



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 24, 2017 – 10:30 AM EDT

PDB ID : 5APM
EMDB ID: : EMD-3137
Title : Multiple capsid-stabilizing protein-RNA and protein-protein interactions revealed in a high-resolution structure of an emerging picornavirus causing neonatal sepsis
Authors : Shakeel, S.; Westerhuis, B.M.; Domanska, A.; Koning, R.I.; Matadeen, R.; Koster, A.J.; Bakker, A.Q.; Beaumont, T.; Wolthers, K.C.; Butcher, S.J.
Deposited on : unknown
Resolution : 4.30 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

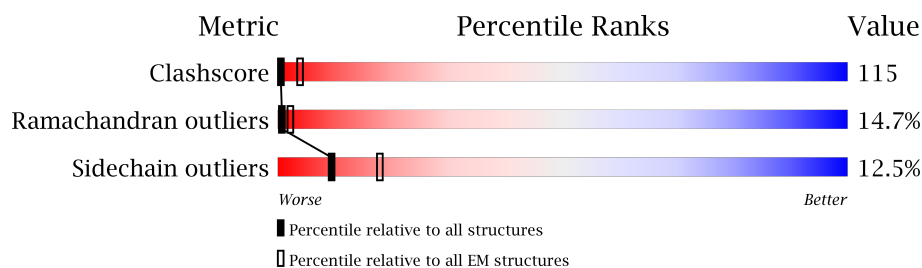
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	198	<div> <div>25%</div> <div>50%</div> <div>21%</div> <div>5%</div> </div>
2	B	237	<div> <div>25%</div> <div>52%</div> <div>19%</div> <div>.</div> </div>
3	C	263	<div> <div>36%</div> <div>45%</div> <div>15%</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5490 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	198	Total	C	N	O	S	0	0
			1577	1006	273	289	9		

- Molecule 2 is a protein called VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	237	Total	C	N	O	S	0	0
			1874	1186	322	354	12		

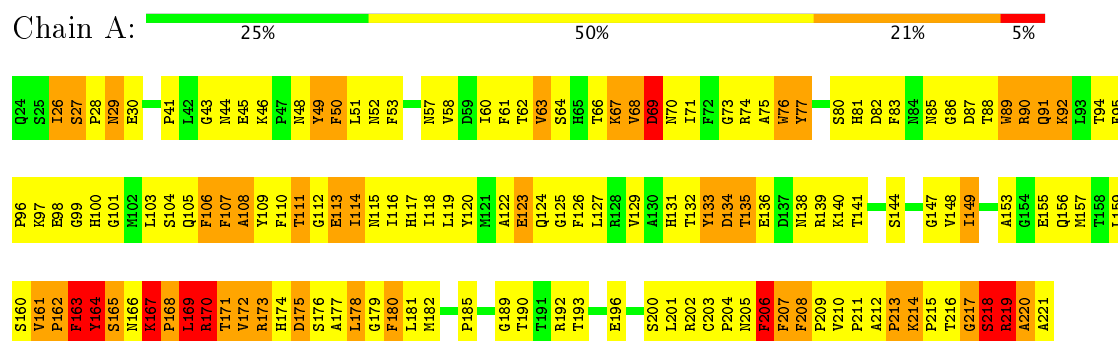
- Molecule 3 is a protein called VP0.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	263	Total	C	N	O	S	0	0
			2039	1283	341	410	5		

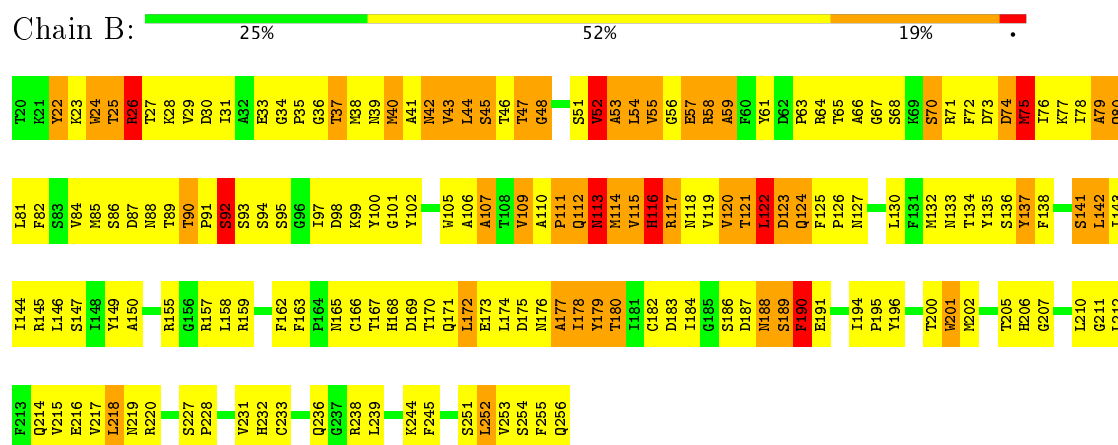
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

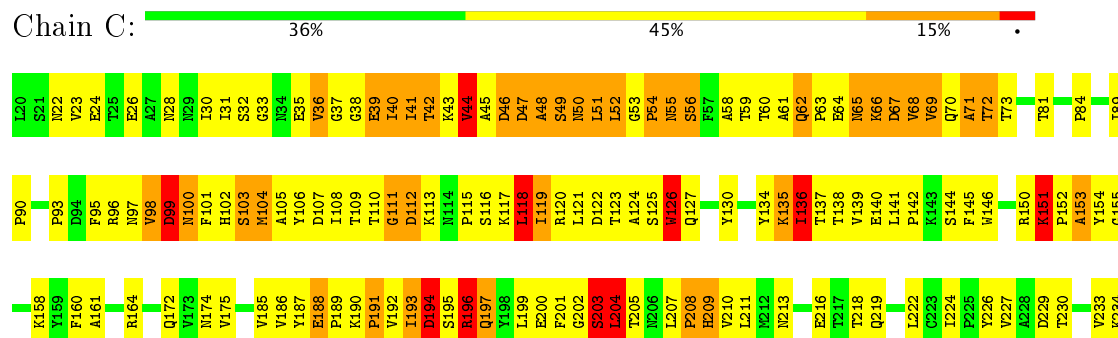
• Molecule 1: VP1



• Molecule 2: VP3



• Molecule 3: VP0



S237	S238	D239	L240	G241	R242	L243	R244	Y245	Y246	Y247	R248	T249	P250	L251	Y261	D262	Y263	T264	Y265	Y266	G267	S268	L269	P277	R278	Y282
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	8889	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	MICROGRAPHS	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	420	Depositor
Maximum defocus (nm)	2340	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.55	0/1623	0.97	3/2204 (0.1%)
2	B	0.50	0/1919	0.88	1/2600 (0.0%)
3	C	0.83	1/2086 (0.0%)	1.04	10/2857 (0.4%)
All	All	0.65	1/5628 (0.0%)	0.96	14/7661 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	118	LEU	C-N	-29.05	0.67	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	118	LEU	O-C-N	-24.50	83.51	122.70
3	C	112	ASP	C-N-CA	-15.45	83.09	121.70
3	C	118	LEU	CA-C-N	15.02	150.25	117.20
3	C	118	LEU	C-N-CA	11.97	151.62	121.70
3	C	112	ASP	CA-C-N	8.65	136.24	117.20
3	C	111	GLY	N-CA-C	-7.19	95.13	113.10
3	C	112	ASP	O-C-N	-5.63	113.69	122.70
1	A	49	TYR	CA-CB-CG	5.39	123.64	113.40
1	A	217	GLY	O-C-N	5.38	131.31	122.70
1	A	161	VAL	C-N-CD	5.35	139.63	128.40
3	C	126	TRP	C-N-CA	5.32	135.00	121.70
3	C	190	LYS	C-N-CD	5.31	139.54	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	218	LEU	CA-CB-CG	5.09	127.00	115.30
3	C	53	GLY	C-N-CD	5.01	138.91	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	118	LEU	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1577	0	1508	482	0
2	B	1874	0	1811	440	0
3	C	2039	0	1961	412	0
All	All	5490	0	5280	1243	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 115.

All (1243) 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:A:109:TYR:CD2	1:A:206:PHE:HZ	1.08	1.70
3:C:110:THR:CG2	3:C:111:GLY:HA2	1.22	1.65
3:C:31:ILE:HG23	3:C:44:VAL:CG1	1.21	1.58
1:A:51:LEU:CD1	1:A:53:PHE:HD2	1.11	1.57
1:A:117:HIS:CE1	2:B:44:LEU:HD21	1.38	1.56
3:C:110:THR:HG22	3:C:111:GLY:CA	1.31	1.55
1:A:51:LEU:CD1	1:A:53:PHE:CD2	1.86	1.54
1:A:174:HIS:CD2	1:A:214:LYS:NZ	1.75	1.53
3:C:145:PHE:C	3:C:153:ALA:HB1	1.22	1.53
1:A:109:TYR:CD2	1:A:206:PHE:CZ	1.98	1.51
3:C:43:LYS:HD2	3:C:49:SER:CB	1.39	1.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:CYS:SG	2:B:190:PHE:CE2	2.07	1.47
1:A:90:ARG:HG2	1:A:182:MET:SD	1.53	1.47
3:C:115:PRO:HA	3:C:152:PRO:CD	1.47	1.44
3:C:60:THR:O	3:C:64:GLU:CG	1.65	1.43
1:A:117:HIS:HE1	2:B:44:LEU:CD2	1.30	1.42
2:B:182:CYS:SG	2:B:190:PHE:HE2	1.40	1.41
1:A:174:HIS:CD2	1:A:214:LYS:HZ2	1.34	1.40
1:A:51:LEU:HD11	1:A:53:PHE:CD2	1.46	1.39
3:C:31:ILE:CG2	3:C:44:VAL:HG11	0.92	1.39
2:B:88:ASN:O	2:B:91:PRO:CB	1.69	1.37
1:A:90:ARG:CG	1:A:182:MET:HE1	1.54	1.37
1:A:174:HIS:HD2	1:A:214:LYS:NZ	0.85	1.34
2:B:88:ASN:C	2:B:91:PRO:HB3	1.48	1.34
2:B:116:HIS:O	2:B:117:ARG:CG	1.75	1.34
3:C:145:PHE:C	3:C:153:ALA:CB	1.97	1.31
1:A:210:VAL:O	1:A:213:PRO:HD2	1.29	1.31
1:A:103:LEU:O	1:A:106:PHE:CZ	1.83	1.31
2:B:56:GLY:HA2	2:B:57:GLU:CG	1.59	1.31
3:C:31:ILE:CG2	3:C:44:VAL:CG1	1.87	1.30
3:C:65:ASN:CA	3:C:67:ASP:N	1.93	1.30
3:C:146:TRP:HA	3:C:153:ALA:O	1.22	1.29
2:B:40:MET:HG2	2:B:43:VAL:O	1.26	1.29
3:C:192:VAL:HG13	3:C:194:ASP:CG	1.53	1.29
2:B:182:CYS:CB	2:B:190:PHE:HE2	1.46	1.28
3:C:65:ASN:HA	3:C:66:LYS:C	1.22	1.28
3:C:188:GLU:OE1	3:C:193:ILE:CD1	1.80	1.27
1:A:90:ARG:HG2	1:A:182:MET:CE	1.64	1.27
3:C:115:PRO:CA	3:C:152:PRO:HG3	1.63	1.26
3:C:192:VAL:HG13	3:C:194:ASP:OD1	1.33	1.26
1:A:90:ARG:CG	1:A:182:MET:CE	2.13	1.26
1:A:67:LYS:HG3	2:B:73:ASP:CB	1.66	1.26
1:A:66:THR:O	2:B:75:MET:HG3	1.29	1.25
1:A:133:TYR:OH	1:A:161:VAL:HG11	1.19	1.25
1:A:66:THR:O	2:B:75:MET:CG	1.84	1.25
3:C:203:SER:O	3:C:205:THR:N	1.69	1.25
1:A:103:LEU:C	1:A:106:PHE:CZ	2.10	1.24
1:A:96:PRO:O	1:A:177:ALA:HB2	1.30	1.24
1:A:67:LYS:HD3	2:B:73:ASP:OD2	1.26	1.24
1:A:172:VAL:HG21	1:A:175:ASP:OD1	1.23	1.24
2:B:40:MET:CG	2:B:43:VAL:O	1.84	1.24
3:C:145:PHE:O	3:C:153:ALA:CB	1.86	1.24

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:GLY:CA	2:B:57:GLU:HG2	1.66	1.23
2:B:22:TYR:HB2	2:B:24:TRP:CA	1.67	1.22
1:A:215:PRO:CB	3:C:203:SER:HA	1.69	1.22
3:C:110:THR:CB	3:C:111:GLY:HA2	1.69	1.22
1:A:109:TYR:CG	1:A:206:PHE:CZ	2.26	1.22
2:B:52:VAL:O	2:B:54:LEU:HD23	1.39	1.21
3:C:115:PRO:CB	3:C:152:PRO:HG3	1.70	1.21
1:A:206:PHE:O	1:A:209:PRO:HD3	1.41	1.20
3:C:118:LEU:CA	3:C:267:GLY:O	1.90	1.20
3:C:43:LYS:CD	3:C:49:SER:OG	1.90	1.20
2:B:114:MET:SD	2:B:115:VAL:N	2.16	1.19
1:A:51:LEU:CG	1:A:52:ASN:H	1.50	1.18
3:C:65:ASN:CA	3:C:66:LYS:C	2.07	1.18
2:B:182:CYS:HA	2:B:190:PHE:CZ	1.77	1.18
2:B:74:ASP:OD2	2:B:77:LYS:CB	1.89	1.18
2:B:74:ASP:OD2	2:B:77:LYS:CG	1.92	1.18
1:A:135:THR:OG1	1:A:136:GLU:HB2	1.44	1.18
1:A:218:SER:C	1:A:220:ALA:H	1.36	1.17
2:B:22:TYR:HB2	2:B:24:TRP:HA	1.24	1.17
3:C:152:PRO:O	3:C:154:TYR:N	1.77	1.17
2:B:23:LYS:HB3	2:B:24:TRP:HA	1.24	1.16
2:B:22:TYR:HB3	2:B:23:LYS:CB	1.76	1.16
1:A:28:PRO:CD	2:B:189:SER:OG	1.91	1.16
1:A:133:TYR:HB2	1:A:134:ASP:HB2	1.24	1.16
3:C:191:PRO:HD2	3:C:193:ILE:HD13	1.23	1.16
1:A:213:PRO:O	1:A:215:PRO:CD	1.93	1.15
2:B:121:THR:O	2:B:210:LEU:HD12	1.47	1.15
2:B:188:ASN:HB2	2:B:189:SER:HA	1.26	1.15
2:B:74:ASP:HA	2:B:75:MET:HB2	1.18	1.15
2:B:74:ASP:OD2	2:B:77:LYS:HG3	1.46	1.15
3:C:188:GLU:OE1	3:C:193:ILE:HD12	1.38	1.15
2:B:182:CYS:CB	2:B:190:PHE:CE2	2.28	1.14
1:A:109:TYR:CG	1:A:206:PHE:HZ	1.61	1.14
1:A:179:GLY:O	1:A:180:PHE:CG	2.00	1.14
1:A:28:PRO:HD3	2:B:189:SER:OG	1.41	1.14
1:A:213:PRO:O	1:A:215:PRO:N	1.82	1.14
1:A:109:TYR:HB2	1:A:206:PHE:CZ	1.83	1.13
3:C:98:VAL:HG13	3:C:99:ASP:HB2	1.20	1.13
2:B:22:TYR:CB	2:B:23:LYS:HB3	1.77	1.13
3:C:99:ASP:HB3	3:C:100:ASN:C	1.68	1.13
3:C:146:TRP:CA	3:C:153:ALA:O	1.97	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:LYS:HD2	3:C:49:SER:OG	1.41	1.12
3:C:50:ASN:O	3:C:52:LEU:N	1.81	1.12
1:A:28:PRO:HG3	2:B:145:ARG:HH22	0.99	1.12
2:B:22:TYR:HB3	2:B:23:LYS:HB3	1.13	1.11
2:B:52:VAL:O	2:B:54:LEU:N	1.82	1.11
3:C:60:THR:O	3:C:64:GLU:HG2	1.36	1.11
3:C:118:LEU:HA	3:C:267:GLY:O	0.95	1.11
1:A:104:SER:HA	1:A:106:PHE:CE1	1.86	1.11
2:B:42:ASN:O	2:B:43:VAL:HG23	1.47	1.11
2:B:120:VAL:CG1	2:B:121:THR:HA	1.80	1.11
2:B:114:MET:HB3	2:B:215:VAL:O	1.49	1.11
1:A:28:PRO:HG3	2:B:145:ARG:NH2	1.66	1.10
1:A:172:VAL:CG2	1:A:175:ASP:OD1	1.98	1.10
1:A:51:LEU:HG	1:A:52:ASN:H	0.98	1.10
1:A:109:TYR:CB	1:A:206:PHE:CZ	2.35	1.10
3:C:145:PHE:O	3:C:153:ALA:HB3	1.49	1.09
3:C:115:PRO:CA	3:C:152:PRO:CG	2.28	1.09
1:A:103:LEU:O	1:A:106:PHE:CE2	2.04	1.09
1:A:210:VAL:O	1:A:213:PRO:CD	2.01	1.09
1:A:90:ARG:HG3	1:A:182:MET:HE1	1.14	1.09
2:B:114:MET:HG3	2:B:215:VAL:HG23	1.28	1.08
3:C:55:ASN:HA	3:C:56:SER:HB2	1.34	1.08
1:A:215:PRO:HB3	3:C:203:SER:HA	1.13	1.08
3:C:145:PHE:HB3	3:C:153:ALA:HB2	1.29	1.08
3:C:65:ASN:HA	3:C:67:ASP:N	1.19	1.08
1:A:51:LEU:HD13	1:A:53:PHE:CD2	1.65	1.07
2:B:123:ASP:HB3	2:B:125:PHE:CE1	1.88	1.07
2:B:23:LYS:HG2	2:B:24:TRP:O	1.52	1.07
2:B:52:VAL:O	2:B:54:LEU:CD2	2.03	1.07
3:C:31:ILE:HG21	3:C:44:VAL:HG11	1.28	1.07
3:C:43:LYS:CD	3:C:49:SER:CB	2.33	1.06
1:A:218:SER:O	1:A:220:ALA:N	1.89	1.06
1:A:118:ILE:O	1:A:157:MET:HA	1.56	1.06
1:A:103:LEU:O	1:A:106:PHE:CE1	2.08	1.06
3:C:146:TRP:N	3:C:153:ALA:HB1	1.68	1.06
1:A:123:GLU:OE1	1:A:189:GLY:HA3	1.55	1.06
3:C:202:GLY:N	3:C:203:SER:OG	1.88	1.05
2:B:123:ASP:HA	2:B:124:GLN:O	1.57	1.05
3:C:151:LYS:HB3	3:C:152:PRO:HD2	1.34	1.05
3:C:192:VAL:CG1	3:C:194:ASP:OD1	2.03	1.04
1:A:206:PHE:CG	1:A:208:PHE:CD1	2.41	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ASN:C	2:B:91:PRO:CB	2.14	1.04
3:C:115:PRO:HA	3:C:152:PRO:HD3	1.06	1.04
2:B:141:SER:O	2:B:239:LEU:HD12	1.57	1.04
1:A:221:ALA:HB2	2:B:256:GLN:HB2	1.05	1.03
1:A:172:VAL:O	1:A:173:ARG:HB3	1.57	1.03
1:A:75:ALA:HB2	1:A:200:SER:HB2	1.35	1.03
1:A:172:VAL:HG21	1:A:175:ASP:CG	1.79	1.03
2:B:116:HIS:O	2:B:117:ARG:HG2	0.86	1.03
2:B:120:VAL:HG13	2:B:121:THR:CA	1.88	1.03
3:C:112:ASP:O	3:C:113:LYS:HD3	1.55	1.03
1:A:213:PRO:O	1:A:215:PRO:HD3	1.58	1.03
1:A:66:THR:O	2:B:75:MET:CB	2.04	1.03
2:B:163:PHE:CE1	2:B:177:ALA:HB3	1.94	1.03
1:A:113:GLU:OE2	2:B:61:TYR:CZ	2.11	1.03
1:A:68:VAL:HG12	1:A:69:ASP:H	1.24	1.03
1:A:210:VAL:HG12	1:A:213:PRO:HG3	1.37	1.02
3:C:110:THR:HG22	3:C:111:GLY:C	1.80	1.02
3:C:136:ILE:HG23	3:C:137:THR:H	1.24	1.02
1:A:74:ARG:NH1	2:B:45:SER:OG	1.93	1.02
3:C:141:LEU:HB3	3:C:239:ASP:HB3	1.38	1.01
3:C:109:THR:HG22	3:C:113:LYS:HB2	1.42	1.01
3:C:115:PRO:HA	3:C:152:PRO:CG	1.87	1.01
3:C:43:LYS:HD2	3:C:49:SER:HB2	1.36	1.01
2:B:22:TYR:CB	2:B:24:TRP:HA	1.90	1.01
1:A:67:LYS:CD	2:B:73:ASP:OD2	2.07	1.01
2:B:40:MET:SD	2:B:42:ASN:ND2	2.34	1.01
3:C:60:THR:O	3:C:64:GLU:HG3	1.59	1.01
3:C:98:VAL:CG1	3:C:99:ASP:HB2	1.89	1.01
3:C:99:ASP:HB3	3:C:100:ASN:CA	1.91	1.00
3:C:115:PRO:CA	3:C:152:PRO:CD	2.37	1.00
1:A:114:ILE:HG22	1:A:115:ASN:N	1.75	1.00
3:C:130:TYR:CD1	3:C:134:TYR:CE2	2.50	1.00
1:A:104:SER:HA	1:A:106:PHE:HE1	1.21	1.00
2:B:182:CYS:HA	2:B:190:PHE:HZ	1.24	0.99
3:C:31:ILE:HG23	3:C:44:VAL:CB	1.93	0.99
3:C:48:ALA:O	3:C:50:ASN:N	1.95	0.99
1:A:51:LEU:HD11	1:A:53:PHE:CE2	1.97	0.99
1:A:89:TRP:NE1	1:A:90:ARG:HD2	1.76	0.99
3:C:192:VAL:CG1	3:C:194:ASP:CG	2.31	0.99
1:A:67:LYS:HG3	2:B:73:ASP:HB3	1.01	0.98
1:A:67:LYS:CG	2:B:73:ASP:HB3	1.92	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ALA:HB2	2:B:78:ILE:HD11	1.45	0.98
1:A:206:PHE:C	1:A:208:PHE:HA	1.84	0.98
2:B:141:SER:O	2:B:239:LEU:CD1	2.12	0.98
1:A:51:LEU:HD12	1:A:52:ASN:N	1.78	0.98
3:C:39:GLU:HA	3:C:40:ILE:HB	1.45	0.98
1:A:133:TYR:OH	1:A:161:VAL:CG1	2.12	0.97
1:A:206:PHE:O	1:A:209:PRO:CD	2.12	0.97
1:A:90:ARG:CG	1:A:182:MET:SD	2.49	0.97
1:A:51:LEU:CG	1:A:52:ASN:N	2.25	0.97
2:B:114:MET:CG	2:B:215:VAL:HG23	1.94	0.97
1:A:174:HIS:CD2	1:A:214:LYS:HZ1	1.55	0.97
2:B:88:ASN:CA	2:B:91:PRO:HB2	1.95	0.97
3:C:145:PHE:CB	3:C:153:ALA:HB2	1.93	0.96
1:A:133:TYR:CB	1:A:134:ASP:HB2	1.96	0.96
3:C:152:PRO:C	3:C:154:TYR:H	1.66	0.96
1:A:68:VAL:HG23	2:B:73:ASP:HA	1.43	0.96
1:A:206:PHE:CG	1:A:208:PHE:HD1	1.71	0.96
2:B:74:ASP:CG	2:B:77:LYS:H	1.69	0.96
3:C:42:THR:HB	3:C:44:VAL:N	1.80	0.96
1:A:167:LYS:HB3	1:A:169:LEU:HD11	1.47	0.96
2:B:23:LYS:CB	2:B:24:TRP:HA	1.96	0.95
1:A:134:ASP:HA	1:A:135:THR:HG22	1.46	0.95
1:A:90:ARG:HG3	1:A:182:MET:CE	1.86	0.95
1:A:218:SER:C	1:A:220:ALA:N	2.09	0.95
2:B:42:ASN:O	2:B:43:VAL:CG2	2.15	0.95
1:A:221:ALA:HB2	2:B:256:GLN:CB	1.97	0.94
2:B:56:GLY:HA2	2:B:57:GLU:HG2	0.94	0.94
1:A:172:VAL:HG11	1:A:175:ASP:OD1	1.67	0.94
3:C:196:ARG:HB2	3:C:196:ARG:HH11	1.30	0.94
1:A:51:LEU:HD13	1:A:53:PHE:HD2	0.77	0.94
2:B:74:ASP:OD2	2:B:77:LYS:HB2	1.64	0.94
2:B:90:THR:N	2:B:91:PRO:HA	1.79	0.94
3:C:43:LYS:HD3	3:C:49:SER:OG	1.68	0.93
1:A:68:VAL:CG2	2:B:73:ASP:HA	1.98	0.93
2:B:88:ASN:O	2:B:91:PRO:HB3	0.75	0.93
2:B:23:LYS:HG2	2:B:24:TRP:C	1.88	0.93
2:B:120:VAL:HG13	2:B:121:THR:HA	0.94	0.93
1:A:115:ASN:HB3	1:A:200:SER:O	1.69	0.93
3:C:115:PRO:C	3:C:152:PRO:HG3	1.88	0.93
3:C:115:PRO:CB	3:C:152:PRO:CG	2.46	0.92
3:C:55:ASN:CA	3:C:56:SER:HB2	1.99	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:PRO:CD	2:B:189:SER:HG	1.76	0.92
3:C:115:PRO:HB3	3:C:152:PRO:HB3	1.52	0.92
2:B:88:ASN:CA	2:B:91:PRO:CB	2.47	0.92
2:B:114:MET:CB	2:B:215:VAL:O	2.17	0.92
1:A:51:LEU:HG	1:A:52:ASN:N	1.84	0.92
1:A:133:TYR:HH	1:A:161:VAL:HG11	1.28	0.91
1:A:51:LEU:CD1	1:A:52:ASN:N	2.33	0.91
1:A:113:GLU:OE1	1:A:113:GLU:N	2.03	0.91
3:C:99:ASP:CB	3:C:100:ASN:CA	2.48	0.91
3:C:98:VAL:HG13	3:C:100:ASN:HA	1.48	0.91
3:C:61:ALA:HA	3:C:64:GLU:CD	1.91	0.91
1:A:162:PRO:O	1:A:163:PHE:HB2	1.71	0.91
3:C:115:PRO:O	3:C:152:PRO:CG	2.19	0.91
3:C:145:PHE:HB3	3:C:153:ALA:CB	2.00	0.91
3:C:203:SER:C	3:C:205:THR:H	1.73	0.90
3:C:110:THR:CG2	3:C:111:GLY:CA	2.10	0.90
2:B:98:ASP:HA	2:B:99:LYS:HB3	1.52	0.90
3:C:42:THR:H	3:C:43:LYS:HA	1.35	0.90
1:A:104:SER:CA	1:A:106:PHE:CE1	2.54	0.90
3:C:99:ASP:CB	3:C:100:ASN:HA	1.99	0.90
3:C:151:LYS:CE	3:C:151:LYS:HA	2.01	0.90
2:B:105:TRP:CZ3	2:B:106:ALA:O	2.24	0.90
2:B:114:MET:HG3	2:B:215:VAL:O	1.71	0.90
2:B:188:ASN:CB	2:B:189:SER:HA	1.99	0.90
3:C:115:PRO:HB2	3:C:152:PRO:HG3	1.52	0.90
1:A:109:TYR:CG	1:A:206:PHE:CE1	2.60	0.89
1:A:118:ILE:O	1:A:157:MET:CA	2.19	0.89
2:B:182:CYS:CA	2:B:190:PHE:CZ	2.55	0.89
1:A:110:PHE:HB3	1:A:173:ARG:HB2	1.55	0.89
3:C:193:ILE:HG22	3:C:196:ARG:NH2	1.87	0.89
1:A:96:PRO:O	1:A:177:ALA:CB	2.19	0.89
2:B:123:ASP:HA	2:B:124:GLN:C	1.92	0.89
2:B:56:GLY:HA2	2:B:57:GLU:CB	2.02	0.89
1:A:134:ASP:HA	1:A:135:THR:CG2	2.03	0.88
2:B:163:PHE:CE1	2:B:177:ALA:CB	2.56	0.88
3:C:145:PHE:CB	3:C:153:ALA:CB	2.51	0.88
1:A:89:TRP:HE1	1:A:90:ARG:HD2	1.35	0.88
1:A:29:ASN:ND2	3:C:211:LEU:HB3	1.88	0.88
2:B:51:SER:C	2:B:54:LEU:HD21	1.94	0.88
3:C:151:LYS:HB3	3:C:152:PRO:CD	2.03	0.88
1:A:221:ALA:CB	2:B:256:GLN:HB2	1.99	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:ASP:O	3:C:113:LYS:CD	2.22	0.87
1:A:215:PRO:HB3	3:C:203:SER:CA	2.02	0.87
2:B:127:ASN:HD21	2:B:238:ARG:HH22	1.22	0.87
3:C:104:MET:O	3:C:106:TYR:N	2.07	0.87
1:A:139:ARG:HH11	1:A:141:THR:HG22	1.40	0.87
1:A:89:TRP:CD1	1:A:90:ARG:HD2	2.09	0.86
3:C:60:THR:O	3:C:64:GLU:CD	2.14	0.86
1:A:207:PHE:HA	2:B:71:ARG:HA	1.57	0.86
3:C:28:ASN:HA	3:C:31:ILE:HD12	1.57	0.86
1:A:103:LEU:CB	1:A:106:PHE:CZ	2.56	0.86
2:B:179:TYR:O	2:B:180:THR:OG1	1.93	0.86
1:A:166:ASN:O	1:A:167:LYS:C	2.11	0.86
2:B:40:MET:HG3	2:B:43:VAL:O	1.73	0.86
3:C:31:ILE:HG22	3:C:44:VAL:HG11	1.51	0.86
1:A:212:ALA:HB2	2:B:78:ILE:CD1	2.06	0.86
2:B:43:VAL:HG12	2:B:44:LEU:H	1.38	0.86
1:A:114:ILE:HG22	1:A:115:ASN:H	1.38	0.86
1:A:168:PRO:O	1:A:170:ARG:N	2.08	0.86
2:B:58:ARG:HG2	2:B:59:ALA:H	1.37	0.86
3:C:116:SER:OG	3:C:269:LEU:O	1.93	0.86
3:C:151:LYS:HA	3:C:151:LYS:HE3	1.57	0.86
1:A:170:ARG:HD3	1:A:171:THR:H	1.38	0.86
2:B:24:TRP:O	2:B:26:ARG:N	2.07	0.86
3:C:99:ASP:HB3	3:C:100:ASN:O	1.74	0.85
3:C:192:VAL:O	3:C:194:ASP:OD1	1.93	0.85
2:B:110:ALA:O	2:B:112:GLN:OE1	1.94	0.85
1:A:206:PHE:O	1:A:208:PHE:HA	1.76	0.85
3:C:145:PHE:O	3:C:153:ALA:HB1	1.58	0.85
1:A:64:SER:HA	1:A:67:LYS:HB3	1.59	0.85
1:A:68:VAL:HG23	2:B:73:ASP:CA	2.07	0.85
1:A:205:ASN:ND2	2:B:63:PRO:HG3	1.91	0.85
1:A:103:LEU:HB3	1:A:106:PHE:HZ	1.42	0.85
3:C:98:VAL:HG22	3:C:99:ASP:CG	1.97	0.85
3:C:98:VAL:HA	3:C:99:ASP:OD1	1.75	0.85
3:C:207:LEU:HD22	3:C:208:PRO:HD2	1.58	0.85
2:B:74:ASP:OD2	2:B:77:LYS:N	2.11	0.84
3:C:141:LEU:HD13	3:C:239:ASP:HB2	1.58	0.84
1:A:114:ILE:CG2	1:A:115:ASN:H	1.90	0.84
1:A:103:LEU:C	1:A:106:PHE:CE1	2.47	0.84
2:B:112:GLN:OE1	2:B:112:GLN:N	2.10	0.84
2:B:92:SER:HB3	2:B:98:ASP:O	1.77	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:TYR:CB	1:A:206:PHE:CE1	2.61	0.84
2:B:114:MET:HG3	2:B:215:VAL:CG2	2.08	0.84
3:C:115:PRO:CA	3:C:152:PRO:HD3	1.99	0.83
3:C:196:ARG:HB2	3:C:196:ARG:NH1	1.93	0.83
1:A:103:LEU:HB3	1:A:106:PHE:CZ	2.13	0.83
3:C:193:ILE:HG22	3:C:196:ARG:CZ	2.08	0.83
3:C:118:LEU:HD23	3:C:268:SER:HB3	1.58	0.83
1:A:205:ASN:O	1:A:207:PHE:N	2.10	0.83
2:B:37:THR:H	2:B:38:MET:HB2	1.44	0.83
2:B:163:PHE:HE1	2:B:177:ALA:HB3	1.40	0.83
1:A:168:PRO:C	1:A:169:LEU:HD13	1.99	0.83
3:C:98:VAL:HG13	3:C:99:ASP:CB	2.07	0.83
1:A:168:PRO:O	1:A:169:LEU:HD22	1.77	0.83
1:A:27:SER:O	1:A:30:GLU:HB2	1.79	0.83
3:C:55:ASN:HA	3:C:56:SER:CB	2.08	0.83
1:A:174:HIS:HD2	1:A:214:LYS:HZ1	0.85	0.82
3:C:38:GLY:O	3:C:40:ILE:HA	1.78	0.82
3:C:65:ASN:OD1	3:C:66:LYS:O	1.97	0.82
1:A:117:HIS:CE1	2:B:44:LEU:CD2	2.21	0.82
1:A:100:HIS:N	1:A:104:SER:OG	2.10	0.82
2:B:51:SER:O	2:B:54:LEU:HD21	1.78	0.82
1:A:66:THR:HG23	2:B:76:ILE:HG23	1.62	0.82
3:C:61:ALA:O	3:C:67:ASP:OD1	1.98	0.82
1:A:109:TYR:HD2	1:A:206:PHE:HZ	0.85	0.82
1:A:88:THR:O	1:A:89:TRP:CB	2.27	0.82
3:C:43:LYS:HD2	3:C:49:SER:HB3	1.60	0.82
1:A:114:ILE:CG2	1:A:115:ASN:N	2.43	0.82
1:A:109:TYR:HD2	1:A:206:PHE:CZ	1.62	0.81
1:A:123:GLU:HB3	1:A:126:PHE:HB3	1.60	0.81
1:A:67:LYS:CG	2:B:73:ASP:CB	2.54	0.81
2:B:165:ASN:HB3	2:B:166:CYS:HA	1.63	0.81
1:A:109:TYR:HE1	1:A:212:ALA:HA	1.44	0.81
2:B:74:ASP:OD1	2:B:76:ILE:CG1	2.29	0.81
1:A:172:VAL:CG1	1:A:175:ASP:OD1	2.29	0.81
2:B:114:MET:HB2	2:B:217:VAL:H	1.45	0.81
1:A:202:ARG:NE	2:B:51:SER:OG	2.12	0.81
2:B:122:LEU:HD13	2:B:132:MET:HG3	1.63	0.81
2:B:158:LEU:O	2:B:182:CYS:HB3	1.81	0.81
2:B:90:THR:HG23	2:B:100:TYR:CE1	2.14	0.81
1:A:134:ASP:CA	1:A:135:THR:HG22	2.10	0.81
1:A:110:PHE:O	1:A:170:ARG:HD2	1.80	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LYS:CG	2:B:73:ASP:CG	2.50	0.80
3:C:61:ALA:HA	3:C:64:GLU:OE1	1.80	0.80
1:A:110:PHE:HD2	1:A:173:ARG:HD2	1.47	0.80
1:A:89:TRP:O	1:A:182:MET:HE3	1.81	0.80
3:C:111:GLY:HA2	3:C:115:PRO:CD	2.11	0.80
1:A:88:THR:O	1:A:89:TRP:HB3	1.78	0.80
2:B:182:CYS:HB2	2:B:190:PHE:CE2	2.13	0.80
2:B:88:ASN:HA	2:B:91:PRO:HB2	1.61	0.80
1:A:179:GLY:O	1:A:180:PHE:CD2	2.34	0.80
2:B:166:CYS:SG	2:B:167:THR:N	2.55	0.80
2:B:74:ASP:HA	2:B:75:MET:CB	2.06	0.80
3:C:61:ALA:HA	3:C:64:GLU:CG	2.12	0.80
2:B:37:THR:HA	2:B:38:MET:C	2.02	0.80
2:B:37:THR:HA	2:B:40:MET:H	1.47	0.80
2:B:114:MET:CG	2:B:215:VAL:O	2.29	0.80
3:C:191:PRO:HD2	3:C:193:ILE:CD1	2.09	0.80
3:C:101:PHE:N	3:C:102:HIS:HA	1.94	0.79
3:C:56:SER:C	3:C:58:ALA:H	1.85	0.79
1:A:28:PRO:HD2	2:B:188:ASN:OD1	1.81	0.79
1:A:28:PRO:HD2	2:B:189:SER:HG	1.47	0.79
1:A:29:ASN:ND2	3:C:211:LEU:CB	2.33	0.79
1:A:133:TYR:HA	1:A:134:ASP:CG	2.03	0.79
2:B:56:GLY:CA	2:B:57:GLU:CG	2.43	0.79
3:C:115:PRO:O	3:C:152:PRO:HG3	1.80	0.79
3:C:50:ASN:C	3:C:52:LEU:H	1.86	0.79
1:A:172:VAL:CB	1:A:175:ASP:OD1	2.31	0.79
1:A:167:LYS:CB	1:A:169:LEU:HD11	2.13	0.78
2:B:43:VAL:C	2:B:44:LEU:HD22	2.03	0.78
2:B:172:LEU:O	2:B:175:ASP:N	2.16	0.78
1:A:112:GLY:C	1:A:113:GLU:OE1	2.22	0.78
1:A:140:LYS:H	1:A:141:THR:HB	1.49	0.78
2:B:102:TYR:HE2	2:B:116:HIS:HA	1.48	0.78
2:B:118:ASN:HB3	2:B:120:VAL:HA	1.65	0.78
2:B:37:THR:N	2:B:38:MET:HB2	1.97	0.78
1:A:213:PRO:HB3	3:C:207:LEU:HD21	1.64	0.78
2:B:88:ASN:HB3	2:B:91:PRO:CB	2.13	0.78
3:C:112:ASP:O	3:C:113:LYS:CG	2.31	0.78
3:C:98:VAL:CB	3:C:99:ASP:HB2	2.14	0.78
2:B:56:GLY:CA	2:B:57:GLU:CB	2.61	0.78
3:C:118:LEU:CD2	3:C:268:SER:HB3	2.14	0.78
1:A:172:VAL:HG21	1:A:175:ASP:CB	2.15	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:233:VAL:HG21	3:C:240:LEU:HD21	1.65	0.77
2:B:105:TRP:CE3	2:B:106:ALA:O	2.36	0.77
1:A:215:PRO:HG2	3:C:204:LEU:N	1.99	0.77
2:B:74:ASP:CA	2:B:75:MET:HB2	2.08	0.77
1:A:219:ARG:HB2	3:C:199:LEU:HD23	1.67	0.77
2:B:90:THR:HG23	2:B:100:TYR:HE1	1.50	0.77
3:C:61:ALA:CA	3:C:64:GLU:HG3	2.13	0.77
3:C:65:ASN:HA	3:C:66:LYS:O	1.85	0.77
1:A:207:PHE:O	2:B:72:PHE:N	2.15	0.77
2:B:58:ARG:O	2:B:59:ALA:O	2.03	0.77
2:B:74:ASP:OD1	2:B:76:ILE:HG12	1.85	0.77
3:C:28:ASN:HD21	3:C:52:LEU:HB3	1.49	0.77
1:A:97:LYS:NZ	1:A:177:ALA:O	2.19	0.76
1:A:85:ASN:HD21	1:A:192:ARG:HA	1.51	0.76
3:C:61:ALA:HA	3:C:64:GLU:HG3	1.66	0.76
1:A:89:TRP:O	1:A:90:ARG:HG3	1.84	0.76
2:B:182:CYS:HB2	2:B:190:PHE:HE2	1.43	0.76
3:C:48:ALA:C	3:C:50:ASN:H	1.88	0.76
1:A:51:LEU:CD1	1:A:53:PHE:CE2	2.62	0.76
3:C:69:VAL:O	3:C:81:THR:O	2.04	0.76
1:A:173:ARG:HH22	1:A:214:LYS:H	1.33	0.76
1:A:167:LYS:HE3	1:A:167:LYS:N	2.02	0.76
2:B:88:ASN:CB	2:B:91:PRO:HB2	2.15	0.75
3:C:146:TRP:O	3:C:153:ALA:O	2.04	0.75
3:C:207:LEU:HD23	3:C:208:PRO:HD3	1.68	0.75
1:A:69:ASP:OD1	1:A:70:ASN:N	2.19	0.75
3:C:186:VAL:HG21	3:C:204:LEU:HD21	1.68	0.75
3:C:62:GLN:HB3	3:C:63:PRO:CD	2.16	0.75
1:A:135:THR:HG1	1:A:136:GLU:HB2	1.48	0.75
3:C:40:ILE:HG13	3:C:41:ILE:HG23	1.68	0.75
2:B:116:HIS:C	2:B:117:ARG:HG2	2.00	0.75
3:C:193:ILE:CG2	3:C:196:ARG:NH2	2.49	0.75
2:B:44:LEU:O	2:B:45:SER:OG	2.04	0.75
2:B:58:ARG:CG	2:B:59:ALA:H	1.99	0.75
3:C:99:ASP:CB	3:C:100:ASN:O	2.35	0.75
3:C:42:THR:N	3:C:43:LYS:HA	1.98	0.75
1:A:215:PRO:CB	3:C:203:SER:CA	2.60	0.75
3:C:187:TYR:CE2	3:C:224:ILE:HG21	2.22	0.75
3:C:35:GLU:C	3:C:37:GLY:H	1.89	0.75
1:A:118:ILE:O	1:A:157:MET:CB	2.35	0.75
1:A:165:SER:HA	1:A:166:ASN:C	2.06	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:THR:O	1:A:173:ARG:N	2.19	0.75
3:C:207:LEU:CD2	3:C:208:PRO:HD2	2.16	0.75
2:B:68:SER:HB3	2:B:70:SER:OG	1.87	0.74
3:C:185:VAL:HG22	3:C:245:VAL:HG22	1.67	0.74
1:A:215:PRO:CG	3:C:203:SER:HA	2.17	0.74
1:A:108:ALA:HB3	1:A:109:TYR:CE1	2.22	0.74
1:A:212:ALA:CB	2:B:78:ILE:HD11	2.16	0.74
3:C:38:GLY:O	3:C:41:ILE:HG22	1.87	0.74
1:A:51:LEU:CD1	1:A:52:ASN:H	1.94	0.74
2:B:37:THR:HA	2:B:39:ASN:N	2.03	0.74
3:C:52:LEU:HD12	3:C:52:LEU:O	1.88	0.74
3:C:135:LYS:HG3	3:C:136:ILE:N	2.01	0.74
2:B:42:ASN:O	2:B:43:VAL:CB	2.36	0.74
1:A:148:VAL:O	1:A:149:ILE:HG12	1.88	0.73
1:A:117:HIS:HA	1:A:157:MET:O	1.88	0.73
1:A:100:HIS:N	1:A:101:GLY:HA2	2.04	0.73
2:B:182:CYS:CA	2:B:190:PHE:CE2	2.71	0.73
3:C:146:TRP:HA	3:C:153:ALA:C	2.08	0.73
3:C:145:PHE:CA	3:C:153:ALA:CB	2.65	0.73
1:A:169:LEU:N	1:A:169:LEU:HD13	2.04	0.73
2:B:162:PHE:HA	2:B:212:LEU:O	1.89	0.73
3:C:35:GLU:O	3:C:37:GLY:N	2.21	0.73
1:A:206:PHE:O	1:A:207:PHE:HB2	1.87	0.73
2:B:114:MET:HB3	2:B:216:GLU:HA	1.70	0.73
2:B:22:TYR:HB2	2:B:24:TRP:CB	2.18	0.73
1:A:133:TYR:HA	1:A:134:ASP:OD2	1.87	0.73
2:B:92:SER:HA	2:B:95:SER:HB3	1.71	0.73
3:C:194:ASP:N	3:C:194:ASP:OD1	2.22	0.73
2:B:37:THR:OG1	2:B:40:MET:O	2.05	0.73
3:C:135:LYS:HG3	3:C:136:ILE:H	1.54	0.73
3:C:138:THR:HG22	3:C:244:ARG:HG2	1.69	0.73
2:B:43:VAL:HG12	2:B:44:LEU:N	2.04	0.73
1:A:28:PRO:CG	2:B:145:ARG:NH2	2.51	0.72
3:C:141:LEU:CD1	3:C:239:ASP:OD2	2.37	0.72
3:C:70:GLN:OE1	3:C:70:GLN:N	2.23	0.72
1:A:172:VAL:O	1:A:173:ARG:CB	2.34	0.72
1:A:67:LYS:HG3	2:B:73:ASP:CG	2.08	0.72
3:C:24:GLU:OE1	3:C:56:SER:OG	2.07	0.72
1:A:118:ILE:N	1:A:157:MET:HB2	2.05	0.72
2:B:22:TYR:CB	2:B:23:LYS:CB	2.53	0.72
3:C:202:GLY:HA2	3:C:203:SER:O	1.90	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:ASN:C	3:C:52:LEU:N	2.42	0.72
1:A:207:PHE:HB2	1:A:208:PHE:C	2.10	0.72
3:C:42:THR:HB	3:C:44:VAL:H	1.51	0.72
1:A:110:PHE:CD2	1:A:173:ARG:HD2	2.25	0.72
3:C:146:TRP:C	3:C:153:ALA:O	2.27	0.71
2:B:75:MET:O	2:B:78:ILE:HG22	1.90	0.71
2:B:86:SER:OG	2:B:89:THR:OG1	2.02	0.71
2:B:123:ASP:HB3	2:B:125:PHE:CD1	2.25	0.71
2:B:92:SER:HA	2:B:95:SER:CB	2.20	0.71
1:A:45:GLU:HB2	1:A:46:LYS:HA	1.72	0.71
1:A:89:TRP:O	1:A:182:MET:CE	2.38	0.71
3:C:191:PRO:O	3:C:194:ASP:OD1	2.08	0.71
2:B:56:GLY:C	2:B:57:GLU:HG2	2.11	0.71
2:B:194:ILE:HD12	2:B:195:PRO:HD2	1.73	0.70
2:B:206:HIS:CG	2:B:207:GLY:H	2.09	0.70
2:B:22:TYR:HB2	2:B:24:TRP:N	2.06	0.70
1:A:103:LEU:O	1:A:106:PHE:CD2	2.44	0.70
1:A:167:LYS:CD	1:A:167:LYS:H	2.03	0.70
3:C:39:GLU:O	3:C:42:THR:HG22	1.91	0.70
1:A:90:ARG:HB3	1:A:91:GLN:C	2.11	0.70
2:B:42:ASN:C	2:B:43:VAL:HG23	2.11	0.70
2:B:58:ARG:HD2	2:B:58:ARG:H	1.55	0.70
3:C:37:GLY:O	3:C:42:THR:HG23	1.92	0.70
1:A:210:VAL:HG12	1:A:213:PRO:CG	2.19	0.70
3:C:110:THR:HB	3:C:111:GLY:HA2	1.71	0.70
3:C:136:ILE:HG23	3:C:137:THR:N	2.04	0.70
1:A:167:LYS:HE3	1:A:167:LYS:H	1.57	0.70
3:C:110:THR:CB	3:C:111:GLY:CA	2.49	0.70
3:C:41:ILE:H	3:C:41:ILE:HD12	1.57	0.70
1:A:110:PHE:HD1	1:A:170:ARG:HD2	1.57	0.69
1:A:167:LYS:H	1:A:167:LYS:HD2	1.57	0.69
1:A:26:ILE:HG22	1:A:27:SER:N	2.06	0.69
2:B:123:ASP:HB3	2:B:125:PHE:HE1	1.54	0.69
1:A:28:PRO:CG	2:B:189:SER:OG	2.40	0.69
2:B:22:TYR:HB2	2:B:23:LYS:HB3	1.74	0.69
2:B:79:ALA:O	2:B:81:LEU:N	2.25	0.69
3:C:130:TYR:CE1	3:C:134:TYR:CE2	2.80	0.69
2:B:109:VAL:HG22	2:B:110:ALA:H	1.57	0.69
2:B:110:ALA:C	2:B:112:GLN:OE1	2.30	0.69
3:C:55:ASN:N	3:C:56:SER:HB2	2.08	0.69
1:A:210:VAL:O	1:A:213:PRO:CG	2.41	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:GLN:C	2:B:113:ASN:ND2	2.46	0.69
2:B:182:CYS:HA	2:B:190:PHE:CE2	2.28	0.69
3:C:191:PRO:CD	3:C:193:ILE:HD13	2.14	0.69
1:A:219:ARG:C	1:A:221:ALA:H	1.93	0.69
2:B:88:ASN:CB	2:B:91:PRO:CB	2.69	0.69
3:C:99:ASP:HB2	3:C:100:ASN:HA	1.74	0.69
1:A:175:ASP:CB	1:A:176:SER:HA	2.21	0.68
3:C:99:ASP:CB	3:C:100:ASN:C	2.56	0.68
2:B:182:CYS:CA	2:B:190:PHE:HZ	1.98	0.68
3:C:141:LEU:HD13	3:C:239:ASP:CB	2.22	0.68
1:A:106:PHE:O	1:A:107:PHE:HB3	1.92	0.68
1:A:123:GLU:OE2	1:A:189:GLY:O	2.12	0.68
1:A:109:TYR:CE1	1:A:212:ALA:HA	2.27	0.68
1:A:67:LYS:HB2	1:A:67:LYS:NZ	2.07	0.68
1:A:91:GLN:CD	1:A:91:GLN:H	1.94	0.68
2:B:74:ASP:OD2	2:B:77:LYS:CA	2.40	0.68
3:C:101:PHE:N	3:C:102:HIS:CA	2.56	0.68
3:C:65:ASN:C	3:C:67:ASP:N	2.46	0.68
1:A:112:GLY:HA2	1:A:113:GLU:OE1	1.93	0.68
1:A:120:TYR:CE2	1:A:122:ALA:HB3	2.28	0.68
1:A:179:GLY:O	1:A:180:PHE:CD1	2.47	0.68
2:B:23:LYS:CB	2:B:24:TRP:CA	2.72	0.68
3:C:93:PRO:HB2	3:C:95:PHE:HD2	1.59	0.68
2:B:117:ARG:NH1	2:B:169:ASP:OD2	2.26	0.68
2:B:165:ASN:H	2:B:166:CYS:HB2	1.59	0.68
3:C:192:VAL:C	3:C:194:ASP:OD1	2.33	0.68
3:C:24:GLU:HB3	3:C:52:LEU:HA	1.74	0.68
3:C:118:LEU:HD23	3:C:267:GLY:O	1.94	0.68
1:A:213:PRO:O	1:A:214:LYS:C	2.31	0.67
1:A:67:LYS:HG2	1:A:68:VAL:N	2.07	0.67
2:B:114:MET:CB	2:B:216:GLU:HA	2.24	0.67
1:A:96:PRO:C	1:A:177:ALA:HB2	2.13	0.67
1:A:155:GLU:HG3	1:A:156:GLN:H	1.60	0.67
2:B:119:VAL:N	2:B:120:VAL:HA	2.09	0.67
1:A:103:LEU:O	1:A:106:PHE:CD1	2.47	0.67
1:A:120:TYR:CZ	1:A:122:ALA:CB	2.78	0.67
1:A:164:TYR:CD1	1:A:166:ASN:ND2	2.62	0.67
1:A:131:HIS:ND1	1:A:182:MET:O	2.28	0.67
3:C:39:GLU:HA	3:C:40:ILE:CB	2.17	0.67
3:C:52:LEU:HD12	3:C:52:LEU:C	2.15	0.67
1:A:66:THR:O	2:B:75:MET:HB3	1.90	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:207:LEU:CD2	3:C:208:PRO:CD	2.72	0.67
1:A:112:GLY:CA	1:A:113:GLU:OE1	2.43	0.66
2:B:58:ARG:O	2:B:59:ALA:C	2.32	0.66
3:C:141:LEU:HD12	3:C:239:ASP:OD2	1.96	0.66
3:C:54:PRO:C	3:C:56:SER:HA	2.15	0.66
3:C:115:PRO:HB3	3:C:152:PRO:CB	2.23	0.66
2:B:34:GLY:O	2:B:36:GLY:N	2.27	0.66
1:A:60:ILE:N	1:A:61:PHE:HA	2.11	0.66
2:B:52:VAL:O	2:B:54:LEU:CG	2.44	0.66
1:A:206:PHE:CD2	1:A:208:PHE:CD1	2.84	0.66
2:B:114:MET:HB2	2:B:217:VAL:N	2.11	0.66
1:A:68:VAL:HG12	1:A:69:ASP:N	2.04	0.66
1:A:116:ILE:HD13	1:A:133:TYR:HE2	1.61	0.65
2:B:30:ASP:HB2	2:B:31:ILE:HA	1.77	0.65
2:B:41:ALA:H	2:B:43:VAL:H	1.44	0.65
3:C:136:ILE:HG21	3:C:245:VAL:HG12	1.78	0.65
2:B:58:ARG:NH1	2:B:58:ARG:H	1.94	0.65
3:C:207:LEU:HD23	3:C:208:PRO:CD	2.26	0.65
2:B:251:SER:HB2	2:B:252:LEU:HA	1.77	0.65
1:A:26:ILE:HG22	1:A:27:SER:H	1.62	0.65
1:A:166:ASN:O	1:A:167:LYS:O	2.14	0.65
2:B:110:ALA:O	2:B:112:GLN:N	2.30	0.65
1:A:110:PHE:CD1	1:A:170:ARG:HD2	2.32	0.65
1:A:210:VAL:CG1	1:A:213:PRO:HG3	2.20	0.65
2:B:102:TYR:CE2	2:B:116:HIS:HA	2.30	0.65
2:B:58:ARG:HG2	2:B:59:ALA:N	2.12	0.65
1:A:117:HIS:HE1	2:B:44:LEU:HD21	0.50	0.65
1:A:167:LYS:H	1:A:167:LYS:CE	2.09	0.65
3:C:100:ASN:CB	3:C:101:PHE:HA	2.27	0.65
3:C:60:THR:C	3:C:64:GLU:HG3	2.18	0.64
1:A:67:LYS:CG	2:B:73:ASP:OD2	2.45	0.64
2:B:114:MET:CG	2:B:115:VAL:H	2.09	0.64
3:C:119:ILE:O	3:C:266:MET:HA	1.98	0.64
3:C:35:GLU:C	3:C:37:GLY:N	2.48	0.64
1:A:219:ARG:NE	1:A:219:ARG:HA	2.11	0.64
1:A:174:HIS:CG	1:A:214:LYS:HZ2	2.06	0.64
1:A:51:LEU:C	1:A:51:LEU:HD12	2.16	0.64
2:B:92:SER:C	2:B:95:SER:HB3	2.18	0.64
3:C:151:LYS:CB	3:C:152:PRO:HD2	2.21	0.64
3:C:195:SER:C	3:C:197:GLN:H	2.00	0.64
3:C:140:GLU:HB3	3:C:144:SER:HB2	1.77	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:207:LEU:O	3:C:209:HIS:N	2.31	0.64
1:A:82:ASP:OD1	1:A:83:PHE:N	2.23	0.64
3:C:161:ALA:HB2	3:C:278:ARG:HD3	1.80	0.64
3:C:233:VAL:HG11	3:C:240:LEU:CD2	2.28	0.64
3:C:118:LEU:HD23	3:C:267:GLY:C	2.17	0.64
1:A:205:ASN:HD22	2:B:63:PRO:HG3	1.62	0.64
1:A:163:PHE:CE1	1:A:166:ASN:HB3	2.32	0.64
1:A:108:ALA:O	1:A:173:ARG:NE	2.31	0.64
1:A:219:ARG:NH2	2:B:256:GLN:HB3	2.13	0.64
3:C:154:TYR:O	3:C:158:LYS:HB3	1.98	0.64
1:A:90:ARG:HB2	1:A:91:GLN:HA	1.79	0.63
2:B:74:ASP:OD1	2:B:76:ILE:HG13	1.98	0.63
2:B:88:ASN:CA	2:B:91:PRO:HB3	2.20	0.63
3:C:115:PRO:CB	3:C:152:PRO:CB	2.77	0.63
1:A:68:VAL:HB	2:B:73:ASP:OD1	1.98	0.63
2:B:41:ALA:HA	2:B:43:VAL:N	2.12	0.63
3:C:109:THR:CG2	3:C:113:LYS:HB2	2.25	0.63
3:C:185:VAL:HB	3:C:210:VAL:HG13	1.81	0.63
1:A:165:SER:HA	1:A:167:LYS:N	2.14	0.63
2:B:52:VAL:C	2:B:54:LEU:H	1.97	0.63
1:A:133:TYR:HB2	1:A:134:ASP:CB	2.15	0.63
2:B:33:GLU:HB3	2:B:34:GLY:C	2.19	0.63
1:A:43:GLY:HA2	1:A:50:PHE:CD2	2.33	0.63
1:A:57:ASN:OD1	2:B:244:LYS:NZ	2.32	0.63
1:A:118:ILE:O	1:A:157:MET:HB3	1.99	0.63
2:B:58:ARG:H	2:B:58:ARG:CD	2.12	0.63
1:A:207:PHE:HD2	1:A:209:PRO:HG3	1.63	0.63
2:B:92:SER:HA	2:B:95:SER:OG	1.98	0.63
1:A:213:PRO:C	1:A:215:PRO:HD3	2.19	0.62
2:B:46:THR:O	2:B:47:THR:HB	1.99	0.62
3:C:145:PHE:CA	3:C:153:ALA:HB1	2.23	0.62
3:C:43:LYS:HB3	3:C:49:SER:HB2	1.80	0.62
1:A:135:THR:OG1	1:A:136:GLU:CB	2.36	0.62
2:B:92:SER:CA	2:B:95:SER:HB3	2.29	0.62
3:C:233:VAL:HG11	3:C:240:LEU:HD22	1.82	0.62
1:A:41:PRO:HA	1:A:51:LEU:HD23	1.81	0.62
3:C:196:ARG:O	3:C:197:GLN:O	2.18	0.62
3:C:42:THR:CB	3:C:44:VAL:N	2.61	0.62
1:A:157:MET:HG2	2:B:41:ALA:HB2	1.82	0.62
1:A:109:TYR:O	1:A:173:ARG:HG3	2.00	0.62
1:A:46:LYS:H	1:A:49:TYR:HB3	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:187:TYR:CE1	3:C:241:GLY:HA3	2.34	0.62
1:A:103:LEU:CA	1:A:106:PHE:CZ	2.81	0.62
2:B:118:ASN:C	2:B:120:VAL:HA	2.21	0.62
2:B:163:PHE:CD1	2:B:177:ALA:CB	2.82	0.61
3:C:115:PRO:C	3:C:152:PRO:CG	2.58	0.61
1:A:113:GLU:OE2	2:B:61:TYR:OH	2.17	0.61
2:B:159:ARG:HD2	2:B:216:GLU:OE1	2.01	0.61
2:B:46:THR:O	2:B:46:THR:HG23	2.00	0.61
3:C:37:GLY:HA3	3:C:39:GLU:OE2	2.00	0.61
2:B:182:CYS:SG	2:B:190:PHE:CZ	2.87	0.61
3:C:192:VAL:HG13	3:C:192:VAL:O	2.00	0.61
1:A:120:TYR:CZ	1:A:122:ALA:HB3	2.35	0.61
2:B:97:ILE:HA	2:B:98:ASP:C	2.20	0.61
1:A:139:ARG:HD2	1:A:141:THR:HG22	1.83	0.61
2:B:141:SER:HB3	2:B:194:ILE:O	2.00	0.61
2:B:41:ALA:N	2:B:43:VAL:H	1.98	0.61
3:C:31:ILE:HG21	3:C:44:VAL:CG1	2.00	0.61
2:B:115:VAL:O	2:B:116:HIS:HB2	1.99	0.61
2:B:155:ARG:HA	2:B:184:ILE:O	2.00	0.61
2:B:167:THR:OG1	2:B:168:HIS:ND1	2.33	0.61
1:A:138:ASN:OD1	1:A:139:ARG:N	2.28	0.61
1:A:66:THR:OG1	2:B:244:LYS:HB2	1.99	0.61
3:C:93:PRO:HB2	3:C:95:PHE:CD2	2.36	0.61
2:B:112:GLN:OE1	2:B:113:ASN:ND2	2.33	0.61
3:C:28:ASN:O	3:C:31:ILE:N	2.34	0.61
1:A:67:LYS:HB2	1:A:67:LYS:HZ3	1.64	0.60
1:A:68:VAL:HG11	1:A:208:PHE:CE1	2.36	0.60
1:A:131:HIS:O	1:A:132:THR:OG1	2.19	0.60
3:C:188:GLU:OE1	3:C:193:ILE:HD11	1.92	0.60
3:C:192:VAL:CG1	3:C:194:ASP:OD2	2.49	0.60
3:C:222:LEU:HD21	3:C:224:ILE:HG12	1.82	0.60
3:C:31:ILE:HA	3:C:44:VAL:HG21	1.84	0.60
3:C:130:TYR:CG	3:C:134:TYR:CE2	2.89	0.60
3:C:115:PRO:O	3:C:152:PRO:HG2	2.01	0.60
2:B:157:ARG:HA	2:B:182:CYS:O	2.01	0.60
3:C:115:PRO:CB	3:C:152:PRO:HB3	2.30	0.60
1:A:219:ARG:HE	1:A:219:ARG:CA	2.15	0.60
3:C:204:LEU:HD11	3:C:246:TYR:HE2	1.65	0.60
2:B:141:SER:O	2:B:239:LEU:HD13	2.00	0.60
3:C:97:ASN:O	3:C:98:VAL:O	2.19	0.60
1:A:119:LEU:HB3	1:A:196:GLU:HB2	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:CD	1:A:182:MET:HE1	2.28	0.60
2:B:22:TYR:CB	2:B:23:LYS:CA	2.80	0.60
3:C:141:LEU:HB3	3:C:239:ASP:CB	2.22	0.59
3:C:151:LYS:CA	3:C:151:LYS:HE3	2.32	0.59
1:A:116:ILE:CD1	1:A:133:TYR:HE2	2.15	0.59
3:C:141:LEU:HD13	3:C:239:ASP:OD2	2.02	0.59
3:C:65:ASN:CG	3:C:67:ASP:HB2	2.19	0.59
2:B:134:THR:HG23	2:B:135:TYR:H	1.66	0.59
2:B:56:GLY:HA2	2:B:57:GLU:HB3	1.84	0.59
3:C:191:PRO:O	3:C:192:VAL:HG12	2.02	0.59
3:C:56:SER:C	3:C:58:ALA:N	2.52	0.59
1:A:68:VAL:HG23	2:B:73:ASP:C	2.23	0.59
2:B:200:THR:HG22	2:B:201:TRP:H	1.67	0.59
3:C:141:LEU:CB	3:C:239:ASP:HB3	2.24	0.59
3:C:98:VAL:HA	3:C:99:ASP:CB	2.31	0.59
2:B:81:LEU:O	2:B:238:ARG:NE	2.34	0.59
1:A:29:ASN:ND2	3:C:211:LEU:N	2.43	0.59
2:B:90:THR:N	2:B:91:PRO:CA	2.61	0.59
2:B:188:ASN:HB2	2:B:189:SER:CA	2.18	0.59
1:A:68:VAL:CG1	1:A:69:ASP:H	2.06	0.58
1:A:85:ASN:ND2	1:A:192:ARG:HA	2.19	0.58
1:A:91:GLN:N	1:A:91:GLN:OE1	2.20	0.58
2:B:22:TYR:HB3	2:B:23:LYS:CA	2.33	0.58
2:B:81:LEU:H	2:B:238:ARG:NE	2.01	0.58
2:B:188:ASN:HD21	3:C:213:ASN:HD22	1.50	0.58
3:C:31:ILE:HG23	3:C:44:VAL:CG2	2.33	0.58
3:C:36:VAL:O	3:C:36:VAL:HG12	2.04	0.58
3:C:96:ARG:HD2	3:C:97:ASN:HB3	1.84	0.58
1:A:170:ARG:HD3	1:A:171:THR:N	2.15	0.58
3:C:204:LEU:O	3:C:204:LEU:HD23	2.04	0.58
1:A:207:PHE:N	1:A:208:PHE:HA	2.17	0.58
1:A:46:LYS:N	1:A:49:TYR:HB3	2.19	0.58
2:B:133:ASN:HD21	2:B:253:VAL:HG22	1.69	0.58
3:C:124:ALA:O	3:C:125:SER:OG	2.19	0.58
3:C:60:THR:C	3:C:64:GLU:CG	2.64	0.57
3:C:100:ASN:HB3	3:C:101:PHE:HA	1.85	0.57
3:C:152:PRO:C	3:C:154:TYR:N	2.39	0.57
3:C:196:ARG:HD3	3:C:244:ARG:HH12	1.70	0.57
1:A:133:TYR:CA	1:A:134:ASP:HB2	2.34	0.57
1:A:80:SER:OG	1:A:81:HIS:N	2.36	0.57
3:C:139:VAL:HB	3:C:243:LEU:HB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:237:SER:O	3:C:239:ASP:OD1	2.22	0.57
1:A:51:LEU:HD12	1:A:53:PHE:N	2.19	0.57
1:A:210:VAL:C	1:A:213:PRO:HD2	2.21	0.57
1:A:90:ARG:CB	1:A:91:GLN:CA	2.83	0.57
2:B:56:GLY:CA	2:B:57:GLU:HB3	2.33	0.57
1:A:104:SER:N	1:A:106:PHE:CE1	2.72	0.57
3:C:38:GLY:O	3:C:41:ILE:HA	2.05	0.57
2:B:56:GLY:C	2:B:57:GLU:CG	2.71	0.57
1:A:132:THR:HG22	1:A:133:TYR:N	2.19	0.57
1:A:46:LYS:H	1:A:49:TYR:CB	2.18	0.57
3:C:97:ASN:O	3:C:98:VAL:C	2.42	0.56
2:B:74:ASP:OD1	2:B:76:ILE:N	2.38	0.56
1:A:163:PHE:CD1	1:A:164:TYR:N	2.73	0.56
1:A:89:TRP:CD1	1:A:90:ARG:CD	2.85	0.56
2:B:127:ASN:O	2:B:130:LEU:HG	2.05	0.56
2:B:25:THR:HG23	2:B:26:ARG:N	2.19	0.56
3:C:98:VAL:CA	3:C:99:ASP:HB2	2.35	0.56
3:C:30:ILE:O	3:C:33:GLY:N	2.39	0.56
2:B:75:MET:HE2	2:B:75:MET:N	2.19	0.56
1:A:133:TYR:HD1	1:A:134:ASP:O	1.89	0.56
1:A:68:VAL:HG11	1:A:208:PHE:HE1	1.69	0.56
3:C:66:LYS:O	3:C:68:VAL:O	2.23	0.56
3:C:43:LYS:CD	3:C:49:SER:HB2	2.16	0.56
2:B:143:ILE:HD11	2:B:191:GLU:HG2	1.87	0.56
2:B:88:ASN:O	2:B:91:PRO:CA	2.52	0.56
3:C:98:VAL:CA	3:C:99:ASP:CB	2.84	0.56
2:B:87:ASP:O	2:B:93:SER:OG	2.23	0.56
3:C:193:ILE:CG2	3:C:196:ARG:CZ	2.82	0.56
3:C:41:ILE:HD13	3:C:41:ILE:O	2.05	0.56
1:A:27:SER:O	1:A:30:GLU:OE1	2.14	0.56
2:B:114:MET:SD	2:B:115:VAL:HG22	2.46	0.56
3:C:244:ARG:NH1	3:C:246:TYR:OH	2.38	0.56
2:B:178:ILE:HG22	2:B:179:TYR:N	2.20	0.56
2:B:88:ASN:C	2:B:91:PRO:CA	2.74	0.56
1:A:133:TYR:CA	1:A:134:ASP:CB	2.84	0.55
1:A:75:ALA:CB	1:A:200:SER:HB2	2.23	0.55
1:A:89:TRP:HD1	1:A:90:ARG:CB	2.19	0.55
1:A:95:PHE:HE2	1:A:97:LYS:HZ2	1.54	0.55
2:B:35:PRO:HA	2:B:38:MET:HG3	1.87	0.55
2:B:40:MET:HG3	2:B:43:VAL:H	1.70	0.55
2:B:75:MET:HA	2:B:75:MET:CE	2.35	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:TYR:CD1	3:C:134:TYR:CD2	2.94	0.55
1:A:177:ALA:O	1:A:178:LEU:HB3	2.05	0.55
1:A:110:PHE:O	1:A:170:ARG:CD	2.45	0.55
1:A:219:ARG:HE	1:A:219:ARG:HA	1.70	0.55
1:A:89:TRP:HD1	1:A:90:ARG:CG	2.19	0.55
2:B:58:ARG:CZ	2:B:58:ARG:H	2.18	0.55
3:C:98:VAL:HA	3:C:99:ASP:CG	2.27	0.55
1:A:206:PHE:O	1:A:207:PHE:CB	2.55	0.55
3:C:164:ARG:CZ	3:C:226:TYR:OH	2.55	0.55
1:A:163:PHE:CD1	1:A:166:ASN:HB3	2.41	0.55
2:B:88:ASN:HA	2:B:92:SER:H	1.70	0.55
3:C:109:THR:HG22	3:C:110:THR:H	1.72	0.55
1:A:83:PHE:CZ	1:A:185:PRO:HG3	2.41	0.55
1:A:89:TRP:C	1:A:90:ARG:HG3	2.27	0.55
2:B:114:MET:SD	2:B:115:VAL:CG2	2.94	0.55
2:B:218:LEU:HD12	2:B:219:ASN:N	2.22	0.55
1:A:68:VAL:HG23	2:B:74:ASP:N	2.20	0.55
3:C:100:ASN:C	3:C:102:HIS:HA	2.27	0.55
1:A:168:PRO:N	1:A:169:LEU:HD13	2.22	0.55
1:A:94:THR:HG22	1:A:180:PHE:HE1	1.72	0.55
3:C:39:GLU:H	3:C:39:GLU:CD	2.09	0.55
3:C:61:ALA:C	3:C:64:GLU:HG3	2.27	0.55
2:B:149:TYR:O	2:B:231:VAL:HG23	2.07	0.55
3:C:187:TYR:CZ	3:C:224:ILE:HG21	2.42	0.55
2:B:150:ALA:HB2	2:B:231:VAL:CG2	2.36	0.54
3:C:112:ASP:C	3:C:113:LYS:HG2	2.28	0.54
1:A:94:THR:HG22	1:A:180:PHE:CE1	2.42	0.54
2:B:165:ASN:CB	2:B:166:CYS:HA	2.36	0.54
3:C:122:ASP:CG	3:C:265:VAL:HG22	2.28	0.54
3:C:103:SER:C	3:C:104:MET:HG2	2.28	0.54
3:C:96:ARG:HB3	3:C:97:ASN:O	2.06	0.54
1:A:111:THR:OG1	1:A:112:GLY:N	2.37	0.54
1:A:43:GLY:N	1:A:44:ASN:O	2.40	0.54
2:B:67:GLY:H	3:C:227:VAL:HG13	1.72	0.54
3:C:62:GLN:CB	3:C:63:PRO:CD	2.85	0.54
3:C:96:ARG:HB3	3:C:97:ASN:HB3	1.90	0.54
1:A:46:LYS:HB3	1:A:49:TYR:CD2	2.43	0.54
3:C:145:PHE:CZ	3:C:269:LEU:HD11	2.43	0.54
3:C:161:ALA:CB	3:C:278:ARG:HD3	2.38	0.54
1:A:212:ALA:HB2	2:B:78:ILE:CG1	2.38	0.54
2:B:109:VAL:HG11	2:B:220:ARG:NH2	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:218:THR:OG1	3:C:219:GLN:OE1	2.14	0.54
2:B:252:LEU:HD13	2:B:255:PHE:HA	1.88	0.54
2:B:163:PHE:CE1	2:B:177:ALA:HB2	2.42	0.54
1:A:161:VAL:CG2	1:A:162:PRO:CD	2.86	0.53
1:A:176:SER:OG	1:A:177:ALA:HB2	2.08	0.53
1:A:179:GLY:O	1:A:180:PHE:CB	2.52	0.53
1:A:189:GLY:O	1:A:190:THR:OG1	2.23	0.53
2:B:183:ASP:H	2:B:190:PHE:HZ	1.56	0.53
2:B:22:TYR:CD1	2:B:24:TRP:HB3	2.42	0.53
2:B:172:LEU:HA	2:B:174:LEU:HG	1.90	0.53
3:C:130:TYR:CG	3:C:134:TYR:CD2	2.97	0.53
1:A:140:LYS:N	1:A:141:THR:HB	2.19	0.53
1:A:219:ARG:NH2	2:B:256:GLN:CB	2.67	0.53
2:B:157:ARG:HG2	2:B:183:ASP:OD1	2.08	0.53
1:A:219:ARG:C	1:A:221:ALA:N	2.60	0.53
1:A:45:GLU:H	1:A:46:LYS:HB2	1.73	0.53
2:B:201:TRP:CE3	2:B:202:MET:HG3	2.44	0.53
2:B:206:HIS:CD2	2:B:207:GLY:H	2.25	0.53
2:B:37:THR:CA	2:B:38:MET:C	2.75	0.53
1:A:115:ASN:OD1	1:A:160:SER:OG	2.19	0.53
1:A:202:ARG:NE	2:B:51:SER:HG	2.07	0.53
2:B:118:ASN:HB3	2:B:120:VAL:CA	2.38	0.53
2:B:87:ASP:OD1	2:B:93:SER:OG	2.18	0.53
1:A:66:THR:CG2	2:B:76:ILE:HG23	2.35	0.53
2:B:116:HIS:O	2:B:117:ARG:CB	2.45	0.53
3:C:112:ASP:C	3:C:113:LYS:CG	2.75	0.53
3:C:61:ALA:O	3:C:64:GLU:HB2	2.06	0.53
1:A:144:SER:HA	1:A:148:VAL:HG12	1.91	0.52
1:A:219:ARG:NE	1:A:219:ARG:CA	2.72	0.52
2:B:40:MET:HG3	2:B:42:ASN:HB3	1.91	0.52
3:C:50:ASN:O	3:C:51:LEU:C	2.42	0.52
2:B:178:ILE:CG2	2:B:179:TYR:N	2.72	0.52
2:B:47:THR:HG22	2:B:48:GLY:N	2.24	0.52
2:B:252:LEU:HD13	2:B:254:SER:H	1.73	0.52
2:B:58:ARG:CZ	2:B:58:ARG:N	2.72	0.52
1:A:113:GLU:OE2	2:B:61:TYR:CE1	2.61	0.52
1:A:140:LYS:HB2	1:A:141:THR:HA	1.91	0.52
1:A:169:LEU:CD1	1:A:169:LEU:N	2.73	0.52
1:A:111:THR:CG2	1:A:206:PHE:HA	2.39	0.52
3:C:22:ASN:O	3:C:26:GLU:HG3	2.09	0.52
3:C:54:PRO:O	3:C:56:SER:HA	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:PRO:CA	1:A:213:PRO:HD2	2.40	0.52
1:A:29:ASN:ND2	3:C:211:LEU:H	2.08	0.52
3:C:135:LYS:HD2	3:C:138:THR:HG23	1.91	0.52
3:C:202:GLY:N	3:C:203:SER:CB	2.72	0.52
3:C:42:THR:N	3:C:43:LYS:CA	2.73	0.52
1:A:202:ARG:HG3	1:A:203:CYS:SG	2.49	0.52
2:B:206:HIS:CG	2:B:207:GLY:N	2.77	0.52
2:B:31:ILE:HG22	2:B:33:GLU:HB2	1.92	0.52
2:B:58:ARG:N	2:B:58:ARG:CD	2.73	0.52
1:A:126:PHE:HD2	1:A:127:LEU:HB2	1.74	0.52
1:A:67:LYS:CG	1:A:68:VAL:N	2.73	0.52
3:C:108:ILE:HG13	3:C:109:THR:HA	1.90	0.52
3:C:122:ASP:HB2	3:C:264:THR:HA	1.91	0.52
1:A:132:THR:HG22	1:A:133:TYR:H	1.75	0.52
2:B:75:MET:CA	2:B:75:MET:CE	2.89	0.52
3:C:195:SER:O	3:C:197:GLN:N	2.43	0.52
3:C:28:ASN:ND2	3:C:52:LEU:HB3	2.22	0.52
2:B:178:ILE:N	2:B:178:ILE:CD1	2.73	0.51
2:B:58:ARG:CG	2:B:59:ALA:N	2.64	0.51
3:C:135:LYS:CG	3:C:136:ILE:N	2.73	0.51
1:A:96:PRO:O	1:A:176:SER:OG	2.28	0.51
2:B:25:THR:CG2	2:B:26:ARG:N	2.73	0.51
3:C:201:PHE:C	3:C:203:SER:OG	2.44	0.51
2:B:163:PHE:HB2	2:B:166:CYS:SG	2.51	0.51
3:C:118:LEU:HD23	3:C:268:SER:CB	2.35	0.51
3:C:185:VAL:HB	3:C:210:VAL:CG1	2.40	0.51
3:C:40:ILE:N	3:C:42:THR:HA	2.25	0.51
3:C:65:ASN:OD1	3:C:67:ASP:HB2	2.10	0.51
1:A:26:ILE:CG2	1:A:27:SER:N	2.73	0.51
1:A:92:LYS:CB	1:A:92:LYS:NZ	2.73	0.51
2:B:42:ASN:O	2:B:43:VAL:HB	2.07	0.51
3:C:72:THR:HG22	3:C:73:THR:N	2.25	0.51
1:A:206:PHE:O	1:A:208:PHE:CA	2.54	0.51
3:C:195:SER:C	3:C:197:GLN:N	2.64	0.51
2:B:73:ASP:O	2:B:74:ASP:HB3	2.11	0.51
1:A:218:SER:O	3:C:199:LEU:HB3	2.09	0.51
3:C:204:LEU:HD11	3:C:246:TYR:CE2	2.44	0.51
3:C:151:LYS:CB	3:C:152:PRO:CD	2.85	0.51
3:C:192:VAL:HG12	3:C:194:ASP:OD1	2.05	0.51
1:A:90:ARG:HB3	1:A:92:LYS:N	2.25	0.51
2:B:187:ASP:O	2:B:188:ASN:O	2.29	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:SER:CB	2:B:252:LEU:HA	2.40	0.51
2:B:72:PHE:CD1	2:B:74:ASP:O	2.64	0.51
2:B:75:MET:CE	2:B:75:MET:N	2.73	0.51
3:C:122:ASP:OD2	3:C:265:VAL:N	2.44	0.51
3:C:126:TRP:HE1	3:C:251:LEU:HB2	1.76	0.51
1:A:161:VAL:HG22	1:A:162:PRO:N	2.26	0.51
1:A:202:ARG:HE	2:B:51:SER:HG	1.58	0.51
1:A:207:PHE:HD1	2:B:71:ARG:CA	2.23	0.51
1:A:70:ASN:O	1:A:73:GLY:N	2.43	0.51
3:C:142:PRO:HG2	3:C:240:LEU:HG	1.92	0.51
3:C:89:ILE:HG22	3:C:90:PRO:O	2.11	0.51
3:C:155:GLY:O	3:C:158:LYS:HG2	2.11	0.50
3:C:229:ASP:OD1	3:C:230:THR:N	2.41	0.50
1:A:172:VAL:CG2	1:A:175:ASP:CG	2.65	0.50
1:A:97:LYS:HG3	1:A:177:ALA:HB3	1.93	0.50
2:B:73:ASP:O	2:B:74:ASP:O	2.29	0.50
2:B:88:ASN:HB3	2:B:91:PRO:HB2	1.83	0.50
3:C:130:TYR:HB3	3:C:134:TYR:HD2	1.75	0.50
1:A:115:ASN:CB	1:A:200:SER:O	2.52	0.50
1:A:89:TRP:CD1	1:A:90:ARG:CG	2.94	0.50
1:A:179:GLY:C	1:A:180:PHE:CG	2.79	0.50
1:A:109:TYR:HE1	1:A:211:PRO:HA	1.77	0.50
1:A:69:ASP:O	1:A:70:ASN:C	2.50	0.50
2:B:23:LYS:CG	2:B:24:TRP:C	2.71	0.50
1:A:120:TYR:CD1	1:A:129:VAL:HG21	2.47	0.50
3:C:96:ARG:CD	3:C:97:ASN:HB3	2.42	0.50
1:A:51:LEU:CD1	1:A:53:PHE:H	2.25	0.50
1:A:105:GLN:HB2	2:B:134:THR:HB	1.93	0.50
2:B:188:ASN:CB	2:B:189:SER:CA	2.79	0.50
1:A:46:LYS:HB3	1:A:49:TYR:CG	2.47	0.50
1:A:96:PRO:C	1:A:177:ALA:CB	2.76	0.50
2:B:80:GLN:N	2:B:238:ARG:HD2	2.27	0.50
3:C:209:HIS:CD2	3:C:209:HIS:C	2.85	0.50
1:A:131:HIS:HE1	1:A:181:LEU:HB3	1.77	0.50
1:A:149:ILE:HG13	1:A:159:LEU:HD21	1.94	0.50
1:A:28:PRO:O	1:A:30:GLU:HG3	2.12	0.50
1:A:48:ASN:HB2	1:A:49:TYR:HA	1.94	0.50
1:A:77:TYR:CD1	1:A:77:TYR:N	2.79	0.50
3:C:130:TYR:HB3	3:C:134:TYR:CD2	2.47	0.50
3:C:196:ARG:N	3:C:196:ARG:NH1	2.60	0.50
1:A:139:ARG:HD2	1:A:141:THR:CG2	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLN:OE1	2:B:41:ALA:HB3	2.12	0.49
1:A:89:TRP:CD1	1:A:89:TRP:C	2.85	0.49
2:B:37:THR:HA	2:B:40:MET:N	2.21	0.49
3:C:151:LYS:CE	3:C:151:LYS:CA	2.85	0.49
1:A:107:PHE:C	1:A:107:PHE:CD1	2.85	0.49
1:A:117:HIS:HB3	1:A:157:MET:SD	2.52	0.49
1:A:77:TYR:HD1	1:A:77:TYR:N	2.10	0.49
3:C:120:ARG:C	3:C:121:LEU:HD12	2.33	0.49
1:A:206:PHE:CD1	1:A:209:PRO:HD3	2.47	0.49
1:A:64:SER:CA	1:A:67:LYS:HB3	2.38	0.49
1:A:90:ARG:CB	1:A:91:GLN:HA	2.43	0.49
1:A:163:PHE:HD1	1:A:164:TYR:N	2.10	0.49
1:A:205:ASN:HD22	2:B:61:TYR:HE2	1.60	0.49
1:A:96:PRO:HB2	1:A:98:GLU:O	2.12	0.49
3:C:107:ASP:OD1	3:C:107:ASP:N	2.46	0.49
1:A:133:TYR:CD1	1:A:133:TYR:C	2.85	0.49
1:A:74:ARG:HG2	1:A:75:ALA:N	2.27	0.49
3:C:249:THR:HG22	3:C:249:THR:O	2.12	0.49
3:C:31:ILE:HG22	3:C:44:VAL:CG1	2.23	0.49
3:C:62:GLN:HG3	3:C:63:PRO:HD3	1.94	0.49
1:A:120:TYR:CZ	1:A:122:ALA:HB2	2.47	0.49
1:A:92:LYS:NZ	1:A:92:LYS:HB2	2.27	0.49
2:B:256:GLN:OE1	2:B:256:GLN:N	2.37	0.49
2:B:58:ARG:NH1	2:B:58:ARG:N	2.60	0.49
3:C:50:ASN:ND2	3:C:50:ASN:N	2.60	0.49
1:A:108:ALA:HB3	1:A:109:TYR:CZ	2.46	0.49
1:A:89:TRP:CD1	1:A:90:ARG:N	2.80	0.49
3:C:64:GLU:O	3:C:65:ASN:O	2.30	0.49
1:A:103:LEU:O	1:A:106:PHE:CG	2.66	0.49
1:A:164:TYR:CD1	1:A:164:TYR:C	2.86	0.49
2:B:112:GLN:O	2:B:113:ASN:CG	2.52	0.49
2:B:22:TYR:HB2	2:B:24:TRP:HB3	1.91	0.49
3:C:24:GLU:OE1	3:C:52:LEU:O	2.31	0.49
3:C:47:ASP:O	3:C:50:ASN:ND2	2.46	0.49
1:A:147:GLY:C	1:A:148:VAL:HG13	2.33	0.48
1:A:206:PHE:CD1	1:A:206:PHE:C	2.85	0.48
1:A:206:PHE:O	1:A:209:PRO:CG	2.60	0.48
1:A:26:ILE:CG2	1:A:27:SER:H	2.24	0.48
1:A:62:THR:O	1:A:63:VAL:HG12	2.13	0.48
2:B:114:MET:HG3	2:B:215:VAL:C	2.30	0.48
3:C:141:LEU:HD23	3:C:241:GLY:O	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:GLN:O	3:C:71:ALA:HB2	2.13	0.48
1:A:109:TYR:CD2	1:A:206:PHE:CE1	2.83	0.48
1:A:161:VAL:HG23	1:A:162:PRO:CD	2.43	0.48
1:A:110:PHE:CB	1:A:170:ARG:HD2	2.43	0.48
2:B:24:TRP:CD1	2:B:24:TRP:C	2.85	0.48
2:B:27:THR:OG1	2:B:28:LYS:N	2.46	0.48
3:C:62:GLN:HB3	3:C:63:PRO:HD3	1.94	0.48
1:A:163:PHE:HD1	1:A:163:PHE:C	2.17	0.48
1:A:149:ILE:HG22	1:A:149:ILE:O	2.13	0.48
1:A:219:ARG:O	1:A:221:ALA:N	2.45	0.48
2:B:113:ASN:N	2:B:113:ASN:ND2	2.60	0.48
1:A:168:PRO:CA	1:A:169:LEU:HD13	2.42	0.48
2:B:82:PHE:HD2	2:B:145:ARG:HH11	1.62	0.48
3:C:193:ILE:HD13	3:C:193:ILE:H	1.77	0.48
1:A:168:PRO:C	1:A:170:ARG:H	2.15	0.48
2:B:183:ASP:N	2:B:190:PHE:HZ	2.12	0.48
2:B:52:VAL:O	2:B:54:LEU:HG	2.14	0.48
3:C:23:VAL:O	3:C:26:GLU:HB2	2.14	0.48
3:C:64:GLU:O	3:C:65:ASN:C	2.52	0.48
1:A:99:GLY:HA3	1:A:100:HIS:HA	1.50	0.48
2:B:94:SER:N	2:B:95:SER:HA	2.28	0.48
1:A:117:HIS:CE1	2:B:44:LEU:HD23	2.35	0.48
1:A:161:VAL:CG2	1:A:162:PRO:HD2	2.44	0.48
2:B:106:ALA:O	2:B:107:ALA:HB2	2.13	0.48
2:B:112:GLN:C	2:B:113:ASN:CG	2.71	0.48
3:C:103:SER:OG	3:C:103:SER:O	2.31	0.48
1:A:215:PRO:HG2	3:C:204:LEU:H	1.76	0.48
1:A:62:THR:C	1:A:64:SER:H	2.15	0.48
2:B:105:TRP:HZ3	2:B:107:ALA:HB2	1.79	0.48
3:C:98:VAL:HG22	3:C:99:ASP:CB	2.43	0.48
3:C:122:ASP:OD2	3:C:265:VAL:HG13	2.14	0.48
1:A:89:TRP:HD1	1:A:90:ARG:N	2.12	0.47
2:B:178:ILE:N	2:B:178:ILE:HD12	2.29	0.47
1:A:67:LYS:HG2	2:B:73:ASP:CG	2.34	0.47
3:C:124:ALA:HA	3:C:262:ASP:HB2	1.96	0.47
1:A:110:PHE:HB2	1:A:170:ARG:HD2	1.97	0.47
3:C:136:ILE:C	3:C:136:ILE:HD12	2.34	0.47
1:A:43:GLY:CA	1:A:50:PHE:CD2	2.96	0.47
1:A:96:PRO:C	1:A:98:GLU:H	2.17	0.47
2:B:171:GLN:O	2:B:173:GLU:N	2.47	0.47
2:B:218:LEU:HD12	2:B:219:ASN:H	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:GLN:O	2:B:81:LEU:HD12	2.14	0.47
3:C:201:PHE:C	3:C:203:SER:CB	2.82	0.47
2:B:187:ASP:C	2:B:188:ASN:O	2.52	0.47
2:B:56:GLY:N	2:B:57:GLU:HB3	2.30	0.47
2:B:196:TYR:OH	2:B:201:TRP:O	2.17	0.47
2:B:91:PRO:O	2:B:92:SER:OG	2.27	0.47
3:C:107:ASP:HA	3:C:108:ILE:HA	1.62	0.47
3:C:201:PHE:O	3:C:203:SER:C	2.52	0.47
1:A:64:SER:O	1:A:67:LYS:N	2.47	0.47
1:A:147:GLY:O	1:A:148:VAL:CG1	2.63	0.47
2:B:167:THR:OG1	2:B:168:HIS:N	2.45	0.47
2:B:23:LYS:HG2	2:B:24:TRP:CA	2.43	0.47
2:B:33:GLU:HB3	2:B:34:GLY:O	2.15	0.47
2:B:55:VAL:HG12	2:B:56:GLY:N	2.29	0.47
3:C:126:TRP:CD1	3:C:127:GLN:N	2.83	0.47
2:B:24:TRP:CD1	2:B:24:TRP:N	2.76	0.47
1:A:62:THR:O	1:A:64:SER:N	2.46	0.47
2:B:146:LEU:HD11	2:B:233:CYS:HB3	1.97	0.47
2:B:88:ASN:HA	2:B:91:PRO:CB	2.33	0.47
1:A:97:LYS:HD2	1:A:177:ALA:HB1	1.97	0.46
2:B:74:ASP:OD1	2:B:77:LYS:N	2.44	0.46
3:C:277:PRO:O	3:C:278:ARG:HG3	2.15	0.46
3:C:31:ILE:HG23	3:C:44:VAL:HG11	0.46	0.46
3:C:196:ARG:NH1	3:C:196:ARG:CB	2.73	0.46
1:A:133:TYR:HA	1:A:134:ASP:CB	2.46	0.46
1:A:163:PHE:C	1:A:163:PHE:CD1	2.88	0.46
1:A:83:PHE:CE2	1:A:85:ASN:HA	2.50	0.46
3:C:174:ASN:OD1	3:C:218:THR:HB	2.16	0.46
3:C:96:ARG:CB	3:C:97:ASN:HB3	2.46	0.46
1:A:111:THR:HG22	1:A:206:PHE:HA	1.96	0.46
2:B:173:GLU:O	2:B:176:ASN:N	2.49	0.46
2:B:194:ILE:HG13	2:B:195:PRO:O	2.16	0.46
1:A:71:ILE:HG13	2:B:135:TYR:OH	2.15	0.46
1:A:74:ARG:HG2	1:A:75:ALA:H	1.79	0.46
2:B:120:VAL:HG21	2:B:211:GLY:N	2.31	0.46
2:B:188:ASN:ND2	3:C:213:ASN:HD22	2.13	0.46
3:C:39:GLU:C	3:C:42:THR:HG22	2.35	0.46
3:C:175:VAL:HG12	3:C:261:VAL:HG11	1.98	0.46
1:A:173:ARG:NH2	1:A:214:LYS:HB2	2.31	0.46
1:A:68:VAL:O	1:A:69:ASP:HB3	2.16	0.46
2:B:163:PHE:HZ	2:B:173:GLU:C	2.19	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ASP:HA	2:B:170:THR:HB	1.98	0.46
2:B:27:THR:OG1	2:B:29:VAL:HG23	2.15	0.46
3:C:109:THR:HG22	3:C:113:LYS:CB	2.30	0.46
1:A:43:GLY:N	1:A:50:PHE:CB	2.79	0.45
1:A:43:GLY:N	1:A:50:PHE:HB2	2.31	0.45
2:B:100:TYR:CG	2:B:101:GLY:N	2.84	0.45
2:B:46:THR:O	2:B:48:GLY:N	2.49	0.45
3:C:58:ALA:HA	3:C:59:THR:HA	1.66	0.45
1:A:163:PHE:HE1	1:A:166:ASN:HB3	1.78	0.45
2:B:136:SER:O	2:B:137:TYR:CG	2.70	0.45
2:B:187:ASP:HB3	3:C:216:GLU:OE2	2.16	0.45
2:B:114:MET:HG2	2:B:215:VAL:HG23	1.93	0.45
1:A:211:PRO:HA	1:A:213:PRO:HD2	1.98	0.45
1:A:109:TYR:HA	1:A:173:ARG:HE	1.82	0.45
1:A:98:GLU:HA	1:A:100:HIS:HA	1.97	0.45
2:B:135:TYR:CD2	2:B:245:PHE:HD2	2.35	0.45
1:A:169:LEU:HD22	1:A:170:ARG:O	2.17	0.45
1:A:175:ASP:HB2	1:A:176:SER:HA	1.97	0.45
1:A:217:GLY:O	1:A:218:SER:C	2.55	0.45
2:B:111:PRO:HA	2:B:218:LEU:HA	1.99	0.45
2:B:22:TYR:N	2:B:23:LYS:C	2.70	0.45
2:B:26:ARG:HA	2:B:27:THR:HA	1.73	0.45
2:B:65:THR:HB	2:B:66:ALA:HA	1.99	0.45
2:B:88:ASN:CB	2:B:91:PRO:HB3	2.44	0.45
1:A:134:ASP:HA	1:A:135:THR:HG23	1.92	0.45
2:B:98:ASP:N	2:B:98:ASP:OD1	2.48	0.45
3:C:226:TYR:H	3:C:226:TYR:HD1	1.64	0.45
3:C:60:THR:O	3:C:64:GLU:OE2	2.35	0.45
3:C:98:VAL:HG13	3:C:100:ASN:CA	2.35	0.45
1:A:161:VAL:HG22	1:A:162:PRO:CD	2.47	0.45
1:A:83:PHE:CD2	1:A:193:THR:HB	2.52	0.45
1:A:201:LEU:HD12	1:A:204:PRO:HG3	1.98	0.45
2:B:189:SER:O	2:B:190:PHE:CG	2.70	0.45
2:B:22:TYR:H	2:B:24:TRP:N	2.15	0.45
1:A:29:ASN:HD22	3:C:211:LEU:HB3	1.76	0.45
2:B:227:SER:HB3	2:B:228:PRO:HD2	1.97	0.45
3:C:28:ASN:HD21	3:C:52:LEU:CB	2.25	0.45
3:C:62:GLN:HB3	3:C:63:PRO:HD2	1.95	0.45
1:A:167:LYS:C	1:A:169:LEU:CD1	2.85	0.44
2:B:41:ALA:CA	2:B:43:VAL:N	2.80	0.44
2:B:43:VAL:CG1	2:B:44:LEU:H	2.13	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:HD12	1:A:53:PHE:H	1.79	0.44
3:C:100:ASN:N	3:C:101:PHE:HA	2.32	0.44
1:A:163:PHE:O	1:A:164:TYR:CD1	2.70	0.44
1:A:163:PHE:O	1:A:164:TYR:CG	2.70	0.44
1:A:214:LYS:O	1:A:216:THR:HG22	2.18	0.44
2:B:109:VAL:HG22	2:B:110:ALA:N	2.29	0.44
2:B:121:THR:O	2:B:122:LEU:HB2	2.18	0.44
2:B:136:SER:O	2:B:137:TYR:CD2	2.71	0.44
2:B:43:VAL:O	2:B:44:LEU:HD22	2.17	0.44
2:B:64:ARG:HG3	2:B:65:THR:O	2.17	0.44
3:C:146:TRP:CA	3:C:153:ALA:HB1	2.44	0.44
3:C:187:TYR:CD2	3:C:187:TYR:O	2.70	0.44
2:B:188:ASN:ND2	3:C:213:ASN:ND2	2.65	0.44
3:C:65:ASN:C	3:C:67:ASP:H	2.21	0.44
3:C:126:TRP:HE1	3:C:251:LEU:CB	2.30	0.44
3:C:41:ILE:C	3:C:41:ILE:CD1	2.86	0.44
1:A:219:ARG:HE	1:A:219:ARG:N	2.16	0.44
2:B:125:PHE:HD2	3:C:199:LEU:HD21	1.82	0.44
2:B:166:CYS:SG	2:B:167:THR:HG22	2.58	0.44
3:C:187:TYR:CG	3:C:187:TYR:O	2.70	0.44
3:C:56:SER:O	3:C:58:ALA:N	2.51	0.44
2:B:61:TYR:HE2	2:B:63:PRO:HG3	1.82	0.44
3:C:59:THR:H	3:C:60:THR:HA	1.83	0.44
1:A:147:GLY:C	1:A:148:VAL:CG1	2.86	0.44
2:B:189:SER:O	2:B:190:PHE:CD1	2.70	0.44
2:B:23:LYS:CG	2:B:24:TRP:CA	2.96	0.44
2:B:90:THR:OG1	2:B:91:PRO:C	2.55	0.44
1:A:173:ARG:HH22	1:A:214:LYS:N	2.08	0.44
2:B:134:THR:HG23	2:B:135:TYR:N	2.32	0.44
1:A:211:PRO:HG3	2:B:72:PHE:CE2	2.53	0.44
1:A:90:ARG:CB	1:A:91:GLN:C	2.85	0.44
2:B:159:ARG:HG2	2:B:216:GLU:HB3	2.00	0.44
3:C:110:THR:HB	3:C:111:GLY:CA	2.35	0.44
2:B:114:MET:HB2	2:B:216:GLU:HA	1.98	0.43
2:B:58:ARG:H	2:B:58:ARG:HH11	1.66	0.43
3:C:43:LYS:CG	3:C:49:SER:HB2	2.48	0.43
1:A:106:PHE:CD1	1:A:106:PHE:O	2.71	0.43
1:A:206:PHE:CB	1:A:208:PHE:HD1	2.26	0.43
2:B:173:GLU:O	2:B:176:ASN:HB3	2.18	0.43
3:C:54:PRO:C	3:C:56:SER:CA	2.85	0.43
1:A:108:ALA:HB3	1:A:109:TYR:CD1	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:NE	1:A:182:MET:HE1	2.33	0.43
3:C:160:PHE:CD1	3:C:160:PHE:N	2.84	0.43
1:A:125:GLY:HA2	1:A:153:ALA:HB3	1.99	0.43
1:A:123:GLU:O	1:A:125:GLY:N	2.52	0.43
1:A:86:GLY:HA2	1:A:87:ASP:HA	1.51	0.43
2:B:120:VAL:CB	2:B:121:THR:HA	2.40	0.43
2:B:123:ASP:CB	2:B:125:PHE:CE1	2.80	0.43
3:C:110:THR:H	3:C:113:LYS:HB2	1.33	0.43
3:C:31:ILE:O	3:C:35:GLU:HG3	2.18	0.43
2:B:57:GLU:O	2:B:58:ARG:NH1	2.51	0.43
2:B:99:LYS:NZ	2:B:232:HIS:CG	2.87	0.43
3:C:233:VAL:HG21	3:C:240:LEU:CD2	2.44	0.43
1:A:132:THR:HG21	1:A:147:GLY:HA3	1.99	0.43
1:A:68:VAL:HG22	2:B:75:MET:HE2	2.00	0.43
2:B:174:LEU:HD12	2:B:175:ASP:N	2.34	0.43
2:B:169:ASP:OD1	2:B:212:LEU:HD11	2.18	0.43
2:B:81:LEU:C	2:B:238:ARG:HE	2.21	0.43
1:A:106:PHE:HD1	1:A:106:PHE:O	2.02	0.43
2:B:74:ASP:CA	2:B:75:MET:CB	2.83	0.43
3:C:100:ASN:H	3:C:101:PHE:HA	1.84	0.43
2:B:114:MET:CG	2:B:115:VAL:N	2.73	0.43
2:B:159:ARG:CG	2:B:216:GLU:HB3	2.49	0.43
2:B:24:TRP:CD1	2:B:25:THR:HG22	2.54	0.43
3:C:197:GLN:HB2	3:C:200:GLU:OE1	2.19	0.43
1:A:207:PHE:CB	1:A:208:PHE:C	2.85	0.43
1:A:173:ARG:NH2	1:A:214:LYS:CB	2.81	0.43
1:A:45:GLU:CB	1:A:46:LYS:HA	2.46	0.43
2:B:168:HIS:O	2:B:169:ASP:HB2	2.19	0.43
1:A:27:SER:O	1:A:30:GLU:CB	2.57	0.42
3:C:43:LYS:CB	3:C:49:SER:HB2	2.47	0.42
3:C:62:GLN:HA	3:C:62:GLN:OE1	2.19	0.42
2:B:35:PRO:HA	2:B:38:MET:CG	2.49	0.42
2:B:72:PHE:HD1	2:B:74:ASP:O	2.01	0.42
3:C:140:GLU:HG3	3:C:141:LEU:N	2.34	0.42
1:A:107:PHE:HD1	1:A:108:ALA:N	2.18	0.42
2:B:110:ALA:C	2:B:112:GLN:H	2.23	0.42
2:B:84:VAL:HA	2:B:236:GLN:HB3	2.01	0.42
3:C:110:THR:HG23	3:C:113:LYS:HA	1.73	0.42
3:C:135:LYS:HD2	3:C:138:THR:CG2	2.49	0.42
3:C:30:ILE:O	3:C:33:GLY:CA	2.67	0.42
2:B:44:LEU:N	2:B:44:LEU:CD2	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:187:TYR:CZ	3:C:241:GLY:HA3	2.55	0.42
3:C:45:ALA:HA	3:C:46:ASP:HA	1.62	0.42
1:A:101:GLY:HA2	1:A:104:SER:OG	2.19	0.42
1:A:166:ASN:C	1:A:167:LYS:O	2.57	0.42
1:A:211:PRO:HA	1:A:212:ALA:HA	1.77	0.42
3:C:136:ILE:CG2	3:C:137:THR:H	2.05	0.42
3:C:121:LEU:HB2	3:C:265:VAL:HG23	2.00	0.42
3:C:37:GLY:C	3:C:39:GLU:N	2.73	0.42
3:C:56:SER:N	3:C:58:ALA:O	2.51	0.42
1:A:110:PHE:HB2	1:A:170:ARG:CD	2.50	0.42
2:B:178:ILE:H	2:B:178:ILE:CD1	2.31	0.42
2:B:255:PHE:N	2:B:256:GLN:CA	2.83	0.42
2:B:57:GLU:HA	2:B:58:ARG:HA	1.72	0.42
3:C:32:SER:HA	3:C:35:GLU:HB2	2.02	0.42
2:B:186:SER:HA	2:B:187:ASP:HA	1.68	0.42
2:B:52:VAL:HB	2:B:53:ALA:H	1.59	0.42
2:B:54:LEU:HA	2:B:55:VAL:HA	1.55	0.42
3:C:118:LEU:C	3:C:119:ILE:HG13	2.40	0.42
3:C:48:ALA:C	3:C:50:ASN:N	2.52	0.42
2:B:98:ASP:HA	2:B:99:LYS:CB	2.32	0.42
3:C:68:VAL:HG21	3:C:84:PRO:HG2	2.01	0.42
3:C:195:SER:C	3:C:196:ARG:NH1	2.73	0.42
3:C:47:ASP:C	3:C:49:SER:N	2.73	0.42
3:C:59:THR:HB	3:C:60:THR:HA	2.02	0.42
1:A:111:THR:HG23	1:A:112:GLY:N	2.35	0.41
1:A:206:PHE:C	1:A:206:PHE:HD1	2.19	0.41
1:A:219:ARG:HE	1:A:219:ARG:H	1.68	0.41
1:A:66:THR:C	2:B:75:MET:HG3	2.24	0.41
3:C:172:GLN:HG2	3:C:219:GLN:HG3	2.01	0.41
1:A:172:VAL:HG21	1:A:175:ASP:CA	2.50	0.41
2:B:138:PHE:HD1	2:B:205:THR:HG22	1.85	0.41
1:A:133:TYR:CD1	1:A:134:ASP:O	2.70	0.41
3:C:117:LYS:O	3:C:119:ILE:HG13	2.20	0.41
2:B:212:LEU:HD21	2:B:214:GLN:NE2	2.35	0.41
2:B:67:GLY:H	3:C:227:VAL:CG1	2.32	0.41
3:C:98:VAL:CG2	3:C:99:ASP:HB2	2.49	0.41
1:A:134:ASP:CB	1:A:135:THR:O	2.68	0.41
1:A:117:HIS:C	1:A:157:MET:HB2	2.41	0.41
2:B:253:VAL:O	2:B:254:SER:OG	2.37	0.41
3:C:41:ILE:HD12	3:C:41:ILE:N	2.24	0.41
2:B:142:LEU:O	2:B:144:ILE:HG12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:SER:N	2:B:255:PHE:HA	2.34	0.41
3:C:123:THR:HB	3:C:124:ALA:H	1.72	0.41
1:A:167:LYS:C	1:A:169:LEU:HD13	2.41	0.41
2:B:137:TYR:O	2:B:138:PHE:HB3	2.21	0.41
1:A:58:VAL:HG11	2:B:201:TRP:CZ3	2.55	0.41
2:B:40:MET:HG3	2:B:41:ALA:H	1.85	0.41
3:C:55:ASN:N	3:C:56:SER:CB	2.82	0.41
1:A:116:ILE:CD1	1:A:133:TYR:CE2	3.01	0.41
3:C:234:LYS:HD3	3:C:237:SER:HB2	2.03	0.41
3:C:59:THR:N	3:C:60:THR:HA	2.36	0.41
1:A:210:VAL:HG12	1:A:210:VAL:O	2.21	0.41
1:A:172:VAL:HG23	1:A:174:HIS:H	1.86	0.41
2:B:122:LEU:CD1	2:B:132:MET:HG3	2.41	0.41
2:B:132:MET:SD	2:B:205:THR:HB	2.60	0.41
1:A:68:VAL:CB	2:B:73:ASP:HA	2.50	0.41
2:B:106:ALA:O	2:B:107:ALA:CB	2.69	0.41
2:B:26:ARG:HA	2:B:27:THR:CB	2.49	0.41
3:C:98:VAL:CG1	3:C:100:ASN:HA	2.36	0.41
3:C:248:TRP:O	3:C:249:THR:HB	2.21	0.41
2:B:147:SER:OG	2:B:189:SER:HB3	2.22	0.40
2:B:41:ALA:N	2:B:42:ASN:HB3	2.36	0.40
3:C:203:SER:O	3:C:205:THR:CA	2.62	0.40
1:A:67:LYS:CB	1:A:67:LYS:NZ	2.73	0.40
2:B:178:ILE:O	2:B:179:TYR:HD1	2.04	0.40
1:A:107:PHE:CD1	1:A:108:ALA:N	2.89	0.40
1:A:144:SER:HA	1:A:148:VAL:CG1	2.51	0.40
1:A:147:GLY:O	1:A:148:VAL:HG12	2.19	0.40
1:A:207:PHE:HB2	1:A:208:PHE:CA	2.51	0.40
1:A:89:TRP:O	1:A:182:MET:HE1	2.21	0.40
2:B:85:MET:O	2:B:89:THR:OG1	2.38	0.40
2:B:97:ILE:HG23	2:B:99:LYS:HB3	2.02	0.40
3:C:46:ASP:C	3:C:48:ALA:N	2.74	0.40
3:C:47:ASP:O	3:C:49:SER:N	2.55	0.40
1:A:114:ILE:HB	1:A:161:VAL:CG1	2.52	0.40
2:B:135:TYR:HD2	2:B:245:PHE:CD2	2.40	0.40
1:A:165:SER:CA	1:A:166:ASN:C	2.84	0.40
1:A:167:LYS:HB3	1:A:169:LEU:CD1	2.35	0.40
1:A:97:LYS:HB2	1:A:177:ALA:CB	2.52	0.40
1:A:92:LYS:HZ2	1:A:92:LYS:HB2	1.87	0.40
2:B:44:LEU:N	2:B:44:LEU:HD22	2.35	0.40
2:B:45:SER:HA	2:B:46:THR:HA	1.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:239:ASP:OD1	3:C:239:ASP:N	2.54	0.40
3:C:31:ILE:HG23	3:C:44:VAL:HG21	2.02	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	196/198 (99%)	124 (63%)	38 (19%)	34 (17%)	0	3
2	B	235/237 (99%)	135 (57%)	65 (28%)	35 (15%)	0	4
3	C	261/263 (99%)	175 (67%)	53 (20%)	33 (13%)	0	6
All	All	692/698 (99%)	434 (63%)	156 (22%)	102 (15%)	1	4

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	63	VAL
1	A	76	TRP
1	A	89	TRP
1	A	111	THR
1	A	114	ILE
1	A	134	ASP
1	A	162	PRO
1	A	163	PHE
1	A	165	SER
1	A	168	PRO
1	A	169	LEU
1	A	172	VAL
1	A	180	PHE
1	A	206	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	207	PHE
1	A	213	PRO
1	A	214	LYS
1	A	219	ARG
2	B	25	THR
2	B	43	VAL
2	B	45	SER
2	B	48	GLY
2	B	53	ALA
2	B	55	VAL
2	B	57	GLU
2	B	59	ALA
2	B	75	MET
2	B	80	GLN
2	B	109	VAL
2	B	116	HIS
2	B	122	LEU
2	B	177	ALA
2	B	180	THR
2	B	188	ASN
3	C	40	ILE
3	C	44	VAL
3	C	49	SER
3	C	51	LEU
3	C	55	ASN
3	C	56	SER
3	C	62	GLN
3	C	65	ASN
3	C	66	LYS
3	C	68	VAL
3	C	71	ALA
3	C	98	VAL
3	C	99	ASP
3	C	105	ALA
3	C	151	LYS
3	C	153	ALA
3	C	193	ILE
3	C	194	ASP
3	C	197	GLN
3	C	204	LEU
1	A	107	PHE
1	A	124	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	135	THR
1	A	149	ILE
1	A	164	TYR
1	A	218	SER
2	B	54	LEU
2	B	107	ALA
2	B	172	LEU
3	C	36	VAL
3	C	72	THR
3	C	119	ILE
3	C	191	PRO
1	A	108	ALA
1	A	220	ALA
2	B	26	ARG
2	B	42	ASN
2	B	74	ASP
2	B	92	SER
2	B	111	PRO
2	B	113	ASN
2	B	117	ARG
2	B	124	GLN
3	C	126	TRP
3	C	135	LYS
3	C	189	PRO
3	C	203	SER
1	A	69	ASP
1	A	170	ARG
1	A	173	ARG
2	B	47	THR
2	B	121	THR
2	B	190	PHE
3	C	196	ARG
1	A	90	ARG
2	B	52	VAL
2	B	126	PRO
2	B	137	TYR
3	C	48	ALA
3	C	208	PRO
1	A	178	LEU
2	B	40	MET
2	B	79	ALA
1	A	68	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	136	ILE
1	A	167	LYS
3	C	54	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/172 (100%)	148 (86%)	24 (14%)	4	25
2	B	208/208 (100%)	181 (87%)	27 (13%)	5	27
3	C	230/230 (100%)	205 (89%)	25 (11%)	7	33
All	All	610/610 (100%)	534 (88%)	76 (12%)	9	29

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	29	ASN
1	A	50	PHE
1	A	67	LYS
1	A	69	ASP
1	A	76	TRP
1	A	77	TYR
1	A	91	GLN
1	A	92	LYS
1	A	106	PHE
1	A	113	GLU
1	A	123	GLU
1	A	133	TYR
1	A	163	PHE
1	A	164	TYR
1	A	167	LYS
1	A	169	LEU
1	A	170	ARG
1	A	171	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	175	ASP
1	A	206	PHE
1	A	208	PHE
1	A	218	SER
1	A	219	ARG
2	B	22	TYR
2	B	24	TRP
2	B	26	ARG
2	B	37	THR
2	B	44	LEU
2	B	52	VAL
2	B	58	ARG
2	B	70	SER
2	B	75	MET
2	B	90	THR
2	B	92	SER
2	B	112	GLN
2	B	113	ASN
2	B	114	MET
2	B	115	VAL
2	B	116	HIS
2	B	120	VAL
2	B	122	LEU
2	B	123	ASP
2	B	141	SER
2	B	142	LEU
2	B	178	ILE
2	B	179	TYR
2	B	189	SER
2	B	190	PHE
2	B	201	TRP
2	B	252	LEU
3	C	39	GLU
3	C	41	ILE
3	C	42	THR
3	C	44	VAL
3	C	46	ASP
3	C	47	ASP
3	C	50	ASN
3	C	52	LEU
3	C	67	ASP
3	C	69	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	99	ASP
3	C	100	ASN
3	C	103	SER
3	C	104	MET
3	C	136	ILE
3	C	150	ARG
3	C	151	LYS
3	C	188	GLU
3	C	194	ASP
3	C	196	ARG
3	C	203	SER
3	C	204	LEU
3	C	209	HIS
3	C	239	ASP
3	C	240	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	A	174	HIS
1	A	205	ASN
2	B	129	ASN
2	B	206	HIS
3	C	50	ASN
3	C	55	ASN
3	C	102	HIS
3	C	209	HIS
3	C	213	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	118:LEU	C	119:ILE	N	0.67