

Integrative Structure Validation Report

July 22, 2024 - 03:51 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	8ZZT
PDB-Dev ID	PDBDEV_00000029
Structure Title	Complex of Ubch5c, 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

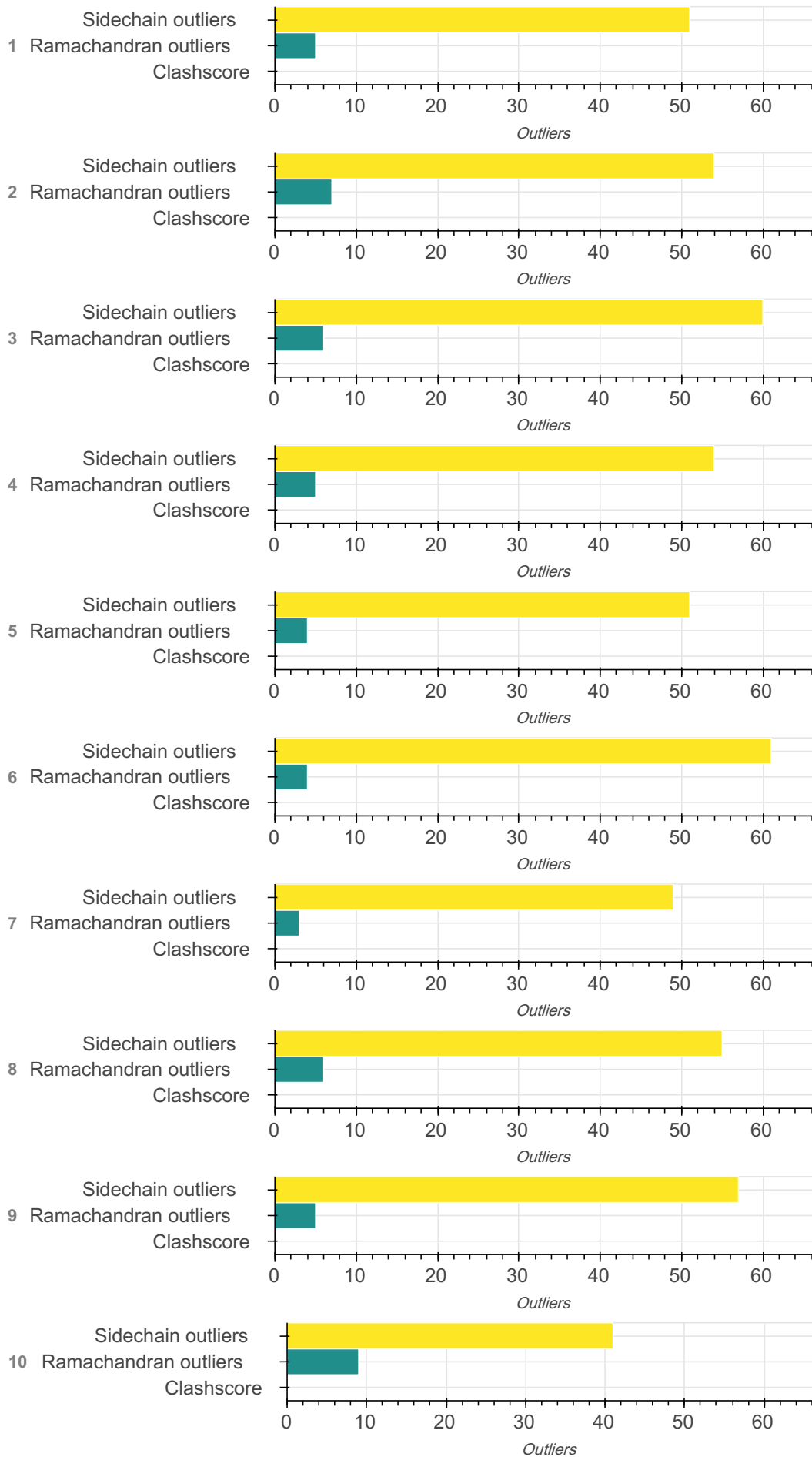
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

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 12 subunits in each model. A total of 3 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 12 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 N18S mutant	C	C	107
1	6	3	H2A N18S mutant	G	G	107
1	7	4	H2B S121A mutant	D	D	95
1	8	4	H2B S121A mutant	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
1	12	8	UbcH5c	L	L	153

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
2	1	1	H3	A	A	99
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 N18S mutant	C	C	107
2	6	3	H2A N18S mutant	G	G	107
2	7	4	H2B S121A mutant	D	D	95
2	8	4	H2B S121A mutant	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
2	12	8	UbcH5c	L	L	153
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 N18S mutant	C	C	107
3	6	3	H2A N18S mutant	G	G	107
3	7	4	H2B S121A mutant	D	D	95
3	8	4	H2B S121A mutant	H	H	95
3	9	5	DNA strand 1	I	I	147
3	10	6	DNA strand 2	J	J	147

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
3	11	7	RNF168 RING domain	K	K	91
3	12	8	UbcH5c	L	L	153
4	1	1	H3	A	A	99
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 N18S mutant	C	C	107
4	6	3	H2A N18S mutant	G	G	107
4	7	4	H2B S121A mutant	D	D	95
4	8	4	H2B S121A mutant	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
4	12	8	UbcH5c	L	L	153
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 N18S mutant	C	C	107
5	6	3	H2A N18S mutant	G	G	107
5	7	4	H2B S121A mutant	D	D	95
5	8	4	H2B S121A mutant	H	H	95

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
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
5	12	8	UbcH5c	L	L	153
6	1	1	H3	A	A	99
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 N18S mutant	C	C	107
6	6	3	H2A N18S mutant	G	G	107
6	7	4	H2B S121A mutant	D	D	95
6	8	4	H2B S121A mutant	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
6	12	8	UbcH5c	L	L	153
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 N18S mutant	C	C	107
7	6	3	H2A N18S mutant	G	G	107

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
7	7	4	H2B S121A mutant	D	D	95
7	8	4	H2B S121A mutant	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
7	12	8	UbcH5c	L	L	153
8	1	1	H3	A	A	99
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 N18S mutant	C	C	107
8	6	3	H2A N18S mutant	G	G	107
8	7	4	H2B S121A mutant	D	D	95
8	8	4	H2B S121A mutant	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
8	12	8	UbcH5c	L	L	153
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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
9	5	3	H2A N18S mutant	C	C	107
9	6	3	H2A N18S mutant	G	G	107
9	7	4	H2B S121A mutant	D	D	95
9	8	4	H2B S121A mutant	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
9	12	8	UbcH5c	L	L	153
10	1	1	H3	A	A	99
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 N18S mutant	C	C	107
10	6	3	H2A N18S mutant	G	G	107
10	7	4	H2B S121A mutant	D	D	95
10	8	4	H2B S121A mutant	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
10	12	8	UbcH5c	L	L	153

Datasets used for modeling ?

There are 3 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Integrative model	PDB-Dev	PDBDEV_00000028
2	Experimental model	PDB	1X23
3	Other	File	10.1038/s41467-019-09756-z

Representation ?

This entry has only one representation and includes 0 rigid bodies and 12 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
L	-	1-153

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 is 1 software package 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/

Data quality ?

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 47340 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
ND2--HD22	0.97	0.86	3
N--H	0.97	0.86	5
N--H	0.98	0.86	8878
ND2--HD22	0.98	0.86	324
NE2--HE22	0.98	0.86	358
NE2--HE2	0.98	0.86	115
C5'--H5''	1.09	0.97	2940
C3'--H3'	1.09	0.97	2940

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
C7--H71	1.09	0.97	870
ND2--HD21	0.98	0.86	295
C7--H73	1.09	0.97	870
C7--H72	1.09	0.97	870
C5'--H5'	1.09	0.97	2940
NE2--HE21	0.98	0.86	253
C1'--H1'	1.09	0.97	2940
C4'--H4'	1.09	0.97	2940
OH--HH	0.96	0.84	169
ND1--HD1	0.98	0.86	76
NE1--HE1	0.98	0.86	40
NE--HE	0.98	0.86	489
OG1--HG1	0.96	0.84	212
OG--HG	0.96	0.84	130
SG--HG	1.32	1.20	2
OG1--HG1	0.97	0.84	360
ND2--HD21	0.99	0.86	45
NE--HE	0.99	0.86	491
N--H	0.99	0.86	607
OG--HG	0.97	0.84	431
OH--HH	0.97	0.84	206
ND1--HD1	0.99	0.86	14
ND2--HD22	0.99	0.86	13

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2--HE21	0.99	0.86	107
SG--HG	1.33	1.20	138
NE1--HE1	0.99	0.86	10
NE2--HE2	0.99	0.86	45
NE2--HE22	0.99	0.86	2
O5'--HO5'	0.97	0.84	10
O3'--HO3'	0.97	0.84	10
OH--HH	0.98	0.84	5
OG1--HG1	0.98	0.84	8
OG--HG	0.98	0.84	9
NE--HE	1.00	0.86	20
NH1--HH12	1.00	0.86	682
NH2--HH22	1.00	0.86	638
NH2--HH21	1.00	0.86	630
NH1--HH11	1.00	0.86	683
NZ--HZ1	1.03	0.89	1
NZ--HZ2	1.03	0.89	2
NH2--HH21	1.01	0.86	342
NH2--HH22	1.01	0.86	345
NH1--HH11	1.01	0.86	298
NH1--HH12	1.01	0.86	295
N6--H62	1.01	0.86	870
NZ--HZ3	1.04	0.89	660

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--HZ1	1.04	0.89	680
NZ--HZ2	1.04	0.89	654
N4--H41	1.01	0.86	592
N6--H61	1.01	0.86	868
N3--H3	1.01	0.86	866
N4--H42	1.01	0.86	589
N2--H21	1.01	0.86	592
N1--H1	1.01	0.86	594
C8--H8	1.08	0.93	1470
N2--H22	1.01	0.86	546
NH2--HH22	1.02	0.86	17
NZ--HZ1	1.05	0.89	29
NH2--HH21	1.02	0.86	28
NH1--HH12	1.02	0.86	23
N3--H3	1.02	0.86	4
N4--H41	1.02	0.86	8
N1--H1	1.02	0.86	6
N2--H22	1.02	0.86	54
NZ--HZ3	1.05	0.89	50
NH1--HH11	1.02	0.86	19
NZ--HZ2	1.05	0.89	54
N4--H42	1.02	0.86	11
N2--H21	1.02	0.86	8

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
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 1022 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'	107.22	120.00	1
C5'-O5'-HO5'	106.77	120.00	1
C5'-O5'-HO5'	106.75	120.00	1
C5'-O5'-HO5'	106.61	120.00	1
C3'-O3'-HO3'	106.57	120.00	1
C5'-O5'-HO5'	106.52	120.00	1
C5'-O5'-HO5'	106.27	120.00	1
C5'-O5'-HO5'	106.00	120.00	1
C3'-O3'-HO3'	106.00	120.00	1
C3'-O3'-HO3'	105.82	120.00	1
C3'-O3'-HO3'	105.81	120.00	1
C5'-O5'-HO5'	105.74	120.00	1
C3'-O3'-HO3'	105.40	120.00	1
C3'-O3'-HO3'	105.11	120.00	1
C3'-O3'-HO3'	105.03	120.00	1
C5'-O5'-HO5'	104.95	120.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5'-O5'-HO5'	104.94	120.00	1
C5'-O5'-HO5'	104.85	120.00	1
C3'-O3'-HO3'	104.80	120.00	1
C3'-O3'-HO3'	103.60	120.00	1
C5-C7-H71	130.97	109.00	1
H71-C7-H72	131.10	109.00	1
H71-C7-H73	131.15	109.00	2
H71-C7-H72	131.16	109.00	1
H72-C7-H73	131.19	109.00	1
C5-C7-H71	131.20	109.00	1
H71-C7-H73	131.20	109.00	1
H72-C7-H73	131.22	109.00	1
H71-C7-H72	131.24	109.00	1
H71-C7-H73	131.25	109.00	1
H71-C7-H73	131.26	109.00	1
H72-C7-H73	131.28	109.00	1
C5-C7-H71	131.29	109.00	1
C5-C7-H72	131.29	109.00	1
H71-C7-H73	131.29	109.00	1
C5-C7-H73	131.29	109.00	1
H71-C7-H73	131.30	109.00	1
H71-C7-H72	131.30	109.00	1
H71-C7-H72	131.31	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H72-C7-H73	131.32	109.00	1
H71-C7-H72	131.33	109.00	1
C5-C7-H72	131.34	109.00	1
H71-C7-H72	131.34	109.00	2
H72-C7-H73	131.34	109.00	1
C5-C7-H72	131.35	109.00	1
H72-C7-H73	131.35	109.00	1
H71-C7-H72	131.36	109.00	1
H71-C7-H73	131.36	109.00	2
C5-C7-H71	131.36	109.00	1
C5-C7-H72	131.36	109.00	1
H72-C7-H73	131.36	109.00	1
C5-C7-H71	131.37	109.00	1
H72-C7-H73	131.37	109.00	1
H71-C7-H72	131.37	109.00	1
C5-C7-H73	131.38	109.00	1
H71-C7-H72	131.38	109.00	2
C5-C7-H72	131.38	109.00	1
H71-C7-H73	131.39	109.00	2
H71-C7-H72	131.39	109.00	2
H72-C7-H73	131.39	109.00	1
H71-C7-H72	131.40	109.00	3
H71-C7-H73	131.40	109.00	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H72	131.40	109.00	1
H72-C7-H73	131.41	109.00	1
C5-C7-H73	131.41	109.00	1
H71-C7-H73	131.41	109.00	1
C5-C7-H71	131.41	109.00	1
H71-C7-H73	131.42	109.00	4
H71-C7-H72	131.42	109.00	1
C5-C7-H71	131.42	109.00	1
C5-C7-H72	131.42	109.00	1
H71-C7-H73	131.43	109.00	1
C5-C7-H71	131.43	109.00	1
H71-C7-H72	131.43	109.00	5
H71-C7-H73	131.44	109.00	4
C5-C7-H73	131.44	109.00	1
C5-C7-H71	131.44	109.00	1
H71-C7-H72	131.44	109.00	1
C5-C7-H72	131.44	109.00	1
H71-C7-H73	131.45	109.00	6
H71-C7-H72	131.45	109.00	1
H71-C7-H73	131.46	109.00	3
C5-C7-H72	131.46	109.00	2
H71-C7-H73	131.47	109.00	2
H72-C7-H73	131.47	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H71-C7-H72	131.47	109.00	1
C5-C7-H73	131.47	109.00	2
C5-C7-H71	131.47	109.00	1
H71-C7-H73	131.48	109.00	1
H71-C7-H72	131.48	109.00	1
C5-C7-H71	131.48	109.00	1
C5-C7-H72	131.48	109.00	1
C5-C7-H72	131.49	109.00	1
H71-C7-H73	131.49	109.00	3
H72-C7-H73	131.49	109.00	1
C5-C7-H73	131.49	109.00	4
H71-C7-H72	131.49	109.00	2
C5-C7-H71	131.49	109.00	1
C5-C7-H72	131.50	109.00	1
H71-C7-H72	131.50	109.00	4
H71-C7-H73	131.50	109.00	2
H72-C7-H73	131.50	109.00	1
H71-C7-H73	131.51	109.00	2
H71-C7-H72	131.51	109.00	1
C5-C7-H72	131.51	109.00	1
C5-C7-H72	131.52	109.00	4
C5-C7-H73	131.52	109.00	1
H71-C7-H73	131.52	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H71	131.52	109.00	1
H71-C7-H73	131.53	109.00	3
H72-C7-H73	131.53	109.00	1
H71-C7-H73	131.54	109.00	1
C5-C7-H72	131.54	109.00	2
C5-C7-H71	131.54	109.00	1
C5-C7-H73	131.54	109.00	1
H71-C7-H72	131.54	109.00	2
H72-C7-H73	131.54	109.00	1
H71-C7-H72	131.55	109.00	1
C5-C7-H71	131.55	109.00	3
H72-C7-H73	131.55	109.00	1
H71-C7-H73	131.55	109.00	1
C5-C7-H72	131.55	109.00	2
C5-C7-H73	131.55	109.00	1
H71-C7-H72	131.56	109.00	1
C5-C7-H73	131.56	109.00	4
H72-C7-H73	131.56	109.00	2
C5-C7-H71	131.56	109.00	2
C5-C7-H72	131.56	109.00	1
H72-C7-H73	131.57	109.00	1
H71-C7-H73	131.57	109.00	3
H71-C7-H72	131.57	109.00	2

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

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H71-C7-H72	131.62	109.00	1
C5-C7-H71	131.62	109.00	1
C5-C7-H72	131.62	109.00	3
C5-C7-H73	131.62	109.00	1
H72-C7-H73	131.63	109.00	1
C5-C7-H73	131.63	109.00	1
C5-C7-H72	131.63	109.00	1
H71-C7-H72	131.63	109.00	2
H71-C7-H73	131.63	109.00	1
H71-C7-H73	131.64	109.00	2
C5-C7-H72	131.64	109.00	5
C5-C7-H73	131.64	109.00	1
H72-C7-H73	131.64	109.00	2
H71-C7-H72	131.64	109.00	1
H71-C7-H73	131.65	109.00	2
C5-C7-H72	131.65	109.00	3
C5-C7-H73	131.65	109.00	1
C5-C7-H71	131.65	109.00	1
C5-C7-H72	131.66	109.00	3
H71-C7-H73	131.66	109.00	1
C5-C7-H71	131.66	109.00	1
C5-C7-H73	131.66	109.00	4
C5-C7-H72	131.67	109.00	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H73	131.67	109.00	3
H72-C7-H73	131.67	109.00	2
H71-C7-H72	131.67	109.00	1
H71-C7-H73	131.68	109.00	2
C5-C7-H73	131.68	109.00	3
C5-C7-H72	131.68	109.00	1
C5-C7-H71	131.68	109.00	2
H71-C7-H72	131.68	109.00	1
C5-C7-H72	131.69	109.00	1
H71-C7-H73	131.69	109.00	1
C5-C7-H73	131.69	109.00	1
C5-C7-H72	131.70	109.00	1
C5-C7-H73	131.70	109.00	1
C5-C7-H73	131.71	109.00	2
H71-C7-H73	131.72	109.00	1
C5-C7-H72	131.72	109.00	2
C5-C7-H71	131.72	109.00	1
H72-C7-H73	131.73	109.00	1
C5-C7-H72	131.73	109.00	6
C5-C7-H71	131.73	109.00	1
H71-C7-H72	131.73	109.00	1
C5-C7-H73	131.73	109.00	1
C5-C7-H73	131.74	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H71-C7-H72	131.74	109.00	2
H71-C7-H72	131.75	109.00	1
C5-C7-H73	131.75	109.00	2
C5-C7-H71	131.75	109.00	1
C5-C7-H72	131.75	109.00	1
C5-C7-H72	131.76	109.00	2
H72-C7-H73	131.76	109.00	1
H71-C7-H73	131.77	109.00	1
C5-C7-H73	131.77	109.00	1
C5-C7-H72	131.77	109.00	1
C5-C7-H73	131.78	109.00	2
C5-C7-H72	131.79	109.00	1
C5-C7-H71	131.80	109.00	1
C5-C7-H73	131.81	109.00	2
C5-C7-H72	131.81	109.00	2
H71-C7-H72	131.81	109.00	1
C5-C7-H72	131.82	109.00	3
C5-C7-H72	131.84	109.00	1
H71-C7-H73	131.85	109.00	1
C5-C7-H73	131.85	109.00	1
C5-C7-H72	131.87	109.00	2
C5-C7-H72	131.88	109.00	1
H71-C7-H72	131.91	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H73	131.91	109.00	1
C5-C7-H72	131.92	109.00	1
C5-C7-H73	131.94	109.00	1
H71-C7-H73	131.98	109.00	1
C5-C7-H73	131.98	109.00	1
C5-C7-H72	131.98	109.00	1
C5-C7-H72	131.99	109.00	1
C5-C7-H72	132.13	109.00	1
C5-C7-H72	132.33	109.00	1
C5-C7-H71	80.81	109.00	1
C5-C7-H71	80.73	109.00	1
C5-C7-H71	80.65	109.00	1
C5-C7-H72	80.61	109.00	1
C5-C7-H72	80.58	109.00	1
C5-C7-H71	80.56	109.00	1
C5-C7-H72	80.56	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-H72	80.54	109.00	1
C5-C7-H71	80.53	109.00	1
C5-C7-H72	80.53	109.00	2
C5-C7-H73	80.53	109.00	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H73	80.52	109.00	1
H72-C7-H73	80.52	109.00	1
C5-C7-H71	80.51	109.00	2
C5-C7-H73	80.51	109.00	1
H71-C7-H72	80.51	109.00	1
C5-C7-H72	80.51	109.00	1
C5-C7-H72	80.50	109.00	4
C5-C7-H71	80.50	109.00	5
C5-C7-H73	80.50	109.00	2
H72-C7-H73	80.50	109.00	1
C5-C7-H72	80.49	109.00	3
C5-C7-H71	80.49	109.00	3
H72-C7-H73	80.49	109.00	1
H71-C7-H72	80.49	109.00	1
C5-C7-H73	80.49	109.00	2
C5-C7-H72	80.48	109.00	5
C5-C7-H71	80.48	109.00	2
C5-C7-H73	80.48	109.00	1
H72-C7-H73	80.48	109.00	1
C5-C7-H73	80.47	109.00	3
C5-C7-H72	80.47	109.00	1
C5-C7-H71	80.47	109.00	1
C5-C7-H73	80.46	109.00	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H71	80.46	109.00	1
C5-C7-H73	80.45	109.00	6
H71-C7-H72	80.45	109.00	1
C5-C7-H72	80.45	109.00	1
C5-C7-H71	80.45	109.00	2
H71-C7-H73	80.45	109.00	1
H72-C7-H73	80.45	109.00	1
H72-C7-H73	80.44	109.00	2
C5-C7-H71	80.44	109.00	3
C5-C7-H72	80.44	109.00	1
C5-C7-H73	80.43	109.00	3
C5-C7-H71	80.43	109.00	4
H72-C7-H73	80.43	109.00	2
C5-C7-H72	80.43	109.00	2
H71-C7-H73	80.43	109.00	1
C5-C7-H71	80.42	109.00	6
H72-C7-H73	80.42	109.00	2
C5-C7-H72	80.42	109.00	9
C5-C7-H73	80.42	109.00	4
C5-C7-H72	80.41	109.00	3
H71-C7-H72	80.41	109.00	2
C5-C7-H73	80.41	109.00	3
C5-C7-H71	80.41	109.00	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H72-C7-H73	80.41	109.00	1
C5-C7-H73	80.40	109.00	1
C5-C7-H72	80.40	109.00	1
H71-C7-H73	80.40	109.00	1
C5-C7-H71	80.40	109.00	3
H72-C7-H73	80.40	109.00	1
C5-C7-H72	80.39	109.00	7
H71-C7-H72	80.39	109.00	2
C5-C7-H71	80.39	109.00	5
C5-C7-H73	80.39	109.00	2
H71-C7-H73	80.39	109.00	3
C5-C7-H71	80.38	109.00	6
H72-C7-H73	80.38	109.00	1
C5-C7-H73	80.38	109.00	2
C5-C7-H72	80.38	109.00	1
C5-C7-H71	80.37	109.00	6
C5-C7-H72	80.37	109.00	2
H71-C7-H72	80.37	109.00	4
C5-C7-H73	80.37	109.00	4
H72-C7-H73	80.37	109.00	1
H71-C7-H73	80.37	109.00	1
C5-C7-H71	80.36	109.00	6
C5-C7-H73	80.36	109.00	4

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H72-C7-H73	80.36	109.00	6
H71-C7-H73	80.36	109.00	1
H71-C7-H72	80.36	109.00	9
C5-C7-H72	80.36	109.00	4
H71-C7-H72	80.35	109.00	4
H71-C7-H73	80.35	109.00	3
C5-C7-H72	80.35	109.00	2
C5-C7-H73	80.35	109.00	3
C5-C7-H71	80.35	109.00	7
H72-C7-H73	80.35	109.00	4
C5-C7-H73	80.34	109.00	8
H72-C7-H73	80.34	109.00	4
H71-C7-H73	80.34	109.00	4
C5-C7-H71	80.34	109.00	6
C5-C7-H72	80.34	109.00	1
H71-C7-H72	80.34	109.00	3
H72-C7-H73	80.33	109.00	11
H71-C7-H73	80.33	109.00	6
C5-C7-H71	80.33	109.00	8
H71-C7-H72	80.33	109.00	5
C5-C7-H72	80.33	109.00	2
C5-C7-H73	80.33	109.00	5
H71-C7-H72	80.32	109.00	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H73	80.32	109.00	4
C5-C7-H71	80.32	109.00	2
C5-C7-H72	80.32	109.00	3
H72-C7-H73	80.32	109.00	2
C5-C7-H71	80.31	109.00	9
H71-C7-H72	80.31	109.00	4
C5-C7-H73	80.31	109.00	4
H71-C7-H73	80.31	109.00	3
H72-C7-H73	80.31	109.00	6
C5-C7-H72	80.31	109.00	1
C5-C7-H71	80.30	109.00	7
H72-C7-H73	80.30	109.00	10
C5-C7-H72	80.30	109.00	5
H71-C7-H72	80.30	109.00	6
C5-C7-H73	80.30	109.00	1
H71-C7-H73	80.30	109.00	2
H72-C7-H73	80.29	109.00	6
C5-C7-H72	80.29	109.00	1
C5-C7-H71	80.29	109.00	5
H71-C7-H73	80.29	109.00	5
H71-C7-H72	80.29	109.00	6
C5-C7-H73	80.29	109.00	5
C5-C7-H73	80.28	109.00	5

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H72-C7-H73	80.28	109.00	6
C5-C7-H71	80.28	109.00	4
H71-C7-H73	80.28	109.00	4
H71-C7-H72	80.28	109.00	2
C5-C7-H72	80.28	109.00	1
H72-C7-H73	80.27	109.00	7
C5-C7-H72	80.27	109.00	2
C5-C7-H71	80.27	109.00	1
H71-C7-H72	80.27	109.00	8
H71-C7-H73	80.27	109.00	8
C5-C7-H73	80.27	109.00	8
C5-C7-H73	80.26	109.00	3
H71-C7-H72	80.26	109.00	6
H72-C7-H73	80.26	109.00	5
H71-C7-H73	80.26	109.00	4
C5-C7-H72	80.26	109.00	2
C5-C7-H71	80.26	109.00	1
C5-C7-H73	80.25	109.00	4
C5-C7-H71	80.25	109.00	3
H72-C7-H73	80.25	109.00	6
H71-C7-H73	80.25	109.00	5
C5-C7-H72	80.25	109.00	2
H71-C7-H72	80.25	109.00	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H71-C7-H73	80.24	109.00	2
H72-C7-H73	80.24	109.00	5
C5-C7-H72	80.24	109.00	3
H71-C7-H72	80.24	109.00	3
C5-C7-H71	80.24	109.00	4
H71-C7-H72	80.23	109.00	7
H71-C7-H73	80.23	109.00	5
C5-C7-H72	80.23	109.00	2
C5-C7-H73	80.23	109.00	3
H72-C7-H73	80.23	109.00	6
C5-C7-H71	80.23	109.00	1
H72-C7-H73	80.22	109.00	3
C5-C7-H72	80.22	109.00	3
C5-C7-H71	80.22	109.00	4
H71-C7-H72	80.22	109.00	1
C5-C7-H73	80.22	109.00	1
H71-C7-H73	80.21	109.00	6
H71-C7-H72	80.21	109.00	5
C5-C7-H73	80.21	109.00	2
H72-C7-H73	80.21	109.00	6
C5-C7-H72	80.21	109.00	1
H72-C7-H73	80.20	109.00	5
H71-C7-H73	80.20	109.00	4

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H72	80.20	109.00	1
H71-C7-H72	80.20	109.00	1
C5-C7-H71	80.20	109.00	4
H71-C7-H73	80.19	109.00	1
H72-C7-H73	80.19	109.00	2
C5-C7-H72	80.19	109.00	1
H71-C7-H72	80.19	109.00	5
C5-C7-H73	80.19	109.00	2
H71-C7-H72	80.18	109.00	1
H71-C7-H73	80.18	109.00	4
H72-C7-H73	80.18	109.00	3
C5-C7-H73	80.18	109.00	2
C5-C7-H72	80.18	109.00	1
H72-C7-H73	80.17	109.00	7
H71-C7-H73	80.17	109.00	2
C5-C7-H73	80.17	109.00	1
C5-C7-H72	80.17	109.00	2
H71-C7-H72	80.17	109.00	4
C5-C7-H71	80.17	109.00	1
H72-C7-H73	80.16	109.00	3
C5-C7-H71	80.16	109.00	2
H71-C7-H72	80.16	109.00	1
C5-C7-H73	80.16	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C7-H72	80.16	109.00	1
C5-C7-H72	80.15	109.00	1
H72-C7-H73	80.15	109.00	1
H71-C7-H73	80.15	109.00	3
H71-C7-H72	80.15	109.00	2
H71-C7-H72	80.14	109.00	3
H71-C7-H73	80.14	109.00	3
H72-C7-H73	80.14	109.00	1
C5-C7-H71	80.14	109.00	1
H72-C7-H73	80.13	109.00	3
H71-C7-H72	80.13	109.00	1
H71-C7-H73	80.13	109.00	3
H71-C7-H72	80.12	109.00	3
C5-C7-H73	80.12	109.00	1
H71-C7-H73	80.12	109.00	1
H72-C7-H73	80.12	109.00	1
H71-C7-H73	80.11	109.00	2
C5-C7-H71	80.10	109.00	1
C5-C7-H73	80.10	109.00	1
H72-C7-H73	80.09	109.00	1
H71-C7-H73	80.09	109.00	1
H71-C7-H72	80.05	109.00	1
H72-C7-H73	80.04	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
H71-C7-H72	80.04	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
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	986	940	41	5
2	986	937	42	7
3	986	929	51	6
4	986	943	38	5
5	986	943	39	4

Model ID	Analyzed	Favored	Allowed	Outliers
6	986	945	37	4
7	986	941	42	3
8	986	938	42	6
9	986	941	40	5
10	986	940	37	9

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	853	743	59	51
2	853	735	64	54
3	853	736	57	60
4	853	740	59	54
5	853	728	74	51
6	853	737	55	61
7	853	749	55	49
8	853	721	77	55
9	853	740	56	57
10	853	744	68	41

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	21	SER
1	A	22	THR
1	A	32	GLN

Model ID	Chain	Residue ID	Residue type
1	A	40	GLN
1	A	50	SER
1	A	51	SER
1	B	51	THR
1	B	52	GLU
1	B	74	THR
1	C	3	SER
1	C	6	SER
1	C	82	LYS
1	C	85	SER
1	D	15	LEU
1	D	22	THR
1	D	61	SER
1	D	92	THR
1	D	93	SER
1	E	22	THR
1	E	23	GLU
1	E	44	THR
1	E	50	SER
1	E	51	SER
1	F	51	THR
1	F	74	THR
1	G	5	SER

Model ID	Chain	Residue ID	Residue type
1	G	63	THR
1	G	85	SER
1	G	88	THR
1	H	61	SER
1	H	92	THR
1	H	93	SER
1	K	1	LEU
1	K	4	ASP
1	K	8	SER
1	K	43	GLU
1	K	57	SER
1	L	3	SER
1	L	13	ASN
1	L	27	CYS
1	L	28	SER
1	L	34	ASP
1	L	42	THR
1	L	76	THR
1	L	86	SER
1	L	89	SER
1	L	104	THR
1	L	106	SER
1	L	113	CYS

Model ID	Chain	Residue ID	Residue type
1	L	135	THR
1	L	147	TRP
2	A	3	HIS
2	A	44	THR
2	A	48	PHE
2	A	51	SER
2	B	39	PHE
2	B	49	THR
2	B	74	THR
2	C	3	SER
2	C	76	ASN
2	C	85	SER
2	D	15	LEU
2	D	22	THR
2	D	26	SER
2	D	61	SER
2	D	85	THR
2	E	3	HIS
2	E	9	THR
2	E	22	THR
2	E	23	GLU
2	E	44	THR
2	E	45	ASP

Model ID	Chain	Residue ID	Residue type
2	E	51	SER
2	F	2	ASP
2	F	74	THR
2	G	3	SER
2	G	63	THR
2	G	85	SER
2	G	88	THR
2	H	6	SER
2	H	22	THR
2	H	61	SER
2	H	65	GLN
2	H	85	THR
2	K	8	SER
2	K	10	SER
2	K	34	CYS
2	K	41	THR
2	K	57	SER
2	K	58	SER
2	K	89	ARG
2	L	13	ASN
2	L	27	CYS
2	L	64	THR
2	L	69	LYS

Model ID	Chain	Residue ID	Residue type
2	L	75	PHE
2	L	81	HIS
2	L	86	SER
2	L	87	ASN
2	L	97	SER
2	L	106	SER
2	L	113	CYS
2	L	118	ASP
2	L	125	LEU
2	L	146	GLU
3	A	3	HIS
3	A	22	THR
3	A	32	GLN
3	A	40	GLN
3	A	44	THR
3	A	51	SER
3	A	56	LEU
3	B	74	THR
3	C	3	SER
3	C	5	SER
3	C	25	ASN
3	C	63	THR
3	C	78	GLU

Model ID	Chain	Residue ID	Residue type
3	C	85	SER
3	C	88	THR
3	D	15	LEU
3	D	26	SER
3	D	29	MET
3	D	57	SER
3	D	61	SER
3	D	93	SER
3	E	22	THR
3	E	44	THR
3	E	45	ASP
3	E	50	SER
3	E	51	SER
3	E	84	MET
3	F	51	THR
3	F	74	THR
3	G	55	ASN
3	G	63	THR
3	G	85	SER
3	H	22	THR
3	H	48	SER
3	H	61	SER
3	H	93	SER

Model ID	Chain	Residue ID	Residue type
3	K	1	LEU
3	K	41	THR
3	K	46	SER
3	K	57	SER
3	K	58	SER
3	K	68	SER
3	L	13	ASN
3	L	18	ASP
3	L	27	CYS
3	L	28	SER
3	L	32	VAL
3	L	34	ASP
3	L	40	GLN
3	L	48	ASP
3	L	59	THR
3	L	64	THR
3	L	75	PHE
3	L	81	HIS
3	L	89	SER
3	L	93	ASP
3	L	97	SER
3	L	106	SER
3	L	113	CYS

Model ID	Chain	Residue ID	Residue type
3	L	114	SER
4	A	3	HIS
4	A	22	THR
4	A	28	LYS
4	A	32	GLN
4	A	41	ASP
4	A	44	THR
4	A	51	SER
4	B	46	ASP
4	B	51	THR
4	B	74	THR
4	C	5	SER
4	C	6	SER
4	C	63	THR
4	C	82	LYS
4	C	85	SER
4	D	26	SER
4	D	61	SER
4	E	9	THR
4	E	13	ARG
4	E	22	THR
4	E	23	GLU
4	E	27	ARG

Model ID	Chain	Residue ID	Residue type
4	E	44	THR
4	E	45	ASP
4	E	50	SER
4	E	51	SER
4	F	51	THR
4	F	74	THR
4	G	3	SER
4	G	63	THR
4	H	21	ASP
4	H	60	THR
4	H	61	SER
4	K	1	LEU
4	K	26	THR
4	K	27	LEU
4	K	41	THR
4	K	47	LEU
4	K	57	SER
4	K	58	SER
4	K	75	TRP
4	L	3	SER
4	L	18	ASP
4	L	27	CYS
4	L	28	SER

Model ID	Chain	Residue ID	Residue type
4	L	34	ASP
4	L	48	ASP
4	L	61	HIS
4	L	81	HIS
4	L	87	ASN
4	L	89	SER
4	L	106	SER
4	L	113	CYS
4	L	138	ASP
5	A	40	GLN
5	A	44	THR
5	A	51	SER
5	B	2	ASP
5	B	12	ILE
5	B	51	THR
5	B	74	THR
5	C	5	SER
5	C	6	SER
5	C	82	LYS
5	C	85	SER
5	D	22	THR
5	D	26	SER
5	D	93	SER

Model ID	Chain	Residue ID	Residue type
5	E	9	THR
5	E	13	ARG
5	E	22	THR
5	E	23	GLU
5	E	27	ARG
5	E	44	THR
5	E	45	ASP
5	F	51	THR
5	G	28	GLU
5	G	63	THR
5	G	85	SER
5	H	57	SER
5	H	61	SER
5	K	10	SER
5	K	14	CYS
5	K	40	SER
5	K	41	THR
5	K	46	SER
5	K	57	SER
5	L	3	SER
5	L	10	LYS
5	L	13	ASN
5	L	18	ASP

Model ID	Chain	Residue ID	Residue type
5	L	34	ASP
5	L	42	THR
5	L	75	PHE
5	L	76	THR
5	L	81	HIS
5	L	93	ASP
5	L	97	SER
5	L	98	GLN
5	L	106	SER
5	L	109	LEU
5	L	113	CYS
5	L	114	SER
5	L	122	ASP
5	L	146	GLU
6	A	21	SER
6	A	40	GLN
6	A	50	SER
6	A	51	SER
6	B	46	ASP
6	B	50	TYR
6	B	51	THR
6	B	74	THR
6	C	5	SER

Model ID	Chain	Residue ID	Residue type
6	C	6	SER
6	C	25	ASN
6	C	63	THR
6	C	82	LYS
6	C	85	SER
6	C	88	THR
6	D	21	ASP
6	D	22	THR
6	D	26	SER
6	D	61	SER
6	D	93	SER
6	E	13	ARG
6	E	22	THR
6	E	23	GLU
6	E	44	THR
6	E	45	ASP
6	E	51	SER
6	F	49	THR
6	F	51	THR
6	F	74	THR
6	G	3	SER
6	G	5	SER
6	G	22	ARG

Model ID	Chain	Residue ID	Residue type
6	G	25	ASN
6	G	63	THR
6	G	76	ASN
6	G	85	SER
6	H	6	SER
6	H	61	SER
6	H	65	GLN
6	K	1	LEU
6	K	8	SER
6	K	29	CYS
6	K	30	ASN
6	K	34	CYS
6	K	41	THR
6	K	52	CYS
6	K	57	SER
6	K	85	GLU
6	K	89	ARG
6	L	3	SER
6	L	13	ASN
6	L	21	ARG
6	L	28	SER
6	L	64	THR
6	L	75	PHE

Model ID	Chain	Residue ID	Residue type
6	L	87	ASN
6	L	91	CYS
6	L	93	ASP
6	L	103	LEU
6	L	106	SER
6	L	113	CYS
7	A	22	THR
7	A	44	THR
7	A	51	SER
7	B	51	THR
7	B	75	LEU
7	C	5	SER
7	C	6	SER
7	C	63	THR
7	C	82	LYS
7	C	85	SER
7	D	26	SER
7	D	61	SER
7	E	13	ARG
7	E	22	THR
7	E	44	THR
7	E	45	ASP
7	F	74	THR

Model ID	Chain	Residue ID	Residue type
7	G	3	SER
7	G	42	MET
7	G	63	THR
7	G	85	SER
7	H	6	SER
7	H	21	ASP
7	H	57	SER
7	H	93	SER
7	K	1	LEU
7	K	10	SER
7	K	34	CYS
7	K	40	SER
7	K	41	THR
7	K	47	LEU
7	K	48	CYS
7	K	52	CYS
7	K	57	SER
7	K	58	SER
7	K	65	ARG
7	K	68	SER
7	L	18	ASP
7	L	27	CYS
7	L	34	ASP

Model ID	Chain	Residue ID	Residue type
7	L	61	HIS
7	L	77	THR
7	L	81	HIS
7	L	93	ASP
7	L	104	THR
7	L	106	SER
7	L	113	CYS
7	L	138	ASP
7	L	146	GLU
8	A	22	THR
8	A	40	GLN
8	A	44	THR
8	A	50	SER
8	A	51	SER
8	B	23	ARG
8	B	46	ASP
8	B	74	THR
8	C	3	SER
8	C	5	SER
8	C	6	SER
8	C	30	VAL
8	C	82	LYS
8	C	85	SER

Model ID	Chain	Residue ID	Residue type
8	C	88	THR
8	D	22	THR
8	D	26	SER
8	D	61	SER
8	D	66	THR
8	D	93	SER
8	E	4	ARG
8	E	9	THR
8	E	13	ARG
8	E	27	ARG
8	E	44	THR
8	E	45	ASP
8	E	51	SER
8	F	51	THR
8	F	74	THR
8	G	3	SER
8	G	5	SER
8	G	25	ASN
8	G	63	THR
8	G	85	SER
8	H	22	THR
8	H	57	SER
8	H	61	SER

Model ID	Chain	Residue ID	Residue type
8	H	93	SER
8	K	10	SER
8	K	14	CYS
8	K	41	THR
8	K	57	SER
8	K	58	SER
8	K	60	THR
8	L	27	CYS
8	L	32	VAL
8	L	34	ASP
8	L	64	THR
8	L	75	PHE
8	L	93	ASP
8	L	97	SER
8	L	104	THR
8	L	106	SER
8	L	113	CYS
8	L	118	ASP
9	A	28	LYS
9	A	41	ASP
9	A	44	THR
9	A	51	SER
9	B	23	ARG

Model ID	Chain	Residue ID	Residue type
9	B	46	ASP
9	B	74	THR
9	C	3	SER
9	C	5	SER
9	C	6	SER
9	C	72	LEU
9	C	82	LYS
9	C	85	SER
9	C	88	THR
9	D	9	ILE
9	D	21	ASP
9	D	26	SER
9	D	46	GLU
9	D	61	SER
9	D	93	SER
9	E	21	SER
9	E	45	ASP
9	E	51	SER
9	E	69	GLU
9	F	46	ASP
9	F	51	THR
9	F	74	THR
9	G	3	SER

Model ID	Chain	Residue ID	Residue type
9	G	5	SER
9	G	55	ASN
9	G	58	ARG
9	G	63	THR
9	G	85	SER
9	H	6	SER
9	H	61	SER
9	H	93	SER
9	K	10	SER
9	K	41	THR
9	K	47	LEU
9	K	57	SER
9	K	58	SER
9	K	62	TYR
9	K	89	ARG
9	L	13	ASN
9	L	18	ASP
9	L	27	CYS
9	L	28	SER
9	L	32	VAL
9	L	75	PHE
9	L	76	THR
9	L	81	HIS

Model ID	Chain	Residue ID	Residue type
9	L	86	SER
9	L	97	SER
9	L	106	SER
9	L	113	CYS
9	L	146	GLU
9	L	153	MET
10	A	22	THR
10	A	28	LYS
10	A	32	GLN
10	A	50	SER
10	B	46	ASP
10	B	51	THR
10	C	6	SER
10	C	85	SER
10	C	88	THR
10	D	21	ASP
10	D	61	SER
10	D	93	SER
10	E	9	THR
10	E	12	LEU
10	E	13	ARG
10	E	44	THR
10	E	45	ASP

Model ID	Chain	Residue ID	Residue type
10	E	51	SER
10	F	51	THR
10	G	3	SER
10	G	55	ASN
10	G	63	THR
10	G	85	SER
10	H	6	SER
10	H	37	ASN
10	H	61	SER
10	K	29	CYS
10	K	41	THR
10	K	47	LEU
10	K	57	SER
10	K	58	SER
10	L	27	CYS
10	L	28	SER
10	L	59	THR
10	L	76	THR
10	L	81	HIS
10	L	89	SER
10	L	97	SER
10	L	106	SER
10	L	113	CYS

Model ID	Chain	Residue ID	Residue type
10	L	153	MET

Fit of model to data used for modeling ?

Fit of model to data used for validation ?

Validation for this section is under development.

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