Full wwPDB EM Validation Report (i)

Sep 1, 2026 – 04:36 pm BST

PDB ID	:	9RL4 / pdb_00009rl4
EMDB ID	:	EMD-54030
Title	:	Structure of BAF in complex with OCT4-SOX2-bound nucleosome - SHL-6
Authors	:	Vecchia, L.; Weiss, J.; Cavadini, S.; Kempf, G.; Kater, L.; Pathare, G.; Thoma, N.H.
Deposited on	:	2025-06-16
Resolution	:	3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

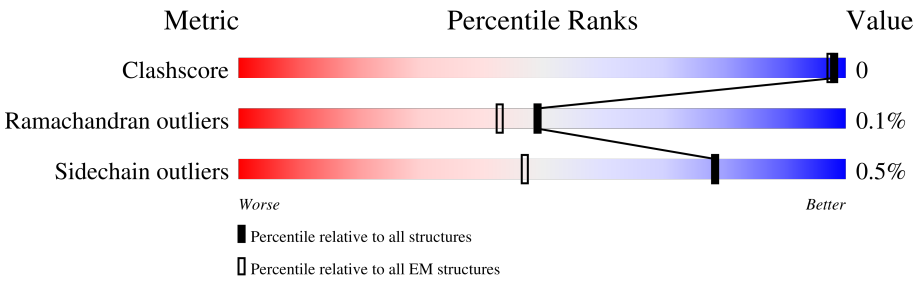
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

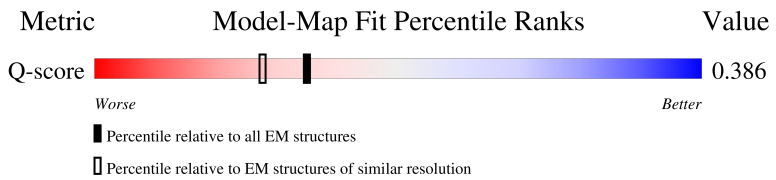
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	139	67% • 32%
1	E	139	68% • 32%
2	B	106	77% 23%
2	F	106	76% 24%

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Mol	Chain	Length	Quality of chain
3	C	133	82% 18%
3	G	133	81% 18%
4	D	128	71% 27%
4	H	128	72% 27%
5	I	1647	8% 46% 54%
6	J	429	91% 7%
7	K	375	95% 5%
8	L	2285	20% 80%
9	M	385	75% 23%
10	N	1214	22% 78%
10	O	1214	27% 73%
11	P	515	7% 73% 26%
12	Q	411	25% 74%
13	R	435	16% 84%
14	V	645	11% 89%
15	W	105	70% 30%
16	X	227	54% 9% 37%
17	Y	227	59% 37%

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 38125 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	94	773	488	147	134	4	0	0
1	E	95	783	494	150	135	4	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P68431
A	-1	SER	-	expression tag	UNP P68431
A	0	HIS	-	expression tag	UNP P68431
E	-2	GLY	-	expression tag	UNP P68431
E	-1	SER	-	expression tag	UNP P68431
E	0	HIS	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	82	653	412	127	113	1	0	0
2	F	81	646	407	126	112	1	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P62805
B	-1	SER	-	expression tag	UNP P62805
B	0	HIS	-	expression tag	UNP P62805
F	-2	GLY	-	expression tag	UNP P62805
F	-1	SER	-	expression tag	UNP P62805
F	0	HIS	-	expression tag	UNP P62805

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	109	837	526	166	145	0	0
3	G	109	840	529	166	145	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P04908
C	-1	SER	-	expression tag	UNP P04908
C	0	HIS	-	expression tag	UNP P04908
G	-2	GLY	-	expression tag	UNP P04908
G	-1	SER	-	expression tag	UNP P04908
G	0	HIS	-	expression tag	UNP P04908

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	93	726	456	130	138	2	0	0
4	H	93	726	456	130	138	2	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP P06899
D	-1	SER	-	expression tag	UNP P06899
D	0	HIS	-	expression tag	UNP P06899
H	-2	GLY	-	expression tag	UNP P06899
H	-1	SER	-	expression tag	UNP P06899
H	0	HIS	-	expression tag	UNP P06899

- Molecule 5 is a protein called Transcription activator BRG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	763	4517	2749	893	872	3	0	0

- Molecule 6 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	400	3109	1967	526	594	22	0	0

- Molecule 7 is a protein called Actin, cytoplasmic 1, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	K	357	2784	1765	465	534	20	0	0

- Molecule 8 is a protein called AT-rich interactive domain-containing protein 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	466	3671	2341	620	689	21	0	0

- Molecule 9 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily B member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	M	295	2375	1496	403	464	12	0	0

- Molecule 10 is a protein called SWI/SNF complex subunit SMARCC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	N	270	2194	1388	387	407	12	0	0
10	O	332	2666	1696	464	493	13	0	0

- Molecule 11 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily D member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	P	381	2744	1722	506	505	11	0	0

- Molecule 12 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Q	105	860	530	161	165	4	0	0

- Molecule 13 is a protein called Zinc finger protein ubi-d4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	R	70	580	361	112	102	5	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	392	GLY	-	expression tag	UNP Q92785
R	393	THR	-	expression tag	UNP Q92785
R	394	LEU	-	expression tag	UNP Q92785
R	395	GLU	-	expression tag	UNP Q92785
R	396	VAL	-	expression tag	UNP Q92785
R	397	LEU	-	expression tag	UNP Q92785
R	398	PHE	-	expression tag	UNP Q92785
R	399	GLN	-	expression tag	UNP Q92785
R	400	GLY	-	expression tag	UNP Q92785
R	401	PRO	-	expression tag	UNP Q92785
R	402	GLY	-	expression tag	UNP Q92785
R	403	GLY	-	expression tag	UNP Q92785
R	404	SER	-	expression tag	UNP Q92785
R	405	GLY	-	expression tag	UNP Q92785
R	406	SER	-	expression tag	UNP Q92785
R	407	ALA	-	expression tag	UNP Q92785
R	408	TRP	-	expression tag	UNP Q92785
R	409	SER	-	expression tag	UNP Q92785
R	410	HIS	-	expression tag	UNP Q92785
R	411	PRO	-	expression tag	UNP Q92785
R	412	GLN	-	expression tag	UNP Q92785
R	413	PHE	-	expression tag	UNP Q92785
R	414	GLU	-	expression tag	UNP Q92785
R	415	LYS	-	expression tag	UNP Q92785
R	416	GLY	-	expression tag	UNP Q92785
R	417	GLY	-	expression tag	UNP Q92785
R	418	GLY	-	expression tag	UNP Q92785
R	419	SER	-	expression tag	UNP Q92785
R	420	GLY	-	expression tag	UNP Q92785
R	421	GLY	-	expression tag	UNP Q92785
R	422	GLY	-	expression tag	UNP Q92785

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Chain	Residue	Modelled	Actual	Comment	Reference
R	423	SER	-	expression tag	UNP Q92785
R	424	GLY	-	expression tag	UNP Q92785
R	425	GLY	-	expression tag	UNP Q92785
R	426	SER	-	expression tag	UNP Q92785
R	427	ALA	-	expression tag	UNP Q92785
R	428	TRP	-	expression tag	UNP Q92785
R	429	SER	-	expression tag	UNP Q92785
R	430	HIS	-	expression tag	UNP Q92785
R	431	PRO	-	expression tag	UNP Q92785
R	432	GLN	-	expression tag	UNP Q92785
R	433	PHE	-	expression tag	UNP Q92785
R	434	GLU	-	expression tag	UNP Q92785
R	435	LYS	-	expression tag	UNP Q92785

- Molecule 14 is a protein called Green fluorescent protein,POU domain, class 5, transcription factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	V	73	363	217	73	73	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-272	MET	-	initiating methionine	UNP P42212
V	-271	ASP	-	expression tag	UNP P42212
V	-270	TRP	-	expression tag	UNP P42212
V	-269	SER	-	expression tag	UNP P42212
V	-268	HIS	-	expression tag	UNP P42212
V	-267	PRO	-	expression tag	UNP P42212
V	-266	GLN	-	expression tag	UNP P42212
V	-265	PHE	-	expression tag	UNP P42212
V	-264	GLU	-	expression tag	UNP P42212
V	-263	LYS	-	expression tag	UNP P42212
V	-262	SER	-	expression tag	UNP P42212
V	-261	ALA	-	expression tag	UNP P42212
V	-260	VAL	-	expression tag	UNP P42212
V	-259	ASP	-	expression tag	UNP P42212
V	-258	GLU	-	expression tag	UNP P42212
V	-257	ASN	-	expression tag	UNP P42212
V	-256	LEU	-	expression tag	UNP P42212
V	-255	TYR	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
V	-254	PHE	-	expression tag	UNP P42212
V	-253	GLN	-	expression tag	UNP P42212
V	-252	GLY	-	expression tag	UNP P42212
V	-251	GLY	-	expression tag	UNP P42212
V	-250	GLY	-	expression tag	UNP P42212
V	-249	ARG	-	expression tag	UNP P42212
V	-248	MET	-	expression tag	UNP P42212
V	-247	VAL	-	expression tag	UNP P42212
V	-184	LEU	PHE	conflict	UNP P42212
V	-183	THR	SER	conflict	UNP P42212
V	-42	LYS	ALA	conflict	UNP P42212
V	-17	LEU	HIS	conflict	UNP P42212
V	-9	GLU	-	linker	UNP P42212
V	-8	ALA	-	linker	UNP P42212
V	-7	ALA	-	linker	UNP P42212
V	-6	ALA	-	linker	UNP P42212
V	-5	LYS	-	linker	UNP P42212
V	-4	GLU	-	linker	UNP P42212
V	-3	ALA	-	linker	UNP P42212
V	-2	ALA	-	linker	UNP P42212
V	-1	ALA	-	linker	UNP P42212
V	0	LYS	-	linker	UNP P42212
V	361	LEU	-	expression tag	UNP Q01860
V	362	PRO	-	expression tag	UNP Q01860
V	363	GLU	-	expression tag	UNP Q01860
V	364	THR	-	expression tag	UNP Q01860
V	365	GLY	-	expression tag	UNP Q01860
V	366	GLY	-	expression tag	UNP Q01860
V	367	HIS	-	expression tag	UNP Q01860
V	368	HIS	-	expression tag	UNP Q01860
V	369	HIS	-	expression tag	UNP Q01860
V	370	HIS	-	expression tag	UNP Q01860
V	371	HIS	-	expression tag	UNP Q01860
V	372	HIS	-	expression tag	UNP Q01860

- Molecule 15 is a protein called Transcription factor SOX-2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	W	74	378	230	74	74	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	14	MET	-	initiating methionine	UNP P48431
W	15	ASP	-	expression tag	UNP P48431
W	16	TRP	-	expression tag	UNP P48431
W	17	SER	-	expression tag	UNP P48431
W	18	HIS	-	expression tag	UNP P48431
W	19	PRO	-	expression tag	UNP P48431
W	20	GLN	-	expression tag	UNP P48431
W	21	PHE	-	expression tag	UNP P48431
W	22	GLU	-	expression tag	UNP P48431
W	23	LYS	-	expression tag	UNP P48431
W	24	SER	-	expression tag	UNP P48431
W	25	ALA	-	expression tag	UNP P48431
W	26	VAL	-	expression tag	UNP P48431
W	27	ASP	-	expression tag	UNP P48431
W	28	GLU	-	expression tag	UNP P48431
W	29	ASN	-	expression tag	UNP P48431
W	30	LEU	-	expression tag	UNP P48431
W	31	TYR	-	expression tag	UNP P48431
W	32	PHE	-	expression tag	UNP P48431
W	33	GLN	-	expression tag	UNP P48431
W	34	GLY	-	expression tag	UNP P48431
W	35	GLY	-	expression tag	UNP P48431
W	36	MET	-	expression tag	UNP P48431

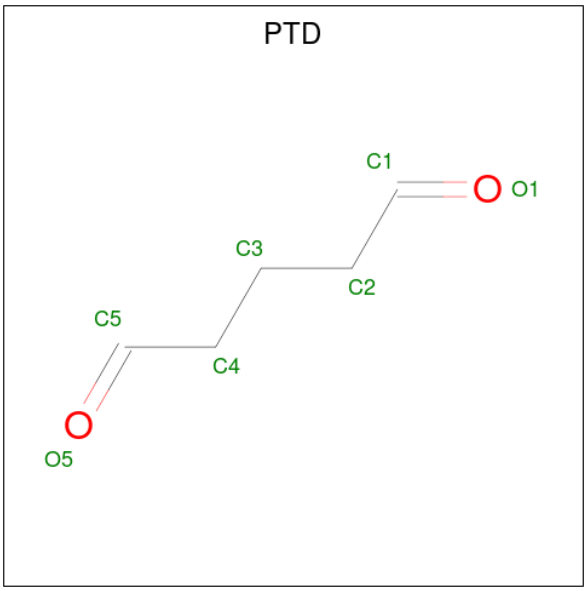
- Molecule 16 is a DNA chain called DNA (148-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	X	142	2889	1377	519	852	141	0	0

- Molecule 17 is a DNA chain called DNA (148-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
17	Y	142	2930	1389	549	850	142	0	0

- Molecule 18 is PENTANEDIAL (CCD ID: PTD) (formula: $C_5H_8O_2$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
18	A	1	5	5	0
18	C	1	5	5	0
18	D	1	5	5	0
18	E	1	5	5	0
18	E	1	5	5	0
18	E	1	5	5	0
18	G	1	5	5	0
18	H	1	5	5	0
18	I	1	5	5	0
18	L	1	5	5	0
18	M	1	5	5	0
18	N	1	5	5	0
18	N	1	5	5	0
18	N	1	5	5	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	C	
18	O	1	5	5	0
			Total	C	
18	P	1	5	5	0

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
19	L	1	1	1	0

3 Residue-property plots (i)

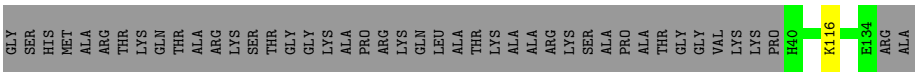
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Histone H3.1

Chain A:

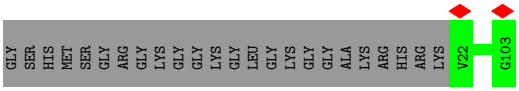
- Molecule 1: Histone H3.1

Chain E:



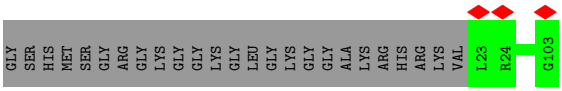
- Molecule 2: Histone H4

Chain B:



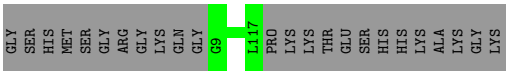
- Molecule 2: Histone H4

Chain F:



- Molecule 3: Histone H2A type 1-B/E

Chain C:



- Molecule 3: Histone H2A type 1-B/E

Chain G: 81% 18%

GLY SER HIS MET SER GLY ARG GLY LYS GLN GLY GLY K10 K37 P118 LYS LYS THR GLU SER HIS HIS LYS ALA LYS GLY LYS

- Molecule 4: Histone H2B type 1-J

Chain D: 71% 27%

GLY SER HIS MET PRO GLU PRO ALA LYS SER ALA PRO ALA PRO LYS LYS GLY SER LYS LYS LYS ALA VAL THR LYS ALA GLN LYS LYS ASP GLY LYS LYS ARG LYS ARG S33 K44 K47 A125

- Molecule 4: Histone H2B type 1-J

Chain H: 72% 27%

GLY SER HIS MET PRO GLU PRO ALA LYS SER ALA PRO ALA PRO LYS LYS GLY SER LYS LYS LYS ALA VAL THR LYS ALA GLN LYS LYS ASP GLY LYS LYS ARG LYS ARG S33 K47 A125

- Molecule 5: Transcription activator BRG1

Chain I: 8% 46% 54%

MET SER THR PRO ASP PRO PRO LEU GLY GLY THR PRO ARG PRO GLY PRO GLY PRO SER PRO GLY ALA ALA MET LEU GLY PRO SER PRO GLY PRO SER PRO GLY SER ALA HIS SER MET MET GLY PRO SER PRO GLY PRO PRO SER ALA GLY HIS PRO ILE PRO THR GLN GLY

PRO GLY GLY TYR PRO GLN ASP ASN MET HIS GLN MET HIS LYS PRO MET GLU SER MET HIS GLU LYS GLY MET SER ASP ASP PRO ARG TYR ASN GLN MET LYS GLY MET GLY MET ARG SER GLY GLY HIS ALA GLY MET GLY PRO PRO PRO SER PRO MET ASP GLN HIS SER GLN GLY TYR

PRO SER PRO LEU GLY GLY SER GLU HIS ALA SER SER PRO VAL PRO ALA SER GLY PRO SER SER GLY PRO GLN MET SER SER GLY PRO GLY GLY ALA PRO LEU ASP GLY ALA ASP PRO GLN ALA LEU GLY GLN GLN ASN ARG GLY PRO THR PRO PHE ASN GLN ASN GLN LEU HIS GLN LEU

ARG ALA GLN ILE MET ALA TYR LYS MET LEU ALA ARG GLY GLN PRO LEU PRO ASP HIS LEU GLN MET ALA VAL GLN GLY LYS ARG PRO MET PRO GLY MET GLN GLN GLN MET PRO THR LEU PRO PRO PRO SER VAL SER ALA THR GLY PRO GLY PRO GLY PRO GLY PRO GLY PRO

GLY PRO GLY PRO ALA PRO PRO ASN TYR SER ARG PRO HIS GLY MET GLY GLY PRO ASN MET PRO PRO PRO GLY PRO SER GLY VAL PRO PRO GLY MET PRO GLY GLN PRO PRO GLY GLY PRO LYS PRO TRP PRO GLU GLY PRO MET ALA ASN ALA ALA ALA PRO THR SER THR PRO GLN

LYS LEU ILE PRO PRO GLN PRO THR GLY ARG PRO SER PRO ALA PRO PRO ALA VAL PRO PRO ALA ALA SER PRO VAL MET PRO PRO GLN THR GLN SER PRO GLY GLN PRO ALA GLN PRO ALA PRO MET VAL PRO LEU HIS GLN LYS GLN S350 K455 K458 T501 Y507 K517

GLU ASN GLU ARG ILE GLU LYS GLU ARG MET ARG ARG LEU MET ALA GLU ASP GLU GLU GLY TYR ARG K540 A551 Y552 L553 L554 Q555 Q556 T557 D558 E559 TYR VAL ALA ASN LEU THR GLU LEU VAL ARG GLN HIS LYS ALA ALA GLN VAL ALA LYS GLU LYS LYS LYS LYS LYS LYS LYS

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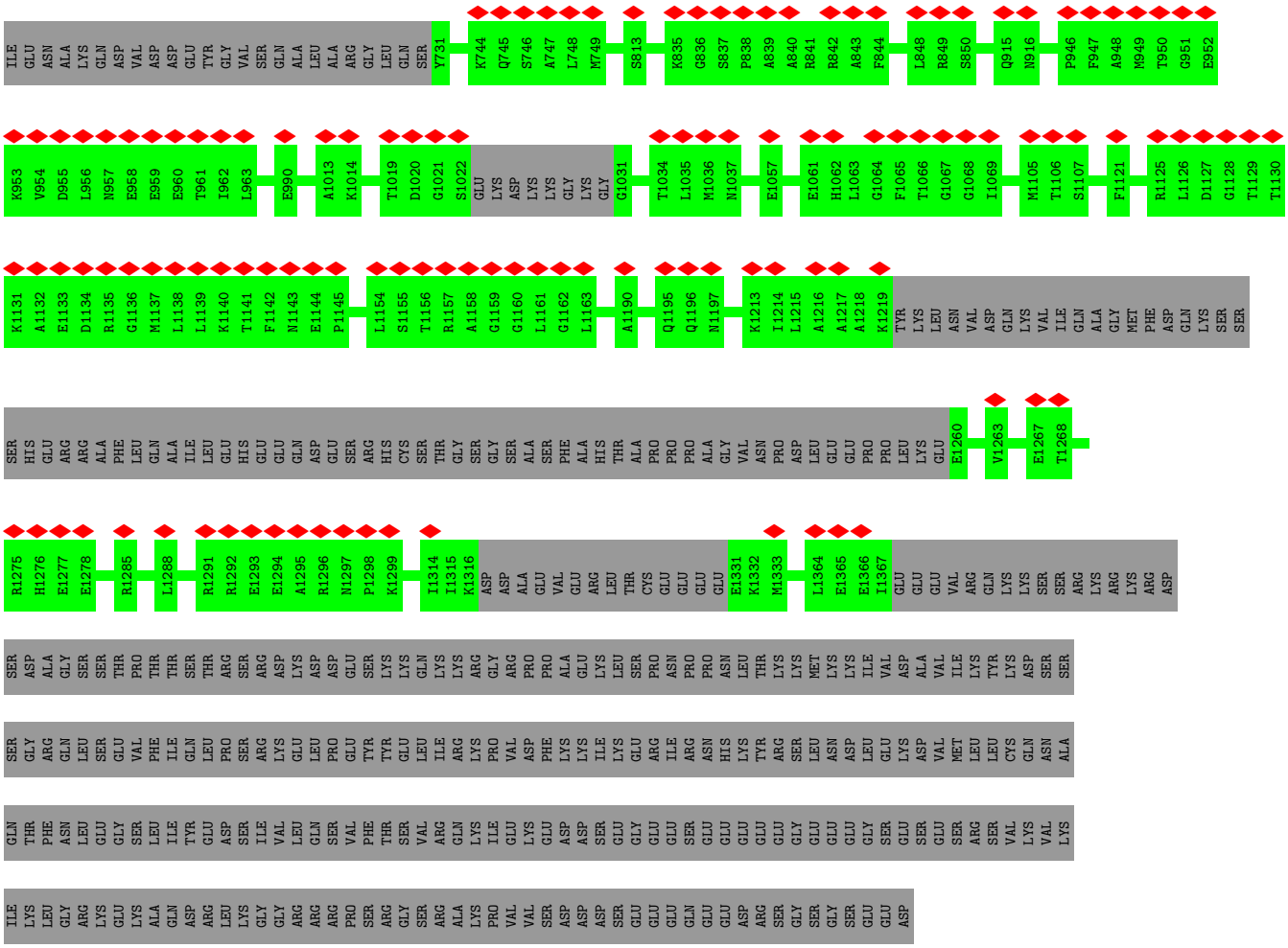
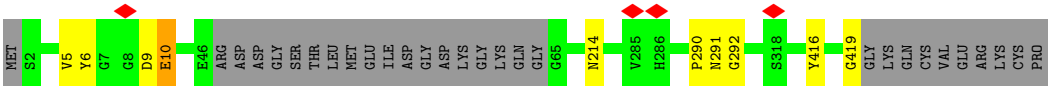


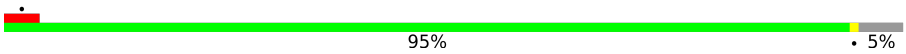
- Molecule 6: Actin-like protein 6A

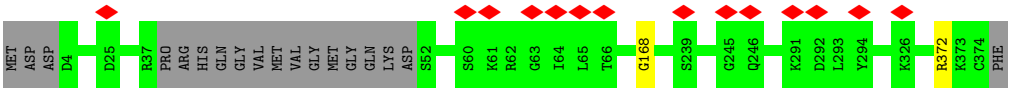
Chain J:



- Molecule 7: Actin, cytoplasmic 1, N-terminally processed

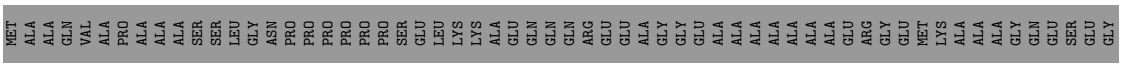
Chain K:





- Molecule 8: AT-rich interactive domain-containing protein 1A

Chain L:



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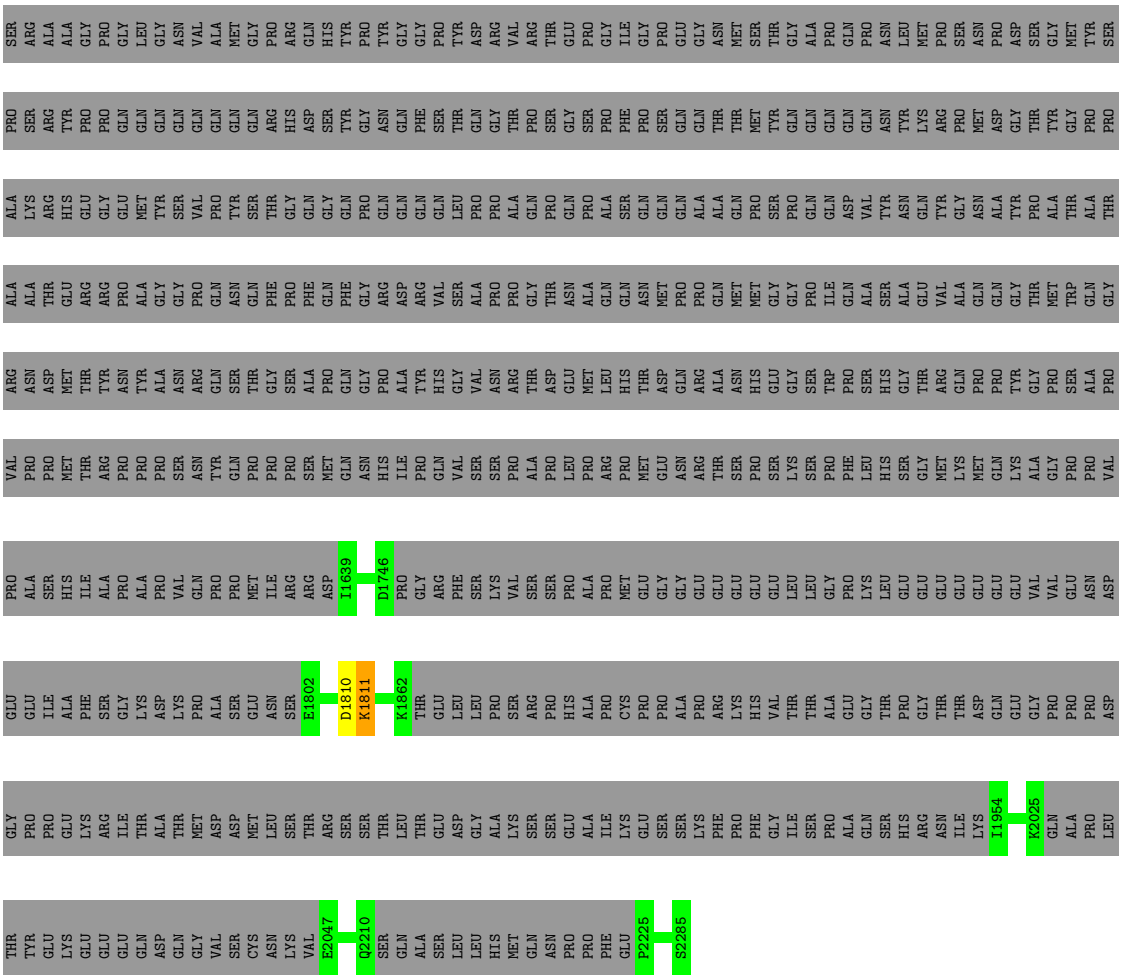
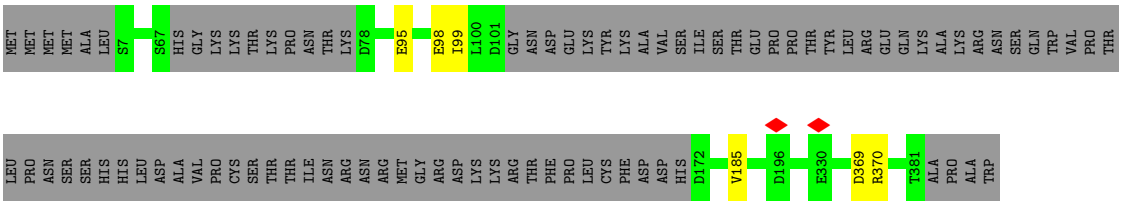


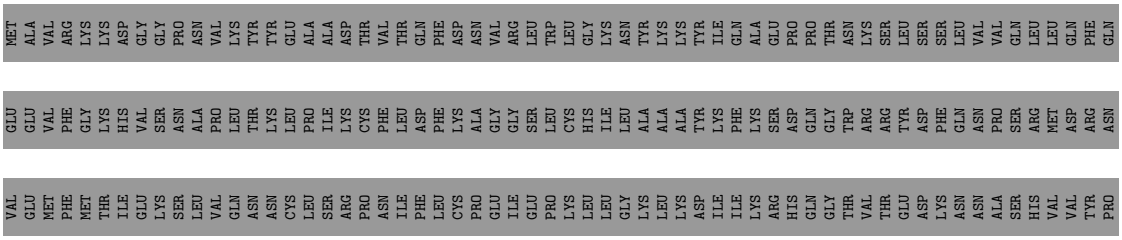
• Molecule 9: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily B member 1

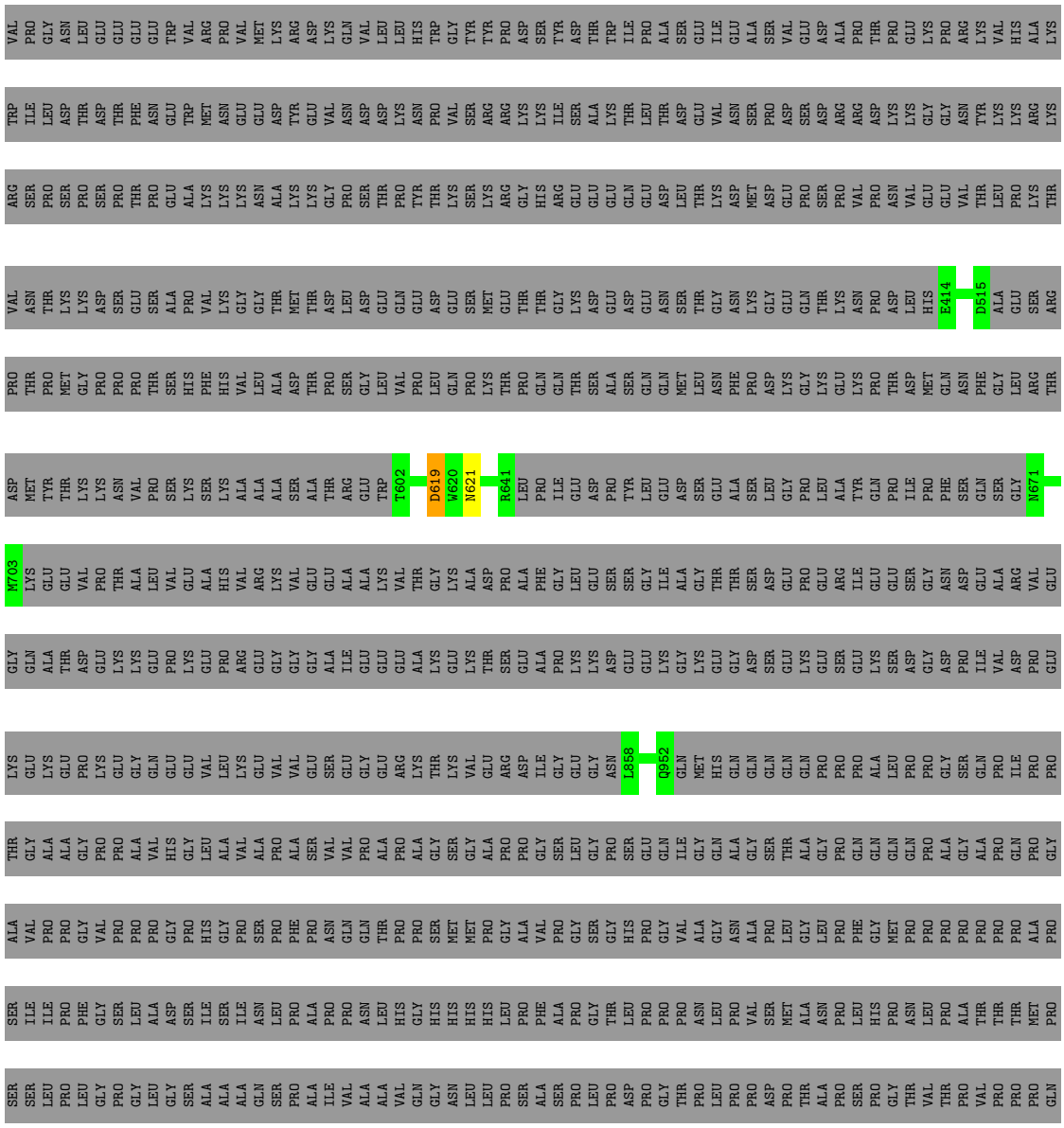
Chain M:



• Molecule 10: SWI/SNF complex subunit SMARCC2

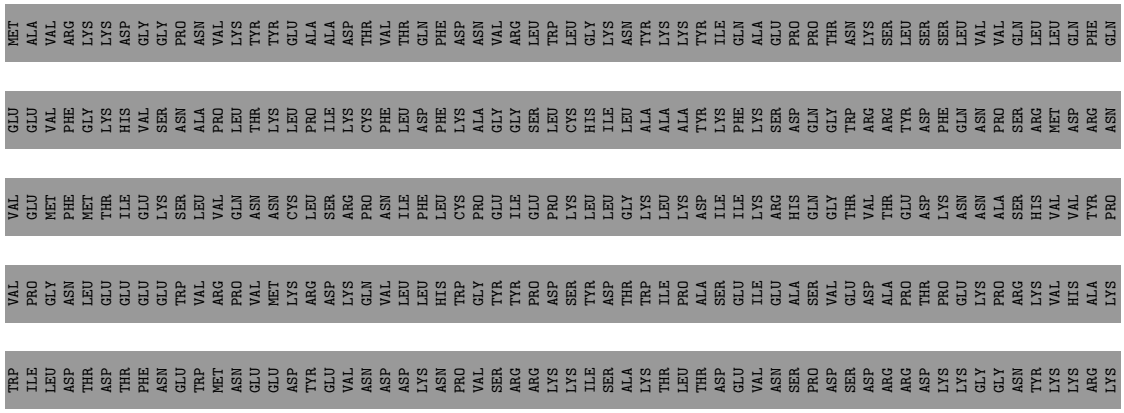
Chain N:

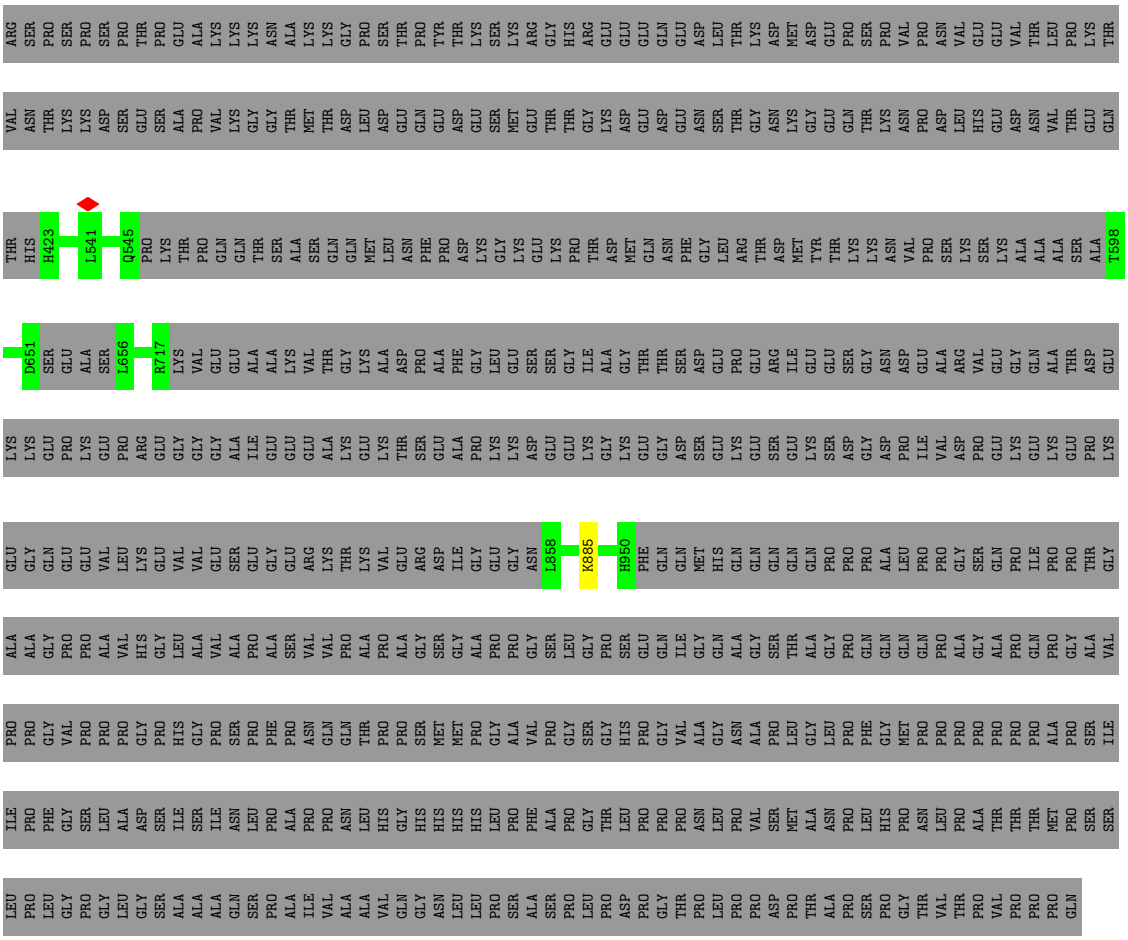




• Molecule 10: SWI/SNF complex subunit SMARCC2

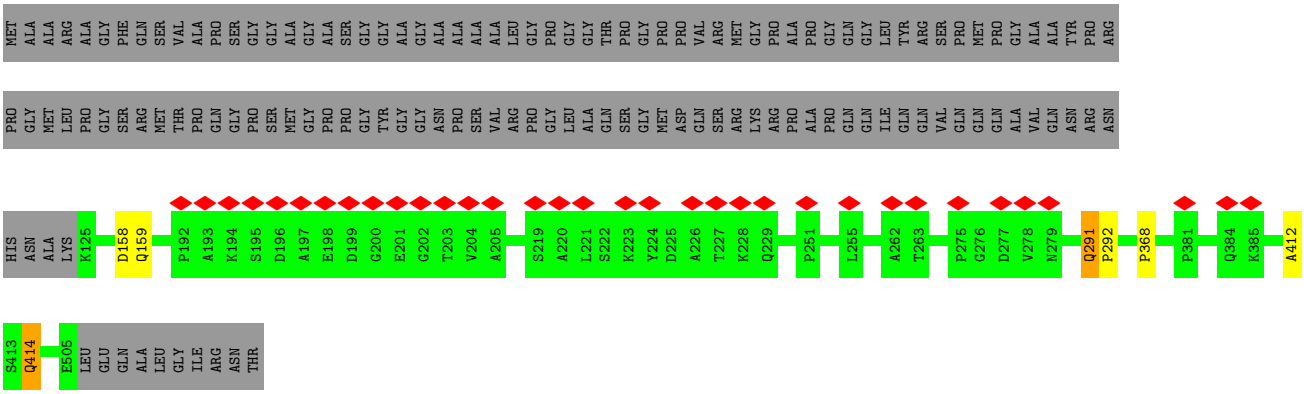
Chain O: 27% 73%





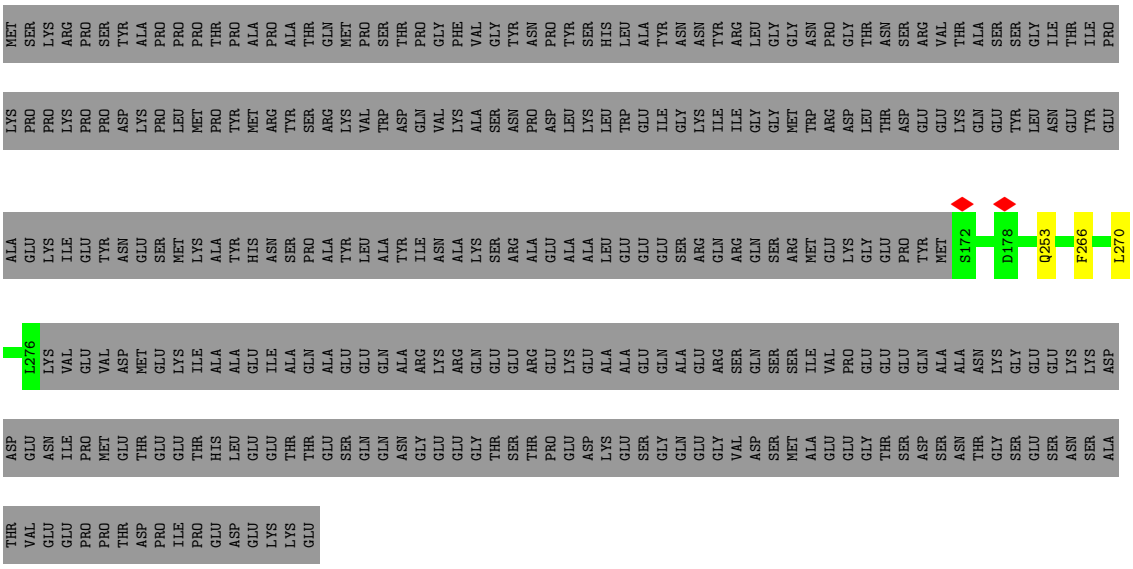
• Molecule 11: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily D member 1

Chain P: 7% 73% • 26%



• Molecule 12: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1

Chain Q: 25% • 74%

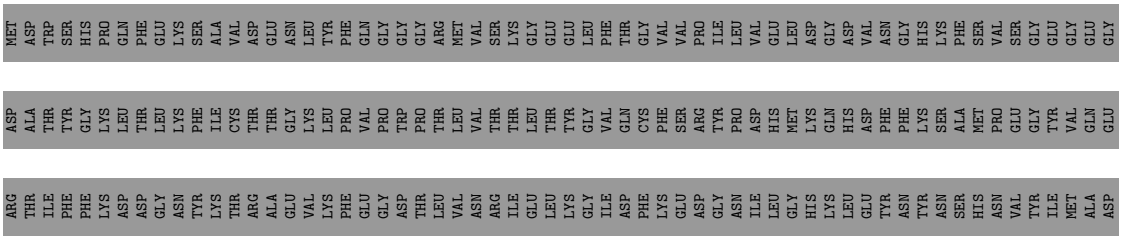


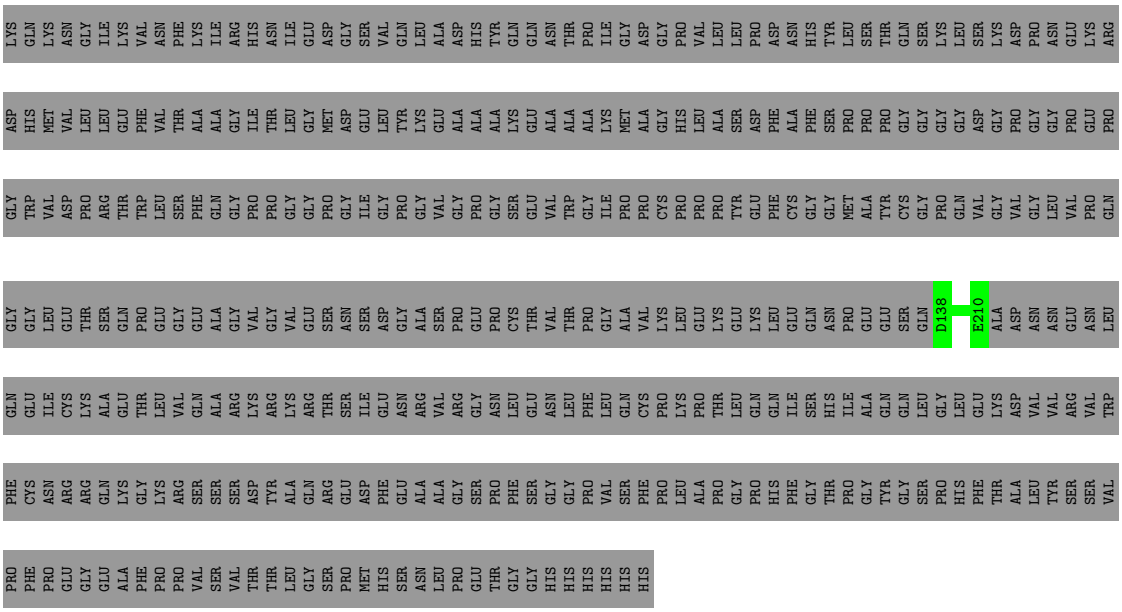
• Molecule 13: Zinc finger protein ubi-d4

Chain R:

• Molecule 14: Green fluorescent protein,POU domain, class 5, transcription factor 1

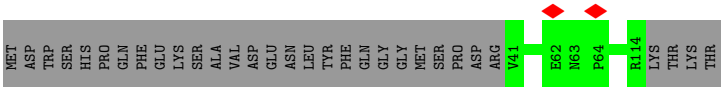
Chain V:





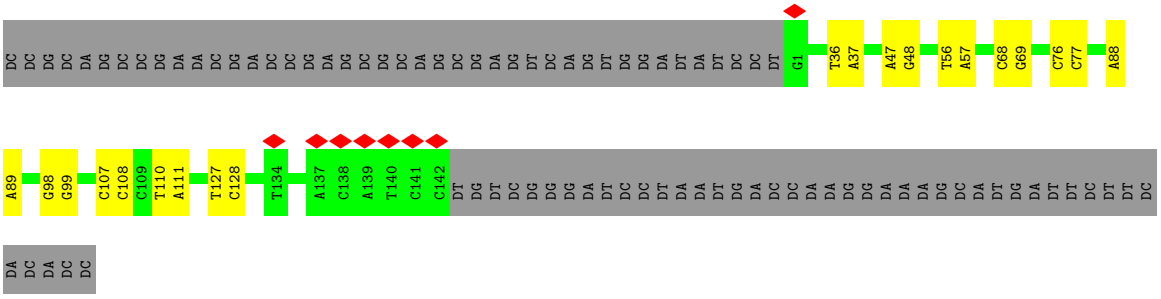
- Molecule 15: Transcription factor SOX-2

Chain W:



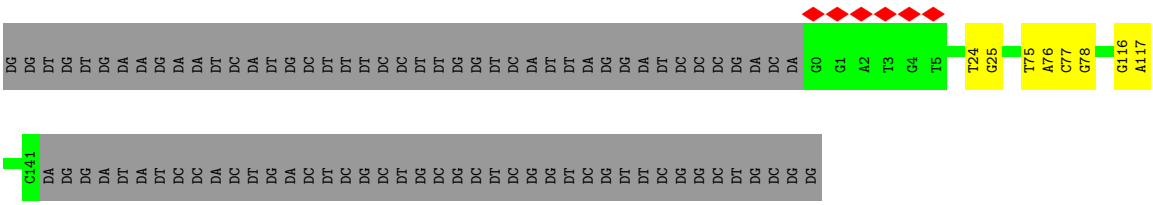
- Molecule 16: DNA (148-MER)

Chain X:



- Molecule 17: DNA (148-MER)

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	179373	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.474	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	405.6, 405.6, 405.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.845, 0.845, 0.845	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PTD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.37	0/783	0.53	1/1050 (0.1%)
1	E	0.36	0/794	0.52	0/1065
2	B	0.32	0/660	0.50	0/883
2	F	0.31	0/653	0.53	0/873
3	C	0.29	0/846	0.47	0/1139
3	G	0.29	0/850	0.45	0/1146
4	D	0.35	0/737	0.47	0/990
4	H	0.36	0/737	0.49	0/990
5	I	0.37	0/4552	0.57	0/6250
6	J	0.25	0/3180	0.49	0/4315
7	K	0.28	0/2843	0.49	0/3852
8	L	0.28	0/3740	0.51	1/5070 (0.0%)
9	M	0.29	0/2418	0.48	0/3269
10	N	0.32	0/2233	0.48	0/3011
10	O	0.27	0/2725	0.49	0/3693
11	P	0.33	0/2792	0.56	0/3797
12	Q	0.27	0/871	0.51	0/1168
13	R	0.34	0/595	0.55	0/799
14	V	0.24	0/363	0.46	0/505
15	W	0.30	0/382	0.51	0/536
16	X	0.40	0/3236	0.71	0/4988
17	Y	0.39	0/3291	0.68	0/5082
All	All	0.32	0/39281	0.55	2/54471 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	1811	LYS	CD-CE-NZ	8.23	138.24	111.90
1	A	123	LYS	N-CA-CB	5.12	117.74	110.06

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	773	0	804	0	0
1	E	783	0	810	0	0
2	B	653	0	694	0	0
2	F	646	0	685	0	0
3	C	837	0	895	0	0
3	G	840	0	900	0	0
4	D	726	0	739	0	0
4	H	726	0	737	0	0
5	I	4517	0	3119	1	0
6	J	3109	0	3039	4	0
7	K	2784	0	2756	2	0
8	L	3671	0	3720	1	0
9	M	2375	0	2337	3	0
10	N	2194	0	2169	1	0
10	O	2666	0	2644	0	0
11	P	2744	0	2403	4	0
12	Q	860	0	864	1	0
13	R	580	0	552	0	0
14	V	363	0	166	0	0
15	W	378	0	189	0	0
16	X	2889	0	1599	10	0
17	Y	2930	0	1596	4	0
18	A	5	0	6	0	0
18	C	5	0	6	0	0
18	D	5	0	6	0	0
18	E	15	0	18	0	0
18	G	5	0	6	0	0
18	H	5	0	6	0	0
18	I	5	0	6	0	0
18	L	5	0	6	0	0
18	M	5	0	6	0	0
18	N	15	0	18	0	0
18	O	5	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	P	5	0	6	0	0
19	L	1	0	0	0	0
All	All	38125	0	33513	29	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:6:TYR:O	7:K:372:ARG:NH1	2.29	0.65
9:M:369:ASP:OD1	9:M:370:ARG:N	2.36	0.59
16:X:88:DA:H2"	16:X:89:DA:C8	2.37	0.58
6:J:416:TYR:O	6:J:419:GLY:N	2.41	0.53
10:N:619:ASP:OD1	10:N:621:ASN:N	2.41	0.52
16:X:110:DT:H2"	16:X:111:DA:C8	2.45	0.52
11:P:291:GLN:HB2	11:P:292:PRO:HD2	1.91	0.52
8:L:1810:ASP:OD1	8:L:1811:LYS:N	2.43	0.52
16:X:76:DC:H2"	16:X:77:DC:C6	2.46	0.51
9:M:369:ASP:OD1	9:M:369:ASP:C	2.54	0.51
16:X:36:DT:H2"	16:X:37:DA:C8	2.47	0.49
17:Y:75:DT:H2"	17:Y:76:DA:C8	2.48	0.48
11:P:412:ALA:O	11:P:414:GLN:NE2	2.43	0.47
16:X:107:DC:H2"	16:X:108:DC:C6	2.50	0.47
17:Y:116:DG:H2"	17:Y:117:DA:C8	2.50	0.47
16:X:47:DA:H2"	16:X:48:DG:C8	2.52	0.45
16:X:127:DT:H2"	16:X:128:DC:C5	2.51	0.45
16:X:68:DC:H2"	16:X:69:DG:C8	2.52	0.45
5:I:501:THR:HG21	7:K:168:GLY:HA3	2.00	0.43
6:J:9:ASP:OD1	6:J:10:GLU:N	2.51	0.43
11:P:291:GLN:CB	11:P:292:PRO:HD2	2.48	0.43
16:X:98:DG:H2"	16:X:99:DG:C8	2.53	0.42
17:Y:24:DT:H2"	17:Y:25:DG:C8	2.54	0.42
12:Q:266:PHE:CZ	12:Q:270:LEU:HD11	2.55	0.42
17:Y:77:DC:H2"	17:Y:78:DG:C8	2.55	0.41
16:X:56:DT:H2"	16:X:57:DA:C8	2.55	0.41
6:J:290:PRO:C	6:J:292:GLY:H	2.29	0.40
11:P:158:ASP:OD1	11:P:159:GLN:N	2.55	0.40
9:M:95:GLU:O	9:M:98:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	92/139 (66%)	92 (100%)	0	0	100	100
1	E	93/139 (67%)	93 (100%)	0	0	100	100
2	B	80/106 (76%)	79 (99%)	1 (1%)	0	100	100
2	F	79/106 (74%)	79 (100%)	0	0	100	100
3	C	107/133 (80%)	105 (98%)	2 (2%)	0	100	100
3	G	107/133 (80%)	104 (97%)	3 (3%)	0	100	100
4	D	91/128 (71%)	89 (98%)	2 (2%)	0	100	100
4	H	91/128 (71%)	91 (100%)	0	0	100	100
5	I	751/1647 (46%)	718 (96%)	33 (4%)	0	100	100
6	J	396/429 (92%)	385 (97%)	9 (2%)	2 (0%)	24	57
7	K	353/375 (94%)	344 (98%)	9 (2%)	0	100	100
8	L	456/2285 (20%)	442 (97%)	14 (3%)	0	100	100
9	M	289/385 (75%)	281 (97%)	8 (3%)	0	100	100
10	N	262/1214 (22%)	261 (100%)	1 (0%)	0	100	100
10	O	324/1214 (27%)	315 (97%)	9 (3%)	0	100	100
11	P	379/515 (74%)	364 (96%)	13 (3%)	2 (0%)	24	57
12	Q	103/411 (25%)	101 (98%)	2 (2%)	0	100	100
13	R	68/435 (16%)	65 (96%)	3 (4%)	0	100	100
14	V	71/645 (11%)	71 (100%)	0	0	100	100
15	W	72/105 (69%)	72 (100%)	0	0	100	100
All	All	4264/10672 (40%)	4151 (97%)	109 (3%)	4 (0%)	49	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	P	291	GLN

Continued on next page...

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Mol	Chain	Res	Type
11	P	368	PRO
6	J	10	GLU
6	J	291	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	82/113 (73%)	82 (100%)	0	100	100
1	E	83/113 (74%)	82 (99%)	1 (1%)	63	73
2	B	67/81 (83%)	67 (100%)	0	100	100
2	F	66/81 (82%)	66 (100%)	0	100	100
3	C	84/102 (82%)	84 (100%)	0	100	100
3	G	85/102 (83%)	84 (99%)	1 (1%)	63	73
4	D	79/106 (74%)	77 (98%)	2 (2%)	42	63
4	H	79/106 (74%)	78 (99%)	1 (1%)	61	72
5	I	204/1422 (14%)	202 (99%)	2 (1%)	68	75
6	J	340/364 (93%)	338 (99%)	2 (1%)	78	79
7	K	303/318 (95%)	303 (100%)	0	100	100
8	L	418/1845 (23%)	418 (100%)	0	100	100
9	M	265/346 (77%)	263 (99%)	2 (1%)	73	77
10	N	231/1030 (22%)	230 (100%)	1 (0%)	84	81
10	O	284/1030 (28%)	283 (100%)	1 (0%)	84	81
11	P	231/442 (52%)	230 (100%)	1 (0%)	84	81
12	Q	98/361 (27%)	97 (99%)	1 (1%)	68	75
13	R	59/373 (16%)	59 (100%)	0	100	100
14	V	1/537 (0%)	1 (100%)	0	100	100
15	W	5/95 (5%)	5 (100%)	0	100	100
All	All	3064/8967 (34%)	3049 (100%)	15 (0%)	78	80

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	44	LYS
4	D	47	LYS
1	E	116	LYS
3	G	37	LYS
4	H	47	LYS
5	I	455	LYS
5	I	458	LYS
6	J	5	VAL
6	J	214	ASN
9	M	99	ILE
9	M	185	VAL
10	N	619	ASP
10	O	885	LYS
11	P	414	GLN
12	Q	253	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
3	G	25	GLN
3	G	39	ASN
5	I	387	ASN
5	I	460	GLN
5	I	490	HIS
5	I	508	HIS
7	K	78	ASN
7	K	92	ASN
7	K	263	GLN
8	L	1692	ASN
8	L	1843	HIS
8	L	1854	HIS
8	L	1986	ASN
8	L	2100	GLN
8	L	2109	ASN
8	L	2115	GLN
8	L	2273	GLN
8	L	2284	GLN
9	M	278	GLN
9	M	348	GLN
10	N	604	GLN

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Mol	Chain	Res	Type
10	O	513	GLN
10	O	626	HIS
10	O	923	GLN
10	O	932	GLN
11	P	432	ASN
11	P	453	ASN
11	P	484	GLN
12	Q	190	HIS
12	Q	197	GLN
12	Q	267	ASN
13	R	23	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	PTD	E	203	1	4,4,6	0.33	0	3,3,5	0.56	0
18	PTD	D	201	4	4,4,6	0.32	0	3,3,5	0.56	0
18	PTD	N	1303	10	4,4,6	0.32	0	3,3,5	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	PTD	O	1301	9,10	4,4,6	0.33	0	3,3,5	0.56	0
18	PTD	E	202	2,1	4,4,6	0.32	0	3,3,5	0.51	0
18	PTD	C	201	3,4	4,4,6	0.33	0	3,3,5	0.51	0
18	PTD	H	201	4	4,4,6	0.30	0	3,3,5	0.60	0
18	PTD	N	1302	10,13	4,4,6	0.33	0	3,3,5	0.52	0
18	PTD	P	601	11,8	4,4,6	0.34	0	3,3,5	0.53	0
18	PTD	M	401	9	4,4,6	0.36	0	3,3,5	0.50	0
18	PTD	G	201	3,4	4,4,6	0.30	0	3,3,5	0.62	0
18	PTD	N	1301	10,11	4,4,6	0.30	0	3,3,5	0.56	0
18	PTD	A	201	2,1	4,4,6	0.30	0	3,3,5	0.56	0
18	PTD	L	2302	13,8	4,4,6	0.32	0	3,3,5	0.53	0
18	PTD	E	201	1	4,4,6	0.30	0	3,3,5	0.63	0
18	PTD	I	1701	5	4,4,6	0.31	0	3,3,5	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	PTD	E	203	1	-	1/2/2/4	-
18	PTD	D	201	4	-	1/2/2/4	-
18	PTD	N	1303	10	-	1/2/2/4	-
18	PTD	O	1301	9,10	-	0/2/2/4	-
18	PTD	E	202	2,1	-	1/2/2/4	-
18	PTD	C	201	3,4	-	1/2/2/4	-
18	PTD	H	201	4	-	0/2/2/4	-
18	PTD	N	1302	10,13	-	2/2/2/4	-
18	PTD	P	601	11,8	-	2/2/2/4	-
18	PTD	M	401	9	-	2/2/2/4	-
18	PTD	G	201	3,4	-	1/2/2/4	-
18	PTD	N	1301	10,11	-	0/2/2/4	-
18	PTD	A	201	2,1	-	1/2/2/4	-
18	PTD	L	2302	13,8	-	0/2/2/4	-
18	PTD	E	201	1	-	0/2/2/4	-
18	PTD	I	1701	5	-	0/2/2/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	P	601	PTD	C1-C2-C3-C4
18	M	401	PTD	C2-C3-C4-C5
18	N	1302	PTD	C1-C2-C3-C4
18	P	601	PTD	C2-C3-C4-C5
18	D	201	PTD	C2-C3-C4-C5
18	G	201	PTD	C2-C3-C4-C5
18	M	401	PTD	C1-C2-C3-C4
18	C	201	PTD	C2-C3-C4-C5
18	E	202	PTD	C2-C3-C4-C5
18	N	1303	PTD	C1-C2-C3-C4
18	A	201	PTD	C2-C3-C4-C5
18	N	1302	PTD	C2-C3-C4-C5
18	E	203	PTD	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

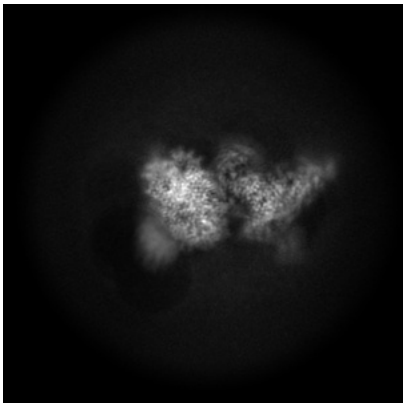
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-54030. These allow visual inspection of the internal detail of the map and identification of artifacts.

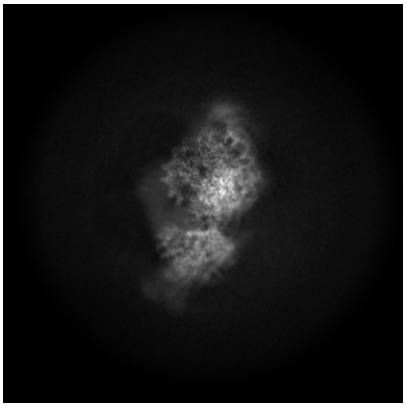
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

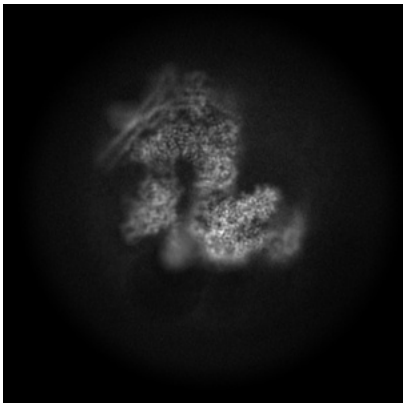
6.1.1 Primary map



X



Y



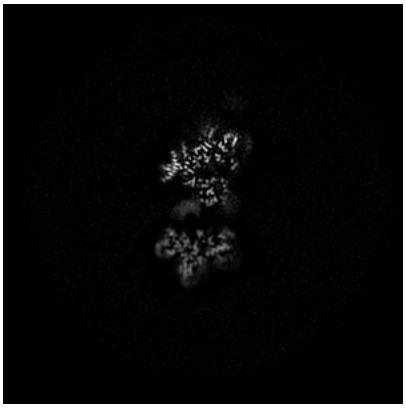
Z

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

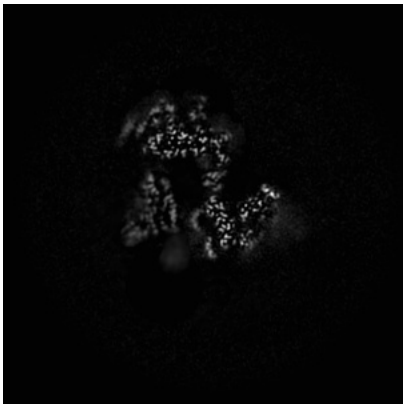
6.2 Central slices (i)

6.2.1 Primary map

X Index: 240



Y Index: 240

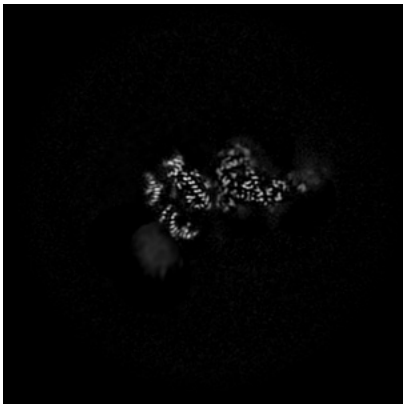


Z Index: 240

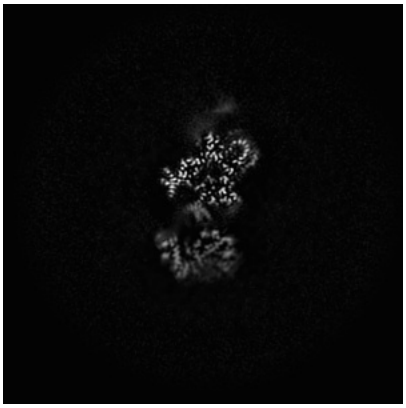
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

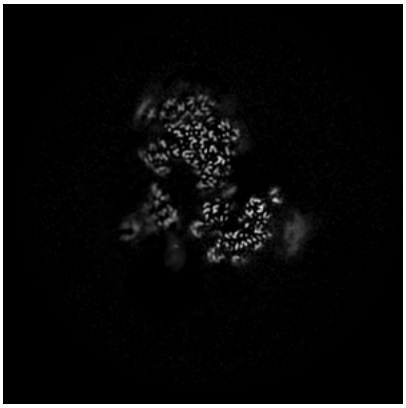
6.3.1 Primary map



X Index: 253



Y Index: 228

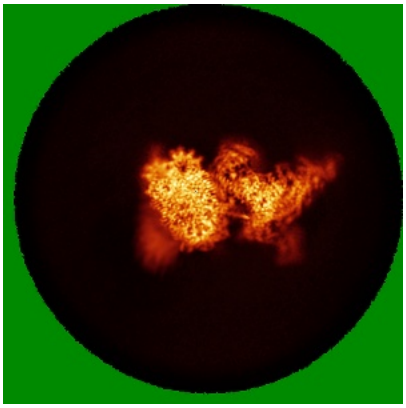


Z Index: 255

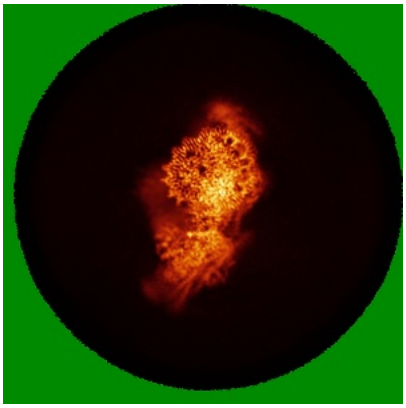
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

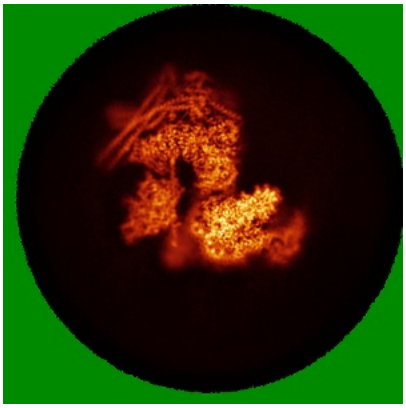
6.4.1 Primary map



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.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

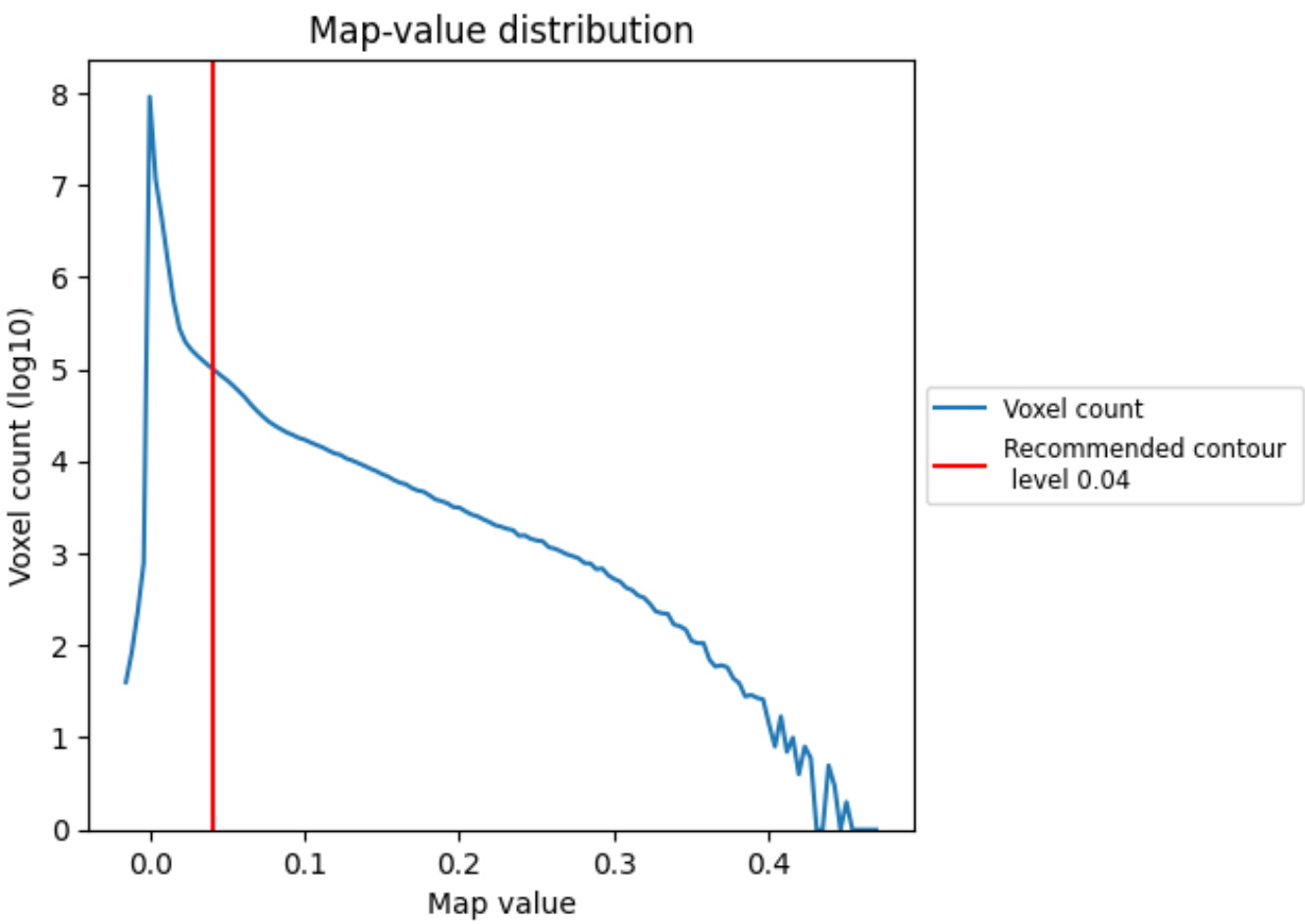
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

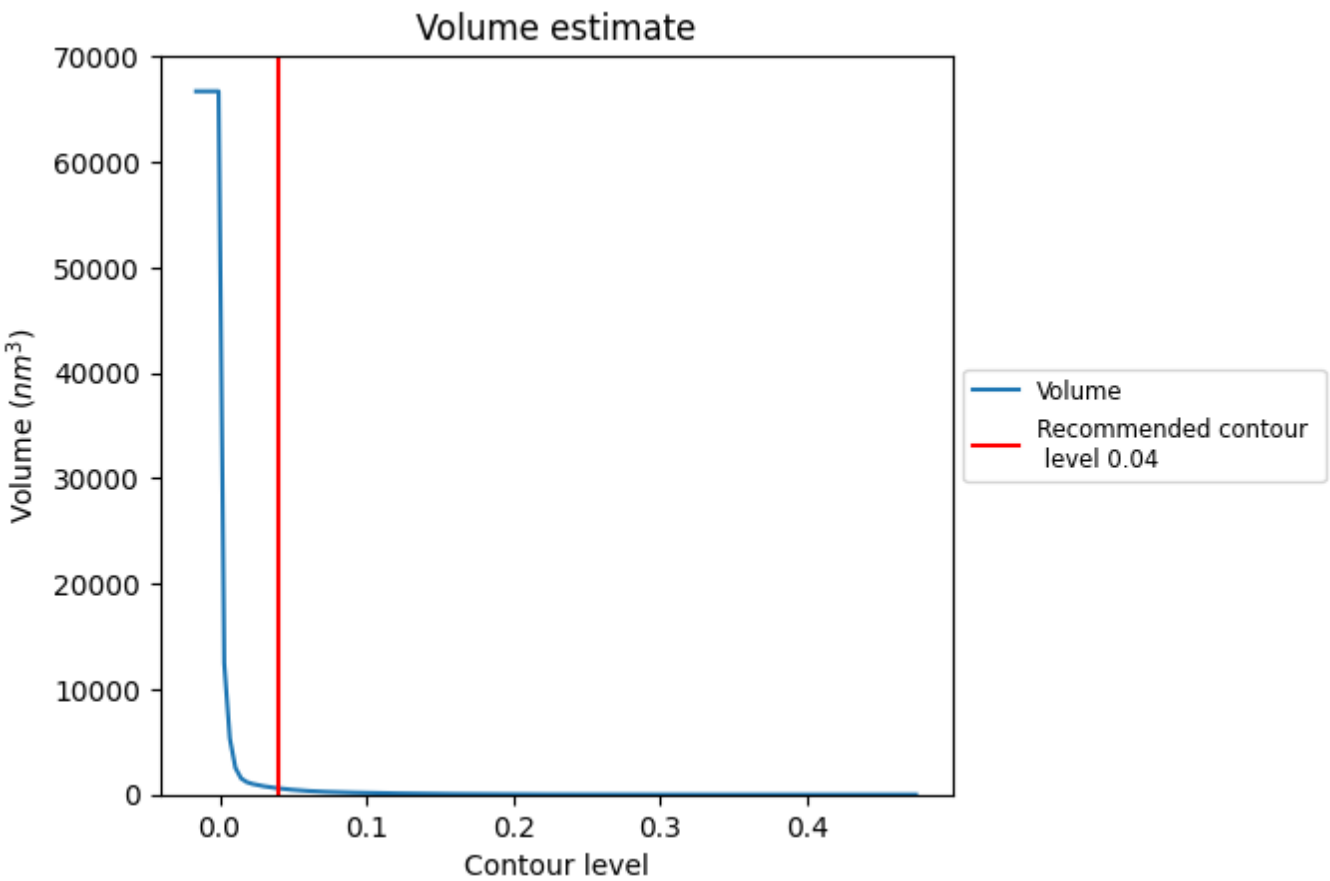
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

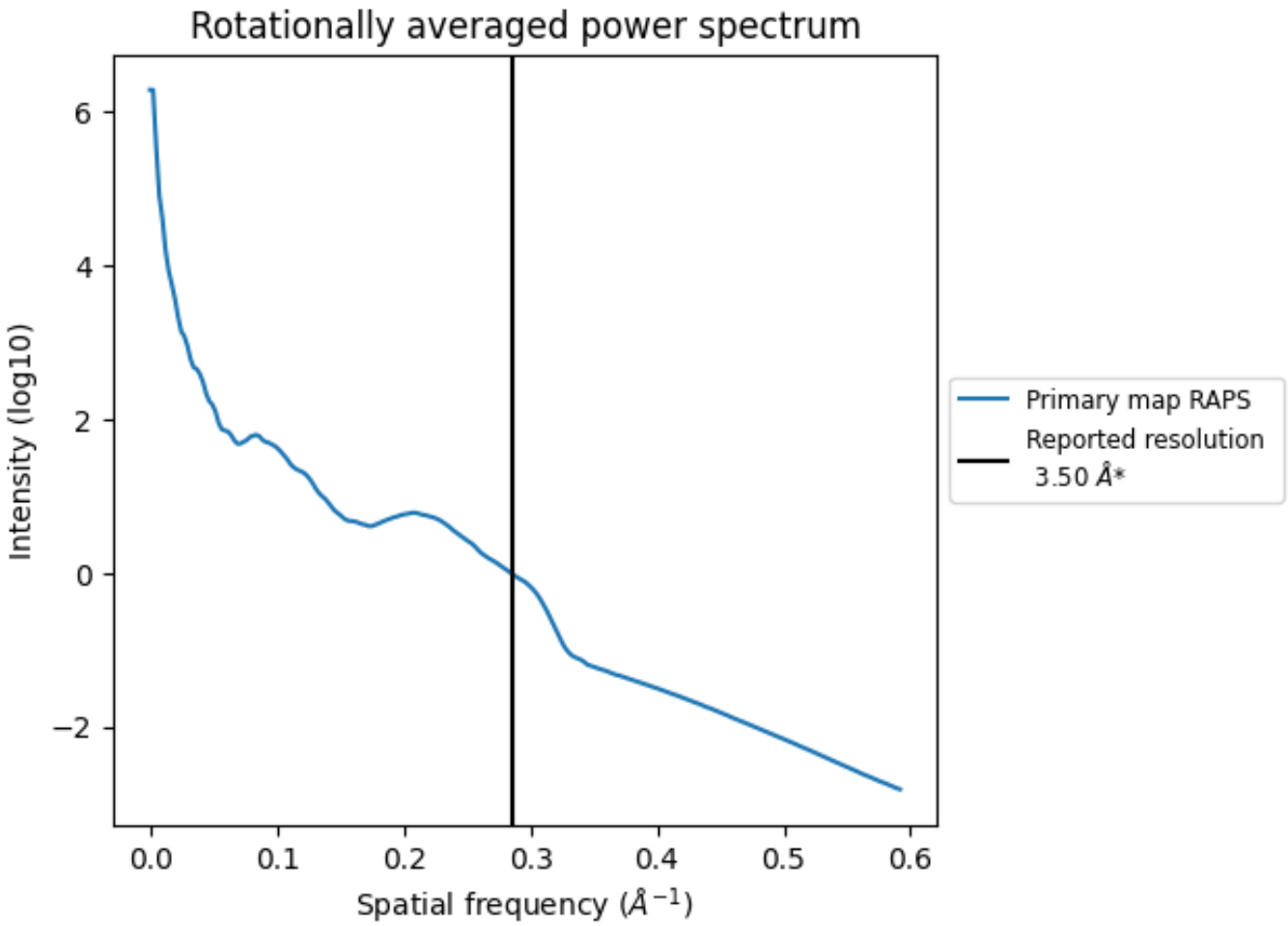
7.2 Volume estimate (i)



The volume at the recommended contour level is 595 nm^3; this corresponds to an approximate mass of 538 kDa.

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.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

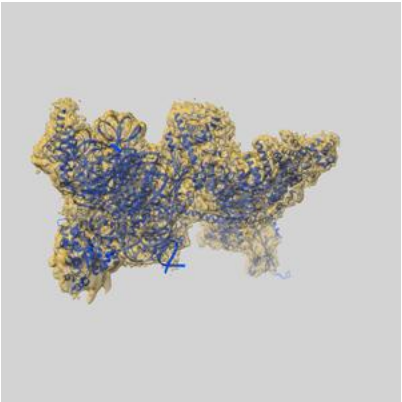
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

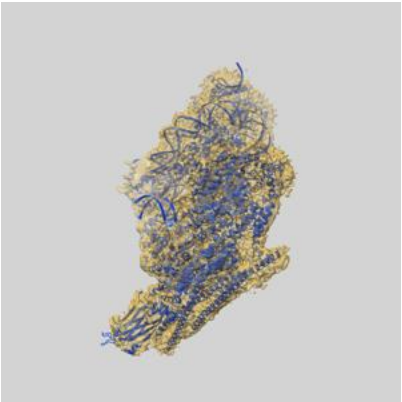
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-54030 and PDB model 9RL4. Per-residue inclusion information can be found in section 3 on page 13.

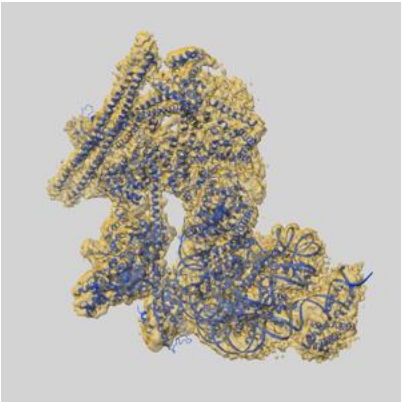
9.1 Map-model overlay (i)



X



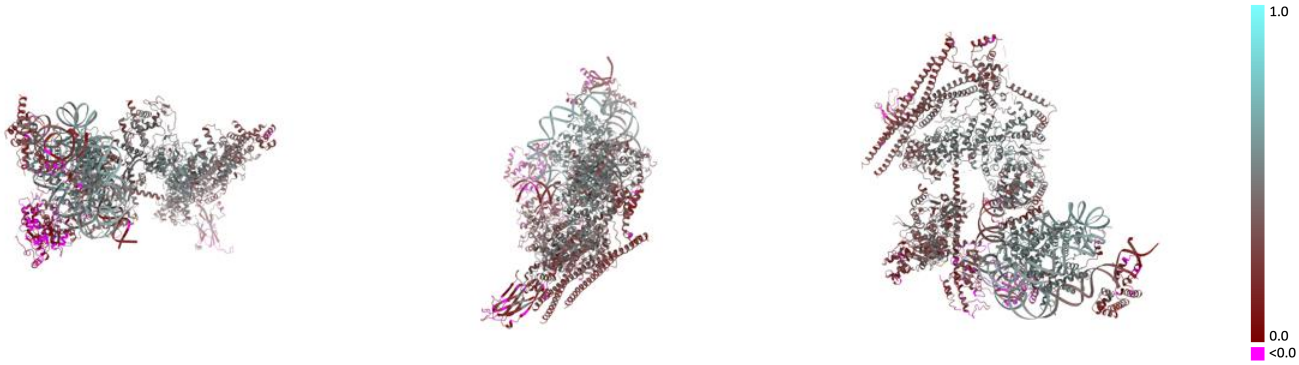
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

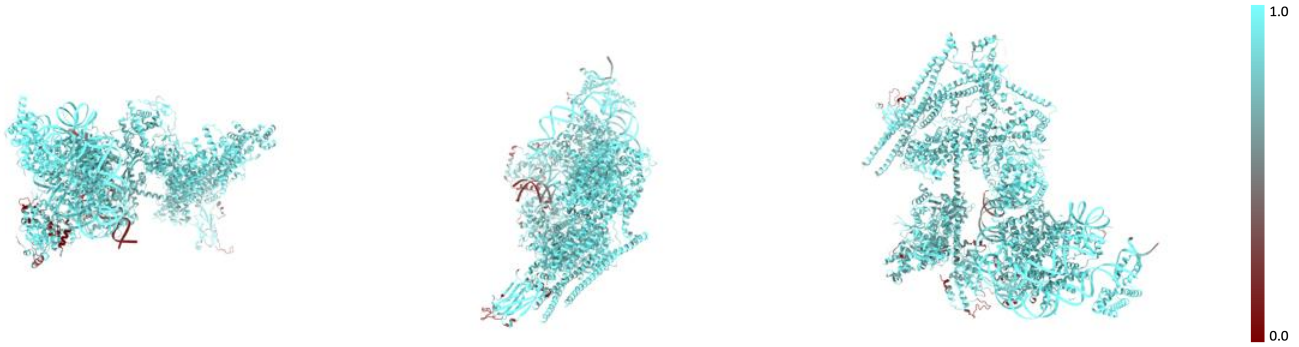
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

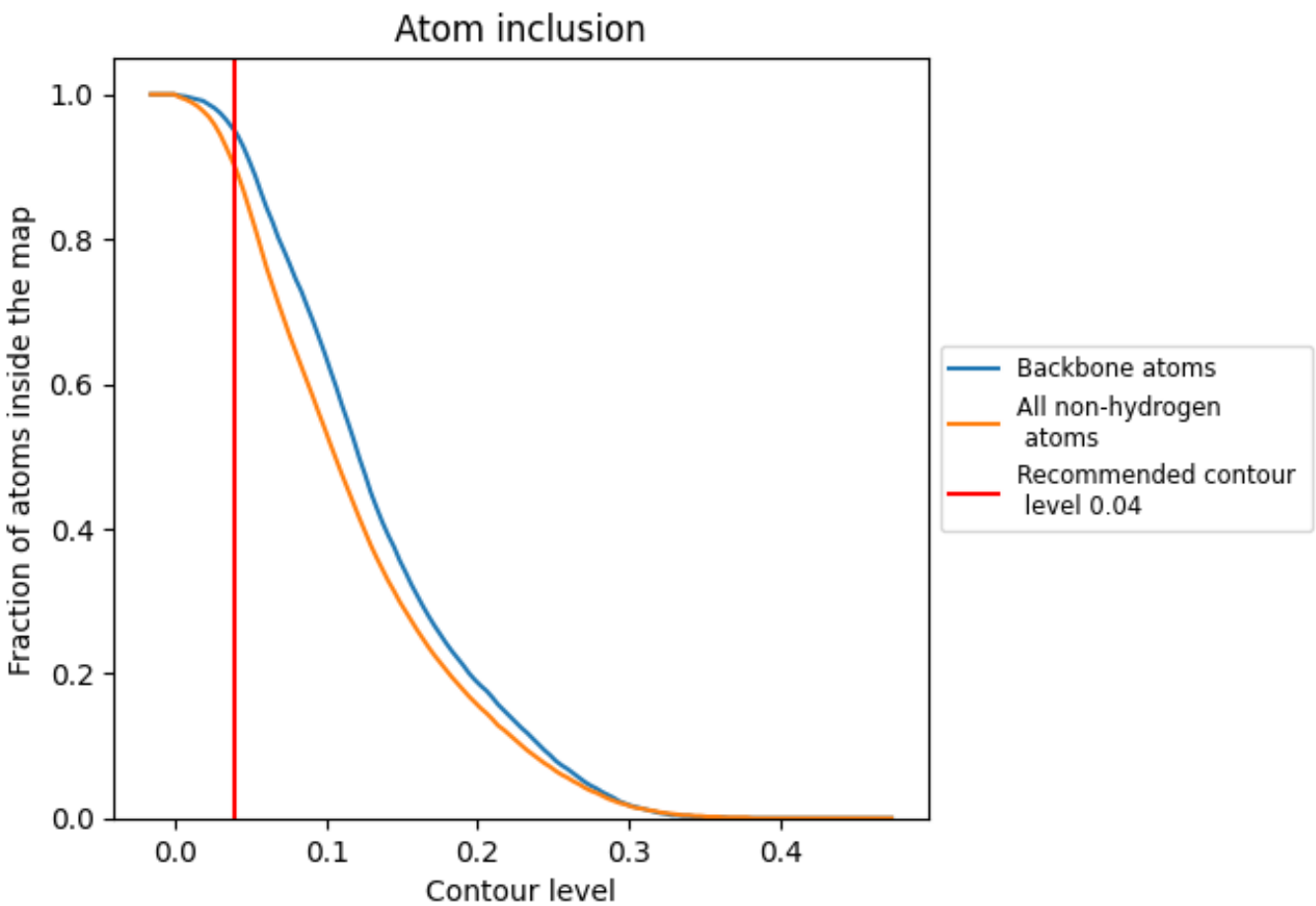
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8980	0.3860
A	0.9610	0.5520
B	0.9490	0.5520
C	0.9660	0.5190
D	0.9760	0.5250
E	0.9730	0.5400
F	0.9520	0.5490
G	0.9310	0.5070
H	0.9580	0.5260
I	0.7940	0.1780
J	0.8900	0.3540
K	0.8420	0.3060
L	0.9240	0.4690
M	0.9120	0.4000
N	0.9120	0.3780
O	0.9040	0.3750
P	0.8490	0.3180
Q	0.8730	0.2980
R	0.9390	0.4550
V	1.0000	0.2740
W	0.9660	0.1580
X	0.9330	0.4630
Y	0.9340	0.4620