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	9A8G
PDB-Dev ID	PDBDEV_00000380
Structure Title	Structural Basis for Mis18 Complex Assembly
Structure Authors	Thamkachy, R.; Medina-Pritchard, B.; Park, S.H.; Chiodi, C.G.; Zou, J.; de la Torre-Barranco, M.; Shimanaka, K.; Abad, M.A.; Paramo, C.G.; Feederle, R.; Ruksenaite, E.; Heun, P.; Davies, O.R.; Rappsilber, J.; Schneidman-Duhovny, D; Cho, U.; Jeyaprakash, A.A.

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

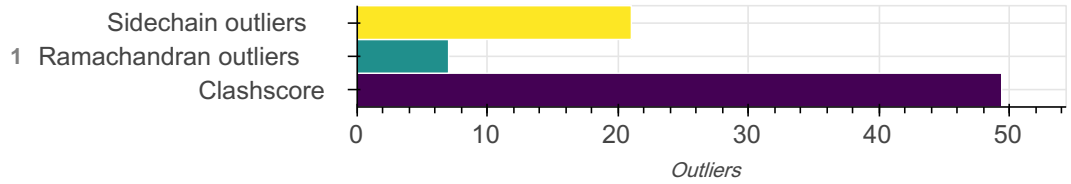
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 18 subunits in each model. A total of 9 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 18 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	Protein Mis18-alpha	A	A	76
1	2	1	Protein Mis18-alpha	A	A	114
1	3	1	Protein Mis18-alpha	A	A	43
1	4	1	Protein Mis18-alpha	D	D	76
1	5	1	Protein Mis18-alpha	D	D	114
1	6	1	Protein Mis18-alpha	D	D	43
1	7	1	Protein Mis18-alpha	E	E	76
1	8	1	Protein Mis18-alpha	E	E	114
1	9	1	Protein Mis18-alpha	E	E	43
1	10	1	Protein Mis18-alpha	F	F	76
1	11	1	Protein Mis18-alpha	F	F	114

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	12	1	Protein Mis18-alpha	F	F	43
1	13	2	Protein Mis18-beta	B	B	187
1	14	2	Protein Mis18-beta	B	B	42
1	15	2	Protein Mis18-beta	G	G	187
1	16	2	Protein Mis18-beta	G	G	42
1	17	3	Mis18-binding protein 1	C	C	130
1	18	3	Mis18-binding protein 1	H	H	130

Datasets used for modeling

There are 9 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
2	3DEM volume	EMDB	EMD-50220
6	3DEM volume	Not available	Not available
7	3DEM volume	Not available	Not available
1	Crosslinking-MS data	PRIDE	PXD047345
3	Experimental model	PDB	7sfz
4	Experimental model	PDB	7sfy
5	De Novo model	AlphaFoldDB	AF-Q9NYP9-F1
8	De Novo model	AlphaFoldDB	AF-O43482-F1
9	De Novo model	AlphaFoldDB	AF-Q6P0N0-F1

Representation

This entry has only one representation and includes 0 rigid bodies and 18 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-76, 77-190, 191-233
B	-	1-187, 188-229
G	-	1-1871-187
D	-	1-76, 77-190, 191-233
E	-	1-76, 77-190, 191-233
F	-	1-76, 77-190, 191-233
C	-	1-130
H	-	1-130

Methodology and software

This entry is a result of 2 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	docking	None	None	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	AlphaFold-Multimer	2.2	model building	https://github.com/google-deepmind/alphafold
2	CombDock	Not available	assembly	http://bioinfo3d.cs.tau.ac.il/CombDock/download/

Data quality

3DEM volume

Validation for this section is under development.

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 136 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
O-C-N	123.00	44.82	1
CA-C-N	116.20	163.17	1
CA-C-O	121.00	163.74	1
CA-C-OXT	121.00	82.52	1
O-C-OXT	118.00	81.24	1
O-C-N	123.00	104.04	1
O-C-N	123.00	104.06	1
O-C-N	123.00	105.25	1
O-C-N	123.00	105.28	1
O-C-N	123.00	106.10	1
O-C-N	123.00	106.12	1
C-N-CA	121.70	139.54	1
C-N-CA	121.70	139.51	1
O-C-N	123.00	107.95	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	107.99	1
C-N-CA	121.70	137.97	1
C-N-CA	121.70	137.89	1
CA-C-N	116.20	133.98	1
CA-C-N	116.20	133.96	1
O-C-N	123.00	137.11	1
O-C-N	123.00	137.06	1
O-C-N	123.00	109.78	2
C-N-CA	121.70	107.30	1
C-N-CA	121.70	107.37	1
C-N-CA	121.70	107.68	1
C-N-CA	121.70	107.73	1
O-C-N	123.00	110.86	1
O-C-N	123.00	110.87	1
O-C-N	123.00	111.07	1
O-C-N	123.00	111.08	1
CA-C-N	116.20	130.74	1
CA-C-N	116.20	130.72	1
CA-C-N	116.20	101.99	1
CA-C-N	116.20	102.00	1
O-C-N	123.00	111.85	1
O-C-N	123.00	111.93	1
CA-C-N	116.20	129.75	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	129.71	1
C-N-CA	121.70	110.46	1
CA-C-N	116.20	103.72	2
C-N-CA	121.70	110.47	1
C-N-CA	121.70	132.91	1
C-N-CA	121.70	110.69	1
C-N-CA	121.70	110.74	1
C-N-CA	121.70	132.65	1
C-N-CA	121.70	132.64	1
CA-C-N	116.20	128.25	1
CA-C-N	116.20	128.20	1
O-C-N	123.00	132.60	1
O-C-N	123.00	132.59	1
CA-C-N	116.20	128.04	2
C-N-CA	121.70	111.11	1
C-N-CA	121.70	111.17	1
CA-C-N	116.20	127.60	1
CA-C-N	116.20	127.57	1
O-C-N	123.00	114.23	2
OE1-CD-NE2	122.60	117.13	1
C-N-CA	121.70	111.91	1
O-C-N	123.00	114.31	1
O-C-N	123.00	114.37	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	131.54	1
O-C-N	123.00	131.53	1
O-C-N	123.00	114.66	1
O-C-N	123.00	131.32	1
O-C-N	123.00	114.68	1
O-C-N	123.00	131.31	1
O-C-N	123.00	131.24	1
CA-C-N	116.20	126.49	1
CA-C-N	116.20	126.47	1
C-N-CA	121.70	112.48	1
C-N-CA	121.70	112.55	1
C-N-CA	121.70	112.56	1
O-C-N	123.00	131.11	1
C-N-CA	121.70	112.58	1
C-N-CA	121.70	112.63	1
C-N-CA	121.70	112.65	1
OE1-CD-NE2	122.60	117.62	1
C-N-CA	121.70	130.65	1
C-N-CA	121.70	130.64	1
OE1-CD-NE2	122.60	117.70	1
OE1-CD-NE2	122.60	117.74	1
OE1-CD-NE2	122.60	117.82	1
C-N-CA	121.70	130.28	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	130.25	2
C-N-CA	121.70	130.23	1
OE1-CD-NE2	122.60	117.87	1
C-N-CA	121.70	113.23	1
O-C-N	123.00	130.51	1
OE1-CD-NE2	122.60	117.91	1
C-N-CA	121.70	113.29	1
O-C-N	123.00	130.44	1
CA-C-N	116.20	106.97	1
OE1-CD-NE2	122.60	118.02	1
CA-C-N	116.20	107.05	1
CA-C-N	116.20	107.17	1
CA-C-N	116.20	107.18	1
C-N-CA	121.70	113.65	1
C-N-CA	121.70	113.67	1
C-N-CA	121.70	113.68	1
CB-CG-CD2	131.20	125.44	1
C-N-CA	121.70	113.75	1
OE1-CD-NE2	122.60	118.20	1
C-CA-CB	110.10	118.42	1
O-C-N	123.00	116.04	2
O-C-N	123.00	129.94	1
C-N-CA	121.70	113.89	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	113.92	1
CB-CG-CD2	131.20	125.59	1
O-C-N	123.00	129.87	1
O-C-N	123.00	129.79	1
C-N-CA	121.70	114.07	1
C-N-CA	121.70	114.12	1
CB-CG-CD2	131.20	125.75	1
O-C-N	123.00	129.68	1
CB-CG-CD2	131.20	125.77	1
CA-C-N	116.20	124.50	2
C-N-CA	121.70	114.28	1
CA-C-N	116.20	107.97	1
C-N-CA	121.70	114.29	1
CA-C-N	116.20	107.98	1
O-C-N	123.00	116.43	2
CA-C-N	116.20	108.06	1
CA-CB-CG	112.60	116.67	1
O-C-N	123.00	116.51	1
CA-C-N	116.20	108.13	1
O-C-N	123.00	116.55	1
C-N-CA	121.70	128.95	1
C-N-CA	121.70	128.92	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	49.37	905

All 905 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	D:215:LEU:HD21	F:52:TRP:CZ3	1.685
1	E:48:TRP:CE2	E:211:VAL:HG13	1.647
1	D:193:PHE:CD2	F:44:LEU:HB2	1.642
1	E:191:GLU:HB3	G:105:VAL:CG1	1.626
1	F:51:MET:HE3	F:211:VAL:CA	1.619
1	B:95:TRP:CE3	F:198:ARG:CD	1.610
1	A:211:VAL:HG13	E:48:TRP:CH2	1.596
1	B:95:TRP:CZ3	F:198:ARG:CD	1.589
1	F:59:ALA:HB1	F:203:LYS:CG	1.582
1	D:215:LEU:CD2	F:52:TRP:CH2	1.577
1	D:215:LEU:CD2	F:52:TRP:CZ3	1.570
1	B:105:VAL:CG1	F:191:GLU:HB3	1.562
1	E:77:GLU:HG3	G:162:PHE:CZ	1.557
1	D:211:VAL:CG2	F:48:TRP:CZ3	1.555
1	E:191:GLU:CD	G:105:VAL:HG21	1.553
1	E:77:GLU:CG	G:162:PHE:CZ	1.548
1	B:105:VAL:HG21	F:191:GLU:CD	1.526
1	F:59:ALA:CB	F:203:LYS:HG3	1.520
1	E:62:ALA:CB	E:203:LYS:HD2	1.515

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:48:TRP:HH2	G:214:MET:SD	1.509
1	F:51:MET:CE	F:211:VAL:HA	1.506
1	E:62:ALA:HB3	E:203:LYS:CD	1.492
1	E:191:GLU:CG	G:163:CYS:SG	1.468
1	D:215:LEU:HD23	F:52:TRP:CH2	1.466
1	A:211:VAL:CG1	E:48:TRP:CH2	1.461
1	E:191:GLU:HG3	G:163:CYS:SG	1.452
1	E:48:TRP:NE1	E:211:VAL:HG13	1.450
1	A:48:TRP:CH2	G:214:MET:SD	1.434
1	B:105:VAL:CG2	F:191:GLU:CD	1.428
1	B:95:TRP:CD2	F:198:ARG:HD3	1.424
1	D:211:VAL:HG22	F:48:TRP:CZ3	1.420
1	B:163:CYS:SG	F:191:GLU:CG	1.410
1	F:48:TRP:CE2	F:211:VAL:CG1	1.409
1	B:163:CYS:SG	F:191:GLU:HG3	1.407
1	F:48:TRP:NE1	F:211:VAL:HG13	1.403
1	E:191:GLU:CD	G:105:VAL:CG2	1.401
1	D:77:GLU:OE1	D:79:ARG:CD	1.395
1	B:95:TRP:CE3	F:198:ARG:HD3	1.395
1	B:95:TRP:CZ3	F:198:ARG:HD3	1.392
1	E:48:TRP:CZ2	E:211:VAL:CG1	1.389
1	F:54:SER:CA	F:57:GLU:HB3	1.387
1	D:193:PHE:CD2	F:44:LEU:CB	1.386

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	F:59:ALA:CB	F:203:LYS:CG	1.369
1	F:59:ALA:O	F:63:ASP:HB2	1.360
1	D:194:ASN:CB	F:37:GLU:HB3	1.341
1	F:48:TRP:CE2	F:211:VAL:HG13	1.339
1	D:207:GLN:OE1	F:41:ARG:NH1	1.330
1	E:54:SER:O	E:58:ASP:N	1.327
1	E:77:GLU:HG3	G:162:PHE:CE2	1.323
1	E:52:TRP:CE3	E:211:VAL:HG21	1.313
1	D:193:PHE:HE2	F:44:LEU:C	1.310
1	D:193:PHE:CE2	F:45:LEU:N	1.309
1	E:48:TRP:CE2	E:211:VAL:CG1	1.307
1	F:51:MET:CE	F:211:VAL:CA	1.303
1	F:55:MET:CA	F:58:ASP:HB2	1.303
1	E:62:ALA:N	E:203:LYS:HZ2	1.303
1	A:38:ASP:O	A:42:HIS:ND1	1.299
1	E:63:ASP:H	E:203:LYS:NZ	1.293
1	E:191:GLU:HA	G:158:LEU:CD2	1.292
1	E:53:SER:O	E:57:GLU:N	1.291
1	F:48:TRP:NE1	F:211:VAL:CG1	1.289
1	F:51:MET:HE3	F:211:VAL:N	1.287
1	E:59:ALA:O	E:63:ASP:HB2	1.278
1	B:95:TRP:CE3	F:198:ARG:HD2	1.276
1	B:158:LEU:CD2	F:191:GLU:HA	1.276

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:193:PHE:HE2	F:45:LEU:N	1.268
1	F:56:SER:O	F:203:LYS:HE3	1.260
1	B:105:VAL:CG1	F:191:GLU:CB	1.258
1	A:52:TRP:CH2	G:218:SER:OG	1.256
1	D:194:ASN:ND2	F:38:ASP:N	1.248
1	E:191:GLU:OE1	G:105:VAL:CG2	1.248
1	B:95:TRP:CH2	F:198:ARG:HD3	1.247
1	D:38:ASP:O	D:42:HIS:ND1	1.244
1	A:211:VAL:CG1	E:48:TRP:CZ2	1.238
1	B:95:TRP:CE2	F:198:ARG:HD3	1.237
1	F:54:SER:HA	F:57:GLU:CB	1.223
1	A:36:SER:O	A:39:SER:OG	1.211
1	D:36:SER:O	D:39:SER:OG	1.209
1	D:194:ASN:HD21	F:38:ASP:CA	1.204
1	D:38:ASP:HB3	D:42:HIS:CE1	1.202
1	A:38:ASP:HB3	A:42:HIS:CE1	1.199
1	B:105:VAL:CG2	F:191:GLU:OE1	1.198
1	E:191:GLU:CG	G:158:LEU:HD13	1.191
1	A:38:ASP:O	A:70:GLU:OE1	1.187
1	A:211:VAL:HG13	E:48:TRP:CZ2	1.184
1	D:38:ASP:O	D:70:GLU:OE1	1.179
1	E:191:GLU:CB	G:105:VAL:CG1	1.176
1	B:158:LEU:HD13	F:191:GLU:CG	1.174

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:53:SER:CB	D:59:ALA:O	1.173
1	D:194:ASN:HD21	F:38:ASP:N	1.171
1	E:57:GLU:HA	E:60:SER:HB3	1.169
1	B:95:TRP:CZ2	F:198:ARG:HD3	1.168
1	A:53:SER:CB	A:59:ALA:O	1.162
1	E:59:ALA:CB	E:207:GLN:NE2	1.162
1	A:215:LEU:HD23	E:52:TRP:HH2	1.161
1	E:191:GLU:CA	G:158:LEU:HD22	1.158
1	E:59:ALA:HB3	E:207:GLN:HE22	1.142
1	B:95:TRP:CH2	F:198:ARG:CD	1.138
1	F:57:GLU:HA	F:60:SER:HB3	1.137
1	B:97:LEU:HD12	F:191:GLU:OE2	1.135
1	E:191:GLU:HB3	G:105:VAL:HG11	1.133
1	E:59:ALA:CB	E:207:GLN:HE22	1.128
1	A:39:SER:HA	A:70:GLU:OE1	1.127
1	A:35:LEU:CD2	A:74:ALA:HA	1.126
1	B:105:VAL:HG13	F:191:GLU:CB	1.124
1	D:35:LEU:CD2	D:74:ALA:HA	1.124
1	F:75:ALA:C	F:78:GLU:HB2	1.123
1	E:48:TRP:NE1	E:211:VAL:CG1	1.123
1	B:158:LEU:HD13	F:191:GLU:HG2	1.121
1	D:194:ASN:HB3	F:37:GLU:HB3	1.121
1	D:65:GLU:OE2	D:220:TRP:CZ2	1.116

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:95:TRP:CH2	F:198:ARG:HG3	1.112
1	E:48:TRP:CZ2	E:211:VAL:HG11	1.111
1	A:43:GLN:O	A:47:LYS:N	1.109
1	D:39:SER:HA	D:70:GLU:OE1	1.108
1	E:191:GLU:HG2	G:158:LEU:HD13	1.106
1	A:48:TRP:HH2	G:214:MET:CE	1.106
1	F:51:MET:HE1	F:211:VAL:HA	1.105
1	D:211:VAL:CB	F:48:TRP:CZ3	1.104
1	E:62:ALA:N	E:203:LYS:NZ	1.103
1	B:158:LEU:HD22	F:191:GLU:CA	1.102
1	B:161:HIS:CD2	F:195:LEU:HB3	1.102
1	B:105:VAL:HG11	F:191:GLU:HB3	1.102
1	B:95:TRP:CD1	F:194:ASN:CB	1.100
1	D:44:LEU:O	D:48:TRP:CB	1.098
1	B:95:TRP:CD2	F:198:ARG:CD	1.097
1	B:97:LEU:HD12	F:191:GLU:CD	1.096
1	A:44:LEU:O	A:48:TRP:CB	1.094
1	A:51:MET:HE1	G:211:LYS:HB3	1.093
1	B:105:VAL:HG21	F:191:GLU:OE1	1.093
1	D:46:GLN:CD	D:63:ASP:O	1.092
1	A:38:ASP:HB3	A:42:HIS:HE1	1.091
1	D:193:PHE:CE2	F:44:LEU:C	1.089
1	D:43:GLN:O	D:47:LYS:N	1.089

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:46:GLN:CD	A:63:ASP:O	1.087
1	E:58:ASP:O	E:203:LYS:NZ	1.087
1	B:95:TRP:CZ3	F:198:ARG:HD2	1.086
1	E:191:GLU:CB	G:105:VAL:HG13	1.079
1	E:194:ASN:CB	G:95:TRP:CD1	1.076
1	F:48:TRP:CD1	F:211:VAL:HG13	1.076
1	D:35:LEU:HD21	D:74:ALA:HA	1.075
1	D:38:ASP:HB3	D:42:HIS:HE1	1.073
1	F:55:MET:HA	F:58:ASP:HB2	1.071
1	B:95:TRP:CD1	F:194:ASN:HB2	1.070
1	A:51:MET:CE	G:211:LYS:HB3	1.069
1	E:195:LEU:HB3	G:161:HIS:CD2	1.069
1	A:211:VAL:HG11	E:48:TRP:CZ2	1.063
1	B:95:TRP:CH2	F:198:ARG:CG	1.063
1	A:35:LEU:HD21	A:74:ALA:HA	1.060
1	F:50:SER:HA	F:53:SER:OG	1.057
1	E:191:GLU:OE2	G:97:LEU:HD12	1.057
1	B:201:GLU:OE2	D:57:GLU:OE1	1.057
1	D:194:ASN:CG	F:37:GLU:HB3	1.055
1	F:59:ALA:HB3	F:203:LYS:CG	1.055
1	F:51:MET:HE2	F:211:VAL:HA	1.055
1	E:50:SER:HA	E:53:SER:OG	1.054
1	E:70:GLU:OE1	E:196:GLU:HG3	1.052

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:194:ASN:HB2	G:95:TRP:CD1	1.041
1	D:46:GLN:HG3	D:66:ARG:HB3	1.037
1	E:191:GLU:CD	G:97:LEU:HD12	1.035
1	A:46:GLN:HG3	A:66:ARG:HB3	1.034
1	E:63:ASP:N	E:203:LYS:NZ	1.033
1	A:52:TRP:CZ2	G:218:SER:OG	1.031
1	B:105:VAL:CG2	F:191:GLU:CG	1.030
1	B:105:VAL:HG11	F:191:GLU:CB	1.029
1	B:161:HIS:NE2	F:195:LEU:HB3	1.029
1	E:61:VAL:N	E:203:LYS:HZ1	1.029
1	E:70:GLU:OE1	E:192:LEU:CD1	1.028
1	E:70:GLU:OE1	E:196:GLU:CG	1.028
1	E:58:ASP:O	E:203:LYS:CE	1.028
1	A:53:SER:O	A:56:SER:O	1.028
1	D:53:SER:O	D:56:SER:O	1.027
1	A:46:GLN:HG2	A:63:ASP:CG	1.024
1	A:215:LEU:HD23	E:52:TRP:CH2	1.022
1	B:107:SER:HB3	F:195:LEU:HD23	1.019
1	E:61:VAL:O	E:65:GLU:N	1.017
1	F:58:ASP:O	F:62:ALA:N	1.015
1	E:52:TRP:HE3	E:211:VAL:CG2	1.013
1	E:58:ASP:O	E:62:ALA:N	1.013
1	F:61:VAL:O	F:65:GLU:N	1.009

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:193:PHE:CE2	F:44:LEU:CB	1.006
1	E:59:ALA:CB	E:203:LYS:HG2	1.004
1	E:191:GLU:CB	G:163:CYS:SG	1.004
1	A:42:HIS:O	A:46:GLN:N	1.003
1	E:50:SER:O	E:54:SER:N	1.003
1	D:46:GLN:HG2	D:63:ASP:CG	0.994
1	A:51:MET:SD	G:211:LYS:HD3	0.994
1	A:44:LEU:O	A:48:TRP:HB3	0.991
1	B:95:TRP:CZ2	F:194:ASN:O	0.991
1	E:59:ALA:O	E:63:ASP:CB	0.991
1	E:191:GLU:OE1	G:105:VAL:HG21	0.990
1	D:42:HIS:O	D:46:GLN:N	0.990
1	E:48:TRP:HE1	E:211:VAL:HG13	0.989
1	F:50:SER:O	F:54:SER:N	0.988
1	B:107:SER:HB3	F:195:LEU:CD2	0.986
1	D:194:ASN:CG	F:38:ASP:N	0.986
1	D:193:PHE:C	F:41:ARG:HB2	0.982
1	D:44:LEU:O	D:48:TRP:HB3	0.979
1	F:59:ALA:HB3	F:203:LYS:HG3	0.979
1	D:215:LEU:CD2	F:52:TRP:HH2	0.979
1	E:191:GLU:HG2	G:163:CYS:SG	0.978
1	E:191:GLU:HB3	G:105:VAL:HG13	0.975
1	E:60:SER:C	E:203:LYS:NZ	0.974

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:48:TRP:CH2	G:214:MET:CE	0.972
1	F:56:SER:O	F:203:LYS:CE	0.970
1	F:59:ALA:O	F:63:ASP:CB	0.970
1	A:51:MET:HE1	G:211:LYS:CB	0.964
1	E:59:ALA:H	E:207:GLN:NE2	0.964
1	E:77:GLU:HG3	G:162:PHE:HZ	0.963
1	B:158:LEU:HD13	F:191:GLU:CD	0.962
1	E:70:GLU:OE1	E:192:LEU:HD11	0.961
1	D:194:ASN:ND2	F:38:ASP:CA	0.961
1	B:105:VAL:HG13	F:191:GLU:HB3	0.959
1	E:195:LEU:HB3	G:161:HIS:NE2	0.955
1	D:39:SER:HA	D:70:GLU:CD	0.951
1	D:194:ASN:CG	F:37:GLU:CB	0.951
1	F:60:SER:O	F:64:MET:N	0.951
1	F:55:MET:N	F:58:ASP:HB2	0.948
1	A:39:SER:HA	A:70:GLU:CD	0.947
1	F:48:TRP:CZ2	F:211:VAL:CG1	0.947
1	E:60:SER:O	E:64:MET:N	0.946
1	D:211:VAL:HG21	F:48:TRP:CZ3	0.941
1	E:60:SER:C	E:203:LYS:HZ3	0.939
1	F:59:ALA:HB2	F:203:LYS:O	0.939
1	F:75:ALA:C	F:78:GLU:CB	0.937
1	D:211:VAL:HG22	F:48:TRP:HZ3	0.937

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:59:ALA:HB2	E:207:GLN:NE2	0.935
1	E:63:ASP:H	E:203:LYS:HZ3	0.934
1	E:191:GLU:CG	G:105:VAL:CG2	0.933
1	B:97:LEU:CD1	F:191:GLU:OE2	0.932
1	E:191:GLU:CD	G:158:LEU:HD13	0.932
1	D:46:GLN:CG	D:63:ASP:O	0.930
1	E:62:ALA:CA	E:203:LYS:HZ2	0.928
1	F:55:MET:N	F:58:ASP:CB	0.928
1	E:44:LEU:CD1	E:218:LYS:HE3	0.927
1	E:191:GLU:CB	G:105:VAL:HG11	0.927
1	B:163:CYS:SG	F:191:GLU:CB	0.927
1	A:211:VAL:HG22	E:48:TRP:CZ3	0.925
1	E:191:GLU:HB2	G:163:CYS:SG	0.924
1	E:195:LEU:HD23	G:107:SER:HB3	0.924
1	A:194:ASN:OD1	E:37:GLU:HB3	0.923
1	A:46:GLN:CG	A:63:ASP:O	0.922
1	E:191:GLU:CG	G:105:VAL:HG22	0.919
1	B:105:VAL:HG22	F:191:GLU:CG	0.918
1	E:44:LEU:CD1	E:218:LYS:CE	0.914
1	F:48:TRP:NE1	F:211:VAL:HG12	0.913
1	F:54:SER:OG	F:58:ASP:CG	0.912
1	F:51:MET:CE	F:210:ASP:C	0.910
1	B:163:CYS:SG	F:191:GLU:HG2	0.910

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	F:55:MET:CA	F:58:ASP:CB	0.906
1	A:38:ASP:C	A:70:GLU:OE1	0.905
1	E:195:LEU:CD2	G:107:SER:HB3	0.901
1	E:59:ALA:HB2	E:207:GLN:CD	0.900
1	B:95:TRP:HZ2	F:194:ASN:O	0.900
1	B:107:SER:CB	F:195:LEU:HD23	0.897
1	D:196:GLU:OE1	F:33:LYS:O	0.896
1	F:54:SER:OG	F:58:ASP:OD1	0.896
1	F:59:ALA:CB	F:203:LYS:HG2	0.893
1	A:39:SER:CA	A:70:GLU:OE1	0.891
1	E:51:MET:CE	E:211:VAL:HA	0.891
1	D:38:ASP:C	D:70:GLU:OE1	0.888
1	E:59:ALA:HB3	E:207:GLN:NE2	0.887
1	D:39:SER:CA	D:70:GLU:OE1	0.886
1	B:95:TRP:CD2	F:194:ASN:HB3	0.884
1	D:193:PHE:CD2	F:44:LEU:HB3	0.884
1	F:59:ALA:HB1	F:203:LYS:CB	0.884
1	D:193:PHE:CE2	F:44:LEU:HB3	0.883
1	F:52:TRP:HE3	F:211:VAL:HG21	0.883
1	E:48:TRP:HZ2	E:211:VAL:CG1	0.882
1	B:158:LEU:CD2	F:191:GLU:CA	0.881
1	D:46:GLN:HG2	D:63:ASP:O	0.879
1	F:55:MET:HA	F:58:ASP:CB	0.879

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	F:48:TRP:CE2	F:211:VAL:HG12	0.878
1	A:46:GLN:HG2	A:63:ASP:O	0.876
1	D:77:GLU:OE1	D:79:ARG:HD2	0.873
1	B:105:VAL:HG11	F:191:GLU:CA	0.872
1	B:105:VAL:HG21	F:191:GLU:CG	0.872
1	F:51:MET:CE	F:211:VAL:N	0.871
1	F:56:SER:O	F:60:SER:N	0.870
1	D:194:ASN:HB3	F:37:GLU:CB	0.866
1	B:95:TRP:CD1	F:194:ASN:HB3	0.864
1	D:53:SER:OG	D:59:ALA:O	0.863
1	B:158:LEU:HD22	F:191:GLU:HA	0.862
1	D:211:VAL:CG2	F:48:TRP:CE3	0.859
1	E:195:LEU:CD2	G:107:SER:N	0.858
1	B:95:TRP:CE2	F:194:ASN:HB3	0.857
1	E:56:SER:O	E:60:SER:N	0.857
1	F:51:MET:O	F:58:ASP:OD2	0.857
1	F:55:MET:CB	F:58:ASP:HB2	0.856
1	B:163:CYS:SG	F:191:GLU:HB2	0.855
1	E:191:GLU:OE1	G:97:LEU:HD12	0.855
1	B:107:SER:N	F:195:LEU:CD2	0.854
1	A:53:SER:OG	A:59:ALA:O	0.854
1	E:77:GLU:HG3	G:162:PHE:CE1	0.853
1	E:194:ASN:HB3	G:95:TRP:CD2	0.851

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	F:59:ALA:HB3	F:203:LYS:HG2	0.851
1	F:75:ALA:O	F:78:GLU:HB2	0.849
1	A:215:LEU:CD2	E:52:TRP:CH2	0.848
1	B:97:LEU:HD12	F:191:GLU:OE1	0.848
1	B:107:SER:CB	F:195:LEU:CD2	0.848
1	E:77:GLU:CB	G:162:PHE:CZ	0.847
1	F:51:MET:HE1	F:211:VAL:CA	0.847
1	E:191:GLU:OE2	G:97:LEU:CD1	0.847
1	E:77:GLU:CG	G:162:PHE:CE1	0.845
1	D:215:LEU:CD2	F:52:TRP:HZ3	0.844
1	F:60:SER:HB2	F:203:LYS:HZ1	0.842
1	E:77:GLU:CB	G:162:PHE:HZ	0.841
1	E:61:VAL:N	E:203:LYS:NZ	0.841
1	E:58:ASP:O	E:62:ALA:CB	0.840
1	B:95:TRP:CZ3	F:198:ARG:CG	0.839
1	E:77:GLU:CD	G:162:PHE:CE1	0.837
1	F:54:SER:CB	F:58:ASP:OD1	0.834
1	F:58:ASP:O	F:62:ALA:CB	0.833
1	D:35:LEU:HD23	D:74:ALA:HA	0.832
1	E:54:SER:HA	E:57:GLU:HB3	0.832
1	E:191:GLU:HA	G:158:LEU:HD22	0.829
1	B:105:VAL:HG22	F:191:GLU:HG3	0.828
1	A:215:LEU:CD2	E:52:TRP:HH2	0.827

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:191:GLU:CD	G:105:VAL:HG22	0.824
1	D:45:LEU:O	D:49:ALA:HB2	0.823
1	E:195:LEU:HD23	G:107:SER:CB	0.822
1	E:63:ASP:H	E:203:LYS:CE	0.822
1	A:45:LEU:O	A:49:ALA:HB2	0.821
1	E:194:ASN:HB3	G:95:TRP:CD1	0.821
1	B:95:TRP:CE2	F:198:ARG:CD	0.820
1	E:191:GLU:CA	G:105:VAL:HG11	0.820
1	F:76:ALA:N	F:78:GLU:N	0.820
1	D:38:ASP:C	D:42:HIS:ND1	0.816
1	F:58:ASP:HA	F:61:VAL:HB	0.816
1	E:70:GLU:OE1	E:192:LEU:HD12	0.815
1	E:70:GLU:OE2	E:196:GLU:HG2	0.814
1	A:38:ASP:C	A:42:HIS:ND1	0.811
1	D:194:ASN:HD21	F:38:ASP:CB	0.811
1	F:52:TRP:CE3	F:211:VAL:HG21	0.811
1	D:44:LEU:O	D:48:TRP:HB2	0.810
1	F:73:ALA:C	F:78:GLU:N	0.808
1	E:77:GLU:CG	G:162:PHE:HZ	0.807
1	F:72:GLU:O	F:76:ALA:N	0.805
1	B:95:TRP:CG	F:194:ASN:HB3	0.804
1	E:62:ALA:H	E:203:LYS:NZ	0.803
1	A:35:LEU:HD23	A:74:ALA:HA	0.802

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:105:VAL:CB	F:191:GLU:HB3	0.799
1	A:211:VAL:CG2	E:48:TRP:CZ3	0.798
1	D:211:VAL:HG21	F:48:TRP:CE3	0.796
1	D:194:ASN:N	F:41:ARG:HB2	0.796
1	E:58:ASP:HA	E:61:VAL:HB	0.794
1	E:194:ASN:HB3	G:95:TRP:CG	0.794
1	E:191:GLU:CD	G:158:LEU:CD1	0.793
1	F:57:GLU:CA	F:60:SER:HB3	0.791
1	A:46:GLN:HG2	A:63:ASP:CA	0.790
1	B:158:LEU:CD1	F:191:GLU:CD	0.790
1	A:35:LEU:HD23	A:74:ALA:CA	0.789
1	D:35:LEU:HD23	D:74:ALA:CA	0.789
1	D:46:GLN:HG2	D:63:ASP:CA	0.789
1	D:193:PHE:CD2	F:41:ARG:O	0.787
1	A:44:LEU:O	A:48:TRP:HB2	0.785
1	F:48:TRP:CD2	F:211:VAL:HG13	0.784
1	F:49:ALA:O	F:53:SER:N	0.782
1	E:57:GLU:HG2	E:61:VAL:HG23	0.780
1	D:35:LEU:CD2	D:74:ALA:CA	0.779
1	E:70:GLU:CD	E:196:GLU:CG	0.779
1	B:95:TRP:CZ2	F:198:ARG:CD	0.778
1	B:97:LEU:CD1	F:191:GLU:CD	0.776
1	F:51:MET:CE	F:210:ASP:O	0.776

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:197:SER:HB2	G:95:TRP:CZ2	0.772
1	E:72:GLU:O	E:76:ALA:N	0.772
1	E:195:LEU:CD2	G:107:SER:CB	0.769
1	F:54:SER:HB2	F:58:ASP:OD1	0.769
1	F:57:GLU:HG2	F:61:VAL:HG23	0.768
1	E:53:SER:C	E:57:GLU:H	0.768
1	E:44:LEU:HD11	E:218:LYS:CE	0.767
1	E:48:TRP:HE1	E:211:VAL:CG1	0.767
1	B:158:LEU:HD22	F:191:GLU:OE1	0.766
1	E:57:GLU:CA	E:60:SER:HB3	0.766
1	F:71:GLU:O	F:75:ALA:N	0.765
1	E:191:GLU:HG2	G:158:LEU:CD1	0.762
1	F:58:ASP:O	F:62:ALA:HB3	0.762
1	E:194:ASN:OD1	G:157:ALA:HB3	0.760
1	A:51:MET:SD	G:211:LYS:CD	0.758
1	B:157:ALA:HB3	F:194:ASN:OD1	0.757
1	E:195:LEU:CD2	G:107:SER:H	0.757
1	A:35:LEU:CD2	A:74:ALA:CA	0.756
1	F:54:SER:HA	F:57:GLU:HB3	0.756
1	E:58:ASP:O	E:62:ALA:HB3	0.755
1	A:48:TRP:CZ3	G:214:MET:SD	0.754
1	B:107:SER:H	F:195:LEU:CD2	0.754
1	E:197:SER:HB2	G:95:TRP:HZ2	0.753

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	F:73:ALA:O	F:78:GLU:O	0.753
1	E:194:ASN:HB3	G:95:TRP:CE2	0.752
1	E:71:GLU:O	E:75:ALA:N	0.752
1	E:44:LEU:HD13	E:218:LYS:CE	0.751
1	F:56:SER:C	F:203:LYS:HE3	0.750
1	E:49:ALA:O	E:53:SER:N	0.750
1	D:196:GLU:OE2	F:37:GLU:HB2	0.749
1	E:59:ALA:N	E:207:GLN:NE2	0.746
1	E:63:ASP:N	E:203:LYS:HZ3	0.746
1	E:191:GLU:HG3	G:105:VAL:HG22	0.745
1	B:158:LEU:CD1	F:191:GLU:HG2	0.744
1	E:52:TRP:O	E:56:SER:N	0.744
1	B:161:HIS:CG	F:191:GLU:O	0.743
1	F:51:MET:HE1	F:210:ASP:O	0.743
1	A:45:LEU:O	A:49:ALA:CB	0.742
1	F:54:SER:C	F:57:GLU:HB3	0.742
1	D:46:GLN:CG	D:63:ASP:CG	0.741
1	E:191:GLU:HB3	G:105:VAL:CB	0.741
1	E:191:GLU:OE1	G:158:LEU:HD22	0.740
1	A:51:MET:HE1	G:211:LYS:C	0.738
1	A:50:SER:HB3	A:63:ASP:HB3	0.737
1	E:191:GLU:C	G:105:VAL:HG11	0.737
1	F:51:MET:SD	F:210:ASP:C	0.737

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:198:ARG:H	G:95:TRP:HZ2	0.737
1	A:46:GLN:HG2	A:63:ASP:C	0.735
1	A:215:LEU:HD21	E:52:TRP:CZ3	0.735
1	B:107:SER:CA	F:195:LEU:HD23	0.734
1	D:194:ASN:CB	F:37:GLU:CB	0.734
1	F:46:GLN:O	F:50:SER:N	0.734
1	D:45:LEU:O	D:49:ALA:CB	0.733
1	D:211:VAL:CG2	F:48:TRP:HZ3	0.733
1	E:195:LEU:HD23	G:107:SER:N	0.732
1	D:46:GLN:HG2	D:63:ASP:C	0.731
1	E:191:GLU:CG	G:105:VAL:HG21	0.731
1	F:70:GLU:O	F:74:ALA:N	0.729
1	B:201:GLU:CD	D:57:GLU:OE1	0.728
1	E:58:ASP:O	E:203:LYS:CD	0.728
1	E:70:GLU:CD	E:196:GLU:HG2	0.727
1	F:48:TRP:CE2	F:211:VAL:HG11	0.727
1	F:51:MET:HA	F:58:ASP:OD2	0.727
1	E:46:GLN:O	E:50:SER:N	0.727
1	E:191:GLU:CA	G:158:LEU:CD2	0.725
1	E:58:ASP:C	E:203:LYS:NZ	0.725
1	E:70:GLU:O	E:74:ALA:N	0.724
1	E:77:GLU:CD	G:162:PHE:CZ	0.721
1	D:50:SER:HB3	D:63:ASP:HB3	0.720

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:38:ASP:O	A:42:HIS:CG	0.718
1	E:191:GLU:O	G:161:HIS:CG	0.718
1	D:38:ASP:O	D:42:HIS:CE1	0.718
1	B:105:VAL:HG11	F:191:GLU:C	0.717
1	E:44:LEU:CD1	E:218:LYS:HE2	0.717
1	D:50:SER:HA	D:53:SER:OG	0.715
1	E:51:MET:HA	E:54:SER:OG	0.715
1	E:51:MET:HE1	E:211:VAL:HA	0.713
1	E:198:ARG:N	G:95:TRP:CZ2	0.713
1	A:50:SER:HA	A:53:SER:OG	0.712
1	E:62:ALA:CA	E:203:LYS:HD2	0.712
1	B:97:LEU:CD1	F:191:GLU:OE1	0.709
1	D:218:LYS:HD3	F:52:TRP:CZ2	0.708
1	F:51:MET:HA	F:54:SER:OG	0.707
1	A:38:ASP:O	A:42:HIS:CE1	0.705
1	B:95:TRP:HZ2	F:197:SER:HB2	0.704
1	E:62:ALA:O	E:66:ARG:HB2	0.703
1	E:47:LYS:HA	E:50:SER:OG	0.701
1	E:195:LEU:HD23	G:107:SER:CA	0.700
1	F:62:ALA:O	F:66:ARG:HB2	0.699
1	E:44:LEU:HD13	E:218:LYS:HE3	0.696
1	F:51:MET:SD	F:210:ASP:HB3	0.695
1	D:38:ASP:O	D:42:HIS:CG	0.694

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:194:ASN:ND2	F:38:ASP:HA	0.694
1	B:107:SER:N	F:195:LEU:HD23	0.691
1	F:59:ALA:H	F:207:GLN:CG	0.691
1	E:61:VAL:C	E:203:LYS:NZ	0.690
1	F:48:TRP:CZ2	F:211:VAL:HG11	0.690
1	F:74:ALA:HB2	F:79:ARG:HG3	0.690
1	A:211:VAL:CG2	E:48:TRP:CH2	0.689
1	B:161:HIS:CE1	F:196:GLU:H	0.688
1	E:74:ALA:N	G:108:ARG:HG2	0.686
1	F:47:LYS:HA	F:50:SER:OG	0.685
1	D:215:LEU:HD21	F:52:TRP:HZ3	0.683
1	A:211:VAL:CB	E:48:TRP:CH2	0.682
1	F:61:VAL:HA	F:64:MET:HB2	0.682
1	F:48:TRP:HE1	F:211:VAL:CG1	0.681
1	D:193:PHE:HD2	F:44:LEU:CB	0.681
1	B:159:ARG:C	F:192:LEU:HB3	0.680
1	E:61:VAL:HA	E:64:MET:HB2	0.680
1	A:55:MET:HB2	G:215:LYS:CD	0.679
1	E:191:GLU:OE1	G:97:LEU:CD1	0.679
1	E:196:GLU:H	G:161:HIS:CE1	0.679
1	D:38:ASP:CB	D:42:HIS:CE1	0.677
1	F:48:TRP:CZ2	F:211:VAL:HG12	0.677
1	F:52:TRP:HE3	F:211:VAL:CG2	0.677

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:55:MET:HB2	G:215:LYS:HG3	0.675
1	E:191:GLU:CD	G:97:LEU:CD1	0.674
1	F:59:ALA:CA	F:203:LYS:HG3	0.674
1	A:194:ASN:CG	E:37:GLU:HB3	0.673
1	E:43:GLN:O	E:47:LYS:HB2	0.673
1	F:48:TRP:NE1	F:211:VAL:O	0.673
1	D:47:LYS:O	D:50:SER:OG	0.672
1	F:43:GLN:O	F:47:LYS:HB2	0.671
1	A:51:MET:SD	G:211:LYS:HB3	0.671
1	B:197:ALA:HB1	D:58:ASP:OD2	0.669
1	E:54:SER:O	E:58:ASP:CB	0.669
1	E:192:LEU:HD12	G:161:HIS:CE1	0.669
1	A:215:LEU:HD21	E:52:TRP:HZ3	0.668
1	D:77:GLU:OE1	D:79:ARG:HD3	0.668
1	E:62:ALA:HB3	E:203:LYS:CG	0.667
1	B:158:LEU:O	F:192:LEU:N	0.666
1	E:52:TRP:CE3	E:211:VAL:CG2	0.665
1	F:74:ALA:CB	F:79:ARG:HG3	0.663
1	F:54:SER:HG	F:58:ASP:CG	0.662
1	F:55:MET:HA	F:59:ALA:H	0.660
1	F:60:SER:HB2	F:203:LYS:NZ	0.660
1	F:48:TRP:HE1	F:211:VAL:HG12	0.660
1	F:50:SER:CA	F:53:SER:OG	0.660

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	F:48:TRP:HE1	F:211:VAL:C	0.658
1	A:211:VAL:CG1	E:48:TRP:HH2	0.658
1	E:54:SER:O	E:58:ASP:CA	0.658
1	F:54:SER:OG	F:58:ASP:OD2	0.656
1	D:35:LEU:HD23	D:74:ALA:CB	0.655
1	E:192:LEU:N	G:158:LEU:O	0.655
1	A:36:SER:C	A:39:SER:HG	0.655
1	E:191:GLU:HB3	G:105:VAL:CG2	0.654
1	E:73:ALA:CB	G:107:SER:C	0.651
1	A:55:MET:HE3	G:215:LYS:C	0.650
1	D:194:ASN:ND2	F:38:ASP:CG	0.650
1	F:73:ALA:C	F:78:GLU:O	0.650
1	A:218:LYS:HD3	E:52:TRP:CZ2	0.649
1	E:69:LEU:HD22	G:92:HIS:HE1	0.649
1	E:192:LEU:HB3	G:159:ARG:C	0.649
1	E:51:MET:HE3	E:211:VAL:HA	0.647
1	E:63:ASP:N	E:203:LYS:HZ2	0.647
1	A:35:LEU:HD23	A:74:ALA:CB	0.646
1	B:158:LEU:HD22	F:191:GLU:CD	0.646
1	B:107:SER:CB	F:195:LEU:HD21	0.644
1	E:59:ALA:CB	E:207:GLN:CD	0.643
1	D:193:PHE:HD2	F:44:LEU:HB2	0.643
1	B:105:VAL:CG2	F:191:GLU:HB3	0.642

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:105:VAL:CG2	F:191:GLU:CB	0.640
1	D:207:GLN:HG2	F:45:LEU:HD11	0.640
1	E:44:LEU:HD11	E:218:LYS:HE2	0.640
1	E:191:GLU:O	G:105:VAL:HG11	0.639
1	A:47:LYS:O	A:50:SER:OG	0.639
1	F:51:MET:SD	F:210:ASP:O	0.639
1	F:48:TRP:CG	F:211:VAL:HG13	0.637
1	F:51:MET:CA	F:58:ASP:OD2	0.635
1	E:77:GLU:OE2	G:162:PHE:CE1	0.634
1	E:50:SER:CA	E:53:SER:OG	0.634
1	A:38:ASP:CB	A:42:HIS:CE1	0.633
1	E:59:ALA:HB2	E:203:LYS:HG2	0.630
1	F:55:MET:HA	F:58:ASP:CA	0.630
1	E:64:MET:O	E:68:GLN:N	0.630
1	A:55:MET:HB2	G:215:LYS:CG	0.629
1	F:54:SER:CA	F:57:GLU:CB	0.629
1	F:55:MET:N	F:58:ASP:CG	0.629
1	E:52:TRP:HE3	E:211:VAL:HG21	0.628
1	B:95:TRP:CZ2	F:197:SER:HB2	0.627
1	D:43:GLN:O	D:47:LYS:HB2	0.625
1	A:43:GLN:O	A:47:LYS:HB2	0.624
1	E:70:GLU:CD	E:196:GLU:HG3	0.624
1	F:76:ALA:H	F:78:GLU:N	0.622

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:193:PHE:CE2	F:44:LEU:CA	0.621
1	F:52:TRP:CE3	F:211:VAL:HG11	0.619
1	E:62:ALA:O	E:66:ARG:N	0.619
1	D:65:GLU:OE2	D:220:TRP:CE2	0.618
1	F:68:GLN:O	F:72:GLU:N	0.618
1	F:102:GLN:HE21	F:109:LEU:HD11	0.617
1	D:193:PHE:CZ	F:45:LEU:HG	0.616
1	F:61:VAL:O	F:65:GLU:HB2	0.616
1	F:77:GLU:HB2	F:78:GLU:HB3	0.616
1	A:211:VAL:HG22	E:48:TRP:HZ3	0.614
1	E:61:VAL:O	E:65:GLU:HB2	0.614
1	E:194:ASN:CB	G:95:TRP:CE2	0.614
1	E:54:SER:O	E:58:ASP:HB2	0.613
1	F:64:MET:O	F:68:GLN:N	0.612
1	E:70:GLU:OE2	E:196:GLU:CG	0.611
1	D:47:LYS:HA	D:50:SER:OG	0.609
1	E:51:MET:HA	E:54:SER:HG	0.609
1	E:191:GLU:CD	G:158:LEU:HD22	0.609
1	D:44:LEU:O	D:48:TRP:N	0.609
1	F:63:ASP:O	F:67:ALA:N	0.608
1	A:52:TRP:CH2	G:218:SER:CB	0.606
1	E:191:GLU:CB	G:105:VAL:CG2	0.604
1	A:44:LEU:O	A:48:TRP:N	0.603

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:47:LYS:HA	A:50:SER:OG	0.602
1	E:53:SER:O	E:57:GLU:HB2	0.602
1	E:58:ASP:O	E:203:LYS:HD2	0.602
1	E:194:ASN:CB	G:95:TRP:CG	0.600
1	F:63:ASP:O	F:67:ALA:CB	0.599
1	F:74:ALA:CB	F:79:ARG:CA	0.596
1	B:95:TRP:HZ2	F:198:ARG:H	0.596
1	E:63:ASP:O	E:67:ALA:N	0.596
1	A:41:ARG:O	A:45:LEU:HG	0.595
1	E:69:LEU:HD22	G:92:HIS:CE1	0.594
1	F:62:ALA:O	F:66:ARG:N	0.594
1	E:63:ASP:O	E:67:ALA:CB	0.593
1	D:194:ASN:HD21	F:38:ASP:CG	0.592
1	A:211:VAL:HG22	E:48:TRP:CH2	0.591
1	D:46:GLN:CG	D:66:ARG:HB3	0.589
1	D:207:GLN:HB3	F:45:LEU:HD21	0.588
1	D:47:LYS:HA	D:63:ASP:OD2	0.587
1	D:46:GLN:CG	D:63:ASP:HA	0.585
1	E:53:SER:O	E:57:GLU:CB	0.585
1	B:161:HIS:HE2	F:195:LEU:HB3	0.585
1	A:46:GLN:CG	A:63:ASP:HA	0.583
1	B:161:HIS:CE1	F:192:LEU:HD12	0.583
1	D:194:ASN:ND2	F:38:ASP:H	0.583

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	F:58:ASP:O	F:62:ALA:CA	0.583
1	A:47:LYS:HA	A:63:ASP:OD2	0.582
1	D:196:GLU:OE2	F:37:GLU:CB	0.582
1	D:65:GLU:OE2	D:220:TRP:HZ2	0.582
1	D:41:ARG:O	D:45:LEU:HG	0.581
1	E:51:MET:HE3	E:211:VAL:CA	0.581
1	E:59:ALA:O	E:63:ASP:N	0.581
1	E:51:MET:O	E:55:MET:N	0.581
1	E:36:SER:HA	E:39:SER:OG	0.579
1	E:58:ASP:O	E:62:ALA:CA	0.579
1	A:46:GLN:CG	A:66:ARG:HB3	0.578
1	E:191:GLU:C	G:105:VAL:CG1	0.578
1	F:36:SER:HA	F:39:SER:OG	0.578
1	E:44:LEU:HD13	E:218:LYS:HE2	0.577
1	E:70:GLU:OE1	E:196:GLU:CD	0.577
1	F:59:ALA:HB2	F:203:LYS:C	0.577
1	F:77:GLU:N	F:78:GLU:HB3	0.577
1	F:59:ALA:O	F:63:ASP:N	0.575
1	E:102:GLN:HE21	E:109:LEU:HD11	0.574
1	E:66:ARG:CB	E:199:VAL:HG11	0.573
1	D:194:ASN:H	F:41:ARG:HD3	0.572
1	E:194:ASN:H	G:157:ALA:C	0.571
1	E:77:GLU:CG	G:162:PHE:CE2	0.571

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:194:ASN:ND2	F:38:ASP:OD1	0.571
1	E:51:MET:SD	E:210:ASP:HB3	0.570
1	E:73:ALA:O	G:108:ARG:HA	0.570
1	A:127:LYS:HE3	C:31:PHE:CE1	0.569
1	E:58:ASP:C	E:203:LYS:HZ1	0.569
1	E:62:ALA:O	E:66:ARG:CB	0.569
1	E:61:VAL:C	E:203:LYS:HZ2	0.569
1	A:35:LEU:HD23	A:74:ALA:HB1	0.568
1	E:195:LEU:HD21	G:107:SER:CB	0.568
1	F:51:MET:HE1	F:211:VAL:C	0.568
1	F:63:ASP:O	F:67:ALA:HB2	0.567
1	F:54:SER:HA	F:57:GLU:CG	0.566
1	F:59:ALA:HB1	F:203:LYS:CA	0.565
1	F:62:ALA:O	F:66:ARG:CB	0.565
1	F:77:GLU:O	F:78:GLU:CB	0.565
1	D:40:SER:O	D:44:LEU:N	0.565
1	E:53:SER:O	E:57:GLU:CA	0.565
1	F:47:LYS:O	F:51:MET:N	0.564
1	F:67:ALA:O	F:71:GLU:N	0.564
1	E:63:ASP:N	E:203:LYS:CD	0.563
1	B:105:VAL:HG11	F:191:GLU:O	0.561
1	D:35:LEU:HD23	D:74:ALA:HB1	0.561
1	F:55:MET:HA	F:59:ALA:N	0.561

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	F:51:MET:C	F:58:ASP:OD2	0.560
1	E:50:SER:O	E:54:SER:OG	0.560
1	A:48:TRP:CZ3	A:209:GLU:OE1	0.559
1	F:56:SER:C	F:60:SER:H	0.559
1	F:51:MET:O	F:55:MET:N	0.558
1	D:193:PHE:CE2	F:45:LEU:CA	0.557
1	D:193:PHE:CZ	F:45:LEU:HD23	0.557
1	E:63:ASP:O	E:67:ALA:HB2	0.557
1	F:55:MET:HB2	F:58:ASP:HB2	0.556
1	B:105:VAL:CG1	F:191:GLU:C	0.555
1	D:36:SER:C	D:39:SER:H	0.555
1	A:36:SER:C	A:39:SER:H	0.552
1	B:158:LEU:CD1	F:191:GLU:OE2	0.552
1	E:67:ALA:O	E:71:GLU:N	0.552
1	D:46:GLN:HG2	D:63:ASP:CB	0.551
1	F:50:SER:O	F:54:SER:OG	0.551
1	A:46:GLN:HG2	A:63:ASP:CB	0.548
1	E:47:LYS:O	E:51:MET:N	0.548
1	A:211:VAL:HG13	E:48:TRP:HH2	0.547
1	E:103:GLU:HG2	H:118:MET:HE2	0.547
1	B:209:ARG:HD2	F:223:GLU:OE1	0.546
1	E:59:ALA:CA	E:207:GLN:NE2	0.545
1	D:53:SER:HB3	D:59:ALA:O	0.544

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:38:ASP:C	A:42:HIS:CE1	0.542
1	A:51:MET:HE1	G:211:LYS:CA	0.542
1	E:194:ASN:N	G:157:ALA:C	0.542
1	E:191:GLU:OE1	G:158:LEU:CD2	0.542
1	D:39:SER:O	D:43:GLN:N	0.542
1	D:38:ASP:C	D:42:HIS:CE1	0.541
1	F:43:GLN:O	F:47:LYS:N	0.541
1	A:46:GLN:CG	A:63:ASP:CA	0.540
1	D:46:GLN:HG2	D:63:ASP:HA	0.539
1	B:190:VAL:O	B:193:SER:N	0.539
1	B:159:ARG:O	F:192:LEU:HB3	0.538
1	E:62:ALA:C	E:203:LYS:HZ2	0.538
1	A:53:SER:HB3	A:59:ALA:O	0.538
1	E:57:GLU:O	E:61:VAL:HG23	0.537
1	B:95:TRP:CZ2	F:198:ARG:CG	0.537
1	E:43:GLN:O	E:47:LYS:N	0.537
1	B:158:LEU:CD2	F:191:GLU:OE1	0.536
1	D:193:PHE:HB2	F:44:LEU:HD12	0.536
1	A:211:VAL:HG11	E:48:TRP:CH2	0.535
1	E:191:GLU:CG	G:158:LEU:CD1	0.535
1	A:215:LEU:CD2	E:52:TRP:CZ3	0.534
1	E:223:GLU:OE1	G:209:ARG:HD2	0.534
1	G:190:VAL:O	G:193:SER:N	0.534

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:192:LEU:HB3	G:159:ARG:O	0.532
1	D:50:SER:HB3	D:63:ASP:CB	0.530
1	E:56:SER:C	E:60:SER:H	0.530
1	F:54:SER:CB	F:58:ASP:CG	0.528
1	F:57:GLU:O	F:61:VAL:HG23	0.528
1	E:198:ARG:N	G:95:TRP:HZ2	0.528
1	F:51:MET:HE3	F:211:VAL:CB	0.527
1	D:211:VAL:C	F:48:TRP:HH2	0.527
1	B:161:HIS:NE2	F:195:LEU:CB	0.526
1	D:46:GLN:CG	D:63:ASP:CA	0.524
1	E:66:ARG:O	E:70:GLU:N	0.522
1	F:66:ARG:O	F:70:GLU:N	0.522
1	E:77:GLU:HB2	G:162:PHE:HZ	0.520
1	E:56:SER:O	E:60:SER:CB	0.519
1	B:160:GLY:N	F:192:LEU:HB3	0.519
1	A:39:SER:O	A:43:GLN:N	0.519
1	B:105:VAL:CB	F:191:GLU:OE1	0.519
1	F:56:SER:O	F:60:SER:CB	0.518
1	F:70:GLU:O	F:74:ALA:CB	0.517
1	B:158:LEU:CD2	F:191:GLU:CD	0.516
1	E:191:GLU:OE2	G:158:LEU:CD1	0.516
1	A:40:SER:O	A:44:LEU:N	0.516
1	D:77:GLU:OE1	D:178:LEU:O	0.516

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:157:ALA:CB	F:194:ASN:OD1	0.514
1	B:161:HIS:HE2	F:196:GLU:N	0.512
1	E:48:TRP:HZ2	E:211:VAL:HG12	0.511
1	E:70:GLU:O	E:74:ALA:CB	0.510
1	A:55:MET:CB	G:215:LYS:HG3	0.508
1	D:31:LEU:O	D:34:ARG:HD3	0.507
1	E:103:GLU:CG	H:114:ILE:HG23	0.507
1	A:193:PHE:HD2	E:44:LEU:HB2	0.506
1	D:211:VAL:CA	F:48:TRP:HH2	0.506
1	E:62:ALA:CB	E:203:LYS:CD	0.505
1	B:107:SER:OG	F:195:LEU:HD21	0.505
1	F:77:GLU:CA	F:78:GLU:HB3	0.504
1	A:50:SER:HB3	A:63:ASP:CB	0.503
1	A:30:LEU:HD21	D:111:ARG:HH22	0.502
1	B:197:ALA:CB	D:58:ASP:OD2	0.502
1	E:63:ASP:N	E:203:LYS:CE	0.502
1	F:52:TRP:HE3	F:211:VAL:HG11	0.502
1	A:46:GLN:NE2	A:63:ASP:O	0.501
1	A:31:LEU:O	A:34:ARG:HD3	0.500
1	E:51:MET:CE	E:211:VAL:CA	0.500
1	E:70:GLU:C	G:108:ARG:HE	0.500
1	D:193:PHE:CZ	F:45:LEU:CD2	0.499
1	B:107:SER:N	F:195:LEU:HD22	0.499

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:42:HIS:O	A:46:GLN:HB2	0.498
1	D:42:HIS:O	D:46:GLN:HB2	0.498
1	B:97:LEU:HD12	B:105:VAL:HG21	0.496
1	E:51:MET:HE3	E:211:VAL:N	0.494
1	A:48:TRP:CH2	G:214:MET:HE2	0.493
1	D:32:GLY:C	D:34:ARG:H	0.493
1	D:46:GLN:HG3	D:63:ASP:HA	0.493
1	E:103:GLU:CD	H:114:ILE:HG23	0.492
1	A:39:SER:N	A:70:GLU:OE1	0.492
1	B:95:TRP:CZ2	F:198:ARG:N	0.491
1	A:127:LYS:HE3	C:31:PHE:CZ	0.490
1	B:158:LEU:HD11	F:191:GLU:OE2	0.490
1	B:95:TRP:CG	F:194:ASN:CB	0.490
1	A:42:HIS:HA	A:45:LEU:HB2	0.489
1	B:157:ALA:C	F:194:ASN:N	0.489
1	E:54:SER:HA	E:57:GLU:CB	0.489
1	D:193:PHE:HZ	F:45:LEU:HD23	0.489
1	D:42:HIS:HA	D:45:LEU:HB2	0.486
1	E:191:GLU:CD	G:158:LEU:CD2	0.486
1	F:59:ALA:HB1	F:203:LYS:HG3	0.486
1	F:53:SER:O	F:57:GLU:CB	0.485
1	F:59:ALA:H	F:207:GLN:HG3	0.483
1	A:32:GLY:C	A:34:ARG:H	0.481

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:95:TRP:CE3	F:198:ARG:NE	0.481
1	F:52:TRP:HE3	F:211:VAL:CB	0.480
1	E:66:ARG:NE	E:199:VAL:C	0.480
1	D:39:SER:N	D:70:GLU:OE1	0.480
1	A:47:LYS:N	A:63:ASP:OD2	0.479
1	D:38:ASP:O	D:42:HIS:N	0.478
1	F:53:SER:O	F:57:GLU:HB2	0.476
1	F:102:GLN:NE2	F:162:LYS:HE2	0.476
1	E:58:ASP:C	E:62:ALA:H	0.476
1	A:46:GLN:HG3	A:63:ASP:HA	0.475
1	B:161:HIS:CD2	F:191:GLU:O	0.475
1	F:59:ALA:CB	F:203:LYS:C	0.474
1	D:194:ASN:HD21	F:38:ASP:H	0.474
1	F:59:ALA:H	F:207:GLN:HG2	0.474
1	E:191:GLU:OE2	G:158:LEU:HD11	0.473
1	E:66:ARG:NH2	E:199:VAL:O	0.473
1	E:60:SER:CA	E:203:LYS:HZ3	0.473
1	E:73:ALA:HB3	G:107:SER:C	0.472
1	D:64:MET:O	D:68:GLN:HG3	0.471
1	G:97:LEU:HD12	G:105:VAL:HG21	0.470
1	A:52:TRP:CZ2	G:218:SER:HG	0.469
1	B:157:ALA:C	F:194:ASN:H	0.468
1	D:47:LYS:CA	D:63:ASP:OD2	0.468

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:66:ARG:HG3	E:199:VAL:HG21	0.468
1	A:64:MET:O	A:68:GLN:HG3	0.467
1	F:55:MET:HA	F:207:GLN:HG2	0.466
1	D:44:LEU:O	D:48:TRP:CA	0.465
1	D:193:PHE:CZ	F:45:LEU:CG	0.464
1	E:102:GLN:NE2	E:162:LYS:HE2	0.464
1	D:194:ASN:CA	F:37:GLU:HB3	0.464
1	F:74:ALA:HB1	F:79:ARG:H	0.464
1	D:127:LYS:HE3	H:31:PHE:CE1	0.463
1	F:48:TRP:CD1	F:211:VAL:O	0.463
1	E:66:ARG:CZ	E:199:VAL:O	0.463
1	A:30:LEU:CD2	D:111:ARG:HH22	0.462
1	F:60:SER:O	F:64:MET:CG	0.462
1	D:47:LYS:N	D:63:ASP:OD2	0.462
1	A:194:ASN:OD1	E:37:GLU:C	0.461
1	E:60:SER:O	E:64:MET:CG	0.461
1	E:191:GLU:O	G:105:VAL:CG1	0.461
1	E:57:GLU:HG2	E:61:VAL:CG2	0.460
1	A:46:GLN:O	A:49:ALA:HB3	0.458
1	E:53:SER:HA	E:56:SER:OG	0.458
1	A:44:LEU:O	A:48:TRP:CA	0.458
1	F:50:SER:O	F:54:SER:CB	0.457
1	B:107:SER:CA	F:195:LEU:CD2	0.457

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:55:MET:C	E:59:ALA:H	0.456
1	D:193:PHE:CD2	F:41:ARG:HA	0.455
1	F:51:MET:O	F:55:MET:HB2	0.455
1	E:191:GLU:OE1	G:105:VAL:CB	0.455
1	E:191:GLU:CB	G:158:LEU:HD22	0.454
1	D:46:GLN:NE2	D:63:ASP:O	0.454
1	A:55:MET:CG	G:219:GLU:HG3	0.453
1	E:51:MET:O	E:55:MET:HB2	0.453
1	A:48:TRP:CH2	G:214:MET:HE1	0.452
1	E:66:ARG:O	E:70:GLU:CB	0.452
1	D:43:GLN:O	D:47:LYS:CB	0.452
1	D:203:LYS:CB	F:41:ARG:NH1	0.451
1	A:38:ASP:O	A:42:HIS:N	0.450
1	E:194:ASN:OD1	G:157:ALA:CB	0.450
1	F:66:ARG:O	F:70:GLU:CB	0.449
1	D:46:GLN:O	D:49:ALA:HB3	0.448
1	E:59:ALA:HB2	E:207:GLN:OE1	0.448
1	F:74:ALA:HB1	F:79:ARG:CA	0.448
1	E:196:GLU:N	G:161:HIS:HE2	0.448
1	E:195:LEU:HD22	G:107:SER:N	0.448
1	E:192:LEU:HB3	G:160:GLY:N	0.448
1	A:43:GLN:O	A:47:LYS:CB	0.448
1	E:195:LEU:HB3	G:161:HIS:HE2	0.447

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:107:SER:HB3	F:195:LEU:HD21	0.446
1	D:193:PHE:CB	F:44:LEU:HD12	0.446
1	A:47:LYS:CA	A:63:ASP:OD2	0.446
1	E:50:SER:O	E:54:SER:CB	0.445
1	A:102:GLN:NE2	A:162:LYS:HE2	0.444
1	F:56:SER:HA	F:59:ALA:HB3	0.443
1	F:59:ALA:N	F:207:GLN:HG3	0.443
1	C:24:LEU:HB2	C:26:MET:HE2	0.442
1	E:56:SER:HA	E:59:ALA:HB3	0.442
1	E:64:MET:HA	E:67:ALA:HB3	0.442
1	F:77:GLU:CB	F:78:GLU:HB3	0.442
1	E:139:LEU:HD21	E:151:VAL:HG23	0.441
1	E:50:SER:C	E:54:SER:HG	0.441
1	A:211:VAL:CG1	E:48:TRP:HZ2	0.440
1	B:76:ALA:CB	B:185:MET:HE1	0.440
1	D:37:GLU:C	D:39:SER:N	0.440
1	F:64:MET:HA	F:67:ALA:HB3	0.440
1	D:46:GLN:O	D:50:SER:N	0.439
1	F:58:ASP:C	F:62:ALA:H	0.439
1	F:69:LEU:O	F:73:ALA:N	0.439
1	A:46:GLN:O	A:50:SER:N	0.438
1	E:48:TRP:CZ2	E:211:VAL:HG12	0.436
1	D:46:GLN:CG	D:63:ASP:C	0.435

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:60:SER:O	E:64:MET:CB	0.435
1	F:139:LEU:HD21	F:151:VAL:HG23	0.435
1	A:52:TRP:CZ3	G:218:SER:CB	0.434
1	A:224:SER:O	A:225:LYS:C	0.433
1	F:72:GLU:O	F:78:GLU:N	0.433
1	E:63:ASP:N	E:203:LYS:HD3	0.432
1	B:158:LEU:HD13	F:191:GLU:OE2	0.431
1	E:195:LEU:CB	G:161:HIS:NE2	0.431
1	F:60:SER:O	F:64:MET:CB	0.428
1	F:56:SER:O	F:203:LYS:NZ	0.428
1	E:191:GLU:CB	G:105:VAL:HG22	0.426
1	G:116:GLU:HG3	G:136:PHE:CE2	0.426
1	D:193:PHE:CD2	F:44:LEU:CA	0.425
1	D:203:LYS:HB2	F:41:ARG:NH1	0.425
1	E:103:GLU:CG	H:118:MET:HE2	0.422
1	B:185:MET:HE2	B:187:ILE:HG12	0.421
1	D:194:ASN:CG	F:38:ASP:CA	0.421
1	F:59:ALA:N	F:207:GLN:CG	0.421
1	E:51:MET:CA	E:54:SER:HG	0.421
1	B:161:HIS:NE2	F:196:GLU:N	0.420
1	E:66:ARG:O	E:70:GLU:HB2	0.419
1	E:36:SER:C	E:39:SER:HG	0.419
1	F:66:ARG:O	F:70:GLU:HB2	0.418

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:62:ALA:N	E:203:LYS:HZ1	0.417
1	D:50:SER:O	D:53:SER:OG	0.417
1	F:56:SER:CA	F:203:LYS:HE3	0.416
1	A:50:SER:O	A:53:SER:OG	0.416
1	E:191:GLU:O	G:161:HIS:CD2	0.416
1	E:62:ALA:HB3	E:203:LYS:HD2	0.415
1	F:57:GLU:HG2	F:61:VAL:CG2	0.415
1	B:116:GLU:HG3	B:136:PHE:CE2	0.414
1	E:48:TRP:HE1	E:211:VAL:C	0.414
1	D:193:PHE:CG	F:41:ARG:HA	0.412
1	E:66:ARG:HB2	E:199:VAL:CG1	0.412
1	F:44:LEU:HD21	F:218:LYS:HE2	0.412
1	B:158:LEU:CD1	F:191:GLU:CG	0.411
1	D:68:GLN:O	D:72:GLU:HB2	0.410
1	A:68:GLN:O	A:72:GLU:HB2	0.409
1	D:224:SER:O	D:225:LYS:C	0.409
1	B:158:LEU:HD22	F:191:GLU:CB	0.408
1	D:211:VAL:CA	F:48:TRP:CH2	0.408
1	F:44:LEU:HD13	F:218:LYS:HG3	0.408
1	G:185:MET:HE2	G:187:ILE:HG23	0.408
1	D:102:GLN:HE21	D:109:LEU:HD11	0.407
1	A:45:LEU:O	A:49:ALA:N	0.407
1	D:81:LEU:CD2	D:177:VAL:HG22	0.406

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	F:51:MET:O	F:55:MET:CB	0.406
1	E:196:GLU:N	G:161:HIS:NE2	0.406
1	E:51:MET:O	E:55:MET:CB	0.406
1	B:220:VAL:HG23	D:198:ARG:HD3	0.405
1	F:48:TRP:NE1	F:211:VAL:C	0.405
1	A:39:SER:O	A:43:GLN:HG3	0.405
1	E:47:LYS:O	E:51:MET:HB2	0.405
1	F:47:LYS:O	F:51:MET:HB2	0.404
1	A:212:LEU:O	A:216:GLN:HG3	0.403
1	F:59:ALA:HB2	F:207:GLN:HG3	0.403
1	C:109:GLU:CD	C:117:ARG:HH22	0.402
1	F:70:GLU:O	F:74:ALA:HB2	0.402

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	1132	1094	31	7

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	1038	956	61	21

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	30	LEU

Model ID	Chain	Residue ID	Residue type
1	A	38	ASP
1	B	101	LEU
1	B	201	GLU
1	B	214	MET
1	B	218	SER
1	C	24	LEU
1	D	30	LEU
1	D	38	ASP
1	E	30	LEU
1	E	56	SER
1	E	64	MET
1	F	30	LEU
1	F	56	SER
1	F	64	MET
1	G	101	LEU
1	G	187	ILE
1	G	201	GLU
1	G	214	MET
1	G	218	SER
1	H	24	LEU

Fit of model to data used for modeling

3DEM volume

Validation for this section is under development.

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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