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	9A37
PDB-Dev ID	PDBDEV_00000192
Structure Title	Model of E. coli OppA 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

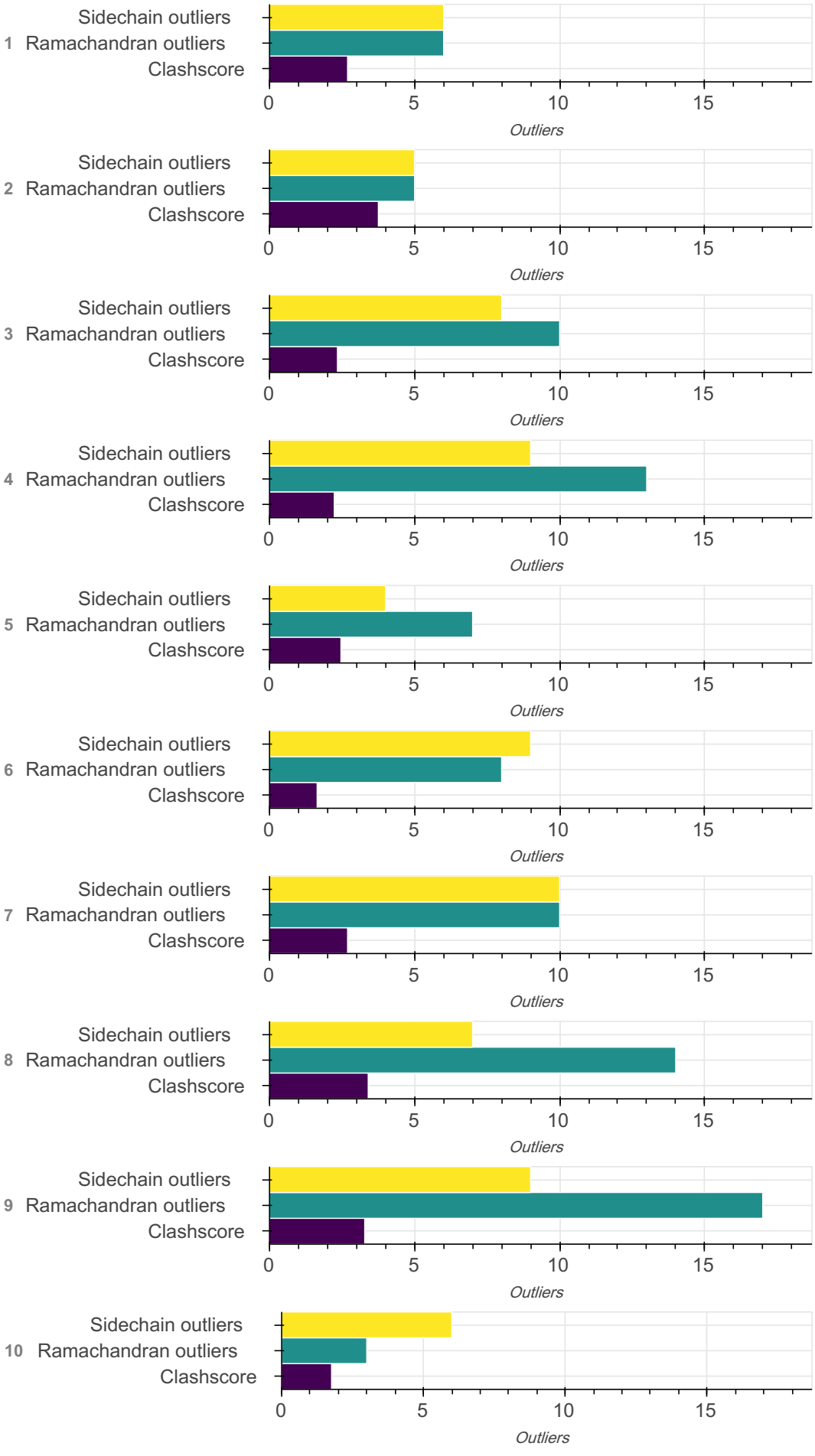
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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
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15
Outliers
Sidechain outliers
2 Ramachandran outliers
Clashscore
0
5
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15
Outliers
Sidechain outliers
3 Ramachandran outliers
Clashscore
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Outliers
Sidechain outliers
4 Ramachandran outliers
Clashscore
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Outliers
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Clashscore
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8 Ramachandran outliers
Clashscore
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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	P23843	A	A	543
2	1	1	P23843	A	A	543
3	1	1	P23843	A	A	543
4	1	1	P23843	A	A	543
5	1	1	P23843	A	A	543
6	1	1	P23843	A	A	543
7	1	1	P23843	A	A	543
8	1	1	P23843	A	A	543
9	1	1	P23843	A	A	543
10	1	1	P23843	A	A	543

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	-	1-543

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 42380 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--HB3	1.09	0.97	4040
CG2--HG21	1.09	0.97	1100
CD--HD2	1.09	0.97	910
CG--HG3	1.09	0.97	1480
CA--HA2	1.09	0.97	290
CB--HB2	1.09	0.97	4040
CA--HA	1.09	0.97	5140
CD2--HD21	1.09	0.97	450
CG1--HG13	1.09	0.97	690
CB--HB	1.09	0.97	1100
CG2--HG22	1.09	0.97	1100
CE--HE2	1.09	0.97	510
CD1--HD13	1.09	0.97	700
CG2--HG23	1.09	0.97	1100
NZ--HZ2	1.01	0.89	410
CE--HE3	1.09	0.97	510
CD--HD3	1.09	0.97	910
CB--HB1	1.09	0.97	460
CD1--HD12	1.09	0.97	700
OG1--HG1	0.96	0.84	410
CD1--HD11	1.09	0.97	700
CG--HG	1.09	0.97	450

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG--HG2	1.09	0.97	1480
NZ--HZ1	1.01	0.89	410
CD2--HD22	1.09	0.97	450
CG1--HG12	1.09	0.97	690
CD2--HD23	1.09	0.97	450
NZ--HZ3	1.01	0.89	410
CE--HE1	1.09	0.97	100
CG1--HG11	1.09	0.97	440
CA--HA3	1.09	0.97	290
OH--HH	0.96	0.84	280
OG--HG	0.96	0.84	300
N--H3	1.01	0.89	10
N--H2	1.01	0.89	10
N--H1	1.01	0.89	10
NE--HE	1.01	0.86	180
N--H	1.01	0.86	5100
ND2--HD21	1.01	0.86	340
NH2--HH21	1.01	0.86	180
CH2--HH2	1.08	0.93	130
NE1--HE1	1.01	0.86	130
CD1--HD1	1.08	0.93	530
CZ2--HZ2	1.08	0.93	130
ND2--HD22	1.01	0.86	340

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD2--HD2	1.08	0.93	510
CE2--HE2	1.08	0.93	400
NH2--HH22	1.01	0.86	180
NH1--HH11	1.01	0.86	180
NE2--HE22	1.01	0.86	170
CE1--HE1	1.08	0.93	509
ND1--HD1	1.01	0.86	90
NE2--HE2	1.01	0.86	19
NH1--HH12	1.01	0.86	180
CE3--HE3	1.08	0.93	130
CZ--HZ	1.08	0.93	120
NE2--HE21	1.01	0.86	170
CZ3--HZ3	1.08	0.93	130
ND1--HD1	1.34	0.86	1
CE1--HE1	2.15	0.93	1

Standard geometry: angle outliers

There are 277 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
ND1-CE1-NE2	108.40	85.01	1
CD2-NE2-CE1	109.00	86.70	1
CG-CD2-NE2	107.20	129.19	1
CG-ND1-CE1	109.30	129.99	1
C-N-CA	121.70	139.22	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	136.76	1
C-N-CA	121.70	135.55	1
C-N-CA	121.70	135.35	1
C-N-CA	121.70	134.33	1
OD1-CG-ND2	122.60	115.75	1
CA-CB-CG	112.60	119.39	1
CA-CB-CG	112.60	119.31	1
OD1-CG-ND2	122.60	116.08	1
C-N-CA	121.70	133.42	1
C-N-CA	121.70	133.28	1
NE-CZ-NH2	119.20	124.87	1
C-N-CA	121.70	133.03	1
OE1-CD-NE2	122.60	116.32	1
C-N-CA	121.70	132.91	1
C-N-CA	121.70	132.72	1
OD1-CG-ND2	122.60	116.65	1
C-N-CA	121.70	132.18	1
OE1-CD-NE2	122.60	116.84	1
C-N-CA	121.70	132.06	1
CA-CB-CG	112.60	106.86	1
C-N-CA	121.70	131.98	1
OE1-CD-NE2	122.60	116.94	1
CA-CB-CG	112.60	106.95	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	117.03	1
C-N-CA	121.70	131.64	1
OD1-CG-ND2	122.60	117.14	1
OD1-CG-ND2	122.60	117.16	1
OE1-CD-NE2	122.60	117.16	1
C-N-CA	121.70	131.45	1
OD1-CG-ND2	122.60	117.21	1
C-N-CA	121.70	131.39	1
C-N-CA	121.70	131.38	1
CA-CB-OG1	109.60	101.60	1
OE1-CD-NE2	122.60	117.27	1
CA-CB-CG	112.60	107.29	1
C-N-CA	121.70	131.11	1
C-N-CA	121.70	131.08	1
OE1-CD-NE2	122.60	117.40	1
C-CA-CB	110.10	119.94	1
OD1-CG-ND2	122.60	117.43	1
OE1-CD-NE2	122.60	117.45	1
C-N-CA	121.70	130.95	1
OD1-CG-ND2	122.60	117.48	1
OE1-CD-NE2	122.60	117.48	1
OD1-CG-ND2	122.60	117.52	1
O-C-N	123.00	114.88	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	117.67	1
C-N-CA	121.70	130.82	1
OD1-CG-ND2	122.60	117.54	1
CA-CB-CG	112.60	117.65	1
OD1-CG-ND2	122.60	117.55	2
OD1-CG-ND2	122.60	117.56	2
OE1-CD-NE2	122.60	117.57	1
OD1-CG-ND2	122.60	117.59	1
C-N-CA	121.70	130.72	1
C-N-CA	121.70	130.69	1
OD1-CG-ND2	122.60	117.62	1
CA-C-N	116.20	126.11	1
C-N-CA	121.70	130.62	1
OE1-CD-NE2	122.60	117.65	1
CA-CB-CG	112.60	117.55	1
OD1-CG-ND2	122.60	117.67	1
CA-CB-CG	112.60	117.50	1
OE1-CD-NE2	122.60	117.71	1
C-CA-CB	110.50	117.83	1
C-N-CA	121.70	130.46	1
OD1-CG-ND2	122.60	117.74	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
OD1-CG-ND2	122.60	117.77	1
CA-CB-CG	112.60	117.42	1
OD1-CG-ND2	122.60	117.80	1
OE1-CD-NE2	122.60	117.81	1
C-N-CA	121.70	130.31	1
OD1-CG-ND2	122.60	117.83	1
OE1-CD-NE2	122.60	117.83	1
N-CA-CB	103.00	108.25	1
C-N-CA	121.70	130.29	1
OE1-CD-NE2	122.60	117.85	1
OE1-CD-NE2	122.60	117.86	1
CA-C-N	116.20	125.65	1
OE1-CD-NE2	122.60	117.88	3
CB-CG-CD2	131.20	125.06	1
C-N-CA	121.70	130.18	1
OE1-CD-NE2	122.60	117.89	1
C-N-CA	121.70	130.17	1
C-N-CA	121.70	130.15	1
CA-CB-CG	112.60	117.29	1
CB-CG-CD2	131.20	125.11	1
C-N-CA	121.70	130.14	1
C-N-CA	121.70	130.12	1
CA-CB-CG	113.80	109.14	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	102.58	1
C-N-CA	121.70	130.07	1
OD1-CG-ND2	122.60	117.96	1
CB-CG-CD2	131.20	125.17	1
CA-CB-CG	112.60	117.24	1
C-N-CA	121.70	130.04	1
OG1-CB-CG2	109.30	100.06	1
C-N-CA	121.70	130.00	1
CB-CG-CD2	131.20	125.21	2
CA-CB-CG	113.80	118.38	1
OE1-CD-NE2	122.60	118.02	1
OE1-CD-NE2	122.60	118.03	1
C-N-CA	121.70	129.92	1
OE1-CD-NE2	122.60	118.04	1
C-N-CA	121.70	129.90	1
CB-CG-CD2	131.20	125.29	1
OE1-CD-NE2	122.60	118.05	1
CB-CG-CD2	131.20	125.30	1
O-C-N	123.00	115.74	1
CA-C-N	116.20	125.26	1
OE1-CD-NE2	122.60	118.08	1
C-N-CA	121.70	129.84	1
OD1-CG-ND2	122.60	118.08	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	115.79	1
NE-CZ-NH2	119.20	123.25	1
OE1-CD-NE2	122.60	118.11	1
C-CA-CB	109.10	118.98	1
OE1-CD-NE2	122.60	118.12	1
C-CA-CB	110.10	118.60	1
OD1-CG-ND2	122.60	118.13	1
OE1-CD-NE2	122.60	118.14	1
OE1-CD-NE2	122.60	118.15	1
CB-CG-CD2	131.20	125.42	1
NE-CZ-NH1	121.50	125.94	1
OE1-CD-NE2	122.60	118.16	1
OD1-CG-ND2	122.60	118.16	1
C-N-CA	121.70	129.69	1
CA-CB-CG	112.60	117.03	1
OD1-CG-ND2	122.60	118.19	1
OE1-CD-NE2	122.60	118.20	1
OE1-CD-NE2	122.60	118.21	2
OD1-CG-ND2	122.60	118.21	1
C-N-CA	121.70	129.59	1
CB-CG-CD2	131.20	125.51	2
OE1-CD-NE2	122.60	118.23	2
CB-CG-CD2	131.20	125.53	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	116.95	1
OE1-CD-NE2	122.60	118.25	1
CA-CB-OG1	109.60	116.13	1
OE1-CD-NE2	122.60	118.26	1
C-N-CA	121.70	129.51	1
CA-CB-CG	112.60	116.93	1
CB-CG-CD2	131.20	125.58	1
CA-CB-CG	112.60	108.28	1
OE1-CD-NE2	122.60	118.29	3
C-N-CA	121.70	129.46	1
OE1-CD-NE2	122.60	118.30	1
CB-CG-CD2	131.20	125.61	1
OE1-CD-NE2	122.60	118.31	2
C-N-CA	121.70	129.41	1
OD1-CG-ND2	122.60	118.32	1
OE1-CD-NE2	122.60	118.32	1
C-N-CA	121.70	129.40	1
C-N-CA	121.70	129.38	1
OE1-CD-NE2	122.60	118.34	2
N-CA-CB	103.00	107.69	1
C-N-CA	121.70	129.37	1
CA-CB-CG	112.60	116.86	2
OD1-CG-ND2	122.60	118.34	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	116.85	1
OE1-CD-NE2	122.60	118.35	1
OE1-CD-NE2	122.60	118.36	3
CB-CG-CD2	131.20	125.69	1
OD1-CG-ND2	122.60	118.37	1
O-C-N	123.00	116.23	1
OE1-CD-NE2	122.60	118.38	2
O-C-N	123.00	116.25	1
C-N-CA	121.70	129.29	1
OE1-CD-NE2	122.60	118.39	1
CA-C-N	116.20	124.60	1
CA-CB-CG	112.60	116.80	1
OE1-CD-NE2	122.60	118.41	1
CB-CG-CD2	131.20	125.76	1
CA-CB-CG	112.60	116.78	1
OE1-CD-NE2	122.60	118.42	1
OE1-CD-NE2	122.60	118.43	3
CA-CB-CG	112.60	116.76	1
OE1-CD-NE2	122.60	118.44	1
OE1-CD-NE2	122.60	118.45	3
CB-CG-CD2	131.20	125.80	1
C-N-CA	121.70	129.17	1
OE1-CD-NE2	122.60	118.46	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	125.82	1
N-CA-C	111.00	122.60	1
OE1-CD-NE2	122.60	118.47	2
CB-CG-CD2	131.20	125.83	1
C-N-CA	121.70	129.13	1
CB-CG-CD2	131.20	125.84	2
OE1-CD-NE2	122.60	118.48	2
C-N-CA	121.70	129.10	1
OE1-CD-NE2	122.60	118.51	3
C-N-CA	121.70	129.05	2
OD1-CG-ND2	122.60	118.52	1
OE1-CD-NE2	122.60	118.52	1
CB-CG-CD2	131.20	125.90	1
CA-C-N	116.20	124.35	1
CA-CB-CG	112.60	108.53	1
CB-CG-CD2	131.20	125.91	2
OE1-CD-NE2	122.60	118.53	2
N-CA-C	111.00	122.39	1
OE1-CD-NE2	122.60	118.54	1
CB-CG-CD2	131.20	125.92	1
CG-CD-CE	111.30	101.96	1
OD1-CG-ND2	122.60	118.54	1
C-CA-CB	110.10	117.78	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.56	1
NH1-CZ-NH2	119.30	114.05	1
OE1-CD-NE2	122.60	118.57	1
CA-CB-CG	112.60	116.63	1
OD1-CG-ND2	122.60	118.58	1
OE1-CD-NE2	122.60	118.59	1
N-CA-C	111.00	122.23	1
CA-CB-OG1	109.60	115.62	1
OD1-CG-ND2	122.60	118.59	1
CB-CG-CD2	131.20	126.00	1
OD1-CG-ND2	122.60	118.60	1
C-N-H	111.78	124.30	1
C-N-H	111.66	124.30	1
C-N-H	111.62	124.30	1
C-N-H	111.44	124.30	1
C-N-H	110.58	124.30	1
C-N-H	110.41	124.30	1
C-N-H	110.22	124.30	1
C-N-H	108.90	124.30	1
C-N-H	108.53	124.30	1
C-N-H	108.45	124.30	1
C-N-H	108.23	124.30	2
C-N-H	108.17	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-H	108.05	124.30	1
C-N-H	107.39	124.30	1
C-N-H	107.19	124.30	1
C-N-H	107.14	124.30	1
C-N-H	107.11	124.30	1
C-N-H	106.98	124.30	1
CG-ND1-HD1	105.15	125.35	1
NE2-CD2-HD2	104.16	126.40	1
ND1-CE1-HE1	62.33	125.80	1
CE1-ND1-HD1	24.84	125.35	1
NE2-CE1-HE1	22.73	125.80	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	2.69	23
2	3.75	32
3	2.34	20
4	2.23	19
5	2.46	21
6	1.64	14
7	2.69	23
8	3.40	29

Model ID	Clash score	Number of clashes
9	3.28	28
10	1.76	15

All 224 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:343:TYR:CD1	A:505:ILE:HD11	0.857
1	A:186:VAL:HG21	A:447:ASN:HD22	0.719
1	A:450:THR:CG2	A:492:TYR:CZ	0.610
1	A:343:TYR:CE1	A:505:ILE:CG1	0.501
1	A:297:CYS:HB2	A:511:TYR:CE1	0.496
1	A:445:ASP:HB3	A:534:TYR:CE2	0.494
1	A:276:ILE:HG21	A:334:ALA:HB1	0.493
1	A:297:CYS:HB2	A:511:TYR:CZ	0.485
1	A:344:THR:HG21	A:351:ALA:CB	0.478
1	A:371:LYS:HE3	A:411:ASN:O	0.477
1	A:392:ASN:ND2	A:423:TRP:CZ3	0.456
1	A:38:LYS:HD3	A:520:TRP:CZ3	0.454
1	A:450:THR:HG22	A:492:TYR:CZ	0.446
1	A:57:ILE:HG23	A:62:GLU:HB2	0.440
1	A:450:THR:HG22	A:492:TYR:CE1	0.439
1	A:488:ARG:HG2	A:492:TYR:CE2	0.431
1	A:333:LYS:HE3	A:509:TYR:CE2	0.427
1	A:217:TYR:CE2	A:541:VAL:CG1	0.424
1	A:69:LEU:HD21	A:230:LEU:HD22	0.422

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:488:ARG:HG2	A:492:TYR:CZ	0.417
1	A:185:LEU:HA	A:190:THR:HG21	0.412
1	A:479:THR:HG21	A:492:TYR:CE1	0.404
1	A:205:TRP:CE2	A:206:THR:HG23	0.402
2	A:535:THR:HA	A:538:MET:HE3	0.777
2	A:276:ILE:HD11	A:334:ALA:HB3	0.670
2	A:35:LEU:HD21	A:543:HIS:HB2	0.630
2	A:247:VAL:HG21	A:539:TYR:OH	0.617
2	A:186:VAL:HG23	A:446:TYR:CZ	0.607
2	A:276:ILE:CD1	A:334:ALA:HB3	0.569
2	A:217:TYR:CE2	A:539:TYR:CE2	0.560
2	A:35:LEU:HD21	A:543:HIS:CG	0.555
2	A:67:ARG:CZ	A:188:PRO:HD3	0.550
2	A:536:ARG:HA	A:539:TYR:CD2	0.539
2	A:126:SER:HB3	A:141:TYR:CE2	0.531
2	A:297:CYS:CB	A:511:TYR:CZ	0.531
2	A:535:THR:HG22	A:539:TYR:CE1	0.510
2	A:444:ALA:HB2	A:452:PHE:CE2	0.505
2	A:186:VAL:HG23	A:446:TYR:CE2	0.496
2	A:186:VAL:CG2	A:446:TYR:CZ	0.493
2	A:13:GLY:O	A:14:VAL:HG23	0.483
2	A:371:LYS:HE3	A:411:ASN:O	0.479
2	A:35:LEU:HD21	A:543:HIS:CB	0.462

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:515:ARG:HH12	A:532:ASN:CA	0.452
2	A:522:GLY:H	A:543:HIS:HE1	0.448
2	A:297:CYS:HB3	A:511:TYR:CZ	0.444
2	A:296:LEU:HD11	A:529:PRO:HG2	0.442
2	A:509:TYR:CE2	A:511:TYR:HB3	0.441
2	A:217:TYR:HE2	A:539:TYR:CE2	0.441
2	A:442:TRP:HB3	A:452:PHE:CE1	0.437
2	A:69:LEU:HD21	A:230:LEU:HD22	0.427
2	A:442:TRP:CD1	A:452:PHE:CD1	0.427
2	A:274:MET:CE	A:279:PHE:HA	0.423
2	A:297:CYS:HB2	A:511:TYR:CZ	0.418
2	A:522:GLY:H	A:543:HIS:CE1	0.412
2	A:535:THR:HB	A:539:TYR:CZ	0.408
3	A:269:MET:HE1	A:524:TYR:CZ	0.794
3	A:340:ALA:HA	A:510:TYR:CE2	0.600
3	A:332:VAL:HG11	A:509:TYR:CD2	0.591
3	A:339:PRO:HG2	A:341:TYR:CE2	0.516
3	A:276:ILE:HD12	A:335:GLN:HG2	0.502
3	A:356:PRO:HD2	A:359:PHE:CE2	0.502
3	A:371:LYS:HE3	A:411:ASN:O	0.477
3	A:332:VAL:HA	A:335:GLN:HG3	0.469
3	A:276:ILE:HB	A:335:GLN:HG2	0.464
3	A:243:VAL:HG21	A:541:VAL:H	0.453

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:69:LEU:HD21	A:230:LEU:HD22	0.451
3	A:333:LYS:HE3	A:339:PRO:HG3	0.443
3	A:96:LYS:HE3	A:174:LEU:O	0.436
3	A:340:ALA:HA	A:510:TYR:CD2	0.427
3	A:354:THR:HG21	A:497:GLN:HE21	0.425
3	A:276:ILE:HG13	A:335:GLN:HA	0.424
3	A:141:TYR:CE1	A:454:ASN:HB3	0.417
3	A:295:TYR:CZ	A:443:CYS:HB3	0.410
3	A:302:GLU:CD	A:430:ARG:HH21	0.406
3	A:297:CYS:HB2	A:511:TYR:CZ	0.406
4	A:55:HIS:CD2	A:55:HIS:NE2	1.162
4	A:55:HIS:CE1	A:55:HIS:ND1	1.161
4	A:55:HIS:HE1	A:122:SER:HA	0.818
4	A:55:HIS:CE1	A:193:VAL:HG22	0.749
4	A:55:HIS:CE1	A:55:HIS:NE2	0.739
4	A:55:HIS:CE1	A:122:SER:HA	0.738
4	A:55:HIS:CE1	A:122:SER:HB3	0.722
4	A:55:HIS:CE1	A:122:SER:CA	0.715
4	A:55:HIS:CE1	A:122:SER:CB	0.656
4	A:55:HIS:NE2	A:191:SER:O	0.638
4	A:55:HIS:HE1	A:122:SER:CA	0.581
4	A:55:HIS:CE1	A:193:VAL:CG2	0.517
4	A:243:VAL:CG2	A:540:ILE:H	0.494

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:69:LEU:HD21	A:230:LEU:HD22	0.450
4	A:33:VAL:CG1	A:38:LYS:HE3	0.420
4	A:371:LYS:HE3	A:411:ASN:O	0.416
4	A:299:TYR:CD1	A:441:GLY:HA3	0.410
4	A:55:HIS:CE1	A:122:SER:O	0.403
4	A:527:LYS:HE2	A:532:ASN:O	0.401
5	A:276:ILE:HG21	A:333:LYS:C	0.778
5	A:462:MET:HA	A:462:MET:HE2	0.698
5	A:135:TYR:CD1	A:462:MET:HE1	0.608
5	A:163:LYS:HE3	A:165:ILE:HD11	0.549
5	A:135:TYR:HD1	A:462:MET:HE1	0.518
5	A:135:TYR:O	A:462:MET:HE3	0.504
5	A:299:TYR:CD2	A:511:TYR:CE1	0.496
5	A:69:LEU:HD21	A:230:LEU:HD22	0.491
5	A:328:ILE:O	A:332:VAL:HG22	0.490
5	A:103:ARG:NH1	A:237:TRP:CE2	0.481
5	A:371:LYS:HE3	A:411:ASN:O	0.475
5	A:64:ASN:ND2	A:271:ASN:HD21	0.471
5	A:350:GLY:O	A:489:THR:HG23	0.468
5	A:527:LYS:HE2	A:532:ASN:OD1	0.461
5	A:276:ILE:HG21	A:333:LYS:O	0.454
5	A:276:ILE:CG1	A:334:ALA:HA	0.452
5	A:33:VAL:HG13	A:541:VAL:HG13	0.443

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:462:MET:CA	A:462:MET:HE2	0.438
5	A:48:GLU:CD	A:225:ASN:H	0.437
5	A:276:ILE:HG23	A:277:GLU:N	0.432
5	A:276:ILE:CB	A:334:ALA:HA	0.405
6	A:295:TYR:CE1	A:512:VAL:HG13	0.512
6	A:299:TYR:CE1	A:439:ARG:NH2	0.512
6	A:69:LEU:HD21	A:230:LEU:HD22	0.495
6	A:333:LYS:HE2	A:396:LEU:HD11	0.489
6	A:520:TRP:HB3	A:543:HIS:CD2	0.482
6	A:371:LYS:HE3	A:411:ASN:O	0.480
6	A:333:LYS:HE2	A:396:LEU:HD21	0.472
6	A:393:THR:HG21	A:422:GLU:OE1	0.463
6	A:140:GLN:HE21	A:187:HIS:CG	0.461
6	A:520:TRP:HA	A:541:VAL:HG22	0.453
6	A:279:PHE:CE1	A:335:GLN:HA	0.429
6	A:274:MET:SD	A:282:LEU:HD12	0.414
6	A:48:GLU:CD	A:225:ASN:H	0.404
6	A:445:ASP:O	A:530:LEU:HD11	0.401
7	A:462:MET:HA	A:462:MET:HE2	0.660
7	A:522:GLY:HA2	A:534:TYR:CE1	0.649
7	A:123:TRP:CD1	A:141:TYR:HH	0.638
7	A:141:TYR:HB2	A:147:ILE:HD12	0.627
7	A:276:ILE:HD13	A:334:ALA:O	0.626

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:123:TRP:CG	A:141:TYR:HH	0.570
7	A:517:VAL:HG21	A:534:TYR:CD2	0.566
7	A:294:PRO:CG	A:531:ASP:HA	0.515
7	A:517:VAL:HG21	A:534:TYR:HD2	0.508
7	A:444:ALA:HB2	A:452:PHE:HE2	0.503
7	A:141:TYR:CD1	A:144:ILE:HD12	0.499
7	A:134:PRO:HB3	A:462:MET:HE3	0.482
7	A:243:VAL:HG21	A:524:TYR:CD1	0.471
7	A:522:GLY:CA	A:534:TYR:CE1	0.463
7	A:371:LYS:HE3	A:411:ASN:O	0.461
7	A:134:PRO:CB	A:462:MET:HE3	0.445
7	A:44:ASN:ND2	A:46:GLY:H	0.442
7	A:67:ARG:CZ	A:188:PRO:HD3	0.434
7	A:297:CYS:HB3	A:511:TYR:CZ	0.424
7	A:269:MET:HG3	A:517:VAL:HG22	0.412
7	A:56:LYS:HA	A:133:SER:HB2	0.407
7	A:294:PRO:HG3	A:531:ASP:HA	0.407
7	A:78:LEU:O	A:528:ASP:HA	0.402
8	A:456:MET:HE1	A:499:LEU:HD22	0.870
8	A:456:MET:HE1	A:499:LEU:CD2	0.583
8	A:323:MET:SD	A:328:ILE:HD11	0.567
8	A:427:LEU:HD22	A:461:SER:HB2	0.559
8	A:299:TYR:CD1	A:439:ARG:NH2	0.558

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:456:MET:CE	A:499:LEU:HD22	0.541
8	A:358:TRP:CH2	A:359:PHE:CE1	0.540
8	A:49:VAL:HG21	A:65:ILE:HD12	0.536
8	A:64:ASN:ND2	A:271:ASN:HD21	0.527
8	A:509:TYR:CE2	A:511:TYR:CE2	0.502
8	A:344:THR:HG23	A:493:THR:HG23	0.499
8	A:341:TYR:CE1	A:359:PHE:CE1	0.487
8	A:48:GLU:CD	A:225:ASN:H	0.461
8	A:371:LYS:HE3	A:411:ASN:O	0.459
8	A:325:ARG:HH12	A:358:TRP:HZ3	0.444
8	A:299:TYR:CE1	A:439:ARG:NH2	0.442
8	A:456:MET:HE1	A:499:LEU:HD13	0.442
8	A:449:PRO:HA	A:492:TYR:CE2	0.438
8	A:439:ARG:C	A:439:ARG:HD3	0.437
8	A:274:MET:HE1	A:516:LEU:HG	0.435
8	A:163:LYS:HE2	A:165:ILE:HD11	0.432
8	A:449:PRO:HG2	A:488:ARG:HE	0.428
8	A:300:TYR:HB2	A:505:ILE:HG23	0.427
8	A:442:TRP:HA	A:462:MET:CE	0.425
8	A:323:MET:HE2	A:408:TRP:CZ2	0.416
8	A:339:PRO:HG2	A:341:TYR:CD2	0.409
8	A:449:PRO:CG	A:488:ARG:HE	0.406
8	A:41:LEU:CD2	A:43:ARG:HE	0.403

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:299:TYR:CD1	A:441:GLY:HA3	0.402
9	A:36:ALA:HB3	A:540:ILE:HG22	0.908
9	A:75:VAL:HG21	A:536:ARG:HH12	0.667
9	A:247:VAL:HG21	A:535:THR:HG21	0.666
9	A:80:GLY:HA2	A:530:LEU:HD12	0.664
9	A:252:ILE:CD1	A:267:ILE:HD11	0.614
9	A:80:GLY:HA2	A:530:LEU:CD1	0.605
9	A:36:ALA:HB3	A:540:ILE:CG2	0.539
9	A:517:VAL:HG21	A:524:TYR:CE1	0.536
9	A:67:ARG:HD2	A:534:TYR:CE1	0.516
9	A:125:ARG:HH11	A:193:VAL:HG21	0.495
9	A:371:LYS:HE3	A:411:ASN:O	0.492
9	A:243:VAL:CG2	A:539:TYR:HA	0.476
9	A:38:LYS:HE2	A:40:THR:O	0.473
9	A:517:VAL:HG21	A:524:TYR:CD1	0.473
9	A:341:TYR:HB3	A:359:PHE:CD2	0.472
9	A:297:CYS:HB3	A:511:TYR:CZ	0.456
9	A:243:VAL:HG21	A:539:TYR:CB	0.455
9	A:133:SER:HB3	A:136:ALA:HB2	0.444
9	A:247:VAL:CG2	A:535:THR:HG21	0.443
9	A:276:ILE:CD1	A:334:ALA:HB3	0.442
9	A:509:TYR:CE2	A:511:TYR:HB3	0.441
9	A:140:GLN:HE22	A:187:HIS:CG	0.438

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:67:ARG:CD	A:534:TYR:CE1	0.431
9	A:69:LEU:HD21	A:230:LEU:HD22	0.427
9	A:341:TYR:HB3	A:359:PHE:CE2	0.419
9	A:297:CYS:CB	A:511:TYR:CZ	0.407
9	A:294:PRO:CG	A:529:PRO:HA	0.401
9	A:88:GLU:CG	A:103:ARG:HB3	0.400
10	A:295:TYR:CZ	A:338:MET:HE2	0.550
10	A:75:VAL:HB	A:536:ARG:HH22	0.524
10	A:296:LEU:HD11	A:444:ALA:O	0.509
10	A:69:LEU:HD21	A:230:LEU:HD22	0.496
10	A:371:LYS:HE3	A:411:ASN:O	0.495
10	A:35:LEU:HD21	A:520:TRP:HB2	0.480
10	A:75:VAL:CB	A:536:ARG:HH22	0.472
10	A:462:MET:HA	A:462:MET:HE2	0.470
10	A:353:LEU:HD13	A:496:GLU:OE1	0.440
10	A:344:THR:HB	A:353:LEU:HD13	0.437
10	A:347:TYR:CE2	A:529:PRO:HD2	0.424
10	A:295:TYR:CE2	A:338:MET:HE2	0.413
10	A:243:VAL:HG21	A:539:TYR:HB3	0.405
10	A:446:TYR:CZ	A:451:SER:HB3	0.402
10	A:488:ARG:HG2	A:492:TYR:CZ	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	541	502	33	6
2	541	511	25	5
3	541	501	30	10
4	541	500	28	13
5	541	515	19	7
6	541	509	24	8
7	541	515	16	10
8	541	500	27	14
9	541	485	39	17
10	541	523	15	3

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	468	457	5	6
2	468	452	11	5
3	468	451	9	8
4	468	447	12	9
5	468	457	7	4
6	468	451	8	9
7	468	448	10	10
8	468	455	6	7
9	468	454	5	9
10	468	453	9	6

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	2	THR
1	A	5	THR
1	A	15	LEU
1	A	448	GLU
1	A	532	ASN
1	A	535	THR
2	A	2	THR
2	A	15	LEU
2	A	18	LEU
2	A	535	THR
2	A	543	HIS
3	A	2	THR
3	A	15	LEU
3	A	35	LEU
3	A	122	SER
3	A	276	ILE
3	A	349	ASP
3	A	446	TYR
3	A	505	ILE
4	A	4	ILE
4	A	5	THR
4	A	15	LEU
4	A	33	VAL

Model ID	Chain	Residue ID	Residue type
4	A	35	LEU
4	A	276	ILE
4	A	295	TYR
4	A	354	THR
4	A	505	ILE
5	A	2	THR
5	A	5	THR
5	A	8	SER
5	A	15	LEU
6	A	2	THR
6	A	5	THR
6	A	15	LEU
6	A	19	MET
6	A	23	VAL
6	A	76	SER
6	A	347	TYR
6	A	439	ARG
6	A	535	THR
7	A	15	LEU
7	A	18	LEU
7	A	19	MET
7	A	35	LEU
7	A	44	ASN

Model ID	Chain	Residue ID	Residue type
7	A	137	SER
7	A	276	ILE
7	A	293	ASP
7	A	394	SER
7	A	531	ASP
8	A	2	THR
8	A	5	THR
8	A	15	LEU
8	A	243	VAL
8	A	344	THR
8	A	449	PRO
8	A	533	THR
9	A	2	THR
9	A	15	LEU
9	A	19	MET
9	A	23	VAL
9	A	273	SER
9	A	335	GLN
9	A	394	SER
9	A	448	GLU
9	A	531	ASP
10	A	2	THR
10	A	5	THR

Model ID	Chain	Residue ID	Residue type
10	A	15	LEU
10	A	35	LEU
10	A	354	THR
10	A	462	MET

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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