Integrative Structure Validation Report

October 09, 2025 - 04:37 PM PDT

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

IHMValidation Version 3.0
Python-IHM Version 2.5
MolProbity Version 4.5.2
EMDB validation analysis Version 0.0.1.dev127
ChimeraX Version 1.9
Chimera Version 1.19
MapQ Version 1.8.1

PDB ID	8ZZE | pdb_00008zze
PDB-Dev ID	PDBDEV_00000014
Structure Title	Structure of 16S rRNA complexed with methyltransferase A small subunit
Structure Authors	van Zundert, G.C.P.; Melquiond, A.S.J.; Bonvin, A.M.J.J.
Deposited on	2018-02-06

This is a PDB-IHM Structure Validation Report.

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.

1. Overview

1.1. Summary

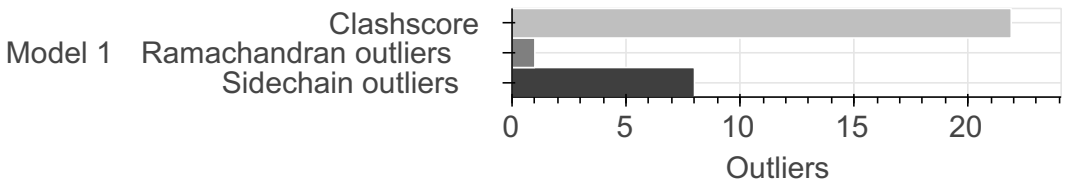
This entry consists of 1 model(s). A total of 4 dataset(s) were used to build this entry.

Name	Type	Count
3DEM volume	Experimental data	1
DNA footprinting data	Experimental data	1
Mutagenesis data	Experimental data	1
Experimental model	Starting model	1

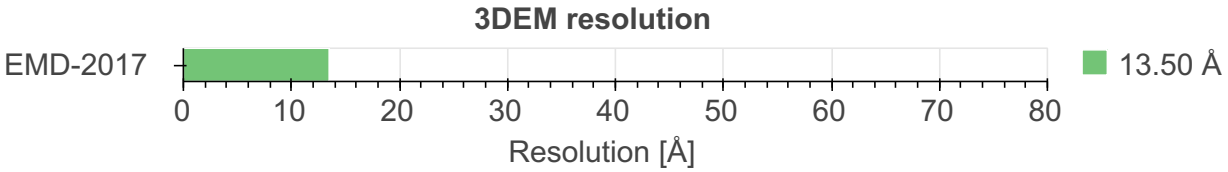
1.2. Overall quality

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.

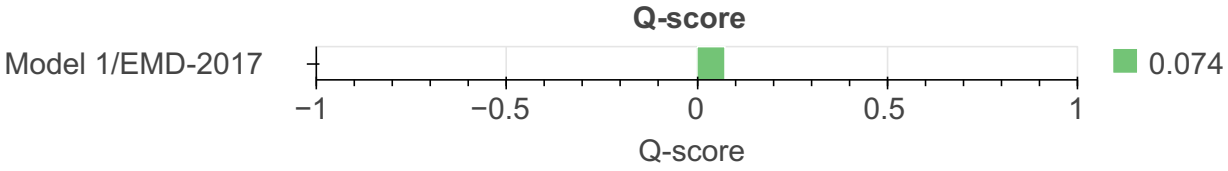
Model Quality: MolProbity Analysis



Data Quality



Fit to Data Used for Modeling



2. Model Details

2.1. Ensemble information

This entry consists of 0 distinct ensemble(s).

2.2. 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

2.3. 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	pdb_00004adv
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

2.4. 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)	Not available	10000	False	False
2	1	Simulated annealing	Semi-flexible SA in HADDOCK (it1)	Not available	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

3. Data quality

3.3. 3DEM

This section describes quality of the 3DEM datasets

EMD-2017

3.3.1. Experimental information

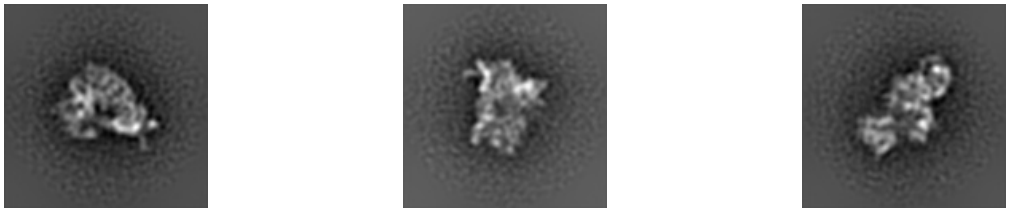
EM reconstruction method:	SINGLE PARTICLE
Resolution:	13.50 Å
Recommended level:	39.000
Estimated volume:	901.89 nm³
Specimen preparation:	Preparation ID 1 Vitrification
Map-only validation report:	wwPDB validation report

3.3.2. Map visualisation

This section contains visualisations of the EMDB entry EMD-2017. These allow visual inspection of the internal detail of the map and identification of artifacts. Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

3.3.2.1. Orthogonal projections

Primary map

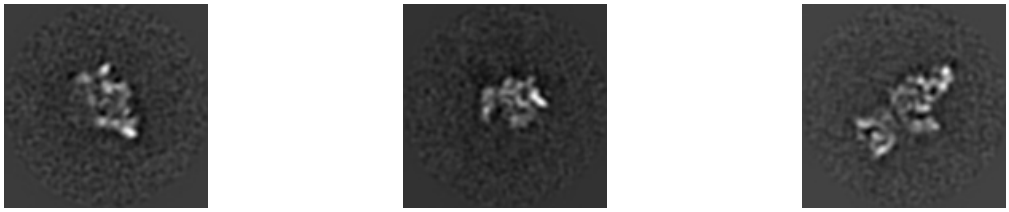


X **Y** **Z**

The images above show the map projected in three orthogonal directions.

3.3.2.2. Central slices

Primary map

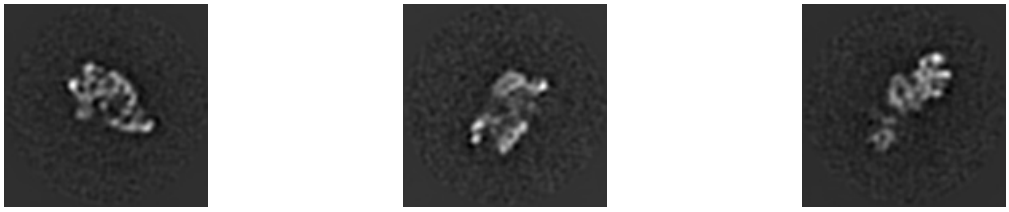


X Index: 64 **Y Index: 64** **Z Index: 64**

The images above show central slices of the map in three orthogonal directions.

3.3.2.3. Largest variance slices

Primary map

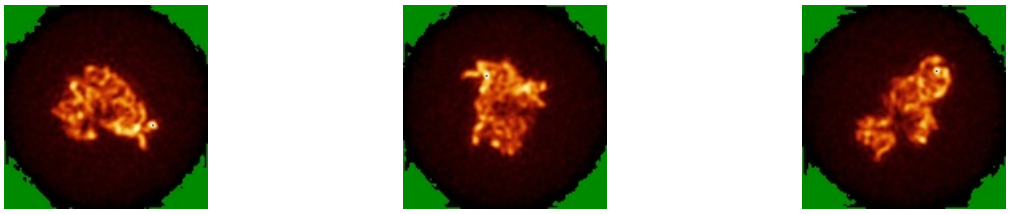


X Index: 75 **Y Index: 53** **Z Index: 51**

The images above show the largest variance slices of the map in three orthogonal directions.

3.3.2.4 Orthogonal standard-deviation projections (false-color)

Primary map

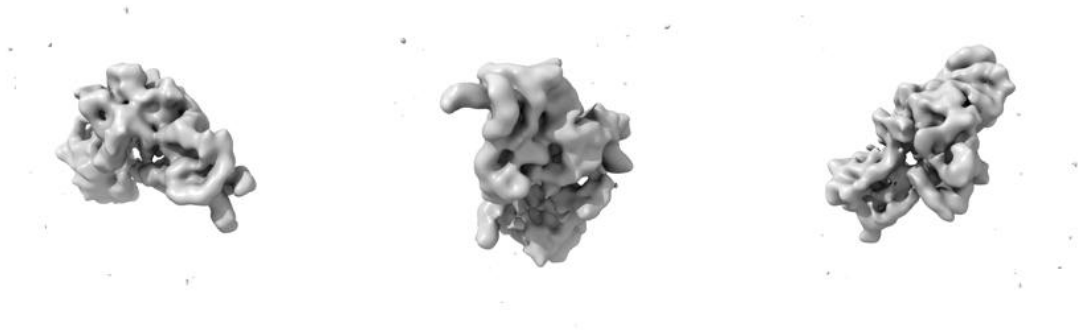


X **Y** **Z**

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

3.3.2.5. Orthogonal surface views

Primary map



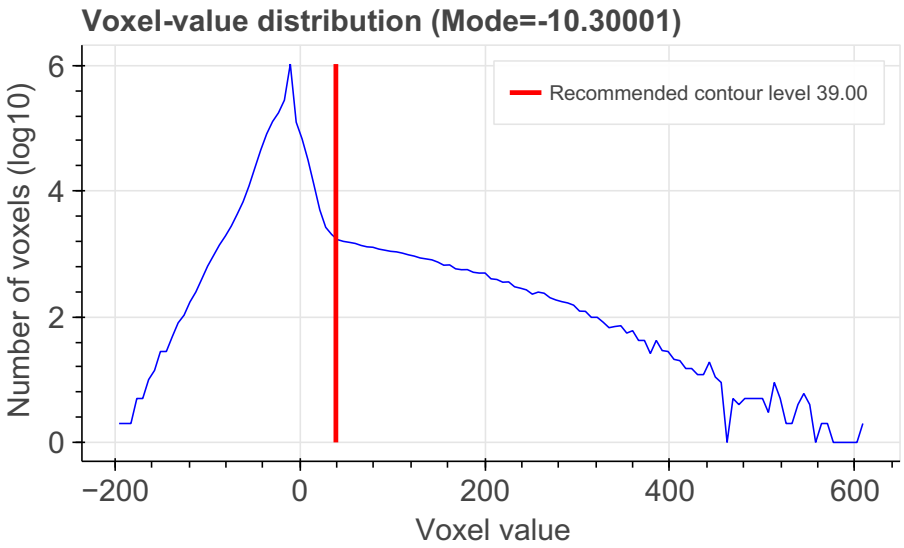
X **Y** **Z**

The images above show the 3D surface view of the map at the recommended contour level 39.000 . These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

3.3.3. Map analysis

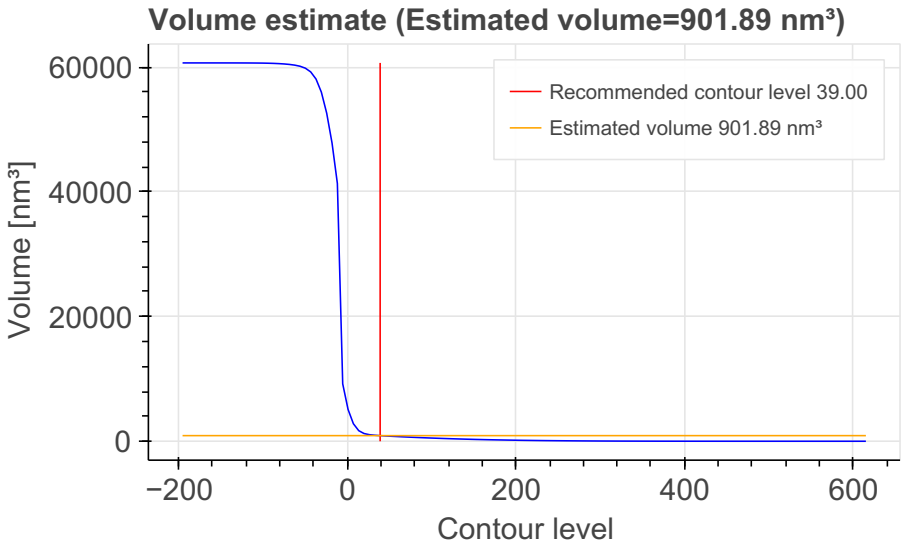
This section contains the results of statistical analysis of the map.

3.3.3.1. Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

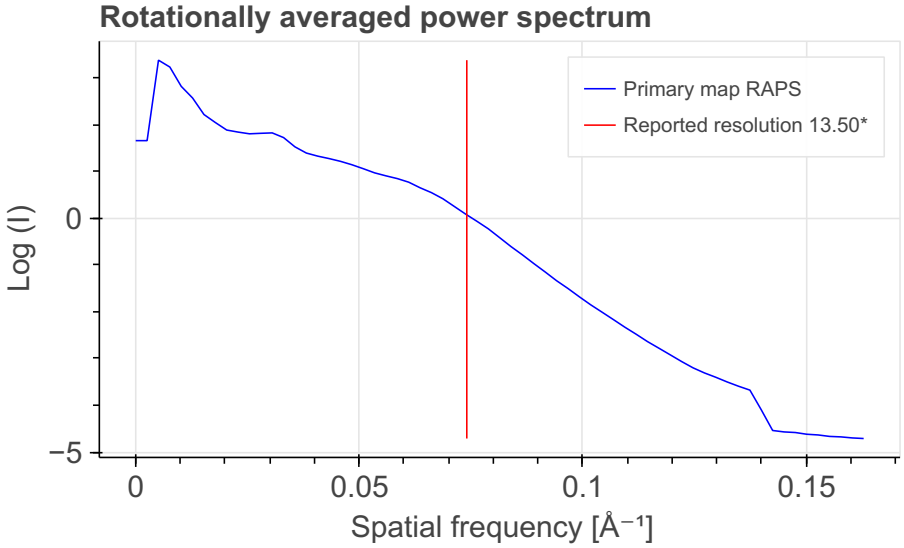
3.3.3.2. Volume estimate



The volume at the recommended contour level is 901.89 nm³.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

3.3.3.3. Rotationally averaged power spectrum



*Reported resolution corresponds to spatial frequency of 0.074 Å^{-1}

3.3.4. Fourier-Shell correlation

3.3.4.2. Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	13.50	-

Author-provided FSC curve is not available.

3.4. Mutagenesis

Validation for this section is under development.

3.4. DNA footprinting

Validation for this section is under development.

4. 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.

4.1b. MolProbity Analysis

Excluded volume satisfaction for the models in the entry are listed below. The Analysed column shows the number of particle-partice or particle-atom pairs for which excluded volume was analysed.

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

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
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
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

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
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
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

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
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

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
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
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

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
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
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

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
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
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

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
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
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

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
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

5. Fit to Data Used for Modeling Assessment

5.3. 3DEM

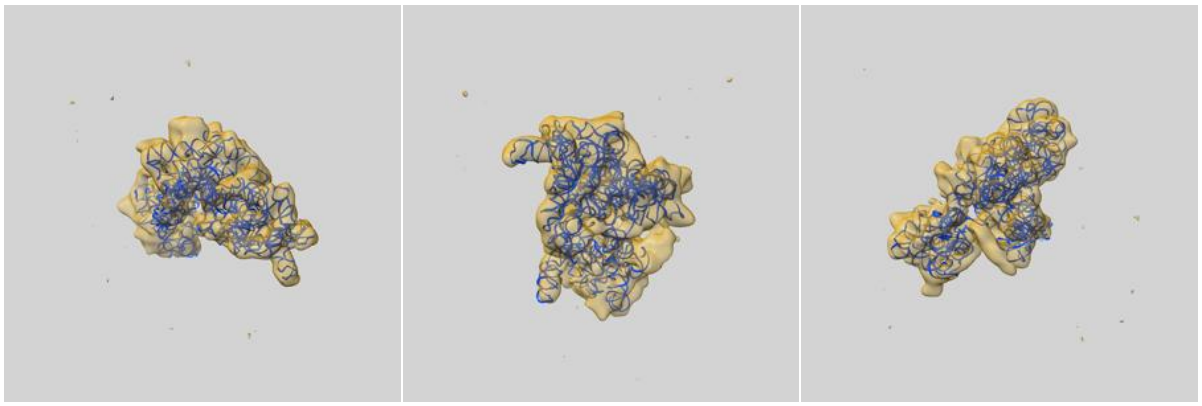
This section describes fit of models to the 3DEM data. Only results for the representative model, selected as a first model with the largest number of asymmetric units.

EMD-2017

5.3.1. Map-model fit

Only results for the representative Model 1 are shown.

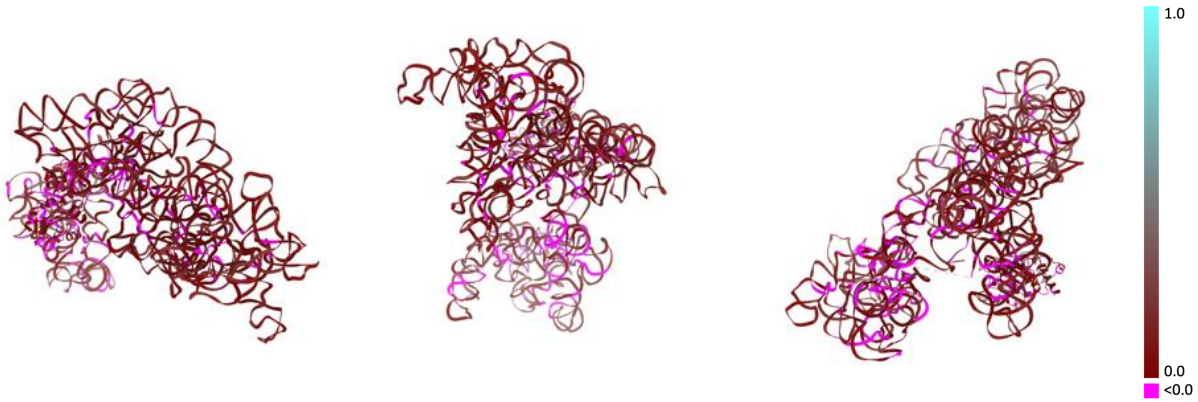
5.3.1.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 39.000 at 50% transparency in yellow overlaid with a ribbon representation of the model colored in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

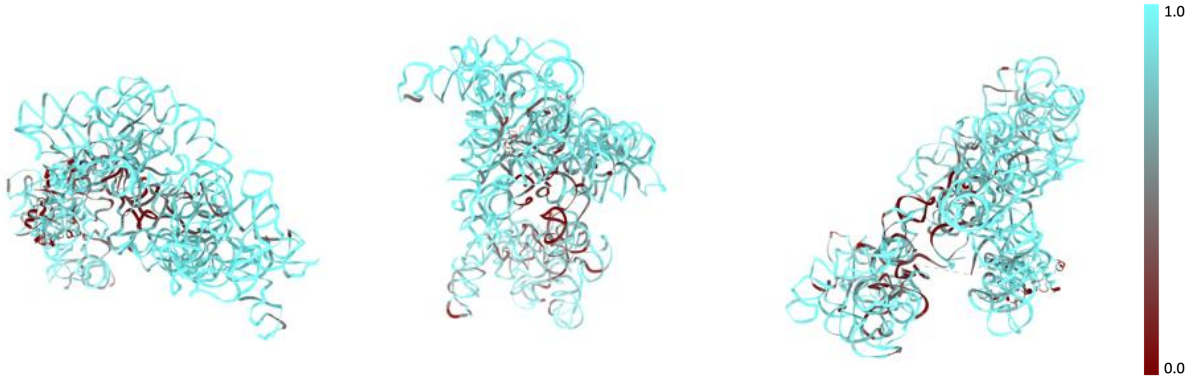
5.3.1.2. Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue colored according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

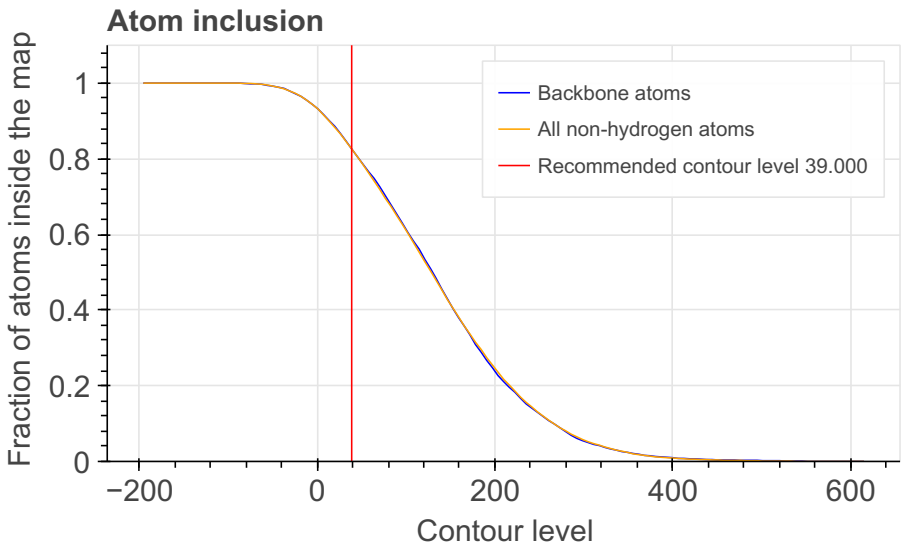
5.3.1.3. Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue colored according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level 39.000 .

5.3.1.4. Atom inclusion



At the recommended contour level, 83% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

5.3.1.5. Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (39.000) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.826	0.074
A	0.834	0.076
B	0.730	0.041

5.4. Mutagenesis

Validation for this section is under development.

5.4. DNA footprinting

Validation for this section is under development.

6. Fit to Data Used for Validation Assessment

Validation for this section is under development.

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