Integrative Structure Validation Report ?

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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	9A2Z
PDB-Dev ID	PDBDEV_00000184
Structure Title	Model of E. coli FepA by in-cell photo-crosslinking MS and deep learning
Structure Authors	Stahl, K.; Graziadei, A.; Dau, T.; Brock, O.; Rappsilber, J.

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
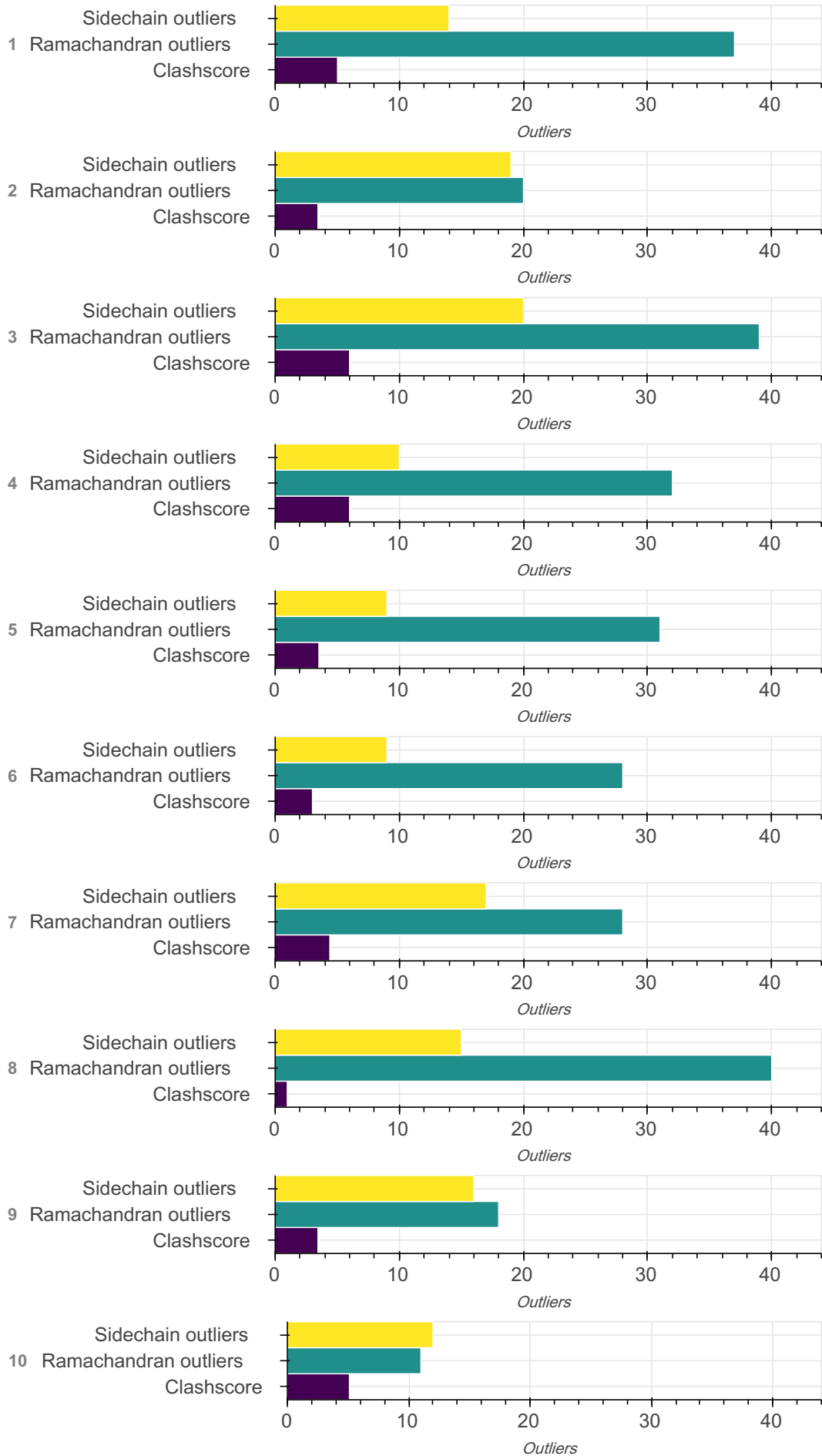
Ensemble information ?

This entry consists of 0 distinct ensemble(s).

Summary ?

This entry consists of 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	P05825	A	A	746
2	1	1	P05825	A	A	746
3	1	1	P05825	A	A	746
4	1	1	P05825	A	A	746
5	1	1	P05825	A	A	746
6	1	1	P05825	A	A	746
7	1	1	P05825	A	A	746
8	1	1	P05825	A	A	746
9	1	1	P05825	A	A	746
10	1	1	P05825	A	A	746

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	-	1-746

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.

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Standard geometry: bond outliers?

There are 55566 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	5230
CG--HG3	1.09	0.97	1820
CB--HB	1.09	0.97	1460
CA--HA2	1.09	0.97	770
CG2--HG21	1.09	0.97	1460
CB--HB2	1.09	0.97	5230
CD2--HD23	1.09	0.97	540
CG1--HG11	1.09	0.97	430
CA--HA	1.09	0.97	6690
CD1--HD12	1.09	0.97	910
CG--HG2	1.09	0.97	1820
CG1--HG13	1.09	0.97	800
OG1--HG1	0.96	0.84	660
CD1--HD11	1.09	0.97	910
CG2--HG22	1.09	0.97	1460
CE--HE3	1.09	0.97	450
CD1--HD13	1.09	0.97	910
NZ--HZ1	1.01	0.89	330
CD2--HD22	1.09	0.97	540
CA--HA3	1.09	0.97	770
CG--HG	1.09	0.97	540
CD--HD3	1.09	0.97	990

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CE--HE2	1.09	0.97	450
CD2--HD21	1.09	0.97	540
CG2--HG23	1.09	0.97	1460
NZ--HZ2	1.01	0.89	330
CB--HB1	1.09	0.97	540
CD--HD2	1.09	0.97	990
CG1--HG12	1.09	0.97	800
OG--HG	0.96	0.84	490
NZ--HZ3	1.01	0.89	330
OH--HH	0.96	0.84	320
N--H2	1.01	0.89	10
N--H3	1.01	0.89	10
CE--HE1	1.09	0.97	120
N--H1	1.01	0.89	10
SG--HG	1.33	1.20	1
SG--HG	1.34	1.20	5
NE2--HE22	1.01	0.86	320
CH2--HH2	1.08	0.93	200
N--H	1.01	0.86	7160
CE1--HE1	1.08	0.93	589
NH2--HH22	1.01	0.86	370
ND2--HD22	1.01	0.86	580
NH2--HH21	1.01	0.86	370

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD2--HD2	1.08	0.93	590
NE2--HE21	1.01	0.86	320
CE3--HE3	1.08	0.93	200
NH1--HH11	1.01	0.86	370
CD1--HD1	1.08	0.93	690
CZ--HZ	1.08	0.93	170
CZ2--HZ2	1.08	0.93	200
CE2--HE2	1.08	0.93	490
NE1--HE1	1.01	0.86	200
ND2--HD21	1.01	0.86	580
CZ3--HZ3	1.08	0.93	200
NH1--HH12	1.01	0.86	370
ND1--HD1	1.01	0.86	92
NE--HE	1.01	0.86	370
NE2--HE2	1.01	0.86	7
ND1--HD1	1.34	0.86	1
CE1--HE1	2.16	0.93	1

Standard geometry: angle outliers ⍰

There are 585 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	84.15	1
CD2-NE2-CE1	109.00	87.45	1
CG-CD2-NE2	107.20	128.70	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-ND1-CE1	109.30	130.81	1
CA-CB-OG1	109.60	125.36	1
C-CA-CB	110.10	127.95	1
C-N-CA	121.70	137.82	1
C-N-CA	121.70	137.67	1
N-CA-CB	110.50	125.45	1
C-N-CA	121.70	137.06	1
C-N-CA	121.70	137.01	1
CA-CB-CG1	110.40	124.13	1
CA-CB-CG	114.10	130.09	1
OE1-CD-NE2	122.60	114.93	1
OD1-CG-ND2	122.60	115.02	1
C-N-CA	121.70	135.29	1
NE-CZ-NH1	121.50	128.86	1
C-N-CA	121.70	134.82	1
C-N-CA	121.70	134.81	1
CB-CG1-CD1	113.80	128.95	1
C-N-CA	121.70	134.54	1
N-CA-CB	110.40	99.71	1
C-N-CA	121.70	134.45	1
N-CA-CB	110.40	99.79	1
C-N-CA	121.70	134.22	1
CA-CB-CG	113.80	120.74	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	115.70	1
C-CA-CB	110.10	122.84	1
C-CA-CB	110.50	120.51	1
OE1-CD-NE2	122.60	115.93	1
C-N-CA	121.70	133.67	1
CA-CB-CG	112.60	119.13	1
CA-N-CD	112.00	102.95	1
C-CA-CB	109.10	123.15	1
C-CA-CB	110.50	101.09	1
OE1-CD-NE2	122.60	116.36	1
OE1-CD-NE2	122.60	116.39	2
C-N-CA	121.70	132.88	1
OE1-CD-NE2	122.60	116.41	1
C-N-CA	121.70	132.80	1
OE1-CD-NE2	122.60	116.46	1
CA-CB-CG	112.60	118.67	1
CA-C-N	116.90	125.94	1
N-CA-C	111.00	94.27	1
C-N-CA	121.70	132.42	1
C-N-CA	121.70	132.38	1
C-N-CA	121.70	132.30	1
NE-CZ-NH1	121.50	127.37	1
CA-CB-CG	112.60	118.47	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	132.23	1
C-N-CA	121.70	132.20	1
C-N-CA	121.70	132.07	1
OE1-CD-NE2	122.60	116.85	1
CA-CB-CG	112.60	118.35	1
OE1-CD-NE2	122.60	116.86	1
CA-CB-CG	112.60	118.32	1
C-N-CA	121.70	131.95	1
C-N-CA	121.70	131.94	1
C-N-CA	121.70	131.91	1
NE-CZ-NH2	119.20	114.10	1
C-N-CA	121.70	131.88	1
OD1-CG-ND2	122.60	116.95	1
C-N-CA	121.70	131.84	1
OE1-CD-NE2	122.60	116.97	2
OE1-CD-NE2	122.60	116.99	1
C-N-CA	121.70	131.79	1
OE1-CD-NE2	122.60	117.01	1
OE1-CD-NE2	122.60	117.03	1
CB-CG-CD2	131.20	123.97	1
NE-CZ-NH2	119.20	124.20	1
C-N-CA	121.70	131.65	1
C-N-CA	121.70	131.58	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	117.14	1
N-CA-CB	110.50	119.75	1
C-N-CA	121.70	131.44	1
CA-CB-CG	112.60	118.00	1
C-N-CA	121.70	131.40	1
OE1-CD-NE2	122.60	117.22	1
C-N-CA	121.70	131.38	1
C-N-CA	121.70	131.36	1
OE1-CD-NE2	122.60	117.23	1
CA-CB-CG	112.60	117.96	1
OE1-CD-NE2	122.60	117.25	1
CA-CB-CG	112.60	117.94	1
C-N-CA	121.70	131.29	1
N-CA-C	111.00	125.92	1
C-N-CA	121.70	131.27	1
C-N-CA	121.70	131.23	1
C-N-CA	121.70	131.18	1
OE1-CD-NE2	122.60	117.33	1
C-N-CA	121.70	131.16	1
C-N-CA	121.70	131.15	1
OD1-CG-ND2	122.60	117.37	1
C-N-CA	121.70	131.09	1
CG1-CB-CG2	110.70	126.34	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	131.07	1
OE1-CD-NE2	122.60	117.40	1
CA-CB-CG	114.10	124.48	1
C-N-CA	121.70	131.04	1
OE1-CD-NE2	122.60	117.42	1
CD1-CG-CD2	110.80	99.49	1
C-N-CA	121.70	130.94	1
CD-NE-CZ	124.40	131.59	1
OE1-CD-NE2	122.60	117.47	1
N-CA-CB	111.50	102.78	1
OE1-CD-NE2	122.60	117.48	1
CA-C-N	116.20	126.44	1
C-N-CA	121.70	130.90	1
CB-CG-CD2	131.20	124.56	1
C-N-CA	121.70	130.89	1
CB-CG-CD	112.60	103.93	1
C-N-CA	121.70	130.87	1
CA-CB-CG	112.60	117.69	1
OE1-CD-NE2	122.60	117.53	1
OE1-CD-NE2	122.60	117.54	1
C-N-CA	121.70	130.79	1
OE1-CD-NE2	122.60	117.55	1
OE1-CD-NE2	122.60	117.57	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	130.76	2
C-N-CA	121.70	130.74	1
CD-NE-CZ	124.40	131.41	1
C-N-CA	121.70	130.70	2
OE1-CD-NE2	122.60	117.61	2
CB-CG-CD2	131.20	124.71	1
CA-CB-CG1	110.40	118.89	1
CA-CB-CG	112.60	117.57	1
C-N-CA	121.70	130.64	3
OE1-CD-NE2	122.60	117.63	1
CA-CB-CG	112.60	117.56	1
OE1-CD-NE2	122.60	117.65	1
CA-CB-CG	112.60	117.55	1
C-N-CA	121.70	130.60	1
OD1-CG-ND2	122.60	117.66	1
OE1-CD-NE2	122.60	117.66	1
C-N-CA	121.70	130.59	1
CA-C-N	116.20	126.07	1
C-N-CA	121.70	130.58	1
OE1-CD-NE2	122.60	117.67	1
C-N-CA	121.70	130.57	1
C-N-CA	121.70	130.56	2
N-CA-CB	110.50	102.14	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	115.15	1
CA-CB-CG2	110.40	118.74	1
NE-CZ-NH2	119.20	123.61	1
OE1-CD-NE2	122.60	117.71	2
NE1-CE2-CZ2	130.10	137.44	1
OD1-CG-ND2	122.60	117.72	1
OE1-CD-NE2	122.60	117.72	2
C-N-CA	121.70	130.47	1
C-N-CA	121.70	130.46	2
CA-CB-CG	112.60	117.47	1
CA-CB-CG	112.60	117.46	1
N-CA-C	111.00	124.60	1
OE1-CD-NE2	122.60	117.75	2
CB-CG-CD2	131.20	124.90	1
C-N-CA	121.70	130.42	1
CB-CG-CD2	131.20	124.91	1
C-CA-CB	110.10	119.29	1
OE1-CD-NE2	122.60	117.76	1
O-C-N	123.00	115.27	1
CB-CG-CD2	131.20	124.92	1
C-N-CA	121.70	130.39	1
OE1-CD-NE2	122.60	117.77	1
O-C-N	123.00	115.28	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	117.42	1
OE1-CD-NE2	122.60	117.78	1
OD1-CG-ND2	122.60	117.79	1
N-CA-C	111.00	124.45	1
CA-CB-CG	112.60	117.40	1
OE1-CD-NE2	122.60	117.80	1
CA-C-N	116.20	125.79	1
OE1-CD-NE2	122.60	117.81	1
C-N-CA	121.70	130.32	1
OE1-CD-NE2	122.60	117.82	1
OD1-CG-ND2	122.60	117.82	1
OD1-CG-ND2	122.60	117.83	1
OE1-CD-NE2	122.60	117.83	1
C-N-CA	121.70	130.29	1
CA-CB-CG1	110.40	118.50	1
C-N-CA	121.70	130.27	1
NE-CZ-NH2	119.20	123.48	1
OE1-CD-NE2	122.60	117.84	1
C-N-CA	121.70	130.26	1
CD2-CE2-NE1	107.40	101.24	1
OE1-CD-NE2	122.60	117.86	1
N-CA-CB	103.00	108.21	1
C-N-CA	121.70	130.21	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.88	1
CA-CB-CG	112.60	117.32	1
CB-CG-CD2	131.20	125.07	1
CA-CB-OG1	109.60	102.52	1
OE1-CD-NE2	122.60	117.89	2
CD-NE-CZ	124.40	130.99	1
C-N-CA	121.70	130.17	1
NE-CZ-NH1	121.50	126.20	1
OE1-CD-NE2	122.60	117.90	1
OE1-CD-NE2	122.60	117.91	1
CB-CG-CD2	131.20	125.11	2
C-N-CA	121.70	130.13	1
OE1-CD-NE2	122.60	117.92	1
OG1-CB-CG2	109.30	99.96	1
OE1-CD-NE2	122.60	117.93	1
C-CA-CB	110.50	117.50	1
C-N-CA	121.70	130.09	2
N-CA-CB	103.00	108.13	1
OE1-CD-NE2	122.60	117.94	1
CB-CG-CD2	131.20	125.14	1
OG1-CB-CG2	109.30	99.98	1
N-CA-C	111.00	124.04	1
OE1-CD-NE2	122.60	117.95	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-N-CD	112.00	105.49	1
O-C-N	123.00	115.56	1
C-N-CA	121.70	130.07	1
OE1-CD-NE2	122.60	117.96	1
OD1-CG-ND2	122.60	117.96	1
N-CA-CB	110.50	102.62	1
CB-CG-CD2	131.20	125.17	1
C-N-CA	121.70	130.03	1
CD-NE-CZ	124.40	130.88	1
OE1-CD-NE2	122.60	117.98	2
C-N-CA	121.70	130.01	1
N-CA-CB	103.00	108.07	1
OD1-CG-ND2	122.60	117.99	2
OE1-CD-NE2	122.60	117.99	1
OE1-CD-NE2	122.60	118.00	3
N-CA-C	111.00	123.89	1
C-CA-CB	110.10	118.84	1
C-N-CA	121.70	129.97	1
OE1-CD-NE2	122.60	118.01	3
CA-CB-CG	112.60	117.19	1
C-N-CA	121.70	129.95	1
CA-C-N	116.20	125.34	1
OE1-CD-NE2	122.60	118.03	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.92	1
OD1-CG-ND2	122.60	118.04	1
OE1-CD-NE2	122.60	118.05	3
OD1-CG-ND2	122.60	118.05	1
CD-NE-CZ	124.40	130.74	1
OE1-CD-NE2	122.60	118.07	1
C-CA-CB	110.10	118.70	1
CA-C-N	116.20	125.24	1
O-C-N	123.00	115.77	1
OE1-CD-NE2	122.60	118.09	7
OD1-CG-ND2	122.60	118.09	1
OE1-CD-NE2	122.60	118.10	2
OD1-CG-ND2	122.60	118.10	2
C-N-CA	121.70	129.80	2
CB-CG-CD2	131.20	125.35	1
C-N-CA	121.70	129.79	1
OE1-CD-NE2	122.60	118.11	1
OE1-CD-NE2	122.60	118.12	2
C-N-CA	121.70	129.76	1
C-CA-CB	110.10	118.61	1
OE1-CD-NE2	122.60	118.13	3
N-CA-C	111.00	123.52	1
C-CA-CB	110.10	118.59	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.13	1
C-N-CA	121.70	129.74	1
OE1-CD-NE2	122.60	118.14	2
C-N-CA	121.70	129.73	1
OD1-CG-ND2	122.60	118.15	1
OE1-CD-NE2	122.60	118.16	4
CA-CB-CG	112.60	117.03	1
OD1-CG-ND2	122.60	118.17	1
OE1-CD-NE2	122.60	118.17	2
CA-C-N	116.90	123.55	1
CB-CG-CD	112.60	120.13	1
OE1-CD-NE2	122.60	118.18	2
C-N-CA	121.70	129.66	1
CA-CB-CG	112.60	117.02	1
N-CA-CB	103.00	107.85	1
C-CA-CB	110.10	118.48	1
OE1-CD-NE2	122.60	118.19	1
N-CA-C	111.00	123.34	1
OD1-CG-ND2	122.60	118.19	1
OE1-CD-NE2	122.60	118.20	1
CA-CB-CG	112.60	117.00	1
NE-CZ-NH1	121.50	125.90	2
C-CA-CB	110.50	117.10	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.61	1
OE1-CD-NE2	122.60	118.21	1
CA-CB-CG	112.60	116.98	1
OD1-CG-ND2	122.60	118.22	1
N-CA-C	111.00	123.25	1
OE1-CD-NE2	122.60	118.23	6
CB-CG-CD2	131.20	125.52	1
OD1-CG-ND2	122.60	118.23	1
OE1-CD-NE2	122.60	118.24	1
C-N-CA	121.70	129.55	1
OD1-CG-ND2	122.60	118.24	1
CA-C-N	116.20	124.91	1
N-CA-C	111.00	123.19	1
OE1-CD-NE2	122.60	118.25	1
OE1-CD-NE2	122.60	118.26	3
OD1-CG-ND2	122.60	118.26	1
NE-CZ-NH2	119.20	123.10	1
CB-CG-CD2	131.20	125.56	1
C-N-CA	121.70	129.50	3
CB-CG-CD2	131.20	125.57	1
C-N-CA	121.70	129.49	1
OD1-CG-ND2	122.60	118.27	1
NH1-CZ-NH2	119.30	113.68	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.47	1
N-CA-CB	103.00	107.75	1
O-C-N	123.00	116.10	1
CB-CG-CD2	131.20	125.59	1
N-CA-CB	110.40	116.86	1
OE1-CD-NE2	122.60	118.29	1
OD1-CG-ND2	122.60	118.30	1
OE1-CD-NE2	122.60	118.30	2
CD-NE-CZ	124.40	130.41	1
CA-CB-CG2	110.50	117.80	1
CA-CB-CG	112.60	116.89	1
CA-C-N	116.20	124.78	1
OE1-CD-NE2	122.60	118.31	3
N-CA-CB	103.00	107.72	1
OD1-CG-ND2	122.60	118.31	1
OE1-CD-NE2	122.60	118.32	4
C-N-CA	121.70	129.41	1
CA-CB-CG	112.60	116.88	1
OE1-CD-NE2	122.60	118.33	2
OD1-CG-ND2	122.60	118.33	1
OE1-CD-NE2	122.60	118.34	2
CA-CB-OG1	109.60	115.99	1
C-N-CA	121.70	129.36	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.34	1
OD1-CG-ND2	122.60	118.36	3
CA-CB-CG	112.60	116.84	1
OE1-CD-NE2	122.60	118.36	1
C-N-CA	121.70	129.32	2
OE1-CD-NE2	122.60	118.37	1
CA-CB-CG	112.60	116.83	1
OD1-CG-ND2	122.60	118.37	1
C-N-CA	121.70	129.30	1
CD-NE-CZ	124.40	130.30	1
O-C-N	123.00	116.26	1
OD1-CG-ND2	122.60	118.39	2
N-CA-CB	110.40	104.09	1
C-N-CA	121.70	129.27	3
OE1-CD-NE2	122.60	118.39	1
CB-CG-CD2	131.20	125.74	1
OE1-CD-NE2	122.60	118.40	3
C-N-CA	121.70	129.26	3
CB-CG-CD2	131.20	125.75	1
CA-CB-CG	112.60	116.79	2
OD1-CG-ND2	122.60	118.41	1
CB-CG-CD2	131.20	125.76	1
OE1-CD-NE2	122.60	118.41	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	103.39	1
OD1-CG-ND2	122.60	118.42	2
OE1-CD-NE2	122.60	118.42	3
C-N-CA	121.70	129.21	2
OE1-CD-NE2	122.60	118.43	3
C-N-CA	121.70	129.20	1
OE1-CD-NE2	122.60	118.44	2
OD1-CG-ND2	122.60	118.44	2
N-CA-C	111.00	122.63	1
OE1-CD-NE2	122.60	118.45	4
NE-CZ-NH2	119.20	122.94	1
CA-CB-CG	112.60	108.45	1
CA-CB-CG	112.60	116.75	1
OE1-CD-NE2	122.60	118.46	1
CA-CB-CG1	110.40	103.36	1
C-N-CA	121.70	129.15	1
OD1-CG-ND2	122.60	118.46	1
CB-CG-CD2	131.20	125.82	1
OE1-CD-NE2	122.60	118.47	2
CA-CB-CG	113.80	117.93	1
NE-CZ-NH2	119.20	122.92	1
CD-NE-CZ	124.40	130.18	1
OD1-CG-ND2	122.60	118.47	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	108.47	1
OE1-CD-NE2	122.60	118.48	2
OD1-CG-ND2	122.60	118.48	2
C-N-CA	121.70	129.10	1
OE1-CD-NE2	122.60	118.49	4
N-CA-CB	110.50	103.51	1
CA-CB-CG	114.10	105.89	1
OD1-CG-ND2	122.60	118.50	2
CA-CB-CG	112.60	116.70	1
NE-CZ-NH2	119.20	122.89	1
CB-CG-CD2	131.20	125.87	1
OE1-CD-NE2	122.60	118.50	1
C-N-CA	121.70	129.07	1
OE1-CD-NE2	122.60	118.51	3
NE-CZ-NH2	119.20	122.88	1
CA-CB-CG	114.10	105.92	1
C-N-CA	121.70	129.06	1
CB-CG-CD2	131.20	125.89	2
OD1-CG-ND2	122.60	118.51	2
C-N-CA	121.70	129.05	1
CA-CB-CG	112.60	116.68	1
OE1-CD-NE2	122.60	118.52	3
OD1-CG-ND2	122.60	118.52	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	117.88	1
OD1-CG-ND2	122.60	118.53	4
OE1-CD-NE2	122.60	118.53	2
NH1-CZ-NH2	119.30	114.00	1
NE-CZ-NH2	119.20	122.87	1
CA-CB-CG	112.60	116.67	1
C-N-CA	121.70	129.02	1
C-N-CA	121.70	129.01	1
CB-CG-CD2	131.20	125.92	1
NH1-CZ-NH2	119.30	114.02	1
OD1-CG-ND2	122.60	118.54	1
OE1-CD-NE2	122.60	118.54	1
C-N-CA	121.70	129.00	1
OE1-CD-NE2	122.60	118.55	1
CB-CG-CD2	131.20	125.93	1
C-N-CA	121.70	128.99	3
OE1-CD-NE2	122.60	118.56	2
OD1-CG-ND2	122.60	118.56	1
N-CA-C	111.00	122.31	1
C-N-CA	121.70	128.97	1
CB-CG-CD2	131.20	125.95	2
OE1-CD-NE2	122.60	118.57	3
OD1-CG-ND2	122.60	118.57	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	125.96	1
C-N-CA	121.70	128.96	1
NH1-CZ-NH2	119.30	114.06	1
CA-CB-CG	112.60	116.63	1
O-C-N	123.00	116.56	1
OE1-CD-NE2	122.60	118.58	2
N-CA-C	111.00	122.26	1
C-N-CA	121.70	128.93	1
C-N-CA	121.70	128.92	2
OE1-CD-NE2	122.60	118.59	2
N-CA-C	111.00	122.23	1
CA-CB-CG	112.60	116.61	1
OD1-CG-ND2	122.60	118.59	1
CB-CG-CD2	131.20	126.00	1
OE1-CD-NE2	122.60	118.60	1
OD1-CG-ND2	122.60	118.60	1
C-N-H	112.14	124.30	1
C-N-H	111.87	124.30	1
HZ1-NZ-HZ3	96.46	109.00	1
C-N-H	111.70	124.30	1
C-N-H	111.68	124.30	1
CB-CA-HA	96.23	109.00	1
C-CA-HA	96.20	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-H	111.45	124.30	1
C-N-H	111.41	124.30	1
HH11-NH1-HH12	107.02	120.00	1
HZ1-NZ-HZ3	95.96	109.00	1
CZ-NH2-HH22	106.94	120.00	1
C-N-H	111.23	124.30	1
C-N-H	111.15	124.30	1
C-N-H	111.11	124.30	1
C-N-H	110.96	124.30	1
C-N-H	110.85	124.30	1
C-N-H	110.61	124.30	1
C-N-H	110.51	124.30	1
HH11-NH1-HH12	106.09	120.00	1
C-N-H	110.34	124.30	1
HH11-NH1-HH12	105.50	120.00	1
N-CA-HA	95.19	110.00	1
HH11-NH1-HH12	105.04	120.00	1
CG-CB-HB3	92.96	108.00	1
C-N-H	108.73	124.30	1
HH11-NH1-HH12	104.40	120.00	1
HH11-NH1-HH12	104.16	120.00	1
HH11-NH1-HH12	103.35	120.00	1
C-CA-HA	92.30	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OG1-CB-HB	92.29	109.00	1
C-N-H	107.43	124.30	1
C-N-H	107.42	124.30	1
HB2-CB-HB3	93.06	110.00	1
HH21-NH2-HH22	102.25	120.00	1
CG-ND1-HD1	106.48	125.35	1
HH21-NH2-HH22	99.52	120.00	1
NE2-CD2-HD2	104.94	126.40	1
ND1-CE1-HE1	61.41	125.80	1
CE1-ND1-HD1	24.44	125.35	1
NE2-CE1-HE1	22.89	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	5.02	57
2	3.44	39
3	5.99	68
4	5.99	68
5	3.52	40
6	3.00	34
7	4.40	50
8	0.97	11

Model ID	Clash score	Number of clashes
9	3.44	39
10	5.11	58

All 464 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:192:GLY:HA2	A:222:ALA:HB2	0.777
1	A:88:ARG:CZ	A:222:ALA:HB3	0.688
1	A:676:TYR:CD2	A:705:LEU:HD11	0.687
1	A:71:ILE:HG22	A:77:VAL:HG11	0.629
1	A:88:ARG:NE	A:222:ALA:HB3	0.620
1	A:623:ILE:HD12	A:728:ALA:HA	0.610
1	A:635:TRP:CE2	A:643:MET:HB2	0.593
1	A:517:TYR:CD2	A:574:LEU:CD1	0.557
1	A:269:LEU:HD11	A:313:LEU:HD11	0.548
1	A:192:GLY:CA	A:222:ALA:HB2	0.532
1	A:635:TRP:HE1	A:637:ALA:HB2	0.505
1	A:627:TYR:CE2	A:651:GLY:CA	0.502
1	A:189:LYS:O	A:222:ALA:HB1	0.497
1	A:37:VAL:HG11	A:147:LEU:HD21	0.493
1	A:635:TRP:CZ2	A:643:MET:SD	0.489
1	A:676:TYR:CG	A:705:LEU:HD21	0.489
1	A:343:LEU:CD1	A:501:ILE:HB	0.484
1	A:35:THR:HG21	A:50:VAL:HG12	0.481
1	A:517:TYR:CD2	A:574:LEU:HD12	0.481

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:134:SER:HB2	A:196:ARG:HH22	0.480
1	A:400:SER:O	A:403:THR:HG23	0.478
1	A:191:GLU:HG3	A:706:TRP:CH2	0.470
1	A:635:TRP:NE1	A:637:ALA:HB2	0.469
1	A:627:TYR:CE2	A:651:GLY:HA2	0.466
1	A:697:VAL:HG22	A:738:TRP:CE3	0.465
1	A:79:LEU:HD13	A:92:ARG:CD	0.463
1	A:82:ASN:HD22	A:126:GLU:CD	0.463
1	A:26:THR:C	A:28:THR:H	0.457
1	A:498:PRO:HA	A:520:GLY:H	0.454
1	A:635:TRP:CD2	A:643:MET:HB2	0.452
1	A:650:TYR:CD2	A:676:TYR:CE2	0.446
1	A:79:LEU:HD13	A:92:ARG:HD3	0.445
1	A:171:GLY:HA2	A:202:THR:CG2	0.444
1	A:108:ILE:HD12	A:135:TRP:CH2	0.442
1	A:508:GLY:C	A:510:TYR:H	0.442
1	A:121:GLN:H	A:338:ARG:NH1	0.442
1	A:402:ASN:ND2	A:501:ILE:HA	0.440
1	A:82:ASN:OD1	A:84:THR:HG23	0.439
1	A:191:GLU:CG	A:706:TRP:CZ3	0.439
1	A:583:ALA:HB1	A:621:LEU:HD11	0.436
1	A:627:TYR:CE2	A:649:TRP:CH2	0.435
1	A:183:PHE:CE1	A:185:ALA:HB2	0.434

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:676:TYR:CD1	A:705:LEU:HD21	0.433
1	A:561:GLY:HA2	A:575:TYR:CD1	0.432
1	A:123:TRP:HB2	A:341:GLU:HB3	0.427
1	A:108:ILE:CD1	A:135:TRP:CH2	0.422
1	A:328:TRP:CE2	A:370:HIS:HB3	0.415
1	A:140:MET:HE2	A:168:THR:CG2	0.410
1	A:140:MET:SD	A:214:TYR:CD2	0.410
1	A:53:ILE:HD13	A:70:ILE:HG22	0.408
1	A:119:VAL:HB	A:336:ASN:ND2	0.405
1	A:609:MET:HG3	A:624:ILE:HD12	0.404
1	A:107:LEU:HD23	A:112:PRO:HA	0.403
1	A:261:TRP:CE3	A:263:PHE:CZ	0.403
1	A:53:ILE:HG12	A:74:MET:HE3	0.402
1	A:155:TYR:CD2	A:163:VAL:HG21	0.401
1	A:498:PRO:HB2	A:518:LEU:HD22	0.400
2	A:99:MET:HE3	A:161:GLY:HA2	0.701
2	A:39:THR:HG22	A:592:LEU:HB2	0.698
2	A:40:ALA:H	A:592:LEU:CA	0.673
2	A:40:ALA:H	A:592:LEU:HA	0.673
2	A:63:VAL:HG22	A:644:GLN:HE22	0.603
2	A:40:ALA:H	A:592:LEU:N	0.601
2	A:39:THR:HA	A:592:LEU:HA	0.599
2	A:45:LEU:HD21	A:539:LYS:HB2	0.545

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:360:VAL:HG13	A:399:LEU:HD13	0.539
2	A:45:LEU:HD11	A:539:LYS:HD2	0.537
2	A:591:SER:HA	A:605:ASN:HA	0.533
2	A:40:ALA:HB1	A:544:LEU:HG	0.528
2	A:37:VAL:O	A:38:VAL:HG23	0.506
2	A:40:ALA:HB2	A:544:LEU:C	0.502
2	A:560:ALA:HB1	A:575:TYR:CE1	0.499
2	A:38:VAL:HG22	A:39:THR:HG23	0.498
2	A:41:ALA:HB2	A:593:ASN:ND2	0.489
2	A:71:ILE:HG22	A:77:VAL:HG11	0.483
2	A:609:MET:HE3	A:624:ILE:HG21	0.480
2	A:63:VAL:HG22	A:644:GLN:NE2	0.478
2	A:11:LEU:HB3	A:12:VAL:HG23	0.477
2	A:41:ALA:HB3	A:44:ASN:CG	0.464
2	A:45:LEU:HD11	A:539:LYS:CD	0.458
2	A:592:LEU:O	A:603:THR:HA	0.454
2	A:46:GLN:C	A:48:PRO:HD2	0.449
2	A:41:ALA:HB3	A:44:ASN:ND2	0.445
2	A:627:TYR:CE2	A:651:GLY:HA2	0.441
2	A:498:PRO:HD2	A:520:GLY:CA	0.440
2	A:108:ILE:HD12	A:135:TRP:CH2	0.437
2	A:38:VAL:HG22	A:39:THR:CG2	0.434
2	A:63:VAL:HG13	A:644:GLN:OE1	0.434

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:379:PHE:C	A:381:VAL:H	0.434
2	A:538:PHE:O	A:544:LEU:HD12	0.434
2	A:261:TRP:CE2	A:263:PHE:HB3	0.429
2	A:65:ARG:HH12	A:743:ASN:N	0.429
2	A:627:TYR:CE2	A:651:GLY:CA	0.427
2	A:38:VAL:HG13	A:39:THR:HB	0.420
2	A:538:PHE:O	A:544:LEU:HA	0.405
2	A:135:TRP:CD1	A:135:TRP:H	0.401
3	A:186:PRO:HD3	A:319:TRP:CH2	0.751
3	A:193:ALA:HA	A:319:TRP:CH2	0.686
3	A:565:VAL:HG21	A:574:LEU:HD12	0.647
3	A:186:PRO:CG	A:319:TRP:CH2	0.625
3	A:82:ASN:HD21	A:84:THR:HG23	0.611
3	A:38:VAL:HG11	A:43:GLN:HE21	0.608
3	A:186:PRO:HG3	A:319:TRP:CH2	0.575
3	A:69:LYS:CE	A:320:ASP:HB3	0.573
3	A:186:PRO:CD	A:319:TRP:CH2	0.571
3	A:192:GLY:C	A:319:TRP:CZ2	0.569
3	A:186:PRO:HG3	A:319:TRP:CZ3	0.562
3	A:330:GLN:HA	A:333:HIS:HB2	0.559
3	A:333:HIS:ND1	A:562:TYR:CE2	0.559
3	A:340:PRO:HG2	A:343:LEU:HD12	0.550
3	A:82:ASN:ND2	A:84:THR:HG23	0.544

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:328:TRP:CZ3	A:332:GLU:HG3	0.533
3	A:635:TRP:CE2	A:643:MET:HB2	0.533
3	A:355:ALA:HB1	A:503:TYR:CD2	0.532
3	A:122:GLY:C	A:124:ARG:H	0.531
3	A:85:SER:C	A:87:GLN:H	0.526
3	A:584:VAL:HB	A:615:LYS:HE3	0.525
3	A:186:PRO:HD3	A:319:TRP:CZ3	0.524
3	A:171:GLY:HA2	A:202:THR:HG22	0.519
3	A:190:GLU:HB3	A:311:TYR:CE2	0.513
3	A:557:LYS:HE3	A:559:GLU:OE1	0.513
3	A:99:MET:SD	A:161:GLY:HA2	0.511
3	A:427:SER:CB	A:497:ASN:HD21	0.500
3	A:99:MET:HE3	A:161:GLY:O	0.497
3	A:107:LEU:HD23	A:112:PRO:HA	0.486
3	A:38:VAL:CG1	A:43:GLN:HE21	0.473
3	A:503:TYR:CE1	A:509:CYS:SG	0.469
3	A:671:LYS:HB2	A:717:LEU:HG	0.465
3	A:355:ALA:CB	A:503:TYR:CD2	0.463
3	A:212:ARG:HH21	A:258:VAL:HG11	0.462
3	A:711:ALA:HB1	A:720:ALA:HA	0.462
3	A:45:LEU:CD2	A:52:THR:HG21	0.457
3	A:184:ASN:CG	A:319:TRP:CE3	0.457
3	A:562:TYR:CE2	A:668:PRO:HD2	0.457

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:71:ILE:HG22	A:77:VAL:HG11	0.455
3	A:115:SER:HB2	A:117:ASN:CG	0.455
3	A:186:PRO:HG3	A:319:TRP:CZ2	0.455
3	A:360:VAL:HG13	A:398:ASP:CG	0.453
3	A:321:ASN:HB3	A:323:VAL:HG23	0.452
3	A:69:LYS:NZ	A:320:ASP:HB3	0.448
3	A:41:ALA:HA	A:154:ARG:HH22	0.444
3	A:608:TYR:CD2	A:627:TYR:CE1	0.441
3	A:211:PHE:CZ	A:213:LEU:HB2	0.437
3	A:652:LYS:HE3	A:672:GLU:CD	0.436
3	A:424:SER:C	A:426:TYR:H	0.435
3	A:192:GLY:O	A:319:TRP:CZ2	0.434
3	A:87:GLN:HE22	A:124:ARG:NH1	0.434
3	A:261:TRP:CE2	A:263:PHE:HB3	0.429
3	A:186:PRO:CG	A:319:TRP:CZ2	0.428
3	A:184:ASN:ND2	A:319:TRP:HB3	0.426
3	A:61:ASN:OD1	A:63:VAL:HG22	0.424
3	A:88:ARG:NH2	A:248:GLU:CD	0.424
3	A:388:GLY:HA3	A:435:PHE:CZ	0.422
3	A:90:ASN:OD1	A:318:GLY:HA3	0.416
3	A:137:PRO:O	A:140:MET:HG2	0.415
3	A:140:MET:SD	A:214:TYR:CD2	0.411
3	A:224:ALA:HB3	A:248:GLU:HB3	0.409

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:717:LEU:CD2	A:721:ASN:HD21	0.409
3	A:576:GLN:HE22	A:661:LYS:NZ	0.405
3	A:114:SER:O	A:115:SER:C	0.405
3	A:652:LYS:HE2	A:654:GLN:NE2	0.404
3	A:186:PRO:CD	A:319:TRP:CZ3	0.402
3	A:333:HIS:ND1	A:575:TYR:CE2	0.402
3	A:711:ALA:CB	A:720:ALA:HA	0.401
4	A:343:LEU:HD11	A:360:VAL:HG11	0.828
4	A:671:LYS:H	A:723:ILE:HG12	0.771
4	A:94:ILE:HD12	A:119:VAL:HG11	0.726
4	A:671:LYS:CG	A:723:ILE:HD13	0.689
4	A:71:ILE:HG22	A:77:VAL:HG11	0.672
4	A:671:LYS:CB	A:723:ILE:HD13	0.642
4	A:515:GLY:O	A:572:THR:HG23	0.629
4	A:40:ALA:CB	A:154:ARG:HH12	0.624
4	A:671:LYS:HB2	A:723:ILE:HD13	0.607
4	A:671:LYS:HB2	A:723:ILE:CG2	0.573
4	A:635:TRP:CH2	A:643:MET:SD	0.563
4	A:235:ARG:HD3	A:240:ALA:HA	0.558
4	A:360:VAL:HG13	A:400:SER:OG	0.541
4	A:405:ALA:HB2	A:420:THR:HG22	0.541
4	A:511:ALA:HB2	A:722:TYR:CE2	0.535
4	A:235:ARG:CB	A:240:ALA:HA	0.533

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:671:LYS:HB2	A:723:ILE:HG21	0.533
4	A:123:TRP:CH2	A:734:PRO:HB3	0.529
4	A:191:GLU:HA	A:224:ALA:HB1	0.524
4	A:513:ALA:HB1	A:572:THR:HA	0.523
4	A:235:ARG:HB3	A:240:ALA:HA	0.522
4	A:8:LEU:HG	A:9:ALA:HB2	0.520
4	A:720:ALA:HA	A:723:ILE:HD12	0.518
4	A:94:ILE:CD1	A:119:VAL:HG11	0.515
4	A:671:LYS:HG3	A:723:ILE:HD13	0.508
4	A:343:LEU:CD1	A:360:VAL:HG11	0.503
4	A:328:TRP:CH2	A:368:MET:HE3	0.502
4	A:99:MET:HE3	A:161:GLY:O	0.497
4	A:261:TRP:CE2	A:263:PHE:HB3	0.496
4	A:40:ALA:HB3	A:154:ARG:HH22	0.488
4	A:230:GLY:HA3	A:729:TYR:CE1	0.487
4	A:727:GLY:HA3	A:729:TYR:CE2	0.484
4	A:31:SER:C	A:33:ASP:H	0.483
4	A:328:TRP:CE2	A:370:HIS:HB3	0.477
4	A:125:GLY:HA2	A:250:VAL:HG21	0.474
4	A:40:ALA:HB3	A:154:ARG:HH12	0.473
4	A:635:TRP:CE3	A:643:MET:HB2	0.472
4	A:226:ASP:CG	A:229:GLN:HB2	0.468
4	A:244:PRO:HD2	A:290:ASN:HA	0.466

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:564:ALA:HB3	A:660:TYR:CD1	0.459
4	A:130:ARG:HH12	A:310:ASN:ND2	0.455
4	A:336:ASN:HD21	A:338:ARG:HH21	0.455
4	A:91:ASN:ND2	A:120:ARG:HH11	0.454
4	A:406:LEU:HD13	A:517:TYR:CD1	0.450
4	A:113:VAL:HG12	A:130:ARG:HD3	0.443
4	A:251:ILE:HD11	A:281:LEU:HD11	0.442
4	A:137:PRO:HD2	A:140:MET:SD	0.440
4	A:508:GLY:HA2	A:658:TYR:CD2	0.437
4	A:635:TRP:HE1	A:637:ALA:HA	0.437
4	A:219:LYS:HE3	A:221:GLN:NE2	0.435
4	A:97:ARG:HB2	A:99:MET:HE2	0.434
4	A:345:GLY:HA3	A:503:TYR:HB3	0.434
4	A:336:ASN:ND2	A:338:ARG:HH21	0.434
4	A:134:SER:HB2	A:196:ARG:NH1	0.429
4	A:244:PRO:CD	A:290:ASN:HA	0.426
4	A:635:TRP:CE2	A:637:ALA:HB2	0.424
4	A:106:ILE:HG13	A:119:VAL:CG2	0.423
4	A:424:SER:HB2	A:497:ASN:HA	0.421
4	A:211:PHE:CE1	A:213:LEU:HB2	0.418
4	A:132:ASP:OD2	A:219:LYS:NZ	0.418
4	A:99:MET:HE3	A:161:GLY:HA2	0.415
4	A:409:THR:HB	A:411:THR:H	0.414

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:563:VAL:CG1	A:661:LYS:HB2	0.409
4	A:725:GLY:O	A:729:TYR:HB2	0.408
4	A:235:ARG:HD3	A:240:ALA:CA	0.405
4	A:43:GLN:HE22	A:384:THR:HG21	0.404
4	A:725:GLY:C	A:729:TYR:O	0.402
4	A:513:ALA:CB	A:572:THR:HA	0.400
5	A:306:LEU:HD11	A:333:HIS:CE1	0.832
5	A:113:VAL:HG21	A:135:TRP:CZ3	0.644
5	A:269:LEU:HD11	A:315:TRP:HE1	0.621
5	A:499:ASN:ND2	A:521:ASN:HD21	0.585
5	A:269:LEU:HD11	A:315:TRP:NE1	0.572
5	A:364:LEU:CD1	A:494:TYR:CE2	0.568
5	A:399:LEU:C	A:403:THR:HG23	0.565
5	A:117:ASN:HB3	A:494:TYR:CD2	0.554
5	A:399:LEU:O	A:403:THR:HG23	0.554
5	A:627:TYR:CE2	A:651:GLY:CA	0.544
5	A:228:ASN:HD22	A:243:LEU:CD1	0.541
5	A:584:VAL:HB	A:615:LYS:HE3	0.541
5	A:132:ASP:HB3	A:135:TRP:CZ2	0.535
5	A:627:TYR:CE2	A:649:TRP:CH2	0.526
5	A:71:ILE:HG22	A:77:VAL:HG11	0.512
5	A:627:TYR:CE2	A:651:GLY:HA2	0.506
5	A:583:ALA:HB1	A:621:LEU:HD11	0.494

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:99:MET:CE	A:161:GLY:HA2	0.488
5	A:123:TRP:CD1	A:572:THR:HG21	0.481
5	A:554:TYR:HB2	A:583:ALA:HB3	0.481
5	A:627:TYR:CE2	A:649:TRP:CZ3	0.474
5	A:99:MET:HE3	A:161:GLY:HA2	0.473
5	A:350:LYS:HG2	A:505:LYS:HD2	0.464
5	A:155:TYR:CD2	A:163:VAL:HG21	0.463
5	A:607:THR:HG22	A:609:MET:HE2	0.453
5	A:93:GLN:HE22	A:127:ARG:HB2	0.449
5	A:120:ARG:HH12	A:339:ILE:HG12	0.441
5	A:364:LEU:HD11	A:494:TYR:CE2	0.434
5	A:302:GLU:CD	A:305:ARG:HH21	0.426
5	A:650:TYR:CD2	A:676:TYR:CE2	0.423
5	A:132:ASP:CG	A:308:ARG:HH12	0.422
5	A:228:ASN:ND2	A:243:LEU:CD1	0.421
5	A:97:ARG:HB2	A:99:MET:HE2	0.419
5	A:99:MET:SD	A:552:ASN:ND2	0.417
5	A:61:ASN:OD1	A:63:VAL:HG22	0.415
5	A:500:TYR:CZ	A:519:GLN:HG2	0.415
5	A:426:TYR:CZ	A:459:ILE:HG23	0.407
5	A:117:ASN:HB3	A:494:TYR:CE2	0.406
5	A:426:TYR:CG	A:459:ILE:HD13	0.406
5	A:498:PRO:HB3	A:518:LEU:HB3	0.402

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:397:LYS:HE2	A:399:LEU:HD21	0.639
6	A:140:MET:HE3	A:212:ARG:HD3	0.578
6	A:111:LYS:HE2	A:314:THR:HG21	0.563
6	A:230:GLY:HA2	A:724:ALA:HB1	0.543
6	A:397:LYS:HE2	A:399:LEU:CD2	0.541
6	A:97:ARG:HB2	A:99:MET:HE2	0.534
6	A:343:LEU:HD21	A:360:VAL:HG11	0.523
6	A:635:TRP:CE2	A:643:MET:HB2	0.504
6	A:711:ALA:HB1	A:730:THR:C	0.503
6	A:707:ARG:C	A:709:GLY:H	0.493
6	A:235:ARG:O	A:240:ALA:HB2	0.488
6	A:44:ASN:ND2	A:154:ARG:HH11	0.488
6	A:406:LEU:HD23	A:501:ILE:HD11	0.475
6	A:99:MET:HE3	A:161:GLY:HA2	0.469
6	A:335:ARG:CG	A:359:PHE:CD1	0.462
6	A:53:ILE:HG13	A:74:MET:HE3	0.455
6	A:37:VAL:HG11	A:143:ARG:NH2	0.439
6	A:335:ARG:HG2	A:359:PHE:CD1	0.439
6	A:99:MET:CE	A:161:GLY:HA2	0.435
6	A:140:MET:CE	A:212:ARG:HD3	0.427
6	A:119:VAL:HG21	A:333:HIS:CD2	0.426
6	A:111:LYS:CE	A:314:THR:HG21	0.426
6	A:113:VAL:HG12	A:116:ARG:HD2	0.421

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:118:SER:HB2	A:494:TYR:CD2	0.419
6	A:188:HIS:CD2	A:704:ARG:NH2	0.419
6	A:235:ARG:C	A:237:GLY:H	0.414
6	A:142:GLU:CD	A:170:LYS:HZ1	0.413
6	A:65:ARG:HB3	A:138:PRO:HG2	0.412
6	A:113:VAL:CG1	A:116:ARG:HD2	0.411
6	A:64:ALA:HB2	A:182:TYR:CE2	0.406
6	A:704:ARG:NH2	A:735:GLY:CA	0.406
6	A:107:LEU:HD23	A:112:PRO:HA	0.404
6	A:261:TRP:CE2	A:263:PHE:HB3	0.402
6	A:44:ASN:HD22	A:154:ARG:HH11	0.402
7	A:72:ARG:HE	A:79:LEU:HD12	0.891
7	A:72:ARG:NE	A:79:LEU:HD12	0.781
7	A:79:LEU:HD13	A:92:ARG:HB3	0.732
7	A:723:ILE:HG22	A:728:ALA:HB3	0.709
7	A:88:ARG:HH12	A:224:ALA:HB2	0.701
7	A:258:VAL:HG22	A:323:VAL:CG2	0.696
7	A:258:VAL:HG22	A:323:VAL:HG21	0.644
7	A:88:ARG:HH22	A:224:ALA:HB2	0.619
7	A:72:ARG:HE	A:79:LEU:CD1	0.611
7	A:303:THR:HG21	A:333:HIS:CE1	0.599
7	A:502:LEU:HD12	A:517:TYR:CE1	0.574
7	A:88:ARG:HH12	A:224:ALA:CB	0.557

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:213:LEU:HD11	A:255:ILE:CG2	0.552
7	A:88:ARG:NH1	A:224:ALA:HB2	0.549
7	A:502:LEU:HB2	A:517:TYR:CZ	0.533
7	A:43:GLN:HE21	A:447:ILE:CG2	0.527
7	A:213:LEU:HD11	A:255:ILE:HG23	0.513
7	A:86:GLY:HA3	A:186:PRO:HG3	0.507
7	A:502:LEU:HD12	A:517:TYR:CZ	0.503
7	A:88:ARG:NH2	A:224:ALA:HB2	0.499
7	A:635:TRP:CE2	A:643:MET:HB2	0.489
7	A:46:GLN:C	A:481:LYS:HZ1	0.485
7	A:202:THR:HG23	A:212:ARG:HG2	0.480
7	A:623:ILE:HB	A:722:TYR:CZ	0.480
7	A:502:LEU:HB2	A:517:TYR:CE2	0.479
7	A:123:TRP:HA	A:335:ARG:NH2	0.477
7	A:182:TYR:CE1	A:184:ASN:HB2	0.471
7	A:61:ASN:OD1	A:63:VAL:HG22	0.468
7	A:426:TYR:HA	A:459:ILE:HD13	0.466
7	A:408:GLY:H	A:519:GLN:NE2	0.464
7	A:71:ILE:HG22	A:77:VAL:HG11	0.457
7	A:399:LEU:HD13	A:423:ARG:HH22	0.456
7	A:502:LEU:CD1	A:517:TYR:CE1	0.442
7	A:623:ILE:HD13	A:722:TYR:CD2	0.441
7	A:185:ALA:HB3	A:738:TRP:CZ2	0.437

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:135:TRP:CE3	A:214:TYR:CE2	0.436
7	A:69:LYS:HG2	A:92:ARG:HH12	0.434
7	A:399:LEU:HD13	A:423:ARG:NH2	0.433
7	A:62:PRO:HB3	A:642:SER:CB	0.430
7	A:326:SER:HB2	A:328:TRP:CD1	0.429
7	A:40:ALA:O	A:41:ALA:C	0.426
7	A:623:ILE:CD1	A:722:TYR:CD2	0.423
7	A:653:GLN:HB2	A:673:ILE:HB	0.419
7	A:307:TYR:HB3	A:329:VAL:HG13	0.417
7	A:623:ILE:HD13	A:722:TYR:CG	0.414
7	A:608:TYR:CD2	A:627:TYR:CE1	0.408
7	A:43:GLN:HE21	A:447:ILE:HG21	0.408
7	A:280:ASN:OD1	A:306:LEU:HD21	0.408
7	A:562:TYR:CD1	A:573:ASP:HB3	0.404
7	A:132:ASP:O	A:135:TRP:CD1	0.401
8	A:119:VAL:HG21	A:278:GLN:CD	0.680
8	A:119:VAL:HG22	A:306:LEU:HD12	0.626
8	A:119:VAL:HG22	A:306:LEU:CD1	0.535
8	A:339:ILE:HG23	A:500:TYR:HA	0.516
8	A:565:VAL:O	A:569:ALA:HB3	0.483
8	A:36:ILE:HG21	A:142:GLU:CD	0.479
8	A:36:ILE:HG22	A:37:VAL:H	0.473
8	A:119:VAL:HG21	A:278:GLN:NE2	0.455

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:71:ILE:HG22	A:77:VAL:HG11	0.436
8	A:86:GLY:H	A:191:GLU:CD	0.422
8	A:297:SER:C	A:299:TYR:H	0.408
9	A:123:TRP:CD2	A:123:TRP:CE3	1.624
9	A:123:TRP:CD2	A:123:TRP:CE2	1.454
9	A:123:TRP:CZ3	A:505:LYS:HA	1.355
9	A:123:TRP:CH2	A:505:LYS:HA	1.295
9	A:176:HIS:CD2	A:176:HIS:NE2	1.159
9	A:123:TRP:CE2	A:505:LYS:CB	1.144
9	A:176:HIS:CE1	A:176:HIS:ND1	1.144
9	A:123:TRP:CE3	A:505:LYS:CB	1.141
9	A:123:TRP:CZ2	A:505:LYS:CB	1.138
9	A:123:TRP:CD2	A:505:LYS:CB	1.128
9	A:123:TRP:CZ3	A:505:LYS:CA	1.128
9	A:123:TRP:CE2	A:505:LYS:CA	1.125
9	A:123:TRP:CE3	A:505:LYS:CA	1.121
9	A:123:TRP:CZ3	A:505:LYS:CB	1.121
9	A:123:TRP:CH2	A:505:LYS:CA	1.118
9	A:123:TRP:CH2	A:505:LYS:CB	1.118
9	A:123:TRP:CZ2	A:505:LYS:CA	1.114
9	A:123:TRP:CD2	A:505:LYS:CA	1.106
9	A:123:TRP:CZ2	A:505:LYS:HB3	0.979
9	A:123:TRP:CD2	A:505:LYS:HB2	0.977

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:123:TRP:CZ3	A:505:LYS:CG	0.820
9	A:123:TRP:CZ2	A:505:LYS:C	0.795
9	A:123:TRP:CE2	A:505:LYS:HB2	0.762
9	A:176:HIS:CE1	A:176:HIS:NE2	0.740
9	A:172:SER:HG	A:176:HIS:HE2	0.707
9	A:123:TRP:CD2	A:505:LYS:N	0.697
9	A:123:TRP:CE3	A:505:LYS:N	0.695
9	A:123:TRP:CE2	A:505:LYS:C	0.633
9	A:123:TRP:CE3	A:505:LYS:CG	0.565
9	A:93:GLN:HE21	A:129:THR:HG21	0.560
9	A:123:TRP:CH2	A:505:LYS:HB3	0.527
9	A:123:TRP:CE3	A:504:SER:C	0.500
9	A:91:ASN:HD21	A:129:THR:HG23	0.488
9	A:123:TRP:CE3	A:505:LYS:HG3	0.484
9	A:174:GLU:HB2	A:176:HIS:NE2	0.468
9	A:99:MET:HE3	A:161:GLY:HA2	0.435
9	A:123:TRP:CZ3	A:505:LYS:HG3	0.434
9	A:172:SER:OG	A:176:HIS:NE2	0.422
9	A:165:ASN:HD21	A:167:ILE:HD11	0.421
10	A:518:LEU:HD12	A:574:LEU:HD12	0.933
10	A:518:LEU:HD12	A:574:LEU:CD1	0.625
10	A:119:VAL:HG22	A:129:THR:HG21	0.619
10	A:119:VAL:HG22	A:129:THR:CG2	0.613

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:71:ILE:HG22	A:77:VAL:HG11	0.572
10	A:99:MET:HE3	A:554:TYR:OH	0.569
10	A:231:HIS:CD2	A:245:ALA:HB3	0.562
10	A:112:PRO:HG2	A:368:MET:HE1	0.555
10	A:65:ARG:HH22	A:743:ASN:HD22	0.555
10	A:120:ARG:HD2	A:338:ARG:HH22	0.554
10	A:120:ARG:HB2	A:338:ARG:HH12	0.547
10	A:99:MET:HE2	A:161:GLY:HA2	0.542
10	A:518:LEU:CD1	A:574:LEU:HD12	0.540
10	A:139:GLU:CD	A:139:GLU:H	0.531
10	A:90:ASN:HD21	A:252:ASN:HD21	0.531
10	A:82:ASN:HA	A:707:ARG:HH22	0.516
10	A:65:ARG:HH11	A:139:GLU:CD	0.502
10	A:345:GLY:HA2	A:572:THR:HG22	0.502
10	A:518:LEU:HD11	A:565:VAL:HG22	0.502
10	A:120:ARG:CD	A:338:ARG:HH22	0.492
10	A:247:ARG:HH12	A:301:ASP:CG	0.483
10	A:84:THR:HG21	A:228:ASN:HD21	0.480
10	A:90:ASN:ND2	A:252:ASN:HD21	0.479
10	A:93:GLN:HE22	A:127:ARG:HB3	0.477
10	A:401:SER:HA	A:499:ASN:HD22	0.473
10	A:261:TRP:CE2	A:263:PHE:HB3	0.472
10	A:222:ALA:CB	A:247:ARG:HE	0.470

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:69:LYS:HE2	A:92:ARG:HH12	0.467
10	A:130:ARG:HH21	A:134:SER:HB2	0.466
10	A:569:ALA:HB1	A:572:THR:HG21	0.465
10	A:584:VAL:HB	A:615:LYS:HE3	0.464
10	A:99:MET:CE	A:161:GLY:HA2	0.458
10	A:328:TRP:CE2	A:370:HIS:HB3	0.457
10	A:116:ARG:O	A:119:VAL:HG23	0.454
10	A:99:MET:HE3	A:554:TYR:CZ	0.452
10	A:98:GLY:HA3	A:624:ILE:HD13	0.446
10	A:119:VAL:CG2	A:129:THR:HG21	0.446
10	A:132:ASP:O	A:135:TRP:CZ3	0.443
10	A:90:ASN:HD21	A:252:ASN:ND2	0.437
10	A:99:MET:HE2	A:161:GLY:CA	0.432
10	A:11:LEU:HB3	A:12:VAL:HG23	0.429
10	A:62:PRO:HB3	A:694:THR:HG21	0.428
10	A:518:LEU:HD12	A:574:LEU:HB2	0.424
10	A:88:ARG:HH22	A:698:ASP:HB2	0.424
10	A:155:TYR:CD2	A:163:VAL:HG21	0.422
10	A:635:TRP:CE2	A:643:MET:HB2	0.422
10	A:124:ARG:HA	A:575:TYR:CE2	0.419
10	A:132:ASP:HA	A:135:TRP:CH2	0.419
10	A:130:ARG:HD3	A:278:GLN:OE1	0.416
10	A:707:ARG:HG3	A:732:ASN:HD21	0.415

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:124:ARG:NH1	A:726:ALA:H	0.414
10	A:139:GLU:CD	A:139:GLU:N	0.411
10	A:491:PRO:HB2	A:496:THR:HG23	0.406
10	A:222:ALA:HA	A:248:GLU:O	0.405
10	A:65:ARG:NH2	A:743:ASN:HD22	0.404
10	A:168:THR:CB	A:212:ARG:HH12	0.403
10	A:119:VAL:HA	A:129:THR:HG23	0.402
10	A:231:HIS:CG	A:245:ALA:HB3	0.401

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	744	644	63	37
2	744	674	50	20
3	744	618	87	39
4	744	647	65	32
5	744	655	58	31
6	744	644	72	28
7	744	670	46	28
8	744	626	78	40
9	744	636	90	18
10	744	655	78	11

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	615	581	20	14
2	615	567	29	19
3	615	568	27	20
4	615	579	26	10
5	615	580	26	9
6	615	590	16	9
7	615	576	22	17
8	615	572	28	15
9	615	562	37	16
10	615	585	18	12

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	7	SER
1	A	10	LEU
1	A	31	SER
1	A	83	SER
1	A	115	SER
1	A	119	VAL
1	A	123	TRP
1	A	129	THR
1	A	238	THR
1	A	295	THR
1	A	347	THR

Model ID	Chain	Residue ID	Residue type
1	A	402	ASN
1	A	501	ILE
1	A	741	SER
2	A	38	VAL
2	A	39	THR
2	A	44	ASN
2	A	84	THR
2	A	108	ILE
2	A	218	ASP
2	A	286	THR
2	A	289	THR
2	A	338	ARG
2	A	347	THR
2	A	369	LEU
2	A	407	THR
2	A	409	THR
2	A	504	SER
2	A	563	VAL
2	A	705	LEU
2	A	713	THR
2	A	730	THR
2	A	737	THR
3	A	8	LEU

Model ID	Chain	Residue ID	Residue type
3	A	10	LEU
3	A	32	HIS
3	A	84	THR
3	A	121	GLN
3	A	139	GLU
3	A	226	ASP
3	A	238	THR
3	A	242	THR
3	A	301	ASP
3	A	303	THR
3	A	307	TYR
3	A	315	TRP
3	A	347	THR
3	A	373	VAL
3	A	409	THR
3	A	419	SER
3	A	421	THR
3	A	622	SER
3	A	717	LEU
4	A	7	SER
4	A	8	LEU
4	A	10	LEU
4	A	11	LEU
Model ID	Chain	Residue ID	Residue type

Model ID	Chain	Residue ID	Residue type
4	A	113	VAL
4	A	325	THR
4	A	529	SER
4	A	635	TRP
4	A	666	VAL
4	A	743	ASN
5	A	8	LEU
5	A	28	THR
5	A	32	HIS
5	A	35	THR
5	A	347	THR
5	A	624	ILE
5	A	646	THR
5	A	706	TRP
5	A	730	THR
6	A	32	HIS
6	A	84	THR
6	A	123	TRP
6	A	170	LYS
6	A	238	THR
6	A	334	THR
6	A	410	ASN
6	A	529	SER
Model ID	Chain	Residue ID	Residue type

Model ID	Chain	Residue ID	Residue type
6	A	723	ILE
7	A	8	LEU
7	A	11	LEU
7	A	19	VAL
7	A	31	SER
7	A	266	LEU
7	A	271	LEU
7	A	286	THR
7	A	314	THR
7	A	335	ARG
7	A	347	THR
7	A	365	ASP
7	A	370	HIS
7	A	385	LEU
7	A	403	THR
7	A	409	THR
7	A	416	ASP
7	A	730	THR
8	A	10	LEU
8	A	14	LEU
8	A	28	THR
8	A	36	ILE
8	A	38	VAL

Model ID	Chain	Residue ID	Residue type
8	A	95	ASP
8	A	200	SER
8	A	238	THR
8	A	242	THR
8	A	286	THR
8	A	347	THR
8	A	399	LEU
8	A	433	SER
8	A	471	SER
8	A	488	TYR
9	A	11	LEU
9	A	38	VAL
9	A	73	THR
9	A	92	ARG
9	A	119	VAL
9	A	191	GLU
9	A	276	SER
9	A	292	ASP
9	A	310	ASN
9	A	337	SER
9	A	496	THR
9	A	503	TYR
9	A	532	LYS

Model ID	Chain	Residue ID	Residue type
9	A	572	THR
9	A	714	THR
9	A	730	THR
10	A	8	LEU
10	A	10	LEU
10	A	12	VAL
10	A	14	LEU
10	A	26	THR
10	A	32	HIS
10	A	286	THR
10	A	347	THR
10	A	421	THR
10	A	502	LEU
10	A	563	VAL
10	A	666	VAL

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.