:HB2	2:E:166:MET:SD	2.52	0.49
2:E:360:TYR:H	2:E:364:THR:HG23	1.78	0.49
3:F:146:GLU:O	3:F:150:ALA:N	2.45	0.49
1:G:151:GLY:HA2	1:G:164:ILE:O	2.13	0.49
1:G:193:TYR:HB3	1:G:207:ARG:NH1	2.27	0.49
2:H:44:VAL:HA	2:H:102:GLN:HA	1.93	0.49
2:H:267:LEU:HD12	2:H:329:ASN:HB2	1.93	0.49
2:H:310:ARG:CZ	2:H:310:ARG:HB2	2.41	0.49
1:J:20:GLU:HB3	1:J:26:PRO:HG3	1.95	0.49
1:J:38:ILE:HB	1:J:269:ALA:HB3	1.94	0.49
2:K:1:ASP:OD1	2:K:4:THR:OG1	2.29	0.49
2:K:41:HIS:O	2:K:131:ARG:HB2	2.13	0.49
2:K:45:ILE:HD12	2:K:102:GLN:HA	1.94	0.49
2:K:85:THR:HG21	2:K:104:PRO:O	2.13	0.49
4:M:18:LEU:O	4:M:83:MET:N	2.45	0.49
1:A:125:HIS:CD2	1:A:125:HIS:N	2.79	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLY:HA2	1:A:164:ILE:O	2.13	0.49
2:B:229:ASP:OD1	2:B:231:LYS:NZ	2.42	0.49
3:C:146:GLU:O	3:C:150:ALA:N	2.45	0.49
1:D:81:PHE:HD2	1:D:102:GLN:HG3	1.77	0.49
2:E:360:TYR:H	2:E:364:THR:CG2	2.26	0.49
2:H:94:HIS:HA	2:H:99:ILE:HA	1.94	0.49
1:J:192:GLU:HB2	1:J:197:LYS:HE2	1.93	0.49
2:K:79:ASP:N	2:K:79:ASP:OD1	2.42	0.49
2:K:394:ILE:HA	2:K:397:TYR:CE2	2.48	0.49
5:P:3:VAL:O	5:P:25:ALA:N	2.45	0.49
4:Q:12:VAL:O	4:Q:115:PRO:HA	2.12	0.49
4:Q:18:LEU:O	4:Q:83:MET:N	2.45	0.49
1:A:81:PHE:HD2	1:A:102:GLN:HG3	1.77	0.49
1:A:124:VAL:HB	1:A:176:ASN:HA	1.95	0.49
2:B:1:ASP:OD1	2:B:4:THR:OG1	2.29	0.49
2:B:19:CYS:O	2:B:27:CYS:N	2.45	0.49
2:B:384:TRP:HE3	2:B:385:LEU:HD22	1.77	0.49
2:E:92:VAL:H	2:E:101:ALA:HA	1.78	0.49
2:E:95:HIS:CB	2:E:157:ARG:HE	2.22	0.49
2:E:138:TYR:CZ	2:E:288:HIS:HB2	2.48	0.49
2:H:187:ILE:HG22	2:H:211:SER:HA	1.94	0.49
1:J:21:ARG:HB3	1:J:24:TYR:HB2	1.95	0.49
2:K:2:LEU:O	2:K:6:PHE:N	2.43	0.49
2:K:315:ASN:OD1	2:K:316:PHE:N	2.46	0.49
4:O:18:LEU:O	4:O:83:MET:N	2.45	0.49
2:B:149:PRO:HA	2:B:262:LYS:HA	1.95	0.49
1:D:21:ARG:HG2	1:D:24:TYR:CG	2.47	0.49
1:D:161:LYS:O	1:D:281:ILE:HA	2.13	0.49
2:E:72:THR:OG1	2:E:73:GLN:N	2.46	0.49
1:G:20:GLU:HB3	1:G:26:PRO:HG3	1.95	0.49
1:G:44:LEU:HA	1:G:122:TYR:HA	1.94	0.49
2:H:45:ILE:HD12	2:H:102:GLN:HA	1.94	0.49
2:H:394:ILE:HA	2:H:397:TYR:CE2	2.48	0.49
1:J:161:LYS:O	1:J:281:ILE:HA	2.13	0.49
2:K:360:TYR:HB2	2:K:364:THR:H	1.77	0.49
4:S:12:VAL:O	4:S:115:PRO:HA	2.12	0.49
1:A:61:LYS:HB2	1:A:101:THR:OG1	2.13	0.49
1:A:137:TYR:O	1:A:140:VAL:N	2.34	0.49
1:A:206:SER:OG	1:A:211:SER:OG	2.30	0.49
2:B:92:VAL:H	2:B:101:ALA:HA	1.78	0.49
2:B:94:HIS:HA	2:B:99:ILE:HA	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:TYR:H	2:B:364:THR:CG2	2.26	0.49
1:D:61:LYS:HB2	1:D:101:THR:OG1	2.13	0.49
1:D:85:TYR:CE2	1:D:98:THR:HA	2.48	0.49
2:E:285:HIS:CG	2:E:311:PRO:HB3	2.48	0.49
1:G:124:VAL:HB	1:G:176:ASN:HA	1.95	0.49
1:G:206:SER:OG	1:G:211:SER:OG	2.30	0.49
1:J:53:THR:HG22	1:J:108:VAL:HG22	1.94	0.49
1:J:331:ILE:HA	1:J:370:VAL:HA	1.95	0.49
2:K:164:VAL:N	2:K:252:LEU:O	2.43	0.49
2:K:187:ILE:HD12	2:K:208:ILE:HD11	1.94	0.49
2:K:276:LYS:NZ	2:K:277:HIS:O	2.40	0.49
2:K:291:LEU:HG	2:K:306:GLN:H	1.77	0.49
5:N:92:ASN:N	5:N:100:GLY:HA2	2.27	0.49
1:A:21:ARG:HB3	1:A:24:TYR:HB2	1.94	0.48
1:A:204:LEU:HA	1:A:214:LEU:HD21	1.94	0.48
1:A:403:ILE:HG12	1:A:408:TRP:CH2	2.48	0.48
1:A:423:VAL:HA	1:A:426:LEU:HD22	1.95	0.48
2:B:85:THR:N	2:B:89:CYS:SG	2.86	0.48
1:D:21:ARG:HB3	1:D:24:TYR:HB2	1.95	0.48
1:D:84:VAL:HB	1:D:86:PRO:HD3	1.95	0.48
1:D:151:GLY:HA2	1:D:164:ILE:O	2.13	0.48
2:E:19:CYS:HB3	2:E:32:ALA:HA	1.95	0.48
2:E:293:THR:O	2:E:325:TYR:HA	2.13	0.48
2:E:310:ARG:NH2	2:E:312:THR:HG23	2.26	0.48
2:E:390:ARG:O	2:E:394:ILE:HG12	2.12	0.48
1:G:23:GLY:O	1:G:290:ARG:NH1	2.44	0.48
1:G:53:THR:HG22	1:G:108:VAL:HG22	1.94	0.48
1:G:319:VAL:N	1:G:353:PHE:O	2.44	0.48
1:G:331:ILE:HA	1:G:370:VAL:HA	1.95	0.48
1:G:403:ILE:HG12	1:G:408:TRP:CH2	2.48	0.48
2:H:293:THR:O	2:H:325:TYR:HA	2.13	0.48
1:J:85:TYR:CE2	1:J:98:THR:HA	2.48	0.48
1:J:193:TYR:HB3	1:J:207:ARG:NH1	2.27	0.48
1:J:206:SER:OG	1:J:211:SER:OG	2.30	0.48
1:J:231:HIS:CD2	1:J:233:PRO:HD3	2.48	0.48
1:J:302:CYS:HB3	1:J:319:VAL:HG12	1.94	0.48
2:K:198:TYR:HD1	2:K:202:PRO:HA	1.77	0.48
5:P:87:TYR:HA	5:P:105:ILE:HA	1.95	0.48
4:Q:22:CYS:O	4:Q:79:LEU:N	2.45	0.48
4:S:22:CYS:O	4:S:79:LEU:N	2.45	0.48
2:B:72:THR:OG1	2:B:73:GLN:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:LYS:HE2	2:B:75:SER:H	1.77	0.48
2:B:85:THR:HG21	2:B:104:PRO:O	2.13	0.48
2:B:177:LEU:HD21	2:B:225:ALA:HB1	1.95	0.48
1:D:38:ILE:HB	1:D:269:ALA:HB3	1.94	0.48
1:G:46:TYR:CD1	1:G:46:TYR:C	2.91	0.48
1:G:118:HIS:H	1:G:120:LYS:NZ	2.10	0.48
1:G:231:HIS:CD2	1:G:233:PRO:HD3	2.48	0.48
2:H:77:LYS:HG3	2:H:79:ASP:N	2.28	0.48
1:J:19:VAL:N	1:J:27:VAL:O	2.36	0.48
1:J:21:ARG:HG2	1:J:24:TYR:CG	2.47	0.48
2:K:285:HIS:CG	2:K:311:PRO:HB3	2.48	0.48
2:K:390:ARG:O	2:K:394:ILE:HG12	2.12	0.48
5:P:92:ASN:N	5:P:100:GLY:HA2	2.27	0.48
5:R:87:TYR:HA	5:R:105:ILE:HA	1.95	0.48
1:A:38:ILE:HD13	1:A:269:ALA:HB3	1.95	0.48
1:A:231:HIS:CD2	1:A:233:PRO:HD3	2.48	0.48
2:B:7:THR:O	2:B:10:LYS:NZ	2.42	0.48
2:B:77:LYS:HG3	2:B:79:ASP:N	2.28	0.48
2:B:360:TYR:HB2	2:B:364:THR:H	1.77	0.48
1:D:41:SER:OG	1:D:125:HIS:HB2	2.13	0.48
1:D:331:ILE:HA	1:D:370:VAL:HA	1.95	0.48
1:G:85:TYR:CE2	1:G:98:THR:HA	2.48	0.48
1:G:95:PHE:HB3	1:G:99:GLU:HG2	1.95	0.48
1:G:404:SER:HA	1:G:408:TRP:CE3	2.49	0.48
2:H:19:CYS:HB3	2:H:32:ALA:HA	1.95	0.48
2:H:198:TYR:HD1	2:H:202:PRO:HA	1.77	0.48
1:J:38:ILE:HD13	1:J:269:ALA:HB3	1.95	0.48
1:J:403:ILE:HG12	1:J:408:TRP:CH2	2.48	0.48
2:K:177:LEU:HD21	2:K:225:ALA:HB1	1.95	0.48
4:O:39:GLN:O	4:O:93:VAL:N	2.47	0.48
1:A:16:LYS:HE2	1:A:18:LEU:N	2.28	0.48
1:A:41:SER:OG	1:A:125:HIS:HB2	2.13	0.48
2:B:315:ASN:OD1	2:B:316:PHE:N	2.46	0.48
2:E:329:ASN:ND2	2:E:329:ASN:H	2.12	0.48
3:F:226:ILE:O	3:F:242:VAL:N	2.42	0.48
1:G:30:GLN:NE2	1:G:32:GLN:HB2	2.23	0.48
1:G:81:PHE:HD2	1:G:102:GLN:HG3	1.77	0.48
1:G:133:VAL:N	1:G:145:ALA:O	2.31	0.48
2:H:19:CYS:O	2:H:27:CYS:N	2.45	0.48
2:H:276:LYS:NZ	2:H:277:HIS:O	2.40	0.48
2:H:281:ILE:HG23	2:H:315:ASN:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:146:GLU:O	3:L:150:ALA:N	2.45	0.48
5:N:152:ALA:O	5:N:194:GLU:HA	2.13	0.48
4:S:39:GLN:O	4:S:93:VAL:N	2.47	0.48
1:A:20:GLU:HB3	1:A:26:PRO:HG3	1.95	0.48
1:A:192:GLU:HB2	1:A:197:LYS:HE2	1.93	0.48
1:A:331:ILE:O	1:A:331:ILE:HG13	2.14	0.48
2:B:11:LEU:HD13	2:B:248:PHE:HZ	1.78	0.48
2:B:149:PRO:CA	2:B:262:LYS:HD2	2.44	0.48
1:D:204:LEU:HA	1:D:214:LEU:HD21	1.94	0.48
2:E:45:ILE:HD12	2:E:102:GLN:HA	1.94	0.48
2:E:46:ARG:HA	2:E:100:LEU:HA	1.93	0.48
2:E:85:THR:N	2:E:89:CYS:SG	2.86	0.48
2:E:164:VAL:N	2:E:252:LEU:O	2.43	0.48
2:E:177:LEU:HD21	2:E:225:ALA:HB1	1.95	0.48
1:G:24:TYR:HA	1:G:289:THR:O	2.14	0.48
1:G:84:VAL:HB	1:G:86:PRO:HD3	1.95	0.48
1:G:161:LYS:O	1:G:281:ILE:HA	2.13	0.48
1:G:237:VAL:HG13	1:G:238:PRO:O	2.13	0.48
2:H:72:THR:OG1	2:H:73:GLN:N	2.46	0.48
2:H:390:ARG:O	2:H:394:ILE:HG12	2.12	0.48
1:J:9:ASN:N	1:J:275:GLY:O	2.31	0.48
1:J:125:HIS:CD2	1:J:125:HIS:N	2.79	0.48
1:J:237:VAL:HG13	1:J:238:PRO:O	2.13	0.48
2:K:11:LEU:HD13	2:K:248:PHE:HZ	1.78	0.48
2:K:138:TYR:CZ	2:K:288:HIS:HB2	2.48	0.48
5:P:152:ALA:O	5:P:194:GLU:HA	2.13	0.48
4:Q:45:LEU:H	5:R:91:CYS:CB	2.26	0.48
5:R:152:ALA:O	5:R:194:GLU:HA	2.14	0.48
1:A:46:TYR:C	1:A:46:TYR:CD1	2.91	0.48
1:A:85:TYR:CE2	1:A:98:THR:HA	2.48	0.48
1:A:261:SER:O	1:A:270:GLU:N	2.42	0.48
2:B:26:ARG:HE	2:B:27:CYS:N	2.12	0.48
2:B:138:TYR:CZ	2:B:288:HIS:HB2	2.48	0.48
2:B:329:ASN:ND2	2:B:329:ASN:H	2.12	0.48
1:D:46:TYR:CD1	1:D:46:TYR:C	2.91	0.48
1:D:118:HIS:H	1:D:120:LYS:NZ	2.11	0.48
1:D:124:VAL:HB	1:D:176:ASN:HA	1.95	0.48
1:D:426:LEU:O	1:D:429:THR:OG1	2.19	0.48
2:E:26:ARG:HE	2:E:27:CYS:N	2.12	0.48
2:E:74:LYS:HE2	2:E:75:SER:H	1.77	0.48
2:E:394:ILE:HA	2:E:397:TYR:CE2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:ARG:HB3	1:G:24:TYR:HB2	1.95	0.48
1:J:118:HIS:H	1:J:120:LYS:HZ2	1.62	0.48
5:N:48:ILE:O	5:N:58:ILE:N	2.47	0.48
5:P:48:ILE:O	5:P:58:ILE:N	2.47	0.48
2:B:285:HIS:CG	2:B:311:PRO:HB3	2.48	0.48
1:D:43:ASN:OD1	1:D:125:HIS:NE2	2.44	0.48
1:D:403:ILE:HG12	1:D:408:TRP:CH2	2.48	0.48
1:D:423:VAL:HA	1:D:426:LEU:HD22	1.95	0.48
2:E:106:GLY:N	2:E:128:VAL:HB	2.29	0.48
2:E:224:ARG:HB3	2:E:226:TYR:HE2	1.79	0.48
1:G:154:PRO:HA	1:G:163:ILE:HD13	1.96	0.48
2:H:224:ARG:HB3	2:H:226:TYR:HE2	1.79	0.48
1:J:30:GLN:NE2	1:J:32:GLN:HB2	2.23	0.48
1:J:117:ASP:HB3	1:J:181:TYR:HE2	1.79	0.48
1:J:208:THR:N	1:J:211:SER:OG	2.27	0.48
1:J:247:ASP:N	1:J:247:ASP:OD1	2.47	0.48
2:K:26:ARG:HE	2:K:27:CYS:N	2.12	0.48
1:A:84:VAL:HB	1:A:86:PRO:HD3	1.95	0.48
2:B:84:ARG:HA	2:B:89:CYS:N	2.27	0.48
2:B:187:ILE:HG22	2:B:211:SER:HA	1.94	0.48
2:B:360:TYR:H	2:B:364:THR:HG23	1.78	0.48
1:D:9:ASN:N	1:D:275:GLY:O	2.30	0.48
1:D:231:HIS:CD2	1:D:233:PRO:HD3	2.48	0.48
1:D:425:GLY:O	1:D:429:THR:HG23	2.13	0.48
2:E:84:ARG:HA	2:E:89:CYS:N	2.27	0.48
2:E:187:ILE:HG22	2:E:211:SER:HA	1.94	0.48
1:G:117:ASP:HB3	1:G:181:TYR:HE2	1.79	0.48
1:G:252:LEU:HA	1:G:255:VAL:HG22	1.96	0.48
1:G:426:LEU:HD23	2:H:385:LEU:HB3	1.96	0.48
2:H:85:THR:HG21	2:H:104:PRO:O	2.13	0.48
2:H:138:TYR:CZ	2:H:288:HIS:HB2	2.48	0.48
2:H:294:THR:HA	2:H:324:GLU:O	2.14	0.48
1:J:24:TYR:HA	1:J:289:THR:O	2.14	0.48
1:J:69:THR:O	1:J:76:TYR:OH	2.24	0.48
1:J:252:LEU:HA	1:J:255:VAL:HG22	1.96	0.48
1:J:295:PRO:HB3	1:J:325:LYS:HG2	1.95	0.48
1:J:331:ILE:HG13	1:J:331:ILE:O	2.14	0.48
2:K:77:LYS:HG3	2:K:79:ASP:N	2.28	0.48
2:K:149:PRO:HA	2:K:262:LYS:HA	1.95	0.48
2:K:181:HIS:N	2:K:184:LYS:O	2.28	0.48
2:K:281:ILE:HG23	2:K:315:ASN:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:294:THR:HA	2:K:324:GLU:O	2.14	0.48
2:K:360:TYR:H	2:K:364:THR:CG2	2.26	0.48
5:T:92:ASN:H	5:T:100:GLY:HA2	1.79	0.48
2:B:56:LYS:NZ	2:B:58:ASP:OD2	2.46	0.48
2:B:62:LEU:HD21	2:B:157:ARG:NH2	2.29	0.48
1:G:41:SER:OG	1:G:125:HIS:HB2	2.13	0.48
1:G:61:LYS:HB2	1:G:101:THR:OG1	2.13	0.48
1:G:302:CYS:HB3	1:G:319:VAL:HG12	1.94	0.48
1:G:425:GLY:O	1:G:429:THR:HG23	2.13	0.48
2:H:85:THR:N	2:H:89:CYS:SG	2.86	0.48
3:I:230:GLY:O	3:I:239:LEU:HA	2.14	0.48
1:J:46:TYR:CD1	1:J:46:TYR:C	2.91	0.48
2:K:19:CYS:HB3	2:K:32:ALA:HA	1.95	0.48
2:K:105:PRO:HA	2:K:128:VAL:HB	1.96	0.48
2:K:187:ILE:HG22	2:K:211:SER:HA	1.94	0.48
2:K:293:THR:O	2:K:325:TYR:HA	2.13	0.48
5:R:92:ASN:H	5:R:100:GLY:HA2	1.79	0.48
5:T:152:ALA:O	5:T:194:GLU:HA	2.14	0.48
2:B:35:GLU:HG2	2:B:48:GLN:HB3	1.96	0.48
3:C:230:GLY:O	3:C:239:LEU:HA	2.14	0.48
1:D:203:ASP:CG	1:D:241:PHE:HB3	2.39	0.48
2:E:85:THR:HG21	2:E:104:PRO:O	2.13	0.48
2:E:277:HIS:ND1	2:E:339:GLU:HB2	2.29	0.48
2:E:388:ARG:O	2:E:392:LEU:HG	2.14	0.48
2:H:84:ARG:HA	2:H:89:CYS:N	2.27	0.48
2:H:85:THR:HG23	2:H:87:ALA:H	1.79	0.48
2:H:177:LEU:HD21	2:H:225:ALA:HB1	1.95	0.48
2:H:360:TYR:H	2:H:364:THR:CG2	2.26	0.48
1:J:84:VAL:HB	1:J:86:PRO:HD3	1.95	0.48
1:J:220:LEU:O	1:J:221:LYS:NZ	2.38	0.48
2:K:72:THR:OG1	2:K:73:GLN:N	2.46	0.48
2:K:85:THR:N	2:K:89:CYS:SG	2.87	0.48
3:L:229:GLY:O	3:L:240:SER:N	2.25	0.48
5:N:87:TYR:HA	5:N:105:ILE:HA	1.95	0.48
5:P:152:ALA:HB1	5:P:155:SER:HA	1.96	0.48
5:T:3:VAL:O	5:T:25:ALA:N	2.45	0.48
1:A:38:ILE:HA	1:A:129:VAL:HA	1.96	0.47
2:B:19:CYS:HB3	2:B:32:ALA:HA	1.96	0.47
2:B:198:TYR:HD1	2:B:202:PRO:HA	1.77	0.47
2:B:394:ILE:HA	2:B:397:TYR:CE2	2.48	0.47
1:D:16:LYS:HE2	1:D:18:LEU:N	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:LEU:HA	1:D:122:TYR:HA	1.94	0.47
1:G:16:LYS:HE2	1:G:18:LEU:N	2.29	0.47
2:H:11:LEU:HD13	2:H:248:PHE:HZ	1.78	0.47
2:H:41:HIS:O	2:H:131:ARG:HB2	2.13	0.47
2:H:285:HIS:CG	2:H:311:PRO:HB3	2.48	0.47
1:J:42:THR:HB	1:J:124:VAL:HG13	1.96	0.47
1:J:124:VAL:HB	1:J:176:ASN:HA	1.95	0.47
4:M:39:GLN:O	4:M:93:VAL:N	2.47	0.47
5:N:92:ASN:H	5:N:100:GLY:HA2	1.79	0.47
4:S:144:ILE:O	4:S:183:LEU:N	2.45	0.47
1:A:117:ASP:HB3	1:A:181:TYR:HE2	1.79	0.47
2:B:277:HIS:ND1	2:B:339:GLU:HB2	2.29	0.47
2:B:291:LEU:HG	2:B:306:GLN:H	1.77	0.47
2:B:293:THR:O	2:B:325:TYR:HA	2.13	0.47
1:D:24:TYR:HA	1:D:289:THR:O	2.14	0.47
1:D:319:VAL:N	1:D:353:PHE:O	2.44	0.47
2:E:62:LEU:HD21	2:E:157:ARG:NH2	2.29	0.47
2:E:77:LYS:HG3	2:E:79:ASP:N	2.28	0.47
1:G:208:THR:N	1:G:211:SER:OG	2.27	0.47
1:G:331:ILE:O	1:G:331:ILE:HG13	2.14	0.47
2:H:106:GLY:N	2:H:128:VAL:HB	2.29	0.47
2:H:181:HIS:N	2:H:184:LYS:O	2.28	0.47
1:J:43:ASN:OD1	1:J:125:HIS:NE2	2.44	0.47
1:J:404:SER:HA	1:J:408:TRP:CE3	2.49	0.47
1:J:425:GLY:O	1:J:429:THR:HG23	2.13	0.47
3:L:230:GLY:O	3:L:239:LEU:HA	2.14	0.47
4:M:159:VAL:O	4:M:162:SER:N	2.47	0.47
5:P:28:SER:HA	5:P:71:PHE:HA	1.96	0.47
4:Q:159:VAL:O	4:Q:162:SER:N	2.47	0.47
5:R:48:ILE:O	5:R:58:ILE:N	2.47	0.47
1:A:404:SER:HA	1:A:408:TRP:CE3	2.49	0.47
1:D:7:MET:SD	1:D:10:LYS:NZ	2.77	0.47
1:D:42:THR:HB	1:D:124:VAL:HG13	1.96	0.47
1:D:95:PHE:HB3	1:D:99:GLU:HG2	1.96	0.47
2:E:56:LYS:NZ	2:E:58:ASP:OD2	2.46	0.47
2:E:85:THR:HG23	2:E:87:ALA:H	1.79	0.47
2:E:294:THR:HA	2:E:324:GLU:O	2.14	0.47
3:F:230:GLY:O	3:F:239:LEU:HA	2.14	0.47
1:G:231:HIS:HB3	2:H:239:ARG:NH2	2.28	0.47
2:H:16:ILE:HG23	2:H:68:MET:SD	2.55	0.47
2:H:149:PRO:CA	2:H:262:LYS:HD2	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:164:VAL:N	2:H:252:LEU:O	2.43	0.47
1:J:41:SER:OG	1:J:125:HIS:HB2	2.13	0.47
1:J:95:PHE:HB3	1:J:99:GLU:HG2	1.96	0.47
1:J:178:VAL:HG22	1:J:187:ASN:HA	1.97	0.47
2:K:35:GLU:HG2	2:K:48:GLN:HB3	1.96	0.47
2:K:85:THR:HG23	2:K:87:ALA:H	1.79	0.47
4:Q:5:VAL:C	4:Q:22:CYS:HA	2.40	0.47
4:Q:39:GLN:O	4:Q:93:VAL:N	2.47	0.47
2:B:387:CYS:SG	2:B:388:ARG:N	2.88	0.47
1:D:331:ILE:O	1:D:331:ILE:HG13	2.14	0.47
2:E:11:LEU:HD13	2:E:248:PHE:HZ	1.78	0.47
2:E:16:ILE:HG23	2:E:68:MET:SD	2.54	0.47
2:E:149:PRO:HA	2:E:262:LYS:HA	1.95	0.47
1:G:41:SER:OG	1:G:127:GLY:N	2.48	0.47
1:J:61:LYS:HB2	1:J:101:THR:OG1	2.13	0.47
2:K:360:TYR:H	2:K:364:THR:HG23	1.78	0.47
4:M:5:VAL:C	4:M:22:CYS:HA	2.40	0.47
5:N:122:GLU:C	5:N:135:LEU:HA	2.40	0.47
4:Q:104:TYR:O	5:R:34:ALA:CB	2.62	0.47
1:A:24:TYR:HA	1:A:289:THR:O	2.14	0.47
1:A:178:VAL:HG22	1:A:187:ASN:HA	1.97	0.47
1:A:203:ASP:CG	1:A:241:PHE:HB3	2.39	0.47
1:D:38:ILE:HD13	1:D:269:ALA:HB3	1.96	0.47
1:D:41:SER:OG	1:D:127:GLY:N	2.48	0.47
1:D:45:GLU:OE2	1:D:123:LYS:N	2.43	0.47
2:E:137:LYS:HB2	2:E:289:PRO:HG2	1.97	0.47
2:E:181:HIS:N	2:E:184:LYS:O	2.28	0.47
2:E:319:THR:OG1	2:E:320:GLY:N	2.48	0.47
1:G:423:VAL:HA	1:G:426:LEU:HD22	1.95	0.47
2:H:56:LYS:NZ	2:H:58:ASP:OD2	2.46	0.47
2:H:62:LEU:HD21	2:H:157:ARG:NH2	2.29	0.47
2:H:81:LEU:HD21	2:H:111:VAL:HB	1.97	0.47
2:H:360:TYR:H	2:H:364:THR:HG23	1.78	0.47
1:J:16:LYS:HE2	1:J:18:LEU:N	2.28	0.47
1:J:208:THR:OG1	1:J:211:SER:N	2.41	0.47
1:J:423:VAL:HA	1:J:426:LEU:HD22	1.95	0.47
2:K:149:PRO:CA	2:K:262:LYS:HD2	2.44	0.47
2:K:277:HIS:ND1	2:K:339:GLU:HB2	2.29	0.47
2:K:329:ASN:H	2:K:329:ASN:ND2	2.12	0.47
5:P:92:ASN:H	5:P:100:GLY:HA2	1.79	0.47
5:P:122:GLU:C	5:P:135:LEU:HA	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:48:ILE:O	5:T:58:ILE:N	2.47	0.47
5:T:122:GLU:C	5:T:135:LEU:HA	2.40	0.47
1:A:42:THR:HB	1:A:124:VAL:HG13	1.96	0.47
1:A:163:ILE:O	1:A:280:SER:N	2.35	0.47
1:A:220:LEU:O	1:A:221:LYS:NZ	2.38	0.47
1:A:303:LYS:N	1:A:318:THR:O	2.48	0.47
2:B:165:GLU:HB3	2:B:251:LYS:HZ2	1.80	0.47
2:B:168:GLN:NE2	2:B:233:TRP:HE1	2.13	0.47
2:B:196:LYS:N	2:B:226:TYR:O	2.48	0.47
2:B:294:THR:HA	2:B:324:GLU:O	2.14	0.47
2:B:310:ARG:H	2:B:310:ARG:HG3	1.44	0.47
2:B:388:ARG:O	2:B:392:LEU:HG	2.14	0.47
2:B:394:ILE:HA	2:B:397:TYR:CZ	2.49	0.47
3:C:243:THR:N	3:C:251:VAL:O	2.38	0.47
2:E:362:LEU:O	2:E:365:ILE:N	2.48	0.47
1:G:178:VAL:HG22	1:G:187:ASN:HA	1.96	0.47
1:G:203:ASP:CG	1:G:241:PHE:HB3	2.39	0.47
2:H:149:PRO:HA	2:H:262:LYS:HA	1.95	0.47
2:H:196:LYS:N	2:H:226:TYR:O	2.48	0.47
2:H:277:HIS:ND1	2:H:339:GLU:HB2	2.29	0.47
2:H:310:ARG:H	2:H:310:ARG:HG3	1.45	0.47
2:K:217:CYS:SG	2:K:222:GLN:HB3	2.55	0.47
1:A:48:THR:N	1:A:119:ALA:HB3	2.30	0.47
1:A:161:LYS:O	1:A:281:ILE:HA	2.13	0.47
1:A:252:LEU:HA	1:A:255:VAL:HG22	1.96	0.47
1:A:331:ILE:HA	1:A:370:VAL:HA	1.95	0.47
1:A:394:GLN:HB2	2:B:336:TRP:CE2	2.49	0.47
1:A:425:GLY:O	1:A:429:THR:HG23	2.13	0.47
2:B:217:CYS:SG	2:B:222:GLN:HB3	2.55	0.47
2:B:281:ILE:HG23	2:B:315:ASN:HB2	1.95	0.47
2:B:292:LEU:HD12	2:B:327:TRP:N	2.30	0.47
2:B:398:LYS:C	2:B:401:PRO:HD2	2.40	0.47
1:D:38:ILE:HA	1:D:129:VAL:HA	1.96	0.47
1:D:237:VAL:HG13	1:D:238:PRO:O	2.13	0.47
1:D:247:ASP:N	1:D:247:ASP:OD1	2.47	0.47
1:D:303:LYS:N	1:D:318:THR:O	2.48	0.47
1:D:328:ASN:HA	1:D:346:THR:HA	1.97	0.47
1:D:404:SER:HA	1:D:408:TRP:CE3	2.48	0.47
2:E:290:THR:OG1	2:E:328:GLY:N	2.48	0.47
2:E:298:GLY:N	2:E:321:GLU:OE1	2.48	0.47
2:E:398:LYS:C	2:E:401:PRO:HD2	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:ILE:HD13	1:G:269:ALA:HB3	1.96	0.47
1:G:38:ILE:HA	1:G:129:VAL:HA	1.96	0.47
1:G:42:THR:HB	1:G:124:VAL:HG13	1.96	0.47
1:G:411:ILE:HD13	1:G:411:ILE:HA	1.74	0.47
2:H:26:ARG:HE	2:H:27:CYS:N	2.12	0.47
2:H:137:LYS:HB2	2:H:289:PRO:HG2	1.97	0.47
2:H:189:VAL:HG21	2:H:208:ILE:O	2.15	0.47
2:H:280:LEU:N	2:H:316:PHE:O	2.39	0.47
1:J:151:GLY:HA2	1:J:164:ILE:O	2.13	0.47
2:K:56:LYS:NZ	2:K:58:ASP:OD2	2.46	0.47
2:K:106:GLY:N	2:K:128:VAL:HB	2.29	0.47
2:K:387:CYS:SG	2:K:388:ARG:N	2.88	0.47
2:K:388:ARG:O	2:K:392:LEU:HG	2.14	0.47
2:K:394:ILE:HA	2:K:397:TYR:CZ	2.50	0.47
4:O:5:VAL:C	4:O:22:CYS:HA	2.40	0.47
5:R:122:GLU:C	5:R:135:LEU:HA	2.40	0.47
4:S:159:VAL:O	4:S:162:SER:N	2.47	0.47
5:T:87:TYR:HA	5:T:105:ILE:HA	1.95	0.47
1:A:208:THR:OG1	1:A:211:SER:N	2.41	0.47
1:D:156:LYS:HZ3	1:D:159:ASP:C	2.23	0.47
1:D:252:LEU:HA	1:D:255:VAL:HG22	1.95	0.47
2:E:35:GLU:HG2	2:E:48:GLN:HB3	1.96	0.47
2:E:196:LYS:N	2:E:226:TYR:O	2.48	0.47
2:E:281:ILE:HG23	2:E:315:ASN:HB2	1.96	0.47
2:H:105:PRO:HA	2:H:128:VAL:HB	1.96	0.47
2:H:168:GLN:NE2	2:H:233:TRP:HE1	2.13	0.47
2:H:168:GLN:OE1	2:H:247:THR:OG1	2.25	0.47
2:H:217:CYS:SG	2:H:222:GLN:HB3	2.55	0.47
2:H:262:LYS:HB3	2:H:262:LYS:HE3	1.58	0.47
1:J:38:ILE:HA	1:J:129:VAL:HA	1.96	0.47
1:J:313:PHE:HA	1:J:358:SER:CB	2.35	0.47
2:K:298:GLY:N	2:K:321:GLU:OE1	2.48	0.47
4:M:114:ILE:O	4:M:116:VAL:N	2.43	0.47
1:A:1:TYR:CE1	1:A:3:HIS:HB2	2.50	0.47
2:B:280:LEU:N	2:B:316:PHE:O	2.39	0.47
1:D:117:ASP:HB3	1:D:181:TYR:HE2	1.79	0.47
2:E:21:ASN:HB3	2:E:27:CYS:HB3	1.97	0.47
1:G:86:PRO:HD2	1:G:99:GLU:CD	2.40	0.47
1:G:322:LYS:HZ1	1:G:350:SER:HB2	1.80	0.47
2:H:30:PRO:HG3	2:H:68:MET:O	2.15	0.47
2:H:220:VAL:HG22	2:H:221:LYS:HZ2	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:388:ARG:O	2:H:392:LEU:HG	2.14	0.47
2:H:398:LYS:C	2:H:401:PRO:HD2	2.40	0.47
1:J:230:VAL:HG21	2:K:240:LEU:C	2.40	0.47
2:K:164:VAL:HG23	2:K:254:VAL:HG12	1.97	0.47
2:K:189:VAL:HG21	2:K:208:ILE:O	2.15	0.47
2:K:319:THR:OG1	2:K:320:GLY:N	2.48	0.47
2:K:362:LEU:O	2:K:365:ILE:N	2.48	0.47
4:S:5:VAL:C	4:S:22:CYS:HA	2.40	0.47
1:A:95:PHE:HB3	1:A:99:GLU:HG2	1.96	0.47
1:A:328:ASN:HA	1:A:346:THR:HA	1.97	0.47
2:B:21:ASN:HB3	2:B:27:CYS:HB3	1.97	0.47
2:B:163:TYR:HA	2:B:253:HIS:HA	1.97	0.47
2:B:362:LEU:O	2:B:365:ILE:N	2.48	0.47
2:E:154:THR:HG22	2:E:257:VAL:O	2.16	0.47
2:E:217:CYS:SG	2:E:222:GLN:HB3	2.55	0.47
2:E:292:LEU:HD12	2:E:327:TRP:N	2.30	0.47
1:G:31:ILE:HA	1:G:31:ILE:HD12	1.77	0.47
2:H:362:LEU:O	2:H:365:ILE:N	2.48	0.47
1:J:41:SER:OG	1:J:127:GLY:N	2.48	0.47
1:J:137:TYR:O	1:J:140:VAL:N	2.34	0.47
1:J:303:LYS:N	1:J:318:THR:O	2.48	0.47
2:K:231:LYS:HD3	2:K:231:LYS:HA	1.65	0.47
4:O:159:VAL:O	4:O:162:SER:N	2.47	0.47
1:A:41:SER:OG	1:A:127:GLY:N	2.48	0.46
1:A:118:HIS:H	1:A:120:LYS:HZ2	1.62	0.46
2:B:91:LEU:HD12	2:B:101:ALA:HB2	1.98	0.46
2:B:298:GLY:N	2:B:321:GLU:OE1	2.48	0.46
2:E:162:HIS:CD2	2:E:257:VAL:HG22	2.50	0.46
2:E:164:VAL:HG23	2:E:254:VAL:HG12	1.97	0.46
2:E:387:CYS:SG	2:E:388:ARG:N	2.88	0.46
1:G:258:PHE:N	2:H:298:GLY:O	2.36	0.46
2:H:181:HIS:O	2:H:182:SER:OG	2.29	0.46
2:H:292:LEU:HD12	2:H:327:TRP:N	2.30	0.46
2:H:387:CYS:SG	2:H:388:ARG:N	2.88	0.46
2:H:394:ILE:HA	2:H:397:TYR:CZ	2.49	0.46
1:J:89:TYR:CE2	2:K:71:LYS:HD3	2.49	0.46
1:J:203:ASP:CG	1:J:241:PHE:HB3	2.39	0.46
2:K:77:LYS:HG3	2:K:79:ASP:H	1.81	0.46
2:K:290:THR:OG1	2:K:328:GLY:N	2.48	0.46
4:O:38:ARG:HA	4:O:94:TYR:HA	1.97	0.46
5:P:30:ALA:O	5:P:34:ALA:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:24:ALA:H	4:Q:78:MET:HA	1.80	0.46
5:R:152:ALA:HB1	5:R:155:SER:HA	1.96	0.46
2:B:16:ILE:HG23	2:B:68:MET:SD	2.54	0.46
2:B:85:THR:HG23	2:B:87:ALA:H	1.79	0.46
1:D:189:ASP:OD1	1:D:190:PHE:N	2.48	0.46
2:E:105:PRO:HA	2:E:128:VAL:HB	1.96	0.46
2:E:149:PRO:CA	2:E:262:LYS:HD2	2.44	0.46
1:J:48:THR:N	1:J:119:ALA:HB3	2.30	0.46
1:J:328:ASN:HA	1:J:346:THR:HA	1.97	0.46
2:K:69:ASN:CG	2:K:74:LYS:HB2	2.41	0.46
2:K:91:LEU:HD12	2:K:101:ALA:HB2	1.98	0.46
1:A:52:LYS:NZ	1:A:110:ARG:O	2.31	0.46
1:A:154:PRO:HA	1:A:163:ILE:HD13	1.96	0.46
1:A:303:LYS:HE3	1:A:305:THR:HA	1.98	0.46
1:A:409:SER:HA	1:A:412:LYS:HE2	1.96	0.46
2:B:106:GLY:N	2:B:128:VAL:HB	2.29	0.46
3:F:243:THR:N	3:F:251:VAL:O	2.38	0.46
1:G:165:GLY:C	1:G:278:PRO:HG2	2.41	0.46
1:G:328:ASN:HA	1:G:346:THR:HA	1.97	0.46
2:H:1:ASP:OD1	2:H:4:THR:OG1	2.29	0.46
2:H:35:GLU:HG2	2:H:48:GLN:HB3	1.96	0.46
2:H:164:VAL:HG23	2:H:254:VAL:HG12	1.98	0.46
2:K:62:LEU:HD21	2:K:157:ARG:NH2	2.29	0.46
2:K:137:LYS:HB2	2:K:289:PRO:HG2	1.97	0.46
2:K:162:HIS:CD2	2:K:257:VAL:HG22	2.50	0.46
2:K:359:ARG:HG2	2:K:360:TYR:H	1.81	0.46
4:O:8:GLY:HA2	4:O:111:GLY:HA3	1.98	0.46
4:O:24:ALA:H	4:O:78:MET:HA	1.80	0.46
4:S:38:ARG:HA	4:S:94:TYR:HA	1.97	0.46
2:B:30:PRO:HG3	2:B:68:MET:O	2.15	0.46
2:B:290:THR:OG1	2:B:328:GLY:N	2.48	0.46
1:D:133:VAL:N	1:D:145:ALA:O	2.31	0.46
1:D:137:TYR:N	1:D:140:VAL:HG12	2.30	0.46
1:D:154:PRO:HA	1:D:163:ILE:HD13	1.96	0.46
2:E:168:GLN:NE2	2:E:233:TRP:HE1	2.13	0.46
2:E:189:VAL:HG21	2:E:208:ILE:O	2.15	0.46
2:E:276:LYS:HZ3	2:E:279:THR:HG22	1.80	0.46
2:E:394:ILE:HA	2:E:397:TYR:CZ	2.49	0.46
1:G:1:TYR:CE1	1:G:3:HIS:HB2	2.50	0.46
1:G:69:THR:O	1:G:76:TYR:OH	2.24	0.46
2:H:162:HIS:CD2	2:H:257:VAL:HG22	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:163:TYR:HA	2:H:253:HIS:HA	1.97	0.46
1:J:133:VAL:N	1:J:145:ALA:O	2.31	0.46
1:J:404:SER:HA	1:J:408:TRP:CZ3	2.51	0.46
2:K:16:ILE:HG23	2:K:68:MET:SD	2.54	0.46
2:K:168:GLN:NE2	2:K:233:TRP:HE1	2.13	0.46
2:K:196:LYS:N	2:K:226:TYR:O	2.48	0.46
2:K:224:ARG:HB3	2:K:226:TYR:HE2	1.79	0.46
4:Q:38:ARG:HA	4:Q:94:TYR:HA	1.97	0.46
5:T:28:SER:HA	5:T:71:PHE:HA	1.96	0.46
5:T:152:ALA:HB1	5:T:155:SER:HA	1.96	0.46
2:B:81:LEU:HD21	2:B:111:VAL:HB	1.97	0.46
2:B:102:GLN:HG2	2:B:103:CYS:N	2.31	0.46
2:B:154:THR:HG22	2:B:257:VAL:O	2.16	0.46
2:B:184:LYS:HZ1	2:B:213:HIS:CD2	2.34	0.46
2:B:189:VAL:HG21	2:B:208:ILE:O	2.15	0.46
2:B:319:THR:OG1	2:B:320:GLY:N	2.48	0.46
2:B:399:LEU:HD12	2:B:400:ALA:N	2.31	0.46
1:D:1:TYR:CE1	1:D:3:HIS:HB2	2.50	0.46
1:D:303:LYS:HE3	1:D:305:THR:HA	1.98	0.46
2:H:69:ASN:CG	2:H:74:LYS:HB2	2.41	0.46
2:H:91:LEU:HD12	2:H:101:ALA:HB2	1.98	0.46
2:H:255:PRO:HG2	2:H:256:PHE:CZ	2.51	0.46
2:H:298:GLY:N	2:H:321:GLU:OE1	2.48	0.46
2:H:329:ASN:ND2	2:H:329:ASN:H	2.12	0.46
1:J:1:TYR:CE1	1:J:3:HIS:HB2	2.50	0.46
1:J:86:PRO:HD2	1:J:99:GLU:CD	2.40	0.46
1:J:154:PRO:HA	1:J:163:ILE:HD13	1.96	0.46
1:J:303:LYS:HE3	1:J:305:THR:HA	1.98	0.46
2:K:81:LEU:HD21	2:K:111:VAL:HB	1.97	0.46
2:K:346:HIS:HA	2:K:352:VAL:HG12	1.97	0.46
2:K:398:LYS:C	2:K:401:PRO:HD2	2.40	0.46
5:N:30:ALA:O	5:N:34:ALA:N	2.49	0.46
4:Q:144:ILE:O	4:Q:183:LEU:N	2.45	0.46
5:R:30:ALA:O	5:R:34:ALA:N	2.49	0.46
1:A:86:PRO:HD2	1:A:99:GLU:CD	2.40	0.46
1:A:165:GLY:C	1:A:278:PRO:HG2	2.40	0.46
2:B:91:LEU:HA	2:B:101:ALA:HB1	1.98	0.46
2:B:105:PRO:HA	2:B:128:VAL:HB	1.96	0.46
2:B:162:HIS:CD2	2:B:257:VAL:HG22	2.51	0.46
1:D:137:TYR:O	1:D:140:VAL:N	2.34	0.46
1:D:150:ASN:O	1:D:153:THR:HG22	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:VAL:HG22	1:D:187:ASN:HA	1.97	0.46
1:G:303:LYS:HE3	1:G:305:THR:HA	1.98	0.46
2:H:22:CYS:HG	2:H:123:THR:HG1	1.53	0.46
1:J:31:ILE:HD12	1:J:31:ILE:HA	1.77	0.46
1:J:121:ALA:HB1	1:J:191:PRO:HG2	1.98	0.46
1:J:409:SER:HA	1:J:412:LYS:HE2	1.97	0.46
2:K:310:ARG:NH2	2:K:312:THR:HG23	2.26	0.46
4:M:8:GLY:HA2	4:M:111:GLY:HA3	1.98	0.46
4:S:8:GLY:HA2	4:S:111:GLY:HA3	1.98	0.46
2:B:231:LYS:HD3	2:B:231:LYS:HA	1.65	0.46
2:B:359:ARG:HG2	2:B:360:TYR:H	1.81	0.46
1:D:409:SER:HA	1:D:412:LYS:HE2	1.97	0.46
2:E:81:LEU:HD21	2:E:111:VAL:HB	1.97	0.46
2:E:165:GLU:HB3	2:E:251:LYS:HZ2	1.81	0.46
2:E:231:LYS:HA	2:E:231:LYS:HD3	1.65	0.46
1:G:44:LEU:HD11	1:G:120:LYS:HA	1.98	0.46
1:G:156:LYS:HB2	1:G:161:LYS:HE2	1.98	0.46
2:H:290:THR:OG1	2:H:328:GLY:N	2.48	0.46
2:H:331:PRO:O	2:H:333:LYS:NZ	2.29	0.46
2:H:359:ARG:HG2	2:H:360:TYR:H	1.81	0.46
2:H:409:LEU:HG	2:H:410:ALA:H	1.81	0.46
1:J:189:ASP:OD1	1:J:190:PHE:N	2.48	0.46
2:K:152:ARG:HH12	2:K:155:HIS:N	2.12	0.46
3:L:215:PRO:HA	3:L:226:ILE:HA	1.98	0.46
5:N:152:ALA:HB1	5:N:155:SER:HA	1.96	0.46
1:A:137:TYR:N	1:A:140:VAL:HG12	2.30	0.46
1:A:150:ASN:O	1:A:153:THR:HG22	2.16	0.46
1:A:247:ASP:N	1:A:247:ASP:OD1	2.47	0.46
2:B:1:ASP:OD1	2:B:158:ALA:HA	2.16	0.46
2:B:224:ARG:HB3	2:B:226:TYR:HE2	1.79	0.46
2:B:255:PRO:HG2	2:B:256:PHE:CZ	2.51	0.46
1:D:201:PHE:O	1:D:241:PHE:HB2	2.16	0.46
1:D:295:PRO:HA	1:D:325:LYS:NZ	2.31	0.46
2:E:18:ASP:HB2	2:E:26:ARG:CD	2.46	0.46
2:E:49:THR:OG1	2:E:50:SER:N	2.49	0.46
3:F:215:PRO:HA	3:F:226:ILE:HA	1.98	0.46
1:G:48:THR:N	1:G:119:ALA:HB3	2.30	0.46
1:G:121:ALA:HB1	1:G:191:PRO:HG2	1.98	0.46
1:G:303:LYS:N	1:G:318:THR:O	2.48	0.46
2:H:165:GLU:HB3	2:H:251:LYS:HZ2	1.80	0.46
1:J:150:ASN:O	1:J:153:THR:HG22	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:181:HIS:HB2	2:K:185:VAL:O	2.16	0.46
4:Q:105:GLU:O	5:R:36:TYR:CB	2.64	0.46
1:A:404:SER:HA	1:A:408:TRP:CZ3	2.51	0.46
2:B:137:LYS:HB2	2:B:289:PRO:HG2	1.97	0.46
1:D:48:THR:N	1:D:119:ALA:HB3	2.30	0.46
1:D:118:HIS:H	1:D:120:LYS:HZ2	1.62	0.46
1:D:165:GLY:C	1:D:278:PRO:HG2	2.40	0.46
1:D:225:PRO:HB3	1:D:231:HIS:O	2.16	0.46
1:D:313:PHE:HA	1:D:358:SER:CB	2.35	0.46
1:G:295:PRO:HA	1:G:325:LYS:NZ	2.31	0.46
1:G:409:SER:HA	1:G:412:LYS:HE2	1.97	0.46
2:H:291:LEU:HD11	2:H:305:ARG:HB3	1.98	0.46
1:J:322:LYS:NZ	1:J:350:SER:HB2	2.31	0.46
2:K:1:ASP:OD1	2:K:158:ALA:HA	2.16	0.46
2:K:255:PRO:HG2	2:K:256:PHE:CZ	2.51	0.46
4:S:24:ALA:H	4:S:78:MET:HA	1.80	0.46
1:A:16:LYS:NZ	1:A:332:HIS:HA	2.31	0.46
1:A:322:LYS:NZ	1:A:350:SER:HB2	2.31	0.46
2:B:184:LYS:HZ1	2:B:213:HIS:HB2	1.80	0.46
3:C:177:TYR:N	3:C:223:VAL:O	2.49	0.46
1:D:16:LYS:NZ	1:D:332:HIS:HA	2.31	0.46
1:G:107:TYR:HD2	1:G:108:VAL:N	2.14	0.46
1:G:130:GLN:HB3	1:G:148:TYR:HA	1.98	0.46
1:J:330:PRO:HA	1:J:344:ASP:HA	1.98	0.46
2:K:102:GLN:HG2	2:K:103:CYS:N	2.31	0.46
1:A:107:TYR:HD2	1:A:108:VAL:N	2.14	0.45
1:A:121:ALA:HB1	1:A:191:PRO:HG2	1.98	0.45
2:B:18:ASP:HB2	2:B:26:ARG:CD	2.46	0.45
2:B:69:ASN:CG	2:B:74:LYS:HB2	2.41	0.45
2:B:165:GLU:HB2	2:B:249:LYS:HA	1.98	0.45
1:D:19:VAL:N	1:D:27:VAL:O	2.36	0.45
1:D:208:THR:N	1:D:211:SER:OG	2.27	0.45
2:E:91:LEU:HD12	2:E:101:ALA:HB2	1.98	0.45
2:E:174:ASP:O	2:E:225:ALA:HB3	2.16	0.45
1:G:423:VAL:O	1:G:427:ILE:HG22	2.16	0.45
2:H:102:GLN:HG2	2:H:103:CYS:N	2.31	0.45
1:J:44:LEU:HD11	1:J:120:LYS:HA	1.98	0.45
1:J:165:GLY:C	1:J:278:PRO:HG2	2.41	0.45
1:J:423:VAL:O	1:J:427:ILE:HG22	2.16	0.45
2:K:29:SER:HB2	2:K:31:ILE:HG12	1.99	0.45
2:K:385:LEU:HD13	2:K:385:LEU:HA	1.83	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:24:ALA:H	4:M:78:MET:HA	1.80	0.45
1:D:107:TYR:HD2	1:D:108:VAL:N	2.14	0.45
1:D:303:LYS:HB3	1:D:318:THR:HG23	1.99	0.45
1:D:322:LYS:HZ1	1:D:350:SER:HB2	1.81	0.45
1:D:339:VAL:HG22	1:D:358:SER:O	2.16	0.45
1:D:404:SER:HA	1:D:408:TRP:CZ3	2.51	0.45
2:E:30:PRO:HG3	2:E:68:MET:O	2.15	0.45
2:E:77:LYS:HG3	2:E:79:ASP:H	1.81	0.45
2:E:359:ARG:HG2	2:E:360:TYR:H	1.81	0.45
1:G:137:TYR:N	1:G:140:VAL:HG12	2.30	0.45
1:G:198:ALA:HA	1:G:217:ASN:ND2	2.32	0.45
1:G:201:PHE:O	1:G:241:PHE:HB2	2.16	0.45
1:G:339:VAL:HG22	1:G:358:SER:O	2.16	0.45
2:H:77:LYS:HG3	2:H:79:ASP:H	1.81	0.45
2:H:189:VAL:HG13	2:H:193:ALA:HB3	1.98	0.45
1:J:16:LYS:NZ	1:J:332:HIS:HA	2.31	0.45
1:J:137:TYR:N	1:J:140:VAL:HG12	2.30	0.45
2:K:18:ASP:HB2	2:K:26:ARG:CD	2.46	0.45
2:K:84:ARG:HA	2:K:89:CYS:N	2.27	0.45
2:K:154:THR:HG22	2:K:257:VAL:O	2.16	0.45
2:K:189:VAL:HG13	2:K:193:ALA:HB3	1.98	0.45
5:N:28:SER:HA	5:N:71:PHE:HA	1.96	0.45
5:R:28:SER:HA	5:R:71:PHE:HA	1.96	0.45
5:R:35:TRP:HA	5:R:92:ASN:HA	1.98	0.45
1:A:315:GLY:O	1:A:356:HIS:HA	2.17	0.45
1:A:339:VAL:HG22	1:A:358:SER:O	2.16	0.45
1:D:44:LEU:HD11	1:D:120:LYS:HA	1.98	0.45
1:D:86:PRO:HD2	1:D:99:GLU:CD	2.40	0.45
2:E:69:ASN:CG	2:E:74:LYS:HB2	2.41	0.45
2:E:102:GLN:HG2	2:E:103:CYS:N	2.31	0.45
2:E:255:PRO:HG2	2:E:256:PHE:CZ	2.51	0.45
2:E:399:LEU:HD12	2:E:400:ALA:N	2.31	0.45
1:G:37:ARG:HE	1:G:130:GLN:CG	2.28	0.45
2:H:11:LEU:HB3	2:H:233:TRP:HE3	1.82	0.45
2:H:174:ASP:O	2:H:225:ALA:HB3	2.16	0.45
2:H:181:HIS:HB2	2:H:185:VAL:O	2.16	0.45
1:J:225:PRO:HB3	1:J:231:HIS:O	2.16	0.45
2:K:21:ASN:HB3	2:K:27:CYS:HB3	1.97	0.45
2:K:30:PRO:HG3	2:K:68:MET:O	2.15	0.45
2:K:272:LEU:O	2:K:283:HIS:HD2	2.00	0.45
2:K:310:ARG:H	2:K:310:ARG:HG3	1.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:35:TRP:HA	5:N:92:ASN:HA	1.98	0.45
2:B:174:ASP:O	2:B:225:ALA:HB3	2.17	0.45
2:B:346:HIS:HA	2:B:352:VAL:HG12	1.97	0.45
1:D:130:GLN:HB3	1:D:148:TYR:HA	1.98	0.45
1:D:208:THR:OG1	1:D:211:SER:N	2.41	0.45
1:G:45:GLU:OE2	1:G:123:LYS:N	2.43	0.45
1:G:298:SER:H	1:G:321:TYR:HE1	1.65	0.45
2:H:346:HIS:HA	2:H:352:VAL:HG12	1.97	0.45
1:J:37:ARG:HE	1:J:130:GLN:CD	2.25	0.45
1:J:107:TYR:HD2	1:J:108:VAL:N	2.14	0.45
1:J:201:PHE:O	1:J:241:PHE:HB2	2.16	0.45
2:K:13:ARG:HB3	2:K:232:LYS:CB	2.44	0.45
2:K:165:GLU:HB3	2:K:251:LYS:HZ2	1.81	0.45
2:K:277:HIS:CE1	2:K:339:GLU:HB2	2.52	0.45
2:K:283:HIS:CD2	2:K:283:HIS:N	2.85	0.45
4:M:38:ARG:HA	4:M:94:TYR:HA	1.97	0.45
5:T:30:ALA:O	5:T:34:ALA:N	2.49	0.45
1:A:37:ARG:HE	1:A:130:GLN:CD	2.25	0.45
1:A:154:PRO:CG	1:D:195:THR:HB	2.43	0.45
1:A:180:VAL:HG23	1:A:184:GLU:O	2.17	0.45
1:A:189:ASP:OD1	1:A:190:PHE:N	2.48	0.45
1:A:225:PRO:HB3	1:A:231:HIS:O	2.16	0.45
1:A:423:VAL:O	1:A:427:ILE:HG22	2.16	0.45
1:D:37:ARG:HH22	1:D:146:ASP:HB2	1.82	0.45
1:G:189:ASP:OD1	1:G:190:PHE:N	2.48	0.45
1:G:330:PRO:HA	1:G:344:ASP:HA	1.98	0.45
1:G:332:HIS:H	1:G:369:GLN:NE2	2.12	0.45
1:G:404:SER:HA	1:G:408:TRP:CZ3	2.51	0.45
2:H:49:THR:OG1	2:H:50:SER:N	2.49	0.45
2:H:272:LEU:O	2:H:283:HIS:HD2	2.00	0.45
2:H:310:ARG:NH2	2:H:312:THR:HG23	2.26	0.45
1:J:77:GLN:NE2	1:J:220:LEU:O	2.50	0.45
1:J:315:GLY:O	1:J:356:HIS:HA	2.17	0.45
2:K:292:LEU:HD12	2:K:327:TRP:N	2.30	0.45
5:P:63:SER:HA	5:P:77:SER:HA	1.99	0.45
1:A:201:PHE:O	1:A:241:PHE:HB2	2.16	0.45
1:A:330:PRO:HA	1:A:344:ASP:HA	1.98	0.45
2:B:49:THR:OG1	2:B:50:SER:N	2.49	0.45
2:B:164:VAL:HG23	2:B:254:VAL:HG12	1.98	0.45
1:D:180:VAL:HG23	1:D:184:GLU:O	2.17	0.45
1:D:207:ARG:HA	1:D:207:ARG:HD3	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:TYR:O	1:D:350:SER:OG	2.31	0.45
1:D:423:VAL:O	1:D:427:ILE:HG22	2.16	0.45
2:E:262:LYS:HE3	2:E:262:LYS:HB3	1.58	0.45
2:E:276:LYS:NZ	2:E:277:HIS:O	2.40	0.45
1:G:16:LYS:NZ	1:G:332:HIS:HA	2.31	0.45
1:G:95:PHE:O	2:H:224:ARG:NE	2.42	0.45
1:G:150:ASN:O	1:G:153:THR:HG22	2.16	0.45
1:G:307:CYS:HB2	1:G:357:PHE:CE2	2.52	0.45
1:G:320:ALA:HA	1:G:352:SER:HB3	1.99	0.45
2:H:277:HIS:CE1	2:H:339:GLU:HB2	2.52	0.45
3:I:215:PRO:HA	3:I:226:ILE:HA	1.98	0.45
1:J:37:ARG:HH22	1:J:146:ASP:HB2	1.82	0.45
1:J:321:TYR:O	1:J:350:SER:OG	2.31	0.45
2:K:51:ALA:HB3	2:K:53:PHE:HE2	1.82	0.45
2:K:163:TYR:HA	2:K:253:HIS:HA	1.97	0.45
2:K:399:LEU:HD12	2:K:400:ALA:N	2.31	0.45
3:L:177:TYR:N	3:L:223:VAL:O	2.49	0.45
5:N:21:LEU:HA	5:N:74:THR:HA	1.99	0.45
4:O:144:ILE:O	4:O:183:LEU:N	2.45	0.45
5:P:35:TRP:HA	5:P:92:ASN:HA	1.99	0.45
4:Q:152:PHE:HA	4:Q:179:ALA:HB2	1.98	0.45
5:R:21:LEU:HA	5:R:74:THR:HA	1.99	0.45
4:S:39:GLN:C	4:S:92:ALA:HB1	2.42	0.45
1:A:156:LYS:HB2	1:A:161:LYS:HE2	1.98	0.45
2:B:398:LYS:HA	2:B:398:LYS:HD3	1.85	0.45
3:C:215:PRO:HA	3:C:226:ILE:HA	1.98	0.45
1:D:322:LYS:NZ	1:D:350:SER:HB2	2.31	0.45
2:E:289:PRO:HA	2:E:308:ILE:O	2.17	0.45
2:E:346:HIS:HA	2:E:352:VAL:HG12	1.97	0.45
1:G:52:LYS:NZ	1:G:110:ARG:O	2.31	0.45
1:G:77:GLN:NE2	1:G:220:LEU:O	2.50	0.45
1:G:165:GLY:HA3	1:G:166:PRO:HA	1.87	0.45
1:G:180:VAL:HG23	1:G:184:GLU:O	2.17	0.45
1:G:225:PRO:HB3	1:G:231:HIS:O	2.16	0.45
2:H:21:ASN:HB3	2:H:27:CYS:HB3	1.97	0.45
2:H:29:SER:HB2	2:H:31:ILE:HG12	1.99	0.45
2:H:154:THR:HG22	2:H:257:VAL:O	2.16	0.45
3:I:177:TYR:N	3:I:223:VAL:O	2.49	0.45
1:J:298:SER:H	1:J:321:TYR:HE1	1.65	0.45
2:K:136:GLU:OE2	2:K:329:ASN:N	2.50	0.45
2:K:280:LEU:N	2:K:316:PHE:O	2.39	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:291:LEU:HD11	2:K:305:ARG:HB3	1.98	0.45
5:P:21:LEU:HA	5:P:74:THR:HA	1.99	0.45
5:T:35:TRP:HA	5:T:92:ASN:HA	1.98	0.45
1:A:37:ARG:HH22	1:A:146:ASP:HB2	1.82	0.45
1:A:59:VAL:HG22	1:A:103:MET:H	1.81	0.45
1:A:75:ASP:CG	1:A:220:LEU:H	2.25	0.45
1:A:245:LYS:HA	1:A:248:LYS:HE3	1.99	0.45
1:A:296:THR:N	1:A:324:SER:OG	2.50	0.45
2:B:181:HIS:HB2	2:B:185:VAL:O	2.16	0.45
1:D:77:GLN:NE2	1:D:220:LEU:O	2.50	0.45
1:D:156:LYS:HB2	1:D:161:LYS:HE2	1.98	0.45
1:D:298:SER:H	1:D:321:TYR:HE1	1.65	0.45
1:D:330:PRO:HA	1:D:344:ASP:HA	1.98	0.45
2:E:163:TYR:HA	2:E:253:HIS:HA	1.97	0.45
2:E:165:GLU:HB2	2:E:249:LYS:HA	1.98	0.45
3:F:177:TYR:N	3:F:223:VAL:O	2.49	0.45
2:H:290:THR:HG1	2:H:327:TRP:NE1	2.15	0.45
1:J:37:ARG:HE	1:J:130:GLN:CG	2.28	0.45
1:J:180:VAL:HG23	1:J:184:GLU:O	2.17	0.45
1:J:339:VAL:HG22	1:J:358:SER:O	2.16	0.45
2:K:174:ASP:O	2:K:225:ALA:HB3	2.16	0.45
2:K:409:LEU:HG	2:K:410:ALA:H	1.81	0.45
4:O:39:GLN:C	4:O:92:ALA:HB1	2.42	0.45
4:S:152:PHE:HA	4:S:179:ALA:HB2	1.98	0.45
1:A:45:GLU:OE2	1:A:123:LYS:N	2.43	0.45
1:A:78:CYS:SG	1:A:103:MET:HB3	2.57	0.45
1:A:198:ALA:HA	1:A:217:ASN:ND2	2.32	0.45
3:C:137:LEU:H	3:C:161:LEU:CA	2.25	0.45
1:D:37:ARG:HE	1:D:130:GLN:CD	2.25	0.45
1:D:121:ALA:HB1	1:D:191:PRO:HG2	1.98	0.45
2:E:52:MET:HG2	2:E:97:TYR:CE2	2.52	0.45
1:G:59:VAL:HG22	1:G:103:MET:H	1.82	0.45
1:G:75:ASP:CG	1:G:220:LEU:H	2.25	0.45
1:G:245:LYS:HA	1:G:248:LYS:HE3	1.99	0.45
1:G:247:ASP:N	1:G:247:ASP:OD1	2.47	0.45
1:G:303:LYS:HB3	1:G:318:THR:HG23	1.99	0.45
2:H:283:HIS:CD2	2:H:283:HIS:N	2.85	0.45
2:H:289:PRO:HA	2:H:308:ILE:O	2.17	0.45
1:J:322:LYS:HZ1	1:J:350:SER:HB2	1.82	0.45
2:K:278:ARG:NH2	2:K:340:SER:O	2.50	0.45
2:K:290:THR:HG1	2:K:327:TRP:CG	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HD11	1:A:120:LYS:HA	1.98	0.45
1:A:130:GLN:HB3	1:A:148:TYR:HA	1.98	0.45
1:A:332:HIS:H	1:A:369:GLN:NE2	2.12	0.45
2:B:11:LEU:HB3	2:B:233:TRP:HE3	1.82	0.45
2:B:77:LYS:HG3	2:B:79:ASP:H	1.81	0.45
2:B:289:PRO:HA	2:B:308:ILE:O	2.17	0.45
1:D:198:ALA:HA	1:D:217:ASN:ND2	2.32	0.45
1:D:315:GLY:O	1:D:356:HIS:HA	2.17	0.45
2:E:1:ASP:OD1	2:E:158:ALA:HA	2.16	0.45
2:E:91:LEU:HA	2:E:101:ALA:HB1	1.98	0.45
2:E:277:HIS:CE1	2:E:339:GLU:HB2	2.52	0.45
1:G:385:LYS:HG3	2:H:339:GLU:HB3	1.99	0.45
1:J:56:PRO:HD2	1:J:105:GLU:HG2	1.99	0.45
1:J:78:CYS:SG	1:J:103:MET:HB3	2.57	0.45
3:L:137:LEU:H	3:L:161:LEU:CA	2.25	0.45
3:L:156:ALA:HB3	3:L:161:LEU:H	1.82	0.45
4:M:152:PHE:HA	4:M:179:ALA:HB2	1.98	0.45
5:N:63:SER:HA	5:N:77:SER:HA	1.99	0.45
4:Q:39:GLN:C	4:Q:92:ALA:HB1	2.42	0.45
2:B:29:SER:HB2	2:B:31:ILE:HG12	1.99	0.44
2:B:189:VAL:HG13	2:B:193:ALA:HB3	1.98	0.44
2:B:409:LEU:HD12	2:B:409:LEU:HA	1.83	0.44
1:D:75:ASP:CG	1:D:220:LEU:H	2.25	0.44
2:H:1:ASP:OD1	2:H:158:ALA:HA	2.16	0.44
2:H:13:ARG:HB3	2:H:232:LYS:CB	2.44	0.44
2:H:136:GLU:OE2	2:H:329:ASN:N	2.50	0.44
2:H:231:LYS:HA	2:H:231:LYS:HD3	1.65	0.44
2:H:319:THR:OG1	2:H:320:GLY:N	2.48	0.44
2:H:399:LEU:HD12	2:H:400:ALA:N	2.31	0.44
1:J:59:VAL:HG22	1:J:103:MET:H	1.82	0.44
1:J:156:LYS:HB2	1:J:161:LYS:HE2	1.98	0.44
1:J:296:THR:N	1:J:324:SER:OG	2.50	0.44
2:K:49:THR:OG1	2:K:50:SER:N	2.49	0.44
2:K:165:GLU:HB2	2:K:249:LYS:HA	1.98	0.44
1:A:37:ARG:HE	1:A:130:GLN:CG	2.28	0.44
1:A:46:TYR:CG	1:A:193:TYR:HD2	2.36	0.44
2:B:15:TYR:HA	2:B:68:MET:SD	2.58	0.44
2:B:277:HIS:CE1	2:B:339:GLU:HB2	2.52	0.44
2:B:283:HIS:CD2	2:B:283:HIS:N	2.85	0.44
2:B:409:LEU:HG	2:B:410:ALA:H	1.81	0.44
3:C:138:HIS:N	3:C:160:ASP:O	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:CYS:SG	1:D:103:MET:HB3	2.57	0.44
1:D:265:GLU:OE2	1:D:268:ARG:NH2	2.50	0.44
2:E:15:TYR:HA	2:E:68:MET:SD	2.58	0.44
2:E:283:HIS:CD2	2:E:283:HIS:N	2.84	0.44
1:G:265:GLU:OE2	1:G:268:ARG:NH2	2.50	0.44
1:G:315:GLY:O	1:G:356:HIS:HA	2.17	0.44
2:H:38:GLY:HA2	2:H:153:TYR:HE1	1.82	0.44
2:H:51:ALA:HB3	2:H:53:PHE:HE2	1.82	0.44
2:K:52:MET:HG2	2:K:97:TYR:CE2	2.52	0.44
2:K:63:ALA:C	2:K:78:ILE:HG13	2.43	0.44
2:K:91:LEU:HA	2:K:101:ALA:HB1	1.98	0.44
2:K:319:THR:C	2:K:321:GLU:H	2.25	0.44
4:M:39:GLN:C	4:M:92:ALA:HB1	2.42	0.44
5:T:21:LEU:HA	5:T:74:THR:HA	1.99	0.44
1:A:359:THR:OG1	1:A:398:SER:OG	2.34	0.44
2:B:272:LEU:O	2:B:283:HIS:HD2	2.00	0.44
2:E:22:CYS:SG	2:E:123:THR:OG1	2.64	0.44
2:E:38:GLY:HA2	2:E:153:TYR:HE1	1.82	0.44
1:G:367:LYS:HB2	1:G:376:THR:HA	1.99	0.44
2:H:18:ASP:HB2	2:H:26:ARG:CD	2.46	0.44
2:H:278:ARG:NH2	2:H:340:SER:O	2.50	0.44
1:J:13:ILE:HD12	1:J:13:ILE:HA	1.89	0.44
1:J:59:VAL:HA	2:K:242:ARG:HG3	2.00	0.44
1:J:102:GLN:C	1:J:103:MET:HE2	2.43	0.44
1:J:322:LYS:HE2	1:J:350:SER:HB2	2.00	0.44
2:K:15:TYR:HA	2:K:68:MET:SD	2.58	0.44
2:K:293:THR:OG1	2:K:324:GLU:OE1	2.29	0.44
2:K:361:PRO:O	2:K:365:ILE:HG12	2.17	0.44
4:O:152:PHE:HA	4:O:179:ALA:HB2	1.98	0.44
1:A:77:GLN:NE2	1:A:220:LEU:O	2.50	0.44
1:A:102:GLN:C	1:A:103:MET:HE2	2.43	0.44
1:A:120:LYS:HB3	1:A:122:TYR:CE2	2.38	0.44
1:A:265:GLU:OE2	1:A:268:ARG:NH2	2.50	0.44
2:B:278:ARG:NH2	2:B:340:SER:O	2.50	0.44
2:B:291:LEU:HD11	2:B:305:ARG:HB3	1.98	0.44
2:B:310:ARG:NH2	2:B:312:THR:HG23	2.26	0.44
1:D:59:VAL:HG22	1:D:103:MET:H	1.81	0.44
2:E:91:LEU:HG	2:E:92:VAL:N	2.33	0.44
2:E:181:HIS:HB2	2:E:185:VAL:O	2.16	0.44
2:E:398:LYS:HA	2:E:398:LYS:HD3	1.85	0.44
1:G:37:ARG:HH22	1:G:146:ASP:HB2	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:SER:H	1:G:224:ARG:HH12	1.66	0.44
1:G:322:LYS:NZ	1:G:350:SER:HB2	2.31	0.44
1:G:426:LEU:HA	2:H:389:THR:HG21	1.98	0.44
2:H:319:THR:C	2:H:321:GLU:H	2.25	0.44
3:I:156:ALA:HB3	3:I:161:LEU:H	1.82	0.44
1:J:162:LEU:HD23	1:J:281:ILE:HG23	2.00	0.44
2:K:13:ARG:CB	2:K:232:LYS:HB2	2.45	0.44
2:K:197:TYR:HE1	2:K:204:VAL:HB	1.83	0.44
5:N:67:SER:O	5:N:74:THR:N	2.51	0.44
4:Q:8:GLY:HA2	4:Q:111:GLY:HA3	1.98	0.44
5:T:151:ASN:HA	5:T:196:THR:HA	2.00	0.44
1:A:48:THR:H	1:A:119:ALA:HB3	1.83	0.44
1:A:320:ALA:HA	1:A:352:SER:HB3	1.99	0.44
1:A:341:LYS:HG2	1:A:342:GLU:CD	2.43	0.44
2:B:197:TYR:HE1	2:B:204:VAL:HB	1.83	0.44
1:D:23:GLY:C	1:D:24:TYR:HD1	2.26	0.44
1:D:296:THR:N	1:D:324:SER:OG	2.50	0.44
1:D:341:LYS:HG2	1:D:342:GLU:CD	2.43	0.44
2:E:136:GLU:OE2	2:E:329:ASN:N	2.50	0.44
1:G:37:ARG:HE	1:G:130:GLN:CD	2.25	0.44
2:H:91:LEU:HA	2:H:101:ALA:HB1	1.98	0.44
2:H:165:GLU:HB2	2:H:249:LYS:HA	1.98	0.44
2:H:198:TYR:CD1	2:H:202:PRO:HA	2.52	0.44
2:H:246:ASP:OD1	2:H:246:ASP:N	2.31	0.44
3:I:137:LEU:H	3:I:161:LEU:CA	2.25	0.44
3:I:138:HIS:N	3:I:160:ASP:O	2.51	0.44
1:J:21:ARG:NH1	1:J:285:ASP:OD1	2.28	0.44
1:J:102:GLN:HG2	1:J:225:PRO:HG2	2.00	0.44
1:J:295:PRO:HA	1:J:325:LYS:NZ	2.31	0.44
1:J:367:LYS:HB2	1:J:376:THR:HA	1.99	0.44
2:K:289:PRO:HA	2:K:308:ILE:O	2.17	0.44
5:T:63:SER:HA	5:T:77:SER:HA	1.99	0.44
2:B:136:GLU:OE2	2:B:329:ASN:N	2.50	0.44
2:B:361:PRO:O	2:B:365:ILE:HG12	2.17	0.44
1:D:13:ILE:HG23	1:D:14:PRO:O	2.18	0.44
1:D:62:CYS:HA	1:D:95:PHE:HA	2.00	0.44
1:D:165:GLY:HA3	1:D:166:PRO:HA	1.87	0.44
2:E:13:ARG:HB3	2:E:232:LYS:CB	2.44	0.44
2:E:61:ASP:O	2:E:64:TYR:N	2.50	0.44
2:E:266:THR:O	2:E:329:ASN:ND2	2.51	0.44
1:G:78:CYS:SG	1:G:103:MET:HB3	2.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:296:THR:N	1:G:324:SER:OG	2.50	0.44
1:G:364:PRO:CD	1:G:382:LYS:HE3	2.48	0.44
2:H:15:TYR:HA	2:H:68:MET:SD	2.58	0.44
2:H:63:ALA:C	2:H:78:ILE:HG13	2.43	0.44
2:H:154:THR:N	2:H:257:VAL:O	2.35	0.44
5:N:151:ASN:HA	5:N:196:THR:HA	2.00	0.44
1:A:303:LYS:HB3	1:A:318:THR:HG23	1.99	0.44
1:A:322:LYS:HZ1	1:A:350:SER:HB2	1.83	0.44
1:D:37:ARG:HE	1:D:130:GLN:CG	2.28	0.44
1:D:59:VAL:HG22	1:D:103:MET:N	2.33	0.44
2:E:272:LEU:HB3	2:E:283:HIS:HB2	2.00	0.44
2:E:272:LEU:O	2:E:283:HIS:HD2	2.00	0.44
3:F:156:ALA:HB3	3:F:161:LEU:H	1.82	0.44
1:G:48:THR:H	1:G:119:ALA:HB3	1.83	0.44
1:G:102:GLN:C	1:G:103:MET:HE2	2.43	0.44
1:G:361:ASN:ND2	1:G:402:ALA:HB1	2.33	0.44
2:H:52:MET:HG2	2:H:97:TYR:CE2	2.52	0.44
2:H:272:LEU:HB3	2:H:283:HIS:HB2	2.00	0.44
1:J:14:PRO:HB3	1:J:30:GLN:NE2	2.33	0.44
1:J:265:GLU:OE2	1:J:268:ARG:NH2	2.50	0.44
1:J:320:ALA:HA	1:J:352:SER:HB3	1.99	0.44
2:K:22:CYS:SG	2:K:123:THR:OG1	2.64	0.44
2:K:162:HIS:O	2:K:253:HIS:HA	2.18	0.44
2:K:198:TYR:CD1	2:K:202:PRO:HA	2.52	0.44
5:R:63:SER:HA	5:R:77:SER:HA	1.99	0.44
5:R:67:SER:O	5:R:74:THR:N	2.51	0.44
4:S:97:ALA:HA	4:S:106:PHE:O	2.18	0.44
4:S:114:ILE:O	4:S:116:VAL:N	2.43	0.44
1:A:208:THR:N	1:A:211:SER:OG	2.27	0.44
1:A:295:PRO:HA	1:A:325:LYS:NZ	2.31	0.44
1:A:364:PRO:CD	1:A:382:LYS:HE3	2.48	0.44
2:B:52:MET:HG2	2:B:97:TYR:CE2	2.52	0.44
2:B:198:TYR:CD1	2:B:202:PRO:HA	2.52	0.44
3:C:156:ALA:HB3	3:C:161:LEU:H	1.82	0.44
1:D:46:TYR:CG	1:D:193:TYR:HD2	2.36	0.44
1:D:52:LYS:NZ	1:D:112:GLU:OE2	2.51	0.44
1:D:143:ARG:HB3	1:D:157:ILE:HD11	2.00	0.44
1:D:257:PRO:HG2	1:D:258:PHE:CE2	2.53	0.44
1:D:320:ALA:HA	1:D:352:SER:HB3	1.99	0.44
1:D:364:PRO:CD	1:D:382:LYS:HE3	2.48	0.44
2:E:13:ARG:CB	2:E:232:LYS:HB2	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:29:SER:HB2	2:E:31:ILE:HG12	1.98	0.44
2:E:278:ARG:NH2	2:E:340:SER:O	2.50	0.44
2:E:291:LEU:HD11	2:E:305:ARG:HB3	1.98	0.44
2:E:300:ASP:N	2:E:300:ASP:OD1	2.51	0.44
2:E:363:THR:HA	2:E:366:ILE:HG12	2.00	0.44
2:E:377:VAL:HA	2:E:380:VAL:HG22	2.00	0.44
2:E:409:LEU:HG	2:E:410:ALA:H	1.81	0.44
1:G:4:THR:OG1	1:G:279:ILE:O	2.20	0.44
1:G:87:PHE:HB2	1:G:93:TYR:CE2	2.53	0.44
1:G:322:LYS:HE2	1:G:350:SER:HB2	2.00	0.44
1:J:87:PHE:HB2	1:J:93:TYR:CE2	2.53	0.44
1:J:257:PRO:HG2	1:J:258:PHE:CE2	2.53	0.44
1:J:260:CYS:HB2	1:J:270:GLU:O	2.18	0.44
2:K:38:GLY:HA2	2:K:153:TYR:HE1	1.82	0.44
2:K:272:LEU:HB3	2:K:283:HIS:HB2	2.00	0.44
3:L:136:PRO:C	3:L:138:HIS:H	2.25	0.44
5:R:147:TRP:HA	5:R:199:GLY:O	2.18	0.44
5:R:151:ASN:HA	5:R:196:THR:HA	2.00	0.44
1:A:45:GLU:HB2	1:A:193:TYR:CZ	2.53	0.44
1:A:82:SER:H	1:A:224:ARG:HH12	1.66	0.44
1:A:361:ASN:OD1	1:A:361:ASN:N	2.51	0.44
2:B:166:MET:O	2:B:233:TRP:HB3	2.18	0.44
2:B:377:VAL:HA	2:B:380:VAL:HG22	2.00	0.44
1:D:23:GLY:C	1:D:291:ILE:HB	2.43	0.44
1:D:385:LYS:HG3	2:E:339:GLU:HB3	1.99	0.44
2:E:51:ALA:HB3	2:E:53:PHE:HE2	1.82	0.44
2:E:149:PRO:HA	2:E:262:LYS:HD2	2.00	0.44
2:E:152:ARG:HH12	2:E:155:HIS:N	2.12	0.44
2:E:374:ILE:HA	2:E:377:VAL:HG22	2.00	0.44
1:G:23:GLY:C	1:G:24:TYR:HD1	2.26	0.44
1:G:102:GLN:HG2	1:G:225:PRO:HG2	2.00	0.44
1:G:341:LYS:HG2	1:G:342:GLU:CD	2.43	0.44
2:H:361:PRO:O	2:H:365:ILE:HG12	2.17	0.44
1:J:48:THR:H	1:J:119:ALA:HB3	1.83	0.44
1:J:130:GLN:HB3	1:J:148:TYR:HA	1.98	0.44
1:J:198:ALA:HA	1:J:217:ASN:ND2	2.32	0.44
1:J:307:CYS:HB2	1:J:357:PHE:CE2	2.52	0.44
1:J:364:PRO:CD	1:J:382:LYS:HE3	2.48	0.44
2:K:91:LEU:HG	2:K:92:VAL:N	2.33	0.44
5:R:138:PHE:HA	5:R:177:THR:O	2.18	0.44
1:A:13:ILE:HG23	1:A:14:PRO:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLY:C	1:A:291:ILE:HB	2.43	0.43
1:A:52:LYS:NZ	1:A:112:GLU:OE2	2.51	0.43
1:A:87:PHE:HB2	1:A:93:TYR:CE2	2.53	0.43
1:A:367:LYS:HB2	1:A:376:THR:HA	1.99	0.43
2:B:91:LEU:HG	2:B:92:VAL:N	2.33	0.43
2:B:319:THR:C	2:B:321:GLU:H	2.25	0.43
3:C:186:TYR:O	3:C:192:ALA:HA	2.17	0.43
1:D:45:GLU:HB2	1:D:193:TYR:CZ	2.53	0.43
1:D:82:SER:H	1:D:224:ARG:HH12	1.66	0.43
1:D:87:PHE:HB2	1:D:93:TYR:CE2	2.53	0.43
1:D:123:LYS:HZ3	1:D:124:VAL:C	2.26	0.43
1:D:307:CYS:HB2	1:D:357:PHE:CE2	2.52	0.43
2:E:197:TYR:HE1	2:E:204:VAL:HB	1.83	0.43
2:E:276:LYS:HD3	2:E:279:THR:HG22	2.00	0.43
3:F:186:TYR:O	3:F:192:ALA:HA	2.18	0.43
1:G:325:LYS:HE3	1:G:325:LYS:HB3	1.88	0.43
2:H:266:THR:O	2:H:329:ASN:ND2	2.51	0.43
2:H:291:LEU:HA	2:H:306:GLN:O	2.18	0.43
2:H:300:ASP:OD1	2:H:300:ASP:N	2.51	0.43
1:J:341:LYS:HG2	1:J:342:GLU:CD	2.43	0.43
2:K:227:LEU:HD23	2:K:228:ILE:N	2.33	0.43
2:K:377:VAL:HA	2:K:380:VAL:HG22	2.00	0.43
5:P:151:ASN:HA	5:P:196:THR:HA	2.00	0.43
1:A:14:PRO:HB3	1:A:30:GLN:NE2	2.33	0.43
1:A:85:TYR:H	1:A:99:GLU:HG3	1.84	0.43
1:A:162:LEU:HD23	1:A:281:ILE:HG23	2.00	0.43
1:A:180:VAL:HB	1:A:185:VAL:HG23	2.00	0.43
1:A:298:SER:H	1:A:321:TYR:HE1	1.65	0.43
1:A:318:THR:HB	1:A:354:THR:HB	2.00	0.43
2:B:38:GLY:HA2	2:B:153:TYR:HE1	1.82	0.43
2:B:61:ASP:O	2:B:64:TYR:N	2.50	0.43
1:D:85:TYR:H	1:D:99:GLU:HG3	1.83	0.43
2:E:162:HIS:O	2:E:253:HIS:HA	2.18	0.43
2:E:361:PRO:O	2:E:365:ILE:HG12	2.17	0.43
1:G:13:ILE:HG23	1:G:14:PRO:O	2.18	0.43
1:G:14:PRO:HB3	1:G:30:GLN:NE2	2.33	0.43
1:G:123:LYS:HZ3	1:G:124:VAL:C	2.26	0.43
2:H:91:LEU:HG	2:H:92:VAL:N	2.33	0.43
2:H:162:HIS:O	2:H:253:HIS:HA	2.18	0.43
2:H:166:MET:O	2:H:233:TRP:HB3	2.18	0.43
2:H:168:GLN:HG2	2:H:245:GLY:HA3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:377:VAL:HA	2:H:380:VAL:HG22	2.00	0.43
1:J:180:VAL:HB	1:J:185:VAL:HG23	2.00	0.43
1:J:245:LYS:HA	1:J:248:LYS:HE3	1.99	0.43
2:K:154:THR:N	2:K:257:VAL:O	2.35	0.43
5:T:67:SER:O	5:T:74:THR:N	2.51	0.43
1:A:23:GLY:C	1:A:24:TYR:HD1	2.26	0.43
1:A:68:CYS:SG	1:A:79:GLN:N	2.92	0.43
1:A:102:GLN:HG2	1:A:225:PRO:HG2	2.00	0.43
1:A:257:PRO:HG2	1:A:258:PHE:CE2	2.53	0.43
1:A:322:LYS:HE2	1:A:350:SER:HB2	2.00	0.43
1:A:367:LYS:CB	1:A:376:THR:HA	2.49	0.43
1:A:412:LYS:HG3	1:A:413:VAL:N	2.34	0.43
2:B:2:LEU:O	2:B:6:PHE:N	2.43	0.43
2:B:63:ALA:C	2:B:78:ILE:HG13	2.43	0.43
2:B:162:HIS:O	2:B:253:HIS:HA	2.18	0.43
2:B:227:LEU:HD23	2:B:228:ILE:N	2.33	0.43
2:B:266:THR:O	2:B:329:ASN:ND2	2.51	0.43
2:B:387:CYS:O	2:B:391:ASN:ND2	2.51	0.43
3:C:136:PRO:C	3:C:138:HIS:H	2.25	0.43
1:D:102:GLN:HG2	1:D:225:PRO:HG2	2.00	0.43
1:D:123:LYS:NZ	1:D:124:VAL:O	2.50	0.43
1:D:162:LEU:HD23	1:D:281:ILE:HG23	2.00	0.43
2:E:1:ASP:OD1	2:E:4:THR:OG1	2.29	0.43
2:E:189:VAL:HG13	2:E:193:ALA:HB3	1.98	0.43
3:F:138:HIS:N	3:F:160:ASP:O	2.51	0.43
1:G:46:TYR:CG	1:G:193:TYR:HD2	2.36	0.43
1:G:257:PRO:HG2	1:G:258:PHE:CE2	2.53	0.43
2:H:363:THR:HA	2:H:366:ILE:HG12	2.00	0.43
3:I:186:TYR:O	3:I:192:ALA:HA	2.18	0.43
1:J:75:ASP:CG	1:J:220:LEU:H	2.25	0.43
1:J:412:LYS:HG3	1:J:413:VAL:N	2.34	0.43
2:K:266:THR:O	2:K:329:ASN:ND2	2.51	0.43
5:N:147:TRP:HA	5:N:199:GLY:O	2.18	0.43
5:P:67:SER:O	5:P:74:THR:N	2.51	0.43
4:Q:7:SER:H	4:Q:21:SER:N	2.16	0.43
1:A:13:ILE:HD12	1:A:13:ILE:HA	1.89	0.43
1:A:59:VAL:HG22	1:A:103:MET:N	2.33	0.43
1:A:116:ILE:H	1:A:116:ILE:HG12	1.47	0.43
2:B:14:PRO:HB3	2:B:66:SER:O	2.18	0.43
2:B:51:ALA:HB3	2:B:53:PHE:HE2	1.82	0.43
2:B:61:ASP:HB3	2:B:64:TYR:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:THR:OG1	2:B:86:SER:N	2.52	0.43
2:B:152:ARG:HH12	2:B:155:HIS:N	2.12	0.43
1:D:245:LYS:HA	1:D:248:LYS:HE3	1.99	0.43
1:D:322:LYS:HE2	1:D:350:SER:HB2	2.00	0.43
1:D:361:ASN:OD1	1:D:361:ASN:N	2.51	0.43
2:E:14:PRO:HB3	2:E:66:SER:O	2.19	0.43
2:E:63:ALA:C	2:E:78:ILE:HG13	2.42	0.43
2:E:227:LEU:HD23	2:E:228:ILE:N	2.33	0.43
1:G:50:LYS:HD3	1:G:51:TYR:O	2.19	0.43
1:G:56:PRO:HD2	1:G:105:GLU:HG2	1.99	0.43
1:G:62:CYS:HA	1:G:95:PHE:HA	2.00	0.43
1:G:85:TYR:H	1:G:99:GLU:HG3	1.83	0.43
1:G:162:LEU:HD23	1:G:281:ILE:HG23	2.00	0.43
1:G:180:VAL:HB	1:G:185:VAL:HG23	2.00	0.43
1:G:367:LYS:CB	1:G:376:THR:HA	2.49	0.43
1:J:13:ILE:HG23	1:J:14:PRO:O	2.18	0.43
1:J:23:GLY:C	1:J:291:ILE:HB	2.43	0.43
1:J:62:CYS:HA	1:J:95:PHE:HA	2.00	0.43
1:J:68:CYS:SG	1:J:79:GLN:N	2.92	0.43
1:J:82:SER:H	1:J:224:ARG:HH12	1.66	0.43
1:J:361:ASN:ND2	1:J:402:ALA:HB1	2.33	0.43
2:K:149:PRO:HA	2:K:262:LYS:HD2	2.00	0.43
2:K:181:HIS:C	2:K:183:ALA:H	2.27	0.43
2:K:374:ILE:HA	2:K:377:VAL:HG22	2.00	0.43
4:O:97:ALA:HA	4:O:106:PHE:O	2.18	0.43
5:P:147:TRP:HA	5:P:199:GLY:O	2.18	0.43
1:A:50:LYS:HD3	1:A:51:TYR:O	2.19	0.43
1:A:69:THR:O	1:A:76:TYR:OH	2.24	0.43
1:A:260:CYS:HB2	1:A:270:GLU:O	2.18	0.43
1:A:307:CYS:HB2	1:A:357:PHE:CE2	2.52	0.43
2:B:187:ILE:HG21	2:B:208:ILE:HD11	2.01	0.43
2:B:300:ASP:N	2:B:300:ASP:OD1	2.51	0.43
2:B:363:THR:HA	2:B:366:ILE:HG12	2.01	0.43
1:D:322:LYS:HD3	1:D:323:SER:H	1.83	0.43
2:E:168:GLN:HG2	2:E:245:GLY:HA3	2.00	0.43
2:E:198:TYR:CD1	2:E:202:PRO:HA	2.52	0.43
3:F:136:PRO:C	3:F:138:HIS:H	2.25	0.43
1:G:19:VAL:N	1:G:27:VAL:O	2.36	0.43
1:G:68:CYS:SG	1:G:79:GLN:N	2.92	0.43
1:G:244:TRP:CZ3	1:G:245:LYS:HG2	2.54	0.43
1:G:311:PHE:HD2	1:G:394:GLN:HB3	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:338:GLN:OE1	2:H:339:GLU:N	2.52	0.43
1:J:303:LYS:HB3	1:J:318:THR:HG23	1.99	0.43
1:J:367:LYS:CB	1:J:376:THR:HA	2.49	0.43
1:J:408:TRP:N	1:J:408:TRP:HD1	2.17	0.43
2:K:61:ASP:HB3	2:K:64:TYR:HB2	2.00	0.43
2:K:168:GLN:HG2	2:K:245:GLY:HA3	2.00	0.43
2:K:187:ILE:HG21	2:K:208:ILE:HD11	2.00	0.43
2:K:291:LEU:HA	2:K:306:GLN:O	2.18	0.43
2:K:300:ASP:OD1	2:K:300:ASP:N	2.51	0.43
3:L:138:HIS:N	3:L:160:ASP:O	2.51	0.43
4:M:97:ALA:HA	4:M:106:PHE:O	2.18	0.43
5:N:138:PHE:HA	5:N:177:THR:O	2.18	0.43
5:T:138:PHE:HA	5:T:177:THR:O	2.18	0.43
1:A:188:TYR:CE2	1:A:191:PRO:HA	2.54	0.43
1:A:322:LYS:HD3	1:A:323:SER:H	1.83	0.43
2:B:338:GLN:OE1	2:B:339:GLU:N	2.52	0.43
1:D:244:TRP:CZ3	1:D:245:LYS:HG2	2.54	0.43
2:E:61:ASP:HB3	2:E:64:TYR:HB2	2.00	0.43
2:E:107:ASP:HA	2:E:127:LYS:HA	2.01	0.43
2:E:168:GLN:OE1	2:E:247:THR:OG1	2.25	0.43
1:G:23:GLY:C	1:G:291:ILE:HB	2.44	0.43
2:H:187:ILE:HG21	2:H:208:ILE:HD11	2.00	0.43
1:J:23:GLY:C	1:J:24:TYR:HD1	2.26	0.43
1:J:36:THR:HB	1:J:271:ASN:H	1.84	0.43
1:J:59:VAL:HG22	1:J:103:MET:N	2.33	0.43
1:J:85:TYR:H	1:J:99:GLU:HG3	1.83	0.43
1:J:307:CYS:HB3	1:J:382:LYS:CE	2.49	0.43
2:K:14:PRO:HB3	2:K:66:SER:O	2.19	0.43
4:Q:97:ALA:HA	4:Q:106:PHE:O	2.18	0.43
5:T:7:SER:H	5:T:23:CYS:H	1.66	0.43
5:T:147:TRP:HA	5:T:199:GLY:O	2.18	0.43
1:A:36:THR:HB	1:A:271:ASN:H	1.84	0.43
1:A:123:LYS:NZ	1:A:124:VAL:O	2.50	0.43
1:A:307:CYS:HB3	1:A:382:LYS:CE	2.49	0.43
1:A:313:PHE:CZ	1:A:341:LYS:HD3	2.54	0.43
2:B:32:ALA:HA	2:B:122:CYS:SG	2.59	0.43
2:B:32:ALA:HB3	2:B:50:SER:HB3	2.01	0.43
2:B:291:LEU:HA	2:B:306:GLN:O	2.18	0.43
1:D:48:THR:H	1:D:119:ALA:HB3	1.83	0.43
1:D:395:HIS:NE2	1:D:396:THR:O	2.52	0.43
2:E:150:CYS:N	2:E:261:ALA:O	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:200:LYS:HB2	2:E:217:CYS:SG	2.59	0.43
2:E:390:ARG:HE	2:E:390:ARG:HB3	1.39	0.43
1:G:143:ARG:HB3	1:G:157:ILE:HD11	2.00	0.43
1:G:167:LEU:HD12	1:G:276:SER:O	2.19	0.43
2:H:229:ASP:OD1	2:H:231:LYS:HG2	2.19	0.43
1:J:244:TRP:C	1:J:247:ASP:H	2.26	0.43
1:J:311:PHE:HD2	1:J:394:GLN:HB3	1.84	0.43
2:K:133:VAL:HG11	2:K:142:PRO:HD3	2.01	0.43
4:M:7:SER:H	4:M:21:SER:N	2.16	0.43
4:M:145:ALA:HB2	5:N:136:ASN:CB	2.48	0.43
1:A:2:GLU:OE2	1:A:281:ILE:N	2.52	0.43
1:A:56:PRO:HD2	1:A:105:GLU:HG2	1.99	0.43
1:A:263:ALA:N	1:A:268:ARG:O	2.50	0.43
1:A:361:ASN:ND2	1:A:402:ALA:HB1	2.33	0.43
1:A:411:ILE:HA	1:A:411:ILE:HD13	1.74	0.43
2:B:107:ASP:HA	2:B:127:LYS:HA	2.01	0.43
2:B:272:LEU:HB3	2:B:283:HIS:HB2	2.00	0.43
2:B:388:ARG:NH2	2:B:391:ASN:OD1	2.52	0.43
1:D:38:ILE:O	1:D:268:ARG:HA	2.19	0.43
1:D:68:CYS:SG	1:D:79:GLN:N	2.92	0.43
1:D:260:CYS:HB2	1:D:270:GLU:O	2.18	0.43
1:D:307:CYS:HB3	1:D:382:LYS:CE	2.49	0.43
1:D:313:PHE:CZ	1:D:341:LYS:HD3	2.54	0.43
2:E:338:GLN:OE1	2:E:339:GLU:N	2.52	0.43
1:G:2:GLU:OE2	1:G:281:ILE:N	2.52	0.43
1:G:52:LYS:NZ	1:G:112:GLU:OE2	2.51	0.43
1:G:395:HIS:NE2	1:G:396:THR:O	2.52	0.43
2:H:13:ARG:CB	2:H:232:LYS:HB2	2.45	0.43
2:H:399:LEU:H	2:H:399:LEU:HG	1.57	0.43
1:J:45:GLU:OE2	1:J:123:LYS:N	2.43	0.43
2:K:61:ASP:O	2:K:64:TYR:N	2.50	0.43
2:K:334:ARG:HE	2:K:334:ARG:HB2	1.61	0.43
3:L:186:TYR:O	3:L:192:ALA:HA	2.18	0.43
4:Q:190:LEU:O	4:Q:194:ALA:N	2.32	0.43
1:A:38:ILE:O	1:A:268:ARG:HA	2.19	0.43
1:A:362:ILE:HB	1:A:403:ILE:O	2.19	0.43
1:A:395:HIS:NE2	1:A:396:THR:O	2.52	0.43
2:B:279:THR:OG1	2:B:316:PHE:O	2.37	0.43
1:D:14:PRO:HB3	1:D:30:GLN:NE2	2.33	0.43
1:D:30:GLN:O	1:D:135:ILE:HA	2.19	0.43
1:D:188:TYR:CE2	1:D:191:PRO:HA	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:THR:HB	1:D:354:THR:HB	2.00	0.43
1:D:361:ASN:ND2	1:D:402:ALA:HB1	2.33	0.43
2:E:166:MET:O	2:E:233:TRP:HB3	2.18	0.43
2:E:184:LYS:HZ1	2:E:213:HIS:CD2	2.37	0.43
2:E:229:ASP:OD1	2:E:231:LYS:HG2	2.19	0.43
1:G:10:LYS:HE3	1:G:15:TYR:CB	2.48	0.43
1:G:57:SER:HB3	2:H:242:ARG:HA	2.00	0.43
1:G:313:PHE:CZ	1:G:341:LYS:HD3	2.54	0.43
2:H:139:ARG:NH2	2:H:140:HIS:HB2	2.34	0.43
2:H:162:HIS:HB2	2:H:254:VAL:HG22	2.01	0.43
2:H:197:TYR:HE1	2:H:204:VAL:HB	1.83	0.43
3:I:136:PRO:C	3:I:138:HIS:H	2.25	0.43
1:J:49:CYS:SG	1:J:204:LEU:HD13	2.59	0.43
1:J:188:TYR:CE2	1:J:191:PRO:HA	2.54	0.43
1:J:362:ILE:HB	1:J:403:ILE:O	2.19	0.43
2:K:139:ARG:NH2	2:K:140:HIS:HB2	2.34	0.43
2:K:162:HIS:HB2	2:K:254:VAL:HG22	2.01	0.43
2:K:166:MET:O	2:K:233:TRP:HB3	2.18	0.43
4:Q:141:ASN:CB	5:R:119:PRO:HA	2.49	0.43
2:B:95:HIS:O	2:B:95:HIS:ND1	2.52	0.43
2:B:200:LYS:HB2	2:B:217:CYS:SG	2.59	0.43
1:D:49:CYS:SG	1:D:204:LEU:HD13	2.59	0.43
1:D:102:GLN:C	1:D:103:MET:HE2	2.43	0.43
1:D:367:LYS:CB	1:D:376:THR:HA	2.49	0.43
2:E:11:LEU:HB3	2:E:233:TRP:HE3	1.82	0.43
2:E:11:LEU:HD12	2:E:166:MET:HE1	2.01	0.43
2:E:162:HIS:HB2	2:E:254:VAL:HG22	2.01	0.43
2:E:246:ASP:OD1	2:E:246:ASP:N	2.31	0.43
2:E:319:THR:C	2:E:321:GLU:H	2.25	0.43
2:E:356:TYR:O	2:E:364:THR:HB	2.19	0.43
2:E:399:LEU:H	2:E:399:LEU:HG	1.57	0.43
1:G:188:TYR:CE2	1:G:191:PRO:HA	2.54	0.43
2:H:14:PRO:HB3	2:H:66:SER:O	2.19	0.43
2:H:37:ARG:HD2	2:H:37:ARG:HA	1.62	0.43
2:H:177:LEU:HD13	2:H:195:VAL:HG21	2.01	0.43
2:H:227:LEU:HD23	2:H:228:ILE:N	2.33	0.43
1:J:30:GLN:O	1:J:135:ILE:HA	2.19	0.43
1:J:143:ARG:HB3	1:J:157:ILE:HD11	2.00	0.43
2:K:338:GLN:OE1	2:K:339:GLU:N	2.52	0.43
2:K:388:ARG:NH2	2:K:391:ASN:OD1	2.52	0.43
5:P:138:PHE:HA	5:P:177:THR:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:TRP:CZ3	1:A:245:LYS:HG2	2.54	0.42
2:B:15:TYR:CD2	2:B:50:SER:HB2	2.54	0.42
2:B:276:LYS:NZ	2:B:277:HIS:O	2.40	0.42
2:B:395:THR:OG1	2:B:396:PRO:HD3	2.19	0.42
1:D:2:GLU:OE2	1:D:281:ILE:N	2.52	0.42
2:E:291:LEU:HA	2:E:306:GLN:O	2.18	0.42
2:E:387:CYS:O	2:E:391:ASN:ND2	2.51	0.42
1:G:45:GLU:HB2	1:G:193:TYR:CZ	2.53	0.42
1:G:59:VAL:HG22	1:G:103:MET:N	2.33	0.42
2:H:133:VAL:HG11	2:H:142:PRO:HD3	2.01	0.42
1:J:38:ILE:O	1:J:268:ARG:HA	2.19	0.42
1:J:313:PHE:CZ	1:J:341:LYS:HD3	2.54	0.42
1:J:395:HIS:NE2	1:J:396:THR:O	2.52	0.42
2:K:11:LEU:HD12	2:K:166:MET:HE1	2.01	0.42
2:K:107:ASP:HA	2:K:127:LYS:HA	2.01	0.42
2:K:153:TYR:HA	2:K:258:PRO:HA	2.01	0.42
2:K:168:GLN:OE1	2:K:247:THR:OG1	2.25	0.42
2:K:363:THR:HA	2:K:366:ILE:HG12	2.00	0.42
4:M:144:ILE:O	4:M:183:LEU:N	2.45	0.42
4:O:7:SER:H	4:O:21:SER:N	2.16	0.42
5:P:7:SER:H	5:P:23:CYS:H	1.66	0.42
1:A:30:GLN:HB3	1:A:136:THR:HB	2.02	0.42
1:A:123:LYS:HZ3	1:A:124:VAL:C	2.27	0.42
1:A:193:TYR:HB3	1:A:207:ARG:NH2	2.34	0.42
2:B:11:LEU:HD12	2:B:166:MET:HE1	2.01	0.42
2:B:37:ARG:HD2	2:B:37:ARG:HA	1.62	0.42
2:B:90:SER:O	2:B:102:GLN:HB3	2.20	0.42
2:B:290:THR:HG1	2:B:327:TRP:CG	2.37	0.42
2:B:374:ILE:HA	2:B:377:VAL:HG22	2.00	0.42
2:B:411:LEU:HD12	2:B:411:LEU:HA	1.86	0.42
1:D:36:THR:HB	1:D:271:ASN:H	1.83	0.42
1:D:50:LYS:HD3	1:D:51:TYR:O	2.18	0.42
1:D:69:THR:O	1:D:76:TYR:OH	2.24	0.42
1:D:180:VAL:HB	1:D:185:VAL:HG23	2.00	0.42
1:D:193:TYR:HB3	1:D:207:ARG:NH2	2.34	0.42
1:D:321:TYR:N	1:D:352:SER:OG	2.49	0.42
1:D:367:LYS:HB2	1:D:376:THR:HA	1.99	0.42
2:E:32:ALA:HA	2:E:122:CYS:SG	2.59	0.42
2:E:95:HIS:O	2:E:95:HIS:ND1	2.52	0.42
2:E:133:VAL:HG11	2:E:142:PRO:HD3	2.01	0.42
2:E:272:LEU:O	2:E:283:HIS:N	2.42	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:279:THR:OG1	2:E:316:PHE:O	2.37	0.42
1:G:223:GLN:HG2	1:G:234:PHE:N	2.34	0.42
1:G:244:TRP:C	1:G:247:ASP:H	2.26	0.42
1:G:322:LYS:HD3	1:G:323:SER:H	1.83	0.42
2:H:107:ASP:HA	2:H:127:LYS:HA	2.01	0.42
2:H:272:LEU:O	2:H:283:HIS:N	2.42	0.42
2:H:284:LEU:HD12	2:H:285:HIS:H	1.84	0.42
2:H:388:ARG:NH2	2:H:391:ASN:OD1	2.52	0.42
1:J:45:GLU:HB2	1:J:193:TYR:CZ	2.53	0.42
1:J:148:TYR:HB2	1:J:150:ASN:ND2	2.34	0.42
2:K:32:ALA:HB3	2:K:50:SER:HB3	2.01	0.42
2:K:347:GLY:N	2:K:351:GLU:OE1	2.52	0.42
1:A:30:GLN:O	1:A:135:ILE:HA	2.19	0.42
1:A:223:GLN:HG2	1:A:234:PHE:N	2.34	0.42
1:A:367:LYS:HZ1	1:A:374:ALA:CB	2.27	0.42
2:B:149:PRO:HA	2:B:262:LYS:HD2	2.00	0.42
2:B:168:GLN:HG2	2:B:245:GLY:HA3	2.00	0.42
2:B:262:LYS:HB3	2:B:262:LYS:HE3	1.58	0.42
1:D:56:PRO:HD2	1:D:105:GLU:HG2	1.99	0.42
1:D:148:TYR:HB2	1:D:150:ASN:ND2	2.34	0.42
1:D:360:ALA:HB2	1:D:397:GLU:HB3	2.01	0.42
1:G:148:TYR:HB2	1:G:150:ASN:ND2	2.34	0.42
1:G:260:CYS:HB2	1:G:270:GLU:O	2.18	0.42
1:G:360:ALA:HB2	1:G:397:GLU:HB3	2.02	0.42
2:H:53:PHE:O	2:H:96:GLY:HA2	2.20	0.42
2:H:290:THR:HG1	2:H:327:TRP:CG	2.37	0.42
1:J:193:TYR:HB3	1:J:207:ARG:NH2	2.34	0.42
2:K:53:PHE:O	2:K:96:GLY:HA2	2.20	0.42
2:K:220:VAL:HG22	2:K:221:LYS:NZ	2.34	0.42
2:K:387:CYS:O	2:K:391:ASN:ND2	2.51	0.42
5:N:7:SER:H	5:N:23:CYS:H	1.66	0.42
1:A:167:LEU:HD12	1:A:276:SER:O	2.19	0.42
2:B:53:PHE:O	2:B:96:GLY:HA2	2.19	0.42
2:B:181:HIS:N	2:B:184:LYS:O	2.28	0.42
2:B:347:GLY:N	2:B:351:GLU:OE1	2.52	0.42
1:D:30:GLN:HB3	1:D:136:THR:HB	2.01	0.42
1:D:88:MET:HE3	1:D:88:MET:HB2	1.95	0.42
1:D:258:PHE:HA	2:E:297:LEU:O	2.19	0.42
1:D:307:CYS:HA	1:D:315:GLY:HA2	2.01	0.42
2:E:395:THR:OG1	2:E:396:PRO:HD3	2.19	0.42
1:G:46:TYR:CE2	1:G:205:GLN:HA	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:263:ALA:N	1:G:268:ARG:O	2.50	0.42
1:G:321:TYR:N	1:G:352:SER:OG	2.49	0.42
1:G:362:ILE:HB	1:G:403:ILE:O	2.19	0.42
2:H:220:VAL:HG22	2:H:221:LYS:NZ	2.34	0.42
3:I:243:THR:N	3:I:251:VAL:O	2.38	0.42
1:J:7:MET:SD	1:J:10:LYS:NZ	2.77	0.42
1:J:10:LYS:HE3	1:J:15:TYR:CB	2.48	0.42
1:J:50:LYS:HD3	1:J:51:TYR:O	2.19	0.42
1:J:167:LEU:HD12	1:J:276:SER:O	2.19	0.42
1:J:307:CYS:HA	1:J:315:GLY:HA2	2.01	0.42
2:K:95:HIS:ND1	2:K:95:HIS:O	2.52	0.42
2:K:284:LEU:HD12	2:K:285:HIS:H	1.84	0.42
5:R:7:SER:H	5:R:23:CYS:H	1.66	0.42
1:A:62:CYS:HA	1:A:95:PHE:HA	2.00	0.42
1:A:207:ARG:HA	1:A:207:ARG:HD3	1.80	0.42
1:A:328:ASN:HA	1:A:347:LEU:N	2.34	0.42
2:B:87:ALA:HB3	2:B:104:PRO:HG2	2.01	0.42
2:B:229:ASP:OD1	2:B:231:LYS:HG2	2.19	0.42
1:D:10:LYS:HE3	1:D:15:TYR:CB	2.48	0.42
1:D:437:PHE:CD1	1:D:437:PHE:N	2.87	0.42
1:G:118:HIS:O	1:G:120:LYS:NZ	2.51	0.42
1:G:313:PHE:HA	1:G:358:SER:CB	2.35	0.42
2:H:15:TYR:CD2	2:H:50:SER:HB2	2.54	0.42
2:H:85:THR:OG1	2:H:86:SER:N	2.52	0.42
2:H:95:HIS:ND1	2:H:95:HIS:O	2.52	0.42
2:H:276:LYS:HD3	2:H:279:THR:HG22	2.00	0.42
1:J:2:GLU:OE2	1:J:281:ILE:N	2.52	0.42
1:J:46:TYR:CG	1:J:193:TYR:HD2	2.36	0.42
2:K:137:LYS:HG3	2:K:307:TRP:CZ3	2.55	0.42
2:K:200:LYS:HB2	2:K:217:CYS:SG	2.59	0.42
4:O:50:VAL:N	4:O:59:TYR:O	2.38	0.42
4:S:7:SER:H	4:S:21:SER:N	2.16	0.42
1:A:31:ILE:HA	1:A:31:ILE:HD12	1.77	0.42
1:A:143:ARG:HB3	1:A:157:ILE:HD11	2.00	0.42
2:B:181:HIS:C	2:B:183:ALA:H	2.27	0.42
1:D:167:LEU:HD12	1:D:276:SER:O	2.19	0.42
2:E:187:ILE:HG21	2:E:208:ILE:HD11	2.01	0.42
1:G:36:THR:HB	1:G:271:ASN:H	1.83	0.42
1:G:220:LEU:C	1:G:221:LYS:HZ3	2.25	0.42
1:G:318:THR:HB	1:G:354:THR:HB	2.00	0.42
1:G:412:LYS:HG3	1:G:413:VAL:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:11:LEU:HD12	2:H:166:MET:HE1	2.01	0.42
2:H:150:CYS:N	2:H:261:ALA:O	2.31	0.42
2:H:326:THR:OG1	2:H:330:HIS:O	2.17	0.42
2:H:387:CYS:O	2:H:391:ASN:ND2	2.51	0.42
1:J:123:LYS:HZ2	1:J:125:HIS:CD2	2.37	0.42
1:J:213:ASP:OD1	1:J:213:ASP:N	2.49	0.42
2:K:177:LEU:HD13	2:K:195:VAL:HG21	2.01	0.42
2:K:274:GLU:O	2:K:280:LEU:HG	2.20	0.42
2:K:276:LYS:HD3	2:K:279:THR:HG22	2.00	0.42
4:M:170:ALA:HB3	4:M:182:ASP:N	2.35	0.42
4:O:190:LEU:O	4:O:194:ALA:N	2.32	0.42
1:A:148:TYR:HB2	1:A:150:ASN:ND2	2.34	0.42
2:B:139:ARG:NH2	2:B:140:HIS:HB2	2.34	0.42
2:B:162:HIS:HB2	2:B:254:VAL:HG22	2.01	0.42
2:B:177:LEU:HD13	2:B:195:VAL:HG21	2.02	0.42
2:B:181:HIS:O	2:B:182:SER:OG	2.29	0.42
2:B:276:LYS:HD3	2:B:279:THR:HG22	2.00	0.42
2:B:277:HIS:O	2:B:278:ARG:HB2	2.20	0.42
1:D:412:LYS:HG3	1:D:413:VAL:N	2.34	0.42
2:E:139:ARG:NH2	2:E:140:HIS:HB2	2.34	0.42
2:E:220:VAL:HG22	2:E:221:LYS:NZ	2.34	0.42
2:E:277:HIS:O	2:E:278:ARG:HB2	2.20	0.42
2:E:388:ARG:NH2	2:E:391:ASN:OD1	2.52	0.42
2:H:90:SER:O	2:H:102:GLN:HB3	2.19	0.42
2:H:137:LYS:HG3	2:H:307:TRP:CZ3	2.55	0.42
2:H:347:GLY:N	2:H:351:GLU:OE1	2.52	0.42
2:H:356:TYR:O	2:H:364:THR:HB	2.19	0.42
1:J:46:TYR:CE2	1:J:205:GLN:HA	2.55	0.42
1:J:318:THR:HB	1:J:354:THR:HB	2.00	0.42
4:M:166:GLN:O	4:M:186:THR:N	2.53	0.42
2:B:168:GLN:OE1	2:B:247:THR:OG1	2.25	0.42
2:B:170:GLY:HA3	2:B:243:GLY:HA3	2.02	0.42
2:B:197:TYR:CE1	2:B:204:VAL:HB	2.55	0.42
1:D:311:PHE:HD2	1:D:394:GLN:HB3	1.84	0.42
1:D:332:HIS:H	1:D:369:GLN:NE2	2.12	0.42
2:E:15:TYR:CD2	2:E:50:SER:HB2	2.54	0.42
2:E:177:LEU:HD13	2:E:195:VAL:HG21	2.02	0.42
2:E:284:LEU:HD12	2:E:285:HIS:H	1.84	0.42
1:G:30:GLN:O	1:G:135:ILE:HA	2.19	0.42
1:G:49:CYS:SG	1:G:204:LEU:HD13	2.59	0.42
2:H:61:ASP:HB3	2:H:64:TYR:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:153:TYR:HA	2:H:258:PRO:HA	2.02	0.42
2:H:184:LYS:HE2	2:H:184:LYS:HB2	1.88	0.42
2:H:200:LYS:HB2	2:H:217:CYS:SG	2.59	0.42
1:J:123:LYS:CD	1:J:176:ASN:HB3	2.49	0.42
1:J:331:ILE:HG22	1:J:370:VAL:HB	2.02	0.42
1:J:338:ALA:HB1	1:J:357:PHE:CD2	2.55	0.42
1:J:339:VAL:HG22	1:J:358:SER:HB3	2.02	0.42
2:K:279:THR:OG1	2:K:316:PHE:O	2.37	0.42
1:A:307:CYS:HA	1:A:315:GLY:HA2	2.01	0.42
2:B:133:VAL:HG11	2:B:142:PRO:HD3	2.01	0.42
2:B:274:GLU:O	2:B:280:LEU:HG	2.20	0.42
1:D:123:LYS:CD	1:D:176:ASN:HB3	2.49	0.42
1:D:223:GLN:HG2	1:D:234:PHE:N	2.34	0.42
2:E:53:PHE:O	2:E:96:GLY:HA2	2.20	0.42
2:E:87:ALA:HB3	2:E:104:PRO:HG2	2.01	0.42
2:E:137:LYS:HG3	2:E:307:TRP:CZ3	2.55	0.42
2:E:217:CYS:HB3	2:E:219:ASP:O	2.20	0.42
1:G:30:GLN:HB3	1:G:136:THR:HB	2.02	0.42
1:G:408:TRP:CH2	2:H:359:ARG:NH1	2.88	0.42
2:H:2:LEU:O	2:H:6:PHE:N	2.43	0.42
2:H:32:ALA:HB3	2:H:50:SER:HB3	2.01	0.42
2:H:87:ALA:HB3	2:H:104:PRO:HG2	2.01	0.42
2:K:85:THR:OG1	2:K:86:SER:N	2.52	0.42
2:K:150:CYS:N	2:K:261:ALA:O	2.31	0.42
2:K:167:HIS:NE2	2:K:246:ASP:HA	2.35	0.42
4:O:170:ALA:HB3	4:O:182:ASP:N	2.35	0.42
2:B:113:PHE:O	2:B:119:ARG:HA	2.20	0.42
2:B:253:HIS:CD2	2:B:255:PRO:HA	2.55	0.42
2:B:272:LEU:O	2:B:283:HIS:N	2.42	0.42
1:D:251:PRO:O	1:D:255:VAL:HG13	2.20	0.42
2:E:32:ALA:HB3	2:E:50:SER:HB3	2.01	0.42
2:E:64:TYR:HD1	2:E:64:TYR:HA	1.67	0.42
1:G:244:TRP:C	1:G:244:TRP:CD2	2.98	0.42
1:G:437:PHE:CD1	1:G:437:PHE:N	2.87	0.42
2:H:179:SER:OG	2:H:186:LYS:O	2.28	0.42
2:H:253:HIS:CD2	2:H:255:PRO:HA	2.55	0.42
1:J:8:PRO:O	1:J:10:LYS:HG2	2.20	0.42
1:J:30:GLN:HB3	1:J:136:THR:HB	2.01	0.42
1:J:223:GLN:HG2	1:J:234:PHE:N	2.34	0.42
1:J:244:TRP:CZ3	1:J:245:LYS:HG2	2.54	0.42
1:J:361:ASN:OD1	1:J:361:ASN:N	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:11:LEU:O	2:K:233:TRP:HE3	2.03	0.42
2:K:171:LEU:H	2:K:171:LEU:HG	1.67	0.42
2:K:229:ASP:OD1	2:K:231:LYS:HG2	2.19	0.42
2:K:282:LEU:HD13	2:K:314:VAL:HG13	2.02	0.42
4:Q:140:GLY:O	4:Q:142:VAL:N	2.53	0.42
1:A:8:PRO:O	1:A:10:LYS:HG2	2.20	0.41
1:A:311:PHE:HD2	1:A:394:GLN:HB3	1.84	0.41
1:A:340:ILE:HA	1:A:357:PHE:HB3	2.02	0.41
2:B:38:GLY:HA2	2:B:45:ILE:HA	2.02	0.41
2:B:282:LEU:HD13	2:B:314:VAL:HG13	2.02	0.41
2:B:356:TYR:O	2:B:364:THR:HB	2.19	0.41
1:D:8:PRO:O	1:D:10:LYS:HG2	2.20	0.41
1:D:46:TYR:CE2	1:D:205:GLN:HA	2.55	0.41
1:D:339:VAL:O	1:D:339:VAL:HG23	2.20	0.41
2:E:90:SER:O	2:E:102:GLN:HB3	2.19	0.41
2:E:229:ASP:OD1	2:E:231:LYS:NZ	2.42	0.41
2:E:253:HIS:CD2	2:E:255:PRO:HA	2.55	0.41
1:G:193:TYR:HB3	1:G:207:ARG:NH2	2.34	0.41
1:G:307:CYS:HB3	1:G:382:LYS:CE	2.49	0.41
1:G:328:ASN:HA	1:G:347:LEU:N	2.34	0.41
2:H:32:ALA:HA	2:H:122:CYS:SG	2.59	0.41
2:H:87:ALA:HB3	2:H:104:PRO:CG	2.50	0.41
2:H:113:PHE:O	2:H:119:ARG:HA	2.20	0.41
2:H:274:GLU:O	2:H:280:LEU:HG	2.20	0.41
2:H:279:THR:OG1	2:H:316:PHE:O	2.37	0.41
2:K:9:TYR:OH	2:K:55:LEU:O	2.37	0.41
2:K:217:CYS:HB3	2:K:219:ASP:O	2.20	0.41
4:Q:108:ASP:HA	5:R:47:LEU:CB	2.50	0.41
1:A:10:LYS:HE3	1:A:15:TYR:CB	2.48	0.41
1:A:49:CYS:SG	1:A:204:LEU:HD13	2.59	0.41
1:A:360:ALA:HB2	1:A:397:GLU:HB3	2.02	0.41
2:B:153:TYR:HA	2:B:258:PRO:HA	2.02	0.41
2:B:167:HIS:NE2	2:B:246:ASP:HA	2.35	0.41
1:D:411:ILE:HA	1:D:411:ILE:HD13	1.74	0.41
2:E:85:THR:OG1	2:E:86:SER:N	2.52	0.41
2:E:304:THR:HB	2:E:306:GLN:OE1	2.20	0.41
1:G:85:TYR:HD1	1:G:95:PHE:CZ	2.38	0.41
1:G:135:ILE:CG2	1:G:143:ARG:HB2	2.50	0.41
1:G:338:ALA:HB1	1:G:357:PHE:CD2	2.55	0.41
2:H:38:GLY:HA2	2:H:45:ILE:HA	2.02	0.41
2:H:181:HIS:C	2:H:183:ALA:H	2.27	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:374:ILE:HA	2:H:377:VAL:HG22	2.00	0.41
2:H:390:ARG:HE	2:H:390:ARG:HB3	1.39	0.41
2:H:395:THR:OG1	2:H:396:PRO:HD3	2.19	0.41
2:K:46:ARG:NH1	2:K:256:PHE:O	2.54	0.41
2:K:64:TYR:HD1	2:K:64:TYR:HA	1.66	0.41
2:K:277:HIS:O	2:K:278:ARG:HB2	2.20	0.41
2:K:393:CYS:C	2:K:396:PRO:HD2	2.45	0.41
4:O:140:GLY:O	4:O:142:VAL:N	2.53	0.41
4:Q:91:THR:HA	4:Q:113:GLY:O	2.21	0.41
2:B:332:PRO:O	2:B:333:LYS:HD3	2.21	0.41
1:D:223:GLN:HG2	1:D:234:PHE:CA	2.51	0.41
1:D:331:ILE:HG22	1:D:370:VAL:HB	2.02	0.41
1:D:340:ILE:HA	1:D:357:PHE:HB3	2.02	0.41
2:E:113:PHE:O	2:E:119:ARG:HA	2.20	0.41
2:E:154:THR:N	2:E:257:VAL:O	2.35	0.41
2:E:332:PRO:O	2:E:333:LYS:HD3	2.21	0.41
2:E:393:CYS:C	2:E:396:PRO:HD2	2.45	0.41
1:G:30:GLN:O	1:G:135:ILE:HD12	2.21	0.41
1:G:46:TYR:CD1	1:G:193:TYR:HD2	2.39	0.41
1:G:361:ASN:OD1	1:G:361:ASN:N	2.51	0.41
2:H:197:TYR:CE1	2:H:204:VAL:HB	2.55	0.41
2:H:277:HIS:O	2:H:278:ARG:HB2	2.20	0.41
2:H:345:PRO:HA	2:H:355:TYR:CD2	2.55	0.41
1:J:251:PRO:O	1:J:255:VAL:HG13	2.20	0.41
1:J:332:HIS:H	1:J:369:GLN:NE2	2.12	0.41
1:J:340:ILE:HA	1:J:357:PHE:HB3	2.02	0.41
1:J:394:GLN:HB2	2:K:336:TRP:CZ2	2.55	0.41
2:K:37:ARG:HA	2:K:37:ARG:HD2	1.62	0.41
5:R:169:ASP:HA	5:R:174:LEU:O	2.21	0.41
1:A:321:TYR:O	1:A:350:SER:OG	2.31	0.41
1:A:339:VAL:O	1:A:339:VAL:HG23	2.20	0.41
2:B:11:LEU:O	2:B:233:TRP:HE3	2.03	0.41
2:B:46:ARG:NH1	2:B:256:PHE:O	2.54	0.41
2:B:87:ALA:HB3	2:B:104:PRO:CG	2.50	0.41
2:B:137:LYS:HG3	2:B:307:TRP:CZ3	2.55	0.41
2:E:181:HIS:C	2:E:183:ALA:H	2.27	0.41
2:E:274:GLU:O	2:E:280:LEU:HG	2.20	0.41
2:E:347:GLY:N	2:E:351:GLU:OE1	2.52	0.41
1:G:38:ILE:O	1:G:268:ARG:HA	2.19	0.41
2:H:152:ARG:HH12	2:H:155:HIS:N	2.12	0.41
2:H:167:HIS:NE2	2:H:246:ASP:HA	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:170:GLY:HA3	2:H:243:GLY:HA3	2.02	0.41
2:H:282:LEU:HD13	2:H:314:VAL:HG13	2.02	0.41
2:H:372:VAL:O	2:H:376:MET:HG2	2.21	0.41
1:J:123:LYS:HZ3	1:J:124:VAL:C	2.26	0.41
1:J:223:GLN:HG2	1:J:234:PHE:CA	2.51	0.41
2:K:15:TYR:CD2	2:K:50:SER:HB2	2.54	0.41
2:K:32:ALA:HA	2:K:122:CYS:SG	2.59	0.41
2:K:372:VAL:O	2:K:376:MET:HG2	2.21	0.41
2:K:395:THR:OG1	2:K:396:PRO:HD3	2.19	0.41
2:K:398:LYS:HA	2:K:398:LYS:HD3	1.85	0.41
4:O:91:THR:HA	4:O:113:GLY:O	2.21	0.41
4:S:154:GLN:HA	4:S:203:VAL:HA	2.03	0.41
1:A:56:PRO:HD2	1:A:105:GLU:O	2.21	0.41
1:A:223:GLN:HG2	1:A:234:PHE:CA	2.50	0.41
1:A:338:ALA:HB1	1:A:357:PHE:CD2	2.55	0.41
1:A:410:TRP:CE3	1:A:411:ILE:HG12	2.56	0.41
1:A:433:ALA:HB1	1:A:437:PHE:CZ	2.56	0.41
2:B:372:VAL:O	2:B:376:MET:HG2	2.21	0.41
2:B:393:CYS:C	2:B:396:PRO:HD2	2.45	0.41
1:D:338:ALA:HB1	1:D:357:PHE:CD2	2.55	0.41
1:D:362:ILE:HB	1:D:403:ILE:O	2.19	0.41
1:G:251:PRO:O	1:G:255:VAL:HG13	2.20	0.41
1:G:307:CYS:HA	1:G:315:GLY:HA2	2.01	0.41
2:H:11:LEU:O	2:H:233:TRP:HE3	2.03	0.41
2:H:149:PRO:HA	2:H:262:LYS:HD2	2.00	0.41
2:H:332:PRO:O	2:H:333:LYS:HD3	2.21	0.41
2:H:393:CYS:C	2:H:396:PRO:HD2	2.45	0.41
1:J:328:ASN:HA	1:J:347:LEU:N	2.34	0.41
1:J:437:PHE:CD1	1:J:437:PHE:N	2.87	0.41
2:K:62:LEU:HD23	2:K:62:LEU:HA	1.94	0.41
2:K:87:ALA:HB3	2:K:104:PRO:HG2	2.01	0.41
2:K:90:SER:O	2:K:102:GLN:HB3	2.19	0.41
2:K:170:GLY:HA3	2:K:243:GLY:HA3	2.02	0.41
2:K:197:TYR:CE1	2:K:204:VAL:HB	2.55	0.41
2:K:373:ALA:O	2:K:377:VAL:HG13	2.21	0.41
4:M:140:GLY:O	4:M:142:VAL:N	2.53	0.41
4:Q:154:GLN:HA	4:Q:203:VAL:HA	2.03	0.41
2:B:279:THR:OG1	2:B:315:ASN:OD1	2.30	0.41
2:B:304:THR:HB	2:B:306:GLN:OE1	2.20	0.41
2:B:390:ARG:NH2	2:B:391:ASN:HD22	2.19	0.41
1:D:85:TYR:HD1	1:D:95:PHE:CZ	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:ALA:HA	1:D:282:ASP:O	2.20	0.41
2:E:11:LEU:O	2:E:233:TRP:HE3	2.03	0.41
2:E:87:ALA:HB3	2:E:104:PRO:CG	2.50	0.41
2:E:167:HIS:NE2	2:E:246:ASP:HA	2.35	0.41
1:G:340:ILE:HA	1:G:357:PHE:HB3	2.02	0.41
1:G:410:TRP:CE3	1:G:411:ILE:HG12	2.56	0.41
2:H:62:LEU:HD23	2:H:62:LEU:HA	1.94	0.41
2:H:115:ASP:C	2:H:117:PRO:HD2	2.46	0.41
2:H:208:ILE:HD12	2:H:212:ASP:H	1.86	0.41
1:J:110:ARG:HD3	1:J:204:LEU:HD11	2.03	0.41
2:K:113:PHE:O	2:K:119:ARG:HA	2.20	0.41
1:A:46:TYR:CE2	1:A:205:GLN:HA	2.55	0.41
1:A:123:LYS:CD	1:A:176:ASN:HB3	2.49	0.41
1:A:160:ALA:HA	1:A:282:ASP:O	2.20	0.41
1:A:252:LEU:H	1:A:252:LEU:HG	1.51	0.41
2:B:13:ARG:HB3	2:B:232:LYS:CB	2.44	0.41
2:B:41:HIS:HB2	2:B:151:ASN:O	2.21	0.41
2:B:217:CYS:HB3	2:B:219:ASP:O	2.20	0.41
3:C:116:ILE:CB	3:C:124:GLY:H	2.34	0.41
1:D:30:GLN:O	1:D:135:ILE:HD12	2.21	0.41
1:D:433:ALA:HB1	1:D:437:PHE:CZ	2.56	0.41
2:E:46:ARG:NH1	2:E:256:PHE:O	2.54	0.41
2:E:129:GLU:OE2	2:E:132:PRO:HD3	2.20	0.41
2:E:153:TYR:HA	2:E:258:PRO:HA	2.01	0.41
2:E:197:TYR:CE1	2:E:204:VAL:HB	2.55	0.41
2:E:291:LEU:HD23	2:E:292:LEU:C	2.46	0.41
3:F:137:LEU:H	3:F:161:LEU:CA	2.25	0.41
1:G:8:PRO:O	1:G:10:LYS:HG2	2.20	0.41
1:G:50:LYS:O	1:G:111:SER:OG	2.39	0.41
1:G:123:LYS:NZ	1:G:124:VAL:O	2.50	0.41
1:G:123:LYS:CD	1:G:176:ASN:HB3	2.49	0.41
1:G:223:GLN:HG2	1:G:234:PHE:CA	2.51	0.41
1:G:290:ARG:NH1	1:G:290:ARG:HA	2.36	0.41
2:H:46:ARG:NH1	2:H:256:PHE:O	2.54	0.41
2:H:76:ILE:HD11	2:H:113:PHE:CE2	2.56	0.41
2:H:224:ARG:HD3	2:H:224:ARG:HA	1.87	0.41
2:H:409:LEU:HD12	2:H:409:LEU:HA	1.83	0.41
1:J:85:TYR:HD1	1:J:95:PHE:CZ	2.38	0.41
1:J:123:LYS:NZ	1:J:124:VAL:O	2.50	0.41
2:K:38:GLY:HA2	2:K:45:ILE:HA	2.02	0.41
2:K:76:ILE:HD11	2:K:113:PHE:CE2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:94:HIS:HB3	2:K:99:ILE:HG23	2.03	0.41
2:K:115:ASP:C	2:K:117:PRO:HD2	2.46	0.41
2:K:200:LYS:HE3	2:K:216:THR:O	2.21	0.41
2:K:208:ILE:HD12	2:K:212:ASP:H	1.86	0.41
2:K:253:HIS:CD2	2:K:255:PRO:HA	2.55	0.41
3:L:116:ILE:CB	3:L:124:GLY:H	2.34	0.41
5:P:38:GLN:HA	5:P:49:TYR:N	2.33	0.41
1:A:119:ALA:C	1:A:120:LYS:HD2	2.46	0.41
1:A:331:ILE:HG22	1:A:370:VAL:HB	2.02	0.41
2:B:76:ILE:HD11	2:B:113:PHE:CE2	2.56	0.41
2:B:164:VAL:N	2:B:252:LEU:O	2.43	0.41
2:B:200:LYS:HE3	2:B:216:THR:O	2.21	0.41
2:B:284:LEU:HD12	2:B:285:HIS:H	1.84	0.41
1:D:50:LYS:HD3	1:D:111:SER:HB3	2.03	0.41
1:D:112:GLU:O	1:D:115:SER:OG	2.32	0.41
1:D:242:GLU:O	1:D:245:LYS:N	2.53	0.41
1:D:339:VAL:HG22	1:D:358:SER:HB3	2.02	0.41
1:D:394:GLN:HB2	2:E:336:TRP:CD2	2.56	0.41
2:E:46:ARG:HH22	2:E:254:VAL:HG21	1.86	0.41
2:E:94:HIS:HB3	2:E:99:ILE:HG23	2.03	0.41
2:E:282:LEU:HD13	2:E:314:VAL:HG13	2.02	0.41
2:E:345:PRO:HA	2:E:355:TYR:CD2	2.55	0.41
3:F:241:VAL:O	3:F:253:ASP:N	2.54	0.41
1:G:433:ALA:HB1	1:G:437:PHE:CZ	2.56	0.41
2:H:61:ASP:O	2:H:64:TYR:N	2.50	0.41
3:I:249:VAL:O	3:I:251:VAL:N	2.54	0.41
1:J:46:TYR:CD1	1:J:193:TYR:HD2	2.39	0.41
1:J:50:LYS:O	1:J:111:SER:OG	2.39	0.41
1:J:92:ALA:H	2:K:173:ALA:HB3	1.86	0.41
1:J:256:ALA:N	2:K:295:ARG:NH2	2.68	0.41
1:J:339:VAL:O	1:J:339:VAL:HG23	2.20	0.41
2:K:102:GLN:HG2	2:K:103:CYS:H	1.86	0.41
2:K:304:THR:HB	2:K:306:GLN:OE1	2.20	0.41
2:K:356:TYR:O	2:K:364:THR:HB	2.19	0.41
2:K:390:ARG:NH2	2:K:391:ASN:HD22	2.19	0.41
3:L:249:VAL:O	3:L:251:VAL:N	2.54	0.41
5:P:169:ASP:HA	5:P:174:LEU:O	2.21	0.41
1:A:85:TYR:HD1	1:A:95:PHE:CZ	2.38	0.41
1:A:110:ARG:HD3	1:A:204:LEU:HD11	2.03	0.41
1:A:156:LYS:HA	1:A:160:ALA:O	2.21	0.41
1:A:191:PRO:O	1:A:193:TYR:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:PRO:O	1:A:255:VAL:HG13	2.20	0.41
1:A:290:ARG:NH1	1:A:290:ARG:HA	2.36	0.41
2:B:46:ARG:HH22	2:B:254:VAL:HG21	1.86	0.41
2:B:102:GLN:HG2	2:B:103:CYS:H	1.86	0.41
2:B:115:ASP:C	2:B:117:PRO:HD2	2.46	0.41
2:B:184:LYS:HE2	2:B:184:LYS:HB2	1.88	0.41
2:B:276:LYS:O	2:B:279:THR:N	2.54	0.41
2:B:291:LEU:HD23	2:B:292:LEU:C	2.46	0.41
2:B:292:LEU:H	2:B:306:GLN:HE21	1.67	0.41
2:B:373:ALA:O	2:B:377:VAL:HG13	2.21	0.41
2:B:385:LEU:HA	2:B:385:LEU:HD13	1.83	0.41
1:D:49:CYS:O	1:D:204:LEU:HB2	2.21	0.41
1:D:56:PRO:HD2	1:D:105:GLU:O	2.21	0.41
2:E:2:LEU:O	2:E:6:PHE:N	2.43	0.41
2:E:76:ILE:HD11	2:E:113:PHE:CE2	2.56	0.41
2:E:115:ASP:C	2:E:117:PRO:HD2	2.46	0.41
2:E:203:ASP:OD1	2:E:203:ASP:N	2.54	0.41
2:E:336:TRP:H	2:E:336:TRP:HE3	1.69	0.41
3:F:195:TYR:H	3:F:200:PHE:HA	1.86	0.41
1:G:49:CYS:O	1:G:204:LEU:HB2	2.21	0.41
1:G:119:ALA:C	1:G:120:LYS:HD2	2.46	0.41
1:G:191:PRO:O	1:G:193:TYR:N	2.54	0.41
2:H:41:HIS:HB2	2:H:151:ASN:O	2.21	0.41
2:H:200:LYS:HE3	2:H:216:THR:O	2.21	0.41
2:H:279:THR:OG1	2:H:315:ASN:OD1	2.30	0.41
2:H:291:LEU:HD23	2:H:292:LEU:C	2.46	0.41
2:H:304:THR:HB	2:H:306:GLN:OE1	2.20	0.41
2:H:390:ARG:NH2	2:H:391:ASN:HD22	2.19	0.41
1:J:52:LYS:NZ	1:J:112:GLU:OE2	2.51	0.41
1:J:56:PRO:HD2	1:J:105:GLU:O	2.21	0.41
1:J:119:ALA:C	1:J:120:LYS:HD2	2.46	0.41
1:J:156:LYS:HA	1:J:160:ALA:O	2.21	0.41
1:J:433:ALA:HB1	1:J:437:PHE:CZ	2.56	0.41
2:K:41:HIS:HB2	2:K:151:ASN:O	2.21	0.41
2:K:55:LEU:O	2:K:66:SER:OG	2.39	0.41
2:K:332:PRO:O	2:K:333:LYS:HD3	2.21	0.41
4:M:91:THR:HA	4:M:113:GLY:O	2.21	0.41
4:O:154:GLN:HA	4:O:203:VAL:HA	2.03	0.41
4:Q:152:PHE:O	4:Q:154:GLN:N	2.49	0.41
1:A:49:CYS:O	1:A:204:LEU:HB2	2.21	0.41
2:B:9:TYR:OH	2:B:55:LEU:O	2.37	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:LEU:O	2:B:66:SER:OG	2.39	0.41
2:B:208:ILE:HD12	2:B:212:ASP:H	1.86	0.41
3:C:195:TYR:H	3:C:200:PHE:HA	1.86	0.41
3:C:199:ARG:CB	3:C:239:LEU:H	2.34	0.41
1:D:239:SER:HB3	1:D:242:GLU:HB2	2.03	0.41
1:G:50:LYS:HD3	1:G:111:SER:HB3	2.03	0.41
1:G:156:LYS:HA	1:G:160:ALA:O	2.21	0.41
1:G:156:LYS:HZ3	1:G:159:ASP:C	2.28	0.41
1:G:205:GLN:HB2	1:G:216:ALA:HB2	2.03	0.41
1:G:339:VAL:HG22	1:G:358:SER:HB3	2.02	0.41
1:G:408:TRP:N	1:G:408:TRP:HD1	2.17	0.41
1:J:323:SER:HB3	1:J:350:SER:H	1.86	0.41
2:K:46:ARG:HH22	2:K:254:VAL:HG21	1.86	0.41
2:K:87:ALA:HB3	2:K:104:PRO:CG	2.50	0.41
2:K:129:GLU:OE2	2:K:132:PRO:HD3	2.20	0.41
3:L:188:TRP:N	3:L:191:GLY:O	2.54	0.41
3:L:243:THR:N	3:L:251:VAL:O	2.38	0.41
4:M:9:GLY:HA2	4:M:112:GLN:C	2.46	0.41
4:M:124:THR:O	4:M:147:LEU:N	2.40	0.41
4:Q:9:GLY:HA2	4:Q:112:GLN:C	2.46	0.41
1:A:118:HIS:C	1:A:120:LYS:HZ2	2.29	0.40
1:A:339:VAL:HG22	1:A:358:SER:HB3	2.02	0.40
2:B:9:TYR:CD1	2:B:57:THR:HA	2.56	0.40
2:B:345:PRO:HA	2:B:355:TYR:CD2	2.55	0.40
1:D:50:LYS:O	1:D:111:SER:OG	2.39	0.40
1:D:119:ALA:C	1:D:120:LYS:HD2	2.46	0.40
2:E:46:ARG:HA	2:E:99:ILE:O	2.22	0.40
2:E:372:VAL:O	2:E:376:MET:HG2	2.21	0.40
2:E:390:ARG:NH2	2:E:391:ASN:HD22	2.19	0.40
3:F:249:VAL:O	3:F:251:VAL:N	2.54	0.40
1:G:56:PRO:HD2	1:G:105:GLU:O	2.21	0.40
1:G:242:GLU:O	1:G:245:LYS:N	2.53	0.40
1:G:321:TYR:O	1:G:350:SER:OG	2.31	0.40
1:G:339:VAL:O	1:G:339:VAL:HG23	2.20	0.40
2:H:9:TYR:CD1	2:H:57:THR:HA	2.56	0.40
2:H:217:CYS:HB3	2:H:219:ASP:O	2.20	0.40
3:I:188:TRP:N	3:I:191:GLY:O	2.54	0.40
1:J:191:PRO:O	1:J:193:TYR:N	2.54	0.40
1:J:322:LYS:HD3	1:J:323:SER:H	1.83	0.40
2:K:11:LEU:HB3	2:K:233:TRP:HE3	1.82	0.40
2:K:345:PRO:HA	2:K:355:TYR:CD2	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:9:GLY:HA2	4:S:112:GLN:C	2.46	0.40
1:A:354:THR:OG1	1:A:355:PHE:N	2.53	0.40
1:A:367:LYS:NZ	1:A:368:LEU:O	2.54	0.40
1:D:37:ARG:NH1	1:D:146:ASP:HB2	2.36	0.40
1:D:46:TYR:CD1	1:D:193:TYR:HD2	2.39	0.40
1:D:290:ARG:NH1	1:D:290:ARG:HA	2.36	0.40
1:D:323:SER:HB3	1:D:350:SER:H	1.86	0.40
2:E:38:GLY:HA2	2:E:45:ILE:HA	2.02	0.40
2:E:55:LEU:O	2:E:66:SER:OG	2.39	0.40
3:F:199:ARG:CB	3:F:239:LEU:H	2.34	0.40
1:G:64:GLY:O	1:G:100:ASN:HB2	2.21	0.40
1:G:160:ALA:HA	1:G:282:ASP:O	2.20	0.40
1:G:331:ILE:HG22	1:G:370:VAL:HB	2.02	0.40
1:G:367:LYS:NZ	1:G:368:LEU:O	2.54	0.40
2:H:129:GLU:OE2	2:H:132:PRO:HD3	2.20	0.40
2:H:276:LYS:HB2	2:H:281:ILE:HD11	2.03	0.40
1:J:30:GLN:O	1:J:135:ILE:HD12	2.21	0.40
1:J:49:CYS:O	1:J:204:LEU:HB2	2.21	0.40
1:J:50:LYS:HD3	1:J:111:SER:HB3	2.03	0.40
1:J:55:VAL:HG22	1:J:56:PRO:O	2.22	0.40
1:J:239:SER:HB3	1:J:242:GLU:HB2	2.03	0.40
1:J:325:LYS:HE3	1:J:325:LYS:HB3	1.88	0.40
1:J:360:ALA:HB2	1:J:397:GLU:HB3	2.02	0.40
2:K:276:LYS:HB2	2:K:281:ILE:HD11	2.03	0.40
4:M:154:GLN:HA	4:M:203:VAL:HA	2.03	0.40
4:O:33:GLY:HA3	4:O:99:ASP:O	2.22	0.40
4:Q:33:GLY:HA3	4:Q:99:ASP:O	2.22	0.40
4:S:33:GLY:HA3	4:S:99:ASP:O	2.22	0.40
1:A:185:VAL:HG13	1:A:252:LEU:HD12	2.03	0.40
2:B:359:ARG:HG2	2:B:360:TYR:N	2.37	0.40
3:C:188:TRP:N	3:C:191:GLY:O	2.54	0.40
1:D:185:VAL:HG13	1:D:252:LEU:HD12	2.03	0.40
1:D:340:ILE:HD11	1:D:368:LEU:HD21	2.04	0.40
1:D:403:ILE:HG12	1:D:408:TRP:HH2	1.86	0.40
2:E:41:HIS:HB2	2:E:151:ASN:O	2.21	0.40
2:E:142:PRO:HD2	2:E:265:ALA:HA	2.03	0.40
2:E:170:GLY:HA3	2:E:243:GLY:HA3	2.02	0.40
2:E:359:ARG:HG2	2:E:360:TYR:N	2.37	0.40
3:F:188:TRP:N	3:F:191:GLY:O	2.54	0.40
1:G:45:GLU:HB2	1:G:193:TYR:CE2	2.56	0.40
1:G:403:ILE:HG12	1:G:408:TRP:HH2	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:VAL:C	2:H:89:CYS:HB2	2.47	0.40
2:H:94:HIS:HB3	2:H:99:ILE:HG23	2.03	0.40
1:J:64:GLY:O	1:J:100:ASN:HB2	2.21	0.40
2:K:46:ARG:HA	2:K:99:ILE:O	2.22	0.40
2:K:48:GLN:CD	2:K:97:TYR:HB3	2.47	0.40
2:K:291:LEU:HD23	2:K:292:LEU:C	2.45	0.40
2:K:359:ARG:HG2	2:K:360:TYR:N	2.37	0.40
3:L:195:TYR:H	3:L:200:PHE:HA	1.86	0.40
3:L:241:VAL:O	3:L:253:ASP:N	2.54	0.40
4:M:97:ALA:HA	4:M:106:PHE:C	2.46	0.40
4:O:97:ALA:HA	4:O:106:PHE:C	2.46	0.40
4:Q:97:ALA:HA	4:Q:106:PHE:C	2.46	0.40
4:S:152:PHE:O	4:S:154:GLN:N	2.49	0.40
1:A:19:VAL:N	1:A:27:VAL:O	2.36	0.40
1:A:55:VAL:HG22	1:A:56:PRO:O	2.22	0.40
1:A:367:LYS:HB3	1:A:376:THR:HG23	2.04	0.40
1:A:408:TRP:N	1:A:408:TRP:HD1	2.17	0.40
2:B:83:VAL:C	2:B:89:CYS:HB2	2.47	0.40
2:B:318:VAL:O	2:B:337:ALA:HB3	2.22	0.40
2:B:322:GLY:HA2	2:B:335:VAL:O	2.22	0.40
3:C:241:VAL:O	3:C:253:ASP:N	2.54	0.40
1:D:83:GLY:H	1:D:100:ASN:HA	1.87	0.40
1:D:110:ARG:HD3	1:D:204:LEU:HD11	2.03	0.40
1:D:135:ILE:CG2	1:D:143:ARG:HB2	2.50	0.40
1:D:244:TRP:CD2	1:D:244:TRP:C	2.98	0.40
2:E:48:GLN:CD	2:E:97:TYR:HB3	2.47	0.40
2:E:83:VAL:C	2:E:89:CYS:HB2	2.47	0.40
2:E:102:GLN:HG2	2:E:103:CYS:H	1.86	0.40
1:G:110:ARG:HD3	1:G:204:LEU:HD11	2.03	0.40
1:G:354:THR:OG1	1:G:355:PHE:N	2.53	0.40
2:H:48:GLN:CD	2:H:97:TYR:HB3	2.47	0.40
2:H:318:VAL:O	2:H:337:ALA:HB3	2.22	0.40
2:H:336:TRP:H	2:H:336:TRP:HE3	1.69	0.40
1:J:160:ALA:HA	1:J:282:ASP:O	2.20	0.40
1:J:242:GLU:O	1:J:245:LYS:N	2.53	0.40
1:J:410:TRP:CE3	1:J:411:ILE:HG12	2.56	0.40
1:J:437:PHE:O	1:J:440:ARG:HB3	2.22	0.40
2:K:165:GLU:HA	2:K:250:GLY:O	2.21	0.40
2:K:322:GLY:HA2	2:K:335:VAL:O	2.22	0.40
5:R:151:ASN:O	5:R:195:VAL:N	2.55	0.40
1:A:30:GLN:O	1:A:135:ILE:HD12	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:CG2	1:A:143:ARG:HB2	2.50	0.40
2:B:40:ALA:CB	2:B:44:VAL:HG22	2.52	0.40
3:C:249:VAL:O	3:C:251:VAL:N	2.54	0.40
1:D:137:TYR:O	1:D:138:GLY:C	2.65	0.40
1:D:408:TRP:N	1:D:408:TRP:HD1	2.17	0.40
2:E:208:ILE:HD12	2:E:212:ASP:H	1.86	0.40
2:E:276:LYS:HB2	2:E:281:ILE:HD11	2.03	0.40
2:E:373:ALA:O	2:E:377:VAL:HG13	2.21	0.40
1:G:44:LEU:HD23	1:G:45:GLU:N	2.37	0.40
1:G:55:VAL:HG22	1:G:56:PRO:O	2.22	0.40
1:G:83:GLY:H	1:G:100:ASN:HA	1.87	0.40
1:G:323:SER:HB3	1:G:350:SER:H	1.86	0.40
2:H:40:ALA:CB	2:H:44:VAL:HG22	2.52	0.40
2:H:154:THR:HG22	2:H:257:VAL:HB	2.04	0.40
2:H:373:ALA:O	2:H:377:VAL:HG13	2.21	0.40
3:I:199:ARG:CB	3:I:239:LEU:H	2.34	0.40
1:J:95:PHE:CD2	1:J:95:PHE:C	3.00	0.40
2:K:333:LYS:HA	2:K:334:ARG:CZ	2.51	0.40
3:L:199:ARG:CB	3:L:239:LEU:H	2.34	0.40
4:M:152:PHE:O	4:M:154:GLN:N	2.49	0.40
5:N:169:ASP:HA	5:N:174:LEU:O	2.21	0.40
4:S:91:THR:HA	4:S:113:GLY:O	2.21	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	429/441 (97%)	359 (84%)	70 (16%)	0	100	100
1	D	429/441 (97%)	359 (84%)	70 (16%)	0	100	100
1	G	429/441 (97%)	361 (84%)	68 (16%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	429/441 (97%)	359 (84%)	70 (16%)	0	100	100
2	B	412/420 (98%)	336 (82%)	76 (18%)	0	100	100
2	E	412/420 (98%)	336 (82%)	76 (18%)	0	100	100
2	H	412/420 (98%)	336 (82%)	76 (18%)	0	100	100
2	K	412/420 (98%)	336 (82%)	76 (18%)	0	100	100
3	C	149/261 (57%)	111 (74%)	38 (26%)	0	100	100
3	F	149/261 (57%)	110 (74%)	39 (26%)	0	100	100
3	I	149/261 (57%)	110 (74%)	39 (26%)	0	100	100
3	L	149/261 (57%)	110 (74%)	39 (26%)	0	100	100
4	M	212/214 (99%)	140 (66%)	72 (34%)	0	100	100
4	O	212/214 (99%)	141 (66%)	71 (34%)	0	100	100
4	Q	212/214 (99%)	141 (66%)	71 (34%)	0	100	100
4	S	212/214 (99%)	141 (66%)	71 (34%)	0	100	100
5	N	211/213 (99%)	161 (76%)	50 (24%)	0	100	100
5	P	211/213 (99%)	161 (76%)	50 (24%)	0	100	100
5	R	211/213 (99%)	161 (76%)	50 (24%)	0	100	100
5	T	211/213 (99%)	160 (76%)	51 (24%)	0	100	100
All	All	5652/6196 (91%)	4429 (78%)	1223 (22%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/371 (98%)	286 (79%)	77 (21%)	1	6
1	D	363/371 (98%)	286 (79%)	77 (21%)	1	6
1	G	363/371 (98%)	286 (79%)	77 (21%)	1	6
1	J	363/371 (98%)	286 (79%)	77 (21%)	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	359/367 (98%)	277 (77%)	82 (23%)	1	6
2	E	359/367 (98%)	277 (77%)	82 (23%)	1	6
2	H	359/367 (98%)	277 (77%)	82 (23%)	1	6
2	K	359/367 (98%)	277 (77%)	82 (23%)	1	6
5	N	1/183 (0%)	1 (100%)	0	100	100
5	P	1/183 (0%)	1 (100%)	0	100	100
5	R	1/183 (0%)	1 (100%)	0	100	100
5	T	1/183 (0%)	1 (100%)	0	100	100
All	All	2892/3684 (78%)	2256 (78%)	636 (22%)	2	6

All (636) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	13	ILE
1	A	20	GLU
1	A	21	ARG
1	A	27	VAL
1	A	29	LEU
1	A	31	ILE
1	A	46	TYR
1	A	48	THR
1	A	52	LYS
1	A	57	SER
1	A	59	VAL
1	A	71	LYS
1	A	80	VAL
1	A	84	VAL
1	A	113	GLU
1	A	116	ILE
1	A	117	ASP
1	A	125	HIS
1	A	126	THR
1	A	140	VAL
1	A	146	ASP
1	A	147	VAL
1	A	153	THR
1	A	157	ILE
1	A	177	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	180	VAL
1	A	181	TYR
1	A	195	THR
1	A	197	LYS
1	A	201	PHE
1	A	215	TYR
1	A	222	LEU
1	A	226	GLN
1	A	230	VAL
1	A	237	VAL
1	A	239	SER
1	A	246	LYS
1	A	247	ASP
1	A	252	LEU
1	A	253	ASN
1	A	254	ASP
1	A	255	VAL
1	A	260	CYS
1	A	264	LEU
1	A	279	ILE
1	A	281	ILE
1	A	282	ASP
1	A	283	ILE
1	A	289	THR
1	A	290	ARG
1	A	291	ILE
1	A	301	GLU
1	A	308	THR
1	A	311	PHE
1	A	316	ILE
1	A	318	THR
1	A	323	SER
1	A	325	LYS
1	A	343	ASN
1	A	356	HIS
1	A	361	ASN
1	A	369	GLN
1	A	370	VAL
1	A	375	VAL
1	A	377	CYS
1	A	385	LYS
1	A	395	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	398	SER
1	A	403	ILE
1	A	408	TRP
1	A	411	ILE
1	A	414	LEU
1	A	426	LEU
1	A	435	VAL
1	A	439	HIS
1	A	441	HIS
2	B	3	ASP
2	B	5	HIS
2	B	8	GLN
2	B	26	ARG
2	B	31	ILE
2	B	33	ILE
2	B	34	GLU
2	B	36	VAL
2	B	44	VAL
2	B	47	ILE
2	B	52	MET
2	B	60	VAL
2	B	64	TYR
2	B	66	SER
2	B	72	THR
2	B	74	LYS
2	B	91	LEU
2	B	94	HIS
2	B	97	TYR
2	B	124	VAL
2	B	126	HIS
2	B	127	LYS
2	B	129	GLU
2	B	130	PHE
2	B	143	GLU
2	B	144	HIS
2	B	148	LEU
2	B	151	ASN
2	B	156	LYS
2	B	163	TYR
2	B	171	LEU
2	B	172	VAL
2	B	184	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	187	ILE
2	B	201	CYS
2	B	203	ASP
2	B	215	THR
2	B	217	CYS
2	B	242	ARG
2	B	246	ASP
2	B	247	THR
2	B	251	LYS
2	B	254	VAL
2	B	256	PHE
2	B	273	VAL
2	B	276	LYS
2	B	281	ILE
2	B	282	LEU
2	B	283	HIS
2	B	287	ASP
2	B	290	THR
2	B	293	THR
2	B	294	THR
2	B	295	ARG
2	B	296	SER
2	B	302	ASN
2	B	309	GLU
2	B	310	ARG
2	B	312	THR
2	B	319	THR
2	B	321	GLU
2	B	323	LEU
2	B	326	THR
2	B	334	ARG
2	B	338	GLN
2	B	339	GLU
2	B	346	HIS
2	B	354	VAL
2	B	362	LEU
2	B	376	MET
2	B	382	SER
2	B	386	LEU
2	B	388	ARG
2	B	390	ARG
2	B	393	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	397	TYR
2	B	398	LYS
2	B	399	LEU
2	B	401	PRO
2	B	405	VAL
2	B	408	LEU
2	B	412	LEU
1	D	11	VAL
1	D	13	ILE
1	D	20	GLU
1	D	21	ARG
1	D	27	VAL
1	D	29	LEU
1	D	31	ILE
1	D	46	TYR
1	D	48	THR
1	D	52	LYS
1	D	57	SER
1	D	59	VAL
1	D	71	LYS
1	D	80	VAL
1	D	84	VAL
1	D	113	GLU
1	D	116	ILE
1	D	117	ASP
1	D	125	HIS
1	D	126	THR
1	D	140	VAL
1	D	146	ASP
1	D	147	VAL
1	D	153	THR
1	D	157	ILE
1	D	177	LYS
1	D	180	VAL
1	D	181	TYR
1	D	195	THR
1	D	197	LYS
1	D	201	PHE
1	D	215	TYR
1	D	222	LEU
1	D	226	GLN
1	D	230	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	237	VAL
1	D	239	SER
1	D	246	LYS
1	D	247	ASP
1	D	252	LEU
1	D	253	ASN
1	D	254	ASP
1	D	255	VAL
1	D	260	CYS
1	D	264	LEU
1	D	279	ILE
1	D	281	ILE
1	D	282	ASP
1	D	283	ILE
1	D	289	THR
1	D	290	ARG
1	D	291	ILE
1	D	301	GLU
1	D	308	THR
1	D	311	PHE
1	D	316	ILE
1	D	318	THR
1	D	323	SER
1	D	325	LYS
1	D	343	ASN
1	D	356	HIS
1	D	361	ASN
1	D	369	GLN
1	D	370	VAL
1	D	375	VAL
1	D	377	CYS
1	D	385	LYS
1	D	395	HIS
1	D	398	SER
1	D	403	ILE
1	D	408	TRP
1	D	411	ILE
1	D	414	LEU
1	D	426	LEU
1	D	435	VAL
1	D	439	HIS
1	D	441	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	3	ASP
2	E	5	HIS
2	E	8	GLN
2	E	26	ARG
2	E	31	ILE
2	E	33	ILE
2	E	34	GLU
2	E	36	VAL
2	E	44	VAL
2	E	47	ILE
2	E	52	MET
2	E	60	VAL
2	E	64	TYR
2	E	66	SER
2	E	72	THR
2	E	74	LYS
2	E	91	LEU
2	E	94	HIS
2	E	97	TYR
2	E	124	VAL
2	E	126	HIS
2	E	127	LYS
2	E	129	GLU
2	E	130	PHE
2	E	143	GLU
2	E	144	HIS
2	E	148	LEU
2	E	151	ASN
2	E	156	LYS
2	E	163	TYR
2	E	171	LEU
2	E	172	VAL
2	E	184	LYS
2	E	187	ILE
2	E	201	CYS
2	E	203	ASP
2	E	215	THR
2	E	217	CYS
2	E	242	ARG
2	E	246	ASP
2	E	247	THR
2	E	251	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	254	VAL
2	E	256	PHE
2	E	273	VAL
2	E	276	LYS
2	E	281	ILE
2	E	282	LEU
2	E	283	HIS
2	E	287	ASP
2	E	290	THR
2	E	293	THR
2	E	294	THR
2	E	295	ARG
2	E	296	SER
2	E	302	ASN
2	E	309	GLU
2	E	310	ARG
2	E	312	THR
2	E	319	THR
2	E	321	GLU
2	E	323	LEU
2	E	326	THR
2	E	334	ARG
2	E	338	GLN
2	E	339	GLU
2	E	346	HIS
2	E	354	VAL
2	E	362	LEU
2	E	376	MET
2	E	382	SER
2	E	386	LEU
2	E	388	ARG
2	E	390	ARG
2	E	393	CYS
2	E	397	TYR
2	E	398	LYS
2	E	399	LEU
2	E	401	PRO
2	E	405	VAL
2	E	408	LEU
2	E	412	LEU
1	G	11	VAL
1	G	13	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	20	GLU
1	G	21	ARG
1	G	27	VAL
1	G	29	LEU
1	G	31	ILE
1	G	46	TYR
1	G	48	THR
1	G	52	LYS
1	G	57	SER
1	G	59	VAL
1	G	71	LYS
1	G	80	VAL
1	G	84	VAL
1	G	113	GLU
1	G	116	ILE
1	G	117	ASP
1	G	125	HIS
1	G	126	THR
1	G	140	VAL
1	G	146	ASP
1	G	147	VAL
1	G	153	THR
1	G	157	ILE
1	G	177	LYS
1	G	180	VAL
1	G	181	TYR
1	G	195	THR
1	G	197	LYS
1	G	201	PHE
1	G	215	TYR
1	G	222	LEU
1	G	226	GLN
1	G	230	VAL
1	G	237	VAL
1	G	239	SER
1	G	246	LYS
1	G	247	ASP
1	G	252	LEU
1	G	253	ASN
1	G	254	ASP
1	G	255	VAL
1	G	260	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	264	LEU
1	G	279	ILE
1	G	281	ILE
1	G	282	ASP
1	G	283	ILE
1	G	289	THR
1	G	290	ARG
1	G	291	ILE
1	G	301	GLU
1	G	308	THR
1	G	311	PHE
1	G	316	ILE
1	G	318	THR
1	G	323	SER
1	G	325	LYS
1	G	343	ASN
1	G	356	HIS
1	G	361	ASN
1	G	369	GLN
1	G	370	VAL
1	G	375	VAL
1	G	377	CYS
1	G	385	LYS
1	G	395	HIS
1	G	398	SER
1	G	403	ILE
1	G	408	TRP
1	G	411	ILE
1	G	414	LEU
1	G	426	LEU
1	G	435	VAL
1	G	439	HIS
1	G	441	HIS
2	H	3	ASP
2	H	5	HIS
2	H	8	GLN
2	H	26	ARG
2	H	31	ILE
2	H	33	ILE
2	H	34	GLU
2	H	36	VAL
2	H	44	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	47	ILE
2	H	52	MET
2	H	60	VAL
2	H	64	TYR
2	H	66	SER
2	H	72	THR
2	H	74	LYS
2	H	91	LEU
2	H	94	HIS
2	H	97	TYR
2	H	124	VAL
2	H	126	HIS
2	H	127	LYS
2	H	129	GLU
2	H	130	PHE
2	H	143	GLU
2	H	144	HIS
2	H	148	LEU
2	H	151	ASN
2	H	156	LYS
2	H	163	TYR
2	H	171	LEU
2	H	172	VAL
2	H	184	LYS
2	H	187	ILE
2	H	201	CYS
2	H	203	ASP
2	H	215	THR
2	H	217	CYS
2	H	242	ARG
2	H	246	ASP
2	H	247	THR
2	H	251	LYS
2	H	254	VAL
2	H	256	PHE
2	H	273	VAL
2	H	276	LYS
2	H	281	ILE
2	H	282	LEU
2	H	283	HIS
2	H	287	ASP
2	H	290	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	293	THR
2	H	294	THR
2	H	295	ARG
2	H	296	SER
2	H	302	ASN
2	H	309	GLU
2	H	310	ARG
2	H	312	THR
2	H	319	THR
2	H	321	GLU
2	H	323	LEU
2	H	326	THR
2	H	334	ARG
2	H	338	GLN
2	H	339	GLU
2	H	346	HIS
2	H	354	VAL
2	H	362	LEU
2	H	376	MET
2	H	382	SER
2	H	386	LEU
2	H	388	ARG
2	H	390	ARG
2	H	393	CYS
2	H	397	TYR
2	H	398	LYS
2	H	399	LEU
2	H	401	PRO
2	H	405	VAL
2	H	408	LEU
2	H	412	LEU
1	J	11	VAL
1	J	13	ILE
1	J	20	GLU
1	J	21	ARG
1	J	27	VAL
1	J	29	LEU
1	J	31	ILE
1	J	46	TYR
1	J	48	THR
1	J	52	LYS
1	J	57	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	59	VAL
1	J	71	LYS
1	J	80	VAL
1	J	84	VAL
1	J	113	GLU
1	J	116	ILE
1	J	117	ASP
1	J	125	HIS
1	J	126	THR
1	J	140	VAL
1	J	146	ASP
1	J	147	VAL
1	J	153	THR
1	J	157	ILE
1	J	177	LYS
1	J	180	VAL
1	J	181	TYR
1	J	195	THR
1	J	197	LYS
1	J	201	PHE
1	J	215	TYR
1	J	222	LEU
1	J	226	GLN
1	J	230	VAL
1	J	237	VAL
1	J	239	SER
1	J	246	LYS
1	J	247	ASP
1	J	252	LEU
1	J	253	ASN
1	J	254	ASP
1	J	255	VAL
1	J	260	CYS
1	J	264	LEU
1	J	279	ILE
1	J	281	ILE
1	J	282	ASP
1	J	283	ILE
1	J	289	THR
1	J	290	ARG
1	J	291	ILE
1	J	301	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	308	THR
1	J	311	PHE
1	J	316	ILE
1	J	318	THR
1	J	323	SER
1	J	325	LYS
1	J	343	ASN
1	J	356	HIS
1	J	361	ASN
1	J	369	GLN
1	J	370	VAL
1	J	375	VAL
1	J	377	CYS
1	J	385	LYS
1	J	395	HIS
1	J	398	SER
1	J	403	ILE
1	J	408	TRP
1	J	411	ILE
1	J	414	LEU
1	J	426	LEU
1	J	435	VAL
1	J	439	HIS
1	J	441	HIS
2	K	3	ASP
2	K	5	HIS
2	K	8	GLN
2	K	26	ARG
2	K	31	ILE
2	K	33	ILE
2	K	34	GLU
2	K	36	VAL
2	K	44	VAL
2	K	47	ILE
2	K	52	MET
2	K	60	VAL
2	K	64	TYR
2	K	66	SER
2	K	72	THR
2	K	74	LYS
2	K	91	LEU
2	K	94	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	97	TYR
2	K	124	VAL
2	K	126	HIS
2	K	127	LYS
2	K	129	GLU
2	K	130	PHE
2	K	143	GLU
2	K	144	HIS
2	K	148	LEU
2	K	151	ASN
2	K	156	LYS
2	K	163	TYR
2	K	171	LEU
2	K	172	VAL
2	K	184	LYS
2	K	187	ILE
2	K	201	CYS
2	K	203	ASP
2	K	215	THR
2	K	217	CYS
2	K	242	ARG
2	K	246	ASP
2	K	247	THR
2	K	251	LYS
2	K	254	VAL
2	K	256	PHE
2	K	273	VAL
2	K	276	LYS
2	K	281	ILE
2	K	282	LEU
2	K	283	HIS
2	K	287	ASP
2	K	290	THR
2	K	293	THR
2	K	294	THR
2	K	295	ARG
2	K	296	SER
2	K	302	ASN
2	K	309	GLU
2	K	310	ARG
2	K	312	THR
2	K	319	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	321	GLU
2	K	323	LEU
2	K	326	THR
2	K	334	ARG
2	K	338	GLN
2	K	339	GLU
2	K	346	HIS
2	K	354	VAL
2	K	362	LEU
2	K	376	MET
2	K	382	SER
2	K	386	LEU
2	K	388	ARG
2	K	390	ARG
2	K	393	CYS
2	K	397	TYR
2	K	398	LYS
2	K	399	LEU
2	K	401	PRO
2	K	405	VAL
2	K	408	LEU
2	K	412	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	212	ASN
1	A	332	HIS
2	B	140	HIS
2	B	160	GLN
2	B	306	GLN
2	B	329	ASN
2	B	346	HIS
1	D	30	GLN
1	D	332	HIS
2	E	160	GLN
2	E	306	GLN
1	G	30	GLN
1	G	332	HIS
2	H	160	GLN
2	H	306	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	329	ASN
1	J	30	GLN
1	J	102	GLN
1	J	212	ASN
1	J	332	HIS
2	K	140	HIS
2	K	160	GLN
2	K	306	GLN
2	K	329	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

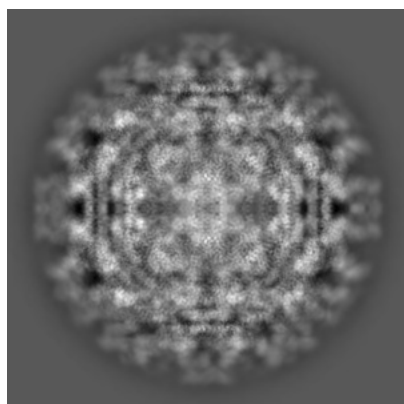
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22277. These allow visual inspection of the internal detail of the map and identification of artifacts.

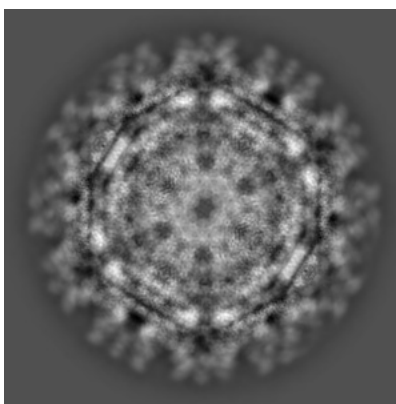
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

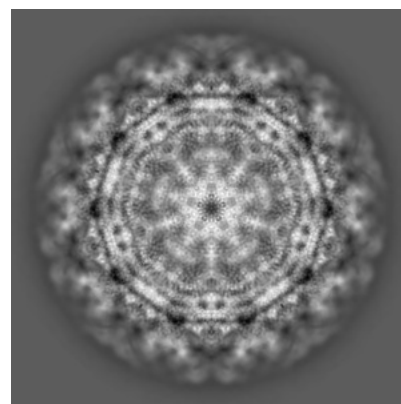
6.1.1 Primary map



X

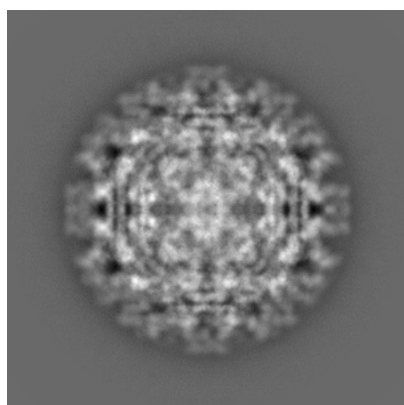


Y

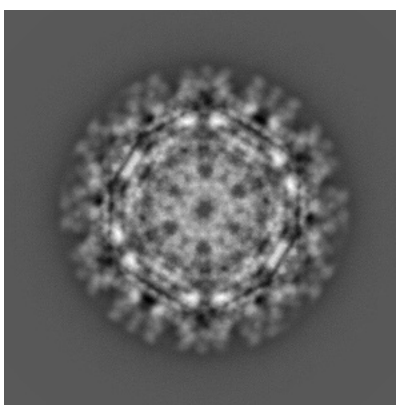


Z

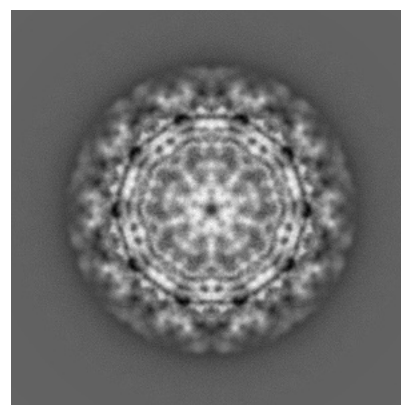
6.1.2 Raw map



X



Y

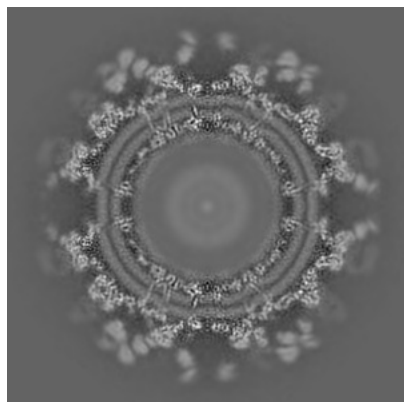


Z

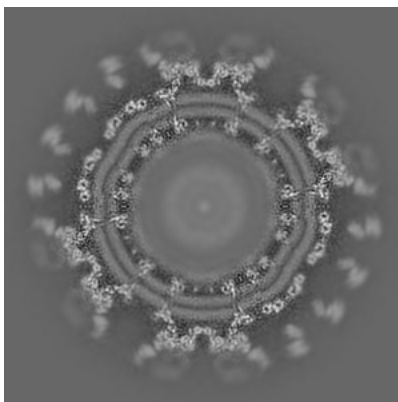
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

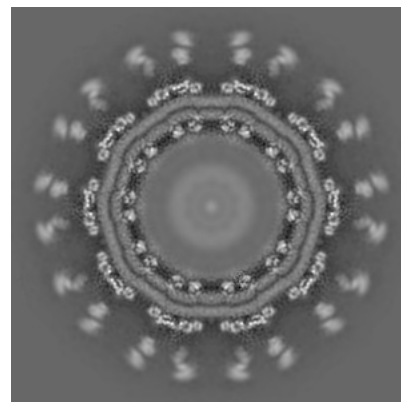
6.2.1 Primary map



X Index: 210

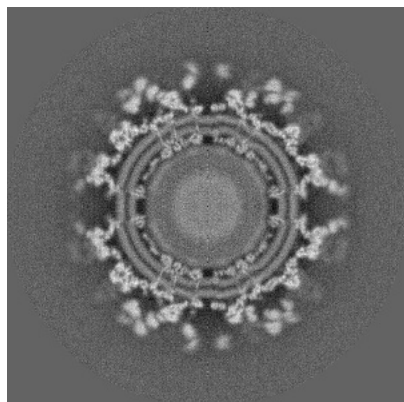


Y Index: 210

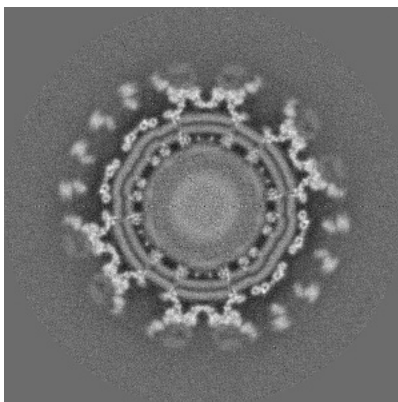


Z Index: 210

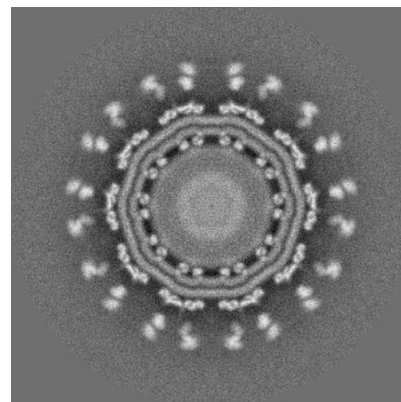
6.2.2 Raw map



X Index: 256



Y Index: 256

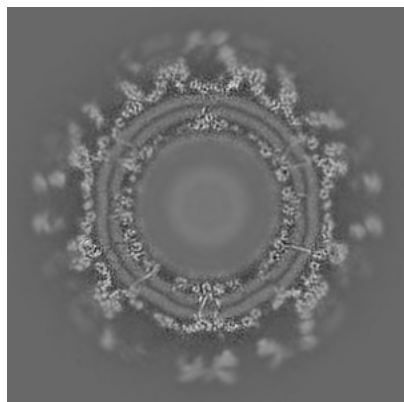


Z Index: 256

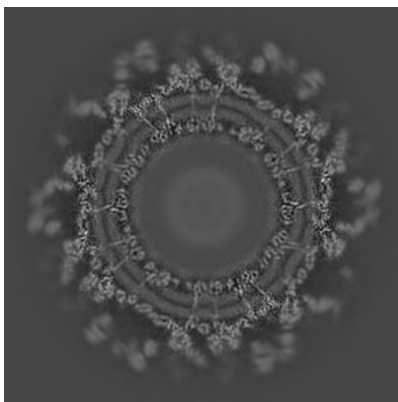
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

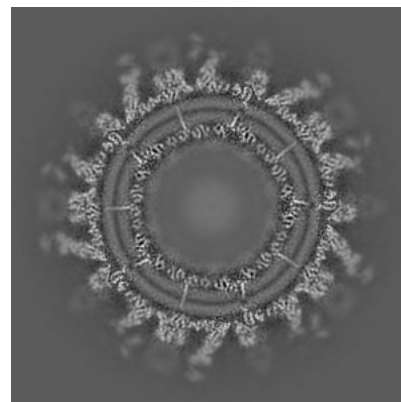
6.3.1 Primary map



X Index: 222

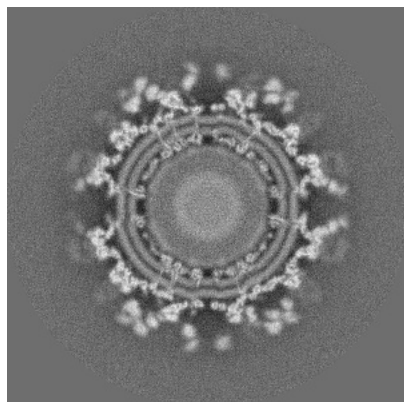


Y Index: 197

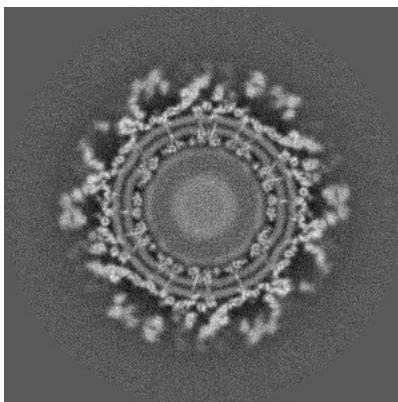


Z Index: 176

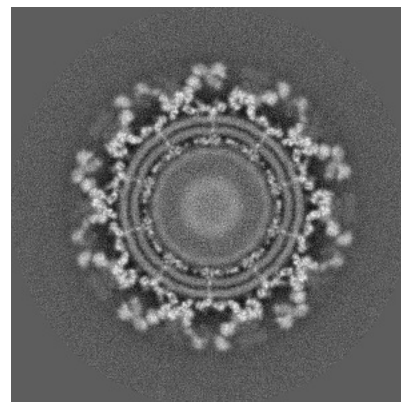
6.3.2 Raw map



X Index: 257



Y Index: 271

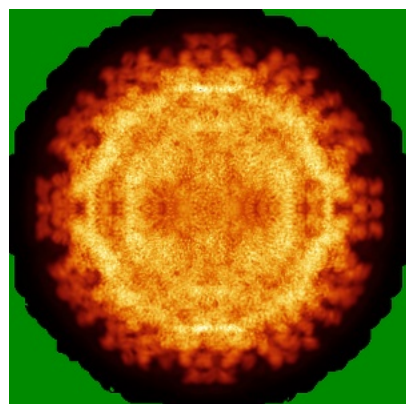


Z Index: 237

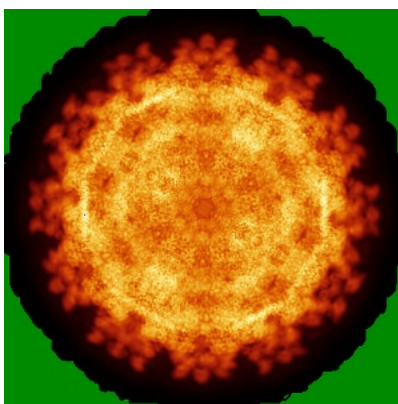
The images above show the largest variance slices of the map in three orthogonal directions.

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

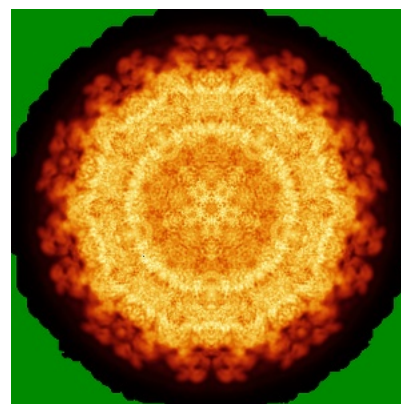
6.4.1 Primary map



X

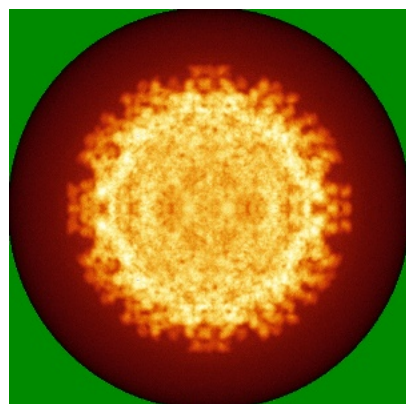


Y

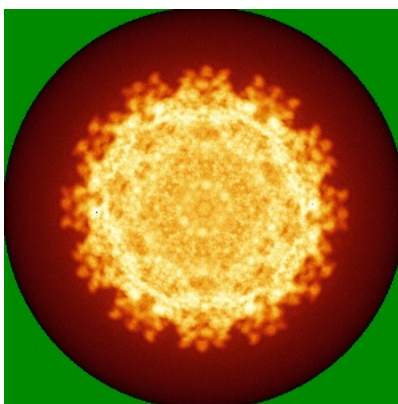


Z

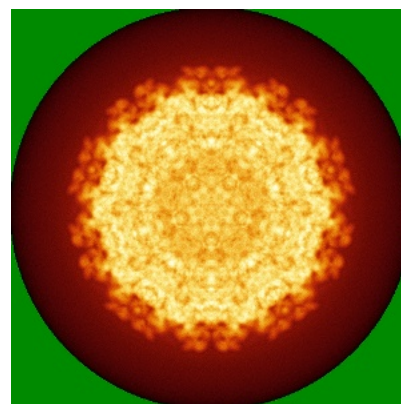
6.4.2 Raw map



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 0.025. 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.

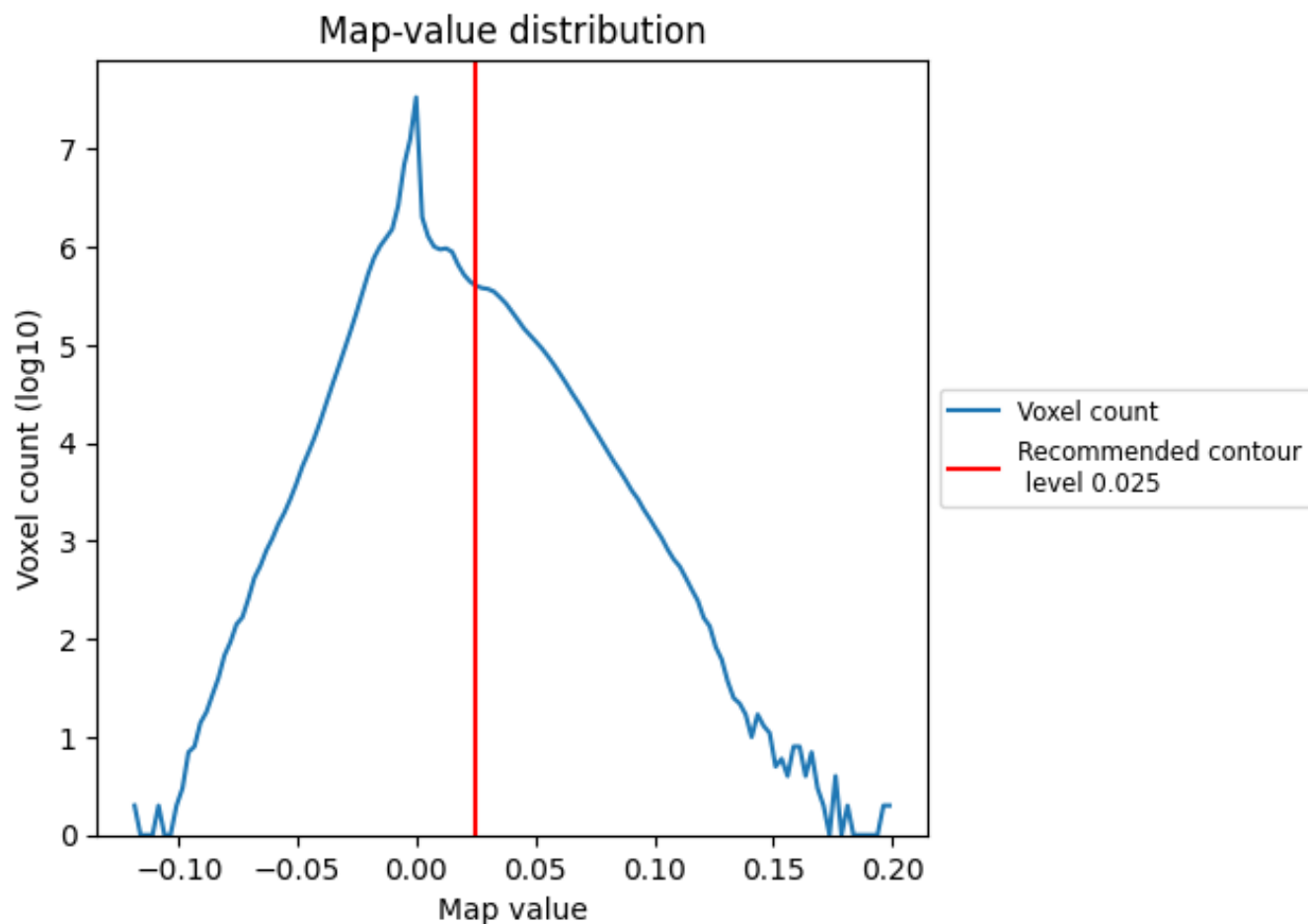
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

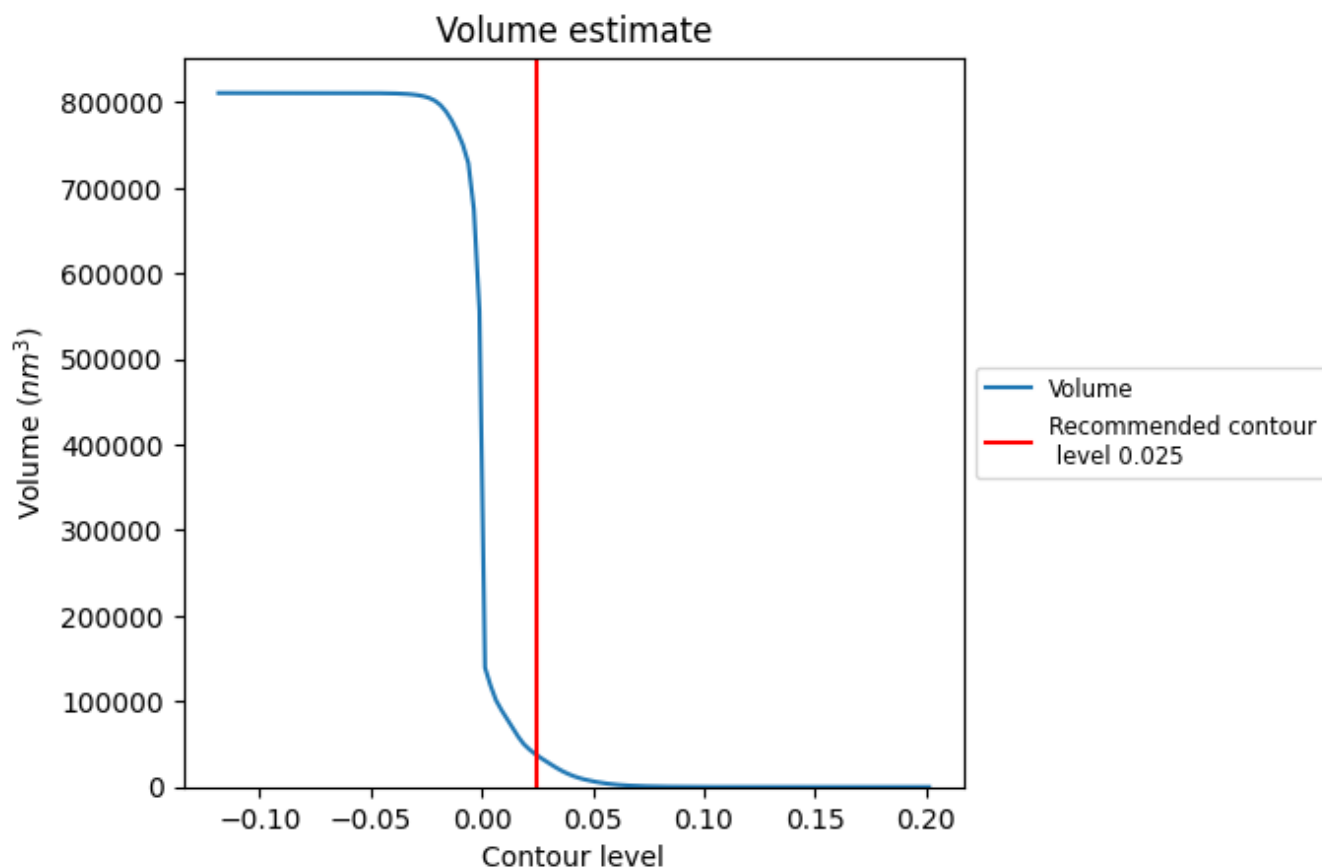
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

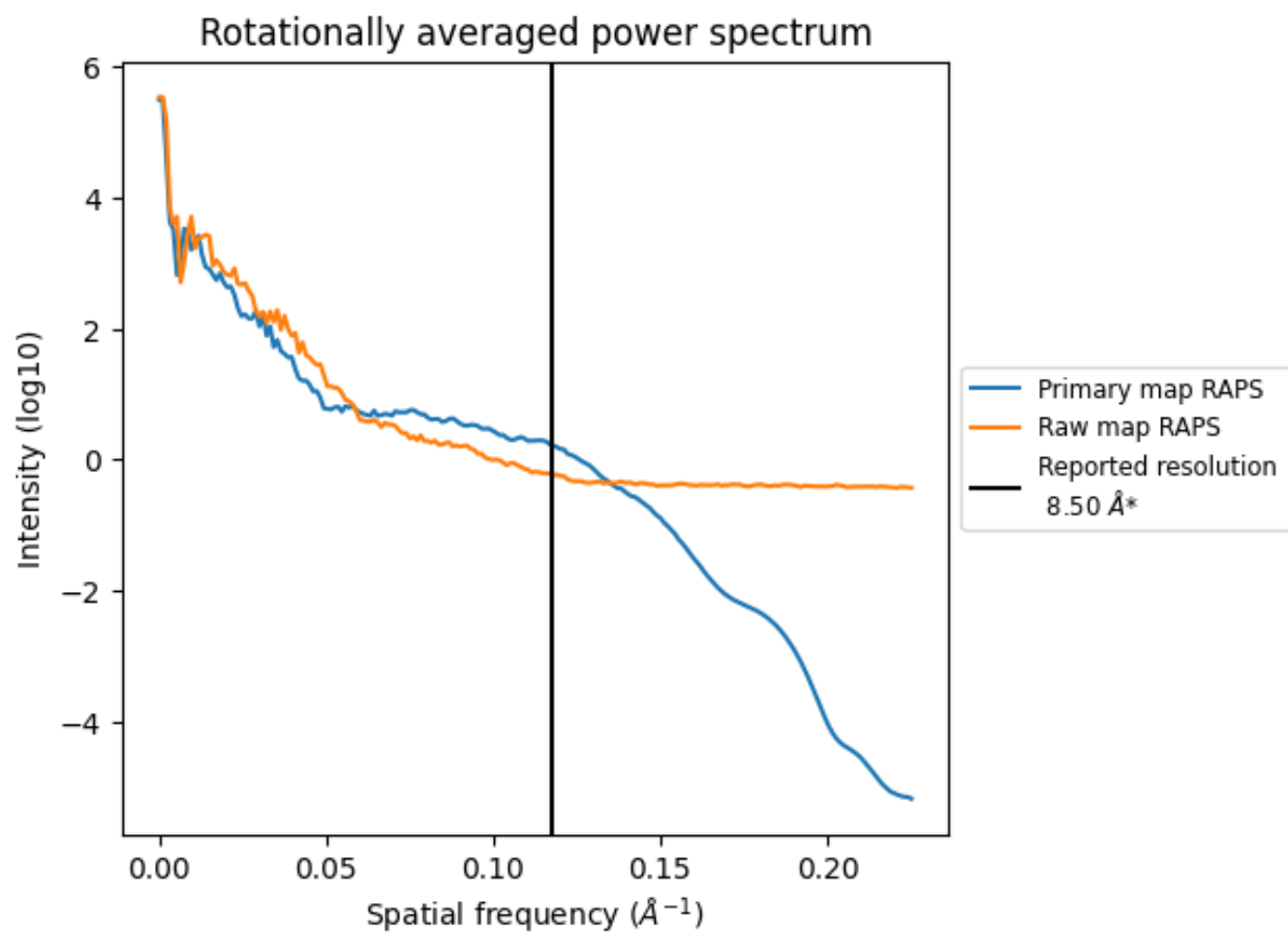
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 36798 nm^3 ; this corresponds to an approximate mass of 33241 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](#)

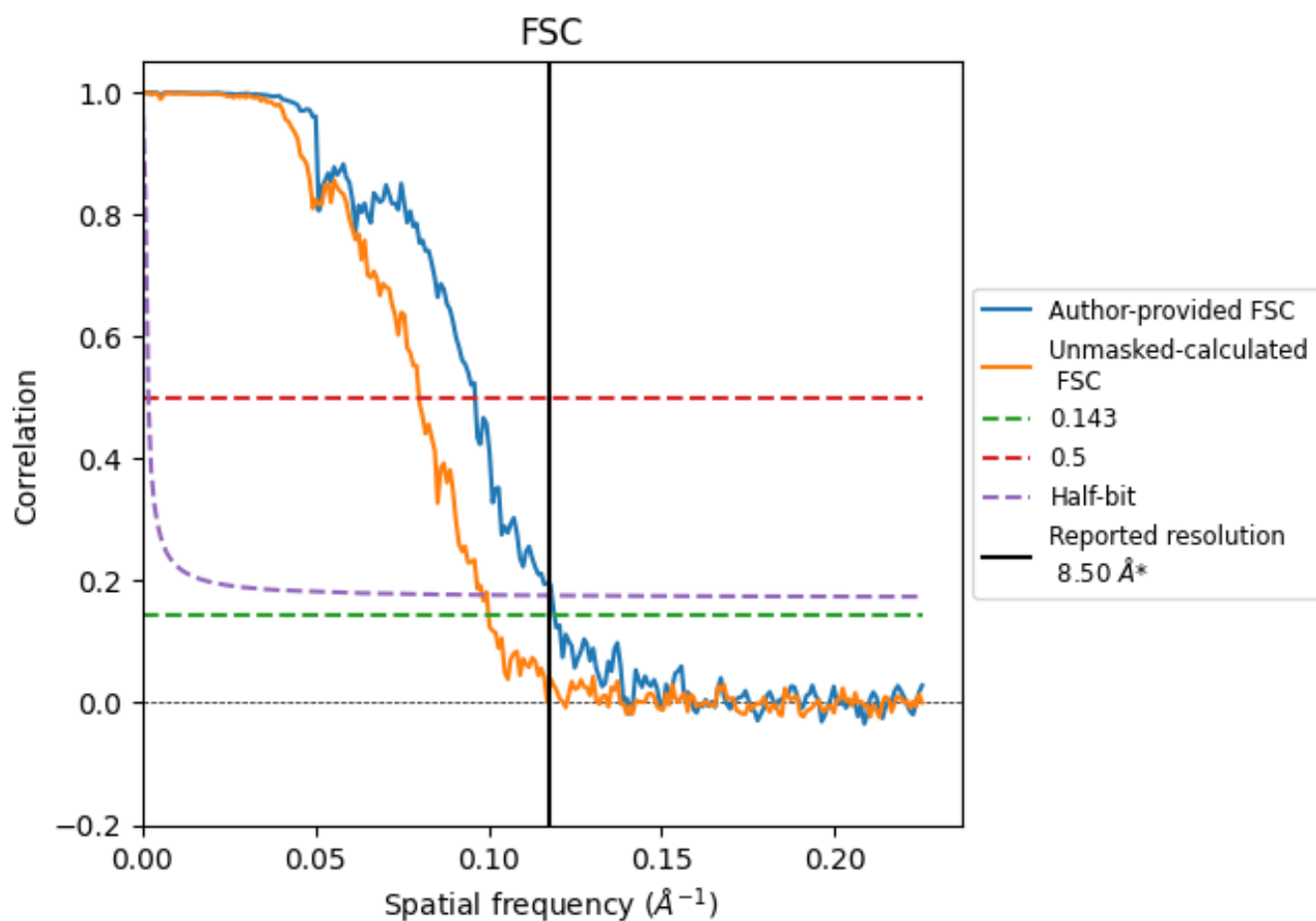


*Reported resolution corresponds to spatial frequency of 0.118 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.118 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.50	-	-
Author-provided FSC curve	8.40	10.41	8.46
Unmasked-calculated*	10.00	12.52	10.18

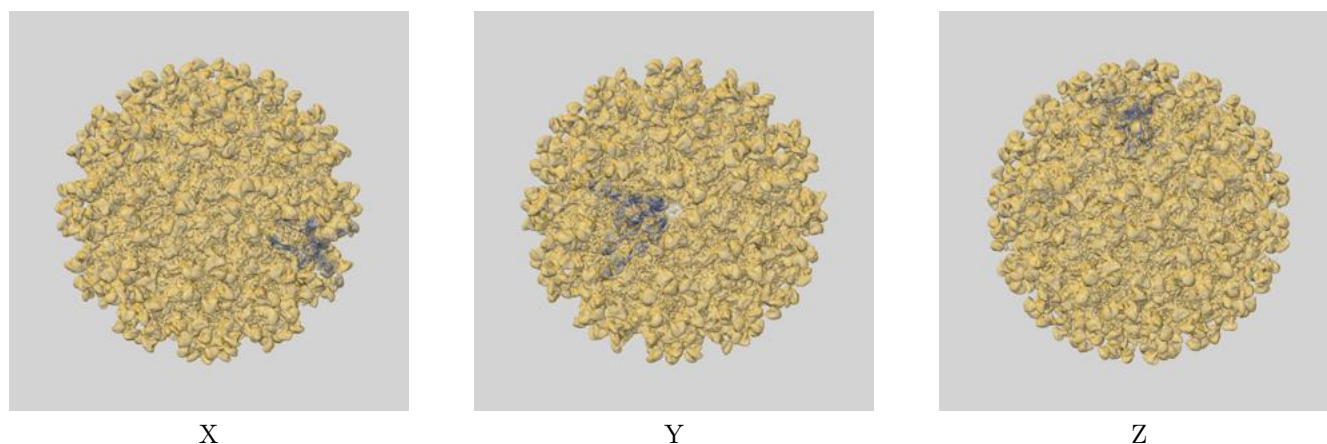
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 10.00 differs from the reported value 8.5 by more than 10 %

9 Map-model fit [i](#)

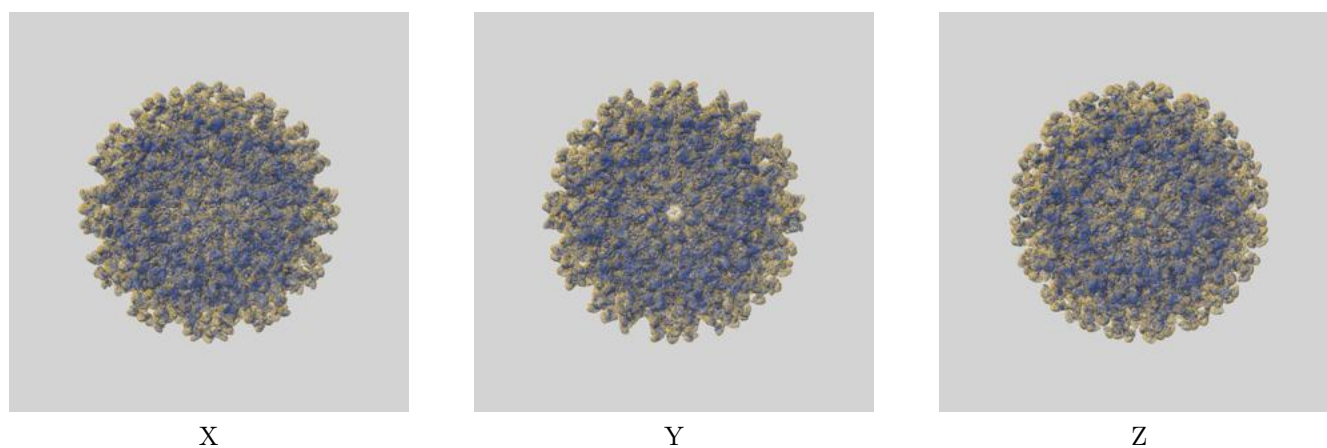
This section contains information regarding the fit between EMDB map EMD-22277 and PDB model 6XOB. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

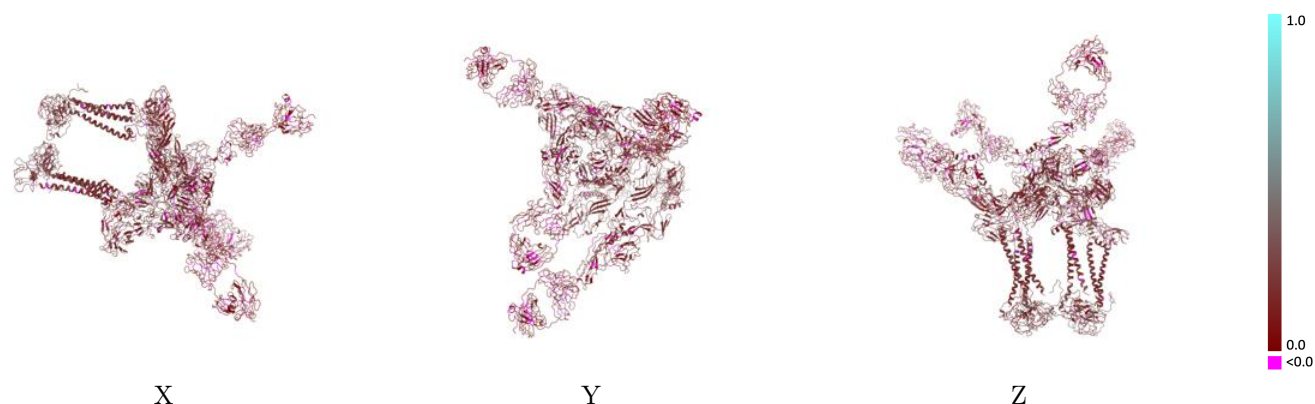


9.1.2 Map-model assembly overlay [i](#)



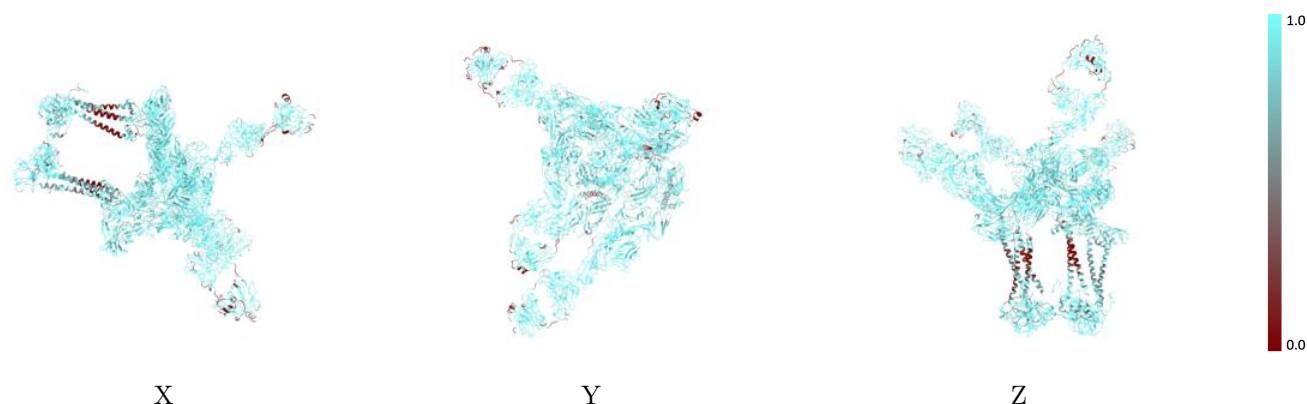
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



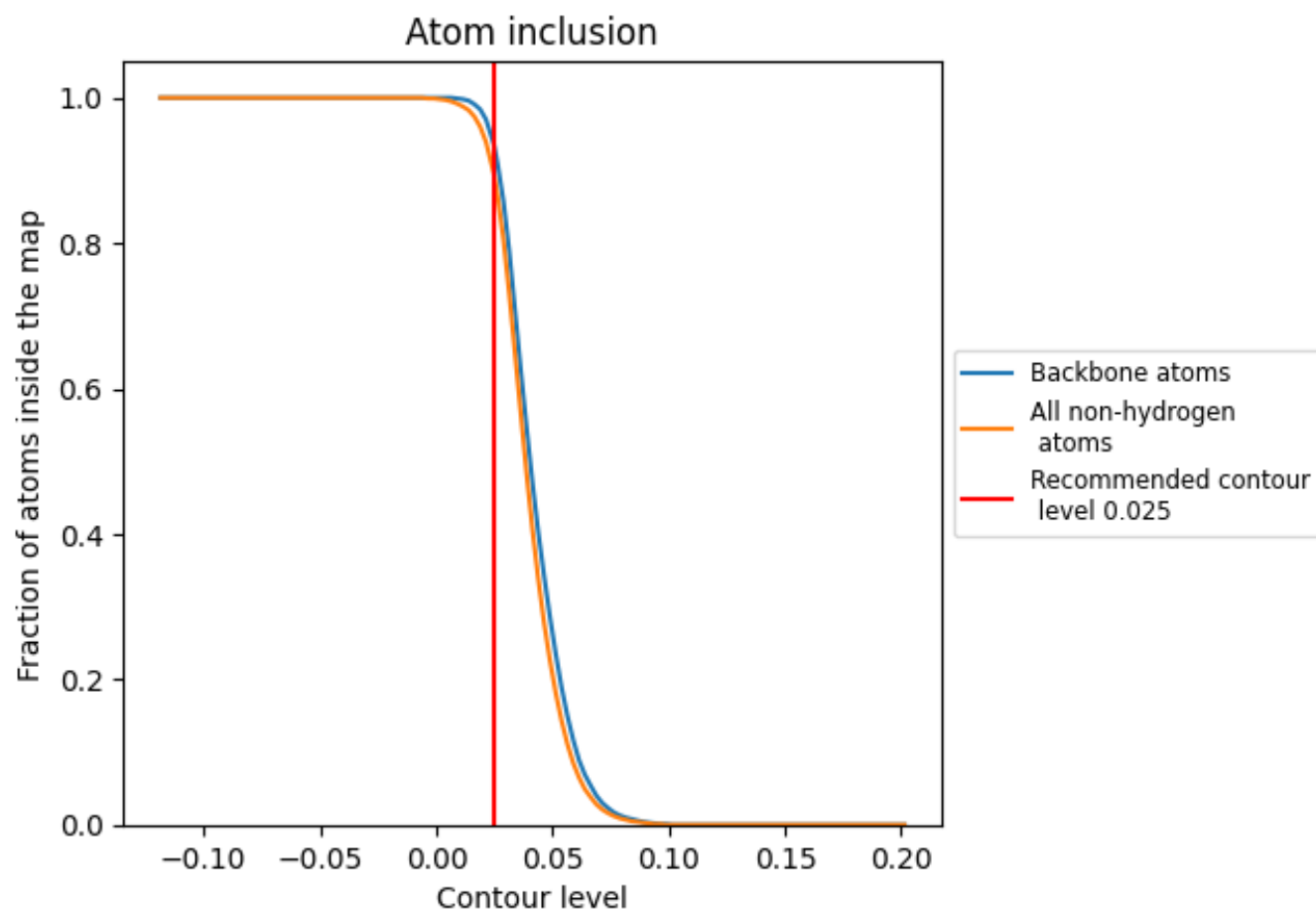
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 89% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8930	 0.1820
A	 0.8980	 0.2050
B	 0.9130	 0.1890
C	 0.8670	 0.2860
D	 0.8900	 0.2020
E	 0.8910	 0.1850
F	 0.8720	 0.2610
G	 0.8760	 0.1980
H	 0.8920	 0.1840
I	 0.8550	 0.2620
J	 0.8980	 0.2030
K	 0.9250	 0.1890
L	 0.9090	 0.2820
M	 0.8840	 0.1190
N	 0.9600	 0.1150
O	 0.8570	 0.1110
P	 0.8540	 0.1110
Q	 0.8110	 0.1080
R	 0.8810	 0.1070
S	 0.8840	 0.1150
T	 0.9320	 0.1220

