

Integrative Structure Validation Report ?

February 18, 2025 - 08:27 AM PST

The following software was used in the production of this report:

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

MolProbity Version 4.5.2

PDB ID	8ZZE
PDB-Dev ID	PDBDEV_00000014
Structure Title	Structure of 16S rRNA complexed with methyltransferase A small subunit
Structure Authors	van Zundert GCP; Melquiond ASJ; Bonvin AMJJ
Deposited on	2018-02-06

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

We welcome your comments at helpdesk@pdb-ihm.org

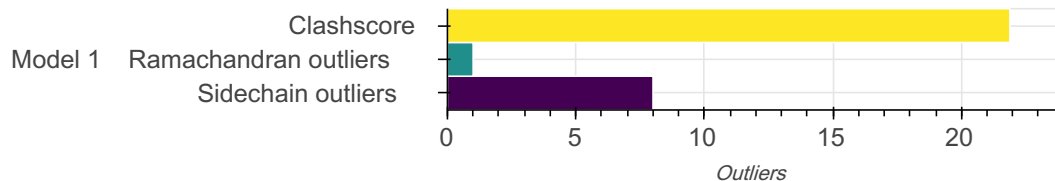
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 and fit to model assessments for SAS and crosslinking-MS 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 1 model(s). A total of 4 datasets were used to build this entry.

Representation ?

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1	1	16Srna	A	1530	1-754, 770-776, 781-785, 790-796, 800-886, 889-893, 899-1507, 1517-1530	755-769, 777-780, 786-789, 797-799, 887-888, 894-898, 1508-1516	100.00 / 100.00	Atomic
		2	ksga	B [V]	252	3-97, 106, 108-123, 129-130, 132-136, 140, 145-161, 163-166, 174-197, 213-214, 216-228, 236-252	1-2, 98-105, 107, 124-128, 131, 137-139, 141-144, 162, 167-173, 198-212, 215, 229-235	100.00 / 100.00	Atomic

Datasets used for modeling ?

There are 4 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	4ADV

ID	Dataset type	Database name	Data access code
2	Mutagenesis data	Not available	10.1074/jbc.M111.318121
3	3DEM volume	EMDB	EMD-2017
4	DNA footprinting data	Not available	10.1038/nsmb.1408

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	Rigid-body minimization	Rigid-body minimization in HADDOCK (it0)	None	10000	False	False
2	1	Simulated annealing	Semi-flexible SA in HADDOCK (it1)	None	400	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	HADDOCK	2.30	molecular docking	http://haddock.science.uu.nl/services/HADDOCK/
2	POWERFIT	2.00	em fitter	https://github.com/haddocking/powerfit

Data quality ?

DNA footprinting

Validation for this section is under development.

3DEM volume

Validation for this section is under development.

Mutagenesis

Validation for this section is under development.

Model quality ?

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

Standard geometry: bond outliers ?

There are 472 bond length outliers in this entry (1.32% of 35889 assessed bonds). A summary is provided below.
The output is limited to 100 rows.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	1074	U	O4'-C1'	119.31	3.80	1.41	1	1
A	1075	G	N7-C5	67.69	2.74	1.39	1	1
A	13	U	C2'-O2'	60.60	2.63	1.42	1	1
A	1074	U	C4-C5	56.79	2.57	1.43	1	1
A	13	U	C4-C5	56.64	2.56	1.43	1	1
A	12	A	C2'-C1'	55.94	2.65	1.53	1	1
A	13	U	C4'-O4'	55.84	2.57	1.45	1	1
A	11	G	C5-C6	52.32	2.47	1.42	1	1
A	1074	U	C3'-C2'	51.43	2.55	1.53	1	1
A	13	U	C5-C6	46.47	0.41	1.34	1	1
A	13	U	C2'-C1'	45.23	2.43	1.53	1	1
A	1076	A	C6-N1	42.22	2.20	1.35	1	1
A	11	G	C6-N1	40.72	0.58	1.39	1	1
A	1075	G	C8-N7	40.08	0.50	1.30	1	1
A	1074	U	C4'-C3'	38.92	2.30	1.52	1	1
A	1074	U	O3'-P	38.40	2.18	1.61	1	1
A	1074	U	N1-C2	37.52	2.13	1.38	1	1
A	12	A	O4'-C1'	35.41	0.70	1.41	1	1
A	12	A	C8-N7	31.59	0.68	1.31	1	1
A	1076	A	N9-C8	30.76	1.99	1.37	1	1
A	13	U	C2-O2	30.39	0.61	1.22	1	1
A	1074	U	C1'-N1	29.83	2.07	1.48	1	1
A	13	U	C4'-C3'	29.30	2.11	1.52	1	1
A	1076	A	N7-C5	28.82	1.96	1.39	1	1
A	11	G	C6-O6	26.94	1.78	1.24	1	1
A	1075	G	O4'-C1'	25.25	1.03	1.41	1	1
A	12	A	C3'-C2'	24.77	1.03	1.53	1	1
A	12	A	C2-N3	24.72	1.83	1.33	1	1
A	11	G	C2-N2	24.59	1.83	1.34	1	1
A	1075	G	C4'-O4'	24.47	1.82	1.45	1	1
A	1074	U	C3'-O3'	24.26	1.90	1.42	1	1
A	1075	G	C5-C4	24.02	0.90	1.38	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	12	A	C3'-O3'	24.00	0.94	1.42	1	1
A	1074	U	C2'-C1'	23.06	1.07	1.53	1	1
A	916	U	C2-O2	21.69	1.65	1.22	1	1
A	11	G	C5-C4	21.50	0.95	1.38	1	1
A	1074	U	N3-C4	19.99	1.78	1.38	1	1
A	13	U	N3-C4	19.98	0.98	1.38	1	1
A	12	A	N3-C4	19.89	1.74	1.34	1	1
A	1075	G	C6-N1	19.65	1.00	1.39	1	1
A	1075	G	C2'-O2'	19.64	1.71	1.42	1	1
A	1075	G	N9-C8	19.50	0.98	1.37	1	1
A	1075	G	N1-C2	18.91	1.75	1.37	1	1
A	1076	A	C2-N3	18.69	1.70	1.33	1	1
A	12	A	C6-N6	18.43	1.70	1.33	1	1
A	13	U	C4-O4	18.02	1.59	1.23	1	1
A	1075	G	C1'-N9	16.38	1.23	1.48	1	1
A	1074	U	C4'-O4'	16.32	1.12	1.45	1	1
A	1075	G	C2'-C1'	15.98	1.77	1.53	1	1
A	12	A	N9-C8	14.49	1.08	1.37	1	1
A	1075	G	O3'-P	14.21	1.39	1.61	1	1
A	14	C	C4'-O4'	14.20	1.66	1.45	1	1
A	1075	G	C5-C6	13.68	1.69	1.42	1	1
A	12	A	C6-N1	13.58	1.62	1.35	1	1
A	12	A	O3'-P	13.57	1.81	1.61	1	1
A	12	A	C4'-O4'	12.97	1.71	1.45	1	1
A	12	A	N1-C2	12.76	1.08	1.34	1	1
A	1075	G	C2-N2	12.52	1.59	1.34	1	1
A	1075	G	N9-C4	12.52	1.63	1.38	1	1
A	13	U	P-O2P	11.86	1.25	1.49	1	1
A	13	U	C1'-N1	11.75	1.71	1.48	1	1
A	12	A	C5-C6	11.30	1.18	1.41	1	1
A	13	U	O3'-P	11.18	1.77	1.61	1	1
A	917	U	O5'-C5'	10.79	1.26	1.42	1	1
A	1074	U	N1-C6	10.70	1.16	1.38	1	1
A	13	U	O4'-C1'	10.64	1.62	1.41	1	1
A	13	U	C5'-C4'	10.38	1.71	1.51	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	1076	A	C5-C6	10.26	1.61	1.41	1	1
A	1074	U	O5'-C5'	9.70	1.23	1.43	1	1
A	755	A	P-OP2	9.56	1.29	1.49	1	1
A	14	C	P-OP1	9.34	1.30	1.49	1	1
A	1074	U	C4-O4	9.12	1.05	1.23	1	1
A	228	G	C4'-O4'	9.12	1.59	1.45	1	1
A	12	A	O5'-C5'	8.94	1.25	1.43	1	1
A	1076	A	C6-N6	8.89	1.16	1.33	1	1
A	1524	U	O3'-P	8.83	1.47	1.61	1	1
A	1524	U	C4'-O4'	8.79	1.59	1.45	1	1
A	12	A	N9-C4	8.54	1.54	1.37	1	1
A	1076	A	C5-C4	8.48	1.21	1.38	1	1
A	13	U	P-O5'	8.36	1.76	1.59	1	1
A	228	G	P-O5'	8.35	1.72	1.59	1	1
A	572	C	C4'-C3'	8.17	1.65	1.53	1	1
A	14	C	C3'-O3'	8.12	1.30	1.42	1	1
A	1074	U	C2-O2	7.86	1.06	1.22	1	1
A	1075	G	C3'-C2'	7.69	1.64	1.52	1	1
A	239	A	C4'-O4'	7.67	1.57	1.45	1	1
A	1061	U	O3'-P	7.48	1.49	1.61	1	1
A	427	A	P-OP2	7.47	1.34	1.49	1	1
A	324	C	O3'-P	7.46	1.50	1.61	1	1
A	1075	G	P-O5'	7.38	1.48	1.59	1	1
A	14	C	P-OP2	7.24	1.63	1.49	1	1
A	239	A	O3'-P	6.93	1.50	1.61	1	1
A	1074	U	C5'-C4'	6.93	1.37	1.51	1	1
A	368	C	C4'-O4'	6.93	1.56	1.45	1	1
A	14	C	P-O5'	6.92	1.70	1.59	1	1
A	1061	U	C4'-O4'	6.82	1.56	1.45	1	1
A	956	U	C2'-O2'	6.74	1.51	1.41	1	1
A	1045	U	O3'-P	6.72	1.51	1.61	1	1
A	1114	U	C4'-O4'	6.69	1.55	1.45	1	1
A	1097	A	C2'-O2'	6.65	1.51	1.41	1	1

Standard geometry: angle outliers ?

There are 294 bond angle outliers in this entry (0.53% of 55586 assessed bonds). A summary is provided below. The

output is limited to 100 rows.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	1074	U	C3'-O3'-P	28.28	77.79	120.20	1	1
A	12	A	O4'-C1'-C2'	23.53	60.35	107.40	1	1
A	12	A	C4'-O4'-C1'	22.48	154.97	110.00	1	1
A	1074	U	O4'-C1'-N1	18.79	52.12	108.50	1	1
A	1074	U	C1'-N1-C2	17.77	64.40	117.70	1	1
A	1075	G	N7-C5-C4	15.89	63.12	110.80	1	1
A	13	U	O2-C2-N3	15.81	74.77	122.20	1	1
A	12	A	O4'-C1'-N9	14.59	137.69	108.50	1	1
A	1074	U	O4-C4-C5	14.55	82.24	125.90	1	1
A	1075	G	C5-C4-N3	14.35	85.55	128.60	1	1
A	12	A	C2'-C1'-N9	13.98	84.45	112.40	1	1
A	13	U	C3'-O3'-P	13.87	99.40	120.20	1	1
A	13	U	N1-C2-O2	13.21	162.43	122.80	1	1
A	1075	G	C6-C5-C4	12.47	156.20	118.80	1	1
A	1075	G	C4'-O4'-C1'	12.29	122.19	109.90	1	1
A	12	A	C4'-C3'-O3'	11.78	136.06	112.50	1	1
A	13	U	O4-C4-C5	11.62	91.04	125.90	1	1
A	12	A	C8-N7-C5	11.55	138.55	103.90	1	1
A	1075	G	C3'-C2'-O2'	11.48	93.48	110.70	1	1
A	12	A	O3'-C3'-C2'	11.39	91.02	113.80	1	1
A	13	U	O2'-C2'-C1'	11.20	74.59	108.20	1	1
A	1074	U	C1'-N1-C6	10.97	154.11	121.20	1	1
A	1074	U	C4'-C3'-O3'	10.96	79.62	112.50	1	1
A	13	U	N3-C4-C5	10.80	82.20	114.60	1	1
A	1076	A	N7-C5-C6	10.52	100.74	132.30	1	1
A	1074	U	O3'-P-O5'	10.29	119.44	104.00	1	1
A	1075	G	C8-N9-C4	10.16	136.89	106.40	1	1
A	13	U	P-O5'-C5'	10.16	90.43	120.90	1	1
A	11	G	C5-C6-O6	10.01	98.57	128.60	1	1
A	324	C	C3'-O3'-P	9.93	135.10	120.20	1	1
A	11	G	N7-C5-C4	9.91	140.53	110.80	1	1
A	1524	U	C3'-O3'-P	9.89	135.03	120.20	1	1
A	12	A	N7-C5-C6	9.72	161.45	132.30	1	1
A	13	U	C4'-C3'-O3'	9.58	83.76	112.50	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	12	A	C3'-O3'-P	9.52	134.48	120.20	1	1
A	1076	A	C2'-C1'-N9	9.41	97.89	112.00	1	1
A	11	G	C6-C5-C4	9.33	90.81	118.80	1	1
A	1074	U	C2'-C1'-N1	9.24	140.12	112.40	1	1
A	1076	A	O4'-C1'-N9	9.00	121.99	108.50	1	1
A	1074	U	O3'-P-O1P	8.99	81.04	108.00	1	1
A	12	A	N7-C5-C4	8.95	83.85	110.70	1	1
A	11	G	C8-N7-C5	8.93	77.51	104.30	1	1
A	12	A	O3'-P-O5'	8.81	117.21	104.00	1	1
A	12	A	O2'-C2'-C1'	8.80	90.61	108.20	1	1
A	11	G	O6-C6-N1	8.79	146.28	119.90	1	1
A	1074	U	C5'-C4'-O4'	8.77	83.18	109.50	1	1
A	1075	G	O2'-C2'-C1'	8.51	121.17	108.40	1	1
A	1075	G	C5-C6-N1	8.48	86.06	111.50	1	1
A	572	C	C3'-O3'-P	8.28	132.62	120.20	1	1
A	964	A	O3'-C3'-C2'	8.21	121.81	109.50	1	1
A	1075	G	C1'-N9-C4	8.10	102.21	126.50	1	1
A	1045	U	C3'-O3'-P	7.98	132.17	120.20	1	1
A	1061	U	C3'-O3'-P	7.92	132.07	120.20	1	1
A	13	U	C3'-C2'-O2'	7.90	133.50	109.80	1	1
A	239	A	C3'-O3'-P	7.86	131.99	120.20	1	1
A	1074	U	C4'-O4'-C1'	7.85	86.45	110.00	1	1
A	1075	G	C5'-C4'-O4'	7.85	121.57	109.80	1	1
A	56	A	C3'-O3'-P	7.83	131.95	120.20	1	1
A	12	A	C1'-N9-C8	7.82	104.25	127.70	1	1
A	572	C	O4'-C4'-C3'	7.74	98.36	106.10	1	1
A	1097	A	C3'-O3'-P	7.42	131.33	120.20	1	1
A	1222	C	C3'-O3'-P	7.41	131.31	120.20	1	1
A	956	U	C3'-O3'-P	7.31	131.17	120.20	1	1
A	916	U	N1-C2-O2	7.13	101.41	122.80	1	1
A	11	G	N9-C4-C5	7.10	84.11	105.40	1	1
A	909	A	C3'-O3'-P	7.08	130.82	120.20	1	1
A	1076	A	C5-C6-N1	7.07	96.50	117.70	1	1
A	1075	G	O4'-C1'-N9	7.06	119.10	108.50	1	1
A	1075	G	N7-C5-C6	7.05	109.25	130.40	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	978	U	C3'-O3'-P	7.01	130.72	120.20	1	1
A	1075	G	N9-C4-N3	7.00	147.01	126.00	1	1
A	12	A	C3'-C2'-O2'	6.96	123.72	109.80	1	1
A	1074	U	N3-C4-C5	6.80	94.20	114.60	1	1
A	362	A	C3'-O3'-P	6.70	130.25	120.20	1	1
A	368	C	C3'-O3'-P	6.66	130.20	120.20	1	1
A	1075	G	O4'-C4'-C3'	6.64	97.36	104.00	1	1
A	1076	A	C5-C6-N6	6.60	143.51	123.70	1	1
A	368	C	O3'-C3'-C2'	6.51	119.26	109.50	1	1
A	1075	G	N9-C4-C5	6.49	124.88	105.40	1	1
A	1177	G	O3'-C3'-C2'	6.46	119.19	109.50	1	1
A	11	G	N7-C5-C6	6.42	111.15	130.40	1	1
A	12	A	N6-C6-N1	6.40	99.41	118.60	1	1
A	13	U	C1'-N1-C2	6.34	98.68	117.70	1	1
A	1135	G	C3'-O3'-P	6.32	129.68	120.20	1	1
A	1074	U	C4'-C3'-C2'	6.26	121.08	102.30	1	1
A	368	C	C3'-C2'-O2'	6.25	105.23	114.60	1	1
A	572	C	O3'-C3'-C2'	6.17	118.75	109.50	1	1
A	1075	G	O1P-P-O2P	6.14	138.03	119.60	1	1
A	116	A	C4'-C3'-O3'	6.10	103.85	113.00	1	1
A	1343	G	O3'-C3'-C2'	6.09	118.64	109.50	1	1
A	47	A	C3'-O3'-P	5.97	129.15	120.20	1	1
A	13	U	O2P-P-O5'	5.97	92.80	110.70	1	1
A	47	A	O2'-C2'-C1'	5.91	102.93	111.80	1	1
A	325	A	O3'-C3'-C2'	5.88	118.33	109.50	1	1
A	480	G	C3'-C2'-O2'	5.85	105.82	114.60	1	1
A	1281	A	O3'-C3'-C2'	5.78	118.17	109.50	1	1
A	1049	G	C3'-O3'-P	5.77	128.86	120.20	1	1
A	480	G	C3'-O3'-P	5.75	128.82	120.20	1	1
A	1177	G	C4'-O4'-C1'	5.69	104.01	109.70	1	1
A	1358	A	O3'-C3'-C2'	5.64	117.97	109.50	1	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 atomic models in this entry.

Model ID	Clash score	Number of clashes
1	21.89	1082

There are 1082 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:11:G:C2	A:11:G:C6	1.64	1	1
A:1075:G:C1'	A:1075:G:C2'	1.61	1	1
A:12:A:C6	A:12:A:N6	1.59	1	1
A:12:A:C4	A:12:A:N3	1.54	1	1
A:1076:A:C2	A:1076:A:N3	1.53	1	1
A:13:U:C1'	A:13:U:N1	1.52	1	1
A:1074:U:C4	A:1074:U:N3	1.49	1	1
A:916:U:C2	A:916:U:O2	1.48	1	1
A:11:G:C2	A:11:G:N2	1.46	1	1
A:12:A:C2	A:12:A:N3	1.45	1	1
A:1075:G:C2'	A:1075:G:O2'	1.38	1	1
A:12:A:C4'	A:12:A:O4'	1.38	1	1
A:11:G:C6	A:11:G:O6	1.36	1	1
A:1076:A:C5	A:1076:A:N7	1.34	1	1
A:1075:G:C2	A:1075:G:N1	1.32	1	1
A:1076:A:C8	A:1076:A:N9	1.29	1	1
A:13:U:C3'	A:13:U:C4'	1.29	1	1
A:1075:G:C4'	A:1075:G:O4'	1.27	1	1
A:14:C:C4'	A:14:C:O4'	1.25	1	1
A:1074:U:C3'	A:1074:U:O3'	1.19	1	1
A:1074:U:C1'	A:1074:U:C2	1.19	1	1
A:1074:U:C2	A:1074:U:N1	1.17	1	1
A:1074:U:C1'	A:1074:U:N1	1.16	1	1
A:1076:A:C5	A:1076:A:C8	1.16	1	1
A:12:A:H1'	A:12:A:O4'	1.14	1	1
A:13:U:C1'	A:13:U:C2	1.11	1	1
A:1076:A:C6	A:1076:A:N1	1.09	1	1
A:1074:U:C3'	A:1074:U:C4'	1.08	1	1
A:12:A:C1'	A:12:A:C4'	1.03	1	1
A:11:G:C5	A:11:G:C6	1.02	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:12:A:C1'	A:12:A:O4'	1.00	1	1
A:1074:U:H1'	A:1074:U:O2	1.00	1	1
A:1074:U:O3'	A:1075:G:P	1.00	1	1
A:1076:A:C2	A:1076:A:C4	0.97	1	1
A:13:U:C1'	A:13:U:C2'	0.96	1	1
A:1074:U:C1'	A:1074:U:O2	0.95	1	1
A:1074:U:C3'	A:1075:G:P	0.93	1	1
A:1074:U:C4	A:1074:U:C5	0.92	1	1
A:13:U:C4	A:13:U:C5	0.91	1	1
A:695:C:H2'	A:696:G:H5"	0.89	1	1
A:239:A:H4'	A:240:U:H5'	0.89	1	1
A:12:A:N9	A:12:A:O4'	0.89	1	1
A:1207:U:H4'	A:1209:A:H1'	0.88	1	1
A:13:U:H2'	A:14:C:O4'	0.88	1	1
A:1076:A:C4	A:1076:A:C8	0.88	1	1
A:1082:U:H3	A:1095:G:H22	0.87	1	1
A:660:G:H22	A:737:G:H1	0.85	1	1
A:11:G:C4	A:11:G:C6	0.84	1	1
A:1319:G:H2'	A:1320:A:C8	0.84	1	1
A:1074:U:C2'	A:1074:U:C3'	0.83	1	1
A:12:A:C2	A:12:A:C4	0.82	1	1
A:61:A:H2'	A:61:A:N3	0.82	1	1
A:836:C:H2'	A:838:U:H5"	0.80	1	1
A:74:A:H2'	A:75:G:C8	0.80	1	1
A:1215:A:H2'	A:1216:G:C8	0.79	1	1
B:210:ARG:HE	B:229:PRO:HB2	0.79	1	1
A:1075:G:C2'	A:1075:G:N9	0.78	1	1
A:1304:U:H2'	A:1305:G:H8	0.78	1	1
A:235:U:H4'	A:235:U:OP1	0.78	1	1
A:11:G:C6	A:11:G:N1	0.78	1	1
A:1304:U:H2'	A:1305:G:C8	0.76	1	1
A:1214:C:H2'	A:1215:A:C8	0.75	1	1
A:942:A:H2'	A:943:G:C8	0.75	1	1
A:497:C:H2'	A:498:A:H8	0.75	1	1
A:1097:A:H4'	A:1098:A:O5'	0.75	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:1121:U:H2'	A:1122:U:H5''	0.75	1	1
A:433:U:H2'	A:434:U:O4'	0.74	1	1
A:1214:C:H2'	A:1215:A:H8	0.74	1	1
A:83:C:H2'	A:84:U:H4'	0.74	1	1
A:12:A:C1'	A:12:A:C2'	0.74	1	1
A:1001:A:H2'	A:1002:G:O4'	0.74	1	1
A:1075:G:C1'	A:1075:G:C3'	0.74	1	1
A:760:C:H3'	A:761:G:H21	0.74	1	1
A:808:G:H2'	A:808:G:N3	0.73	1	1
A:1074:U:C2	A:1074:U:C4	0.73	1	1
A:996:A:H2'	A:997:C:C6	0.73	1	1
A:386:U:H2'	A:387:G:C8	0.72	1	1
A:469:U:H2'	A:470:G:H8	0.72	1	1
A:1322:U:H2'	A:1323:C:C6	0.72	1	1
A:1073:G:N2	A:1075:G:H3'	0.72	1	1
A:1247:A:H2'	A:1248:A:C8	0.72	1	1
A:918:G:H2'	A:919:A:C8	0.72	1	1
A:13:U:C4'	A:13:U:O3'	0.72	1	1
A:669:A:H2'	A:670:G:C8	0.72	1	1
A:1204:C:H2'	A:1205:C:O4'	0.72	1	1
A:12:A:C2'	A:12:A:O4'	0.72	1	1
A:1232:A:H4'	A:1300:G:H4'	0.71	1	1
A:497:C:H2'	A:498:A:C8	0.71	1	1
A:264:U:H2'	A:265:C:C6	0.71	1	1
A:514:C:H2'	A:526:G:C8	0.70	1	1
A:1075:G:C1'	A:1075:G:C4'	0.70	1	1
A:1022:G:H2'	A:1023:C:C6	0.70	1	1
A:963:C:H3'	A:964:A:H5'	0.70	1	1
A:1056:U:H2'	A:1057:G:H8	0.70	1	1
A:1076:A:N7	A:1077:A:H1'	0.70	1	1
A:266:A:H2'	A:267:C:C6	0.69	1	1
A:13:U:C2'	A:14:C:O4'	0.69	1	1
A:1067:C:H2'	A:1068:G:H8	0.69	1	1
A:1076:A:C8	A:1077:A:O4'	0.69	1	1
A:1326:U:H2'	A:1327:G:H5'	0.69	1	1

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	250	246	3	1

There are 1 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
B	114	THR	1

Torsion angles : Protein sidechains ?

In the following table, sidechain rotameric outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analysed	Favored	Allowed	Outliers
1	216	194	14	8

There are 8 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
B	1	GLN	1
B	5	ASN	1
B	21	LYS	1
B	65	LEU	1
B	75	ASP	1
B	139	LYS	1
B	189	LYS	1
B	215	ASN	1

Fit of model to data used for modeling ?

DNA footprinting

Validation for this section is under development.

3DEM volume

Validation for this section is under development.

Mutagenesis

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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