Integrative Structure Validation Report

July 22, 2024 - 05:03 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	9A2O
PDB-Dev ID	PDBDEV_00000173
Structure Title	Model of E. coli BamA 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

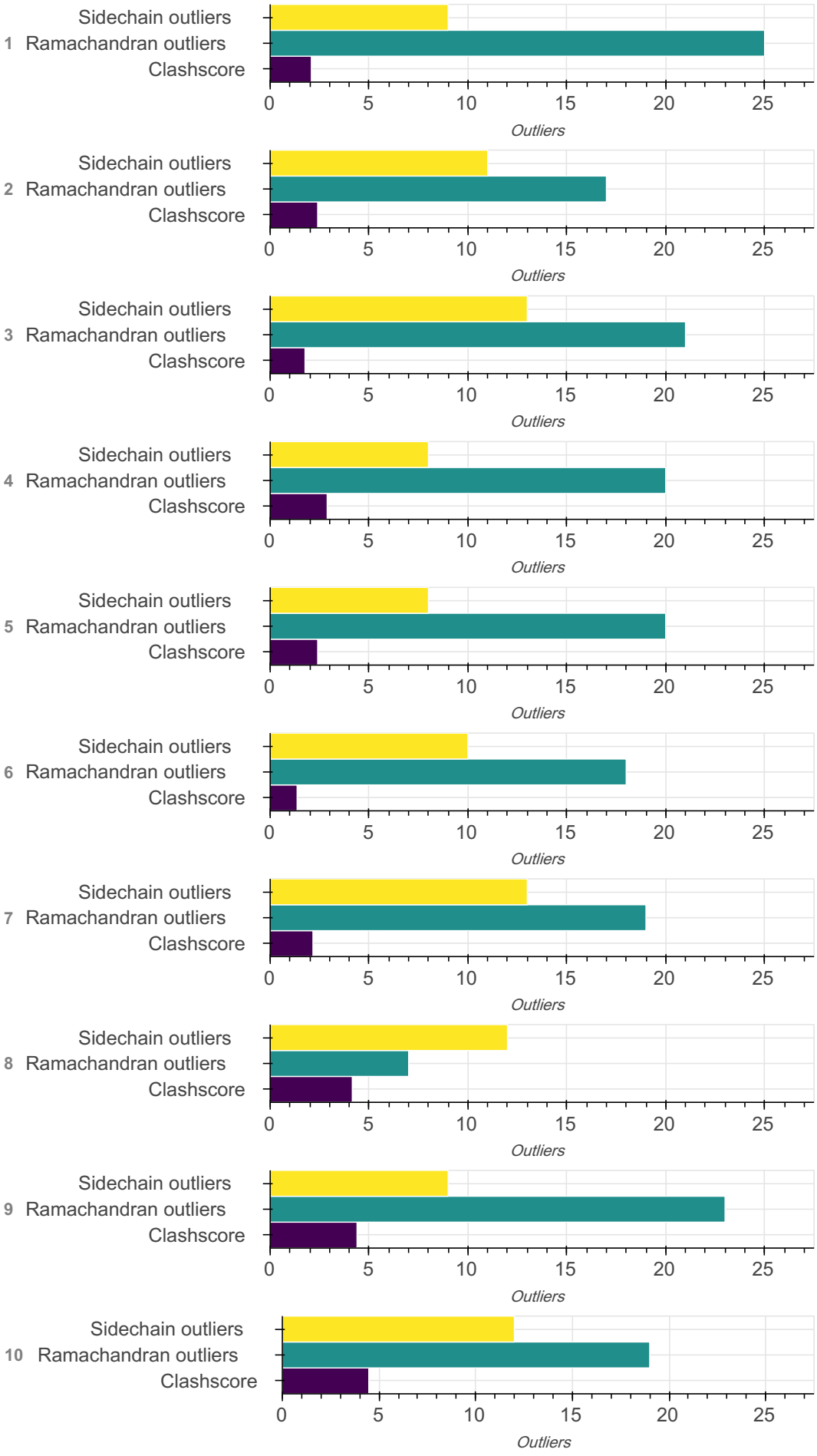
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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


1
2
3
4
5
6
7
8
9
10
Sidechain outliers
Ramachandran outliers
Clashscore
0
5
10
15
20
25
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	P0A940	A	A	810
2	1	1	P0A940	A	A	810
3	1	1	P0A940	A	A	810
4	1	1	P0A940	A	A	810
5	1	1	P0A940	A	A	810
6	1	1	P0A940	A	A	810
7	1	1	P0A940	A	A	810
8	1	1	P0A940	A	A	810
9	1	1	P0A940	A	A	810
10	1	1	P0A940	A	A	810

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	-	1-810

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 61222 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
CB--HB2	1.09	0.97	5820
CA--HA	1.09	0.97	7350
CD--HD3	1.09	0.97	1120
CB--HB3	1.09	0.97	5820
CG--HG3	1.09	0.97	1990
CG--HG2	1.09	0.97	1990
CD--HD2	1.09	0.97	1120
CD2--HD22	1.09	0.97	570
CD2--HD21	1.09	0.97	570
CD1--HD11	1.09	0.97	880
CG2--HG23	1.09	0.97	1530
CD1--HD13	1.09	0.97	880
NZ--HZ1	1.01	0.89	450
CD1--HD12	1.09	0.97	880
CE--HE3	1.09	0.97	610
CG1--HG13	1.09	0.97	970
CE--HE2	1.09	0.97	610
OG--HG	0.96	0.84	580
CG2--HG22	1.09	0.97	1530
OH--HH	0.96	0.84	470
CG1--HG11	1.09	0.97	660
CB--HB1	1.09	0.97	470

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG2--HG21	1.09	0.97	1530
CG1--HG12	1.09	0.97	970
OG1--HG1	0.96	0.84	560
CA--HA3	1.09	0.97	750
CA--HA2	1.09	0.97	750
CB--HB	1.09	0.97	1530
CD2--HD23	1.09	0.97	570
NZ--HZ2	1.01	0.89	450
CG--HG	1.09	0.97	570
NZ--HZ3	1.01	0.89	450
CE--HE1	1.09	0.97	160
N--H2	1.01	0.89	10
N--H1	1.01	0.89	10
N--H3	1.01	0.89	10
SG--HG	1.33	1.20	1
SG--HG	1.34	1.20	11
N--H	1.01	0.86	7800
NH2--HH22	1.01	0.86	380
NE--HE	1.01	0.86	380
ND2--HD22	1.01	0.86	430
CZ--HZ	1.08	0.93	380
CD2--HD2	1.08	0.93	930
CE1--HE1	1.08	0.93	930

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CE2--HE2	1.08	0.93	850
NH1--HH12	1.01	0.86	380
NH1--HH11	1.01	0.86	380
CD1--HD1	1.08	0.93	980
NE2--HE21	1.01	0.86	330
ND2--HD21	1.01	0.86	430
NH2--HH21	1.01	0.86	380
NE2--HE22	1.01	0.86	330
CH2--HH2	1.08	0.93	130
CE3--HE3	1.08	0.93	130
NE1--HE1	1.01	0.86	130
CZ3--HZ3	1.08	0.93	130
ND1--HD1	1.01	0.86	80
CZ2--HZ2	1.08	0.93	130

Standard geometry: angle outliers

There are 386 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	135.96	1
C-N-CA	121.70	135.81	1
OE1-CD-NE2	122.60	115.05	1
C-N-CA	121.70	135.25	1
C-N-CA	121.70	134.71	1
OD1-CG-ND2	122.60	115.68	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	119.35	1
NE-CZ-NH2	119.20	125.22	1
N-CA-CB	103.00	110.30	1
C-N-CA	121.70	133.62	1
C-CA-CB	110.10	122.53	1
CA-CB-CG	112.60	119.13	1
C-N-CA	121.70	133.33	1
CA-CB-CG	112.60	118.98	1
CD-NE-CZ	124.40	133.32	1
CA-CB-CG	112.60	118.81	1
CA-CB-CG	112.60	118.74	1
CA-N-CD	112.00	103.45	1
C-N-CA	121.70	132.62	1
C-CA-CB	110.50	119.46	1
C-N-CA	121.70	132.42	1
C-N-CA	121.70	132.31	1
CA-CB-CG	112.60	118.45	1
C-N-CA	121.70	132.18	1
C-N-CA	121.70	132.14	1
OE1-CD-NE2	122.60	116.87	1
CA-CB-CG	112.60	118.32	1
C-N-CA	121.70	131.95	1
N-CA-CB	110.50	100.82	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	120.02	1
OE1-CD-NE2	122.60	117.00	1
CA-CB-CG	112.60	118.13	1
OE1-CD-NE2	122.60	117.07	1
N-CA-CB	110.40	102.11	1
C-N-CA	121.70	131.60	1
CA-C-N	116.90	125.08	1
CD-NE-CZ	124.40	132.00	1
OE1-CD-NE2	122.60	117.18	1
NE-CZ-NH2	119.20	124.05	1
CA-CB-CG	112.60	117.89	1
OE1-CD-NE2	122.60	117.34	1
C-N-CA	121.70	131.14	1
C-N-CA	121.70	131.13	1
OE1-CD-NE2	122.60	117.37	2
C-N-CA	121.70	131.11	1
CA-CB-CG	113.60	123.52	1
OE1-CD-NE2	122.60	117.38	1
OD1-CG-ND2	122.60	117.39	1
OE1-CD-NE2	122.60	117.40	1
C-N-CA	121.70	131.03	1
C-N-CA	121.70	131.02	1
OE1-CD-NE2	122.60	117.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.50	118.20	1
C-N-CA	121.70	130.94	1
OE1-CD-NE2	122.60	117.48	1
CA-CB-CG	112.60	117.70	1
OE1-CD-NE2	122.60	117.51	1
NE-CZ-NH2	119.20	123.78	1
C-N-CA	121.70	130.85	1
N-CA-C	111.00	125.14	1
CA-CB-CG	112.60	117.65	1
C-N-CA	121.70	130.76	1
OD1-CG-ND2	122.60	117.58	1
OE1-CD-NE2	122.60	117.61	1
N-CA-CB	103.00	108.47	1
OD1-CG-ND2	122.60	117.64	1
OE1-CD-NE2	122.60	117.66	2
C-N-CA	121.70	130.59	1
O-C-N	123.00	115.11	1
N-CA-CB	110.50	102.13	1
CA-C-N	116.20	126.00	1
C-N-CA	121.70	130.51	1
OE1-CD-NE2	122.60	117.72	1
CA-CB-CG	112.60	117.47	1
C-CA-CB	110.10	119.36	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.75	1
OE1-CD-NE2	122.60	117.76	1
C-N-CA	121.70	130.40	1
OE1-CD-NE2	122.60	117.77	1
C-N-CA	121.70	130.38	1
OE1-CD-NE2	122.60	117.78	1
OE1-CD-NE2	122.60	117.79	2
N-CA-C	111.00	124.45	1
CA-CB-CG2	110.40	118.56	1
CA-CB-CG	112.60	117.40	1
OE1-CD-NE2	122.60	117.81	2
CB-CG-CD2	131.20	124.97	1
OD1-CG-ND2	122.60	117.81	1
N-CA-CB	110.40	103.22	1
CA-CB-CG	112.60	117.39	1
N-CA-CB	110.50	102.36	1
OE1-CD-NE2	122.60	117.82	1
OE1-CD-NE2	122.60	117.83	1
N-CA-CB	111.50	103.39	1
C-CA-CB	111.60	121.12	1
OE1-CD-NE2	122.60	117.85	1
OE1-CD-NE2	122.60	117.86	2
OE1-CD-NE2	122.60	117.87	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	108.20	1
O-C-N	123.00	115.44	1
OE1-CD-NE2	122.60	117.88	3
C-CA-CB	110.10	119.05	1
CA-CB-CG	112.60	117.31	1
OE1-CD-NE2	122.60	117.90	2
OD1-CG-ND2	122.60	117.90	1
CA-CB-CG	112.60	117.30	1
OE1-CD-NE2	122.60	117.91	2
OE1-CD-NE2	122.60	117.93	4
OE1-CD-NE2	122.60	117.94	2
CD-NE-CZ	124.40	130.92	1
OE1-CD-NE2	122.60	117.95	2
OE1-CD-NE2	122.60	117.97	2
CA-CB-CG	112.60	117.23	1
OE1-CD-NE2	122.60	117.98	2
CA-CB-CG	112.60	117.22	1
OE1-CD-NE2	122.60	117.99	1
O-C-N	123.00	115.63	1
C-N-CA	121.70	113.40	1
OD1-CG-ND2	122.60	118.00	1
OE1-CD-NE2	122.60	118.01	3
C-N-CA	121.70	129.96	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.02	1
C-N-CA	121.70	129.93	1
OE1-CD-NE2	122.60	118.03	2
OD1-CG-ND2	122.60	118.04	1
C-N-CA	121.70	129.90	1
OE1-CD-NE2	122.60	118.05	1
N-CA-CB	110.50	102.79	1
CA-CB-CG	112.60	117.13	1
CA-CB-CG	112.60	117.12	1
C-N-CA	121.70	129.84	1
OE1-CD-NE2	122.60	118.08	2
OE1-CD-NE2	122.60	118.09	3
C-N-CA	121.70	129.81	2
OE1-CD-NE2	122.60	118.10	3
OE1-CD-NE2	122.60	118.11	3
C-N-CA	121.70	129.79	1
C-CA-CB	110.50	117.23	1
C-CA-CB	110.10	118.62	1
C-N-CA	121.70	129.76	1
OE1-CD-NE2	122.60	118.13	1
CA-CB-CG	112.60	117.06	1
OE1-CD-NE2	122.60	118.14	1
OE1-CD-NE2	122.60	118.15	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.70	1
OE1-CD-NE2	122.60	118.16	3
C-N-CA	121.70	129.68	1
OE1-CD-NE2	122.60	118.17	1
OE1-CD-NE2	122.60	118.18	2
CA-CB-CG	112.60	117.02	1
C-N-CA	121.70	129.65	1
CA-CB-CG	113.80	118.21	1
OD1-CG-ND2	122.60	118.19	1
OE1-CD-NE2	122.60	118.20	4
C-N-CA	121.70	129.61	1
OE1-CD-NE2	122.60	118.21	3
C-N-CA	121.70	129.60	1
CA-CB-CG	112.60	116.99	1
OE1-CD-NE2	122.60	118.22	1
OE1-CD-NE2	122.60	118.23	3
CB-CG-CD2	131.20	125.53	1
OD1-CG-ND2	122.60	118.24	1
OE1-CD-NE2	122.60	118.24	1
C-N-CA	121.70	129.54	1
OE1-CD-NE2	122.60	118.25	1
OE1-CD-NE2	122.60	118.26	4
OE1-CD-NE2	122.60	118.27	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	118.13	1
CB-CG-CD2	131.20	125.58	1
C-N-CA	121.70	129.48	1
OD1-CG-ND2	122.60	118.28	1
OE1-CD-NE2	122.60	118.28	1
N-CA-CB	110.50	103.17	1
OD1-CG-ND2	122.60	118.29	1
OE1-CD-NE2	122.60	118.29	3
C-N-CA	121.70	129.45	1
OE1-CD-NE2	122.60	118.30	4
C-N-CA	121.70	129.44	1
OE1-CD-NE2	122.60	118.31	4
CG1-CB-CG2	110.80	101.38	1
CB-CG-CD	112.60	105.32	1
NE1-CE2-CZ2	130.10	136.51	1
O-C-N	123.00	116.17	1
OE1-CD-NE2	122.60	118.33	1
C-N-CA	121.70	129.38	1
OD1-CG-ND2	122.60	118.34	1
CA-CB-CG	112.60	116.86	1
OE1-CD-NE2	122.60	118.34	2
CA-CB-CG	114.10	105.59	1
CA-CB-CG	112.60	116.84	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.34	1
OE1-CD-NE2	122.60	118.36	2
OE1-CD-NE2	122.60	118.37	2
C-N-CA	121.70	129.31	1
OD1-CG-ND2	122.60	118.37	1
CA-CB-OG1	109.60	103.26	1
C-CA-CB	110.10	118.12	1
C-N-CA	121.70	129.29	1
C-N-CA	121.70	129.27	1
CD-NE-CZ	124.40	130.29	1
OD1-CG-ND2	122.60	118.39	1
OE1-CD-NE2	122.60	118.40	3
CA-CB-CG	112.60	116.80	1
OD1-CG-ND2	122.60	118.40	1
CB-CG-CD2	131.20	125.74	1
NH1-CZ-NH2	119.30	113.85	1
C-N-CA	121.70	129.25	1
OE1-CD-NE2	122.60	118.41	1
OD1-CG-ND2	122.60	118.42	1
CA-CB-CG	112.60	116.78	1
OE1-CD-NE2	122.60	118.42	3
N-CA-CB	110.50	103.41	1
OD1-CG-ND2	122.60	118.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.43	2
C-N-CA	121.70	129.20	1
OE1-CD-NE2	122.60	118.44	2
C-N-CA	121.70	129.19	1
OE1-CD-NE2	122.60	118.45	4
CA-N-CD	112.00	106.19	1
OD1-CG-ND2	122.60	118.45	1
OE1-CD-NE2	122.60	118.46	4
CA-CB-CG	112.60	116.74	2
OD1-CG-ND2	122.60	118.46	1
N-CA-CB	103.00	107.55	1
OE1-CD-NE2	122.60	118.47	3
CA-CB-CG	112.60	116.73	1
N-CA-CB	110.50	103.48	1
OD1-CG-ND2	122.60	118.47	1
OE1-CD-NE2	122.60	118.48	5
CA-CB-CG	112.60	116.72	1
OD1-CG-ND2	122.60	118.48	1
CA-CB-CG2	110.50	117.50	1
OD1-CG-ND2	122.60	118.49	1
CA-CB-CG	112.60	116.71	2
OE1-CD-NE2	122.60	118.49	3
OE1-CD-NE2	122.60	118.50	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.08	1
N-CA-CB	103.00	107.51	1
C-N-CA	121.70	129.07	2
OD1-CG-ND2	122.60	118.51	1
CA-CB-CG	112.60	116.69	1
OD1-CG-ND2	122.60	118.52	2
OE1-CD-NE2	122.60	118.52	2
CA-CB-CG	113.80	117.88	1
C-CA-CB	110.10	117.85	1
OE1-CD-NE2	122.60	118.53	3
C-N-CA	121.70	129.02	1
OE1-CD-NE2	122.60	118.54	4
N-CA-C	111.00	99.64	1
N-CA-CB	103.00	107.46	1
CB-CG-CD2	131.20	125.93	1
CA-C-N	116.20	124.31	1
OD1-CG-ND2	122.60	118.55	1
OE1-CD-NE2	122.60	118.55	3
NE-CZ-NH2	119.20	122.84	1
CD-NE-CZ	124.40	118.73	1
CA-CB-CG	112.60	116.65	1
OD1-CG-ND2	122.60	118.56	1
OE1-CD-NE2	122.60	118.56	4

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	116.64	2
CA-CB-CG	113.80	117.84	1
OD1-CG-ND2	122.60	118.57	1
OE1-CD-NE2	122.60	118.57	4
C-N-CA	121.70	128.95	1
OE1-CD-NE2	122.60	118.58	1
CA-C-N	116.20	124.23	1
OD1-CG-ND2	122.60	118.59	1
C-CA-CB	110.10	117.72	1
C-N-CA	121.70	128.92	1
OE1-CD-NE2	122.60	118.59	1
OE1-CD-NE2	122.60	118.60	1
CA-C-N	116.20	124.20	1
CB-CG-CD2	131.20	126.00	1
CG-ND2-HD21	107.97	120.00	1
C-N-H	112.07	124.30	1
HH21-NH2-HH22	107.74	120.00	1
HB2-CB-HB3	97.69	110.00	1
C-N-H	111.45	124.30	1
C-N-H	110.82	124.30	1
C-N-H	110.77	124.30	1
HH11-NH1-HH12	106.28	120.00	1
C-N-H	110.39	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-H	110.36	124.30	1
HH21-NH2-HH22	105.93	120.00	1
C-N-H	110.23	124.30	1
HZ1-NZ-HZ2	94.52	109.00	1
C-N-H	109.81	124.30	1
C-N-H	109.00	124.30	1
N-CA-HA	94.66	110.00	1
C-N-H	108.75	124.30	1
C-N-H	107.80	124.30	1
C-N-H	106.76	124.30	1
C-N-H	105.86	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	2.08	26
2	2.40	30
3	1.76	22
4	2.88	36
5	2.40	30
6	1.36	17
7	2.16	27
8	4.15	52

Model ID	Clash score	Number of clashes
9	4.39	55
10	4.47	56

All 351 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:502:SER:HB2	A:543:VAL:HG22	0.886
1	A:592:ARG:HH21	A:594:ASN:ND2	0.554
1	A:177:ILE:HD11	A:199:LEU:HD22	0.543
1	A:586:PHE:CE2	A:719:ILE:HG22	0.514
1	A:548:TYR:CZ	A:647:PRO:HD2	0.504
1	A:470:GLU:CD	A:488:ARG:HD2	0.496
1	A:606:ASN:OD1	A:646:MET:HE2	0.490
1	A:747:THR:C	A:749:TRP:H	0.487
1	A:654:ALA:HA	A:740:ASP:CG	0.480
1	A:705:ALA:HB1	A:744:VAL:CG1	0.469
1	A:705:ALA:HB1	A:744:VAL:HG12	0.468
1	A:504:TYR:CD2	A:536:LEU:HD11	0.466
1	A:592:ARG:HE	A:594:ASN:ND2	0.465
1	A:565:PHE:CZ	A:606:ASN:HB2	0.456
1	A:592:ARG:HH21	A:594:ASN:HD21	0.453
1	A:572:PHE:CZ	A:597:GLY:HA3	0.447
1	A:190:THR:HG22	A:194:ILE:HD12	0.431
1	A:304:MET:HE1	A:337:LEU:HD21	0.427
1	A:540:GLN:O	A:543:VAL:HG23	0.422

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:544:ALA:CB	A:673:VAL:HB	0.414
1	A:678:GLN:NE2	A:688:TYR:CE1	0.409
1	A:568:ASP:HB3	A:601:ILE:HD12	0.404
1	A:652:PHE:CE2	A:744:VAL:HG22	0.402
1	A:673:VAL:HG11	A:675:PHE:CE2	0.402
1	A:203:VAL:HG11	A:207:ASN:HD22	0.401
1	A:650:GLU:O	A:651:ASN:C	0.401
2	A:586:PHE:CZ	A:719:ILE:HG22	0.666
2	A:653:TYR:HB3	A:666:ASN:HD21	0.665
2	A:369:MET:HE1	A:385:GLY:O	0.614
2	A:369:MET:HE1	A:385:GLY:C	0.586
2	A:673:VAL:HG22	A:704:ASP:H	0.554
2	A:586:PHE:HZ	A:719:ILE:HG22	0.535
2	A:653:TYR:HB3	A:666:ASN:ND2	0.513
2	A:369:MET:HE1	A:385:GLY:CA	0.510
2	A:147:TYR:CE2	A:254:ILE:HD11	0.506
2	A:673:VAL:HG21	A:747:THR:OG1	0.489
2	A:190:THR:HG22	A:194:ILE:HD12	0.488
2	A:529:LEU:HD22	A:570:PHE:CZ	0.487
2	A:144:VAL:C	A:213:LYS:HD3	0.485
2	A:673:VAL:HG22	A:702:SER:O	0.481
2	A:496:ALA:HB1	A:501:LEU:HB2	0.474
2	A:211:ASP:C	A:213:LYS:H	0.472

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:348:TYR:CZ	A:376:TRP:CH2	0.464
2	A:581:LEU:CD2	A:587:PRO:HA	0.462
2	A:432:TYR:HB3	A:804:PHE:CE1	0.458
2	A:581:LEU:HD21	A:587:PRO:HA	0.455
2	A:663:PHE:CE1	A:784:VAL:HG11	0.455
2	A:352:ILE:HD13	A:369:MET:HB3	0.446
2	A:364:VAL:HG13	A:367:ARG:NH2	0.435
2	A:610:LYS:HE3	A:652:PHE:CE1	0.431
2	A:541:PRO:HA	A:544:ALA:HB3	0.425
2	A:626:LYS:O	A:721:PRO:HD3	0.421
2	A:496:ALA:HB3	A:502:SER:OG	0.414
2	A:652:PHE:CE1	A:711:MET:HE2	0.413
2	A:529:LEU:HD22	A:570:PHE:HZ	0.405
2	A:653:TYR:CB	A:666:ASN:HD21	0.405
3	A:364:VAL:HG13	A:367:ARG:HH21	0.827
3	A:705:ALA:HB2	A:767:ARG:HH22	0.743
3	A:352:ILE:HD11	A:372:MET:HB2	0.648
3	A:610:LYS:HE3	A:649:TYR:CE1	0.640
3	A:610:LYS:HE3	A:649:TYR:CZ	0.599
3	A:369:MET:HE1	A:385:GLY:O	0.574
3	A:653:TYR:HB3	A:665:SER:HB2	0.565
3	A:177:ILE:HD11	A:214:TYR:CD2	0.542
3	A:610:LYS:CE	A:649:TYR:CE1	0.510

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:565:PHE:CE1	A:567:THR:HG23	0.507
3	A:364:VAL:HG13	A:367:ARG:NH2	0.489
3	A:364:VAL:CG1	A:367:ARG:HH21	0.484
3	A:702:SER:C	A:704:ASP:H	0.478
3	A:632:ARG:CZ	A:659:THR:HG22	0.456
3	A:648:PHE:CD2	A:673:VAL:HG13	0.451
3	A:652:PHE:CZ	A:767:ARG:HD2	0.437
3	A:185:ASN:HB3	A:260:ILE:HD11	0.428
3	A:352:ILE:HD11	A:372:MET:CB	0.417
3	A:266:TYR:HB3	A:335:VAL:HG23	0.408
3	A:632:ARG:NH2	A:659:THR:HG22	0.408
3	A:491:TYR:CD2	A:509:TYR:CE1	0.407
3	A:188:PHE:CZ	A:233:ARG:HD3	0.402
4	A:514:THR:HG21	A:526:ARG:HE	0.880
4	A:177:ILE:HD11	A:199:LEU:HD22	0.673
4	A:514:THR:HG21	A:526:ARG:NE	0.648
4	A:608:TYR:CD1	A:648:PHE:CZ	0.620
4	A:548:TYR:CE1	A:556:PRO:CD	0.616
4	A:465:TYR:CZ	A:657:SER:HB2	0.598
4	A:548:TYR:CE1	A:556:PRO:HD2	0.594
4	A:652:PHE:CD1	A:663:PHE:HB3	0.569
4	A:661:ARG:HH21	A:773:ALA:CB	0.562
4	A:547:ARG:HH22	A:670:PRO:CB	0.528

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:543:VAL:HG12	A:547:ARG:HE	0.518
4	A:661:ARG:HH21	A:773:ALA:HB3	0.514
4	A:548:TYR:CZ	A:556:PRO:CD	0.497
4	A:548:TYR:CE1	A:556:PRO:HD3	0.489
4	A:649:TYR:CD1	A:709:ASN:ND2	0.487
4	A:666:ASN:C	A:667:THR:HG23	0.476
4	A:547:ARG:NH2	A:670:PRO:CB	0.465
4	A:652:PHE:CG	A:663:PHE:HB3	0.462
4	A:190:THR:HG22	A:194:ILE:HD12	0.459
4	A:318:ALA:HB2	A:377:LEU:HD23	0.456
4	A:266:TYR:HB3	A:335:VAL:HG23	0.454
4	A:733:VAL:HG22	A:776:TRP:CD1	0.448
4	A:608:TYR:CD1	A:648:PHE:CE1	0.446
4	A:618:TYR:CE1	A:630:LEU:HD22	0.442
4	A:652:PHE:CD1	A:663:PHE:CB	0.440
4	A:725:ILE:CD1	A:733:VAL:HG11	0.438
4	A:600:THR:CG2	A:608:TYR:CE1	0.436
4	A:608:TYR:CE1	A:648:PHE:CE1	0.436
4	A:572:PHE:CZ	A:597:GLY:HA3	0.432
4	A:586:PHE:HB3	A:734:ARG:CZ	0.421
4	A:547:ARG:HH22	A:670:PRO:HB3	0.413
4	A:753:GLN:C	A:755:SER:H	0.408
4	A:207:ASN:C	A:209:VAL:H	0.406

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:776:TRP:CE3	A:783:LEU:HD12	0.406
4	A:710:ALA:HB3	A:745:TRP:CE2	0.403
4	A:278:ALA:HB1	A:317:TYR:CZ	0.402
5	A:783:LEU:HD21	A:785:PHE:CE2	0.833
5	A:658:SER:HB2	A:711:MET:HE1	0.696
5	A:586:PHE:CE2	A:777:MET:HE3	0.672
5	A:526:ARG:HH22	A:596:THR:CG2	0.605
5	A:369:MET:HE1	A:416:TYR:CE2	0.602
5	A:609:TYR:CE1	A:637:TYR:HB3	0.585
5	A:526:ARG:HH22	A:596:THR:HG22	0.578
5	A:783:LEU:HD21	A:785:PHE:CD2	0.531
5	A:519:ILE:HD11	A:525:LEU:HG	0.510
5	A:790:PRO:HB2	A:793:LYS:HE2	0.501
5	A:188:PHE:CE1	A:233:ARG:HD3	0.491
5	A:668:ILE:HB	A:744:VAL:HG23	0.486
5	A:676:PRO:O	A:677:HIS:CG	0.470
5	A:369:MET:HE1	A:416:TYR:CD2	0.469
5	A:354:PHE:CE1	A:369:MET:HE2	0.459
5	A:783:LEU:C	A:783:LEU:HD23	0.452
5	A:366:ARG:HH12	A:373:GLU:CD	0.448
5	A:354:PHE:CZ	A:369:MET:HE2	0.442
5	A:637:TYR:CE2	A:706:VAL:HG13	0.433
5	A:190:THR:HG22	A:194:ILE:HD12	0.428

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:785:PHE:CE1	A:804:PHE:CD2	0.426
5	A:177:ILE:HD11	A:199:LEU:HD22	0.425
5	A:691:ALA:C	A:693:GLN:H	0.423
5	A:203:VAL:HG11	A:210:GLY:HA3	0.421
5	A:230:TYR:CE2	A:260:ILE:HD13	0.419
5	A:188:PHE:CZ	A:233:ARG:HD3	0.410
5	A:668:ILE:HG23	A:767:ARG:NH1	0.409
5	A:636:GLY:HA3	A:652:PHE:CE2	0.407
5	A:560:ASP:C	A:562:ASP:H	0.406
5	A:768:MET:HB3	A:791:PHE:CZ	0.403
6	A:648:PHE:CE1	A:777:MET:HE3	0.859
6	A:706:VAL:HG13	A:760:TYR:CE1	0.837
6	A:608:TYR:CE1	A:646:MET:HE3	0.695
6	A:706:VAL:HG13	A:760:TYR:CZ	0.685
6	A:177:ILE:HD11	A:199:LEU:HD22	0.606
6	A:687:ASP:C	A:689:GLU:H	0.600
6	A:652:PHE:CE2	A:719:ILE:HD12	0.581
6	A:657:SER:C	A:659:THR:H	0.543
6	A:702:SER:C	A:704:ASP:H	0.532
6	A:685:ASP:C	A:687:ASP:H	0.489
6	A:300:LYS:HE2	A:685:ASP:OD2	0.482
6	A:211:ASP:C	A:213:LYS:H	0.469
6	A:470:GLU:CD	A:488:ARG:HD2	0.467

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:679:ALA:C	A:681:ASN:H	0.450
6	A:186:HIS:H	A:262:GLU:CD	0.438
6	A:393:GLY:HA2	A:582:ASP:O	0.429
6	A:587:PRO:HB2	A:618:TYR:CE1	0.405
7	A:621:ILE:HD11	A:629:VAL:HG23	0.639
7	A:672:ALA:HB2	A:701:LYS:HE2	0.631
7	A:541:PRO:CB	A:546:TRP:HE1	0.556
7	A:659:THR:HB	A:663:PHE:CD2	0.553
7	A:494:PHE:CE1	A:496:ALA:HB2	0.551
7	A:348:TYR:CE2	A:411:GLN:HG2	0.524
7	A:676:PRO:HD2	A:757:TYR:CZ	0.512
7	A:359:THR:HG21	A:449:TRP:CZ3	0.510
7	A:504:TYR:CE1	A:648:PHE:CE2	0.507
7	A:663:PHE:CZ	A:738:PHE:HB2	0.502
7	A:666:ASN:HD21	A:769:SER:N	0.502
7	A:452:THR:HA	A:477:TYR:O	0.499
7	A:541:PRO:CA	A:546:TRP:HE1	0.479
7	A:545:MET:HE1	A:648:PHE:CZ	0.475
7	A:673:VAL:HG22	A:760:TYR:CE2	0.470
7	A:470:GLU:CD	A:488:ARG:HD2	0.469
7	A:767:ARG:NH1	A:794:TYR:CD2	0.459
7	A:504:TYR:CZ	A:648:PHE:HE2	0.453
7	A:670:PRO:HA	A:703:ASP:O	0.437

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:677:HIS:CB	A:698:ASP:HB2	0.425
7	A:677:HIS:HB3	A:698:ASP:HB2	0.424
7	A:348:TYR:CZ	A:411:GLN:HG2	0.421
7	A:496:ALA:HB3	A:502:SER:O	0.421
7	A:186:HIS:H	A:262:GLU:CD	0.414
7	A:731:ASN:HA	A:777:MET:O	0.412
7	A:661:ARG:HH12	A:805:ASN:HB3	0.412
7	A:554:GLU:HG3	A:565:PHE:CE2	0.409
8	A:536:LEU:HD21	A:670:PRO:HB3	0.929
8	A:547:ARG:HH12	A:679:ALA:HB3	0.793
8	A:547:ARG:NH1	A:679:ALA:HB3	0.710
8	A:360:SER:HA	A:450:LEU:HD11	0.694
8	A:392:LEU:HD22	A:449:TRP:CE2	0.683
8	A:204:PRO:HB2	A:206:TRP:CE3	0.668
8	A:348:TYR:CZ	A:376:TRP:CZ3	0.657
8	A:205:TRP:CG	A:254:ILE:HD13	0.622
8	A:652:PHE:CD2	A:767:ARG:HD2	0.620
8	A:392:LEU:HD22	A:449:TRP:CD2	0.600
8	A:204:PRO:HG2	A:206:TRP:CH2	0.576
8	A:204:PRO:HB2	A:206:TRP:CZ3	0.565
8	A:706:VAL:HG21	A:767:ARG:HH12	0.525
8	A:370:ARG:HH12	A:521:GLU:N	0.524
8	A:607:GLU:HB3	A:641:LEU:HD12	0.521

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:394:PHE:CD2	A:449:TRP:HB2	0.519
8	A:348:TYR:CE1	A:376:TRP:CZ3	0.513
8	A:370:ARG:HH22	A:520:ASN:C	0.512
8	A:201:ASP:HB2	A:203:VAL:HG23	0.510
8	A:201:ASP:C	A:203:VAL:H	0.502
8	A:522:TYR:CD1	A:580:LYS:HA	0.493
8	A:706:VAL:HG22	A:760:TYR:CE1	0.492
8	A:652:PHE:CD2	A:767:ARG:CD	0.491
8	A:680:SER:HB3	A:688:TYR:CE1	0.490
8	A:141:TYR:HA	A:144:VAL:HG22	0.479
8	A:465:TYR:CE1	A:497:ASP:OD1	0.474
8	A:205:TRP:CH2	A:254:ILE:HG21	0.473
8	A:352:ILE:HG21	A:369:MET:SD	0.473
8	A:203:VAL:CG1	A:207:ASN:HD22	0.469
8	A:352:ILE:HD13	A:369:MET:CE	0.467
8	A:536:LEU:CD2	A:670:PRO:HB3	0.462
8	A:205:TRP:CZ2	A:254:ILE:HG21	0.460
8	A:392:LEU:HA	A:449:TRP:CZ3	0.453
8	A:501:LEU:HD23	A:675:PHE:CZ	0.450
8	A:426:PHE:CD1	A:444:VAL:HG12	0.445
8	A:652:PHE:HB3	A:663:PHE:CE1	0.444
8	A:536:LEU:HD21	A:670:PRO:CB	0.437
8	A:565:PHE:CE2	A:605:ASP:HB2	0.430

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:18:VAL:O	A:19:TYR:CD2	0.424
8	A:360:SER:HA	A:450:LEU:CD1	0.422
8	A:205:TRP:CZ2	A:209:VAL:CG2	0.420
8	A:565:PHE:CE2	A:605:ASP:CB	0.419
8	A:660:VAL:HG21	A:784:VAL:HG11	0.419
8	A:587:PRO:HB2	A:618:TYR:CE1	0.415
8	A:395:PHE:CD1	A:418:VAL:HB	0.411
8	A:501:LEU:O	A:502:SER:C	0.408
8	A:346:ARG:HD3	A:376:TRP:CZ3	0.405
8	A:610:LYS:HE2	A:612:THR:HG23	0.405
8	A:268:LEU:HB3	A:290:ILE:HD12	0.403
8	A:145:GLY:HA3	A:206:TRP:HB3	0.402
8	A:652:PHE:CG	A:767:ARG:CD	0.401
8	A:371:GLN:HE22	A:382:VAL:HG22	0.400
9	A:621:ILE:HD11	A:629:VAL:HG23	0.663
9	A:790:PRO:HG2	A:793:LYS:HE2	0.651
9	A:610:LYS:CE	A:646:MET:HE1	0.638
9	A:504:TYR:CD1	A:652:PHE:CE2	0.636
9	A:488:ARG:HH21	A:526:ARG:NH2	0.587
9	A:610:LYS:HE3	A:646:MET:HE1	0.586
9	A:506:ASN:HD21	A:532:VAL:HG13	0.585
9	A:543:VAL:HG22	A:675:PHE:CZ	0.577
9	A:506:ASN:HD21	A:532:VAL:CG1	0.561

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:790:PRO:CG	A:793:LYS:HE2	0.552
9	A:659:THR:HG21	A:767:ARG:HD3	0.551
9	A:668:ILE:CG2	A:709:ASN:HA	0.546
9	A:803:GLN:NE2	A:805:ASN:HD21	0.529
9	A:488:ARG:HH21	A:526:ARG:CZ	0.521
9	A:185:ASN:HB3	A:260:ILE:HD11	0.518
9	A:211:ASP:OD2	A:213:LYS:HE3	0.518
9	A:610:LYS:HE2	A:646:MET:HE1	0.517
9	A:504:TYR:CG	A:652:PHE:CZ	0.516
9	A:504:TYR:CG	A:652:PHE:CE2	0.511
9	A:649:TYR:O	A:652:PHE:CE2	0.511
9	A:666:ASN:HA	A:667:THR:HG23	0.507
9	A:388:ARG:HH12	A:521:GLU:CD	0.495
9	A:548:TYR:CZ	A:555:HIS:HA	0.495
9	A:548:TYR:CE2	A:555:HIS:HA	0.490
9	A:565:PHE:CE1	A:567:THR:HG23	0.490
9	A:610:LYS:HE3	A:646:MET:CE	0.487
9	A:653:TYR:CE1	A:656:GLY:N	0.487
9	A:658:SER:HA	A:662:GLY:HA3	0.485
9	A:729:TYR:C	A:731:ASN:H	0.475
9	A:174:SER:OG	A:213:LYS:HE2	0.469
9	A:512:ASP:CG	A:526:ARG:HE	0.467
9	A:504:TYR:CB	A:652:PHE:CZ	0.460

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:674:TYR:CE1	A:757:TYR:CD1	0.460
9	A:662:GLY:C	A:664:GLN:H	0.457
9	A:668:ILE:HG23	A:709:ASN:C	0.456
9	A:278:ALA:HB1	A:317:TYR:CZ	0.451
9	A:674:TYR:CE2	A:749:TRP:CH2	0.449
9	A:612:THR:OG1	A:667:THR:HG22	0.447
9	A:586:PHE:CE2	A:777:MET:HG2	0.443
9	A:504:TYR:CE1	A:652:PHE:CE2	0.437
9	A:654:ALA:HB3	A:706:VAL:O	0.437
9	A:147:TYR:CE2	A:254:ILE:HD11	0.434
9	A:658:SER:HB2	A:662:GLY:C	0.430
9	A:649:TYR:C	A:652:PHE:CE2	0.428
9	A:562:ASP:C	A:564:SER:H	0.427
9	A:660:VAL:HG21	A:740:ASP:HB3	0.424
9	A:674:TYR:HB3	A:699:LEU:HB3	0.424
9	A:634:ARG:HE	A:711:MET:HE1	0.424
9	A:649:TYR:O	A:652:PHE:CD2	0.421
9	A:190:THR:HG22	A:194:ILE:HD12	0.412
9	A:177:ILE:HD11	A:199:LEU:HD22	0.410
9	A:557:SER:C	A:559:SER:H	0.407
9	A:660:VAL:CG1	A:715:SER:HB2	0.407
9	A:348:TYR:CZ	A:376:TRP:CH2	0.406
9	A:674:TYR:CE2	A:749:TRP:HH2	0.401

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:394:PHE:CE1	A:449:TRP:HA	0.888
10	A:449:TRP:CD1	A:477:TYR:HH	0.863
10	A:392:LEU:HB3	A:394:PHE:CZ	0.821
10	A:548:TYR:CE1	A:556:PRO:HG3	0.740
10	A:394:PHE:CZ	A:449:TRP:HA	0.698
10	A:501:LEU:HD21	A:678:GLN:HG2	0.698
10	A:392:LEU:HD13	A:394:PHE:CE2	0.660
10	A:548:TYR:CZ	A:556:PRO:HG3	0.639
10	A:548:TYR:CE1	A:556:PRO:CG	0.626
10	A:802:PHE:CE1	A:804:PHE:CE2	0.625
10	A:394:PHE:CZ	A:449:TRP:HB2	0.579
10	A:394:PHE:CE2	A:449:TRP:HB2	0.575
10	A:548:TYR:CZ	A:556:PRO:CG	0.550
10	A:367:ARG:CZ	A:449:TRP:CZ2	0.543
10	A:394:PHE:CZ	A:449:TRP:CA	0.537
10	A:689:GLU:C	A:691:ALA:H	0.532
10	A:802:PHE:CE1	A:804:PHE:CZ	0.527
10	A:367:ARG:NH2	A:449:TRP:CE2	0.524
10	A:394:PHE:CD1	A:394:PHE:N	0.515
10	A:394:PHE:CD1	A:449:TRP:HA	0.504
10	A:185:ASN:HB3	A:260:ILE:HD11	0.503
10	A:392:LEU:HD13	A:394:PHE:CZ	0.498
10	A:392:LEU:CB	A:394:PHE:CZ	0.497

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:436:SER:HB3	A:668:ILE:HG23	0.494
10	A:394:PHE:CE1	A:449:TRP:CA	0.493
10	A:390:ASN:HB3	A:583:ARG:HH22	0.481
10	A:177:ILE:HD11	A:199:LEU:HD22	0.476
10	A:501:LEU:HD11	A:678:GLN:HG3	0.474
10	A:190:THR:HG22	A:194:ILE:HD12	0.471
10	A:422:ASN:HB3	A:810:TRP:C	0.470
10	A:749:TRP:CD1	A:760:TYR:H	0.470
10	A:449:TRP:CH2	A:450:LEU:HD21	0.464
10	A:661:ARG:HH21	A:717:GLU:CD	0.464
10	A:586:PHE:HB2	A:734:ARG:CZ	0.463
10	A:392:LEU:HD13	A:394:PHE:HE2	0.461
10	A:491:TYR:CD2	A:509:TYR:CE1	0.460
10	A:367:ARG:CZ	A:449:TRP:CH2	0.454
10	A:348:TYR:CZ	A:376:TRP:CH2	0.453
10	A:668:ILE:O	A:668:ILE:HG22	0.443
10	A:565:PHE:CZ	A:606:ASN:HB2	0.442
10	A:660:VAL:HG21	A:773:ALA:HB2	0.437
10	A:501:LEU:HD21	A:678:GLN:CG	0.435
10	A:663:PHE:CE2	A:784:VAL:HG11	0.433
10	A:646:MET:HE1	A:746:ASP:OD2	0.432
10	A:278:ALA:HB1	A:317:TYR:CZ	0.429
10	A:206:TRP:CZ2	A:724:PHE:CE2	0.425

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:448:ASN:CG	A:452:THR:O	0.416
10	A:810:TRP:C	A:810:TRP:CD1	0.414
10	A:395:PHE:CD1	A:418:VAL:HB	0.413
10	A:552:MET:C	A:554:GLU:H	0.412
10	A:394:PHE:CE1	A:449:TRP:C	0.411
10	A:609:TYR:CE1	A:639:ASP:HB3	0.408
10	A:207:ASN:C	A:209:VAL:H	0.408
10	A:586:PHE:CZ	A:775:GLN:NE2	0.407
10	A:548:TYR:CE1	A:552:MET:HE2	0.403
10	A:660:VAL:HG21	A:773:ALA:CB	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	808	751	32	25
2	808	748	43	17
3	808	752	35	21
4	808	752	36	20
5	808	749	39	20
6	808	740	50	18
7	808	746	43	19
8	808	768	33	7
9	808	754	31	23
10	808	762	27	19

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	688	658	21	9
2	688	662	15	11
3	688	662	13	13
4	688	662	18	8
5	688	671	9	8
6	688	657	21	10
7	688	661	14	13
8	688	661	15	12
9	688	664	15	9
10	688	660	16	12

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	6	LEU
1	A	7	LEU
1	A	10	SER
1	A	17	THR
1	A	211	ASP
1	A	557	SER
1	A	677	HIS
1	A	711	MET
1	A	727	ASP

Model ID	Chain	Residue ID	Residue type
2	A	6	LEU
2	A	7	LEU
2	A	17	THR
2	A	173	VAL
2	A	209	VAL
2	A	247	LEU
2	A	436	SER
2	A	545	MET
2	A	581	LEU
2	A	754	TYR
2	A	784	VAL
3	A	6	LEU
3	A	7	LEU
3	A	10	SER
3	A	11	LEU
3	A	93	THR
3	A	174	SER
3	A	247	LEU
3	A	480	VAL
3	A	562	ASP
3	A	581	LEU
3	A	646	MET
3	A	659	THR

Model ID	Chain	Residue ID	Residue type
3	A	682	TYR
4	A	1	MET
4	A	6	LEU
4	A	7	LEU
4	A	11	LEU
4	A	14	SER
4	A	562	ASP
4	A	693	GLN
4	A	706	VAL
5	A	1	MET
5	A	6	LEU
5	A	7	LEU
5	A	11	LEU
5	A	15	SER
5	A	17	THR
5	A	726	SER
5	A	732	SER
6	A	3	MET
6	A	6	LEU
6	A	10	SER
6	A	209	VAL
6	A	247	LEU
6	A	362	ASP

Model ID	Chain	Residue ID	Residue type
6	A	505	THR
6	A	649	TYR
6	A	732	SER
6	A	772	ILE
7	A	3	MET
7	A	6	LEU
7	A	7	LEU
7	A	11	LEU
7	A	14	SER
7	A	17	THR
7	A	209	VAL
7	A	359	THR
7	A	562	ASP
7	A	665	SER
7	A	692	THR
7	A	706	VAL
7	A	722	THR
8	A	6	LEU
8	A	7	LEU
8	A	10	SER
8	A	17	THR
8	A	129	THR
8	A	211	ASP

Model ID	Chain	Residue ID	Residue type
8	A	474	THR
8	A	658	SER
8	A	660	VAL
8	A	667	THR
8	A	688	TYR
8	A	784	VAL
9	A	3	MET
9	A	6	LEU
9	A	7	LEU
9	A	11	LEU
9	A	17	THR
9	A	209	VAL
9	A	434	THR
9	A	500	ASP
9	A	658	SER
10	A	6	LEU
10	A	7	LEU
10	A	14	SER
10	A	209	VAL
10	A	247	LEU
10	A	364	VAL
10	A	392	LEU
10	A	394	PHE

Model ID	Chain	Residue ID	Residue type
10	A	542	GLN
10	A	548	TYR
10	A	700	CYS
10	A	739	TRP

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.

Acknowledgements

Development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures, are funded by NSF ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The PDB-Dev team and members of Sali labcontributed model validation metrics and software packages.

Implementation of validation methods for SAS data and SAS-based models are funded byRCSB PDB (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from RCSB PDB, Dr. Jill Trewhella, Dr. Dina Schneidman, and members of the SASBDB repository are acknowledged for their advice and support in implementing SAS validation methods.

Members of the wwPDB Integrative/Hybrid Methods Task Force provided recommendations and community support for the project.