Integrative Structure Validation Report

July 22, 2024 - 05:42 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	9A8D
PDB-Dev ID	PDBDEV_00000536
Structure Title	Integrative model of SARS-CoV-2 Replicase polyprotein 1ab
Structure Authors	Schneidman, D; Kalisman, N

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

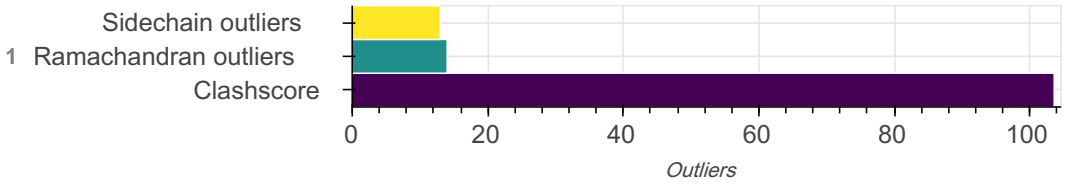
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 1 subunits in each model. A total of 4 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 8 flexible or non-rigid units.

Entry composition

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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	SARS-CoV-2 Replicase polyprotein 1ab	A	A	638

Datasets used for modeling

There are 4 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	PRIDE	PXD023487
2	De Novo model	Not available	Not available
3	Comparative model	Not available	Not available
4	Experimental model	PDB	3LD1

Representation

This entry has only one representation and includes 0 rigid bodies and 8 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	346-437, 1-104, 105-132, 133-275, 276-345, 346-358, 359-511, 512-638

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	Modeling with CombDock	CombDock with AlphaFold2 domains and crosslinks as an input	None	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	UCSF ChimeraX	1.2/v9	model building	https://www.rbvi.ucsf.edu/chimerax/
2	CombDock	Not available	assembly	http://bioinfo3d.cs.tau.ac.il/CombDock/download/

Data quality

Crosslinking-MS

Validation for this section is under development.

Model quality

For models with atomic structures, molprobity 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 161 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	158.64	1
C-N-CA	121.70	145.98	1
CA-CB-CG	113.80	101.15	1
C-N-CA	121.70	143.80	1
C-N-CA	121.70	141.61	1
N-CA-CB	110.50	128.78	1
CA-CB-CG	112.60	102.11	1
C-N-CA	121.70	139.92	1
CA-C-N	116.90	131.88	1
C-N-CA	121.70	138.68	1
C-CA-CB	110.10	92.38	1
C-CA-CB	110.10	93.26	1
CA-CB-CG	112.60	103.91	1
CA-CB-CG	113.90	98.87	1
CA-CB-CG	113.80	105.73	1
C-N-CA	121.70	107.33	1
N-CA-C	111.00	133.28	1
CA-CB-CG	113.80	105.85	1
CA-CB-CG	113.80	105.93	1
CA-C-N	116.20	131.76	1
CA-CB-CG	112.60	105.05	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	107.99	1
N-CA-C	111.00	90.26	1
CA-CB-CG	113.80	106.53	1
N-CA-C	111.00	131.32	1
CA-C-N	116.20	101.95	1
N-CA-CB	110.50	122.36	1
CA-CB-CG	113.80	106.90	1
C-N-CA	121.70	109.28	1
CA-CB-CG	112.60	105.70	1
N-CA-CB	110.50	121.60	1
C-CA-CB	110.10	97.84	1
N-CA-CB	110.50	121.43	1
CA-CB-CG	114.10	126.70	1
C-CA-CB	110.10	98.18	1
C-CA-CB	110.10	98.27	1
CA-CB-CG	112.60	106.46	1
CA-CB-CG	113.80	107.75	1
CA-CB-CG	112.60	106.57	1
CA-C-N	116.20	128.12	1
CA-CB-CG	112.60	106.64	1
CA-CB-CG	113.80	108.03	1
C-CA-CB	110.10	121.03	1
CA-CB-CG	112.60	106.85	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	106.88	1
CA-CB-CG	113.90	103.62	1
C-CA-CB	110.10	99.34	1
N-CA-CB	111.50	121.09	1
C-CA-CB	110.10	99.39	1
C-N-CA	121.70	131.84	1
C-N-CA	121.70	111.59	1
CA-CB-CG	112.60	107.03	1
CA-CB-CG	113.80	108.26	1
CA-CB-CG	113.80	108.31	1
CA-CB-CG	112.60	107.17	1
CA-CB-CG	112.60	107.18	1
C-N-CA	121.70	112.00	1
CB-CG-CD	112.60	103.53	1
CA-CB-CG	112.60	107.28	1
C-CA-CB	110.10	100.05	1
CA-CB-CG	113.80	108.51	1
C-N-CA	121.70	131.21	1
N-CA-C	111.00	125.77	1
N-CA-CB	110.50	119.47	1
C-N-CA	121.70	131.14	1
O-C-N	123.00	114.65	1
CA-CB-CG	112.60	107.39	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	100.26	1
C-N-CA	121.70	131.00	1
CB-CG-CD	112.60	103.82	1
N-CA-CB	110.50	119.22	1
CA-CB-OG	111.10	121.34	1
CA-CB-CG	113.80	108.70	1
CA-CB-CG	112.60	107.51	1
C-CA-CB	110.50	102.93	1
CA-CB-CG	112.60	107.62	1
C-CA-CB	110.10	100.70	1
N-CA-C	111.00	124.72	1
N-CA-CB	110.50	118.72	1
CD2-NE2-CE1	109.00	104.19	1
CA-CB-CG	112.60	107.80	1
CA-CB-CG	112.60	107.81	1
CA-CB-CG	113.80	109.03	1
CA-C-O	120.80	112.74	1
CB-CG-CD	112.60	104.57	1
C-CA-CB	110.10	101.13	1
CB-CG-CD	112.60	120.61	1
C-CA-CB	110.10	101.16	1
CA-CB-CG	113.80	109.12	1
CA-CB-CG	113.80	109.14	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	101.26	1
CA-CB-CG	112.60	107.96	1
C-N-CA	121.70	130.03	1
CD2-NE2-CE1	109.00	104.40	1
C-N-CA	121.70	113.43	1
CA-CB-CG	112.60	108.01	1
C-CA-CB	110.10	101.39	1
CD-NE-CZ	124.40	117.98	1
CA-C-N	116.90	123.77	1
C-N-CA	121.70	113.46	1
CA-CB-CG	112.60	108.04	1
CA-C-O	120.80	113.05	1
CA-CB-CG2	110.50	102.83	1
CA-C-O	120.80	113.14	1
C-N-CA	121.70	129.80	1
CA-CB-CG	112.60	108.10	1
C-CA-CB	110.10	101.56	1
CB-CG-CD	112.60	104.98	1
CD2-NE2-CE1	109.00	104.52	1
CA-CB-CG	112.60	108.13	1
C-N-CA	121.70	113.66	1
CD2-NE2-CE1	109.00	104.53	1
CA-CB-CG	113.80	109.34	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD2-NE2-CE1	109.00	104.55	1
CD-NE-CZ	124.40	118.17	1
C-CA-CB	110.10	118.55	1
C-CA-CB	111.40	102.96	1
CD2-NE2-CE1	109.00	104.56	1
C-CA-CB	110.10	101.73	1
C-CA-CB	110.10	118.47	1
C-CA-CB	110.10	118.43	1
N-CA-CB	110.50	117.94	1
C-CA-CB	110.10	101.78	1
CB-CG-CD	112.60	105.18	1
CA-CB-CG	114.10	105.37	1
C-CA-CB	110.10	101.81	1
CA-CB-CG	113.80	109.45	1
C-CA-CB	110.10	101.83	1
C-N-CA	121.70	113.93	1
CA-C-O	120.80	113.47	1
CD2-NE2-CE1	109.00	104.71	1
C-N-CA	121.70	129.42	1
C-CA-CB	110.10	118.23	1
CD2-NE2-CE1	109.00	104.73	1
C-N-CA	121.70	114.04	1
C-CA-CB	110.10	102.03	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	124.64	1
C-N-CA	121.70	129.23	1
CD2-NE2-CE1	109.00	104.83	1
CA-CB-CG	112.60	108.43	1
CB-CG-CD	112.60	105.53	1
C-CA-CB	111.40	103.50	1
C-CA-CB	110.50	104.28	1
C-N-CA	121.70	129.16	1
ND1-CE1-NE2	108.40	112.54	1
C-N-CA	121.70	114.26	1
CA-CB-CG	112.60	108.47	1
N-CA-C	111.00	122.55	1
CG1-CB-CG2	110.80	119.86	1
CA-CB-CG	112.60	108.49	1
C-N-CA	121.70	129.10	1
CB-CG-CD	112.60	105.62	1
C-CA-CB	110.10	102.31	1
N-CA-CB	103.00	107.50	1
CA-C-N	116.20	124.35	1
CD-NE-CZ	124.40	118.72	1
CA-CB-OG1	109.60	103.51	1
C-N-CA	121.70	114.40	1
CA-CB-CG	112.60	108.55	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	109.10	117.99	1
N-CA-C	112.10	122.12	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	103.58	1028

All 1028 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	A:348:SER:CA	A:348:SER:N	1.563
1	A:410:LEU:HD12	A:412:THR:HG22	1.159
1	A:96:PRO:HD3	A:259:VAL:HG12	1.124
1	A:453:GLU:HB3	A:557:LYS:HB3	1.116
1	A:347:LYS:CB	A:444:LEU:HD11	1.113
1	A:338:LYS:HE2	A:539:LYS:HB2	1.110
1	A:377:ASN:HB2	A:380:ARG:HG3	1.109
1	A:381:VAL:HA	A:384:LYS:HB2	1.109
1	A:489:LYS:HD3	A:502:VAL:HG21	1.108
1	A:556:PRO:HG3	A:607:GLY:HA2	1.108
1	A:347:LYS:HB2	A:444:LEU:HD11	1.106
1	A:453:GLU:HG3	A:558:GLU:HB2	1.099
1	A:347:LYS:CA	A:426:VAL:HG11	1.095
1	A:389:ILE:HG21	A:398:LEU:HD21	1.085
1	A:103:THR:HG21	A:106:PRO:HD3	1.083

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:275:GLN:HB2	A:277:GLU:H	1.082
1	A:505:PHE:HA	A:514:ILE:HD12	1.074
1	A:251:ILE:HB	A:271:LEU:HD21	1.073
1	A:577:VAL:HG12	A:603:VAL:HG12	1.068
1	A:485:VAL:HG22	A:491:ILE:HD11	1.067
1	A:132:CYS:HA	A:183:ASN:HB2	1.065
1	A:338:LYS:HE3	A:445:LYS:HB2	1.065
1	A:341:TRP:HB2	A:348:SER:HB3	1.060
1	A:443:LYS:HE3	A:513:ILE:HG22	1.055
1	A:375:ALA:HA	A:382:LEU:HD21	1.053
1	A:520:LEU:HD13	A:534:LYS:HE2	1.048
1	A:335:LYS:HG2	A:546:GLU:HB2	1.040
1	A:96:PRO:HB3	A:259:VAL:HA	1.037
1	A:341:TRP:HB2	A:348:SER:CB	1.028
1	A:381:VAL:HG12	A:385:ALA:HB2	1.021
1	A:116:PHE:HB2	A:234:VAL:HA	1.019
1	A:94:VAL:HA	A:225:ALA:HB1	1.008
1	A:258:VAL:HG21	A:266:LEU:HD23	0.998
1	A:465:GLY:HA2	A:468:ILE:HG12	0.998
1	A:34:THR:HG21	A:548:GLY:HA3	0.989
1	A:338:LYS:HD2	A:541:VAL:HG23	0.984
1	A:415:LEU:HA	A:418:MET:HE2	0.983
1	A:505:PHE:CD2	A:514:ILE:HB	0.982

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:446:PRO:HD3	A:539:LYS:HD3	0.980
1	A:447:VAL:HG22	A:448:LEU:HD22	0.980
1	A:338:LYS:HG3	A:445:LYS:CG	0.977
1	A:490:GLU:HA	A:495:VAL:HB	0.977
1	A:347:LYS:HA	A:426:VAL:HG11	0.974
1	A:348:SER:HA	A:348:SER:N	0.974
1	A:348:SER:HA	A:441:TYR:OH	0.970
1	A:398:LEU:HD23	A:405:MET:HG3	0.962
1	A:14:ASP:HB3	A:216:ILE:HD12	0.958
1	A:94:VAL:HG21	A:230:VAL:CG2	0.955
1	A:338:LYS:CD	A:541:VAL:HG23	0.947
1	A:338:LYS:HG3	A:445:LYS:HG2	0.945
1	A:374:THR:HG22	A:381:VAL:HG11	0.944
1	A:75:PHE:HB3	A:106:PRO:HD2	0.942
1	A:488:ALA:HA	A:496:GLN:HB3	0.941
1	A:95:PHE:HB3	A:96:PRO:HD2	0.940
1	A:116:PHE:CG	A:234:VAL:HG13	0.939
1	A:486:THR:H	A:503:ASN:HD21	0.933
1	A:445:LYS:HD3	A:539:LYS:CD	0.929
1	A:570:GLU:HB3	A:599:VAL:HG12	0.928
1	A:341:TRP:CZ2	A:427:GLN:HG2	0.927
1	A:410:LEU:CD1	A:412:THR:HG22	0.927
1	A:347:LYS:HB3	A:444:LEU:HD21	0.923

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:515:ILE:HD12	A:520:LEU:HD12	0.923
1	A:338:LYS:HG2	A:539:LYS:HG3	0.922
1	A:377:ASN:HB2	A:380:ARG:CG	0.914
1	A:338:LYS:HD2	A:541:VAL:CG2	0.912
1	A:22:LYS:HD3	A:219:LYS:CE	0.911
1	A:415:LEU:CA	A:418:MET:HE2	0.909
1	A:483:GLN:HG2	A:507:ALA:HA	0.909
1	A:489:LYS:HD3	A:502:VAL:CG2	0.908
1	A:455:PHE:CZ	A:472:ILE:HB	0.907
1	A:116:PHE:CD1	A:234:VAL:HG22	0.906
1	A:341:TRP:CB	A:348:SER:HB3	0.906
1	A:258:VAL:HG21	A:266:LEU:CD2	0.903
1	A:451:LEU:HD12	A:502:VAL:HG12	0.903
1	A:491:ILE:HD13	A:503:ASN:HB3	0.901
1	A:341:TRP:HA	A:347:LYS:C	0.899
1	A:508:LEU:HD11	A:519:LYS:CD	0.899
1	A:116:PHE:HE2	A:129:PRO:HG3	0.898
1	A:336:ALA:HB2	A:346:GLN:HG3	0.895
1	A:490:GLU:CA	A:495:VAL:HB	0.895
1	A:132:CYS:HA	A:183:ASN:CB	0.894
1	A:290:ASN:HB2	A:420:TYR:CZ	0.894
1	A:96:PRO:CB	A:259:VAL:HA	0.892
1	A:381:VAL:CG1	A:385:ALA:HB2	0.891

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:531:THR:HB	A:534:LYS:HD3	0.891
1	A:275:GLN:HB2	A:277:GLU:N	0.890
1	A:520:LEU:CD1	A:534:LYS:HE2	0.889
1	A:347:LYS:HD3	A:449:ASP:CA	0.884
1	A:338:LYS:CE	A:445:LYS:HB2	0.883
1	A:341:TRP:HA	A:347:LYS:O	0.883
1	A:116:PHE:CD2	A:234:VAL:HG13	0.881
1	A:389:ILE:HG23	A:393:ILE:HG13	0.878
1	A:348:SER:HA	A:441:TYR:CZ	0.874
1	A:418:MET:SD	A:472:ILE:HG21	0.870
1	A:486:THR:HB	A:489:LYS:HD2	0.870
1	A:476:ALA:HB3	A:487:CYS:SG	0.862
1	A:251:ILE:HB	A:271:LEU:CD2	0.861
1	A:75:PHE:CD1	A:106:PRO:HG2	0.858
1	A:103:THR:CG2	A:106:PRO:HD3	0.858
1	A:335:LYS:HG2	A:546:GLU:CB	0.858
1	A:447:VAL:HG13	A:448:LEU:H	0.856
1	A:274:LEU:HB3	A:277:GLU:CD	0.848
1	A:508:LEU:HD11	A:519:LYS:HD3	0.848
1	A:508:LEU:CD2	A:519:LYS:HB2	0.841
1	A:414:ASN:O	A:418:MET:HG3	0.840
1	A:415:LEU:HA	A:418:MET:CE	0.839
1	A:445:LYS:HD3	A:539:LYS:HD3	0.839

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:389:ILE:CG2	A:398:LEU:HD21	0.836
1	A:499:PHE:O	A:502:VAL:HG22	0.836
1	A:276:LYS:HZ1	A:527:GLU:HG3	0.836
1	A:111:LYS:H	A:111:LYS:HD3	0.835
1	A:400:LEU:HD22	A:421:ILE:HD11	0.835
1	A:96:PRO:CD	A:259:VAL:HG12	0.834
1	A:60:TRP:HD1	A:97:LEU:HD11	0.834
1	A:346:GLN:HB3	A:449:ASP:OD1	0.834
1	A:348:SER:H	A:426:VAL:CG2	0.834
1	A:449:ASP:O	A:453:GLU:HG2	0.833
1	A:103:THR:HB	A:105:GLN:HA	0.831
1	A:338:LYS:HE3	A:446:PRO:HD3	0.829
1	A:94:VAL:HG23	A:225:ALA:HB1	0.828
1	A:338:LYS:HE2	A:539:LYS:CB	0.828
1	A:610:LEU:HD23	A:621:ALA:HA	0.828
1	A:537:TYR:CE2	A:562:LEU:HB3	0.827
1	A:338:LYS:HB2	A:541:VAL:N	0.826
1	A:377:ASN:CB	A:380:ARG:HG3	0.825
1	A:338:LYS:HB2	A:540:CYS:HA	0.824
1	A:347:LYS:HG3	A:426:VAL:HG12	0.824
1	A:469:VAL:O	A:472:ILE:HG22	0.824
1	A:22:LYS:HD3	A:219:LYS:HD2	0.823
1	A:342:ASN:HB2	A:347:LYS:H	0.823

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:389:ILE:HG21	A:398:LEU:CD2	0.821
1	A:464:ASP:O	A:468:ILE:HG23	0.820
1	A:488:ALA:HA	A:496:GLN:CB	0.820
1	A:547:THR:HG21	A:559:ILE:HD11	0.820
1	A:103:THR:HB	A:105:GLN:CG	0.817
1	A:94:VAL:HG21	A:230:VAL:HG22	0.815
1	A:346:GLN:C	A:347:LYS:HD2	0.815
1	A:374:THR:HA	A:381:VAL:HB	0.815
1	A:486:THR:CB	A:489:LYS:HD2	0.815
1	A:157:VAL:HG12	A:158:LYS:HG3	0.814
1	A:275:GLN:HB3	A:277:GLU:OE1	0.814
1	A:74:PRO:CG	A:230:VAL:HG21	0.813
1	A:613:ILE:HG13	A:616:THR:OG1	0.813
1	A:338:LYS:HA	A:541:VAL:HB	0.811
1	A:349:ILE:HA	A:430:SER:OG	0.810
1	A:426:VAL:O	A:429:THR:HG22	0.810
1	A:342:ASN:HB2	A:346:GLN:HB2	0.806
1	A:19:GLU:HA	A:22:LYS:HD2	0.804
1	A:342:ASN:HB2	A:347:LYS:N	0.804
1	A:347:LYS:HD3	A:449:ASP:HA	0.804
1	A:465:GLY:CA	A:468:ILE:HG12	0.804
1	A:425:VAL:HG23	A:428:LEU:HD12	0.803
1	A:414:ASN:ND2	A:469:VAL:HB	0.803

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:231:PHE:CE2	A:245:PRO:HG3	0.802
1	A:341:TRP:CD1	A:348:SER:N	0.802
1	A:283:ILE:HD13	A:287:PHE:HD1	0.800
1	A:8:ASN:HD22	A:627:MET:HE1	0.799
1	A:75:PHE:CG	A:106:PRO:HG2	0.796
1	A:22:LYS:HD3	A:219:LYS:CD	0.795
1	A:12:GLY:HA3	A:218:ARG:HH21	0.792
1	A:83:PHE:CD2	A:85:THR:HG22	0.791
1	A:323:VAL:HG12	A:329:PHE:HB2	0.790
1	A:338:LYS:HE3	A:539:LYS:HD3	0.789
1	A:534:LYS:HB3	A:631:ASN:ND2	0.787
1	A:403:ALA:O	A:407:THR:HG22	0.786
1	A:251:ILE:HD13	A:255:HIS:O	0.785
1	A:282:ASN:OD1	A:332:THR:HG23	0.785
1	A:489:LYS:HG2	A:499:PHE:CB	0.785
1	A:152:GLN:HE22	A:168:ASN:HD22	0.785
1	A:94:VAL:HG21	A:230:VAL:HG23	0.784
1	A:140:LEU:HB3	A:175:THR:HG22	0.784
1	A:274:LEU:HB3	A:277:GLU:OE2	0.783
1	A:397:SER:O	A:403:ALA:HB1	0.782
1	A:119:ARG:HG3	A:246:ARG:CZ	0.776
1	A:119:ARG:HG3	A:246:ARG:NE	0.770
1	A:446:PRO:HG3	A:539:LYS:HE3	0.770

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:512:SER:HB3	A:520:LEU:O	0.770
1	A:176:THR:HG21	A:226:PHE:CE1	0.769
1	A:103:THR:C	A:105:GLN:H	0.767
1	A:445:LYS:HB3	A:541:VAL:CG2	0.767
1	A:485:VAL:CG1	A:491:ILE:HG12	0.767
1	A:338:LYS:CE	A:539:LYS:HB2	0.766
1	A:67:LYS:HD2	A:76:GLU:OE2	0.765
1	A:453:GLU:CG	A:558:GLU:HB2	0.765
1	A:554:LYS:HG2	A:578:LEU:HD21	0.765
1	A:348:SER:N	A:441:TYR:OH	0.765
1	A:339:GLY:HA2	A:445:LYS:HE2	0.764
1	A:348:SER:H	A:426:VAL:HG21	0.764
1	A:423:GLY:O	A:426:VAL:HG22	0.764
1	A:611:LEU:HB2	A:622:LEU:HD21	0.764
1	A:258:VAL:CG2	A:266:LEU:HD23	0.763
1	A:505:PHE:HA	A:514:ILE:CD1	0.763
1	A:96:PRO:HG2	A:99:SER:CB	0.762
1	A:363:VAL:HG12	A:367:ILE:HD13	0.762
1	A:485:VAL:HG11	A:491:ILE:HG12	0.761
1	A:443:LYS:CE	A:513:ILE:HG22	0.760
1	A:96:PRO:HG2	A:99:SER:HB3	0.758
1	A:523:LEU:HB2	A:530:VAL:HG22	0.758
1	A:339:GLY:N	A:445:LYS:HG2	0.754

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:140:LEU:HB3	A:175:THR:CG2	0.752
1	A:347:LYS:CB	A:426:VAL:HG11	0.752
1	A:120:ILE:HD13	A:244:VAL:HG11	0.751
1	A:318:ALA:O	A:322:ILE:HG12	0.751
1	A:577:VAL:CG1	A:603:VAL:HG12	0.751
1	A:132:CYS:SG	A:183:ASN:HB3	0.750
1	A:338:LYS:HB2	A:540:CYS:CA	0.750
1	A:348:SER:O	A:427:GLN:HA	0.750
1	A:552:PRO:O	A:554:LYS:HG3	0.749
1	A:116:PHE:HE1	A:244:VAL:HG11	0.746
1	A:75:PHE:CD1	A:247:ALA:HB2	0.745
1	A:292:GLU:HG2	A:424:GLY:HA2	0.744
1	A:342:ASN:CB	A:346:GLN:HB2	0.744
1	A:537:TYR:CD2	A:562:LEU:HB3	0.744
1	A:338:LYS:CG	A:539:LYS:HG3	0.743
1	A:158:LYS:HD2	A:167:GLU:OE1	0.742
1	A:292:GLU:OE2	A:343:ILE:HD13	0.740
1	A:185:VAL:HG12	A:244:VAL:HG12	0.739
1	A:338:LYS:HG3	A:445:LYS:CB	0.739
1	A:451:LEU:HD12	A:502:VAL:CG1	0.738
1	A:94:VAL:CA	A:225:ALA:HB1	0.737
1	A:551:MET:HB3	A:554:LYS:HD2	0.737
1	A:447:VAL:CG2	A:448:LEU:HD22	0.736

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:531:THR:HB	A:534:LYS:CD	0.736
1	A:429:THR:O	A:433:LEU:HG	0.734
1	A:490:GLU:HA	A:495:VAL:CB	0.734
1	A:79:LEU:HD12	A:99:SER:O	0.733
1	A:508:LEU:HD11	A:519:LYS:CG	0.733
1	A:63:GLU:OE2	A:563:GLU:HB3	0.733
1	A:103:THR:CB	A:105:GLN:HA	0.732
1	A:389:ILE:CG2	A:393:ILE:HG13	0.732
1	A:415:LEU:HD11	A:456:LYS:O	0.732
1	A:520:LEU:HD22	A:534:LYS:CE	0.732
1	A:36:SER:HB3	A:626:MET:HB2	0.729
1	A:198:VAL:CG1	A:202:HIS:HB3	0.729
1	A:525:LEU:HB2	A:528:THR:HG23	0.729
1	A:338:LYS:HB2	A:541:VAL:H	0.728
1	A:347:LYS:HG3	A:426:VAL:CG1	0.728
1	A:368:PHE:O	A:371:THR:HG22	0.727
1	A:453:GLU:O	A:457:GLU:HG3	0.727
1	A:520:LEU:HD13	A:534:LYS:CE	0.725
1	A:276:LYS:NZ	A:527:GLU:HG3	0.725
1	A:286:ASP:H	A:387:ILE:HG12	0.724
1	A:508:LEU:HD22	A:514:ILE:HG12	0.724
1	A:445:LYS:H	A:445:LYS:HD2	0.723
1	A:41:PHE:CZ	A:45:LYS:HE2	0.722

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:347:LYS:HA	A:426:VAL:CG1	0.722
1	A:8:ASN:HD22	A:627:MET:CE	0.722
1	A:399:ARG:O	A:403:ALA:HB3	0.720
1	A:495:VAL:HG12	A:496:GLN:H	0.720
1	A:94:VAL:HA	A:225:ALA:CB	0.719
1	A:443:LYS:HE2	A:505:PHE:CZ	0.718
1	A:63:GLU:CD	A:563:GLU:HB3	0.716
1	A:335:LYS:HB2	A:546:GLU:CD	0.716
1	A:587:GLU:HG3	A:588:GLN:HG3	0.716
1	A:103:THR:O	A:105:GLN:HG3	0.715
1	A:425:VAL:HA	A:428:LEU:HG	0.715
1	A:83:PHE:HD2	A:85:THR:HG22	0.709
1	A:488:ALA:CA	A:496:GLN:HB3	0.709
1	A:338:LYS:CA	A:541:VAL:HB	0.707
1	A:81:LYS:C	A:97:LEU:HD12	0.706
1	A:103:THR:HG22	A:105:GLN:N	0.706
1	A:292:GLU:OE1	A:343:ILE:HG23	0.706
1	A:489:LYS:HA	A:497:THR:OG1	0.706
1	A:612:GLU:HA	A:619:TYR:HD1	0.705
1	A:508:LEU:HD22	A:514:ILE:CG1	0.704
1	A:94:VAL:HG13	A:95:PHE:CD2	0.703
1	A:414:ASN:HD22	A:469:VAL:HB	0.703
1	A:450:TRP:CZ2	A:451:LEU:HD21	0.702

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:129:PRO:O	A:132:CYS:HB2	0.701
1	A:436:ILE:HG23	A:437:PHE:CD2	0.699
1	A:468:ILE:HG13	A:469:VAL:N	0.699
1	A:74:PRO:CB	A:230:VAL:HG21	0.698
1	A:554:LYS:HE2	A:556:PRO:O	0.698
1	A:446:PRO:HG3	A:539:LYS:CE	0.695
1	A:508:LEU:HD22	A:519:LYS:HB2	0.695
1	A:428:LEU:O	A:431:GLN:HG2	0.694
1	A:251:ILE:HD12	A:257:GLY:CA	0.693
1	A:341:TRP:HZ2	A:427:GLN:HG2	0.693
1	A:329:PHE:CE2	A:349:ILE:HD11	0.692
1	A:377:ASN:HD22	A:380:ARG:HD2	0.692
1	A:22:LYS:HD3	A:219:LYS:NZ	0.690
1	A:505:PHE:HD2	A:514:ILE:HB	0.690
1	A:401:ILE:HG13	A:402:ASP:N	0.688
1	A:143:CYS:HB3	A:146:CYS:SG	0.686
1	A:116:PHE:HE1	A:244:VAL:CG1	0.686
1	A:520:LEU:CG	A:534:LYS:HE2	0.686
1	A:489:LYS:CD	A:502:VAL:HG21	0.685
1	A:119:ARG:HG2	A:232:SER:OG	0.684
1	A:120:ILE:HD13	A:244:VAL:CG1	0.684
1	A:374:THR:HG22	A:381:VAL:CG1	0.683
1	A:286:ASP:O	A:387:ILE:HD11	0.682

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:525:LEU:HB2	A:528:THR:CG2	0.682
1	A:531:THR:CB	A:534:LYS:HD3	0.682
1	A:601:THR:HG23	A:602:PRO:HD2	0.682
1	A:335:LYS:HE3	A:546:GLU:HG3	0.681
1	A:338:LYS:HG2	A:539:LYS:C	0.681
1	A:443:LYS:CG	A:505:PHE:HE1	0.681
1	A:448:LEU:HB3	A:452:GLU:OE1	0.681
1	A:102:LYS:HB3	A:330:LYS:HE2	0.680
1	A:490:GLU:HG2	A:495:VAL:O	0.680
1	A:185:VAL:HG12	A:244:VAL:CG1	0.679
1	A:569:THR:OG1	A:628:VAL:HG23	0.678
1	A:490:GLU:HG2	A:495:VAL:C	0.675
1	A:94:VAL:HG23	A:225:ALA:CB	0.674
1	A:347:LYS:HB3	A:444:LEU:CD2	0.674
1	A:415:LEU:HD21	A:456:LYS:HB3	0.674
1	A:413:ASN:O	A:417:VAL:HG23	0.674
1	A:74:PRO:HB2	A:247:ALA:CB	0.673
1	A:172:GLU:OE2	A:214:LYS:HG3	0.673
1	A:556:PRO:HG3	A:607:GLY:CA	0.673
1	A:628:VAL:HG12	A:629:THR:O	0.672
1	A:329:PHE:HE2	A:349:ILE:HD11	0.671
1	A:520:LEU:CD2	A:585:PRO:HG3	0.671
1	A:275:GLN:HB3	A:277:GLU:CG	0.670

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:290:ASN:HB2	A:420:TYR:CE1	0.670
1	A:292:GLU:HA	A:427:GLN:OE1	0.669
1	A:341:TRP:HZ2	A:427:GLN:HE21	0.669
1	A:275:GLN:CA	A:277:GLU:HG3	0.667
1	A:336:ALA:CB	A:346:GLN:HG3	0.667
1	A:347:LYS:CB	A:444:LEU:HD21	0.667
1	A:347:LYS:HA	A:426:VAL:HG21	0.665
1	A:432:TRP:CD1	A:477:CYS:H	0.664
1	A:571:VAL:HG13	A:602:PRO:HD3	0.663
1	A:253:CYS:H	A:278:LYS:HE3	0.660
1	A:464:ASP:C	A:468:ILE:HG23	0.660
1	A:288:LYS:HD3	A:387:ILE:O	0.659
1	A:620:CYS:HB3	A:628:VAL:CG1	0.659
1	A:382:LEU:HD22	A:416:VAL:CG1	0.658
1	A:612:GLU:HG3	A:619:TYR:CE1	0.658
1	A:523:LEU:HG	A:530:VAL:HG23	0.657
1	A:341:TRP:CD1	A:348:SER:H	0.654
1	A:422:THR:O	A:426:VAL:HG13	0.654
1	A:445:LYS:HB3	A:541:VAL:HG23	0.654
1	A:489:LYS:H	A:497:THR:HG23	0.654
1	A:375:ALA:HA	A:382:LEU:CD2	0.653
1	A:102:LYS:HB2	A:250:ASN:HB3	0.652
1	A:523:LEU:HB2	A:530:VAL:CG2	0.652

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:342:ASN:CB	A:347:LYS:H	0.651
1	A:103:THR:C	A:105:GLN:HG3	0.650
1	A:195:ASN:OD1	A:198:VAL:HB	0.650
1	A:341:TRP:CG	A:348:SER:CA	0.650
1	A:488:ALA:HA	A:496:GLN:CD	0.650
1	A:278:LYS:HA	A:328:ASN:O	0.649
1	A:508:LEU:CD1	A:519:LYS:HB2	0.649
1	A:534:LYS:HA	A:631:ASN:OD1	0.649
1	A:448:LEU:HD11	A:489:LYS:NZ	0.648
1	A:4:ARG:NH1	A:218:ARG:HH12	0.648
1	A:198:VAL:HG11	A:202:HIS:HB3	0.646
1	A:342:ASN:HB2	A:346:GLN:CB	0.646
1	A:405:MET:HB3	A:417:VAL:HG11	0.645
1	A:554:LYS:HA	A:578:LEU:HD22	0.645
1	A:96:PRO:CA	A:259:VAL:HA	0.642
1	A:119:ARG:NH1	A:232:SER:HB2	0.641
1	A:75:PHE:HD1	A:247:ALA:HB2	0.641
1	A:501:LEU:O	A:504:LYS:HG2	0.640
1	A:103:THR:HG22	A:104:ILE:N	0.639
1	A:125:PRO:HB2	A:317:LYS:HE2	0.639
1	A:415:LEU:O	A:415:LEU:HD23	0.639
1	A:94:VAL:CG2	A:225:ALA:HB1	0.638
1	A:283:ILE:HD13	A:287:PHE:CD1	0.638

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:422:THR:HA	A:425:VAL:HG12	0.638
1	A:66:GLU:HA	A:66:GLU:OE1	0.636
1	A:103:THR:HG21	A:106:PRO:CD	0.636
1	A:275:GLN:HB3	A:277:GLU:CD	0.636
1	A:476:ALA:HB3	A:487:CYS:HG	0.636
1	A:601:THR:CG2	A:602:PRO:HD2	0.636
1	A:485:VAL:CG2	A:491:ILE:HD11	0.634
1	A:486:THR:H	A:503:ASN:ND2	0.634
1	A:126:VAL:HA	A:131:GLU:OE1	0.633
1	A:208:HIS:CD2	A:222:ARG:HD2	0.633
1	A:74:PRO:HG2	A:230:VAL:HG21	0.632
1	A:470:LYS:HE3	A:471:PHE:CE1	0.632
1	A:542:LYS:HE3	A:624:PRO:HB3	0.632
1	A:74:PRO:HG2	A:230:VAL:HG11	0.630
1	A:534:LYS:HB3	A:631:ASN:HD21	0.629
1	A:448:LEU:HD11	A:489:LYS:HZ1	0.628
1	A:338:LYS:CE	A:539:LYS:HD3	0.627
1	A:445:LYS:HB3	A:541:VAL:HG21	0.627
1	A:34:THR:CG2	A:548:GLY:HA3	0.626
1	A:135:MET:HE2	A:137:LEU:CD2	0.625
1	A:10:PHE:HB3	A:21:ILE:CD1	0.624
1	A:292:GLU:OE2	A:343:ILE:HA	0.624
1	A:505:PHE:CE2	A:514:ILE:HB	0.624

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:215:THR:OG1	A:222:ARG:HD3	0.623
1	A:338:LYS:HB2	A:540:CYS:C	0.623
1	A:384:LYS:O	A:387:ILE:HG22	0.622
1	A:103:THR:HG23	A:248:SER:O	0.621
1	A:386:ALA:HA	A:389:ILE:HD11	0.620
1	A:513:ILE:HD12	A:515:ILE:HD11	0.620
1	A:295:ILE:CG2	A:427:GLN:HE22	0.619
1	A:490:GLU:O	A:500:LYS:HA	0.619
1	A:338:LYS:HG2	A:539:LYS:O	0.618
1	A:393:ILE:HG21	A:398:LEU:CD2	0.618
1	A:519:LYS:HE3	A:521:LYS:HD3	0.618
1	A:22:LYS:CD	A:219:LYS:HD2	0.617
1	A:347:LYS:CB	A:444:LEU:CD1	0.617
1	A:363:VAL:HG11	A:393:ILE:CD1	0.617
1	A:116:PHE:HA	A:119:ARG:HE	0.616
1	A:116:PHE:CE2	A:129:PRO:HG3	0.616
1	A:348:SER:CA	A:441:TYR:OH	0.615
1	A:341:TRP:CZ3	A:349:ILE:HG13	0.614
1	A:126:VAL:HG11	A:183:ASN:CG	0.613
1	A:103:THR:CG2	A:105:GLN:HA	0.612
1	A:465:GLY:HA2	A:468:ILE:CG1	0.611
1	A:513:ILE:HG21	A:529:PHE:CD2	0.611
1	A:82:LYS:N	A:97:LEU:HD12	0.610

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:463:ARG:HA	A:463:ARG:HE	0.610
1	A:505:PHE:HE2	A:514:ILE:O	0.610
1	A:410:LEU:HD13	A:412:THR:H	0.609
1	A:490:GLU:HA	A:495:VAL:CG1	0.609
1	A:536:LEU:N	A:536:LEU:HD12	0.609
1	A:608:LEU:CD2	A:610:LEU:HD21	0.609
1	A:96:PRO:HG2	A:99:SER:OG	0.608
1	A:75:PHE:HD1	A:247:ALA:CB	0.608
1	A:381:VAL:HG12	A:385:ALA:CB	0.608
1	A:418:MET:O	A:421:ILE:HG22	0.607
1	A:286:ASP:N	A:387:ILE:HG12	0.606
1	A:341:TRP:HZ2	A:427:GLN:NE2	0.606
1	A:508:LEU:O	A:511:ASP:HB2	0.605
1	A:5:TYR:CD2	A:91:PRO:HG3	0.604
1	A:620:CYS:HA	A:631:ASN:O	0.603
1	A:376:GLN:OE1	A:380:ARG:HD2	0.602
1	A:520:LEU:HD22	A:534:LYS:HE2	0.602
1	A:453:GLU:HA	A:453:GLU:OE1	0.600
1	A:444:LEU:C	A:444:LEU:HD13	0.599
1	A:489:LYS:O	A:495:VAL:HG12	0.599
1	A:116:PHE:HB2	A:234:VAL:CA	0.597
1	A:102:LYS:HB2	A:250:ASN:O	0.596
1	A:447:VAL:HG22	A:448:LEU:N	0.596

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:483:GLN:HG2	A:507:ALA:CA	0.596
1	A:612:GLU:CG	A:619:TYR:HE1	0.596
1	A:635:LEU:HB2	A:638:GLY:OXT	0.595
1	A:22:LYS:CE	A:219:LYS:HD2	0.594
1	A:348:SER:N	A:426:VAL:HG21	0.594
1	A:490:GLU:CB	A:495:VAL:HB	0.594
1	A:92:ASN:CG	A:173:GLY:HA2	0.593
1	A:98:ASN:HB2	A:264:GLU:CB	0.593
1	A:445:LYS:HD3	A:539:LYS:HD2	0.593
1	A:459:VAL:HG23	A:460:GLU:N	0.593
1	A:337:LYS:HA	A:541:VAL:O	0.592
1	A:36:SER:HB3	A:626:MET:CB	0.591
1	A:385:ALA:O	A:389:ILE:HG13	0.591
1	A:410:LEU:HD13	A:411:ALA:N	0.591
1	A:446:PRO:CD	A:539:LYS:HD3	0.591
1	A:103:THR:HB	A:105:GLN:HG2	0.589
1	A:493:GLU:HG3	A:494:SER:N	0.589
1	A:96:PRO:HB3	A:259:VAL:CA	0.587
1	A:104:ILE:O	A:104:ILE:HG22	0.587
1	A:142:LYS:HG3	A:142:LYS:O	0.587
1	A:111:LYS:HD3	A:111:LYS:N	0.586
1	A:347:LYS:HD3	A:449:ASP:CB	0.586
1	A:103:THR:HB	A:105:GLN:HG3	0.585

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:520:LEU:HD23	A:585:PRO:HG3	0.585
1	A:216:ILE:HG22	A:218:ARG:HG2	0.584
1	A:284:VAL:HG22	A:343:ILE:O	0.584
1	A:387:ILE:HG23	A:388:THR:HG23	0.584
1	A:531:THR:CG2	A:534:LYS:HD3	0.583
1	A:372:LEU:H	A:372:LEU:HD12	0.582
1	A:483:GLN:HG3	A:510:ALA:HB2	0.582
1	A:316:TYR:CE1	A:333:LYS:HB2	0.581
1	A:82:LYS:HE3	A:86:PHE:HD2	0.580
1	A:296:ILE:HA	A:350:LEU:HD13	0.580
1	A:425:VAL:HA	A:428:LEU:CG	0.580
1	A:489:LYS:HG2	A:499:PHE:CG	0.580
1	A:338:LYS:HD3	A:540:CYS:N	0.579
1	A:372:LEU:N	A:372:LEU:HD12	0.579
1	A:339:GLY:H	A:445:LYS:HG2	0.579
1	A:341:TRP:CB	A:348:SER:CB	0.578
1	A:135:MET:HE2	A:137:LEU:HD23	0.576
1	A:452:GLU:O	A:455:PHE:HB3	0.576
1	A:495:VAL:HG12	A:496:GLN:N	0.576
1	A:36:SER:HB3	A:626:MET:CG	0.575
1	A:103:THR:C	A:105:GLN:N	0.575
1	A:605:ILE:HD12	A:610:LEU:HD12	0.575
1	A:498:PHE:C	A:500:LYS:H	0.574

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:347:LYS:CD	A:449:ASP:HA	0.573
1	A:534:LYS:H	A:534:LYS:HD2	0.573
1	A:598:LEU:HD23	A:613:ILE:HG21	0.573
1	A:371:THR:CG2	A:372:LEU:HD12	0.572
1	A:443:LYS:HG2	A:505:PHE:HE1	0.571
1	A:455:PHE:O	A:468:ILE:HD12	0.571
1	A:508:LEU:HD21	A:519:LYS:HD3	0.571
1	A:338:LYS:N	A:541:VAL:HB	0.571
1	A:94:VAL:CB	A:225:ALA:HB1	0.570
1	A:569:THR:HG21	A:611:LEU:HD22	0.570
1	A:275:GLN:HA	A:277:GLU:HG3	0.568
1	A:335:LYS:CD	A:546:GLU:HG3	0.568
1	A:496:GLN:HG2	A:497:THR:CG2	0.568
1	A:519:LYS:HE3	A:521:LYS:CD	0.568
1	A:338:LYS:NZ	A:560:ILE:HG12	0.568
1	A:421:ILE:HG21	A:472:ILE:HD11	0.567
1	A:373:GLU:HG3	A:374:THR:N	0.566
1	A:393:ILE:CG2	A:397:SER:HB2	0.565
1	A:135:MET:HG3	A:179:TYR:O	0.564
1	A:537:TYR:CD2	A:562:LEU:HD12	0.564
1	A:152:GLN:HE22	A:168:ASN:ND2	0.564
1	A:348:SER:HB2	A:441:TYR:CE2	0.563
1	A:339:GLY:H	A:445:LYS:CG	0.562

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:389:ILE:HG22	A:398:LEU:HD11	0.561
1	A:103:THR:HB	A:105:GLN:CA	0.560
1	A:120:ILE:HG23	A:121:ARG:N	0.560
1	A:276:LYS:HE2	A:442:GLU:CG	0.560
1	A:398:LEU:HA	A:405:MET:HB2	0.560
1	A:608:LEU:HD21	A:610:LEU:HD21	0.560
1	A:176:THR:HG21	A:226:PHE:CZ	0.559
1	A:180:LEU:N	A:180:LEU:HD12	0.559
1	A:496:GLN:HG2	A:497:THR:HG22	0.559
1	A:425:VAL:HA	A:428:LEU:CD1	0.558
1	A:116:PHE:CE1	A:244:VAL:HG11	0.557
1	A:347:LYS:CA	A:426:VAL:CG1	0.557
1	A:119:ARG:CG	A:246:ARG:HG2	0.556
1	A:618:LYS:HG2	A:632:THR:HG21	0.556
1	A:22:LYS:HB3	A:219:LYS:HZ1	0.555
1	A:76:GLU:HA	A:76:GLU:OE1	0.555
1	A:347:LYS:C	A:441:TYR:OH	0.555
1	A:434:THR:HG22	A:435:ASN:N	0.555
1	A:347:LYS:CG	A:426:VAL:HG11	0.554
1	A:378:SER:HA	A:382:LEU:HD12	0.554
1	A:501:LEU:HD12	A:504:LYS:CE	0.554
1	A:508:LEU:CD2	A:514:ILE:HG13	0.554
1	A:537:TYR:HE2	A:562:LEU:HB3	0.554

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:36:SER:OG	A:626:MET:HG2	0.554
1	A:432:TRP:NE1	A:477:CYS:H	0.554
1	A:347:LYS:CG	A:444:LEU:HD21	0.553
1	A:377:ASN:ND2	A:380:ARG:HD2	0.553
1	A:447:VAL:HG13	A:448:LEU:N	0.553
1	A:515:ILE:HG22	A:608:LEU:HD22	0.552
1	A:520:LEU:CD2	A:534:LYS:HE2	0.552
1	A:506:LEU:O	A:509:CYS:HB3	0.551
1	A:5:TYR:CG	A:91:PRO:HG3	0.550
1	A:180:LEU:CD1	A:256:THR:HG23	0.550
1	A:501:LEU:HD12	A:504:LYS:HE3	0.550
1	A:300:PHE:HZ	A:329:PHE:CE1	0.549
1	A:490:GLU:HG3	A:497:THR:O	0.549
1	A:293:ILE:HG21	A:314:LEU:HD21	0.548
1	A:379:VAL:HG12	A:545:GLU:OE2	0.548
1	A:387:ILE:HG23	A:388:THR:N	0.548
1	A:74:PRO:HB2	A:247:ALA:HB3	0.547
1	A:335:LYS:CE	A:546:GLU:HG3	0.547
1	A:179:TYR:C	A:180:LEU:HD12	0.546
1	A:223:THR:HG21	A:230:VAL:CG1	0.546
1	A:610:LEU:CD2	A:621:ALA:HA	0.546
1	A:424:GLY:O	A:427:GLN:HB2	0.545
1	A:338:LYS:HZ2	A:560:ILE:HG12	0.545

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:338:LYS:HD3	A:540:CYS:C	0.544
1	A:347:LYS:CG	A:426:VAL:CG1	0.544
1	A:410:LEU:C	A:410:LEU:HD13	0.544
1	A:465:GLY:O	A:468:ILE:HG12	0.544
1	A:489:LYS:HG2	A:499:PHE:HB2	0.544
1	A:290:ASN:ND2	A:420:TYR:HE1	0.544
1	A:393:ILE:HG22	A:397:SER:HB2	0.543
1	A:465:GLY:C	A:468:ILE:HG12	0.543
1	A:612:GLU:HG3	A:619:TYR:HE1	0.543
1	A:399:ARG:HB3	A:403:ALA:HB2	0.542
1	A:42:ILE:O	A:45:LYS:HB2	0.541
1	A:386:ALA:HA	A:389:ILE:CD1	0.541
1	A:341:TRP:CE2	A:427:GLN:HG2	0.541
1	A:423:GLY:O	A:427:GLN:HG3	0.541
1	A:335:LYS:CG	A:546:GLU:HB2	0.541
1	A:104:ILE:N	A:104:ILE:HD12	0.539
1	A:103:THR:O	A:330:LYS:HE3	0.539
1	A:436:ILE:HG23	A:437:PHE:N	0.539
1	A:16:TYR:HE1	A:230:VAL:HG11	0.537
1	A:269:ASN:HA	A:272:GLU:HG2	0.537
1	A:342:ASN:HB2	A:346:GLN:C	0.537
1	A:399:ARG:NE	A:401:ILE:HD11	0.537
1	A:348:SER:N	A:426:VAL:CG2	0.537

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:489:LYS:HA	A:499:PHE:HB2	0.537
1	A:336:ALA:O	A:542:LYS:HA	0.537
1	A:38:GLN:O	A:42:ILE:HG13	0.536
1	A:341:TRP:CG	A:348:SER:N	0.536
1	A:342:ASN:CB	A:346:GLN:CB	0.536
1	A:348:SER:CB	A:441:TYR:CE2	0.535
1	A:101:ILE:N	A:101:ILE:HD12	0.534
1	A:169:LEU:N	A:169:LEU:HD12	0.534
1	A:445:LYS:HB2	A:446:PRO:HD3	0.534
1	A:125:PRO:CB	A:317:LYS:HE2	0.533
1	A:75:PHE:HB3	A:106:PRO:CD	0.532
1	A:490:GLU:H	A:500:LYS:HA	0.532
1	A:198:VAL:HG11	A:202:HIS:CB	0.531
1	A:347:LYS:HE2	A:448:LEU:HB3	0.530
1	A:374:THR:CG2	A:381:VAL:HG11	0.530
1	A:472:ILE:O	A:472:ILE:HG23	0.530
1	A:534:LYS:HD2	A:534:LYS:N	0.530
1	A:22:LYS:HD3	A:219:LYS:HZ2	0.529
1	A:198:VAL:HG12	A:202:HIS:HB3	0.529
1	A:290:ASN:CB	A:420:TYR:CE1	0.529
1	A:464:ASP:HB3	A:468:ILE:CG2	0.529
1	A:508:LEU:HB2	A:514:ILE:HD11	0.529
1	A:554:LYS:HZ1	A:559:ILE:HG21	0.529

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:94:VAL:O	A:94:VAL:HG22	0.528
1	A:60:TRP:CD1	A:97:LEU:HD11	0.527
1	A:103:THR:CA	A:105:GLN:HG3	0.527
1	A:442:GLU:C	A:444:LEU:H	0.527
1	A:444:LEU:HA	A:447:VAL:HG12	0.527
1	A:508:LEU:CD1	A:519:LYS:HD3	0.527
1	A:412:THR:O	A:416:VAL:HG22	0.525
1	A:422:THR:O	A:425:VAL:HG12	0.525
1	A:462:LEU:C	A:464:ASP:H	0.525
1	A:569:THR:HG23	A:598:LEU:O	0.525
1	A:620:CYS:HB3	A:628:VAL:HG13	0.525
1	A:117:MET:O	A:120:ILE:HG22	0.524
1	A:125:PRO:HB2	A:317:LYS:CE	0.523
1	A:335:LYS:HB3	A:543:SER:OG	0.523
1	A:389:ILE:HG22	A:393:ILE:HB	0.523
1	A:21:ILE:O	A:25:LEU:HG	0.521
1	A:433:LEU:O	A:434:THR:HB	0.521
1	A:341:TRP:HZ2	A:427:GLN:CG	0.521
1	A:18:LEU:O	A:22:LYS:HG3	0.520
1	A:342:ASN:HB2	A:346:GLN:CA	0.520
1	A:444:LEU:O	A:444:LEU:HD13	0.520
1	A:98:ASN:HB2	A:264:GLU:HB3	0.519
1	A:382:LEU:HD22	A:416:VAL:HG11	0.519

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:525:LEU:HB2	A:528:THR:O	0.519
1	A:348:SER:H	A:426:VAL:HG23	0.519
1	A:18:LEU:HD23	A:218:ARG:CZ	0.518
1	A:512:SER:OG	A:521:LYS:HD2	0.518
1	A:126:VAL:O	A:126:VAL:HG23	0.517
1	A:463:ARG:HA	A:463:ARG:NE	0.517
1	A:502:VAL:HG23	A:503:ASN:N	0.517
1	A:508:LEU:HD11	A:519:LYS:NZ	0.517
1	A:152:GLN:HE21	A:161:CYS:HA	0.516
1	A:191:PRO:HG3	A:211:SER:HA	0.516
1	A:386:ALA:O	A:389:ILE:HG13	0.516
1	A:405:MET:HB3	A:417:VAL:HG21	0.516
1	A:419:ALA:HA	A:456:LYS:HD2	0.516
1	A:497:THR:OG1	A:499:PHE:HD1	0.516
1	A:443:LYS:HE2	A:505:PHE:CE1	0.515
1	A:444:LEU:C	A:447:VAL:HG12	0.515
1	A:92:ASN:OD1	A:173:GLY:HA2	0.514
1	A:363:VAL:HG11	A:393:ILE:HD12	0.514
1	A:401:ILE:HG13	A:402:ASP:H	0.514
1	A:389:ILE:CG2	A:398:LEU:HD11	0.512
1	A:406:PHE:CE1	A:418:MET:HA	0.512
1	A:512:SER:HB2	A:519:LYS:HD3	0.512
1	A:448:LEU:HD12	A:452:GLU:CD	0.511

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:432:TRP:HD1	A:477:CYS:HB2	0.511
1	A:531:THR:OG1	A:534:LYS:HB2	0.510
1	A:618:LYS:CG	A:632:THR:HG21	0.510
1	A:443:LYS:HG3	A:505:PHE:CE1	0.509
1	A:443:LYS:HE2	A:505:PHE:HZ	0.509
1	A:82:LYS:HD2	A:90:CYS:SG	0.508
1	A:396:TYR:O	A:403:ALA:HB2	0.508
1	A:323:VAL:HG12	A:329:PHE:CB	0.507
1	A:372:LEU:CD1	A:372:LEU:H	0.507
1	A:554:LYS:HB3	A:556:PRO:O	0.506
1	A:338:LYS:H	A:541:VAL:H	0.506
1	A:61:TYR:CE1	A:566:THR:CG2	0.505
1	A:275:GLN:CB	A:277:GLU:HG3	0.505
1	A:347:LYS:HA	A:426:VAL:CG2	0.505
1	A:135:MET:HE3	A:180:LEU:CD1	0.504
1	A:489:LYS:C	A:497:THR:H	0.504
1	A:251:ILE:HD12	A:257:GLY:N	0.503
1	A:253:CYS:H	A:278:LYS:CE	0.503
1	A:444:LEU:O	A:447:VAL:HG12	0.503
1	A:292:GLU:H	A:420:TYR:HH	0.503
1	A:289:LEU:HD13	A:314:LEU:HD23	0.502
1	A:338:LYS:HG2	A:539:LYS:CG	0.502
1	A:103:THR:HG22	A:105:GLN:H	0.500

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:135:MET:HB2	A:184:ALA:HB1	0.500
1	A:292:GLU:O	A:296:ILE:HG13	0.500
1	A:443:LYS:HG3	A:505:PHE:HE1	0.500
1	A:22:LYS:HZ2	A:219:LYS:HG3	0.499
1	A:489:LYS:CB	A:499:PHE:HB2	0.499
1	A:251:ILE:H	A:251:ILE:HD13	0.498
1	A:208:HIS:CE1	A:222:ARG:HD2	0.497
1	A:341:TRP:CD1	A:426:VAL:HG21	0.497
1	A:502:VAL:O	A:506:LEU:HG	0.497
1	A:22:LYS:HD3	A:219:LYS:HE3	0.496
1	A:347:LYS:NZ	A:449:ASP:HA	0.496
1	A:450:TRP:CZ2	A:451:LEU:CD2	0.496
1	A:113:LEU:HD12	A:121:ARG:HD2	0.495
1	A:518:ALA:HB2	A:583:LEU:HB2	0.495
1	A:119:ARG:HD2	A:246:ARG:NH1	0.494
1	A:485:VAL:HG22	A:491:ILE:CD1	0.493
1	A:573:THR:HG22	A:601:THR:HG23	0.493
1	A:363:VAL:HG12	A:367:ILE:CD1	0.492
1	A:374:THR:CA	A:381:VAL:HB	0.492
1	A:386:ALA:HA	A:389:ILE:CG1	0.492
1	A:428:LEU:HA	A:431:GLN:NE2	0.492
1	A:625:ASN:HD21	A:627:MET:HE2	0.492
1	A:386:ALA:HA	A:389:ILE:HG13	0.491

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:562:LEU:HD23	A:608:LEU:HD11	0.491
1	A:399:ARG:HG2	A:401:ILE:HG12	0.490
1	A:448:LEU:HD12	A:452:GLU:OE1	0.490
1	A:464:ASP:HB3	A:468:ILE:HG21	0.490
1	A:449:ASP:OD2	A:541:VAL:HG11	0.490
1	A:592:GLU:HG2	A:594:VAL:CG1	0.490
1	A:274:LEU:O	A:277:GLU:HG3	0.489
1	A:549:LEU:HD11	A:626:MET:HE2	0.489
1	A:547:THR:CG2	A:559:ILE:HD11	0.489
1	A:103:THR:HG22	A:104:ILE:H	0.488
1	A:309:GLU:HA	A:312:LYS:HD2	0.488
1	A:534:LYS:C	A:537:TYR:CE1	0.487
1	A:202:HIS:CE1	A:207:TYR:HB2	0.486
1	A:275:GLN:CB	A:277:GLU:CG	0.484
1	A:335:LYS:HB2	A:546:GLU:OE1	0.484
1	A:348:SER:HB2	A:441:TYR:HE2	0.484
1	A:363:VAL:O	A:367:ILE:HD13	0.484
1	A:425:VAL:HA	A:428:LEU:HD12	0.484
1	A:104:ILE:H	A:104:ILE:HD12	0.483
1	A:444:LEU:HA	A:447:VAL:CG1	0.483
1	A:17:PRO:HB2	A:69:TYR:CE2	0.482
1	A:96:PRO:HB3	A:258:VAL:O	0.482
1	A:192:ALA:HB3	A:202:HIS:CD2	0.482

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:208:HIS:CG	A:222:ARG:HD2	0.482
1	A:569:THR:HG22	A:570:GLU:N	0.482
1	A:103:THR:CB	A:105:GLN:HG3	0.481
1	A:513:ILE:HG21	A:529:PHE:CE2	0.481
1	A:152:GLN:HE21	A:161:CYS:CA	0.480
1	A:556:PRO:CG	A:607:GLY:HA2	0.480
1	A:348:SER:CA	A:348:SER:H	0.479
1	A:338:LYS:CG	A:445:LYS:CB	0.479
1	A:484:ILE:O	A:484:ILE:HG23	0.479
1	A:445:LYS:HZ2	A:539:LYS:HG3	0.479
1	A:592:GLU:HG2	A:594:VAL:HG13	0.479
1	A:232:SER:HB3	A:246:ARG:HD2	0.478
1	A:347:LYS:HB3	A:444:LEU:CG	0.478
1	A:491:ILE:H	A:495:VAL:HG21	0.477
1	A:390:LEU:HD12	A:393:ILE:O	0.476
1	A:428:LEU:HA	A:431:GLN:HG2	0.476
1	A:116:PHE:CD1	A:234:VAL:CG2	0.475
1	A:455:PHE:C	A:455:PHE:CD2	0.474
1	A:100:ILE:O	A:100:ILE:HG13	0.473
1	A:371:THR:HG23	A:372:LEU:N	0.473
1	A:569:THR:CG2	A:611:LEU:HD22	0.473
1	A:97:LEU:N	A:97:LEU:HD22	0.472
1	A:180:LEU:HD13	A:256:THR:HG23	0.472

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:347:LYS:HD3	A:449:ASP:N	0.472
1	A:453:GLU:CD	A:557:LYS:HZ2	0.472
1	A:338:LYS:CB	A:540:CYS:HA	0.472
1	A:35:LEU:O	A:39:LEU:HG	0.471
1	A:75:PHE:CE1	A:246:ARG:C	0.471
1	A:410:LEU:CD1	A:412:THR:H	0.471
1	A:292:GLU:O	A:295:ILE:HG22	0.470
1	A:445:LYS:N	A:446:PRO:HD2	0.470
1	A:119:ARG:HG3	A:246:ARG:CD	0.469
1	A:345:GLU:HB3	A:346:GLN:CD	0.469
1	A:371:THR:HG23	A:372:LEU:HD12	0.469
1	A:620:CYS:CB	A:628:VAL:CG1	0.469
1	A:132:CYS:HA	A:183:ASN:HB3	0.468
1	A:223:THR:CG2	A:230:VAL:CG1	0.468
1	A:276:LYS:HA	A:276:LYS:HD2	0.468
1	A:16:TYR:HB3	A:17:PRO:HD2	0.467
1	A:4:ARG:NH2	A:18:LEU:HD22	0.467
1	A:296:ILE:HG22	A:300:PHE:HE2	0.467
1	A:338:LYS:CB	A:541:VAL:N	0.467
1	A:191:PRO:HD2	A:207:TYR:HE1	0.466
1	A:422:THR:HG23	A:425:VAL:HG11	0.466
1	A:10:PHE:HB3	A:21:ILE:HD13	0.465
1	A:338:LYS:CE	A:539:LYS:CD	0.465

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:386:ALA:CA	A:389:ILE:HG13	0.465
1	A:612:GLU:CG	A:619:TYR:CE1	0.465
1	A:377:ASN:HD22	A:380:ARG:CD	0.465
1	A:36:SER:CB	A:626:MET:CG	0.464
1	A:64:ARG:NH1	A:77:ILE:HG12	0.464
1	A:429:THR:HG23	A:430:SER:N	0.464
1	A:618:LYS:HB3	A:632:THR:HG23	0.464
1	A:58:ILE:HG21	A:83:PHE:CE1	0.463
1	A:81:LYS:HZ3	A:565:GLU:HB2	0.463
1	A:618:LYS:HB3	A:632:THR:CG2	0.463
1	A:320:LYS:HG3	A:331:VAL:HB	0.462
1	A:436:ILE:CG2	A:437:PHE:CD2	0.462
1	A:504:LYS:HG3	A:505:PHE:N	0.462
1	A:424:GLY:HA2	A:427:GLN:OE1	0.461
1	A:96:PRO:HA	A:260:GLY:H	0.460
1	A:371:THR:HG22	A:372:LEU:HD12	0.459
1	A:347:LYS:HB3	A:444:LEU:HD11	0.459
1	A:338:LYS:CD	A:445:LYS:HB2	0.459
1	A:455:PHE:HE1	A:468:ILE:O	0.459
1	A:176:THR:O	A:259:VAL:HG22	0.458
1	A:347:LYS:CB	A:426:VAL:CG1	0.458
1	A:341:TRP:HZ3	A:349:ILE:HG13	0.458
1	A:386:ALA:C	A:389:ILE:HG13	0.458

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:342:ASN:H	A:347:LYS:H	0.458
1	A:275:GLN:HB3	A:277:GLU:HG3	0.457
1	A:338:LYS:HE2	A:539:LYS:NZ	0.457
1	A:508:LEU:HD21	A:519:LYS:HB2	0.457
1	A:119:ARG:CG	A:246:ARG:CD	0.456
1	A:135:MET:CE	A:180:LEU:HD11	0.456
1	A:289:LEU:O	A:390:LEU:HD22	0.456
1	A:393:ILE:CG2	A:398:LEU:HG	0.456
1	A:135:MET:HE3	A:180:LEU:HD12	0.455
1	A:116:PHE:CB	A:234:VAL:HG13	0.455
1	A:338:LYS:CG	A:539:LYS:C	0.455
1	A:341:TRP:CG	A:348:SER:HB3	0.455
1	A:354:TYR:O	A:355:ALA:HB2	0.455
1	A:467:GLU:HG2	A:471:PHE:CD1	0.455
1	A:501:LEU:CD1	A:504:LYS:CE	0.455
1	A:536:LEU:C	A:537:TYR:CD1	0.455
1	A:14:ASP:OD2	A:218:ARG:HG3	0.454
1	A:275:GLN:CB	A:277:GLU:CB	0.454
1	A:555:ALA:H	A:578:LEU:HD22	0.454
1	A:180:LEU:HA	A:181:PRO:HD2	0.453
1	A:400:LEU:HA	A:406:PHE:HB2	0.453
1	A:404:MET:HB3	A:408:SER:OG	0.453
1	A:180:LEU:CD1	A:256:THR:CG2	0.451

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:335:LYS:HD3	A:546:GLU:HG3	0.451
1	A:525:LEU:HD12	A:528:THR:HG23	0.451
1	A:18:LEU:CD2	A:218:ARG:CZ	0.450
1	A:22:LYS:HB3	A:219:LYS:NZ	0.450
1	A:94:VAL:CG2	A:230:VAL:HG22	0.450
1	A:276:LYS:HE2	A:442:GLU:CD	0.450
1	A:562:LEU:CD2	A:608:LEU:HD11	0.450
1	A:573:THR:CG2	A:601:THR:HG23	0.450
1	A:628:VAL:HG12	A:629:THR:N	0.450
1	A:321:GLN:HB2	A:321:GLN:HE21	0.450
1	A:554:LYS:HZ1	A:559:ILE:CG2	0.450
1	A:102:LYS:HG3	A:250:ASN:O	0.449
1	A:415:LEU:C	A:415:LEU:HD23	0.449
1	A:489:LYS:HG2	A:499:PHE:HB3	0.449
1	A:515:ILE:HD12	A:520:LEU:CD1	0.449
1	A:119:ARG:HG2	A:246:ARG:HG2	0.448
1	A:365:ARG:C	A:365:ARG:HD2	0.448
1	A:530:VAL:O	A:530:VAL:HG23	0.448
1	A:238:ASN:O	A:239:LYS:HB2	0.447
1	A:470:LYS:HE3	A:471:PHE:HE1	0.447
1	A:115:GLY:O	A:119:ARG:HD3	0.446
1	A:428:LEU:C	A:431:GLN:HG2	0.446
1	A:338:LYS:CD	A:445:LYS:CB	0.445

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:404:MET:HB2	A:404:MET:HE2	0.444
1	A:439:THR:O	A:442:GLU:HG2	0.444
1	A:501:LEU:N	A:501:LEU:HD22	0.444
1	A:566:THR:CB	A:627:MET:HE3	0.444
1	A:586:LEU:HD21	A:618:LYS:HE2	0.444
1	A:95:PHE:CB	A:96:PRO:HD2	0.443
1	A:486:THR:HG22	A:488:ALA:O	0.443
1	A:95:PHE:HB3	A:96:PRO:CD	0.442
1	A:14:ASP:CB	A:216:ILE:HD12	0.442
1	A:363:VAL:CG1	A:393:ILE:CD1	0.442
1	A:445:LYS:HB2	A:446:PRO:CD	0.442
1	A:161:CYS:HB3	A:164:CYS:SG	0.441
1	A:432:TRP:CD1	A:477:CYS:N	0.441
1	A:103:THR:CG2	A:105:GLN:CA	0.440
1	A:338:LYS:HE2	A:539:LYS:CG	0.440
1	A:368:PHE:CE1	A:371:THR:HG21	0.440
1	A:446:PRO:HD3	A:539:LYS:CD	0.440
1	A:537:TYR:HD2	A:562:LEU:HD12	0.440
1	A:23:ASP:HB3	A:27:ARG:HH12	0.439
1	A:61:TYR:CE1	A:566:THR:HG23	0.439
1	A:269:ASN:O	A:272:GLU:HG2	0.439
1	A:292:GLU:HA	A:427:GLN:CD	0.439
1	A:296:ILE:CG2	A:300:PHE:HE2	0.439

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:444:LEU:CA	A:447:VAL:HG12	0.439
1	A:456:LYS:HB2	A:456:LYS:HE2	0.439
1	A:542:LYS:O	A:558:GLU:HG3	0.439
1	A:571:VAL:CG1	A:602:PRO:HD3	0.439
1	A:258:VAL:HG21	A:266:LEU:HD21	0.438
1	A:381:VAL:O	A:381:VAL:HG12	0.438
1	A:393:ILE:HG22	A:394:SER:O	0.438
1	A:586:LEU:N	A:586:LEU:HD12	0.438
1	A:75:PHE:CD1	A:75:PHE:N	0.437
1	A:103:THR:CB	A:105:GLN:CA	0.437
1	A:445:LYS:CD	A:445:LYS:H	0.437
1	A:583:LEU:HD23	A:635:LEU:HD23	0.437
1	A:275:GLN:HB3	A:277:GLU:CB	0.436
1	A:399:ARG:C	A:406:PHE:HD2	0.436
1	A:508:LEU:CD1	A:519:LYS:CB	0.436
1	A:519:LYS:HG3	A:519:LYS:O	0.436
1	A:434:THR:CG2	A:435:ASN:N	0.436
1	A:94:VAL:CB	A:225:ALA:CB	0.435
1	A:96:PRO:HG3	A:258:VAL:O	0.435
1	A:113:LEU:O	A:118:GLY:HA3	0.435
1	A:126:VAL:CG1	A:183:ASN:CG	0.435
1	A:289:LEU:HD13	A:314:LEU:CD2	0.435
1	A:426:VAL:HG23	A:427:GLN:N	0.435

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:467:GLU:HG2	A:471:PHE:CE1	0.435
1	A:525:LEU:CB	A:528:THR:CG2	0.435
1	A:534:LYS:HB3	A:631:ASN:CG	0.435
1	A:283:ILE:CD1	A:287:PHE:HD1	0.435
1	A:490:GLU:HG3	A:497:THR:N	0.434
1	A:39:LEU:HD23	A:42:ILE:HD12	0.433
1	A:492:LYS:HG3	A:493:GLU:H	0.433
1	A:180:LEU:HD11	A:256:THR:CG2	0.432
1	A:251:ILE:HD12	A:257:GLY:HA2	0.432
1	A:269:ASN:O	A:273:ILE:HG12	0.432
1	A:290:ASN:ND2	A:420:TYR:CE1	0.432
1	A:523:LEU:CG	A:530:VAL:HG23	0.432
1	A:405:MET:HB3	A:417:VAL:CG1	0.431
1	A:513:ILE:O	A:513:ILE:HG13	0.431
1	A:467:GLU:CG	A:471:PHE:CE1	0.430
1	A:406:PHE:HZ	A:420:TYR:HD2	0.430
1	A:420:TYR:CD1	A:420:TYR:O	0.429
1	A:290:ASN:CB	A:420:TYR:CZ	0.429
1	A:429:THR:CG2	A:430:SER:N	0.429
1	A:175:THR:O	A:175:THR:HG23	0.429
1	A:102:LYS:O	A:249:ALA:HA	0.428
1	A:338:LYS:HE2	A:539:LYS:CD	0.428
1	A:431:GLN:HG3	A:432:TRP:N	0.428

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:537:TYR:HD2	A:562:LEU:HB3	0.428
1	A:566:THR:OG1	A:627:MET:HE3	0.428
1	A:339:GLY:N	A:445:LYS:CG	0.428
1	A:379:VAL:HG23	A:380:ARG:N	0.428
1	A:116:PHE:CE1	A:244:VAL:HG21	0.427
1	A:282:ASN:CG	A:332:THR:HG23	0.427
1	A:346:GLN:HA	A:347:LYS:NZ	0.427
1	A:498:PHE:C	A:500:LYS:N	0.427
1	A:625:ASN:ND2	A:627:MET:HE2	0.427
1	A:6:VAL:HG23	A:58:ILE:HD13	0.426
1	A:116:PHE:CE1	A:244:VAL:CG1	0.426
1	A:279:VAL:HG11	A:349:ILE:HG12	0.426
1	A:393:ILE:HG21	A:398:LEU:HD21	0.426
1	A:405:MET:CB	A:417:VAL:HG11	0.426
1	A:478:GLU:C	A:479:ILE:HD12	0.426
1	A:525:LEU:CB	A:528:THR:HG23	0.426
1	A:399:ARG:HD2	A:399:ARG:HH11	0.426
1	A:187:LYS:HE2	A:242:TYR:CE2	0.425
1	A:296:ILE:HG22	A:300:PHE:CE2	0.425
1	A:319:PHE:CZ	A:323:VAL:HG21	0.425
1	A:341:TRP:CD2	A:348:SER:C	0.425
1	A:348:SER:OG	A:349:ILE:HG23	0.425
1	A:467:GLU:O	A:470:LYS:HB3	0.425

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:78:LYS:HE2	A:563:GLU:OE2	0.424
1	A:75:PHE:CE1	A:247:ALA:HB2	0.424
1	A:296:ILE:HA	A:350:LEU:CD1	0.424
1	A:393:ILE:HD12	A:405:MET:HE3	0.424
1	A:455:PHE:CE1	A:468:ILE:O	0.424
1	A:485:VAL:HG21	A:491:ILE:HG13	0.424
1	A:534:LYS:O	A:537:TYR:CE1	0.424
1	A:550:LEU:O	A:552:PRO:HD3	0.424
1	A:502:VAL:CG2	A:503:ASN:N	0.424
1	A:323:VAL:CG1	A:329:PHE:HB2	0.423
1	A:346:GLN:HA	A:347:LYS:HZ2	0.423
1	A:347:LYS:CE	A:449:ASP:HA	0.423
1	A:399:ARG:CB	A:403:ALA:HB2	0.423
1	A:453:GLU:HB3	A:557:LYS:CB	0.423
1	A:425:VAL:CG1	A:426:VAL:N	0.423
1	A:341:TRP:CH2	A:349:ILE:O	0.422
1	A:198:VAL:CG1	A:202:HIS:CB	0.421
1	A:554:LYS:HA	A:578:LEU:CD2	0.421
1	A:467:GLU:OE1	A:498:PHE:CE2	0.420
1	A:489:LYS:CG	A:499:PHE:HB2	0.420
1	A:436:ILE:CG2	A:437:PHE:N	0.420
1	A:39:LEU:HA	A:42:ILE:HD12	0.419
1	A:61:TYR:CZ	A:566:THR:HG23	0.419

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:152:GLN:NE2	A:161:CYS:HA	0.419
1	A:132:CYS:HB3	A:183:ASN:O	0.418
1	A:191:PRO:HD2	A:207:TYR:CE1	0.418
1	A:290:ASN:OD1	A:293:ILE:HG12	0.418
1	A:341:TRP:HA	A:348:SER:N	0.418
1	A:450:TRP:CH2	A:451:LEU:HD21	0.418
1	A:119:ARG:CG	A:246:ARG:CZ	0.417
1	A:381:VAL:CA	A:384:LYS:HB2	0.417
1	A:410:LEU:C	A:410:LEU:CD1	0.417
1	A:422:THR:CG2	A:452:GLU:CD	0.417
1	A:120:ILE:CG2	A:121:ARG:N	0.417
1	A:234:VAL:HG23	A:242:TYR:O	0.416
1	A:442:GLU:O	A:445:LYS:HE3	0.416
1	A:491:ILE:N	A:495:VAL:HG21	0.416
1	A:81:LYS:NZ	A:565:GLU:HB2	0.416
1	A:103:THR:CG2	A:104:ILE:N	0.416
1	A:406:PHE:CD1	A:418:MET:HA	0.415
1	A:276:LYS:NZ	A:442:GLU:HG3	0.415
1	A:534:LYS:C	A:537:TYR:HE1	0.415
1	A:36:SER:CB	A:626:MET:HB2	0.415
1	A:224:ILE:CG2	A:231:PHE:HB2	0.414
1	A:347:LYS:C	A:426:VAL:HG21	0.414
1	A:422:THR:HA	A:425:VAL:CG1	0.414

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:489:LYS:CG	A:499:PHE:CB	0.414
1	A:505:PHE:C	A:505:PHE:CD1	0.414
1	A:622:LEU:HD13	A:626:MET:SD	0.414
1	A:342:ASN:H	A:347:LYS:N	0.414
1	A:251:ILE:CD1	A:257:GLY:N	0.413
1	A:308:VAL:O	A:311:VAL:HG22	0.413
1	A:323:VAL:CG1	A:329:PHE:CB	0.413
1	A:347:LYS:HD2	A:347:LYS:N	0.413
1	A:439:THR:HG23	A:440:VAL:N	0.413
1	A:338:LYS:CG	A:445:LYS:HG2	0.413
1	A:618:LYS:CG	A:632:THR:CG2	0.413
1	A:98:ASN:HD22	A:264:GLU:HB3	0.413
1	A:17:PRO:HG2	A:22:LYS:HE2	0.412
1	A:338:LYS:CD	A:540:CYS:C	0.412
1	A:344:GLY:O	A:345:GLU:HB2	0.412
1	A:398:LEU:O	A:406:PHE:CD2	0.412
1	A:415:LEU:C	A:415:LEU:CD2	0.412
1	A:462:LEU:O	A:463:ARG:HB2	0.412
1	A:485:VAL:HG13	A:503:ASN:ND2	0.412
1	A:620:CYS:CB	A:628:VAL:HG11	0.412
1	A:58:ILE:CG2	A:83:PHE:CD1	0.411
1	A:75:PHE:CE1	A:246:ARG:O	0.411
1	A:485:VAL:HG13	A:491:ILE:HG12	0.411

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:361:ALA:O	A:362:ARG:HB3	0.411
1	A:223:THR:HG22	A:231:PHE:O	0.410
1	A:276:LYS:HE2	A:442:GLU:HG3	0.410
1	A:434:THR:HG22	A:436:ILE:H	0.410
1	A:508:LEU:HD13	A:519:LYS:HB2	0.410
1	A:525:LEU:HB2	A:528:THR:HG22	0.410
1	A:338:LYS:N	A:541:VAL:H	0.410
1	A:116:PHE:CD1	A:116:PHE:O	0.408
1	A:132:CYS:CB	A:183:ASN:O	0.408
1	A:169:LEU:CD1	A:169:LEU:N	0.408
1	A:450:TRP:CH2	A:451:LEU:CD2	0.408
1	A:586:LEU:CD2	A:618:LYS:HE2	0.408
1	A:421:ILE:CG2	A:422:THR:N	0.408
1	A:350:LEU:HA	A:350:LEU:HD23	0.407
1	A:467:GLU:CG	A:471:PHE:HE1	0.407
1	A:520:LEU:HB3	A:534:LYS:HE2	0.407
1	A:445:LYS:HZ2	A:539:LYS:CG	0.407
1	A:98:ASN:CB	A:264:GLU:HB2	0.406
1	A:347:LYS:HA	A:426:VAL:CB	0.406
1	A:508:LEU:HD11	A:519:LYS:HG2	0.406
1	A:111:LYS:HG2	A:111:LYS:O	0.406
1	A:346:GLN:O	A:426:VAL:HG11	0.405
1	A:441:TYR:CE1	A:444:LEU:HD23	0.405

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:152:GLN:HE21	A:161:CYS:N	0.405
1	A:338:LYS:NZ	A:560:ILE:HG23	0.405
1	A:234:VAL:HB	A:242:TYR:O	0.404
1	A:251:ILE:HD13	A:255:HIS:C	0.404
1	A:508:LEU:CD1	A:519:LYS:CG	0.404
1	A:459:VAL:CG2	A:460:GLU:N	0.404
1	A:614:LYS:HG2	A:615:ASP:OD2	0.404
1	A:462:LEU:C	A:464:ASP:N	0.403
1	A:488:ALA:O	A:489:LYS:HG3	0.403
1	A:501:LEU:HD12	A:504:LYS:HE2	0.403
1	A:505:PHE:CE2	A:514:ILE:N	0.403
1	A:455:PHE:CD2	A:456:LYS:N	0.403
1	A:534:LYS:O	A:537:TYR:HE1	0.403
1	A:92:ASN:CG	A:173:GLY:CA	0.402
1	A:338:LYS:HG3	A:445:LYS:CD	0.402
1	A:443:LYS:CG	A:505:PHE:CE1	0.402
1	A:490:GLU:HB2	A:500:LYS:HB2	0.402
1	A:487:CYS:SG	A:488:ALA:N	0.402
1	A:22:LYS:NZ	A:219:LYS:HG3	0.401
1	A:491:ILE:HB	A:495:VAL:HG21	0.401
1	A:555:ALA:HB3	A:556:PRO:HD3	0.401
1	A:433:LEU:O	A:437:PHE:CD2	0.401
1	A:292:GLU:CD	A:423:GLY:C	0.400

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:457:GLU:O	A:460:GLU:HG2	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	636	593	29	14

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	545	496	36	13

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	75	PHE
1	A	111	LYS
1	A	223	THR
1	A	251	ILE
1	A	346	GLN
1	A	347	LYS
1	A	364	VAL
1	A	408	SER
1	A	422	THR
1	A	445	LYS
1	A	519	LYS
1	A	539	LYS

Model ID	Chain	Residue ID	Residue type
1	A	558	GLU

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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