Integrative Structure Validation Report

July 22, 2024 - 05:15 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	9A38
PDB-Dev ID	PDBDEV_00000193
Structure Title	Model of E. coli MetQ by in-cell photo-crosslinking MS and deep learning
Structure Authors	Stahl, K.; Graziadei, A.; Dau, T.; Brock, O.; Rappsilber, J.

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

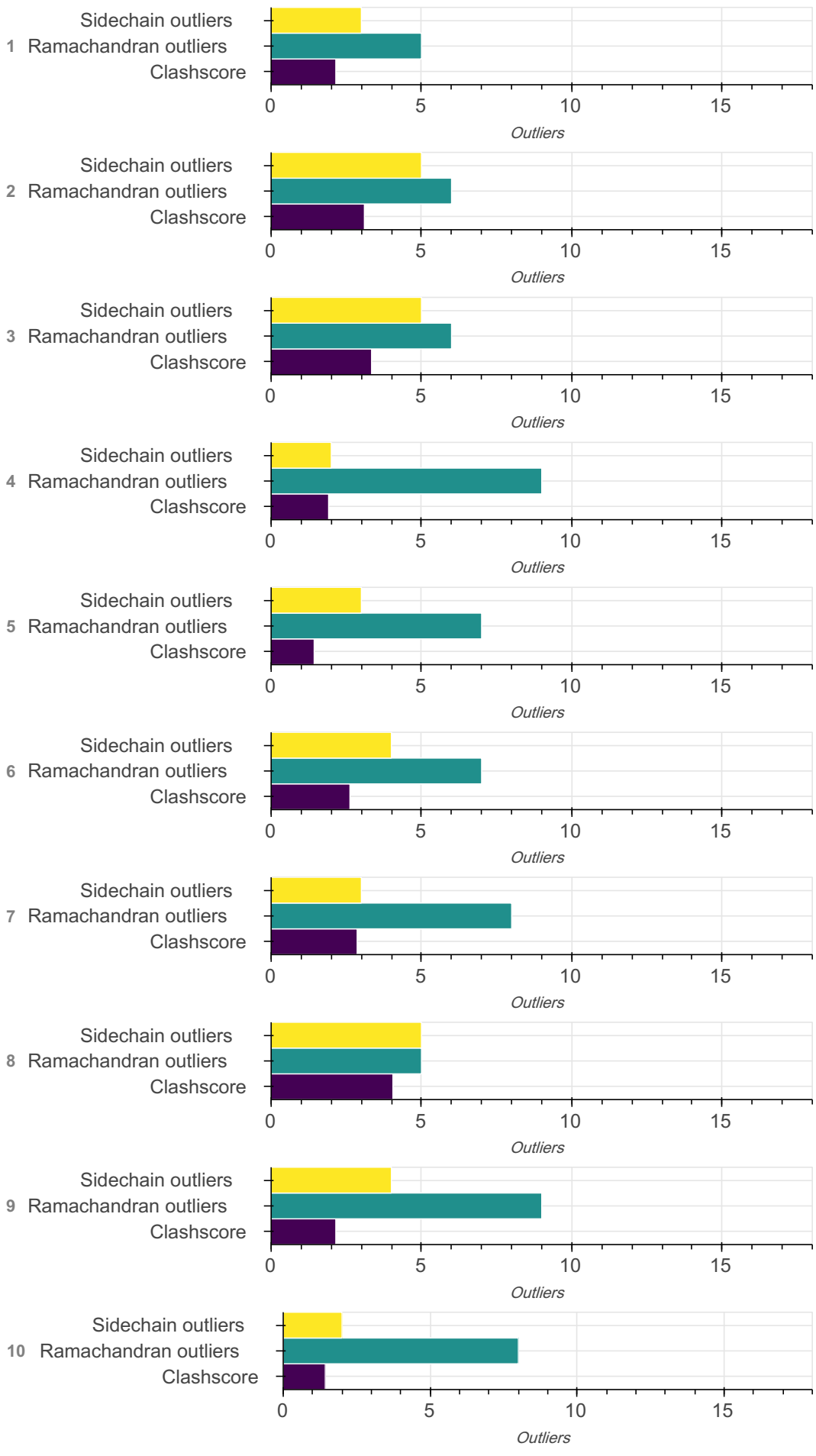
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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


Sidechain outliers
1 Ramachandran outliers
Clashscore
0
5
10
15
Outliers
Sidechain outliers
2 Ramachandran outliers
Clashscore
0
5
10
15
Outliers
Sidechain outliers
3 Ramachandran outliers
Clashscore
0
5
10
15
Outliers
Sidechain outliers
4 Ramachandran outliers
Clashscore
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Outliers
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Outliers
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8 Ramachandran outliers
Clashscore
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15
Outliers
Sidechain outliers
9 Ramachandran outliers
Clashscore
0
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Outliers
Sidechain outliers
10 Ramachandran outliers
Clashscore
0
5
10
15
Outliers

Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 10 unique models, with 1 subunits in each model. A total of 1 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 1 flexible or non-rigid units.

Entry composition

There are 10 unique types of models in this entry.These models are titled None, None, None, None, None, None, None, None, None, None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	P28635	A	A	271
2	1	1	P28635	A	A	271
3	1	1	P28635	A	A	271
4	1	1	P28635	A	A	271
5	1	1	P28635	A	A	271
6	1	1	P28635	A	A	271
7	1	1	P28635	A	A	271
8	1	1	P28635	A	A	271
9	1	1	P28635	A	A	271
10	1	1	P28635	A	A	271

Datasets used for modeling

There is 1 unique dataset used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	jPOSTrepo	JPST001851

Representation

This entry has only one representation and includes 0 rigid bodies and 1 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-271

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	AlphaLink with 10 msa subsamples	AlphaLink	None	10	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	AlphaLink	1.0	model building	https://github.com/lhatsk/AlphaLink

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

There are 21160 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG--HG3	1.09	0.97	730
CG2--HG22	1.09	0.97	530
CB--HB3	1.09	0.97	1970
CA--HA	1.09	0.97	2500
CG2--HG23	1.09	0.97	530
CD1--HD13	1.09	0.97	420
CG--HG	1.09	0.97	290
CG2--HG21	1.09	0.97	530
CD2--HD21	1.09	0.97	290
CG--HG2	1.09	0.97	730
CG1--HG12	1.09	0.97	440
NZ--HZ3	1.01	0.89	260
CA--HA3	1.09	0.97	210
CD1--HD11	1.09	0.97	420
CB--HB2	1.09	0.97	1970
CG1--HG11	1.09	0.97	310
CD2--HD22	1.09	0.97	290
CD--HD2	1.09	0.97	420
OG--HG	0.96	0.84	100
CB--HB1	1.09	0.97	260
CB--HB	1.09	0.97	530
CD--HD3	1.09	0.97	420

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CE--HE3	1.09	0.97	270
CD2--HD23	1.09	0.97	290
OH--HH	0.96	0.84	100
CD1--HD12	1.09	0.97	420
CG1--HG13	1.09	0.97	440
NZ--HZ2	1.01	0.89	260
CE--HE2	1.09	0.97	270
CA--HA2	1.09	0.97	210
OG1--HG1	0.96	0.84	90
NZ--HZ1	1.01	0.89	260
N--H2	1.01	0.89	10
N--H3	1.01	0.89	10
CE--HE1	1.09	0.97	10
N--H1	1.01	0.89	10
SG--HG	1.33	1.20	3
SG--HG	1.34	1.20	7
CD2--HD2	1.08	0.93	210
N--H	1.01	0.86	2580
CZ2--HZ2	1.08	0.93	10
ND1--HD1	1.01	0.86	20
CE2--HE2	1.08	0.93	190
NE2--HE22	1.01	0.86	150
CZ--HZ	1.08	0.93	90

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
ND2--HD22	1.01	0.86	150
NH1--HH11	1.01	0.86	40
CE1--HE1	1.08	0.93	210
NH2--HH22	1.01	0.86	40
CD1--HD1	1.08	0.93	200
CH2--HH2	1.08	0.93	10
NE2--HE21	1.01	0.86	150
NE--HE	1.01	0.86	40
ND2--HD21	1.01	0.86	150
NH2--HH21	1.01	0.86	40
NE1--HE1	1.01	0.86	10
CZ3--HZ3	1.08	0.93	10
CE3--HE3	1.08	0.93	10
NH1--HH12	1.01	0.86	40

Standard geometry: angle outliers

There are 141 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
CA-CB-CG	113.80	107.38	1
OE1-CD-NE2	122.60	116.42	1
OE1-CD-NE2	122.60	116.49	1
CA-CB-CG	112.60	118.45	1
C-N-CA	121.70	132.01	1
OE1-CD-NE2	122.60	116.93	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	131.88	1
OE1-CD-NE2	122.60	116.97	1
OE1-CD-NE2	122.60	117.02	1
C-N-CA	121.70	131.44	1
CA-CB-CG	112.60	117.98	1
OE1-CD-NE2	122.60	117.28	1
C-N-CA	121.70	131.04	1
OE1-CD-NE2	122.60	117.41	1
OE1-CD-NE2	122.60	117.43	1
C-N-CA	121.70	131.00	1
OE1-CD-NE2	122.60	117.49	1
CA-CB-CG	112.60	117.71	1
OE1-CD-NE2	122.60	117.52	1
C-N-CA	121.70	130.79	1
OE1-CD-NE2	122.60	117.58	1
CA-CB-CG	112.60	107.59	1
CA-CB-CG	112.60	117.61	1
OE1-CD-NE2	122.60	117.61	2
OE1-CD-NE2	122.60	117.62	1
C-N-CA	121.70	130.66	1
OE1-CD-NE2	122.60	117.66	1
OE1-CD-NE2	122.60	117.75	1
OE1-CD-NE2	122.60	117.76	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	130.35	1
C-N-CA	121.70	130.32	1
OE1-CD-NE2	122.60	117.81	1
OE1-CD-NE2	122.60	117.82	2
OE1-CD-NE2	122.60	117.89	1
C-N-CA	121.70	130.16	2
OE1-CD-NE2	122.60	118.00	1
OE1-CD-NE2	122.60	118.03	1
OE1-CD-NE2	122.60	118.06	1
CA-CB-OG1	109.60	116.38	1
OE1-CD-NE2	122.60	118.08	1
OE1-CD-NE2	122.60	118.09	2
OE1-CD-NE2	122.60	118.10	1
C-N-CA	121.70	129.79	1
OE1-CD-NE2	122.60	118.11	1
OE1-CD-NE2	122.60	118.12	1
OE1-CD-NE2	122.60	118.13	2
OE1-CD-NE2	122.60	118.14	3
OE1-CD-NE2	122.60	118.15	1
C-N-CA	121.70	129.70	1
OE1-CD-NE2	122.60	118.16	2
OE1-CD-NE2	122.60	118.17	1
OE1-CD-NE2	122.60	118.18	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.20	1
OE1-CD-NE2	122.60	118.22	2
OE1-CD-NE2	122.60	118.23	1
CB-CG-CD2	131.20	125.52	1
CB-CG-CD2	131.20	125.53	1
CB-CG-CD2	131.20	125.54	3
OE1-CD-NE2	122.60	118.25	3
OE1-CD-NE2	122.60	118.26	1
OE1-CD-NE2	122.60	118.28	3
OE1-CD-NE2	122.60	118.29	1
CB-CG-CD2	131.20	125.60	1
CB-CG-CD2	131.20	125.61	1
OE1-CD-NE2	122.60	118.30	1
CB-CG-CD2	131.20	125.62	1
OE1-CD-NE2	122.60	118.31	2
CB-CG-CD2	131.20	125.64	1
OE1-CD-NE2	122.60	118.33	1
CA-CB-CG	112.60	116.87	1
C-N-CA	121.70	129.37	1
OE1-CD-NE2	122.60	118.34	1
OE1-CD-NE2	122.60	118.36	1
OE1-CD-NE2	122.60	118.38	4
OD1-CG-ND2	122.60	118.40	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.41	1
OE1-CD-NE2	122.60	118.42	1
CA-CB-CG	113.80	109.62	1
OE1-CD-NE2	122.60	118.43	2
CB-CG-CD2	131.20	125.78	1
OD1-CG-ND2	122.60	118.44	1
OE1-CD-NE2	122.60	118.44	1
C-N-CA	121.70	129.19	1
OE1-CD-NE2	122.60	118.45	1
OD1-CG-ND2	122.60	118.46	1
OD1-CG-ND2	122.60	118.47	1
CA-CB-CG2	110.50	117.53	1
OE1-CD-NE2	122.60	118.47	1
CA-CB-CG	112.60	116.73	1
C-N-CA	121.70	129.12	1
OE1-CD-NE2	122.60	118.48	1
OE1-CD-NE2	122.60	118.49	2
CA-CB-CG	112.60	116.71	1
OE1-CD-NE2	122.60	118.50	1
OE1-CD-NE2	122.60	118.51	1
CA-CB-CG	112.60	116.68	1
N-CA-C	113.30	101.47	2
OE1-CD-NE2	122.60	118.52	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	125.90	2
OE1-CD-NE2	122.60	118.53	2
OD1-CG-ND2	122.60	118.53	1
OE1-CD-NE2	122.60	118.54	1
OE1-CD-NE2	122.60	118.56	2
N-CA-C	113.30	101.62	1
OE1-CD-NE2	122.60	118.58	4
OD1-CG-ND2	122.60	118.58	1
OE1-CD-NE2	122.60	118.60	3
C-N-H	111.85	124.30	1
C-N-H	111.66	124.30	1
C-N-H	110.91	124.30	1
C-N-H	108.82	124.30	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	2.15	9
2	3.10	13
3	3.34	14
4	1.91	8
5	1.43	6
6	2.62	11

Model ID	Clash score	Number of clashes
7	2.86	12
8	4.05	17
9	2.15	9
10	1.43	6

All 105 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:163:LEU:HD22	A:226:PRO:CG	0.659
1	A:69:TYR:CD1	A:86:PHE:CE1	0.567
1	A:163:LEU:HD22	A:226:PRO:HG3	0.557
1	A:114:ILE:HG22	A:202:ASN:HA	0.538
1	A:69:TYR:CE1	A:86:PHE:CE1	0.477
1	A:69:TYR:CE1	A:86:PHE:CZ	0.472
1	A:163:LEU:HD22	A:226:PRO:HG2	0.448
1	A:269:LYS:HE3	A:271:TRP:CE2	0.429
1	A:144:ARG:HE	A:221:GLU:CD	0.402
2	A:112:TYR:CE1	A:263:PHE:CZ	0.642
2	A:110:PHE:CE2	A:112:TYR:CZ	0.615
2	A:110:PHE:CE2	A:112:TYR:CE1	0.565
2	A:110:PHE:HE2	A:112:TYR:CZ	0.492
2	A:90:PRO:HG3	A:163:LEU:HD13	0.470
2	A:110:PHE:C	A:110:PHE:CD2	0.433
2	A:94:GLN:HE21	A:98:ASP:CG	0.424
2	A:269:LYS:HE3	A:271:TRP:CE2	0.421

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:66:PHE:CG	A:72:PRO:HG3	0.415
2	A:112:TYR:HE1	A:263:PHE:CE2	0.411
2	A:72:PRO:HG2	A:86:PHE:CZ	0.408
2	A:114:ILE:CG2	A:200:VAL:HG12	0.407
2	A:41:ALA:HB1	A:263:PHE:CZ	0.401
3	A:110:PHE:CE2	A:112:TYR:CZ	0.633
3	A:110:PHE:CE2	A:112:TYR:CE2	0.602
3	A:112:TYR:CZ	A:263:PHE:CZ	0.549
3	A:88:HIS:CD2	A:140:THR:HG21	0.523
3	A:112:TYR:CZ	A:263:PHE:CE2	0.517
3	A:72:PRO:HG2	A:86:PHE:CE2	0.480
3	A:72:PRO:CG	A:86:PHE:CZ	0.463
3	A:72:PRO:HG2	A:86:PHE:CZ	0.453
3	A:112:TYR:OH	A:263:PHE:CE2	0.444
3	A:38:ILE:HG12	A:86:PHE:CD2	0.431
3	A:110:PHE:CD2	A:112:TYR:CZ	0.431
3	A:110:PHE:C	A:110:PHE:CD2	0.416
3	A:99:ARG:HD2	A:101:TYR:CE2	0.414
3	A:163:LEU:HD22	A:226:PRO:CG	0.410
4	A:269:LYS:HE3	A:271:TRP:CE2	0.519
4	A:144:ARG:HD2	A:227:TYR:CD2	0.516
4	A:88:HIS:CE1	A:91:TYR:HB2	0.512
4	A:92:LEU:HA	A:96:LEU:HD12	0.457

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:163:LEU:HD22	A:226:PRO:CG	0.448
4	A:151:LYS:HZ3	A:222:ASP:CG	0.436
4	A:163:LEU:HD22	A:226:PRO:HG3	0.424
4	A:251:GLN:HA	A:271:TRP:CZ2	0.420
5	A:73:ASN:ND2	A:95:GLN:HE22	0.544
5	A:69:TYR:CE1	A:86:PHE:CE1	0.500
5	A:116:GLY:HA3	A:219:PHE:CE1	0.452
5	A:114:ILE:CG2	A:200:VAL:HG12	0.432
5	A:111:VAL:HG22	A:228:VAL:HG23	0.416
5	A:112:TYR:CE2	A:263:PHE:CD1	0.411
6	A:69:TYR:CE1	A:86:PHE:CE1	0.597
6	A:92:LEU:HD11	A:232:VAL:HG11	0.521
6	A:114:ILE:HG22	A:202:ASN:HA	0.481
6	A:88:HIS:CE1	A:91:TYR:HB2	0.474
6	A:73:ASN:HD21	A:87:GLN:NE2	0.443
6	A:70:VAL:HG22	A:91:TYR:OH	0.439
6	A:163:LEU:HD22	A:226:PRO:CG	0.434
6	A:96:LEU:HD21	A:102:LYS:HA	0.432
6	A:269:LYS:HE3	A:271:TRP:CE2	0.431
6	A:45:VAL:HG11	A:110:PHE:CE1	0.414
6	A:184:ALA:HB1	A:205:TYR:CE2	0.406
7	A:69:TYR:CE1	A:86:PHE:CE1	0.588
7	A:88:HIS:CE1	A:91:TYR:HB2	0.532

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:163:LEU:HD22	A:226:PRO:HG3	0.495
7	A:114:ILE:HG22	A:202:ASN:HA	0.488
7	A:96:LEU:HD21	A:103:LEU:H	0.484
7	A:90:PRO:HG3	A:163:LEU:HD13	0.475
7	A:251:GLN:HA	A:271:TRP:CZ2	0.453
7	A:69:TYR:HE1	A:86:PHE:CE1	0.437
7	A:110:PHE:CE1	A:271:TRP:CH2	0.432
7	A:110:PHE:CE1	A:271:TRP:HH2	0.429
7	A:94:GLN:HE21	A:98:ASP:CG	0.426
7	A:42:GLU:OE2	A:86:PHE:CD2	0.411
8	A:144:ARG:HD2	A:227:TYR:CZ	0.817
8	A:144:ARG:HD2	A:227:TYR:CE1	0.642
8	A:140:THR:HG22	A:227:TYR:CZ	0.618
8	A:144:ARG:HD2	A:227:TYR:CE2	0.559
8	A:88:HIS:CE1	A:229:ASN:OD1	0.534
8	A:109:THR:OG1	A:229:ASN:HB3	0.474
8	A:87:GLN:NE2	A:91:TYR:CD1	0.463
8	A:144:ARG:CD	A:227:TYR:CZ	0.455
8	A:88:HIS:CG	A:227:TYR:CE1	0.452
8	A:251:GLN:HA	A:271:TRP:CZ2	0.448
8	A:38:ILE:HG13	A:69:TYR:CE1	0.430
8	A:163:LEU:HD13	A:226:PRO:HG2	0.427
8	A:163:LEU:CD2	A:226:PRO:HG3	0.416

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:114:ILE:HG23	A:144:ARG:CZ	0.413
8	A:72:PRO:HB2	A:86:PHE:HZ	0.409
8	A:88:HIS:CE1	A:227:TYR:CE1	0.402
8	A:114:ILE:HG22	A:202:ASN:HA	0.402
9	A:69:TYR:CE1	A:86:PHE:CE1	0.600
9	A:38:ILE:HG13	A:86:PHE:CE1	0.538
9	A:69:TYR:CE1	A:86:PHE:CZ	0.527
9	A:212:THR:HG21	A:264:ASN:HB3	0.469
9	A:112:TYR:CE1	A:263:PHE:CE2	0.442
9	A:163:LEU:HD22	A:226:PRO:HG3	0.418
9	A:144:ARG:NH2	A:221:GLU:OE2	0.416
9	A:269:LYS:HE2	A:271:TRP:NE1	0.413
9	A:69:TYR:CD1	A:86:PHE:CE1	0.407
10	A:96:LEU:HD13	A:103:LEU:HD12	0.735
10	A:69:TYR:CE1	A:86:PHE:CE1	0.546
10	A:111:VAL:HG11	A:271:TRP:CH2	0.470
10	A:114:ILE:HG22	A:202:ASN:HA	0.469
10	A:73:ASN:HD21	A:87:GLN:NE2	0.433
10	A:88:HIS:CE1	A:229:ASN:OD1	0.403

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	269	251	13	5

Model ID	Analyzed	Favored	Allowed	Outliers
2	269	248	15	6
3	269	247	16	6
4	269	249	11	9
5	269	250	12	7
6	269	249	13	7
7	269	250	11	8
8	269	248	16	5
9	269	248	12	9
10	269	246	15	8

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	224	215	6	3
2	224	219	0	5
3	224	216	3	5
4	224	215	7	2
5	224	217	4	3
6	224	215	5	4
7	224	217	4	3
8	224	217	2	5
9	224	217	3	4
10	224	219	3	2

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	7	THR
1	A	14	LEU
1	A	17	SER
2	A	5	PHE
2	A	7	THR
2	A	14	LEU
2	A	18	LEU
2	A	91	TYR
3	A	7	THR
3	A	14	LEU
3	A	17	SER
3	A	18	LEU
3	A	91	TYR
4	A	7	THR
4	A	14	LEU
5	A	7	THR
5	A	14	LEU
5	A	18	LEU
6	A	5	PHE
6	A	7	THR
6	A	14	LEU
6	A	17	SER
7	A	7	THR

Model ID	Chain	Residue ID	Residue type
7	A	14	LEU
7	A	17	SER
8	A	7	THR
8	A	14	LEU
8	A	18	LEU
8	A	140	THR
8	A	227	TYR
9	A	7	THR
9	A	14	LEU
9	A	17	SER
9	A	18	LEU
10	A	7	THR
10	A	14	LEU

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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