

Integrative Structure Validation Report

July 22, 2024 - 04:11 PM PDT

The following software was used in the production of this report:

Python-IHM Version 1.3

MolProbity Version 4.5.2

Integrative Modeling Validation Version 1.2

PDB ID	9A0M
PDB-Dev ID	PDBDEV_00000058
Structure Title	Integrative structure of cGMP-GAFab complex
Structure Authors	Gupta R; Liu Y; Wang H; Nordyke CT; Puterbaugh RZ; Cui W; Varga K; Chu F; Ke H; Vashisth H; Cote RH

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

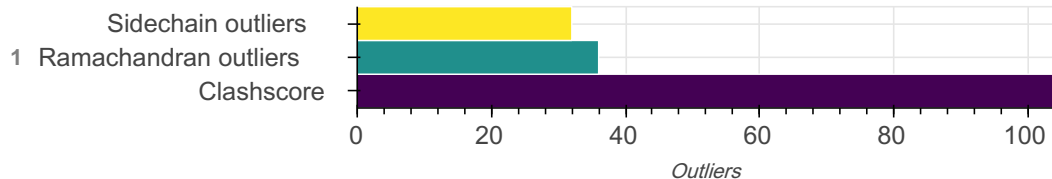
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

List of references used to build this report is available [here](#).

Overall quality

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis



Ensemble information ?

This entry consists of 0 distinct ensemble(s).

Summary ?

This entry consists of 1 unique models, with 4 subunits in each model. A total of 3 datasets or restraints were used to build this entry. Each model is represented by 2 rigid bodies and 2 flexible or non-rigid units.

Entry composition ?

There is 1 unique type of models in this entry. This model is titled None/Best scoring model.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	GAFab	A	A	399
1	2	1	GAFab	B	B	399
1	3	2	GUANOSINE-3',5'-MONOPHOSPHATE	C	A	Not available
1	4	2	GUANOSINE-3',5'-MONOPHOSPHATE	D	B	Not available

Datasets used for modeling ?

There are 3 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	PRIDE	PXD020817
2	Experimental model	PDB	6X88

ID	Dataset type	Database name	Data access code
3	Experimental model	PDB	6MZB

Representation ?

This entry has only one representation and includes 2 rigid bodies and 2 flexible units

Chain ID	Rigid bodies	Non-rigid segments
C	None-None	-
D	None-None	-
A	-	1-399
B	-	1-399

Methodology and software ?

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	None	None	None	None	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Integrative Modeling Platform (IMP)	Not available	integrative model building	https://integrativemodeling.org
2	Modeller	Not available	model building	https://salilab.org/modeller/

Data quality ?

Crosslinking-MS

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobability analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers ?

Bond length outliers can not be evaluated for this model

Standard geometry: angle outliers ?

There are 304 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found [here](#).

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	85.27	1
C-N-CA	121.70	155.86	1
CA-C-N	116.20	80.66	1
C-N-CA	121.70	147.57	1
C-N-CA	121.70	146.44	1
C-N-CA	121.70	146.09	1
C-N-CA	121.70	145.07	1
C-N-CA	121.70	98.53	1
CA-CB-CG	113.80	101.41	1
C-N-CA	121.70	99.77	1
N-CA-C	112.10	142.48	1
N-CA-C	112.10	142.28	1
C-N-CA	121.70	143.35	1
C-N-CA	121.70	101.11	1
CA-C-O	120.80	101.53	1
C-N-CA	121.70	141.73	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	141.06	1
C-N-CA	121.70	102.96	1
C-N-CA	121.70	103.11	1
CA-C-O	120.80	103.29	1
C-N-CA	121.70	140.18	1
N-CA-C	111.00	139.73	1
CA-C-O	120.80	138.24	1
N-CA-C	111.00	139.71	1
CA-CB-CG	113.80	103.85	1
C-N-CA	121.70	103.83	1
C-CA-CB	110.10	91.25	1
C-N-CA	121.70	139.54	1
CA-CB-CG	113.80	104.04	1
C-N-CA	121.70	139.02	1
CA-C-N	116.20	135.18	1
N-CA-C	111.00	84.75	1
CA-C-N	116.20	134.87	1
CA-C-N	116.20	134.79	1
CA-C-N	116.20	134.57	1
C-CA-CB	110.10	92.76	1
CA-CB-CG	114.10	96.11	1
N-CA-C	111.00	85.84	1
O-C-N	123.00	108.74	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	137.59	1
C-CA-CB	110.10	93.49	1
CA-CB-CG	113.80	105.10	2
C-CA-CB	110.10	93.65	1
N-CA-C	111.00	86.84	1
O-C-N	123.00	109.24	1
CA-CB-CG	113.80	105.54	1
CA-C-O	120.80	106.81	1
N-CA-C	111.00	133.33	1
C-N-CA	121.70	107.96	1
C-N-CA	121.70	135.43	1
C-N-CA	121.70	108.11	1
CA-C-N	116.20	101.16	1
CB-CG-CD	112.60	99.83	1
CG-SD-CE	100.90	84.41	1
C-N-CA	121.70	135.18	1
CA-CB-CG	113.80	106.35	1
CA-CB-CG	112.60	105.17	1
C-CA-CB	110.10	124.20	1
N-CA-C	111.00	131.51	1
N-CA-C	111.00	131.42	1
C-N-CA	121.70	134.61	1
CA-C-O	120.80	132.99	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	101.93	1
CA-C-N	116.20	102.00	1
CA-CB-CG	113.80	106.72	1
N-CA-C	112.10	129.64	1
CA-CB-CG	113.90	101.37	1
CA-CB-CG	113.80	106.94	1
C-N-CA	121.70	133.98	1
N-CA-C	111.00	129.77	1
CA-C-N	116.20	129.59	1
N-CA-C	111.00	92.26	1
CA-CB-CG	112.60	105.92	1
CA-C-N	116.90	126.84	1
N-CA-C	112.10	128.62	1
CA-CB-CG	113.80	107.22	1
C-N-CA	121.70	109.88	1
CA-CB-CG	113.80	107.27	1
C-CA-CB	110.10	97.74	1
CA-CB-CG	113.90	102.28	1
CA-CB-CG	113.80	107.37	1
CA-CB-CG	113.90	102.35	1
C-N-CA	121.70	110.18	1
CA-CB-CG	113.80	107.42	1
CA-CB-CG	113.90	102.49	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	98.11	1
CA-CB-CG	113.80	107.51	1
C-CA-CB	110.10	98.22	1
CA-CB-CG	112.60	106.44	1
C-N-CA	121.70	110.67	1
C-CA-CB	110.10	98.47	1
C-CA-CB	110.10	98.49	1
C-CA-CB	110.50	101.34	1
CA-C-N	116.90	126.01	1
C-N-CA	121.70	110.81	1
CA-C-O	120.80	110.58	1
O-C-N	123.00	113.39	1
CA-C-N	116.90	125.77	1
C-N-CA	121.70	132.32	1
O-C-N	123.00	132.41	1
CB-CG-CD	112.60	102.64	1
C-CA-CB	110.10	98.99	1
CA-CB-CG	112.60	106.76	1
O-C-N	123.00	113.68	1
C-N-CA	121.70	132.13	1
C-CA-CB	110.10	99.09	1
CA-CB-CG	112.60	106.81	2
CA-CB-CG	112.60	106.82	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	106.83	1
CA-CB-CG	113.90	103.57	1
C-N-CA	121.70	111.38	1
CA-CB-CG	112.60	106.88	1
CA-C-N	116.20	104.81	1
C-N-CA	121.70	131.94	1
CA-CB-CG	114.10	125.43	1
CA-C-O	120.80	111.42	1
CA-CB-CG	113.90	103.98	1
C-N-CA	121.70	111.83	1
CA-CB-CG	112.60	107.12	1
C-CA-CB	110.10	99.72	1
CA-CB-CG	112.60	107.15	1
CA-CB-CG	113.80	108.36	1
CA-CB-CG	112.60	107.17	1
C-CA-CB	111.60	100.77	1
C-N-CA	121.70	111.99	1
N-CA-C	111.00	126.09	1
N-CA-CB	110.50	119.65	1
CA-CB-CG	112.60	107.24	1
C-N-CA	121.70	112.11	1
CA-C-O	120.80	111.75	1
C-CA-CB	110.10	100.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	131.48	1
N-CA-C	111.00	125.83	1
C-CA-CB	110.10	100.05	1
CA-CB-CG	113.80	108.53	1
O-C-N	123.00	131.41	1
N-CA-C	111.00	125.65	1
C-CA-CB	110.10	100.17	1
C-N-CA	121.70	131.08	1
CA-CB-CG	112.60	107.39	1
C-N-CA	121.70	112.35	1
C-CA-CB	110.10	100.25	1
C-CA-CB	110.10	100.26	1
C-CA-CB	110.50	102.73	1
C-N-CA	121.70	131.01	1
CA-C-N	116.20	105.87	1
CD-NE-CZ	124.40	117.18	1
C-N-CA	121.70	112.45	1
CA-CB-CG	112.60	107.47	1
CA-CB-CG	113.80	108.67	1
N-CA-C	111.00	96.68	1
C-CA-CB	110.10	100.38	1
CA-CB-CG	112.60	107.50	1
CA-CB-CG	113.80	108.72	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	126.34	1
CA-C-O	120.80	112.19	1
C-N-CA	121.70	130.77	1
C-N-CA	121.70	130.71	1
N-CA-C	111.00	124.92	1
CA-CB-CG	112.60	107.63	1
CA-CB-CG	112.60	107.65	2
CA-CB-CG	113.80	108.85	1
CA-CB-CG	112.60	107.66	1
N-CA-C	111.00	97.17	1
CG-SD-CE	100.90	90.04	1
C-N-CA	121.70	130.56	1
CA-CB-CG	112.60	107.68	1
CA-CB-CG	113.80	108.89	2
C-N-CA	121.70	112.89	1
CA-CB-CG	112.60	107.71	1
C-CA-CB	110.10	100.87	1
CA-CB-CG	113.80	108.95	1
CA-C-N	116.20	125.89	1
C-N-CA	121.70	113.04	1
N-CA-C	111.00	124.46	1
CA-CB-CG	112.60	107.83	3
CA-C-O	120.80	112.77	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	101.13	1
CA-C-N	116.20	125.64	1
C-N-CA	121.70	130.19	1
CA-CB-CG	113.80	109.09	1
CA-CB-CG	113.90	105.44	1
N-CA-C	111.00	97.87	1
CA-CB-CG	113.90	105.47	1
C-CA-CB	110.10	101.21	1
CA-CB-CG	112.60	107.93	1
CA-CB-CG	112.60	107.94	3
N-CA-C	111.00	124.05	1
N-CA-CB	110.50	118.40	1
CA-CB-CG	113.80	109.16	1
C-N-CA	121.70	130.05	1
C-N-CA	121.70	130.04	1
C-N-CA	121.70	113.39	1
C-N-CA	121.70	113.40	1
N-CA-CB	110.50	118.30	1
CA-CB-CG	113.90	105.69	1
C-N-CA	121.70	129.90	1
CA-CB-CG	113.80	109.27	1
N-CA-C	111.00	98.37	1
CA-C-O	120.80	128.42	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.77	1
N-CA-C	111.00	98.46	1
CA-C-N	116.20	125.14	1
CA-CB-CG	112.60	108.13	1
CD2-NE2-CE1	109.00	104.53	1
CB-CG-CD	112.60	105.01	1
CA-CB-CG	112.60	108.14	1
CD2-NE2-CE1	109.00	104.54	1
CA-C-O	120.80	113.25	1
CD2-NE2-CE1	109.00	104.56	1
N-CA-C	111.00	123.42	1
CD2-NE2-CE1	109.00	104.57	2
CD2-NE2-CE1	109.00	104.58	2
N-CA-CB	110.50	118.01	1
CD2-NE2-CE1	109.00	104.59	1
CD2-NE2-CE1	109.00	104.60	2
CD2-NE2-CE1	109.00	104.61	2
CA-C-O	120.80	113.35	1
CA-C-N	116.90	123.45	1
CD2-NE2-CE1	109.00	104.63	1
N-CA-C	111.00	123.21	1
CD2-NE2-CE1	109.00	104.64	1
N-CA-CB	110.50	117.88	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	113.43	1
CA-CB-CG	112.60	108.27	1
N-CA-C	111.00	123.13	1
CA-C-N	116.20	124.86	1
N-CA-CB	110.50	117.85	1
CA-CB-CG	112.60	108.28	1
CA-C-N	116.20	124.83	1
CA-CB-CG	112.60	108.29	1
C-CA-CB	110.10	101.91	1
N-CA-CB	111.50	118.82	1
C-CA-CB	111.60	103.00	1
CB-CG-CD	112.60	105.29	1
C-CA-CB	111.60	103.01	1
CD2-NE2-CE1	109.00	104.70	1
N-CA-C	111.00	98.98	1
N-CA-C	111.00	99.01	1
CB-CG-CD	112.60	105.32	1
CD2-NE2-CE1	109.00	104.72	1
C-N-CA	121.70	129.40	1
O-C-N	123.00	116.16	1
CA-C-N	116.20	124.74	1
C-CA-CB	110.10	101.99	1
CA-CB-CG	112.60	108.34	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	122.88	1
CA-CB-CG	112.60	108.37	2
CB-CG-CD	112.60	105.41	1
C-N-CA	121.70	129.31	1
CA-C-O	120.80	127.95	1
C-N-CD	125.00	107.77	1
C-CA-CB	111.60	103.20	1
CA-CB-CG	112.60	108.40	1
N-CA-C	111.00	122.75	1
C-N-CA	121.70	129.25	1
N-CA-C	113.30	125.45	1
CA-C-N	116.20	124.58	1
C-N-CA	121.70	129.21	2
N-CA-CB	110.50	117.60	1
C-CA-CB	110.10	102.17	1
CA-CB-CG	112.60	108.43	1
C-CA-CB	110.10	102.18	2
CA-CB-CG	112.60	108.44	1
C-N-CD	125.00	107.98	1
C-CA-CB	110.10	102.21	1
N-CA-CB	110.50	117.52	1
CA-CB-CG	113.90	106.46	1
CA-CB-CG	113.90	106.47	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	107.98	1
CA-CB-CG2	110.50	103.53	1
C-CA-CB	110.10	102.32	1
CA-C-N	116.20	124.37	1
CG-SD-CE	100.90	91.91	1
C-N-CA	121.70	114.37	1
CA-CB-CG	113.90	106.58	1
N-CA-C	111.00	99.63	1
N-CA-C	113.30	125.05	1
C-N-CA	121.70	128.99	1
N-CA-CB	110.50	117.38	1
CB-CG-CD	112.60	105.72	1
CA-CB-CG2	110.50	103.63	1
CD-NE-CZ	124.40	118.74	1
C-N-CA	121.70	128.98	1
CA-CB-CG	112.60	108.56	1
CD-NE-CZ	124.40	118.75	1
N-CA-C	111.00	99.72	1
CA-C-N	116.20	124.25	1
N-CA-C	111.00	99.79	1

Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	Clash score	Number of clashes
1	104.67	1365

All 1365 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:254:LYS:C	B:254:LYS:CA	1.590
1	A:254:LYS:C	A:254:LYS:CA	1.568
1	B:396:ASP:CA	B:396:ASP:N	1.537
1	A:122:THR:HG23	C:1:35G:C2	1.506
1	B:110:PHE:CZ	D:1:35G:O2'	1.364
1	B:111:SER:O	D:1:35G:H4'	1.334
1	B:143:LEU:CD2	D:1:35G:O6	1.333
1	B:396:ASP:N	B:397:ILE:N	1.287
1	B:143:LEU:HD21	D:1:35G:O6	1.267
1	A:122:THR:HG21	C:1:35G:C6	1.259
1	A:115:ASP:OD2	C:1:35G:C1'	1.258
1	A:115:ASP:OD2	C:1:35G:H1'	1.191
1	A:122:THR:CG2	C:1:35G:N1	1.182
1	A:115:ASP:CG	C:1:35G:N3	1.169
1	A:115:ASP:OD2	C:1:35G:N3	1.166
1	A:122:THR:CG2	C:1:35G:C2	1.140
1	B:188:MET:HG2	B:214:ILE:HD11	1.134
1	B:396:ASP:N	B:397:ILE:H	1.134
1	B:128:ILE:HG21	B:163:LEU:HD13	1.133
1	A:342:LYS:H	A:342:LYS:HD2	1.132

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:88:ILE:N	D:1:35G:O2P	1.123
1	A:232:LYS:HB2	A:260:GLU:HG2	1.121
1	A:181:ILE:HG23	A:367:ILE:HD11	1.115
1	A:340:ASN:HD21	A:343:GLU:HB2	1.104
1	B:289:CYS:HA	B:320:LYS:HE2	1.099
1	A:338:ILE:HG22	A:372:THR:HG23	1.093
1	A:126:MET:HE1	A:156:GLU:HA	1.078
1	B:230:MET:HA	B:230:MET:HE2	1.077
1	A:395:LYS:HB2	B:391:LEU:HD23	1.070
1	B:240:TRP:HB2	B:243:ARG:HD2	1.068
1	B:257:ASP:HB2	B:301:ASN:HA	1.068
1	A:64:THR:HG23	A:67:SER:H	1.064
1	B:286:ASP:HA	B:291:ILE:HD11	1.060
1	B:181:ILE:HD13	B:363:TYR:HB3	1.055
1	A:115:ASP:HB2	C:1:35G:O4'	1.033
1	A:115:ASP:OD1	C:1:35G:N3	1.032
1	A:339:VAL:HG11	A:342:LYS:HA	1.020
1	B:340:ASN:HD21	B:343:GLU:HB2	1.020
1	A:122:THR:HG21	A:143:LEU:HD23	1.019
1	B:392:GLU:HG3	B:398:ALA:HB3	1.019
1	A:195:LYS:HD2	A:209:LYS:HG2	1.011
1	A:294:LEU:HD11	A:307:MET:HE1	1.011
1	A:395:LYS:HG2	A:398:ALA:HB2	1.000

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:257:ASP:HB2	A:301:ASN:HA	0.996
1	A:288:TRP:HE3	A:320:LYS:HA	0.995
1	A:289:CYS:HA	A:320:LYS:HE2	0.992
1	B:87:GLY:HA2	B:111:SER:HB3	0.988
1	B:319:GLN:HG2	B:330:ILE:H	0.985
1	B:110:PHE:CE1	D:1:35G:O2'	0.970
1	A:288:TRP:CE3	A:320:LYS:HA	0.967
1	B:321:GLY:HA3	B:328:TRP:CE3	0.959
1	A:294:LEU:HA	A:315:TYR:CE1	0.956
1	A:395:LYS:HG2	B:391:LEU:HB2	0.956
1	B:200:LEU:HD12	B:385:TYR:HD1	0.953
1	B:58:THR:HG21	B:61:LEU:HD11	0.951
1	A:82:PHE:HZ	A:114:LEU:HB2	0.950
1	A:388:MET:HA	A:391:LEU:CD1	0.950
1	A:118:THR:HG23	A:120:TYR:H	0.946
1	A:87:GLY:HA2	A:111:SER:HB3	0.943
1	B:225:VAL:HG12	B:267:ILE:HG12	0.940
1	A:297:TYR:CD1	A:314:GLU:HB2	0.939
1	B:291:ILE:HB	B:318:PHE:CE1	0.939
1	A:175:THR:HG23	B:175:THR:HG21	0.936
1	B:392:GLU:HG3	B:398:ALA:CB	0.936
1	A:339:VAL:CG1	A:342:LYS:HA	0.934
1	A:187:GLN:HA	A:187:GLN:HE21	0.931

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:267:ILE:CD1	A:279:VAL:HG22	0.923
1	A:319:GLN:HB3	A:330:ILE:HB	0.919
1	A:388:MET:HA	A:391:LEU:HD12	0.918
1	B:313:ASP:HB2	B:315:TYR:CE2	0.918
1	A:181:ILE:HG23	A:367:ILE:CD1	0.917
1	B:95:THR:CB	B:97:LYS:HG2	0.917
1	A:111:SER:O	C:1:35G:H4'	0.915
1	A:122:THR:HG21	C:1:35G:N1	0.913
1	B:294:LEU:HB3	B:295:PRO:HD3	0.913
1	A:122:THR:CG2	C:1:35G:C6	0.912
1	A:319:GLN:HG2	A:330:ILE:H	0.910
1	B:297:TYR:CD2	B:314:GLU:HB2	0.910
1	B:235:GLU:HB2	B:257:ASP:CA	0.902
1	B:319:GLN:HB2	B:322:PRO:HG3	0.900
1	A:95:THR:HB	A:97:LYS:HG2	0.897
1	A:95:THR:CB	A:97:LYS:HG2	0.894
1	B:339:VAL:HG11	B:342:LYS:HA	0.892
1	A:371:LEU:HD13	A:375:LEU:HD23	0.891
1	A:294:LEU:HB3	A:295:PRO:HD3	0.886
1	A:128:ILE:CD1	A:163:LEU:HD13	0.885
1	B:111:SER:O	D:1:35G:C4'	0.885
1	A:321:GLY:HA3	A:328:TRP:CE3	0.884
1	B:319:GLN:HG2	B:330:ILE:N	0.884

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:291:ILE:HD13	A:318:PHE:CE1	0.883
1	B:159:PHE:CE2	B:163:LEU:HD11	0.882
1	A:9:PHE:CG	B:161:LYS:HD2	0.880
1	B:339:VAL:CG1	B:342:LYS:HA	0.879
1	A:340:ASN:ND2	A:343:GLU:HB2	0.877
1	A:98:PHE:CD1	A:128:ILE:HG22	0.873
1	A:228:LEU:HD22	A:261:VAL:HG13	0.872
1	A:82:PHE:CZ	A:114:LEU:HB2	0.871
1	B:87:GLY:CA	B:111:SER:HB3	0.871
1	A:395:LYS:CG	B:391:LEU:HB2	0.869
1	B:304:ILE:HG12	B:336:LEU:HD12	0.869
1	A:319:GLN:HB2	A:322:PRO:HD3	0.868
1	B:294:LEU:HA	B:315:TYR:CE1	0.868
1	A:122:THR:HG23	C:1:35G:N1	0.867
1	B:200:LEU:HD12	B:385:TYR:CD1	0.866
1	B:289:CYS:HA	B:320:LYS:CE	0.866
1	A:338:ILE:HA	A:372:THR:CG2	0.864
1	B:286:ASP:HA	B:291:ILE:CD1	0.863
1	A:257:ASP:HB2	A:301:ASN:CA	0.862
1	B:321:GLY:HA3	B:328:TRP:HE3	0.862
1	B:228:LEU:HD12	B:261:VAL:HG13	0.861
1	A:394:ARG:HE	B:395:LYS:HD3	0.860
1	B:251:LYS:H	B:251:LYS:HE2	0.859

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:317:THR:HG22	B:318:PHE:O	0.859
1	A:256:PRO:HB3	A:297:TYR:CD1	0.857
1	B:289:CYS:CA	B:320:LYS:HE2	0.856
1	A:115:ASP:CB	C:1:35G:O4'	0.854
1	A:381:ASN:O	A:384:THR:HG22	0.854
1	B:319:GLN:HB3	B:330:ILE:HB	0.854
1	A:187:GLN:HG2	A:217:TYR:CZ	0.853
1	A:130:ILE:HD13	A:170:LEU:HD12	0.851
1	A:255:THR:HB	A:256:PRO:HD2	0.850
1	B:233:GLU:HB3	B:344:GLU:OE2	0.848
1	B:340:ASN:ND2	B:343:GLU:HB2	0.847
1	B:367:ILE:HG23	B:368:ILE:HD12	0.845
1	A:87:GLY:CA	A:111:SER:HB3	0.844
1	B:319:GLN:C	B:330:ILE:HD12	0.844
1	A:33:LEU:HD21	A:162:TYR:CB	0.843
1	B:333:VAL:HG22	B:352:TYR:CD1	0.843
1	A:175:THR:HG23	B:175:THR:CG2	0.842
1	B:241:PRO:C	B:242:ILE:HD13	0.841
1	A:288:TRP:O	A:291:ILE:HG22	0.840
1	A:398:ALA:HB2	B:391:LEU:HG	0.840
1	A:319:GLN:CB	A:330:ILE:HB	0.839
1	A:336:LEU:CD2	A:368:ILE:HG22	0.838
1	B:257:ASP:HB2	B:301:ASN:CA	0.838

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:337:PRO:O	B:372:THR:HG21	0.838
1	B:228:LEU:CD2	B:347:GLY:HA2	0.837
1	A:337:PRO:O	A:372:THR:HG21	0.835
1	A:391:LEU:HD13	B:398:ALA:HB1	0.835
1	A:115:ASP:CG	C:1:35G:C1'	0.834
1	A:321:GLY:HA3	A:328:TRP:CZ3	0.833
1	B:110:PHE:HZ	D:1:35G:O2'	0.833
1	A:319:GLN:HG2	A:330:ILE:N	0.832
1	B:256:PRO:HB3	B:297:TYR:CD2	0.829
1	B:320:LYS:HG2	B:352:TYR:CZ	0.829
1	B:101:ILE:HG22	B:125:MET:O	0.826
1	B:143:LEU:HD21	D:1:35G:C6	0.826
1	A:298:VAL:HG21	A:348:VAL:HG13	0.824
1	B:319:GLN:O	B:320:LYS:HD2	0.824
1	A:122:THR:CG2	A:143:LEU:HD23	0.823
1	B:73:LEU:HD23	B:74:VAL:N	0.822
1	B:166:ILE:O	B:169:VAL:HG12	0.822
1	B:338:ILE:HA	B:372:THR:CG2	0.822
1	A:232:LYS:CB	A:260:GLU:HG2	0.821
1	A:57:ALA:HB2	A:81:VAL:HG22	0.819
1	B:26:VAL:HG13	B:166:ILE:HD11	0.818
1	A:115:ASP:OD2	C:1:35G:C4	0.817
1	B:143:LEU:CD2	D:1:35G:C6	0.815

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:126:MET:HE3	A:156:GLU:HG2	0.814
1	A:294:LEU:HG	A:315:TYR:CZ	0.814
1	B:115:ASP:O	B:118:THR:HG22	0.814
1	B:235:GLU:HB2	B:257:ASP:CB	0.814
1	A:319:GLN:O	A:330:ILE:HD12	0.812
1	A:179:TYR:CE1	B:178:LEU:HB3	0.810
1	B:391:LEU:HD13	B:392:GLU:N	0.810
1	A:92:VAL:HG12	A:129:PRO:HG3	0.809
1	A:195:LYS:HD2	A:209:LYS:CG	0.808
1	A:398:ALA:CB	B:391:LEU:HG	0.808
1	B:10:GLU:O	B:13:THR:HG22	0.807
1	A:174:HIS:O	A:178:LEU:HD13	0.805
1	A:115:ASP:O	A:118:THR:HG22	0.804
1	A:338:ILE:CG2	A:372:THR:HG23	0.804
1	B:185:ARG:HD3	B:367:ILE:HA	0.804
1	B:287:HIS:CD2	B:290:LEU:HD23	0.803
1	B:294:LEU:CD1	B:333:VAL:HG11	0.803
1	A:395:LYS:CB	B:391:LEU:HD23	0.801
1	B:320:LYS:HG2	B:352:TYR:CE2	0.800
1	A:195:LYS:CD	A:209:LYS:HG2	0.799
1	A:339:VAL:HG13	A:344:GLU:O	0.798
1	B:328:TRP:CZ3	B:330:ILE:HD11	0.798
1	B:181:ILE:CD1	B:363:TYR:HB3	0.797

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:319:GLN:CB	B:330:ILE:HB	0.797
1	B:26:VAL:O	B:29:THR:HG22	0.796
1	A:235:GLU:HB3	A:257:ASP:OD1	0.795
1	A:292:SER:HB3	A:320:LYS:NZ	0.795
1	A:341:LYS:O	A:343:GLU:HG3	0.795
1	B:91:TRP:CE2	B:95:THR:HG21	0.794
1	B:267:ILE:HG22	B:279:VAL:HG22	0.794
1	A:298:VAL:HG21	A:348:VAL:CG1	0.793
1	B:288:TRP:CE3	B:320:LYS:HA	0.792
1	A:234:LYS:O	A:257:ASP:HB3	0.789
1	A:257:ASP:CB	A:301:ASN:HA	0.788
1	A:98:PHE:HD1	A:128:ILE:HG22	0.787
1	B:319:GLN:HB2	B:322:PRO:CG	0.786
1	B:155:ASP:O	B:158:VAL:HG12	0.784
1	A:10:GLU:O	A:13:THR:HG22	0.781
1	A:336:LEU:HD22	A:368:ILE:HG22	0.780
1	B:33:LEU:CD1	B:37:LEU:HG	0.777
1	B:234:LYS:O	B:257:ASP:HB3	0.777
1	B:336:LEU:HD21	B:368:ILE:HG21	0.776
1	A:254:LYS:C	A:254:LYS:N	0.774
1	B:130:ILE:HG21	B:170:LEU:HD13	0.774
1	B:177:TYR:HA	B:180:ASN:ND2	0.772
1	B:292:SER:O	B:315:TYR:HB3	0.772

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:204:GLU:HG3	B:265:LYS:HE2	0.771
1	B:297:TYR:CB	B:315:TYR:HE1	0.771
1	A:8:LEU:HD23	B:8:LEU:HD23	0.769
1	B:57:ALA:HB2	B:81:VAL:HG22	0.769
1	B:185:ARG:HD2	B:370:THR:OG1	0.769
1	B:297:TYR:HD2	B:314:GLU:HB2	0.769
1	B:391:LEU:O	B:391:LEU:HD22	0.768
1	B:392:GLU:CG	B:398:ALA:HB3	0.766
1	B:231:THR:C	B:232:LYS:HD2	0.765
1	A:48:ARG:HH22	A:81:VAL:HG21	0.764
1	B:67:SER:HB2	B:72:ASN:HD21	0.764
1	A:22:MET:HE1	A:170:LEU:HD22	0.763
1	B:200:LEU:CD1	B:385:TYR:HB2	0.760
1	A:130:ILE:HD13	A:170:LEU:CD1	0.758
1	A:155:ASP:O	A:158:VAL:HG12	0.758
1	A:294:LEU:CD1	A:307:MET:HE1	0.758
1	A:50:ARG:HH22	A:359:PRO:HB2	0.758
1	B:254:LYS:C	B:254:LYS:N	0.758
1	B:392:GLU:CD	B:399:GLN:HB3	0.758
1	A:104:VAL:HG22	A:123:VAL:O	0.757
1	A:395:LYS:CD	B:391:LEU:HB2	0.755
1	B:255:THR:HB	B:256:PRO:HD2	0.755
1	A:163:LEU:O	A:166:ILE:HG22	0.754

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:388:MET:HE1	A:399:GLN:N	0.754
1	B:76:PRO:HG3	B:358:LYS:HD3	0.752
1	A:7:ILE:HG23	A:32:ARG:HH11	0.751
1	B:38:ALA:O	B:145:LYS:HD2	0.751
1	B:308:MET:HA	B:332:ASN:OD1	0.751
1	A:289:CYS:CA	A:320:LYS:HE2	0.750
1	A:388:MET:SD	A:399:GLN:HA	0.750
1	B:319:GLN:HB3	B:330:ILE:CB	0.750
1	B:388:MET:O	B:391:LEU:HB3	0.750
1	A:128:ILE:HD13	A:163:LEU:HD13	0.749
1	B:95:THR:HB	B:97:LYS:HG2	0.749
1	A:314:GLU:HB3	A:315:TYR:CD1	0.748
1	A:380:LEU:HD22	B:197:PHE:O	0.748
1	B:36:LEU:CD2	B:158:VAL:HG21	0.748
1	B:222:ARG:HG3	B:328:TRP:CZ3	0.748
1	B:228:LEU:HD23	B:347:GLY:HA2	0.748
1	A:37:LEU:O	A:37:LEU:HD23	0.747
1	A:197:PHE:HA	B:380:LEU:HD22	0.745
1	A:80:THR:HG21	A:114:LEU:HD23	0.744
1	A:313:ASP:HB2	A:315:TYR:CE2	0.744
1	B:92:VAL:CG1	B:129:PRO:HD3	0.744
1	B:339:VAL:HG13	B:344:GLU:O	0.744
1	A:185:ARG:HB3	A:367:ILE:HG23	0.743

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:172:ASN:O	A:175:THR:HG22	0.742
1	A:291:ILE:HD13	A:318:PHE:HE1	0.739
1	B:181:ILE:HD13	B:363:TYR:CB	0.739
1	B:228:LEU:HD12	B:261:VAL:CG1	0.739
1	A:126:MET:HE1	A:156:GLU:CA	0.738
1	A:267:ILE:HD13	A:279:VAL:HG22	0.738
1	A:291:ILE:HG21	A:318:PHE:CE1	0.738
1	B:292:SER:HB3	B:320:LYS:NZ	0.737
1	B:319:GLN:HB3	B:330:ILE:CG1	0.737
1	B:380:LEU:HG	B:380:LEU:O	0.736
1	A:304:ILE:HG13	A:336:LEU:HG	0.734
1	A:37:LEU:HD22	A:39:ALA:HB2	0.733
1	A:254:LYS:C	A:254:LYS:CB	0.733
1	A:319:GLN:O	A:320:LYS:HD2	0.733
1	A:319:GLN:H	A:322:PRO:HG3	0.733
1	A:168:LEU:HD23	B:168:LEU:HD23	0.732
1	B:56:VAL:O	B:81:VAL:HG13	0.732
1	A:319:GLN:CG	A:330:ILE:HB	0.731
1	B:299:ALA:O	B:345:ILE:HD12	0.730
1	B:204:GLU:CG	B:265:LYS:HE2	0.729
1	A:48:ARG:NH2	A:81:VAL:HG21	0.728
1	B:114:LEU:O	B:114:LEU:HD13	0.728
1	B:58:THR:HG21	B:61:LEU:CD1	0.726

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:292:SER:HA	A:316:PHE:O	0.725
1	B:204:GLU:HG3	B:265:LYS:CE	0.725
1	A:7:ILE:HG23	A:32:ARG:NH1	0.724
1	B:392:GLU:OE1	B:399:GLN:HB3	0.724
1	B:304:ILE:HG23	B:336:LEU:CD1	0.723
1	B:395:LYS:C	B:397:ILE:H	0.722
1	A:289:CYS:HA	A:320:LYS:CE	0.721
1	B:233:GLU:O	B:234:LYS:HG3	0.721
1	B:36:LEU:HD23	B:158:VAL:HG21	0.720
1	B:104:VAL:HG12	B:123:VAL:O	0.720
1	A:55:GLU:OE1	A:81:VAL:HG11	0.718
1	A:97:LYS:HB3	A:99:PHE:CD2	0.718
1	A:330:ILE:CD1	A:352:TYR:HB3	0.717
1	A:159:PHE:CZ	A:163:LEU:HD11	0.716
1	A:179:TYR:CD1	B:178:LEU:HB3	0.716
1	B:118:THR:HG23	B:120:TYR:H	0.716
1	B:214:ILE:HD12	B:217:TYR:HD2	0.716
1	B:291:ILE:HB	B:318:PHE:HE1	0.716
1	A:23:GLU:CG	A:59:ARG:HH21	0.715
1	A:126:MET:CE	A:156:GLU:HG2	0.715
1	A:181:ILE:CG2	A:367:ILE:HD11	0.715
1	B:76:PRO:O	B:79:GLU:HG2	0.715
1	A:391:LEU:HD13	B:398:ALA:CB	0.714

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:204:GLU:HG3	B:265:LYS:NZ	0.714
1	B:254:LYS:CE	B:254:LYS:HA	0.714
1	B:319:GLN:CG	B:330:ILE:HB	0.714
1	B:319:GLN:HB2	B:322:PRO:HD3	0.714
1	A:80:THR:HG21	A:114:LEU:CD2	0.713
1	B:33:LEU:O	B:33:LEU:HD13	0.713
1	B:254:LYS:HA	B:254:LYS:NZ	0.713
1	A:118:THR:HG23	A:120:TYR:N	0.712
1	A:319:GLN:HB3	A:330:ILE:CB	0.712
1	A:319:GLN:N	A:322:PRO:HG3	0.712
1	A:395:LYS:HB2	B:391:LEU:CD2	0.712
1	B:97:LYS:HB3	B:99:PHE:CE2	0.712
1	B:301:ASN:HD21	B:303:PHE:HB2	0.712
1	B:174:HIS:O	B:178:LEU:HD13	0.711
1	A:304:ILE:CD1	A:336:LEU:HG	0.710
1	A:319:GLN:HG2	A:330:ILE:CA	0.710
1	B:231:THR:O	B:232:LYS:HD2	0.710
1	B:310:ALA:O	B:317:THR:HB	0.710
1	B:342:LYS:CD	B:342:LYS:H	0.710
1	B:395:LYS:O	B:397:ILE:HG13	0.710
1	B:163:LEU:O	B:166:ILE:HG22	0.709
1	A:33:LEU:HD21	A:162:TYR:CG	0.708
1	A:50:ARG:O	A:53:ILE:HG22	0.708

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:251:LYS:CE	B:251:LYS:H	0.708
1	A:258:GLY:N	A:300:GLU:HB3	0.707
1	A:380:LEU:HG	A:380:LEU:O	0.707
1	A:97:LYS:HB3	A:99:PHE:CE2	0.705
1	A:319:GLN:C	A:320:LYS:HD2	0.705
1	B:214:ILE:HD12	B:217:TYR:CD2	0.705
1	A:195:LYS:HE2	A:213:THR:OG1	0.703
1	A:395:LYS:CE	B:391:LEU:HB2	0.703
1	A:201:THR:HG22	A:202:ASP:H	0.702
1	B:128:ILE:CG2	B:163:LEU:HD13	0.702
1	B:257:ASP:N	B:301:ASN:HB2	0.702
1	A:141:MET:SD	C:1:35G:N7	0.701
1	B:46:ILE:HG12	B:59:ARG:HB2	0.700
1	B:188:MET:HG2	B:214:ILE:CD1	0.700
1	A:92:VAL:HA	A:97:LYS:HB2	0.699
1	B:230:MET:CE	B:230:MET:HA	0.699
1	A:122:THR:HG21	C:1:35G:C5	0.698
1	B:254:LYS:C	B:254:LYS:CB	0.698
1	B:257:ASP:H	B:301:ASN:HB2	0.698
1	A:189:LEU:HD21	A:370:THR:CG2	0.697
1	A:228:LEU:HD22	A:261:VAL:CG1	0.697
1	A:266:ILE:HD13	A:287:HIS:NE2	0.697
1	A:92:VAL:CG1	A:129:PRO:HG3	0.696

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:126:MET:CE	A:156:GLU:HA	0.696
1	B:60:LEU:C	B:61:LEU:HD22	0.696
1	B:82:PHE:HZ	B:114:LEU:CB	0.696
1	A:115:ASP:CG	C:1:35G:C4	0.695
1	A:297:TYR:CB	A:315:TYR:HE1	0.695
1	B:286:ASP:CA	B:291:ILE:HD11	0.695
1	A:256:PRO:HA	A:301:ASN:ND2	0.694
1	A:256:PRO:HB3	A:297:TYR:HD1	0.693
1	A:295:PRO:O	A:298:VAL:HG22	0.692
1	A:191:TRP:CE3	A:191:TRP:HA	0.691
1	B:185:ARG:O	B:189:LEU:HD13	0.691
1	A:320:LYS:HG2	A:352:TYR:CZ	0.690
1	B:363:TYR:O	B:366:GLN:HG2	0.689
1	A:168:LEU:HD23	B:168:LEU:CD2	0.688
1	A:342:LYS:HD2	A:342:LYS:N	0.688
1	B:393:ASN:O	B:396:ASP:HB2	0.688
1	A:317:THR:HG22	A:318:PHE:O	0.687
1	A:206:GLN:HE22	A:378:SER:HB2	0.687
1	B:320:LYS:O	B:322:PRO:HD2	0.686
1	B:319:GLN:HB2	B:322:PRO:CD	0.685
1	A:167:SER:HB2	B:16:GLN:HE22	0.684
1	B:298:VAL:CG1	B:337:PRO:HD3	0.684
1	B:333:VAL:HG22	B:352:TYR:HD1	0.684

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:201:THR:CG2	A:205:ARG:HB2	0.682
1	B:342:LYS:H	B:342:LYS:HD3	0.682
1	A:232:LYS:HB2	A:260:GLU:CG	0.681
1	B:297:TYR:HB2	B:314:GLU:OE1	0.681
1	B:392:GLU:HG2	B:399:GLN:NE2	0.681
1	A:177:TYR:O	A:181:ILE:HD13	0.680
1	A:395:LYS:HE3	A:397:ILE:CD1	0.680
1	B:22:MET:O	B:25:ILE:HG22	0.680
1	A:377:TRP:HH2	B:190:LEU:HD11	0.679
1	B:319:GLN:HG2	B:330:ILE:CA	0.679
1	B:67:SER:CB	B:72:ASN:HD21	0.678
1	A:181:ILE:HG23	A:367:ILE:CG1	0.677
1	B:291:ILE:HB	B:318:PHE:CZ	0.675
1	B:258:GLY:N	B:300:GLU:HB3	0.675
1	A:97:LYS:O	A:129:PRO:HD3	0.674
1	B:92:VAL:HA	B:97:LYS:HB2	0.674
1	B:88:ILE:CA	D:1:35G:O2P	0.674
1	A:76:PRO:O	A:79:GLU:HG2	0.673
1	A:395:LYS:HG2	A:398:ALA:CB	0.673
1	B:185:ARG:HD2	B:370:THR:CB	0.673
1	A:319:GLN:CB	A:322:PRO:HD3	0.672
1	A:197:PHE:CD2	B:377:TRP:HB3	0.671
1	B:97:LYS:HB3	B:99:PHE:CD2	0.670

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:336:LEU:CD2	B:368:ILE:HG21	0.670
1	A:115:ASP:OD1	C:1:35G:C2	0.670
1	A:185:ARG:CB	A:367:ILE:HG23	0.669
1	A:319:GLN:HB2	A:322:PRO:CD	0.669
1	B:288:TRP:HE3	B:320:LYS:HA	0.669
1	A:200:LEU:HD11	B:384:THR:HB	0.668
1	A:395:LYS:HE3	A:397:ILE:HD11	0.668
1	B:170:LEU:O	B:170:LEU:HD23	0.668
1	A:9:PHE:CD1	B:161:LYS:HG2	0.667
1	B:82:PHE:HZ	B:114:LEU:HB3	0.667
1	B:396:ASP:CA	B:396:ASP:H	0.667
1	A:235:GLU:HB2	A:257:ASP:CA	0.666
1	A:398:ALA:HB2	B:391:LEU:CG	0.666
1	B:339:VAL:O	B:376:GLY:HA3	0.666
1	A:289:CYS:HA	A:320:LYS:HG3	0.665
1	A:361:ASP:O	A:365:GLU:HG2	0.665
1	B:76:PRO:CG	B:358:LYS:HD3	0.665
1	B:123:VAL:HG22	B:144:ASN:OD1	0.664
1	A:1:ARG:HG3	A:2:LEU:N	0.663
1	A:122:THR:HG21	A:143:LEU:CD2	0.663
1	A:201:THR:HG22	A:205:ARG:HB2	0.663
1	A:339:VAL:O	A:376:GLY:HA3	0.663
1	A:22:MET:HE1	A:170:LEU:CD2	0.661

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:185:ARG:HD3	B:186:SER:HB2	0.661
1	B:4:GLU:HB3	B:162:TYR:OH	0.661
1	A:201:THR:HG22	A:202:ASP:N	0.660
1	B:257:ASP:CB	B:301:ASN:HA	0.660
1	A:9:PHE:CE1	B:8:LEU:HD22	0.659
1	A:381:ASN:HB2	B:197:PHE:HE1	0.659
1	B:41:ARG:HD2	B:62:ASN:HB3	0.659
1	B:341:LYS:C	B:343:GLU:H	0.659
1	A:130:ILE:HG21	A:170:LEU:HD12	0.658
1	A:259:ARG:HB3	A:259:ARG:NH1	0.658
1	A:297:TYR:HB3	A:315:TYR:HE1	0.658
1	B:333:VAL:HG22	B:352:TYR:CE1	0.658
1	A:194:ASN:HB2	B:377:TRP:CZ3	0.657
1	A:395:LYS:HE2	B:391:LEU:CA	0.657
1	B:48:ARG:NH2	B:81:VAL:HG21	0.657
1	B:95:THR:OG1	B:97:LYS:HG2	0.657
1	A:73:LEU:HD22	A:74:VAL:H	0.656
1	A:395:LYS:NZ	A:397:ILE:HD11	0.656
1	A:398:ALA:HB2	B:391:LEU:CB	0.656
1	B:33:LEU:HD13	B:37:LEU:HG	0.656
1	B:339:VAL:HG12	B:340:ASN:OD1	0.656
1	B:241:PRO:O	B:242:ILE:HD13	0.655
1	A:266:ILE:HD13	A:287:HIS:CD2	0.654

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:388:MET:HE2	A:388:MET:O	0.654
1	A:395:LYS:HZ1	A:397:ILE:HD11	0.654
1	B:59:ARG:O	B:74:VAL:HG12	0.654
1	B:97:LYS:HG3	B:99:PHE:CE2	0.654
1	B:335:SER:OG	B:350:THR:HG22	0.653
1	A:64:THR:HG23	A:67:SER:N	0.650
1	A:200:LEU:HG	B:384:THR:HG21	0.650
1	B:314:GLU:HB3	B:315:TYR:CE1	0.650
1	A:190:LEU:HD11	B:377:TRP:HH2	0.649
1	A:194:ASN:HB2	B:377:TRP:CH2	0.649
1	B:53:ILE:HG22	B:54:PRO:O	0.649
1	B:153:LYS:C	B:153:LYS:HD3	0.649
1	B:257:ASP:C	B:300:GLU:HB3	0.649
1	A:319:GLN:CG	A:330:ILE:H	0.649
1	A:197:PHE:C	B:380:LEU:HD22	0.648
1	A:320:LYS:O	A:328:TRP:HZ3	0.648
1	B:33:LEU:HD11	B:37:LEU:HG	0.647
1	A:128:ILE:CG1	A:163:LEU:HD13	0.646
1	A:169:VAL:HA	A:172:ASN:ND2	0.646
1	B:256:PRO:HG3	B:314:GLU:HG3	0.645
1	B:383:ASP:HA	B:386:ASP:OD1	0.644
1	A:394:ARG:NE	B:395:LYS:HD3	0.644
1	A:87:GLY:HA2	C:1:35G:P	0.643

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:45:PHE:CE2	A:58:THR:HG22	0.642
1	A:115:ASP:CG	C:1:35G:O4'	0.642
1	A:231:THR:HG23	A:232:LYS:N	0.642
1	A:388:MET:HG2	A:391:LEU:HD12	0.642
1	B:333:VAL:HG13	B:352:TYR:CE1	0.642
1	B:143:LEU:HD23	D:1:35G:O6	0.641
1	A:200:LEU:CD1	B:384:THR:HB	0.640
1	A:333:VAL:HG22	A:352:TYR:HD1	0.640
1	A:395:LYS:CE	A:397:ILE:HD11	0.640
1	B:101:ILE:HD13	B:104:VAL:HA	0.640
1	A:206:GLN:NE2	A:378:SER:HB2	0.638
1	B:294:LEU:HD21	B:305:CYS:SG	0.638
1	B:115:ASP:OD2	D:1:35G:O2'	0.638
1	B:321:GLY:HA3	B:328:TRP:CZ3	0.637
1	A:256:PRO:HA	A:301:ASN:HD21	0.636
1	A:320:LYS:HG2	A:352:TYR:CE1	0.635
1	A:375:LEU:O	A:379:VAL:HG23	0.635
1	A:122:THR:HG23	C:1:35G:N3	0.634
1	B:87:GLY:HA2	B:111:SER:CB	0.634
1	A:292:SER:HB3	A:320:LYS:HZ2	0.633
1	B:7:ILE:O	B:10:GLU:HG2	0.633
1	A:322:PRO:HA	A:328:TRP:O	0.632
1	B:380:LEU:O	B:384:THR:HG23	0.632

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:341:LYS:C	A:343:GLU:H	0.631
1	B:195:LYS:HA	B:195:LYS:HE2	0.631
1	B:203:ILE:HA	B:382:THR:HG21	0.631
1	A:182:GLU:OE2	A:185:ARG:HD2	0.630
1	A:64:THR:CG2	A:67:SER:H	0.630
1	B:101:ILE:CD1	B:104:VAL:HA	0.629
1	B:274:LYS:HG3	B:274:LYS:O	0.629
1	B:298:VAL:HG13	B:337:PRO:HD3	0.629
1	A:336:LEU:CD1	A:368:ILE:HG21	0.628
1	B:188:MET:CG	B:214:ILE:HD11	0.627
1	A:178:LEU:HB3	B:179:TYR:CE1	0.626
1	A:195:LYS:HB3	A:209:LYS:HG2	0.626
1	B:294:LEU:O	B:294:LEU:HD23	0.626
1	B:88:ILE:H	D:1:35G:P	0.626
1	A:104:VAL:HG11	A:125:MET:HE3	0.625
1	A:242:ILE:O	A:242:ILE:HG13	0.624
1	B:232:LYS:HB2	B:260:GLU:HG2	0.624
1	A:229:ASP:HB2	A:262:ASN:HD22	0.622
1	A:391:LEU:HD22	B:395:LYS:HB3	0.622
1	B:110:PHE:CE2	B:112:ASP:HA	0.622
1	A:320:LYS:HG2	A:352:TYR:OH	0.621
1	B:76:PRO:HG3	B:358:LYS:CD	0.621
1	A:26:VAL:HG13	A:166:ILE:HD11	0.620

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:172:ASN:HA	B:172:ASN:OD1	0.620
1	A:231:THR:C	A:232:LYS:HG3	0.620
1	A:304:ILE:CG1	A:336:LEU:HG	0.620
1	A:362:GLU:HG3	A:363:TYR:CD2	0.619
1	B:391:LEU:HD13	B:392:GLU:CA	0.619
1	A:57:ALA:CB	A:81:VAL:HG22	0.618
1	A:222:ARG:HH21	A:321:GLY:HA2	0.618
1	B:244:LEU:HD22	B:245:GLY:H	0.618
1	B:33:LEU:O	B:37:LEU:HD23	0.617
1	A:197:PHE:O	B:380:LEU:HD22	0.617
1	A:394:ARG:HH21	B:395:LYS:CE	0.617
1	A:197:PHE:CA	B:380:LEU:HD22	0.616
1	A:212:TYR:O	A:215:ARG:HG3	0.616
1	B:123:VAL:HG23	B:124:ASN:ND2	0.616
1	B:305:CYS:SG	B:335:SER:HB2	0.615
1	B:215:ARG:HB2	B:271:LEU:HD11	0.614
1	B:69:PHE:HZ	B:73:LEU:HD12	0.613
1	A:179:TYR:CE1	B:182:GLU:HG2	0.611
1	A:188:MET:CE	A:367:ILE:HG22	0.611
1	A:228:LEU:HD12	A:345:ILE:O	0.611
1	A:338:ILE:HG12	A:347:GLY:C	0.611
1	A:21:SER:O	A:24:LYS:HG3	0.610
1	A:339:VAL:HB	A:342:LYS:NZ	0.610

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:76:PRO:HG3	B:358:LYS:NZ	0.610
1	B:376:GLY:O	B:379:VAL:HB	0.610
1	A:128:ILE:HG12	A:163:LEU:HD13	0.609
1	A:182:GLU:HG2	B:183:SER:N	0.609
1	A:291:ILE:HG21	A:318:PHE:CD1	0.609
1	A:2:LEU:C	A:2:LEU:HD13	0.608
1	A:6:ASN:O	A:10:GLU:HG3	0.608
1	A:392:GLU:HG2	A:396:ASP:HA	0.608
1	B:157:GLU:HA	B:157:GLU:OE1	0.608
1	B:225:VAL:HG12	B:267:ILE:CG1	0.608
1	A:197:PHE:HE1	B:381:ASN:CG	0.608
1	A:350:THR:HG22	A:352:TYR:CE1	0.606
1	B:292:SER:HB3	B:320:LYS:HZ3	0.606
1	A:9:PHE:CD1	B:161:LYS:HD2	0.605
1	A:371:LEU:HD13	A:375:LEU:CD2	0.605
1	B:33:LEU:O	B:37:LEU:HB2	0.605
1	B:297:TYR:HB3	B:315:TYR:HE1	0.605
1	B:342:LYS:HE2	B:342:LYS:N	0.604
1	A:50:ARG:HH22	A:359:PRO:CB	0.603
1	B:370:THR:O	B:373:GLN:HG2	0.603
1	A:33:LEU:HD21	A:162:TYR:HB2	0.601
1	A:336:LEU:HD11	A:368:ILE:HG21	0.601
1	A:376:GLY:O	A:379:VAL:HB	0.600

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:222:ARG:CD	A:270:ILE:HG13	0.599
1	A:294:LEU:HG	A:315:TYR:CE2	0.599
1	A:294:LEU:O	A:294:LEU:HD23	0.599
1	A:392:GLU:CG	A:396:ASP:HA	0.598
1	B:91:TRP:CZ2	B:95:THR:HG21	0.598
1	B:391:LEU:HD22	B:394:ARG:HD2	0.598
1	B:96:LYS:HA	B:129:PRO:HG3	0.597
1	B:73:LEU:C	B:73:LEU:HD23	0.596
1	B:313:ASP:HB2	B:315:TYR:CZ	0.596
1	B:301:ASN:OD1	B:303:PHE:HD2	0.596
1	B:145:LYS:CG	B:148:ALA:HB2	0.595
1	A:228:LEU:HD21	A:263:PHE:CE2	0.594
1	A:339:VAL:HG11	A:342:LYS:CA	0.594
1	B:308:MET:HG2	B:359:PRO:HB3	0.594
1	A:50:ARG:HD2	A:55:GLU:OE2	0.593
1	A:203:ILE:HG23	A:204:GLU:N	0.592
1	B:58:THR:CG2	B:61:LEU:HD21	0.592
1	B:118:THR:HG23	B:120:TYR:N	0.592
1	A:40:ASP:HB3	A:144:ASN:OD1	0.591
1	B:193:ALA:O	B:196:VAL:HG22	0.591
1	A:122:THR:HG23	C:1:35G:N2	0.590
1	A:159:PHE:CE2	A:163:LEU:HD11	0.590
1	A:305:CYS:HB3	A:313:ASP:OD2	0.590

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:395:LYS:HG3	A:398:ALA:H	0.590
1	B:128:ILE:HG21	B:163:LEU:CD1	0.590
1	B:143:LEU:HD23	D:1:35G:C6	0.589
1	A:97:LYS:HG3	A:99:PHE:HE2	0.588
1	A:115:ASP:HB2	C:1:35G:C4'	0.588
1	A:145:LYS:HD3	A:148:ALA:HB3	0.586
1	A:158:VAL:HG23	A:161:LYS:HZ2	0.586
1	B:73:LEU:HD23	B:74:VAL:C	0.586
1	A:338:ILE:HG22	A:372:THR:CG2	0.585
1	B:314:GLU:HB3	B:315:TYR:CD1	0.585
1	A:8:LEU:O	A:12:LEU:HD13	0.584
1	A:41:ARG:O	A:143:LEU:HB2	0.584
1	A:271:LEU:N	A:271:LEU:HD22	0.584
1	B:304:ILE:CG1	B:336:LEU:HD12	0.584
1	A:161:LYS:HD3	B:9:PHE:CE1	0.583
1	B:190:LEU:C	B:190:LEU:HD13	0.583
1	B:274:LYS:HE3	B:276:GLU:HG2	0.583
1	A:228:LEU:HD23	A:263:PHE:CD2	0.582
1	B:181:ILE:HD12	B:366:GLN:HE21	0.582
1	B:251:LYS:HD2	B:251:LYS:O	0.582
1	A:123:VAL:HG23	A:124:ASN:N	0.581
1	A:228:LEU:CD2	A:261:VAL:HG13	0.581
1	A:292:SER:O	A:315:TYR:HB3	0.581

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:344:GLU:HG2	A:345:ILE:N	0.581
1	B:195:LYS:HG3	B:210:ALA:HA	0.581
1	B:355:LYS:O	B:356:ASP:HB3	0.581
1	A:190:LEU:HD11	B:377:TRP:CH2	0.580
1	A:395:LYS:HG2	B:391:LEU:CB	0.580
1	B:288:TRP:CE3	B:320:LYS:CA	0.580
1	B:305:CYS:HB2	B:313:ASP:OD2	0.580
1	A:200:LEU:HD11	B:384:THR:CB	0.579
1	A:97:LYS:CG	A:99:PHE:HE2	0.578
1	A:203:ILE:HA	A:382:THR:HG21	0.578
1	B:97:LYS:HG3	B:99:PHE:HE2	0.578
1	B:310:ALA:HB2	B:319:GLN:HE21	0.578
1	A:41:ARG:HH12	A:122:THR:HG22	0.577
1	A:267:ILE:O	A:267:ILE:HG23	0.577
1	A:330:ILE:HD13	A:352:TYR:HB3	0.577
1	A:336:LEU:HD21	A:368:ILE:HG22	0.577
1	B:254:LYS:HA	B:254:LYS:HE3	0.577
1	A:114:LEU:O	A:114:LEU:HD13	0.576
1	A:339:VAL:HG12	A:340:ASN:N	0.576
1	A:294:LEU:HG	A:315:TYR:OH	0.575
1	B:48:ARG:HH22	B:81:VAL:HG21	0.574
1	B:271:LEU:N	B:271:LEU:HD22	0.574
1	A:294:LEU:HA	A:315:TYR:CZ	0.573

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:297:TYR:CG	A:315:TYR:HE1	0.573
1	A:320:LYS:HE3	A:320:LYS:N	0.573
1	B:342:LYS:CE	B:342:LYS:H	0.573
1	B:141:MET:HG3	B:143:LEU:HD11	0.572
1	A:377:TRP:HH2	B:190:LEU:CD1	0.572
1	B:328:TRP:CH2	B:330:ILE:HG12	0.572
1	B:375:LEU:O	B:379:VAL:HG23	0.571
1	A:321:GLY:HA3	A:328:TRP:HE3	0.570
1	B:83:PRO:HB2	B:85:ASP:OD1	0.570
1	B:319:GLN:CB	B:322:PRO:HG3	0.570
1	B:364:ASP:O	B:368:ILE:HD13	0.570
1	B:50:ARG:HD3	B:55:GLU:OE1	0.569
1	B:320:LYS:HE3	B:320:LYS:N	0.569
1	A:323:VAL:O	A:324:ASP:HB2	0.568
1	B:202:ASP:OD1	B:205:ARG:HB2	0.568
1	B:319:GLN:CB	B:322:PRO:HD3	0.568
1	A:185:ARG:HG3	A:186:SER:N	0.567
1	B:177:TYR:HA	B:180:ASN:HD21	0.567
1	A:189:LEU:HD21	A:370:THR:HG22	0.566
1	A:297:TYR:HE2	A:305:CYS:HG	0.566
1	A:45:PHE:HB3	A:56:VAL:HG22	0.565
1	A:56:VAL:O	A:81:VAL:HG13	0.565
1	B:38:ALA:HB3	B:145:LYS:HE3	0.565

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:350:THR:HB	A:352:TYR:OH	0.563
1	B:57:ALA:CB	B:81:VAL:HG22	0.563
1	B:123:VAL:HG23	B:124:ASN:N	0.563
1	A:211:LEU:HA	A:214:ILE:HG12	0.562
1	B:251:LYS:HE2	B:251:LYS:N	0.562
1	B:101:ILE:CG2	B:125:MET:H	0.561
1	B:153:LYS:HD3	B:153:LYS:O	0.561
1	B:235:GLU:HB2	B:257:ASP:HB3	0.561
1	B:320:LYS:CA	B:320:LYS:HE3	0.561
1	B:319:GLN:OE1	B:322:PRO:HG3	0.561
1	B:339:VAL:HG12	B:340:ASN:N	0.560
1	B:319:GLN:CG	B:330:ILE:H	0.560
1	A:392:GLU:O	A:396:ASP:HB3	0.559
1	B:294:LEU:HD13	B:333:VAL:HG11	0.559
1	B:320:LYS:CG	B:352:TYR:CZ	0.559
1	A:297:TYR:HE2	A:305:CYS:SG	0.559
1	A:174:HIS:CE1	A:178:LEU:HD11	0.558
1	A:187:GLN:HA	A:187:GLN:NE2	0.558
1	A:215:ARG:HB3	A:271:LEU:HD11	0.558
1	A:255:THR:HB	A:256:PRO:CD	0.558
1	A:395:LYS:HE2	B:391:LEU:CB	0.558
1	A:67:SER:CB	A:72:ASN:HD21	0.557
1	A:206:GLN:HG2	A:382:THR:HG22	0.557

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:228:LEU:HD21	A:263:PHE:CZ	0.557
1	A:392:GLU:OE1	A:399:GLN:HB3	0.557
1	B:95:THR:HB	B:97:LYS:CE	0.557
1	B:288:TRP:CZ3	B:320:LYS:HA	0.556
1	A:15:ILE:HG21	B:168:LEU:HD13	0.555
1	A:182:GLU:HG2	B:182:GLU:C	0.555
1	A:190:LEU:HD22	B:377:TRP:CZ3	0.555
1	A:395:LYS:HE2	B:391:LEU:HA	0.555
1	B:36:LEU:HD21	B:158:VAL:HG21	0.555
1	A:355:LYS:O	A:356:ASP:HB2	0.554
1	B:304:ILE:HG23	B:336:LEU:HD13	0.554
1	B:319:GLN:O	B:330:ILE:HD12	0.554
1	A:115:ASP:CG	C:1:35G:H1'	0.554
1	B:136:VAL:O	B:136:VAL:HG13	0.553
1	A:257:ASP:C	A:300:GLU:HB3	0.551
1	B:339:VAL:HG11	B:342:LYS:CA	0.551
1	A:190:LEU:O	B:377:TRP:HZ3	0.551
1	A:104:VAL:HG23	A:105:LYS:N	0.550
1	B:221:GLU:O	B:271:LEU:HB2	0.550
1	A:91:TRP:CE2	A:95:THR:HG21	0.549
1	A:185:ARG:HD3	B:186:SER:CB	0.549
1	A:190:LEU:HD21	B:373:GLN:HG3	0.549
1	B:386:ASP:O	B:389:ASN:HB2	0.549

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:226:GLY:CA	B:266:ILE:HD12	0.548
1	B:319:GLN:C	B:320:LYS:HD2	0.548
1	A:397:ILE:C	A:397:ILE:HD12	0.547
1	B:188:MET:HE3	B:367:ILE:HD11	0.547
1	A:339:VAL:HG12	A:340:ASN:OD1	0.546
1	A:395:LYS:HE2	B:391:LEU:HB2	0.546
1	B:266:ILE:O	B:266:ILE:HG23	0.546
1	B:64:THR:CG2	B:65:PRO:HD2	0.545
1	B:101:ILE:HG22	B:125:MET:H	0.545
1	B:114:LEU:C	B:114:LEU:HD13	0.545
1	A:319:GLN:HB2	A:322:PRO:CG	0.544
1	B:33:LEU:HD22	B:37:LEU:CD2	0.544
1	A:114:LEU:C	A:114:LEU:HD13	0.543
1	A:136:VAL:O	A:136:VAL:HG13	0.543
1	A:320:LYS:CB	A:352:TYR:CZ	0.543
1	A:350:THR:HG22	A:352:TYR:CZ	0.543
1	A:369:GLU:O	A:373:GLN:HG3	0.543
1	A:377:TRP:CH2	B:190:LEU:HD11	0.543
1	B:11:LEU:HA	B:14:GLU:HG2	0.543
1	B:189:LEU:HD21	B:370:THR:CG2	0.543
1	B:319:GLN:HB3	B:330:ILE:HD12	0.543
1	A:388:MET:HE1	A:398:ALA:CB	0.542
1	A:151:PHE:HB3	A:155:ASP:OD2	0.541

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:330:ILE:HD11	A:352:TYR:HB3	0.541
1	A:308:MET:O	A:309:ASN:HB2	0.540
1	B:294:LEU:HA	B:315:TYR:CZ	0.540
1	A:115:ASP:OD2	C:1:35G:N9	0.540
1	A:73:LEU:C	A:73:LEU:HD13	0.539
1	B:126:MET:HE3	B:151:PHE:CB	0.539
1	B:336:LEU:N	B:336:LEU:HD22	0.539
1	A:64:THR:HG22	A:67:SER:HB3	0.538
1	A:73:LEU:HD22	A:74:VAL:N	0.538
1	A:104:VAL:HG21	A:122:THR:O	0.538
1	A:235:GLU:HB2	A:257:ASP:C	0.538
1	A:319:GLN:H	A:322:PRO:CG	0.538
1	B:97:LYS:CE	B:97:LYS:HA	0.538
1	B:294:LEU:HD21	B:335:SER:HB2	0.538
1	B:341:LYS:O	B:343:GLU:HG3	0.538
1	A:291:ILE:HD13	A:318:PHE:CZ	0.537
1	A:294:LEU:CD1	A:333:VAL:HG11	0.537
1	A:388:MET:SD	B:388:MET:HG2	0.537
1	A:381:ASN:HB2	B:197:PHE:CE1	0.536
1	B:203:ILE:HA	B:382:THR:CG2	0.536
1	B:228:LEU:HD23	B:347:GLY:CA	0.536
1	A:195:LYS:O	A:209:LYS:HD2	0.535
1	A:319:GLN:HB3	A:330:ILE:CG1	0.535

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:15:ILE:HD11	B:165:PHE:HZ	0.535
1	B:33:LEU:HD13	B:37:LEU:CG	0.535
1	B:69:PHE:CZ	B:73:LEU:HD12	0.535
1	B:148:ALA:HB3	B:149:SER:HA	0.535
1	B:228:LEU:CD1	B:261:VAL:HG13	0.535
1	B:306:ASN:HD21	B:360:PHE:C	0.535
1	A:256:PRO:HB3	A:297:TYR:CE1	0.534
1	A:257:ASP:HB2	A:300:GLU:C	0.534
1	B:230:MET:CA	B:230:MET:HE2	0.534
1	B:267:ILE:CG2	B:279:VAL:HG22	0.534
1	B:294:LEU:HG	B:315:TYR:CZ	0.534
1	B:308:MET:SD	B:359:PRO:HG3	0.534
1	A:190:LEU:C	A:190:LEU:HD13	0.533
1	A:243:ARG:C	A:244:LEU:HD12	0.533
1	A:282:THR:O	A:282:THR:HG22	0.533
1	A:185:ARG:HH22	A:366:GLN:HB3	0.533
1	B:41:ARG:CD	B:62:ASN:HB3	0.532
1	A:95:THR:OG1	A:97:LYS:HG2	0.531
1	A:319:GLN:O	A:320:LYS:HB2	0.531
1	B:284:PRO:HB2	B:286:ASP:OD1	0.531
1	B:391:LEU:C	B:391:LEU:HD13	0.531
1	A:145:LYS:NZ	A:152:SER:H	0.531
1	A:267:ILE:HD12	A:279:VAL:HG22	0.530

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:292:SER:HB3	A:320:LYS:HZ3	0.530
1	B:218:LEU:HD12	B:223:TYR:CE1	0.530
1	B:225:VAL:CG1	B:267:ILE:HD11	0.530
1	B:257:ASP:HB2	B:300:GLU:C	0.530
1	A:394:ARG:HH21	B:395:LYS:HE3	0.530
1	B:340:ASN:HD21	B:343:GLU:CB	0.530
1	A:314:GLU:HG2	A:314:GLU:O	0.529
1	A:23:GLU:HG3	A:59:ARG:HH21	0.529
1	A:298:VAL:HG11	A:335:SER:OG	0.528
1	A:364:ASP:O	A:368:ILE:HD13	0.528
1	B:229:ASP:HB2	B:262:ASN:HD22	0.528
1	B:265:LYS:NZ	B:267:ILE:HD12	0.528
1	A:145:LYS:HD3	A:150:GLU:O	0.527
1	A:256:PRO:CD	A:297:TYR:HE1	0.527
1	B:207:PHE:O	B:211:LEU:HD13	0.527
1	A:145:LYS:HD2	A:151:PHE:HA	0.526
1	B:210:ALA:O	B:214:ILE:HG22	0.526
1	B:317:THR:HG22	B:318:PHE:C	0.526
1	B:328:TRP:CH2	B:330:ILE:HD11	0.526
1	B:350:THR:HB	B:352:TYR:OH	0.526
1	A:145:LYS:HB2	A:151:PHE:CE1	0.525
1	A:198:GLU:HA	B:341:LYS:NZ	0.525
1	B:354:ARG:HG3	B:356:ASP:O	0.525

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:339:VAL:HB	A:342:LYS:HZ2	0.524
1	A:395:LYS:HG3	A:398:ALA:N	0.523
1	A:341:LYS:HB3	A:341:LYS:NZ	0.522
1	B:95:THR:O	B:96:LYS:HB2	0.522
1	B:97:LYS:CB	B:99:PHE:CE2	0.522
1	B:222:ARG:CD	B:270:ILE:HG13	0.522
1	B:256:PRO:HG3	B:314:GLU:CG	0.522
1	B:328:TRP:HZ3	B:330:ILE:HD11	0.522
1	A:97:LYS:CG	A:99:PHE:CE2	0.521
1	A:104:VAL:CG1	A:125:MET:HE3	0.521
1	A:321:GLY:HA3	A:328:TRP:HZ3	0.521
1	B:92:VAL:HG13	B:129:PRO:HD3	0.521
1	A:182:GLU:HB3	B:182:GLU:HB3	0.520
1	B:53:ILE:N	B:53:ILE:HD12	0.520
1	B:391:LEU:C	B:391:LEU:HD22	0.520
1	B:396:ASP:CB	B:396:ASP:N	0.519
1	A:22:MET:O	A:25:ILE:HG22	0.516
1	A:87:GLY:HA2	A:111:SER:CB	0.516
1	A:181:ILE:HG12	A:363:TYR:HB3	0.516
1	A:288:TRP:CE3	A:320:LYS:CA	0.516
1	B:61:LEU:CD2	B:74:VAL:HB	0.516
1	B:342:LYS:H	B:342:LYS:HE2	0.516
1	A:146:LEU:C	A:146:LEU:HD13	0.515

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:189:LEU:HD21	A:370:THR:HG21	0.515
1	B:33:LEU:HD22	B:37:LEU:HD23	0.515
1	B:256:PRO:HB3	B:297:TYR:HD2	0.515
1	B:321:GLY:H	B:328:TRP:HZ3	0.515
1	A:88:ILE:O	A:92:VAL:HG23	0.514
1	A:319:GLN:HB2	A:322:PRO:HG3	0.514
1	B:22:MET:O	B:26:VAL:HG23	0.514
1	B:41:ARG:HD2	B:62:ASN:CB	0.514
1	B:200:LEU:HD11	B:385:TYR:HB2	0.514
1	A:203:ILE:HA	A:382:THR:CG2	0.513
1	B:59:ARG:HA	B:74:VAL:HG12	0.513
1	B:185:ARG:CB	B:367:ILE:HG13	0.513
1	B:195:LYS:HD2	B:213:THR:OG1	0.513
1	B:237:TYR:O	B:238:ASP:HB3	0.513
1	B:395:LYS:C	B:397:ILE:N	0.513
1	A:41:ARG:HD3	A:62:ASN:HA	0.512
1	B:92:VAL:HG13	B:97:LYS:O	0.512
1	A:187:GLN:HG2	A:217:TYR:OH	0.511
1	A:291:ILE:CG2	A:318:PHE:CE1	0.511
1	A:388:MET:HE1	A:398:ALA:HB3	0.511
1	B:15:ILE:HD11	B:165:PHE:CZ	0.511
1	B:102:PRO:HB3	B:150:GLU:HG2	0.511
1	A:372:THR:O	A:372:THR:HG22	0.511

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:159:PHE:CE2	A:163:LEU:CD1	0.510
1	B:130:ILE:O	B:136:VAL:HG23	0.510
1	B:290:LEU:N	B:290:LEU:HD22	0.510
1	A:141:MET:HG3	A:143:LEU:HD11	0.509
1	B:148:ALA:CB	B:149:SER:HA	0.509
1	B:257:ASP:HB2	B:300:GLU:O	0.509
1	B:319:GLN:HB3	B:330:ILE:CD1	0.509
1	A:22:MET:CE	A:170:LEU:HD22	0.508
1	B:123:VAL:HG23	B:124:ASN:HD22	0.508
1	B:222:ARG:HG3	B:328:TRP:CH2	0.508
1	A:7:ILE:HG21	A:32:ARG:HG2	0.507
1	A:9:PHE:CD1	B:161:LYS:CG	0.506
1	A:41:ARG:HD3	A:62:ASN:CB	0.506
1	A:391:LEU:CD1	B:398:ALA:HB1	0.506
1	A:14:GLU:CD	A:24:LYS:HZ2	0.505
1	A:151:PHE:HB3	A:155:ASP:CG	0.505
1	A:169:VAL:HA	A:172:ASN:HD21	0.505
1	A:377:TRP:CH2	B:194:ASN:HB2	0.505
1	B:96:LYS:C	B:129:PRO:HG3	0.505
1	A:143:LEU:N	A:143:LEU:HD12	0.504
1	A:190:LEU:CD1	B:377:TRP:CH2	0.504
1	A:298:VAL:HG23	A:348:VAL:HG22	0.504
1	B:64:THR:HG22	B:65:PRO:HD2	0.504

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:391:LEU:O	B:394:ARG:HD2	0.504
1	B:394:ARG:O	B:395:LYS:C	0.504
1	A:394:ARG:NH2	B:395:LYS:HE3	0.504
1	B:372:THR:O	B:372:THR:HG22	0.504
1	A:295:PRO:HA	A:348:VAL:HG11	0.503
1	A:371:LEU:C	A:371:LEU:HD13	0.503
1	B:254:LYS:CA	B:254:LYS:O	0.503
1	A:338:ILE:HA	A:372:THR:HG22	0.502
1	A:388:MET:CA	A:391:LEU:HD12	0.502
1	B:294:LEU:HB3	B:295:PRO:CD	0.502
1	A:297:TYR:CE2	A:305:CYS:SG	0.501
1	A:297:TYR:HB3	A:315:TYR:CE1	0.501
1	B:58:THR:HG22	B:61:LEU:HD21	0.501
1	B:214:ILE:HD11	B:217:TYR:HB2	0.501
1	B:297:TYR:HB2	B:315:TYR:HE1	0.501
1	A:91:TRP:CE2	A:95:THR:CG2	0.500
1	A:395:LYS:C	A:397:ILE:H	0.500
1	B:80:THR:HG21	B:114:LEU:HD23	0.500
1	B:185:ARG:HD2	B:370:THR:HB	0.500
1	A:97:LYS:CB	A:99:PHE:CE2	0.499
1	A:121:THR:CA	C:1:35G:N2	0.499
1	A:190:LEU:CD2	B:377:TRP:CZ3	0.499
1	A:257:ASP:HB2	A:300:GLU:O	0.499

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:291:ILE:CB	B:318:PHE:CZ	0.499
1	B:307:MET:HE2	B:313:ASP:OD2	0.499
1	A:201:THR:HG21	A:205:ARG:CB	0.498
1	A:209:LYS:HB2	A:209:LYS:NZ	0.498
1	A:211:LEU:CD2	A:225:VAL:HG21	0.498
1	A:388:MET:HA	A:391:LEU:HD11	0.498
1	A:391:LEU:CD1	B:398:ALA:CB	0.498
1	B:189:LEU:HD11	B:370:THR:HG22	0.498
1	B:392:GLU:O	B:396:ASP:HB2	0.498
1	A:190:LEU:CD1	B:377:TRP:HH2	0.498
1	A:43:SER:HB2	A:61:LEU:HD23	0.497
1	A:91:TRP:CZ2	A:95:THR:CG2	0.497
1	A:41:ARG:NH1	A:122:THR:HG22	0.497
1	A:218:LEU:HB3	A:220:CYS:SG	0.497
1	A:294:LEU:HB3	A:295:PRO:CD	0.497
1	B:97:LYS:CG	B:99:PHE:CE2	0.497
1	A:258:GLY:N	A:300:GLU:CB	0.497
1	A:44:MET:SD	A:59:ARG:HD3	0.496
1	A:313:ASP:HB3	A:315:TYR:CZ	0.496
1	B:41:ARG:HB3	B:62:ASN:HA	0.496
1	B:333:VAL:HG12	B:334:LEU:N	0.496
1	A:44:MET:HE3	A:138:ALA:CB	0.495
1	A:345:ILE:N	A:345:ILE:HD12	0.495

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:178:LEU:HA	B:181:ILE:HG12	0.495
1	B:254:LYS:HA	B:254:LYS:HZ1	0.495
1	A:291:ILE:CG2	A:318:PHE:CD1	0.494
1	B:308:MET:O	B:309:ASN:HB2	0.494
1	A:84:LEU:N	A:84:LEU:HD12	0.493
1	A:320:LYS:CB	A:352:TYR:CE1	0.493
1	B:267:ILE:N	B:267:ILE:HD13	0.493
1	B:294:LEU:HG	B:315:TYR:CE2	0.493
1	A:195:LYS:CB	A:209:LYS:HG2	0.492
1	A:228:LEU:CD2	A:263:PHE:CE2	0.492
1	B:291:ILE:HG13	B:318:PHE:HZ	0.492
1	B:49:SER:O	B:362:GLU:HB2	0.492
1	A:388:MET:HE1	A:398:ALA:C	0.491
1	B:288:TRP:HZ3	B:320:LYS:CB	0.491
1	B:392:GLU:CG	B:399:GLN:H	0.490
1	A:319:GLN:OE1	A:322:PRO:HG3	0.489
1	B:244:LEU:HD22	B:245:GLY:N	0.489
1	A:362:GLU:HA	A:365:GLU:HG2	0.488
1	A:377:TRP:CH2	B:190:LEU:CD1	0.488
1	B:82:PHE:CZ	B:114:LEU:CB	0.488
1	B:322:PRO:HA	B:328:TRP:O	0.488
1	A:254:LYS:CA	A:254:LYS:O	0.487
1	A:371:LEU:CD1	A:375:LEU:HD23	0.487

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:110:PHE:CE1	D:1:35G:C2'	0.487
1	B:190:LEU:O	B:190:LEU:HD13	0.487
1	B:333:VAL:CG2	B:352:TYR:CE1	0.487
1	A:270:ILE:O	A:275:GLU:HG3	0.486
1	A:258:GLY:H	A:300:GLU:HB3	0.486
1	B:319:GLN:N	B:322:PRO:HG3	0.486
1	A:49:SER:HB2	A:362:GLU:HB3	0.485
1	B:292:SER:HB3	B:320:LYS:HZ1	0.485
1	B:395:LYS:HE2	B:395:LYS:O	0.485
1	A:336:LEU:N	A:336:LEU:HD12	0.484
1	A:338:ILE:HA	A:372:THR:HG21	0.484
1	B:244:LEU:HD13	B:259:ARG:HH22	0.484
1	A:158:VAL:HG13	A:159:PHE:N	0.483
1	A:296:THR:O	A:300:GLU:HG3	0.483
1	B:104:VAL:HG11	B:122:THR:O	0.483
1	B:391:LEU:CD2	B:394:ARG:HD2	0.483
1	A:95:THR:O	A:96:LYS:HB2	0.482
1	A:97:LYS:HD2	A:99:PHE:CE2	0.482
1	A:297:TYR:CB	A:315:TYR:CE1	0.482
1	A:313:ASP:CB	A:315:TYR:CE2	0.482
1	B:84:LEU:HD22	B:93:ALA:HB3	0.482
1	B:362:GLU:HA	B:365:GLU:HG2	0.482
1	B:362:GLU:O	B:365:GLU:HG2	0.482

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:182:GLU:HB3	B:182:GLU:CB	0.481
1	B:391:LEU:HD11	B:398:ALA:CB	0.481
1	A:330:ILE:CD1	A:352:TYR:CD1	0.480
1	A:151:PHE:HB3	A:155:ASP:OD1	0.479
1	A:320:LYS:HB2	A:352:TYR:CE1	0.479
1	B:148:ALA:HB1	B:150:GLU:N	0.479
1	B:255:THR:HB	B:256:PRO:CD	0.479
1	B:330:ILE:HA	B:353:ASN:HD21	0.479
1	B:338:ILE:HA	B:372:THR:HG22	0.479
1	A:266:ILE:HG22	A:280:ILE:HB	0.478
1	A:304:ILE:HD12	A:336:LEU:CD2	0.478
1	A:320:LYS:CG	A:352:TYR:CZ	0.478
1	B:51:ASN:C	B:53:ILE:H	0.478
1	B:338:ILE:HG12	B:372:THR:HG23	0.478
1	A:330:ILE:HD13	A:352:TYR:CD1	0.477
1	B:52:GLY:C	B:53:ILE:HD12	0.477
1	B:91:TRP:CZ2	B:95:THR:CG2	0.477
1	B:96:LYS:CA	B:129:PRO:HG3	0.477
1	B:298:VAL:O	B:298:VAL:HG12	0.477
1	B:310:ALA:CB	B:319:GLN:HE21	0.477
1	B:328:TRP:CH2	B:330:ILE:CG1	0.477
1	B:335:SER:CB	B:350:THR:HG22	0.477
1	B:145:LYS:HG2	B:148:ALA:HB2	0.476

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:395:LYS:CG	A:398:ALA:H	0.476
1	A:189:LEU:CD1	A:374:PHE:HB2	0.475
1	A:319:GLN:C	A:330:ILE:HD12	0.475
1	A:306:ASN:HD21	A:360:PHE:C	0.475
1	B:152:SER:OG	B:154:GLU:HG2	0.475
1	B:185:ARG:HB2	B:367:ILE:HG13	0.475
1	A:49:SER:HA	A:54:PRO:HA	0.474
1	A:218:LEU:HD12	A:223:TYR:CE2	0.474
1	B:97:LYS:O	B:129:PRO:HD3	0.474
1	B:225:VAL:HG13	B:267:ILE:HD11	0.474
1	B:128:ILE:HG12	B:129:PRO:O	0.473
1	B:158:VAL:HG13	B:159:PHE:N	0.473
1	B:228:LEU:HD13	B:263:PHE:CD1	0.473
1	B:328:TRP:CZ3	B:330:ILE:CD1	0.473
1	B:333:VAL:CG1	B:352:TYR:CE1	0.473
1	A:128:ILE:HD13	A:163:LEU:CD1	0.472
1	A:235:GLU:CB	A:257:ASP:CA	0.472
1	A:304:ILE:HG13	A:335:SER:O	0.472
1	B:25:ILE:HG23	B:26:VAL:N	0.472
1	B:58:THR:HG21	B:61:LEU:HD21	0.472
1	B:254:LYS:C	B:255:THR:HG23	0.472
1	B:258:GLY:N	B:300:GLU:CB	0.472
1	B:288:TRP:HZ3	B:320:LYS:HB3	0.472

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:259:ARG:HB3	A:259:ARG:HH11	0.471
1	B:57:ALA:HA	B:80:THR:O	0.471
1	B:211:LEU:HA	B:214:ILE:CG2	0.471
1	A:146:LEU:O	A:146:LEU:HD13	0.470
1	B:287:HIS:CD2	B:289:CYS:H	0.470
1	A:28:LYS:HB2	A:28:LYS:NZ	0.469
1	B:7:ILE:HD13	B:32:ARG:HD2	0.469
1	B:229:ASP:HB2	B:262:ASN:ND2	0.469
1	B:330:ILE:HD13	B:352:TYR:CD1	0.469
1	B:340:ASN:CG	B:344:GLU:H	0.469
1	A:177:TYR:CE1	A:181:ILE:HD11	0.468
1	B:148:ALA:HB1	B:149:SER:C	0.468
1	B:228:LEU:HD11	B:263:PHE:CZ	0.468
1	B:242:ILE:O	B:243:ARG:HG2	0.467
1	A:256:PRO:N	A:297:TYR:HE1	0.467
1	A:50:ARG:O	A:51:ASN:HB2	0.466
1	A:371:LEU:O	A:375:LEU:HD23	0.466
1	B:211:LEU:HA	B:214:ILE:HG22	0.466
1	A:40:ASP:HB3	A:144:ASN:CG	0.465
1	A:231:THR:O	A:232:LYS:HG3	0.465
1	B:37:LEU:HD21	B:158:VAL:HG13	0.465
1	B:267:ILE:CG2	B:279:VAL:HG13	0.465
1	A:267:ILE:HD12	A:278:LYS:O	0.464

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:309:ASN:HB3	A:311:PRO:HD2	0.464
1	A:321:GLY:N	A:322:PRO:HD2	0.464
1	A:330:ILE:HD11	A:352:TYR:CB	0.464
1	B:61:LEU:HD23	B:74:VAL:HB	0.464
1	B:181:ILE:CD1	B:363:TYR:CD1	0.464
1	B:288:TRP:CZ3	B:320:LYS:CA	0.464
1	A:59:ARG:HB3	A:59:ARG:NH1	0.463
1	A:88:ILE:HD12	A:125:MET:HE1	0.463
1	A:92:VAL:HG13	A:97:LYS:O	0.463
1	A:167:SER:O	A:171:ARG:HG2	0.463
1	B:49:SER:HA	B:54:PRO:HA	0.463
1	A:328:TRP:CH2	A:330:ILE:CG1	0.462
1	A:388:MET:HG2	A:391:LEU:CD1	0.462
1	B:101:ILE:O	B:101:ILE:HG23	0.462
1	A:391:LEU:HD13	B:391:LEU:HD11	0.461
1	B:386:ASP:HA	B:389:ASN:OD1	0.461
1	A:45:PHE:CZ	A:58:THR:HG22	0.460
1	A:191:TRP:HA	A:191:TRP:HE3	0.460
1	A:387:LYS:O	A:391:LEU:HG	0.460
1	B:88:ILE:O	B:92:VAL:HG23	0.460
1	B:225:VAL:CG1	B:267:ILE:CD1	0.460
1	B:242:ILE:O	B:242:ILE:HG12	0.460
1	B:339:VAL:HG12	B:342:LYS:HA	0.460

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:274:LYS:HD3	A:275:GLU:N	0.459
1	A:298:VAL:CG2	A:348:VAL:CG2	0.459
1	A:320:LYS:HB3	A:352:TYR:CZ	0.459
1	B:70:GLU:CD	B:70:GLU:H	0.459
1	B:307:MET:HE2	B:313:ASP:CG	0.458
1	B:26:VAL:O	B:30:LEU:HG	0.457
1	A:337:PRO:HB3	A:345:ILE:CG2	0.456
1	A:374:PHE:C	A:374:PHE:CD1	0.456
1	B:82:PHE:CZ	B:114:LEU:HB2	0.455
1	B:148:ALA:CB	B:149:SER:CA	0.455
1	B:166:ILE:HG23	B:167:SER:N	0.455
1	B:298:VAL:O	B:345:ILE:HD13	0.455
1	A:7:ILE:CG2	A:32:ARG:HG2	0.454
1	A:237:TYR:CD1	A:237:TYR:N	0.454
1	A:244:LEU:N	A:244:LEU:HD12	0.454
1	A:266:ILE:CG2	A:280:ILE:HB	0.454
1	A:314:GLU:HB3	A:315:TYR:CE1	0.454
1	A:388:MET:CE	A:398:ALA:CB	0.454
1	B:15:ILE:CG1	B:25:ILE:CD1	0.454
1	B:204:GLU:HB2	B:265:LYS:HE2	0.454
1	B:184:ARG:NH1	B:367:ILE:HD13	0.454
1	A:146:LEU:HD12	A:147:ASN:OD1	0.453
1	A:174:HIS:NE2	A:178:LEU:HD11	0.453

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:98:PHE:C	B:98:PHE:CD1	0.453
1	B:294:LEU:HD22	B:335:SER:CB	0.453
1	A:197:PHE:O	B:380:LEU:HD13	0.453
1	A:130:ILE:HD11	A:140:VAL:HG21	0.452
1	A:197:PHE:HA	B:380:LEU:CD2	0.452
1	A:391:LEU:CD2	B:395:LYS:CG	0.452
1	B:256:PRO:HB3	B:297:TYR:CE2	0.452
1	A:12:LEU:HD23	B:165:PHE:HA	0.451
1	A:104:VAL:HG11	A:125:MET:CE	0.451
1	A:22:MET:CE	A:170:LEU:CD2	0.451
1	A:328:TRP:CZ3	A:330:ILE:HG13	0.451
1	A:371:LEU:CD1	A:375:LEU:CD2	0.451
1	A:222:ARG:O	A:352:TYR:HD2	0.451
1	A:201:THR:CG2	A:202:ASP:N	0.451
1	B:22:MET:SD	B:26:VAL:HG21	0.450
1	B:95:THR:HB	B:97:LYS:HE3	0.450
1	B:189:LEU:HD11	B:370:THR:CG2	0.450
1	A:107:ASN:HD21	A:109:HIS:HD2	0.450
1	A:166:ILE:HG23	A:167:SER:N	0.449
1	A:22:MET:SD	A:170:LEU:HD23	0.449
1	A:187:GLN:HG2	A:217:TYR:CE1	0.449
1	A:254:LYS:C	A:255:THR:HG23	0.449
1	A:268:ASP:CG	A:288:TRP:CZ2	0.449

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:138:ALA:HB2	B:170:LEU:HD11	0.449
1	B:53:ILE:CG2	B:54:PRO:N	0.449
1	A:12:LEU:HD23	B:165:PHE:CA	0.448
1	A:97:LYS:CB	A:99:PHE:HE2	0.448
1	A:288:TRP:O	A:320:LYS:HE2	0.448
1	A:391:LEU:HD21	B:398:ALA:HA	0.448
1	B:34:SER:OG	B:65:PRO:HD3	0.448
1	B:97:LYS:HA	B:97:LYS:HE2	0.448
1	B:145:LYS:HB3	B:148:ALA:HB2	0.448
1	A:338:ILE:O	A:338:ILE:HG13	0.448
1	A:130:ILE:HD11	A:140:VAL:CG2	0.447
1	B:58:THR:CG2	B:61:LEU:CD2	0.447
1	B:58:THR:CG2	B:61:LEU:CD1	0.447
1	B:222:ARG:HD3	B:270:ILE:HG13	0.447
1	B:235:GLU:HB3	B:257:ASP:OD1	0.447
1	A:201:THR:CG2	A:202:ASP:H	0.447
1	A:98:PHE:C	A:98:PHE:CD2	0.446
1	A:163:LEU:C	A:166:ILE:HG22	0.446
1	A:350:THR:CG2	A:352:TYR:CZ	0.446
1	B:294:LEU:O	B:298:VAL:HG23	0.446
1	A:9:PHE:CD1	B:161:LYS:CD	0.445
1	A:270:ILE:N	A:270:ILE:HD12	0.445
1	A:294:LEU:CD2	A:335:SER:CB	0.445

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:350:THR:CG2	A:352:TYR:CE1	0.445
1	B:191:TRP:CE3	B:213:THR:HG21	0.445
1	B:294:LEU:CD2	B:335:SER:HB2	0.445
1	B:384:THR:O	B:388:MET:HG3	0.445
1	B:395:LYS:HZ3	B:397:ILE:HG13	0.445
1	A:122:THR:OG1	C:1:35G:C4	0.445
1	B:193:ALA:O	B:197:PHE:HD2	0.445
1	A:67:SER:HB2	A:72:ASN:HD21	0.444
1	A:126:MET:HE3	A:156:GLU:CG	0.444
1	A:161:LYS:HG3	A:162:TYR:N	0.444
1	B:310:ALA:HB3	B:311:PRO:HD3	0.444
1	A:85:ASP:O	A:86:ILE:HG12	0.443
1	B:68:LYS:HB3	B:70:GLU:OE2	0.443
1	B:91:TRP:CE2	B:95:THR:CG2	0.443
1	B:294:LEU:CD2	B:335:SER:CB	0.443
1	B:336:LEU:HG	B:368:ILE:HG22	0.443
1	B:244:LEU:CD2	B:245:GLY:H	0.443
1	A:36:LEU:HD23	A:158:VAL:HG21	0.442
1	A:104:VAL:HG22	A:123:VAL:C	0.442
1	A:231:THR:HG23	A:260:GLU:OE1	0.442
1	B:110:PHE:CE1	D:1:35G:O3'	0.442
1	B:141:MET:HG3	B:143:LEU:CD1	0.442
1	A:339:VAL:CG1	A:340:ASN:N	0.442

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:91:TRP:CE2	A:109:HIS:CE1	0.441
1	B:211:LEU:HD23	B:223:TYR:HE2	0.441
1	B:212:TYR:CE2	B:215:ARG:NH2	0.441
1	B:225:VAL:CG1	B:267:ILE:HG12	0.441
1	B:399:GLN:HG2	B:399:GLN:O	0.441
1	A:60:LEU:HD23	A:73:LEU:HA	0.440
1	A:335:SER:C	A:336:LEU:HD12	0.440
1	A:336:LEU:CD1	A:368:ILE:CG2	0.440
1	A:391:LEU:CD2	B:395:LYS:HG3	0.440
1	A:130:ILE:O	A:136:VAL:HG23	0.439
1	A:319:GLN:HG2	A:330:ILE:CB	0.439
1	A:362:GLU:HA	A:365:GLU:CG	0.439
1	A:391:LEU:CD2	B:397:ILE:HD12	0.439
1	B:196:VAL:HG23	B:197:PHE:N	0.439
1	B:252:GLY:N	B:253:PRO:HD3	0.439
1	B:387:LYS:HB2	B:387:LYS:HE2	0.439
1	A:145:LYS:HD3	A:148:ALA:CB	0.438
1	A:132:GLN:HE21	A:171:ARG:HB2	0.438
1	A:201:THR:HG21	A:205:ARG:HB2	0.438
1	A:320:LYS:CG	A:352:TYR:CE1	0.438
1	A:391:LEU:CD2	B:397:ILE:CD1	0.438
1	A:391:LEU:HD23	B:395:LYS:HG3	0.438
1	B:226:GLY:HA2	B:266:ILE:HD12	0.438

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:235:GLU:HB2	B:257:ASP:C	0.438
1	B:388:MET:HB3	B:392:GLU:OE2	0.438
1	B:391:LEU:HD13	B:392:GLU:HA	0.438
1	A:34:SER:HB2	A:65:PRO:HG3	0.437
1	A:88:ILE:HG13	C:1:35G:O3'	0.437
1	B:110:PHE:CD1	D:1:35G:O3'	0.437
1	B:267:ILE:HG23	B:279:VAL:HG13	0.437
1	B:391:LEU:HD11	B:398:ALA:HB1	0.437
1	A:50:ARG:HG2	A:55:GLU:OE2	0.436
1	A:96:LYS:C	A:129:PRO:HG2	0.436
1	A:280:ILE:N	A:280:ILE:HD12	0.436
1	B:59:ARG:C	B:74:VAL:HG12	0.436
1	B:244:LEU:CD2	B:245:GLY:N	0.436
1	B:268:ASP:CG	B:288:TRP:CZ2	0.436
1	A:201:THR:HG23	A:205:ARG:CZ	0.435
1	A:257:ASP:CB	A:300:GLU:O	0.435
1	B:163:LEU:HA	B:166:ILE:HG22	0.435
1	B:295:PRO:HG3	B:350:THR:HG21	0.435
1	A:178:LEU:HB3	B:179:TYR:CD1	0.434
1	A:201:THR:CG2	A:205:ARG:CB	0.434
1	A:234:LYS:HG3	A:235:GLU:OE1	0.434
1	A:320:LYS:CD	A:320:LYS:N	0.434
1	B:24:LYS:O	B:28:LYS:HG2	0.434

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:41:ARG:O	B:143:LEU:HB2	0.434
1	A:291:ILE:CD1	A:318:PHE:HE1	0.434
1	A:1:ARG:HG3	A:2:LEU:H	0.433
1	A:227:LEU:N	A:227:LEU:HD12	0.433
1	A:391:LEU:HD21	B:397:ILE:HD12	0.433
1	B:289:CYS:C	B:320:LYS:HE2	0.433
1	A:59:ARG:CZ	A:59:ARG:HB2	0.432
1	A:188:MET:CE	A:367:ILE:CG2	0.432
1	A:225:VAL:O	A:267:ILE:HG22	0.432
1	A:313:ASP:CB	A:315:TYR:CZ	0.432
1	A:391:LEU:HD21	B:397:ILE:CD1	0.432
1	B:33:LEU:CD2	B:37:LEU:HD21	0.432
1	B:170:LEU:C	B:170:LEU:HD23	0.432
1	B:320:LYS:CA	B:320:LYS:CE	0.432
1	A:53:ILE:HA	A:54:PRO:HD2	0.431
1	B:69:PHE:C	B:69:PHE:CD2	0.431
1	A:336:LEU:HD13	A:368:ILE:HG21	0.430
1	A:398:ALA:HB2	B:391:LEU:HB2	0.430
1	B:138:ALA:CB	B:170:LEU:HD11	0.430
1	B:297:TYR:C	B:297:TYR:CD1	0.430
1	B:303:PHE:CD2	B:303:PHE:N	0.430
1	A:163:LEU:HA	A:166:ILE:HG22	0.429
1	B:211:LEU:HD23	B:223:TYR:CE2	0.429

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:285:ALA:O	B:291:ILE:HD13	0.429
1	B:377:TRP:O	B:380:LEU:HB3	0.429
1	B:53:ILE:HG22	B:54:PRO:N	0.429
1	A:218:LEU:CB	A:220:CYS:SG	0.428
1	A:259:ARG:H	A:300:GLU:HG2	0.428
1	B:204:GLU:CB	B:265:LYS:HE2	0.428
1	B:336:LEU:CD2	B:368:ILE:CG2	0.428
1	B:397:ILE:HD12	B:398:ALA:N	0.428
1	A:14:GLU:HG3	A:25:ILE:HD13	0.427
1	A:168:LEU:HD13	B:15:ILE:HG21	0.427
1	A:235:GLU:HB3	A:257:ASP:CG	0.427
1	A:257:ASP:HB2	A:301:ASN:N	0.427
1	A:168:LEU:CD2	B:168:LEU:CD2	0.427
1	A:391:LEU:O	A:394:ARG:HB2	0.426
1	B:33:LEU:C	B:33:LEU:HD13	0.426
1	B:225:VAL:CG1	B:267:ILE:CG1	0.426
1	B:319:GLN:CG	B:330:ILE:CB	0.426
1	B:320:LYS:HG2	B:352:TYR:HH	0.426
1	B:344:GLU:HG3	B:345:ILE:N	0.426
1	B:237:TYR:CG	B:237:TYR:O	0.426
1	B:143:LEU:HD22	D:1:35G:O6	0.426
1	A:80:THR:HG21	A:114:LEU:HD21	0.425
1	A:201:THR:HG21	A:205:ARG:HB3	0.425

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:391:LEU:HA	B:395:LYS:HG2	0.425
1	A:2:LEU:O	A:2:LEU:HD22	0.424
1	A:73:LEU:HD13	A:74:VAL:N	0.424
1	A:22:MET:SD	A:170:LEU:CD2	0.424
1	A:193:ALA:O	A:197:PHE:CD2	0.424
1	A:211:LEU:HD22	A:225:VAL:HG21	0.424
1	A:228:LEU:CD2	A:261:VAL:CG1	0.424
1	B:64:THR:HG22	B:65:PRO:CD	0.424
1	A:166:ILE:CG2	A:167:SER:N	0.424
1	B:158:VAL:CG1	B:159:PHE:N	0.424
1	A:294:LEU:HD21	A:335:SER:CB	0.423
1	B:185:ARG:N	B:367:ILE:CD1	0.423
1	A:145:LYS:HZ2	A:152:SER:H	0.423
1	B:169:VAL:CG1	B:170:LEU:N	0.423
1	A:82:PHE:CZ	A:114:LEU:CB	0.422
1	A:206:GLN:CG	A:382:THR:HG22	0.422
1	A:254:LYS:O	A:255:THR:HG23	0.422
1	A:256:PRO:HD3	A:297:TYR:HE1	0.422
1	B:58:THR:CG2	B:61:LEU:HD11	0.422
1	A:104:VAL:CG2	A:105:LYS:N	0.422
1	A:291:ILE:CG2	A:292:SER:N	0.422
1	A:384:THR:CG2	A:385:TYR:N	0.422
1	A:212:TYR:CZ	A:215:ARG:NH1	0.421

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:304:ILE:HD11	A:336:LEU:HG	0.421
1	A:391:LEU:HD23	B:395:LYS:CG	0.421
1	B:189:LEU:HD21	B:370:THR:HG21	0.421
1	B:362:GLU:CA	B:365:GLU:HG2	0.421
1	A:291:ILE:HG23	A:292:SER:N	0.421
1	B:290:LEU:CD2	B:290:LEU:N	0.421
1	B:388:MET:O	B:391:LEU:N	0.421
1	A:395:LYS:C	A:397:ILE:N	0.420
1	B:22:MET:HB2	B:173:HIS:CD2	0.420
1	B:228:LEU:CD1	B:261:VAL:CG1	0.420
1	B:200:LEU:CD1	B:385:TYR:CD1	0.420
1	A:11:LEU:O	A:14:GLU:HG2	0.419
1	A:8:LEU:CD2	B:8:LEU:HD23	0.419
1	B:104:VAL:HG12	B:123:VAL:C	0.419
1	B:228:LEU:HD22	B:347:GLY:HA2	0.419
1	A:320:LYS:CE	A:320:LYS:N	0.419
1	A:4:GLU:HB3	A:162:TYR:OH	0.418
1	A:145:LYS:HD2	A:151:PHE:CD1	0.418
1	A:185:ARG:CA	A:367:ILE:HG23	0.418
1	B:185:ARG:HA	B:367:ILE:HG13	0.418
1	A:298:VAL:HG23	A:348:VAL:CG2	0.417
1	B:11:LEU:O	B:14:GLU:HG2	0.417
1	B:211:LEU:HD22	B:269:TYR:CE1	0.417

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:254:LYS:O	B:255:THR:HG23	0.417
1	B:294:LEU:HD23	B:298:VAL:HG23	0.417
1	B:296:THR:O	B:300:GLU:HG3	0.417
1	B:220:CYS:SG	B:351:PHE:HB3	0.417
1	A:158:VAL:CG1	A:159:PHE:N	0.417
1	B:251:LYS:CD	B:251:LYS:H	0.417
1	B:379:VAL:O	B:379:VAL:HG12	0.417
1	A:185:ARG:HA	A:367:ILE:HG23	0.416
1	B:37:LEU:O	B:38:ALA:HB3	0.416
1	B:288:TRP:CZ3	B:320:LYS:CB	0.416
1	B:166:ILE:CG2	B:167:SER:N	0.416
1	A:41:ARG:HD3	A:62:ASN:CA	0.415
1	A:195:LYS:CG	A:209:LYS:HG2	0.415
1	A:319:GLN:HG2	A:330:ILE:HB	0.415
1	A:362:GLU:CA	A:365:GLU:HG2	0.415
1	B:132:GLN:HB2	B:137:LEU:HD11	0.415
1	B:204:GLU:HG3	B:265:LYS:HZ1	0.415
1	B:257:ASP:HB2	B:301:ASN:N	0.415
1	B:257:ASP:CA	B:300:GLU:HB3	0.415
1	A:200:LEU:HB3	A:385:TYR:CD1	0.414
1	B:159:PHE:CE2	B:163:LEU:CD1	0.414
1	B:218:LEU:O	B:219:ASN:HB2	0.414
1	A:201:THR:HG23	A:205:ARG:NE	0.413

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:188:MET:HA	B:214:ILE:HD13	0.413
1	B:250:TYR:CD2	B:251:LYS:O	0.413
1	B:333:VAL:CG1	B:334:LEU:N	0.413
1	B:339:VAL:CG1	B:340:ASN:N	0.413
1	A:166:ILE:O	A:170:LEU:HG	0.412
1	A:222:ARG:C	A:352:TYR:HD2	0.412
1	A:254:LYS:HB3	A:254:LYS:O	0.412
1	A:319:GLN:CG	A:330:ILE:CB	0.412
1	B:61:LEU:N	B:61:LEU:HD22	0.412
1	B:76:PRO:HG3	B:358:LYS:CE	0.412
1	A:168:LEU:CD2	B:168:LEU:HD23	0.412
1	A:59:ARG:CB	A:59:ARG:CZ	0.411
1	A:97:LYS:HA	A:97:LYS:HD3	0.411
1	A:351:PHE:CD1	A:351:PHE:N	0.411
1	A:385:TYR:HE1	A:399:GLN:HB2	0.411
1	B:64:THR:HG22	B:65:PRO:N	0.411
1	B:214:ILE:CD1	B:217:TYR:HB2	0.411
1	B:392:GLU:O	B:393:ASN:C	0.411
1	B:320:LYS:CE	B:320:LYS:N	0.411
1	B:393:ASN:O	B:394:ARG:C	0.411
1	A:26:VAL:O	A:30:LEU:HG	0.410
1	A:283:PRO:HA	A:284:PRO:HD3	0.410
1	B:287:HIS:CG	B:290:LEU:HD23	0.410

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:122:THR:CG2	C:1:35G:C5	0.410
1	A:203:ILE:CG2	A:204:GLU:N	0.410
1	A:237:TYR:CD2	A:237:TYR:O	0.409
1	B:174:HIS:NE2	B:178:LEU:HD11	0.409
1	B:240:TRP:CB	B:243:ARG:HD2	0.409
1	A:288:TRP:CD1	A:288:TRP:H	0.408
1	A:222:ARG:O	A:352:TYR:CD2	0.408
1	B:320:LYS:C	B:322:PRO:HD2	0.408
1	B:104:VAL:HG13	B:105:LYS:N	0.408
1	B:111:SER:O	D:1:35G:C5'	0.408
1	A:33:LEU:CD2	A:162:TYR:CD2	0.407
1	A:211:LEU:HD21	A:225:VAL:HG21	0.407
1	A:318:PHE:O	A:319:GLN:HG3	0.407
1	A:288:TRP:CZ3	A:320:LYS:HA	0.407
1	A:340:ASN:CG	A:344:GLU:H	0.407
1	B:266:ILE:CG2	B:280:ILE:HB	0.407
1	B:397:ILE:C	B:397:ILE:HD12	0.407
1	B:256:PRO:N	B:297:TYR:HE2	0.407
1	B:340:ASN:O	B:342:LYS:N	0.407
1	A:337:PRO:HB3	A:345:ILE:HG23	0.406
1	A:206:GLN:CD	A:382:THR:CG2	0.406
1	B:58:THR:HG22	B:61:LEU:CD2	0.406
1	A:297:TYR:HD1	A:314:GLU:HB2	0.405

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:201:THR:HG23	B:206:GLN:HB2	0.405
1	B:256:PRO:CD	B:297:TYR:HE2	0.405
1	B:228:LEU:N	B:228:LEU:HD22	0.405
1	A:124:ASN:OD1	A:151:PHE:CE2	0.405
1	A:188:MET:HE1	A:367:ILE:HG22	0.404
1	A:225:VAL:HB	A:267:ILE:CG2	0.404
1	A:257:ASP:CG	A:301:ASN:HA	0.404
1	B:319:GLN:HB3	B:330:ILE:HG13	0.404
1	B:320:LYS:CD	B:320:LYS:N	0.404
1	B:200:LEU:CD1	B:385:TYR:CB	0.403
1	B:374:PHE:C	B:374:PHE:CD1	0.403
1	A:147:ASN:O	A:148:ALA:HB2	0.403
1	A:21:SER:HB3	A:24:LYS:CG	0.402
1	A:114:LEU:C	A:114:LEU:CD1	0.402
1	A:145:LYS:HB2	A:151:PHE:CZ	0.402
1	A:256:PRO:CB	A:297:TYR:CE1	0.402
1	A:391:LEU:HD22	B:395:LYS:CB	0.402
1	A:395:LYS:CE	A:397:ILE:CD1	0.402
1	B:5:CYS:O	B:9:PHE:CD2	0.402
1	B:319:GLN:HG2	B:330:ILE:CB	0.402
1	A:13:THR:HG23	A:14:GLU:N	0.402
1	A:385:TYR:CE2	A:389:ASN:OD1	0.402
1	A:87:GLY:CA	C:1:35G:P	0.402

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:84:LEU:C	A:86:ILE:H	0.401
1	A:294:LEU:C	A:294:LEU:CD2	0.401
1	A:378:SER:HA	B:197:PHE:CE1	0.401
1	B:33:LEU:HD11	B:159:PHE:HD1	0.401
1	B:170:LEU:C	B:170:LEU:CD2	0.401
1	B:257:ASP:CB	B:300:GLU:O	0.401
1	B:304:ILE:CG2	B:336:LEU:CD1	0.401
1	A:18:GLU:HG3	B:171:ARG:NH1	0.400
1	A:338:ILE:HG12	A:347:GLY:CA	0.400
1	A:297:TYR:CD2	A:315:TYR:HE1	0.400
1	B:67:SER:HB3	B:72:ASN:HD21	0.400

Torsion angles: Protein backbone ?

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	794	716	42	36

Detailed list of outliers are tabulated below.

Torsion angles: Protein sidechains ?

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	724	620	72	32

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	22	MET
1	A	28	LYS

Model ID	Chain	Residue ID	Residue type
1	A	50	ARG
1	A	56	VAL
1	A	187	GLN
1	A	209	LYS
1	A	222	ARG
1	A	235	GLU
1	A	251	LYS
1	A	254	LYS
1	A	260	GLU
1	A	315	TYR
1	A	320	LYS
1	A	342	LYS
1	A	388	MET
1	A	399	GLN
1	B	107	ASN
1	B	200	LEU
1	B	233	GLU
1	B	242	ILE
1	B	251	LYS
1	B	254	LYS
1	B	267	ILE
1	B	274	LYS
1	B	315	TYR

Model ID	Chain	Residue ID	Residue type
1	B	320	LYS
1	B	336	LEU
1	B	390	LYS
1	B	391	LEU
1	B	395	LYS
1	B	397	ILE
1	B	399	GLN

Fit of model to data used for modeling ?

Crosslinking-MS

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

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