wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Nov 5, 2019 – 10:53 AM EST

PDB ID	:	6K15
EMDB ID:	:	EMD-9905
Title	:	RSC substrate-recruitment module
Authors	:	Ye, Y.P.; Wu, H.; Chen, K.J.; Verma, N.; Cairns, B.; Gao, N.; Chen, Z.C.
Deposited on	:	2019-05-09
Resolution	:	3.40 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB 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.

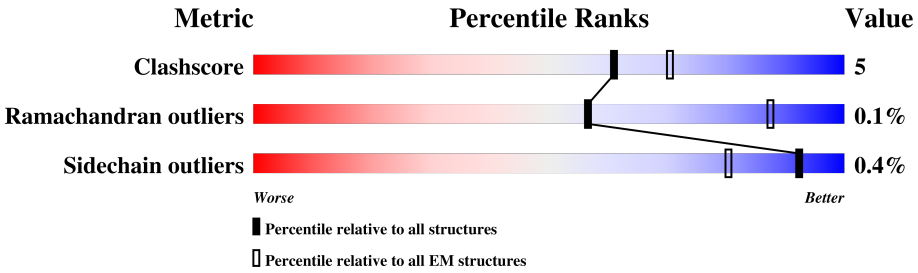
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

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 3.40 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)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

Mol	Chain	Length	Quality of chain
1	F	435	25% · 73%
2	D	557	48% 7% 45%
2	H	557	62% 9% 29%
3	M	581	62% · 34%
4	I	483	46% 5% 49%
5	G	426	47% 11% 42%
6	A	502	62% 11% 27%
7	J	1359	15% · 83%
8	E	78	64% 10% 26%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	C	883	96%
10	K	885	5% 95%
11	X	625	19% 76%
12	L	889	8% 90%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 21486 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 Chromatin structure-remodeling complex subunit RSC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	118	Total	C	N	O	S	0	0
			964	601	164	197	2		

- Molecule 2 is a protein called Chromatin structure-remodeling complex protein RSC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	393	Total	C	N	O	S	0	0
			3215	2036	552	613	14		
2	D	305	Total	C	N	O	S	0	0
			2510	1613	416	471	10		

- Molecule 3 is a protein called Chromatin structure-remodeling complex subunit RSC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	384	Total	C	N	O	S	0	0
			3058	1970	497	574	17		

- Molecule 4 is a protein called Chromatin structure-remodeling complex protein RSC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	244	Total	C	N	O	S	0	0
			1944	1234	328	377	5		

- Molecule 5 is a protein called Chromatin structure-remodeling complex subunit SFH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	246	Total	C	N	O	S	0	0
			1991	1268	335	380	8		

- Molecule 6 is a protein called Chromatin structure-remodeling complex protein RSC58.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	365	Total	C	N	O	S	0	0
			3007	1942	509	547	9		

- Molecule 7 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	235	Total	C	N	O	S	0	0
			1814	1136	327	349	2		

- Molecule 8 is a protein called High temperature lethal protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	58	Total	C	N	O	S	0	0
			477	295	86	92	4		

- Molecule 9 is a protein called Chromatin structure-remodeling complex protein RSC30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	33	Total	C	N	O	S	0	0
			269	177	39	52	1		

- Molecule 10 is a protein called Chromatin structure-remodeling complex protein RSC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	42	Total	C	N	O	S	0	0
			347	225	57	63	2		

- Molecule 11 is a protein called Chromatin structure-remodeling complex subunit RSC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	147	Total	C	N	O	S	0	0
			1220	776	202	234	8		

- Molecule 12 is a protein called Chromatin structure-remodeling complex subunit RSC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	85	Total	C	N	O	S	0	0
			669	428	120	119	2		

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

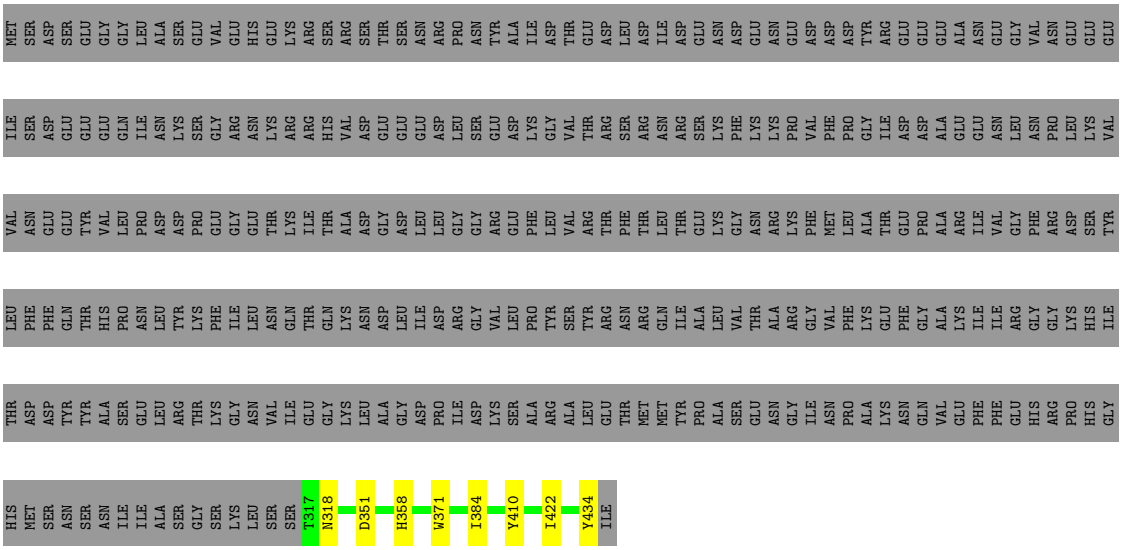
Mol	Chain	Residues	Atoms		AltConf
13	H	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

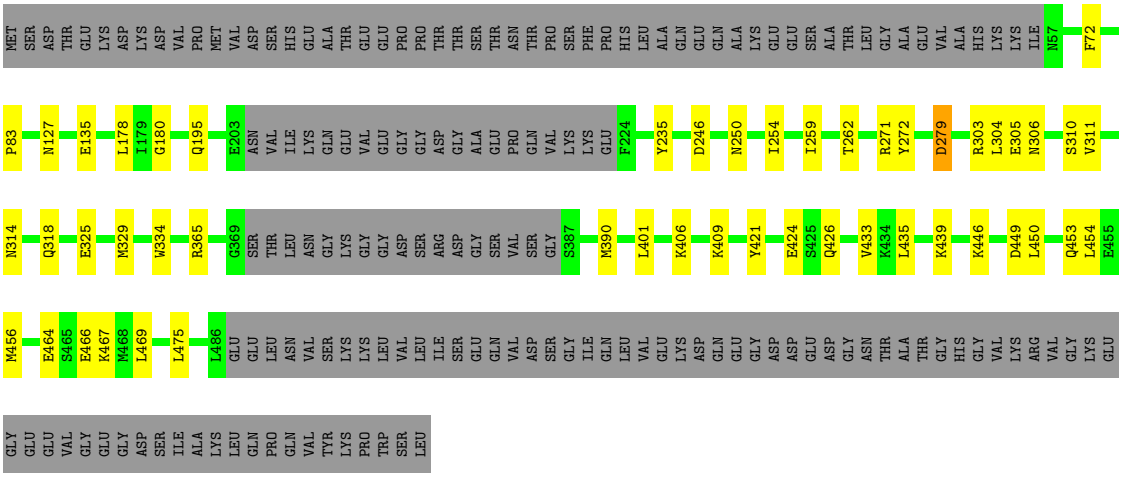
• Molecule 1: Chromatin structure-remodeling complex subunit RSC7

Chain F:



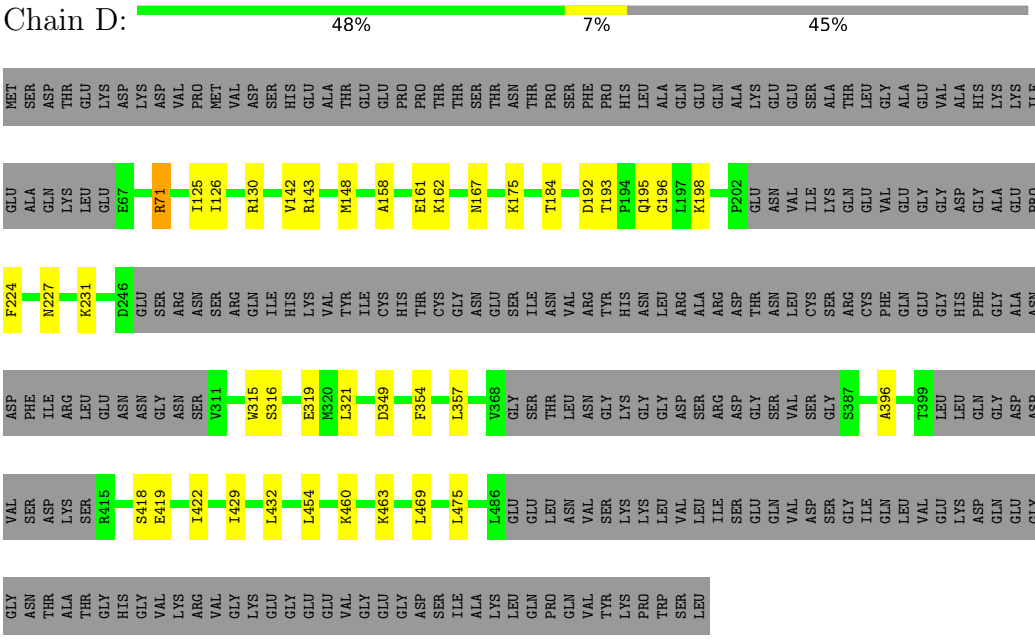
• Molecule 2: Chromatin structure-remodeling complex protein RSC8

Chain H:



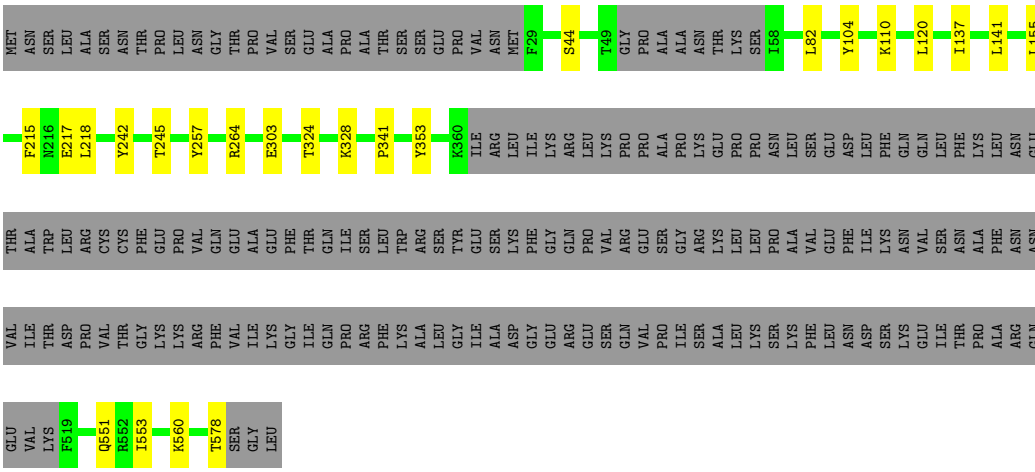
• Molecule 2: Chromatin structure-remodeling complex protein RSC8

Chain D:



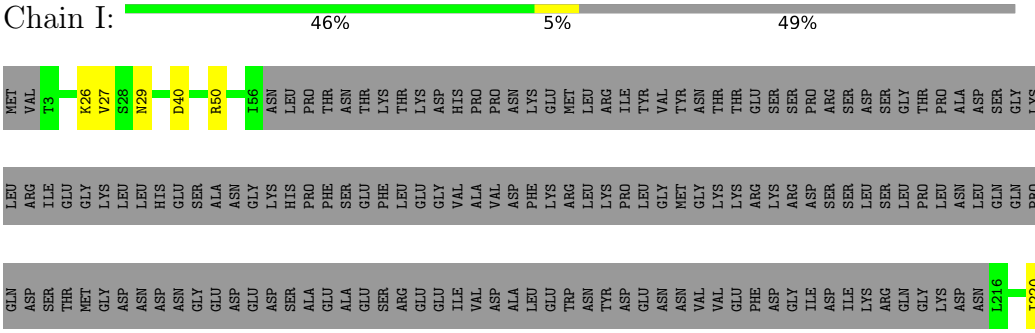
• Molecule 3: Chromatin structure-remodeling complex subunit RSC9

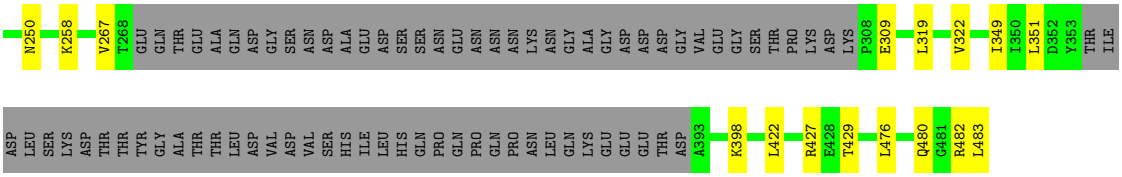
Chain M:



• Molecule 4: Chromatin structure-remodeling complex protein RSC6

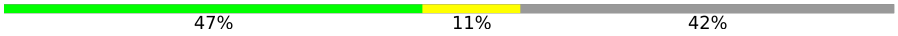
Chain I:

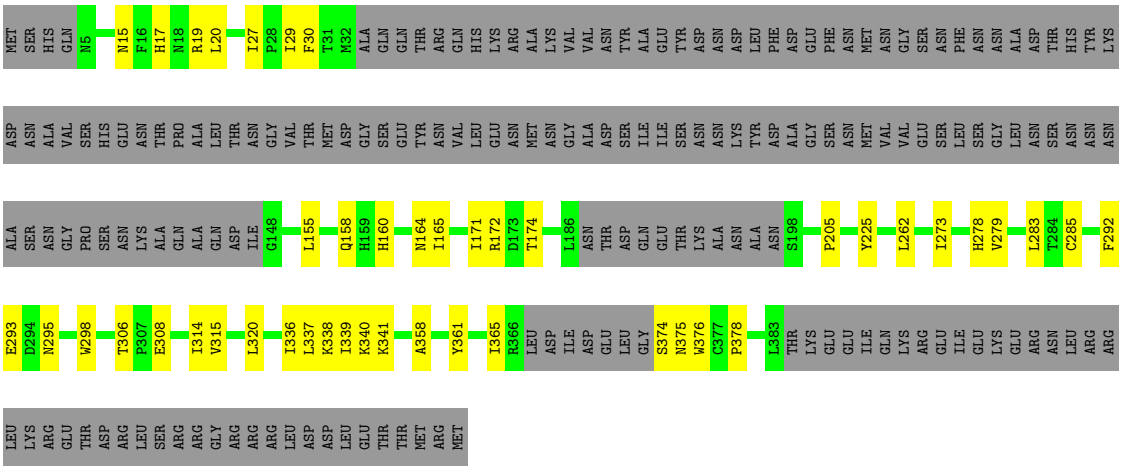




• Molecule 5: Chromatin structure-remodeling complex subunit SFH1

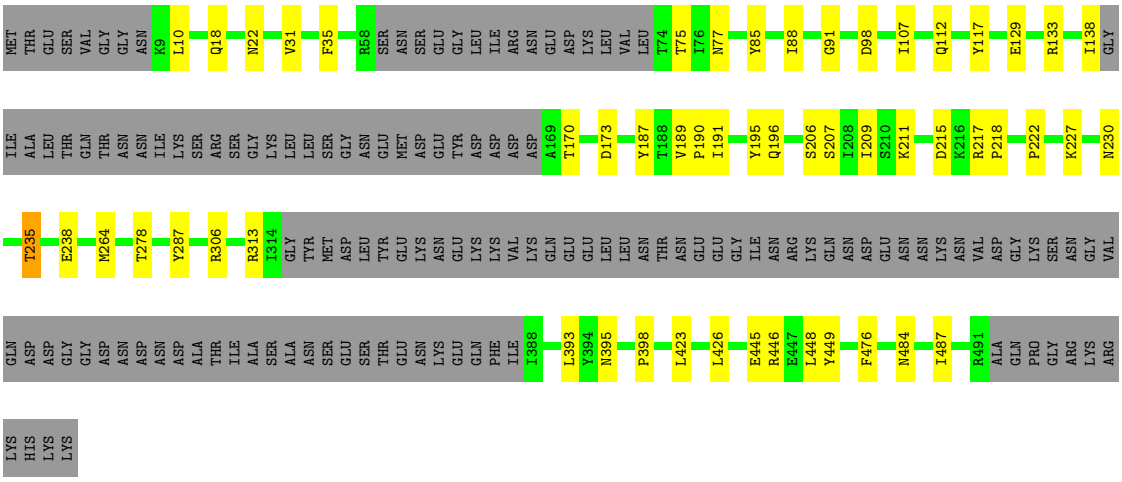
Chain G:





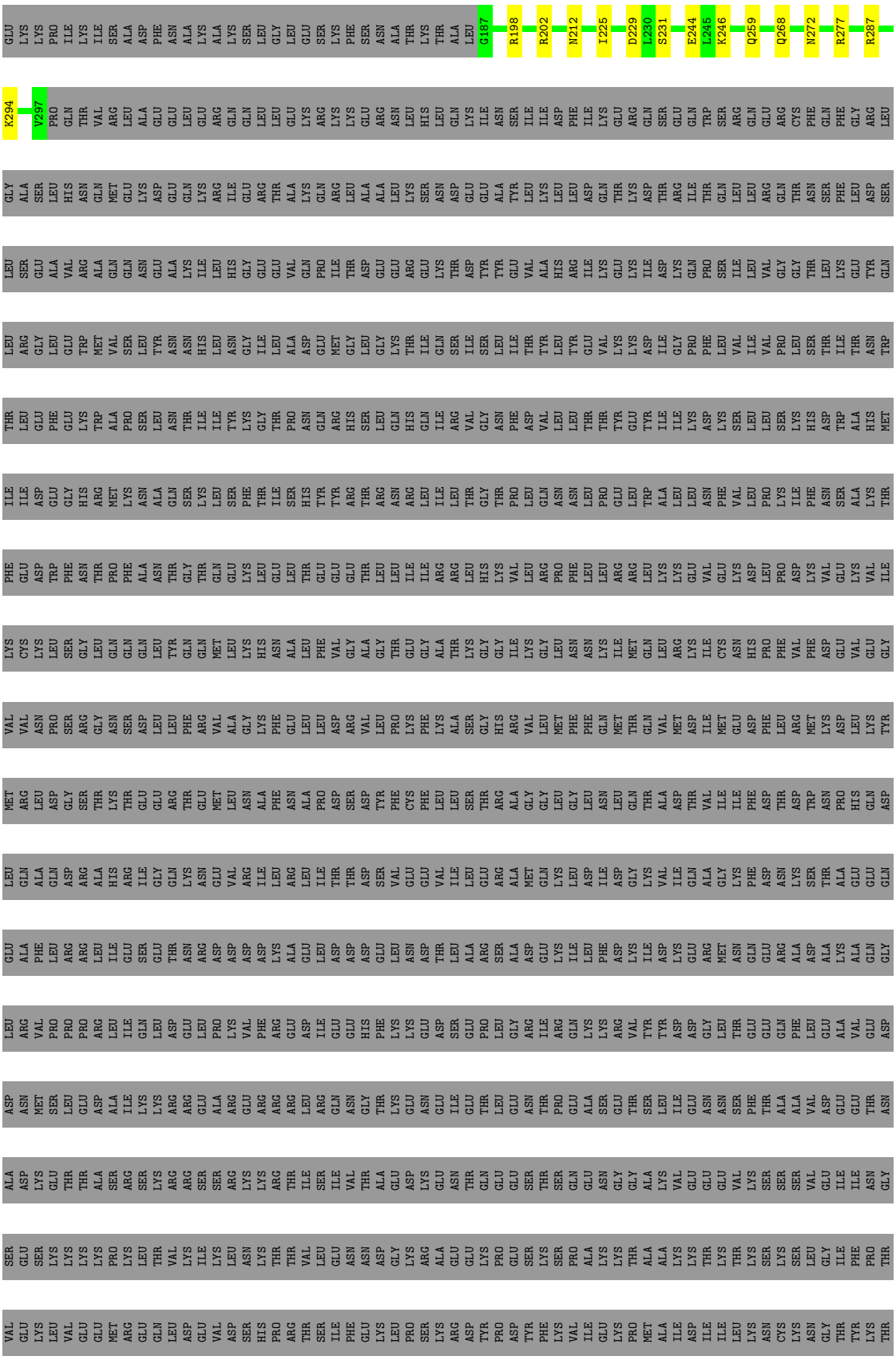
• Molecule 6: Chromatin structure-remodeling complex protein RSC58

Chain A:



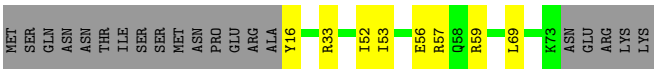
• Molecule 7: Nuclear protein STH1/NPS1

Chain J:


G187
R198
R202
N212
T225
D229
L230
S231
E244
L245
K246
Q259
Q268
N272
R277
R287
K294
V297

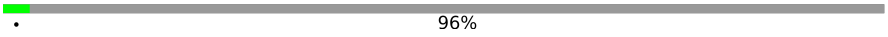
• Molecule 8: High temperature lethal protein 1

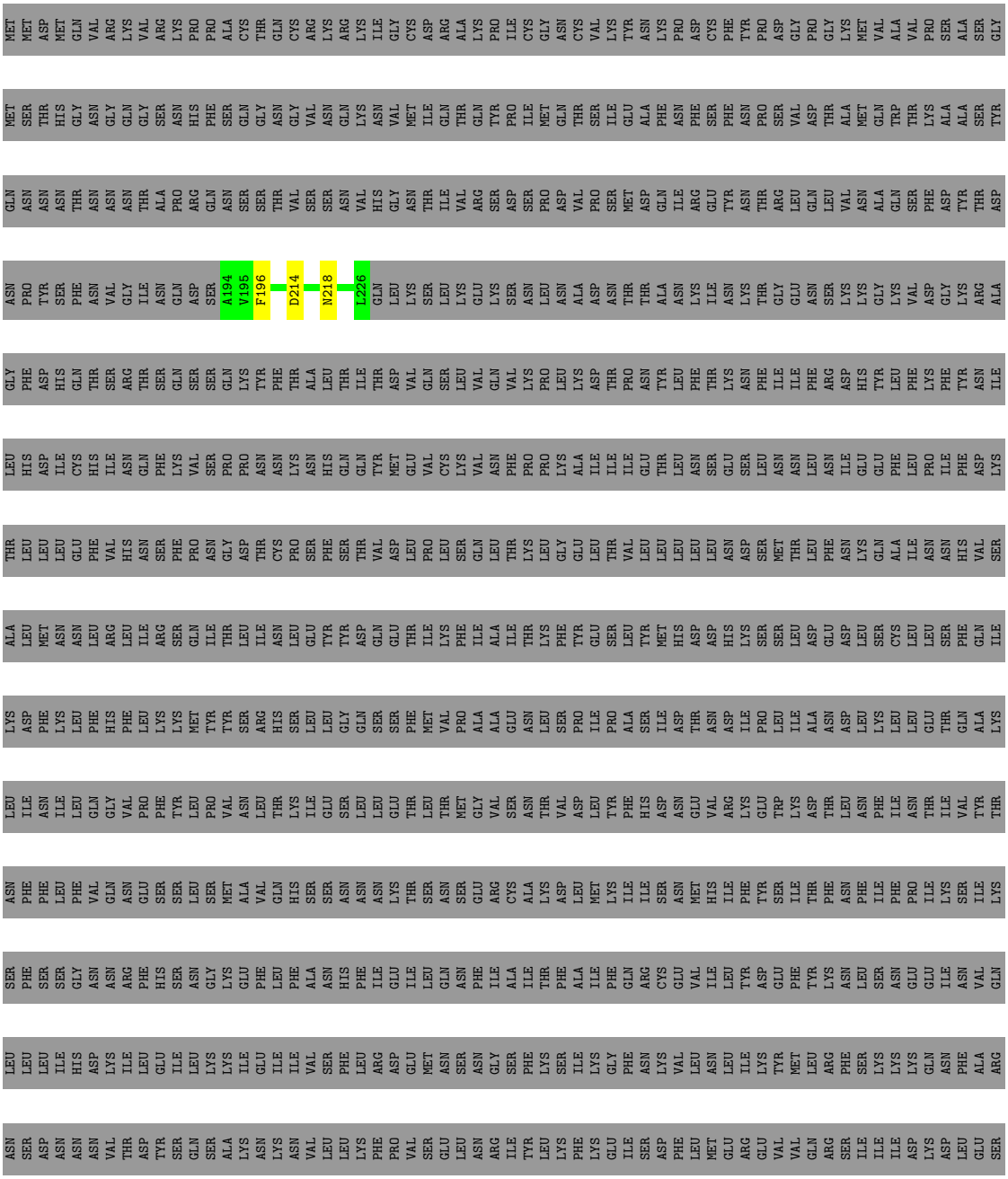
Chain E:

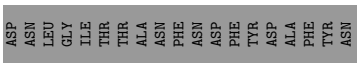


• Molecule 9: Chromatin structure-remodeling complex protein RSC30

Chain C:

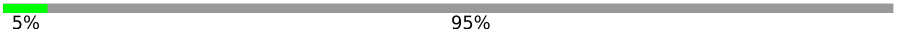


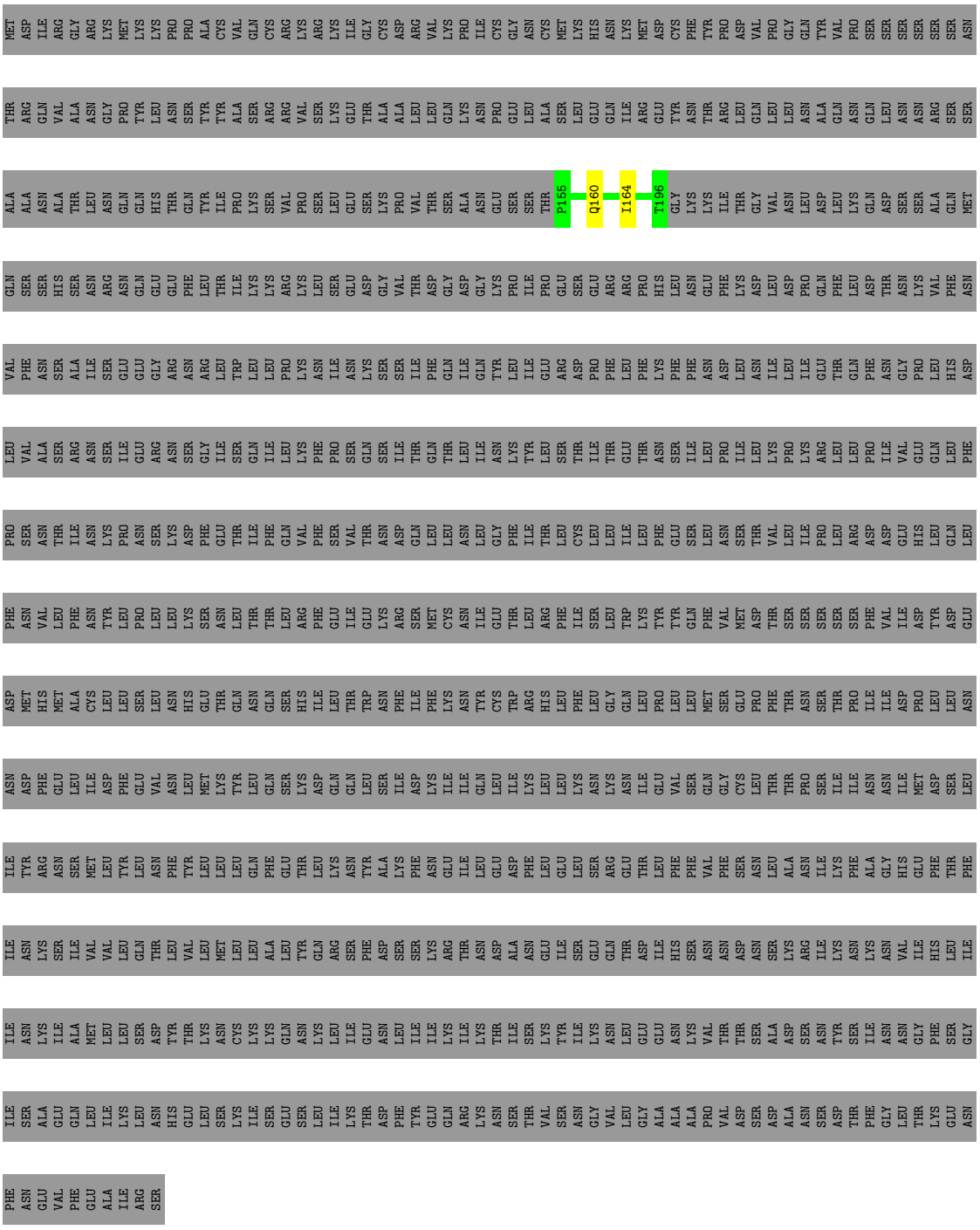




• Molecule 10: Chromatin structure-remodeling complex protein RSC3

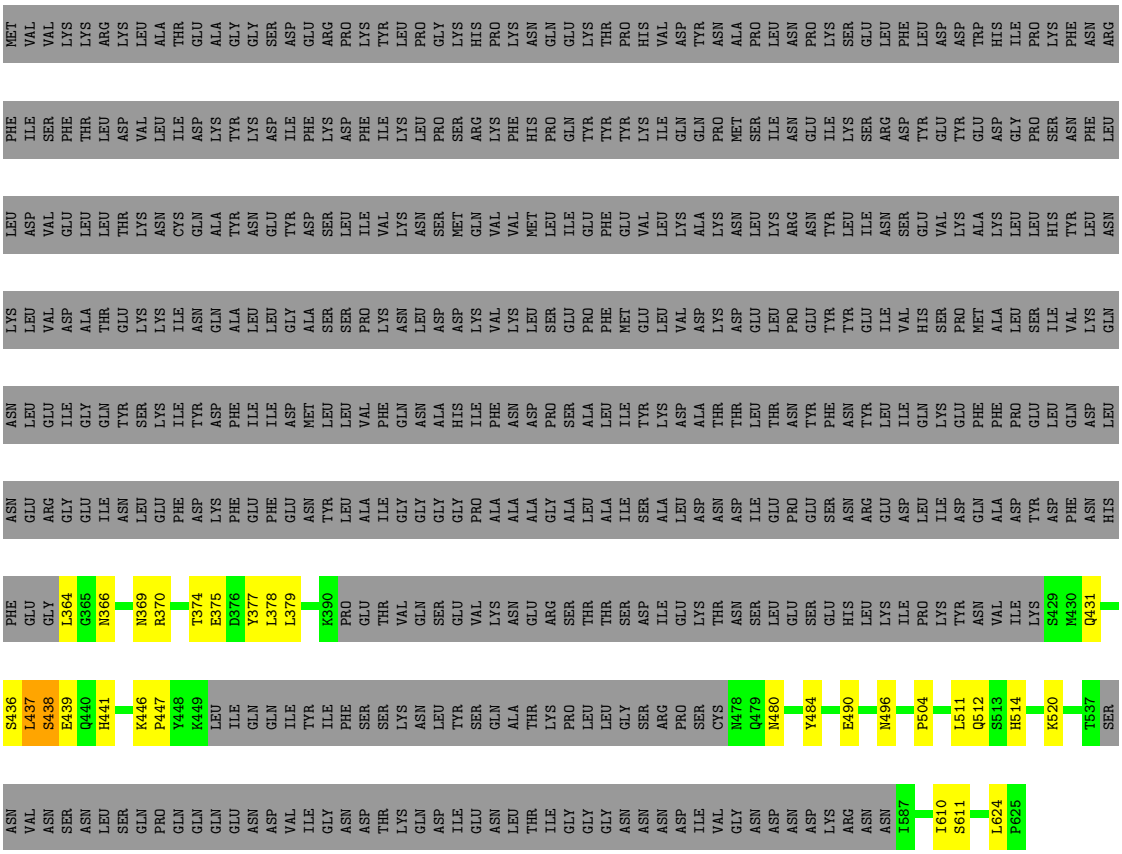
Chain K:





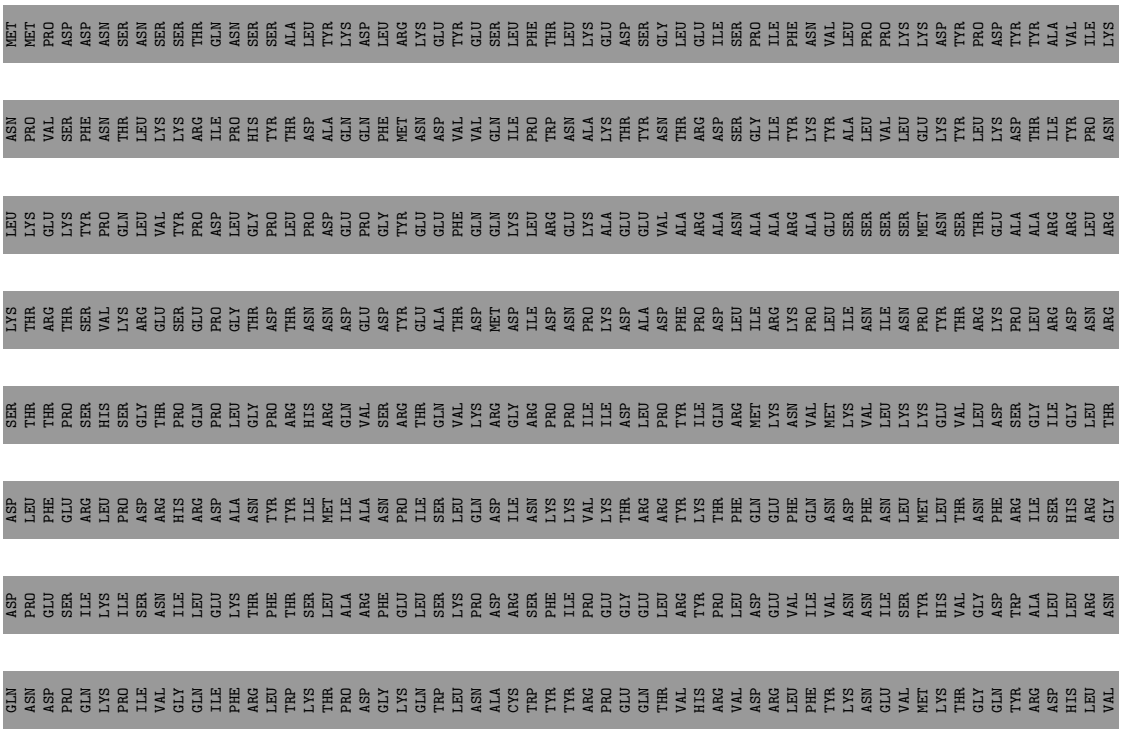
• Molecule 11: Chromatin structure-remodeling complex subunit RSC4

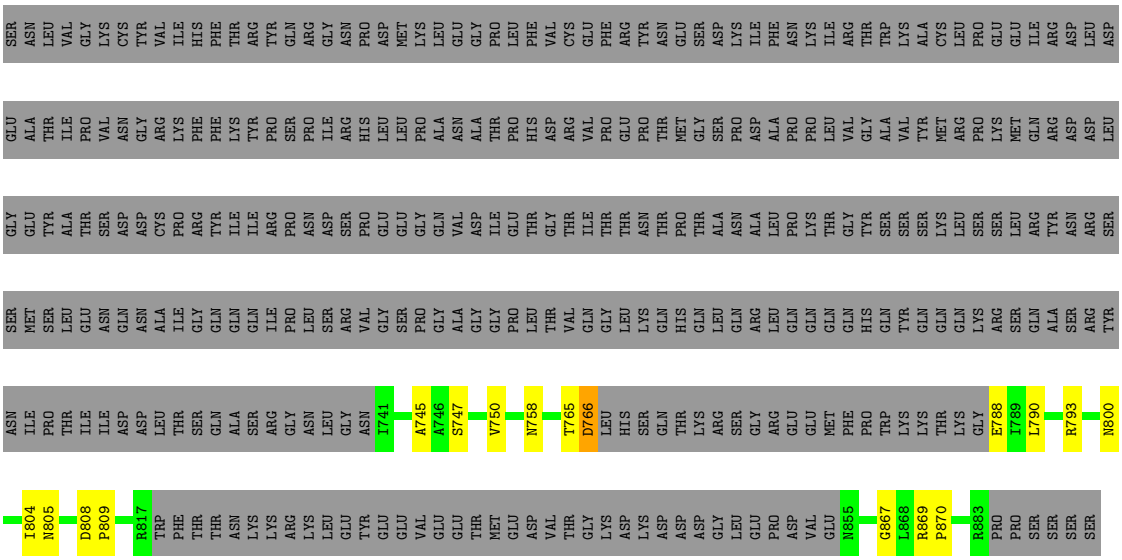
Chain X:



• Molecule 12: Chromatin structure-remodeling complex subunit RSC2

Chain L: 8% 90%




SER ASN LEU VAL GLY LYS CYS TYR VAL ILE HIS PHE THR ARG TYR GLN ARG GLY ASN PRO ASP MET LYS LEU GLU GLY PRO LEU PHE VAL CYS GLU PHE ARG TYR ASN GLU SER ASP LYS ILE PHE ASN LYS ILE ARG THR TRP LYS ALA CYS LEU PRO GLU GLU ILE ARG ASP LEU ASP
GLU ALA THR ILE PRO VAL ASN GLY ARG LYS PHE PHE LYS TYR PRO SER PRO ILE ARG HIS LEU LEU PRO ALA ASN ALA THR PRO HIS ASP ARG VAL PRO GLU PRO THR MET GLY SER PRO ASP ALA PRO PRO LEU VAL GLY ALA VAL TYR MET ARG PRO LYS MET GLN ARG ASP ASP LEU
GLY GLU TYR ALA THR SER ASP ASP CYS PRO ARG TYR ILE ILE ARG PRO ASN ASP SER PRO GLU GLU GLY GLN VAL ASP ILE GLU THR GLY THR ILE THR THR ASN THR PRO THR ALA ASN ALA LEU PRO LYS THR GLY TYR SER SER SER LYS LEU SER SER LEU ARG TYR ASN ARG SER
SER MET SER LEU GLU ASN GLN ASN ALA ILE GLY GLN GLN GLN ILE PRO LEU SER ARG VAL GLY SER PRO GLY ALA GLY GLY PRO LEU THR VAL GLN GLY LEU LYS GLN HIS GLN LEU GLN ARG LEU GLN GLN GLN GLN HIS GLN TYR GLN GLN GLN GLN LYS ARG SER GLN ALA SER ARG TYR
ASN ILE PRO THR ILE ILE ASP LEU THR SER GLN ALA SER ARG GLY ASN LEU GLY ASN I741 A745 A746 S747 V750 N758 T765 D766 LEU HIS SER GLN THR LYS ARG SER GLY ARG GLU GLU MET PHE PRO TRP LYS LYS THR LYS GLY E788 T789 L790 R793 N800
I804 N805 D808 P809 R817 TRP PHE THR THR ASN LYS LYS ARG LYS LEU GLU TYR GLU GLU VAL GLU GLU THR MET GLU ASP VAL THR GLY LYS ASP LYS ASP ASP GLY LEU GLU PRO ASP VAL GLU N855 G867 L868 R869 P870 R883 PRO PRO SER SER SER SER SER

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	280000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	F	0.28	0/983	0.57	0/1337
10	K	0.27	0/356	0.50	0/483
11	X	0.31	0/1243	0.57	0/1672
12	L	0.28	0/681	0.62	1/921 (0.1%)
2	D	0.29	0/2557	0.50	0/3442
2	H	0.30	0/3275	0.53	1/4409 (0.0%)
3	M	0.31	0/3113	0.58	0/4215
4	I	0.28	0/1976	0.56	0/2685
5	G	0.29	0/2033	0.57	0/2761
6	A	0.30	0/3077	0.54	0/4169
7	J	0.29	0/1836	0.55	1/2480 (0.0%)
8	E	0.27	0/480	0.56	0/643
9	C	0.28	0/272	0.44	0/366
All	All	0.29	0/21882	0.55	3/29583 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	J	17	PRO	N-CA-CB	5.80	110.26	103.30
12	L	766	ASP	CB-CG-OD2	5.20	122.98	118.30
2	H	279	ASP	CB-CG-OD2	5.19	122.97	118.30

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	F	964	0	919	5	0
2	D	2510	0	2542	33	0
2	H	3215	0	3195	45	0
3	M	3058	0	3127	16	0
4	I	1944	0	1964	22	0
5	G	1991	0	1943	29	0
6	A	3007	0	3045	51	0
7	J	1814	0	1777	23	0
8	E	477	0	491	6	0
9	C	269	0	279	2	0
10	K	347	0	342	2	0
11	X	1220	0	1192	31	0
12	L	669	0	693	17	0
13	H	1	0	0	0	0
All	All	21486	0	21509	213	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 5.

The worst 5 of 213 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)
11:X:439:GLU:OE1	11:X:490:GLU:CG	1.64	1.46
6:A:238:GLU:OE2	7:J:212:ASN:ND2	1.71	1.21
12:L:765:THR:HG22	12:L:790:LEU:HD21	1.23	1.16
11:X:439:GLU:OE1	11:X:490:GLU:HG2	0.91	1.07
6:A:187:TYR:OH	6:A:235:THR:HG21	1.56	1.04

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	F	116/435 (27%)	102 (88%)	14 (12%)	0	100	100
2	D	295/557 (53%)	280 (95%)	15 (5%)	0	100	100
2	H	387/557 (70%)	356 (92%)	31 (8%)	0	100	100
3	M	378/581 (65%)	349 (92%)	29 (8%)	0	100	100
4	I	236/483 (49%)	218 (92%)	18 (8%)	0	100	100
5	G	238/426 (56%)	213 (90%)	25 (10%)	0	100	100
6	A	357/502 (71%)	321 (90%)	36 (10%)	0	100	100
7	J	229/1359 (17%)	201 (88%)	27 (12%)	1 (0%)	36	73
8	E	56/78 (72%)	53 (95%)	3 (5%)	0	100	100
9	C	31/883 (4%)	31 (100%)	0	0	100	100
10	K	40/885 (4%)	38 (95%)	2 (5%)	0	100	100
11	X	139/625 (22%)	126 (91%)	13 (9%)	0	100	100
12	L	79/889 (9%)	69 (87%)	9 (11%)	1 (1%)	13	50
All	All	2581/8260 (31%)	2357 (91%)	222 (9%)	2 (0%)	56	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	J	17	PRO
12	L	809	PRO

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	F	111/388 (29%)	111 (100%)	0	100 100
2	D	285/500 (57%)	284 (100%)	1 (0%)	92 96
2	H	363/500 (73%)	361 (99%)	2 (1%)	87 94
3	M	349/521 (67%)	348 (100%)	1 (0%)	93 97
4	I	223/435 (51%)	223 (100%)	0	100 100
5	G	225/384 (59%)	224 (100%)	1 (0%)	92 96
6	A	343/462 (74%)	342 (100%)	1 (0%)	93 97
7	J	187/1228 (15%)	186 (100%)	1 (0%)	90 95
8	E	56/75 (75%)	56 (100%)	0	100 100
9	C	32/824 (4%)	32 (100%)	0	100 100
10	K	39/832 (5%)	39 (100%)	0	100 100
11	X	141/578 (24%)	139 (99%)	2 (1%)	69 87
12	L	77/810 (10%)	77 (100%)	0	100 100
All	All	2431/7537 (32%)	2422 (100%)	9 (0%)	92 96

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	G	172	ARG
11	X	438	SER
7	J	277	ARG
2	D	71	ARG
6	A	235	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
4	I	463	ASN
6	A	112	GLN
11	X	494	ASN
4	I	480	GLN
2	H	314	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.