

Integrative Structure Validation Report

July 22, 2024 - 03:50 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	8ZZS
PDB-Dev ID	PDBDEV_00000028
Structure Title	Complex of RNF168-RING domain and the nucleosome
Structure Authors	Horn V; Uckelmann M; Zhang H; Eerland J; Aarsman I; le Paige UB; Davidovich C; Sixma TK; van Ingen H

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

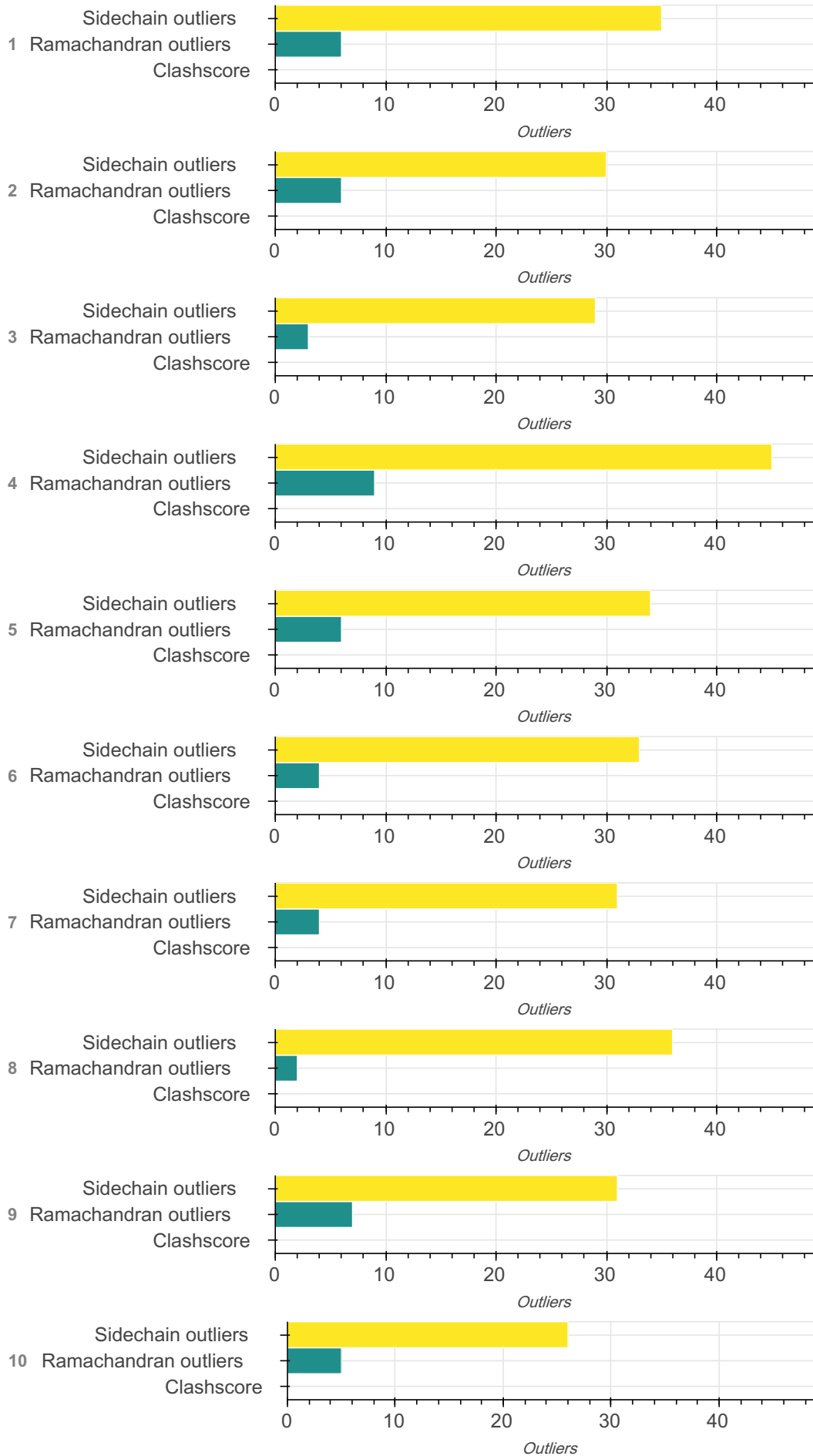
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

List of references used to build this report is available [here](#).

Overall quality

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis



Ensemble information ?

This entry consists of 0 distinct ensemble(s).

Summary ?

This entry consists of 10 unique models, with 11 subunits in each model. A total of 7 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 11 flexible or non-rigid units.

Entry composition ?

There are 10 unique types of models in this entry. These models are titled Best Scoring Model cluster 1, no.2 Scoring Model cluster 1, no.3 Scoring Model cluster 1, no.4 Scoring Model cluster 1, no.5 Scoring Model cluster 1, no.6 Scoring Model cluster 1, no.7 Scoring Model cluster 1, no.8 Scoring Model cluster 1, no.9 Scoring Model cluster 1, no.10 Scoring Model cluster 1 respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	H3	A	A	99
1	2	1	H3	E	E	99
1	3	2	H4	B	B	80
1	4	2	H4	F	F	80
1	5	3	H2A	C	C	107
1	6	3	H2A	G	G	107
1	7	4	H2B	D	D	95
1	8	4	H2B	H	H	95
1	9	5	DNA strand 1	I	I	147
1	10	6	DNA strand 2	J	J	147
1	11	7	RNF168 RING domain	K	K	91
2	1	1	H3	A	A	99

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
2	2	1	H3	E	E	99
2	3	2	H4	B	B	80
2	4	2	H4	F	F	80
2	5	3	H2A	C	C	107
2	6	3	H2A	G	G	107
2	7	4	H2B	D	D	95
2	8	4	H2B	H	H	95
2	9	5	DNA strand 1	I	I	147
2	10	6	DNA strand 2	J	J	147
2	11	7	RNF168 RING domain	K	K	91
3	1	1	H3	A	A	99
3	2	1	H3	E	E	99
3	3	2	H4	B	B	80
3	4	2	H4	F	F	80
3	5	3	H2A	C	C	107
3	6	3	H2A	G	G	107
3	7	4	H2B	D	D	95
3	8	4	H2B	H	H	95
3	9	5	DNA strand 1	I	I	147
3	10	6	DNA strand 2	J	J	147
3	11	7	RNF168 RING domain	K	K	91
4	1	1	H3	A	A	99

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
4	2	1	H3	E	E	99
4	3	2	H4	B	B	80
4	4	2	H4	F	F	80
4	5	3	H2A	C	C	107
4	6	3	H2A	G	G	107
4	7	4	H2B	D	D	95
4	8	4	H2B	H	H	95
4	9	5	DNA strand 1	I	I	147
4	10	6	DNA strand 2	J	J	147
4	11	7	RNF168 RING domain	K	K	91
5	1	1	H3	A	A	99
5	2	1	H3	E	E	99
5	3	2	H4	B	B	80
5	4	2	H4	F	F	80
5	5	3	H2A	C	C	107
5	6	3	H2A	G	G	107
5	7	4	H2B	D	D	95
5	8	4	H2B	H	H	95
5	9	5	DNA strand 1	I	I	147
5	10	6	DNA strand 2	J	J	147
5	11	7	RNF168 RING domain	K	K	91
6	1	1	H3	A	A	99

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
6	2	1	H3	E	E	99
6	3	2	H4	B	B	80
6	4	2	H4	F	F	80
6	5	3	H2A	C	C	107
6	6	3	H2A	G	G	107
6	7	4	H2B	D	D	95
6	8	4	H2B	H	H	95
6	9	5	DNA strand 1	I	I	147
6	10	6	DNA strand 2	J	J	147
6	11	7	RNF168 RING domain	K	K	91
7	1	1	H3	A	A	99
7	2	1	H3	E	E	99
7	3	2	H4	B	B	80
7	4	2	H4	F	F	80
7	5	3	H2A	C	C	107
7	6	3	H2A	G	G	107
7	7	4	H2B	D	D	95
7	8	4	H2B	H	H	95
7	9	5	DNA strand 1	I	I	147
7	10	6	DNA strand 2	J	J	147
7	11	7	RNF168 RING domain	K	K	91
8	1	1	H3	A	A	99

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
8	2	1	H3	E	E	99
8	3	2	H4	B	B	80
8	4	2	H4	F	F	80
8	5	3	H2A	C	C	107
8	6	3	H2A	G	G	107
8	7	4	H2B	D	D	95
8	8	4	H2B	H	H	95
8	9	5	DNA strand 1	I	I	147
8	10	6	DNA strand 2	J	J	147
8	11	7	RNF168 RING domain	K	K	91
9	1	1	H3	A	A	99
9	2	1	H3	E	E	99
9	3	2	H4	B	B	80
9	4	2	H4	F	F	80
9	5	3	H2A	C	C	107
9	6	3	H2A	G	G	107
9	7	4	H2B	D	D	95
9	8	4	H2B	H	H	95
9	9	5	DNA strand 1	I	I	147
9	10	6	DNA strand 2	J	J	147
9	11	7	RNF168 RING domain	K	K	91
10	1	1	H3	A	A	99

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
10	2	1	H3	E	E	99
10	3	2	H4	B	B	80
10	4	2	H4	F	F	80
10	5	3	H2A	C	C	107
10	6	3	H2A	G	G	107
10	7	4	H2B	D	D	95
10	8	4	H2B	H	H	95
10	9	5	DNA strand 1	I	I	147
10	10	6	DNA strand 2	J	J	147
10	11	7	RNF168 RING domain	K	K	91

Datasets used for modeling

There are 7 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	2PYO
2	Experimental model	PDB	4GB0
3	Mutagenesis data	File	10.1038/s41467-019-09756-z
4	NMR data	BMRB	27786
5	NMR data	BMRB	27791
6	NMR data	BMRB	27792
7	Crosslinking-MS data	PRIDE	PXD012723

Representation ?

This entry has only one representation and includes 0 rigid bodies and 11 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-99
B	-	1-80
C	-	1-107
D	-	1-95
E	-	1-99
F	-	1-80
G	-	1-107
H	-	1-95
I	-	1-147
J	-	1-147
K	-	1-91

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	None	None	None	None	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	HADDOCK	2.2	molecular docking	http://haddock.science.uu.nl/services/HADDOCK/
2	JWALK	1.1	XL-MS validation	http://jwalk.ismb.lon.ac.uk/jwalk/download/

Data quality ?

Mutagenesis

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

NMR

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobit analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers ?

There are 50660 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
N--H	0.97	0.86	4
N--H	0.98	0.86	7535
NE2--HE2	0.98	0.86	79
ND2--HD22	0.98	0.86	288
NE2--HE22	0.98	0.86	306
C2'--H2'	1.09	0.97	2940
C3'--H3'	1.09	0.97	2940
C5'--H5"	1.09	0.97	2940
ND2--HD21	0.98	0.86	259
C5'--H5'	1.09	0.97	2940
C2'--H2"	1.09	0.97	2940
C7--H71	1.09	0.97	870

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
C7--H72	1.09	0.97	870
OH--HH	0.96	0.84	142
C7--H73	1.09	0.97	870
NE2--HE21	0.98	0.86	214
C1'--H1'	1.09	0.97	2940
C4'--H4'	1.09	0.97	2940
ND1--HD1	0.98	0.86	38
NE--HE	0.98	0.86	420
OG--HG	0.96	0.84	121
OG1--HG1	0.96	0.84	164
NE1--HE1	0.98	0.86	19
SG--HG	1.32	1.20	4
N--H	0.99	0.86	591
NE--HE	0.99	0.86	474
SG--HG	1.33	1.20	116
OG1--HG1	0.97	0.84	324
NE2--HE2	0.99	0.86	51
ND2--HD21	0.99	0.86	30
OH--HH	0.97	0.84	163
OG--HG	0.97	0.84	337
ND2--HD22	0.99	0.86	2
ND1--HD1	0.99	0.86	22
NE2--HE21	0.99	0.86	96

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2--HE22	0.99	0.86	4
O5'--HO5'	0.97	0.84	10
O3'--HO3'	0.97	0.84	10
NE1--HE1	0.99	0.86	1
NE--HE	1.00	0.86	26
ND2--HD21	1.00	0.86	1
OG1--HG1	0.98	0.84	12
OH--HH	0.98	0.84	15
OG--HG	0.98	0.84	2
NH1--HH12	1.00	0.86	615
NH1--HH11	1.00	0.86	637
NH2--HH21	1.00	0.86	624
NH2--HH22	1.00	0.86	549
NH1--HH11	1.01	0.86	275
NH1--HH12	1.01	0.86	286
NH2--HH22	1.01	0.86	338
NH2--HH21	1.01	0.86	290
NZ--HZ2	1.04	0.89	604
NZ--HZ1	1.04	0.89	596
NZ--HZ3	1.04	0.89	592
N6--H62	1.01	0.86	870
N2--H21	1.01	0.86	593
N6--H61	1.01	0.86	868

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
N4--H41	1.01	0.86	594
N4--H42	1.01	0.86	598
N3--H3	1.01	0.86	867
C8--H8	1.08	0.93	1470
N1--H1	1.01	0.86	594
N2--H22	1.01	0.86	496
NZ--HZ2	1.05	0.89	26
N2--H22	1.02	0.86	104
NZ--HZ3	1.05	0.89	38
N3--H3	1.02	0.86	3
NH2--HH21	1.02	0.86	6
N1--H1	1.02	0.86	6
NH2--HH22	1.02	0.86	33
N4--H42	1.02	0.86	2
NH1--HH11	1.02	0.86	8
N2--H21	1.02	0.86	7
NH1--HH12	1.02	0.86	19
N4--H41	1.02	0.86	6
NZ--HZ1	1.05	0.89	34
N6--H61	1.02	0.86	2
C6--H6	1.09	0.93	1470
C5--H5	1.09	0.93	600
C2--H2	1.09	0.93	870

Standard geometry: angle outliers 

There are 1637 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
C3'-O3'-HO3'	107.88	120.00	1
C3'-O3'-HO3'	107.77	120.00	1
C3'-O3'-HO3'	107.71	120.00	1
C3'-O3'-HO3'	107.70	120.00	1
C3'-O3'-HO3'	107.59	120.00	1
C3'-O3'-HO3'	107.38	120.00	1
C3'-O3'-HO3'	107.34	120.00	1
C5'-O5'-HO5'	107.07	120.00	1
C5'-O5'-HO5'	106.48	120.00	1
C5'-O5'-HO5'	105.61	120.00	1
C5'-O5'-HO5'	105.53	120.00	1
C5'-O5'-HO5'	105.52	120.00	1
C5'-O5'-HO5'	105.36	120.00	1
C5'-O5'-HO5'	104.78	120.00	1
C5'-O5'-HO5'	104.55	120.00	1
C5'-O5'-HO5'	103.44	120.00	1
C5'-O5'-HO5'	102.70	120.00	1
H72-C7-H73	131.14	109.00	1
H72-C7-H73	131.15	109.00	1
H71-C7-H73	131.18	109.00	1
H72-C7-H73	131.19	109.00	1
C5-C7-H71	131.26	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H71-C7-H72	131.28	109.00	1
H71-C7-H73	131.30	109.00	1
H71-C7-H72	131.30	109.00	2
H72-C7-H73	131.30	109.00	1
C5-C7-H71	131.31	109.00	1
H71-C7-H72	131.31	109.00	1
H71-C7-H73	131.31	109.00	1
C5-C7-H72	131.32	109.00	1
H71-C7-H72	131.32	109.00	2
H72-C7-H73	131.33	109.00	1
H71-C7-H73	131.33	109.00	3
C5-C7-H72	131.33	109.00	2
C5-C7-H72	131.34	109.00	1
H72-C7-H73	131.34	109.00	1
H71-C7-H73	131.35	109.00	2
C5-C7-H71	131.35	109.00	1
H72-C7-H73	131.35	109.00	3
H71-C7-H72	131.35	109.00	2
H71-C7-H72	131.36	109.00	3
C5-C7-H72	131.36	109.00	1
H72-C7-H73	131.37	109.00	2
H71-C7-H73	131.37	109.00	1
C5-C7-H72	131.37	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H73	131.38	109.00	1
H71-C7-H73	131.38	109.00	4
H71-C7-H72	131.38	109.00	2
C5-C7-H71	131.38	109.00	2
C5-C7-H71	131.39	109.00	2
H72-C7-H73	131.39	109.00	2
H71-C7-H73	131.39	109.00	2
H71-C7-H72	131.39	109.00	2
C5-C7-H71	131.40	109.00	2
H72-C7-H73	131.40	109.00	3
H71-C7-H73	131.40	109.00	2
H71-C7-H72	131.40	109.00	1
H72-C7-H73	131.41	109.00	1
C5-C7-H72	131.41	109.00	2
H71-C7-H73	131.41	109.00	6
H71-C7-H73	131.42	109.00	5
H72-C7-H73	131.42	109.00	2
H72-C7-H73	131.43	109.00	3
H71-C7-H72	131.43	109.00	4
C5-C7-H71	131.43	109.00	2
H71-C7-H73	131.43	109.00	2
H71-C7-H72	131.44	109.00	2
C5-C7-H72	131.44	109.00	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H73	131.44	109.00	2
H72-C7-H73	131.44	109.00	3
H71-C7-H73	131.44	109.00	9
H71-C7-H72	131.45	109.00	2
H72-C7-H73	131.45	109.00	2
C5-C7-H71	131.45	109.00	2
H71-C7-H73	131.45	109.00	2
C5-C7-H71	131.46	109.00	3
H71-C7-H73	131.46	109.00	4
H71-C7-H72	131.46	109.00	3
C5-C7-H72	131.46	109.00	2
C5-C7-H73	131.46	109.00	1
H71-C7-H73	131.47	109.00	6
H72-C7-H73	131.47	109.00	7
C5-C7-H71	131.47	109.00	1
C5-C7-H72	131.47	109.00	1
H71-C7-H72	131.47	109.00	2
C5-C7-H73	131.47	109.00	1
C5-C7-H73	131.48	109.00	1
H71-C7-H73	131.48	109.00	3
C5-C7-H71	131.48	109.00	2
H72-C7-H73	131.48	109.00	1
H71-C7-H72	131.48	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H71-C7-H72	131.49	109.00	2
H72-C7-H73	131.49	109.00	4
H71-C7-H73	131.49	109.00	4
C5-C7-H73	131.49	109.00	3
C5-C7-H71	131.49	109.00	2
H71-C7-H73	131.50	109.00	2
C5-C7-H71	131.50	109.00	3
C5-C7-H72	131.50	109.00	1
H71-C7-H72	131.50	109.00	3
C5-C7-H73	131.50	109.00	1
H72-C7-H73	131.50	109.00	1
H71-C7-H73	131.51	109.00	5
C5-C7-H73	131.51	109.00	1
C5-C7-H72	131.51	109.00	4
C5-C7-H71	131.51	109.00	3
H71-C7-H72	131.51	109.00	1
C5-C7-H73	131.52	109.00	2
H71-C7-H73	131.52	109.00	2
H72-C7-H73	131.52	109.00	2
C5-C7-H72	131.52	109.00	2
H71-C7-H73	131.53	109.00	2
H71-C7-H72	131.53	109.00	6
H72-C7-H73	131.53	109.00	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H71	131.53	109.00	3
C5-C7-H72	131.53	109.00	1
C5-C7-H73	131.53	109.00	2
H72-C7-H73	131.54	109.00	5
C5-C7-H72	131.54	109.00	2
H71-C7-H72	131.54	109.00	3
C5-C7-H73	131.54	109.00	4
C5-C7-H71	131.54	109.00	2
C5-C7-H73	131.55	109.00	3
C5-C7-H72	131.55	109.00	2
H71-C7-H72	131.55	109.00	3
C5-C7-H71	131.55	109.00	1
H72-C7-H73	131.55	109.00	4
H71-C7-H73	131.55	109.00	1
C5-C7-H72	131.56	109.00	1
C5-C7-H71	131.56	109.00	3
C5-C7-H73	131.56	109.00	4
H72-C7-H73	131.56	109.00	2
C5-C7-H72	131.57	109.00	3
C5-C7-H71	131.57	109.00	2
H72-C7-H73	131.57	109.00	2
C5-C7-H73	131.57	109.00	7
H71-C7-H73	131.57	109.00	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H71-C7-H72	131.57	109.00	3
C5-C7-H72	131.58	109.00	5
H71-C7-H72	131.58	109.00	2
H72-C7-H73	131.58	109.00	5
H71-C7-H73	131.58	109.00	2
C5-C7-H71	131.58	109.00	1
H72-C7-H73	131.59	109.00	3
C5-C7-H73	131.59	109.00	2
C5-C7-H71	131.59	109.00	4
C5-C7-H72	131.59	109.00	2
H71-C7-H72	131.59	109.00	3
H71-C7-H72	131.60	109.00	4
C5-C7-H73	131.60	109.00	2
C5-C7-H71	131.60	109.00	2
C5-C7-H72	131.60	109.00	3
H71-C7-H73	131.60	109.00	1
C5-C7-H71	131.61	109.00	3
C5-C7-H72	131.61	109.00	2
H72-C7-H73	131.61	109.00	5
C5-C7-H73	131.61	109.00	5
H71-C7-H73	131.61	109.00	2
H72-C7-H73	131.62	109.00	4
C5-C7-H71	131.62	109.00	4

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H72	131.62	109.00	4
C5-C7-H73	131.62	109.00	3
H71-C7-H72	131.62	109.00	2
H71-C7-H73	131.62	109.00	1
H71-C7-H72	131.63	109.00	2
C5-C7-H72	131.63	109.00	3
H72-C7-H73	131.63	109.00	1
C5-C7-H73	131.63	109.00	3
C5-C7-H71	131.63	109.00	1
H72-C7-H73	131.64	109.00	2
C5-C7-H72	131.64	109.00	3
H71-C7-H73	131.64	109.00	5
C5-C7-H73	131.64	109.00	2
C5-C7-H71	131.64	109.00	2
H71-C7-H72	131.64	109.00	1
C5-C7-H72	131.65	109.00	5
C5-C7-H71	131.65	109.00	6
C5-C7-H73	131.65	109.00	3
H71-C7-H73	131.65	109.00	1
H72-C7-H73	131.65	109.00	1
H71-C7-H72	131.65	109.00	1
H71-C7-H73	131.66	109.00	1
H71-C7-H72	131.66	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H72	131.66	109.00	2
C5-C7-H71	131.66	109.00	1
C5-C7-H73	131.66	109.00	1
H72-C7-H73	131.66	109.00	2
C5-C7-H73	131.67	109.00	4
C5-C7-H71	131.67	109.00	1
H71-C7-H72	131.67	109.00	1
H71-C7-H72	131.68	109.00	3
C5-C7-H72	131.68	109.00	1
C5-C7-H71	131.68	109.00	1
C5-C7-H72	131.69	109.00	4
H71-C7-H72	131.69	109.00	2
C5-C7-H73	131.69	109.00	3
H71-C7-H73	131.69	109.00	4
C5-C7-H71	131.69	109.00	2
C5-C7-H72	131.70	109.00	5
C5-C7-H71	131.70	109.00	4
C5-C7-H73	131.70	109.00	1
H71-C7-H72	131.70	109.00	3
C5-C7-H73	131.71	109.00	1
H72-C7-H73	131.71	109.00	2
H71-C7-H73	131.71	109.00	1
H71-C7-H72	131.71	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H72	131.71	109.00	1
C5-C7-H71	131.71	109.00	1
C5-C7-H71	131.72	109.00	2
C5-C7-H72	131.72	109.00	5
H71-C7-H73	131.72	109.00	2
H72-C7-H73	131.72	109.00	1
C5-C7-H73	131.72	109.00	1
C5-C7-H73	131.73	109.00	3
C5-C7-H72	131.73	109.00	1
H72-C7-H73	131.73	109.00	1
H71-C7-H72	131.74	109.00	1
H72-C7-H73	131.74	109.00	2
C5-C7-H73	131.74	109.00	2
C5-C7-H72	131.74	109.00	1
H71-C7-H73	131.75	109.00	1
C5-C7-H73	131.75	109.00	3
C5-C7-H72	131.75	109.00	2
C5-C7-H71	131.75	109.00	2
H71-C7-H72	131.75	109.00	1
H71-C7-H72	131.76	109.00	1
H72-C7-H73	131.76	109.00	1
C5-C7-H73	131.76	109.00	1
H71-C7-H73	131.76	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H72	131.76	109.00	1
C5-C7-H71	131.76	109.00	1
C5-C7-H73	131.77	109.00	2
C5-C7-H71	131.77	109.00	4
H71-C7-H73	131.78	109.00	2
C5-C7-H72	131.78	109.00	2
C5-C7-H71	131.78	109.00	3
H72-C7-H73	131.78	109.00	2
C5-C7-H73	131.79	109.00	1
C5-C7-H72	131.79	109.00	2
C5-C7-H71	131.79	109.00	1
C5-C7-H72	131.80	109.00	1
C5-C7-H73	131.80	109.00	1
C5-C7-H71	131.80	109.00	1
C5-C7-H72	131.81	109.00	3
C5-C7-H73	131.81	109.00	1
C5-C7-H71	131.82	109.00	2
H71-C7-H73	131.82	109.00	2
C5-C7-H72	131.82	109.00	1
C5-C7-H71	131.83	109.00	1
C5-C7-H72	131.83	109.00	1
H71-C7-H73	131.83	109.00	1
C5-C7-H71	131.84	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H72	131.84	109.00	2
C5-C7-H73	131.86	109.00	1
C5-C7-H72	131.86	109.00	1
C5-C7-H72	131.87	109.00	3
C5-C7-H72	131.90	109.00	1
C5-C7-H72	131.91	109.00	1
C5-C7-H72	131.92	109.00	1
C5-C7-H71	131.96	109.00	1
C5-C7-H72	131.98	109.00	1
C5-C7-H73	132.00	109.00	1
C5-C7-H73	80.67	109.00	1
C5-C7-H73	80.66	109.00	1
C5-C7-H73	80.65	109.00	1
C5-C7-H73	80.64	109.00	1
C5-C7-H71	80.62	109.00	1
C5-C7-H72	80.61	109.00	2
C5-C7-H71	80.60	109.00	1
C5-C7-H73	80.60	109.00	1
C5-C7-H71	80.59	109.00	1
C5-C7-H72	80.58	109.00	1
C5-C7-H71	80.56	109.00	2
C5-C7-H73	80.55	109.00	2
C5-C7-H72	80.55	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H71-C7-H73	80.55	109.00	1
C5-C7-H71	80.55	109.00	1
C5-C7-H71	80.54	109.00	1
C5-C7-H73	80.54	109.00	1
C5-C7-H71	80.53	109.00	2
C5-C7-H72	80.53	109.00	1
C5-C7-H73	80.53	109.00	2
C5-C7-H73	80.52	109.00	4
H71-C7-H73	80.52	109.00	1
C5-C7-H71	80.52	109.00	1
C5-C7-H71	80.51	109.00	4
C5-C7-H72	80.51	109.00	2
C5-C7-H73	80.51	109.00	1
C5-C7-H73	80.50	109.00	1
C5-C7-H71	80.50	109.00	1
C5-C7-H72	80.50	109.00	1
C5-C7-H73	80.49	109.00	7
C5-C7-H72	80.49	109.00	1
C5-C7-H71	80.49	109.00	2
C5-C7-H73	80.48	109.00	5
C5-C7-H72	80.48	109.00	5
C5-C7-H71	80.48	109.00	2
C5-C7-H73	80.47	109.00	6

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H71	80.47	109.00	4
C5-C7-H72	80.47	109.00	2
H71-C7-H73	80.46	109.00	1
C5-C7-H73	80.46	109.00	2
H72-C7-H73	80.46	109.00	1
C5-C7-H72	80.46	109.00	4
C5-C7-H71	80.46	109.00	2
C5-C7-H73	80.45	109.00	6
C5-C7-H71	80.45	109.00	3
C5-C7-H72	80.45	109.00	1
C5-C7-H71	80.44	109.00	5
C5-C7-H73	80.44	109.00	5
C5-C7-H72	80.44	109.00	6
H71-C7-H72	80.43	109.00	1
C5-C7-H72	80.43	109.00	8
H72-C7-H73	80.43	109.00	1
C5-C7-H73	80.43	109.00	3
C5-C7-H71	80.43	109.00	3
C5-C7-H71	80.42	109.00	10
C5-C7-H72	80.42	109.00	10
C5-C7-H73	80.42	109.00	5
H71-C7-H72	80.42	109.00	2
H71-C7-H73	80.42	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H72-C7-H73	80.42	109.00	3
H71-C7-H73	80.41	109.00	3
C5-C7-H72	80.41	109.00	8
C5-C7-H73	80.41	109.00	8
H72-C7-H73	80.41	109.00	1
C5-C7-H71	80.41	109.00	10
H71-C7-H72	80.41	109.00	1
C5-C7-H72	80.40	109.00	7
C5-C7-H71	80.40	109.00	8
C5-C7-H73	80.40	109.00	4
H72-C7-H73	80.40	109.00	4
H71-C7-H72	80.40	109.00	1
H71-C7-H73	80.40	109.00	3
C5-C7-H71	80.39	109.00	10
H72-C7-H73	80.39	109.00	4
C5-C7-H73	80.39	109.00	9
H71-C7-H72	80.39	109.00	2
C5-C7-H72	80.39	109.00	7
H71-C7-H73	80.39	109.00	2
H71-C7-H73	80.38	109.00	2
H72-C7-H73	80.38	109.00	3
C5-C7-H73	80.38	109.00	10
H71-C7-H72	80.38	109.00	5

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H71	80.38	109.00	9
C5-C7-H72	80.38	109.00	3
C5-C7-H71	80.37	109.00	5
H72-C7-H73	80.37	109.00	3
C5-C7-H73	80.37	109.00	4
C5-C7-H72	80.37	109.00	6
H71-C7-H73	80.37	109.00	2
H71-C7-H72	80.37	109.00	3
H72-C7-H73	80.36	109.00	8
H71-C7-H72	80.36	109.00	7
C5-C7-H73	80.36	109.00	6
C5-C7-H72	80.36	109.00	8
H71-C7-H73	80.36	109.00	3
C5-C7-H71	80.36	109.00	6
H71-C7-H73	80.35	109.00	1
H71-C7-H72	80.35	109.00	3
H72-C7-H73	80.35	109.00	9
C5-C7-H72	80.35	109.00	8
C5-C7-H73	80.35	109.00	7
C5-C7-H71	80.35	109.00	9
C5-C7-H72	80.34	109.00	12
C5-C7-H71	80.34	109.00	4
H71-C7-H72	80.34	109.00	7

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H73	80.34	109.00	3
H71-C7-H73	80.34	109.00	4
H72-C7-H73	80.34	109.00	4
C5-C7-H72	80.33	109.00	13
C5-C7-H71	80.33	109.00	8
H72-C7-H73	80.33	109.00	11
H71-C7-H72	80.33	109.00	9
C5-C7-H73	80.33	109.00	14
H71-C7-H73	80.33	109.00	12
C5-C7-H71	80.32	109.00	2
C5-C7-H72	80.32	109.00	5
C5-C7-H73	80.32	109.00	6
H72-C7-H73	80.32	109.00	2
H71-C7-H72	80.32	109.00	1
H71-C7-H73	80.32	109.00	3
H71-C7-H73	80.31	109.00	10
H72-C7-H73	80.31	109.00	9
C5-C7-H73	80.31	109.00	12
C5-C7-H71	80.31	109.00	8
H71-C7-H72	80.31	109.00	9
C5-C7-H72	80.31	109.00	5
H71-C7-H73	80.30	109.00	9
C5-C7-H72	80.30	109.00	5

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H71	80.30	109.00	7
H71-C7-H72	80.30	109.00	12
H72-C7-H73	80.30	109.00	8
C5-C7-H73	80.30	109.00	5
C5-C7-H73	80.29	109.00	5
H71-C7-H72	80.29	109.00	10
H71-C7-H73	80.29	109.00	11
C5-C7-H72	80.29	109.00	4
H72-C7-H73	80.29	109.00	6
C5-C7-H71	80.29	109.00	3
H72-C7-H73	80.28	109.00	21
C5-C7-H71	80.28	109.00	10
H71-C7-H72	80.28	109.00	11
H71-C7-H73	80.28	109.00	9
C5-C7-H72	80.28	109.00	10
C5-C7-H73	80.28	109.00	6
H72-C7-H73	80.27	109.00	7
C5-C7-H71	80.27	109.00	3
H71-C7-H73	80.27	109.00	6
H71-C7-H72	80.27	109.00	11
C5-C7-H72	80.27	109.00	3
C5-C7-H73	80.27	109.00	4
H71-C7-H73	80.26	109.00	6

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H72-C7-H73	80.26	109.00	12
C5-C7-H71	80.26	109.00	4
H71-C7-H72	80.26	109.00	13
C5-C7-H72	80.26	109.00	4
C5-C7-H73	80.26	109.00	3
H72-C7-H73	80.25	109.00	9
H71-C7-H73	80.25	109.00	13
H71-C7-H72	80.25	109.00	12
C5-C7-H73	80.25	109.00	4
C5-C7-H71	80.25	109.00	7
C5-C7-H72	80.25	109.00	2
H72-C7-H73	80.24	109.00	6
C5-C7-H73	80.24	109.00	5
H71-C7-H72	80.24	109.00	9
H71-C7-H73	80.24	109.00	5
C5-C7-H71	80.24	109.00	3
C5-C7-H72	80.24	109.00	2
H71-C7-H73	80.23	109.00	10
H71-C7-H72	80.23	109.00	9
C5-C7-H71	80.23	109.00	2
C5-C7-H73	80.23	109.00	4
C5-C7-H72	80.23	109.00	2
H72-C7-H73	80.23	109.00	7

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H72-C7-H73	80.22	109.00	5
H71-C7-H72	80.22	109.00	10
C5-C7-H71	80.22	109.00	7
C5-C7-H73	80.22	109.00	6
H71-C7-H73	80.22	109.00	10
C5-C7-H72	80.22	109.00	3
H71-C7-H72	80.21	109.00	4
C5-C7-H73	80.21	109.00	2
H72-C7-H73	80.21	109.00	3
H71-C7-H73	80.21	109.00	5
C5-C7-H71	80.21	109.00	3
C5-C7-H72	80.21	109.00	2
H71-C7-H73	80.20	109.00	12
H72-C7-H73	80.20	109.00	5
H71-C7-H72	80.20	109.00	3
C5-C7-H71	80.20	109.00	3
C5-C7-H73	80.20	109.00	2
C5-C7-H72	80.19	109.00	2
H72-C7-H73	80.19	109.00	9
H71-C7-H73	80.19	109.00	7
H71-C7-H72	80.19	109.00	5
H72-C7-H73	80.18	109.00	5
C5-C7-H73	80.18	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H71-C7-H72	80.18	109.00	2
H71-C7-H73	80.18	109.00	5
C5-C7-H72	80.18	109.00	1
H72-C7-H73	80.17	109.00	4
C5-C7-H73	80.17	109.00	2
H71-C7-H73	80.17	109.00	3
H71-C7-H72	80.17	109.00	6
C5-C7-H72	80.17	109.00	1
C5-C7-H71	80.16	109.00	2
H71-C7-H72	80.16	109.00	2
H71-C7-H73	80.16	109.00	4
H72-C7-H73	80.16	109.00	3
H72-C7-H73	80.15	109.00	1
H71-C7-H72	80.15	109.00	3
C5-C7-H73	80.15	109.00	1
H71-C7-H73	80.15	109.00	1
H71-C7-H72	80.14	109.00	3
H72-C7-H73	80.14	109.00	1
H71-C7-H72	80.13	109.00	3
H71-C7-H73	80.13	109.00	1
H71-C7-H73	80.12	109.00	2
H72-C7-H73	80.12	109.00	1
H71-C7-H72	80.12	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H72	80.12	109.00	1
C5-C7-H73	80.12	109.00	1
H71-C7-H72	80.11	109.00	2
H71-C7-H73	80.11	109.00	1
C5-C7-H73	80.11	109.00	1
H72-C7-H73	80.11	109.00	1
H71-C7-H72	80.10	109.00	2
H72-C7-H73	80.10	109.00	1
H71-C7-H73	80.09	109.00	1
C5-C7-H71	80.08	109.00	1
H71-C7-H72	80.08	109.00	2
H72-C7-H73	80.08	109.00	1
H71-C7-H72	80.07	109.00	3
H72-C7-H73	80.05	109.00	1
C5-C7-H72	80.04	109.00	1
H71-C7-H72	80.03	109.00	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	0.00	0
2	0.00	0
3	0.00	0

Model ID	Clash score	Number of clashes
4	0.00	0
5	0.00	0
6	0.00	0
7	0.00	0
8	0.00	0
9	0.00	0
10	0.00	0

All 0 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	Analysed	Favored	Allowed	Outliers
1	835	802	27	6
2	835	801	28	6
3	835	798	34	3
4	835	798	28	9
5	835	803	26	6
6	835	800	31	4
7	835	802	29	4
8	835	804	29	2
9	835	793	35	7
10	835	797	33	5

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	719	641	43	35
2	719	648	41	30
3	719	636	54	29
4	719	625	49	45
5	719	648	37	34
6	719	640	46	33
7	719	641	47	31
8	719	630	53	36
9	719	646	42	31
10	719	643	50	26

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	4	ARG
1	A	40	GLN
1	A	44	THR
1	A	51	SER
1	A	79	LYS
1	B	51	THR
1	C	3	SER
1	C	63	THR
1	C	76	ASN
1	C	85	SER
1	C	87	VAL

Model ID	Chain	Residue ID	Residue type
1	C	88	THR
1	D	5	GLU
1	D	22	THR
1	D	61	SER
1	D	86	LYS
1	E	22	THR
1	E	27	ARG
1	E	44	THR
1	E	45	ASP
1	E	51	SER
1	F	74	THR
1	G	85	SER
1	H	57	SER
1	H	61	SER
1	K	1	LEU
1	K	10	SER
1	K	17	CYS
1	K	29	CYS
1	K	30	ASN
1	K	34	CYS
1	K	41	THR
1	K	47	LEU
1	K	52	CYS

Model ID	Chain	Residue ID	Residue type
1	K	57	SER
2	A	40	GLN
2	A	44	THR
2	A	50	SER
2	A	51	SER
2	B	12	ILE
2	B	74	THR
2	C	5	SER
2	C	25	ASN
2	C	42	MET
2	C	63	THR
2	C	85	SER
2	D	22	THR
2	D	37	ASN
2	D	48	SER
2	D	61	SER
2	D	86	LYS
2	E	22	THR
2	E	44	THR
2	E	51	SER
2	F	74	THR
2	G	63	THR
2	G	85	SER

Model ID	Chain	Residue ID	Residue type
2	H	54	ASN
2	H	61	SER
2	H	93	SER
2	H	95	LYS
2	K	1	LEU
2	K	10	SER
2	K	29	CYS
2	K	68	SER
3	A	22	THR
3	A	32	GLN
3	A	44	THR
3	B	51	THR
3	C	7	ARG
3	C	29	ARG
3	C	85	SER
3	C	88	THR
3	D	37	ASN
3	E	22	THR
3	E	23	GLU
3	E	27	ARG
3	E	44	THR
3	E	51	SER
3	F	74	THR

Model ID	Chain	Residue ID	Residue type
3	G	3	SER
3	G	5	SER
3	G	6	ASN
3	G	63	THR
3	G	85	SER
3	H	57	SER
3	H	61	SER
3	K	1	LEU
3	K	10	SER
3	K	29	CYS
3	K	41	THR
3	K	43	GLU
3	K	46	SER
3	K	52	CYS
4	A	22	THR
4	A	40	GLN
4	A	44	THR
4	A	51	SER
4	B	48	VAL
4	B	49	THR
4	B	51	THR
4	B	52	GLU
4	C	51	GLU

Model ID	Chain	Residue ID	Residue type
4	C	88	THR
4	D	26	SER
4	D	56	ARG
4	D	57	SER
4	D	61	SER
4	D	83	GLU
4	D	92	THR
4	D	93	SER
4	E	22	THR
4	E	44	THR
4	E	48	PHE
4	F	51	THR
4	G	3	SER
4	G	5	SER
4	G	6	ASN
4	G	12	PHE
4	G	21	LEU
4	G	59	ASP
4	G	63	THR
4	G	85	SER
4	H	61	SER
4	H	66	THR
4	H	82	SER

Model ID	Chain	Residue ID	Residue type
4	H	93	SER
4	K	1	LEU
4	K	4	ASP
4	K	10	SER
4	K	34	CYS
4	K	46	SER
4	K	47	LEU
4	K	55	ARG
4	K	57	SER
4	K	58	SER
4	K	68	SER
4	K	75	TRP
4	K	89	ARG
5	A	40	GLN
5	A	41	ASP
5	A	44	THR
5	A	50	SER
5	B	51	THR
5	C	3	SER
5	C	51	GLU
5	C	88	THR
5	D	14	VAL
5	D	22	THR

Model ID	Chain	Residue ID	Residue type
5	D	57	SER
5	D	58	THR
5	D	61	SER
5	D	86	LYS
5	E	21	SER
5	E	44	THR
5	E	50	SER
5	E	51	SER
5	F	51	THR
5	F	74	THR
5	F	75	LEU
5	G	3	SER
5	G	5	SER
5	G	37	TYR
5	G	59	ASP
5	G	76	ASN
5	G	85	SER
5	H	61	SER
5	K	1	LEU
5	K	10	SER
5	K	29	CYS
5	K	30	ASN
5	K	57	SER

Model ID	Chain	Residue ID	Residue type
5	K	68	SER
6	A	22	THR
6	A	23	GLU
6	A	37	GLU
6	A	40	GLN
6	A	44	THR
6	A	51	SER
6	B	46	ASP
6	B	52	GLU
6	B	74	THR
6	C	58	ARG
6	C	59	ASP
6	C	63	THR
6	C	82	LYS
6	C	88	THR
6	D	61	SER
6	E	22	THR
6	E	23	GLU
6	E	44	THR
6	E	50	SER
6	F	24	ILE
6	F	36	LEU
6	F	52	GLU

Model ID	Chain	Residue ID	Residue type
6	G	63	THR
6	G	76	ASN
6	G	85	SER
6	H	22	THR
6	H	61	SER
6	H	93	SER
6	K	1	LEU
6	K	10	SER
6	K	20	ILE
6	K	41	THR
6	K	55	ARG
7	A	28	LYS
7	A	44	THR
7	B	51	THR
7	B	74	THR
7	C	45	LEU
7	C	63	THR
7	C	85	SER
7	C	88	THR
7	D	6	SER
7	D	57	SER
7	D	61	SER
7	E	4	ARG

Model ID	Chain	Residue ID	Residue type
7	E	21	SER
7	E	44	THR
7	E	50	SER
7	E	51	SER
7	E	79	LYS
7	F	74	THR
7	G	5	SER
7	G	63	THR
7	G	85	SER
7	H	3	ARG
7	H	21	ASP
7	H	57	SER
7	H	61	SER
7	K	1	LEU
7	K	4	ASP
7	K	10	SER
7	K	32	THR
7	K	57	SER
7	K	68	SER
8	A	4	ARG
8	A	22	THR
8	A	32	GLN
8	A	41	ASP

Model ID	Chain	Residue ID	Residue type
8	A	50	SER
8	A	51	SER
8	B	51	THR
8	B	74	THR
8	C	3	SER
8	C	63	THR
8	C	85	SER
8	C	94	VAL
8	D	61	SER
8	D	92	THR
8	E	41	ASP
8	E	44	THR
8	E	45	ASP
8	E	50	SER
8	E	51	SER
8	F	8	THR
8	F	51	THR
8	F	74	THR
8	G	5	SER
8	G	25	ASN
8	G	63	THR
8	G	85	SER
8	G	88	THR

Model ID	Chain	Residue ID	Residue type
8	H	15	LEU
8	H	61	SER
8	K	1	LEU
8	K	19	GLU
8	K	29	CYS
8	K	30	ASN
8	K	47	LEU
8	K	57	SER
8	K	68	SER
9	A	51	SER
9	B	51	THR
9	B	74	THR
9	C	3	SER
9	C	59	ASP
9	C	63	THR
9	D	22	THR
9	D	61	SER
9	D	92	THR
9	E	22	THR
9	E	23	GLU
9	E	41	ASP
9	E	44	THR
9	E	49	GLN

Model ID	Chain	Residue ID	Residue type
9	E	51	SER
9	E	69	GLU
9	F	51	THR
9	F	74	THR
9	G	60	ASN
9	G	85	SER
9	H	92	THR
9	H	93	SER
9	K	1	LEU
9	K	4	ASP
9	K	10	SER
9	K	23	GLU
9	K	41	THR
9	K	46	SER
9	K	57	SER
9	K	68	SER
9	K	75	TRP
10	A	40	GLN
10	A	44	THR
10	A	50	SER
10	B	51	THR
10	B	74	THR
10	C	5	SER

Model ID	Chain	Residue ID	Residue type
10	C	63	THR
10	C	85	SER
10	C	88	THR
10	D	21	ASP
10	D	61	SER
10	E	22	THR
10	E	50	SER
10	E	51	SER
10	G	3	SER
10	G	63	THR
10	G	76	ASN
10	G	85	SER
10	H	21	ASP
10	H	30	SER
10	H	61	SER
10	K	1	LEU
10	K	26	THR
10	K	57	SER
10	K	68	SER
10	K	89	ARG

Fit of model to data used for modeling ?

Mutagenesis

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

NMR

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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