wwPDB EM Validation Summary Report ⓘ

Dec 17, 2023 – 12:07 AM JST

PDB ID	:	8HXY
EMDB ID	:	EMD-35082
Title	:	Cryo-EM structure of the histone deacetylase complex Rpd3S in complex with nucleosome
Authors	:	Cui, H.; Wang, H.
Deposited on	:	2023-01-05
Resolution	:	3.10 Å(reported)

This is a wwPDB EM Validation Summary 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 ⓘ 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 ⓘ) were used in the production of this report:

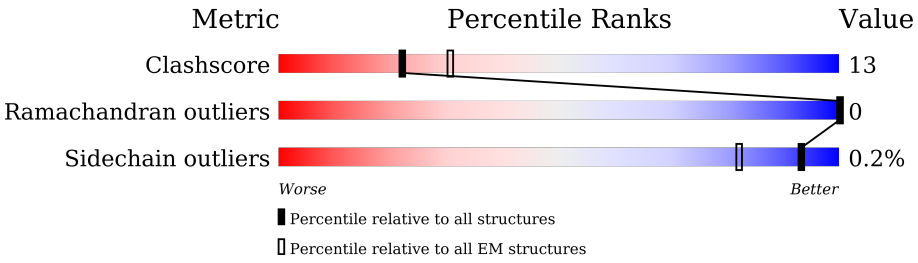
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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%

Mol	Chain	Length	Quality of chain
1	A	135	36% 40% 24%
1	E	135	36% 50% 14%
2	B	102	29% 49% 22%
2	F	102	47% 30% 23%
3	C	129	50% 34% 16%
3	G	129	47% 35% 18%
4	D	122	43% 36% 21%
4	H	122	51% 26% 23%
5	I	352	40% 9% 52%

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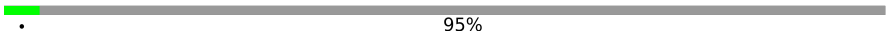
Mol	Chain	Length	Quality of chain
6	J	352	
7	K	1536	
8	L	433	
9	M	401	
10	N	684	
10	P	684	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 26263 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	102	Total	C	N	O	S	0	0
			837	529	162	143	3		
1	E	116	Total	C	N	O	S	0	0
			945	591	189	163	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1
E	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	80	Total	C	N	O	S	0	0
			641	405	125	110	1		
2	F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	109	Total	C	N	O	0	0
			843	531	167	145		
3	G	106	Total	C	N	O	0	0
			818	516	160	142		

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total	C	N	O	S	0	0
			757	475	140	140	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	94	Total	C	N	O	S	0	0
			736	463	132	139	2		

- Molecule 5 is a DNA chain called DNA (352-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	170	Total	C	N	O	P	0	0
			3466	1648	623	1025	170		

- Molecule 6 is a DNA chain called DNA (352-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	170	Total	C	N	O	P	0	0
			3504	1659	660	1015	170		

- Molecule 7 is a protein called Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	549	Total	C	N	O	S	0	0
			4597	2954	774	854	15		

- Molecule 8 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	384	Total	C	N	O	S	0	0
			3048	1941	512	569	26		

- Molecule 9 is a protein called Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	294	Total	C	N	O	S	0	0
			2398	1541	394	449	14		

- Molecule 10 is a protein called Transcriptional regulatory protein RCO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	340	Total	C	N	O	S	0	0
			2769	1752	480	520	17		
10	P	31	Total	C	N	O	S	0	0
			272	178	42	51	1		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

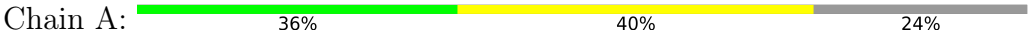
Mol	Chain	Residues	Atoms	AltConf
11	L	1	Total Zn 1 1	0
11	N	4	Total Zn 4 4	0

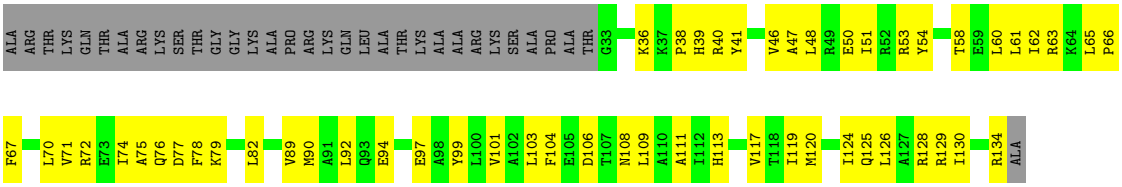
3 Residue-property plots (i)

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. 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: Histone H3

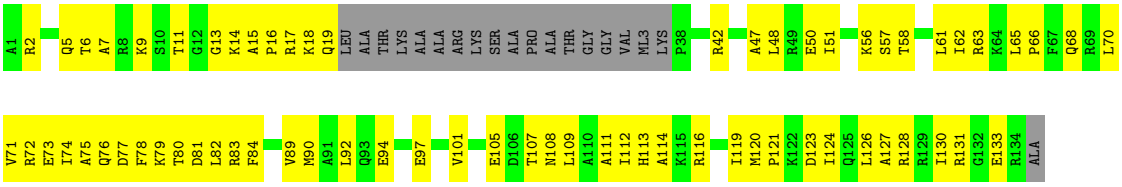
Chain A:





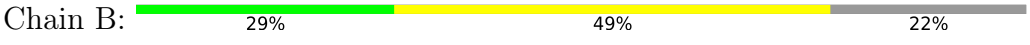
• Molecule 1: Histone H3

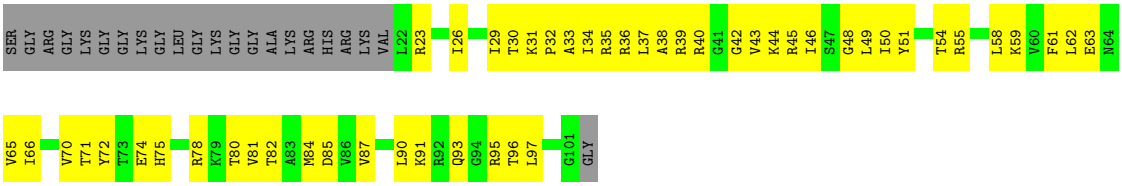
Chain E:



• Molecule 2: Histone H4

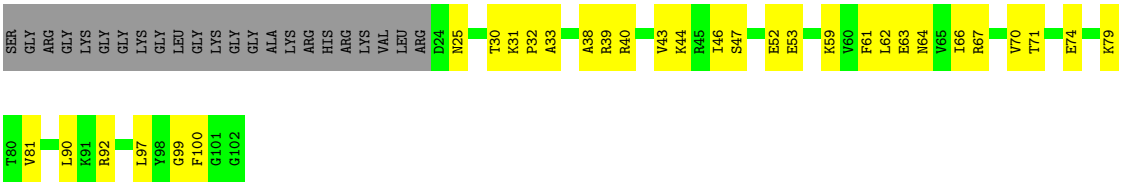
Chain B:





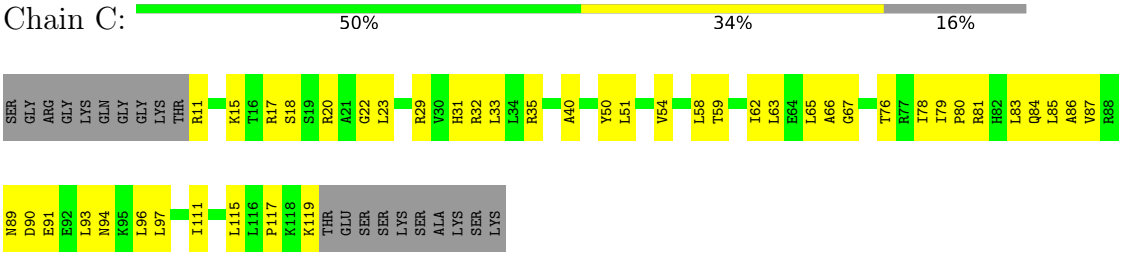
• Molecule 2: Histone H4

Chain F:



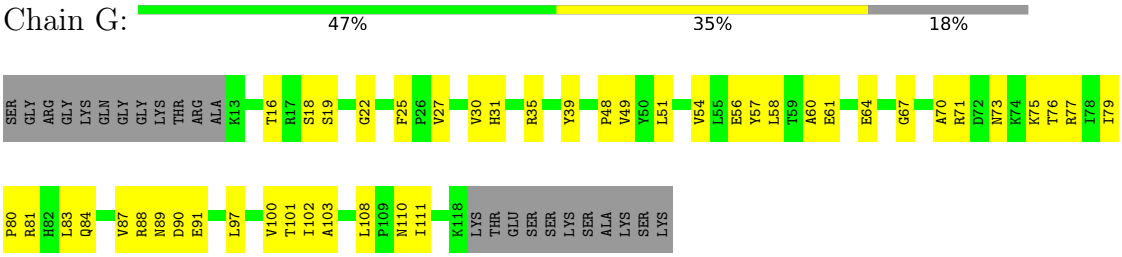
• Molecule 3: Histone H2A

Chain C:



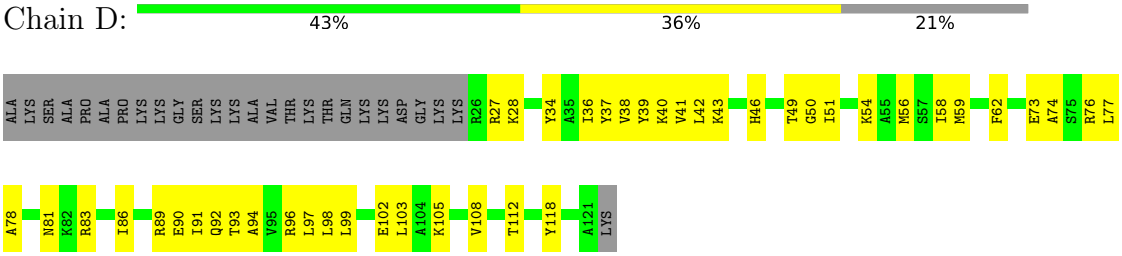
• Molecule 3: Histone H2A

Chain G:



• Molecule 4: Histone H2B

Chain D:

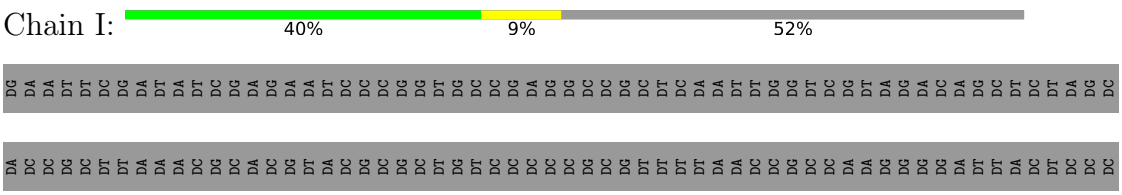


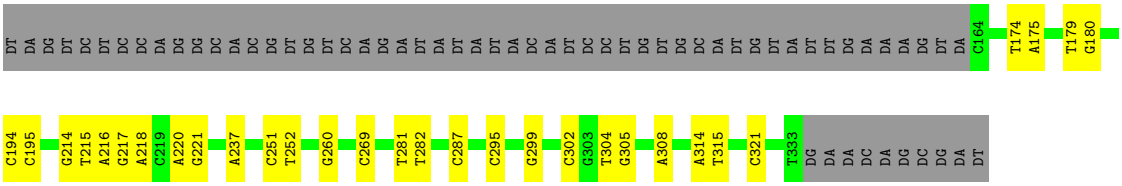
• Molecule 4: Histone H2B

Chain H:

• Molecule 5: DNA (352-MER)

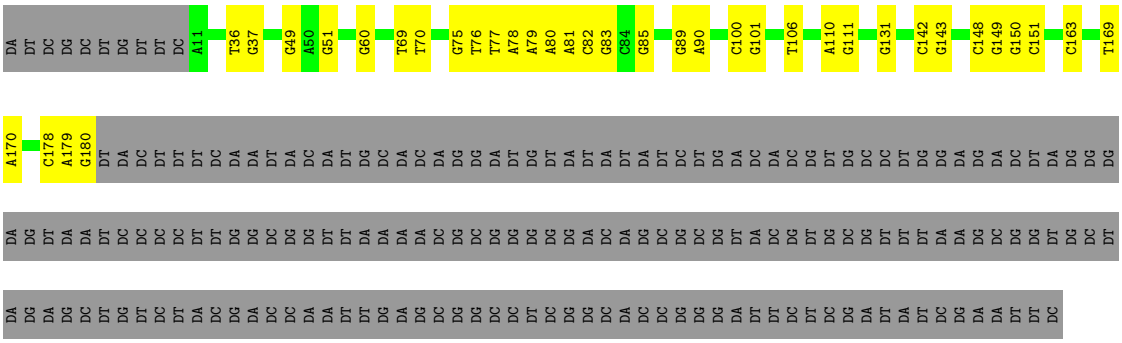
Chain I:





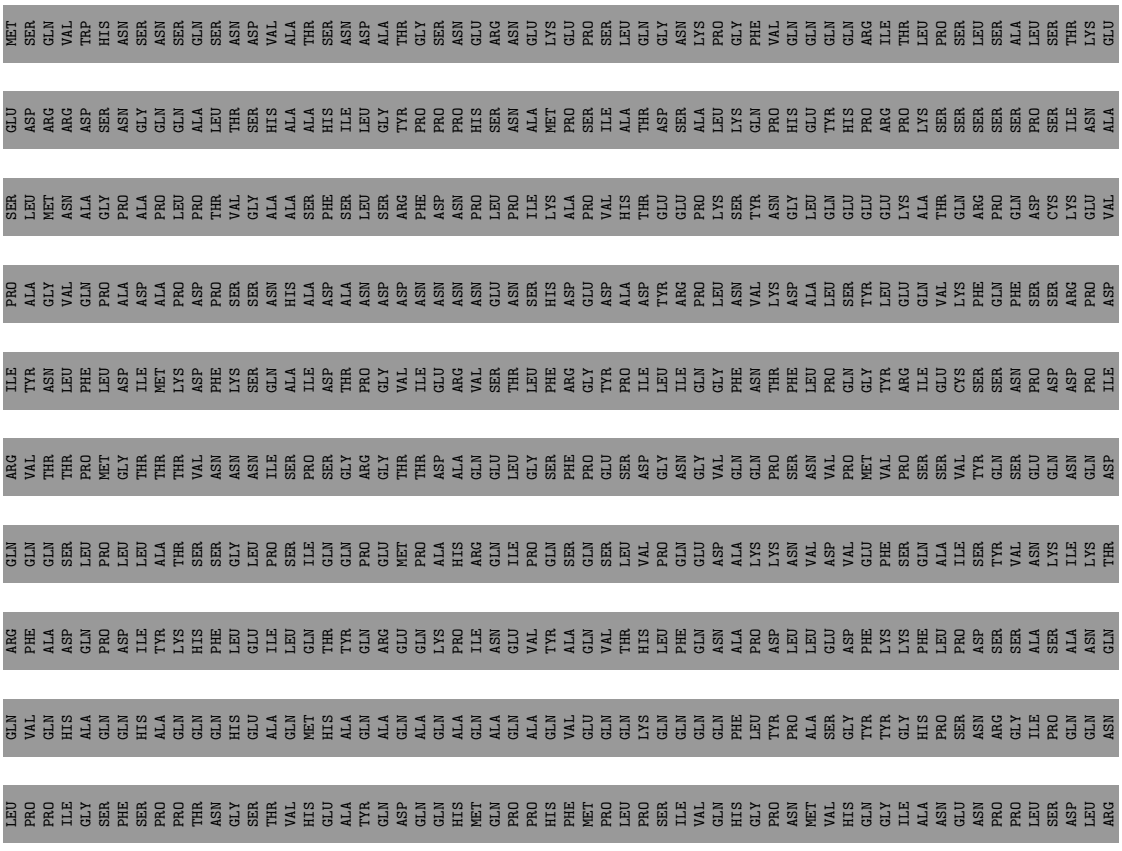
• Molecule 6: DNA (352-MER)

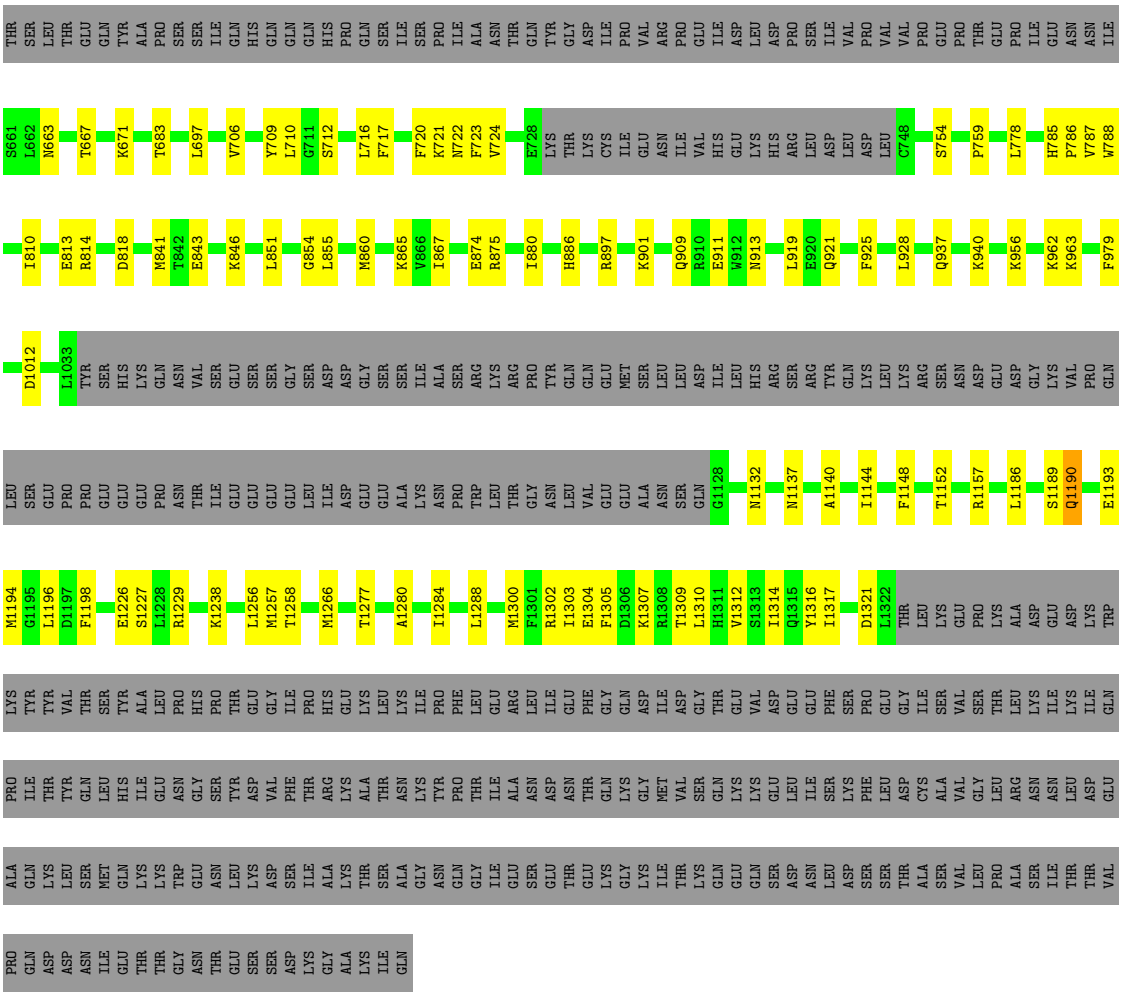
Chain J:



• Molecule 7: Transcriptional regulatory protein SIN3

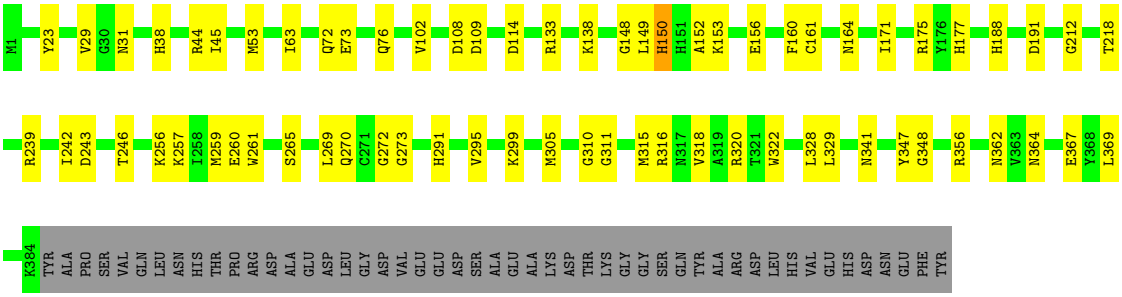
Chain K:





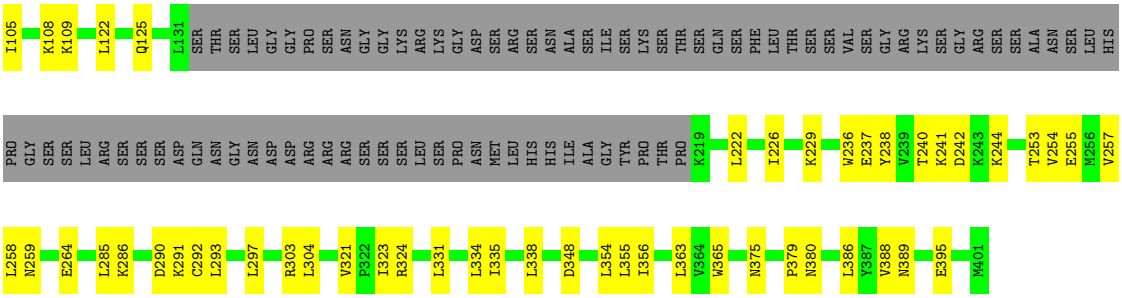
• Molecule 8: Histone deacetylase RPD3

Chain L:



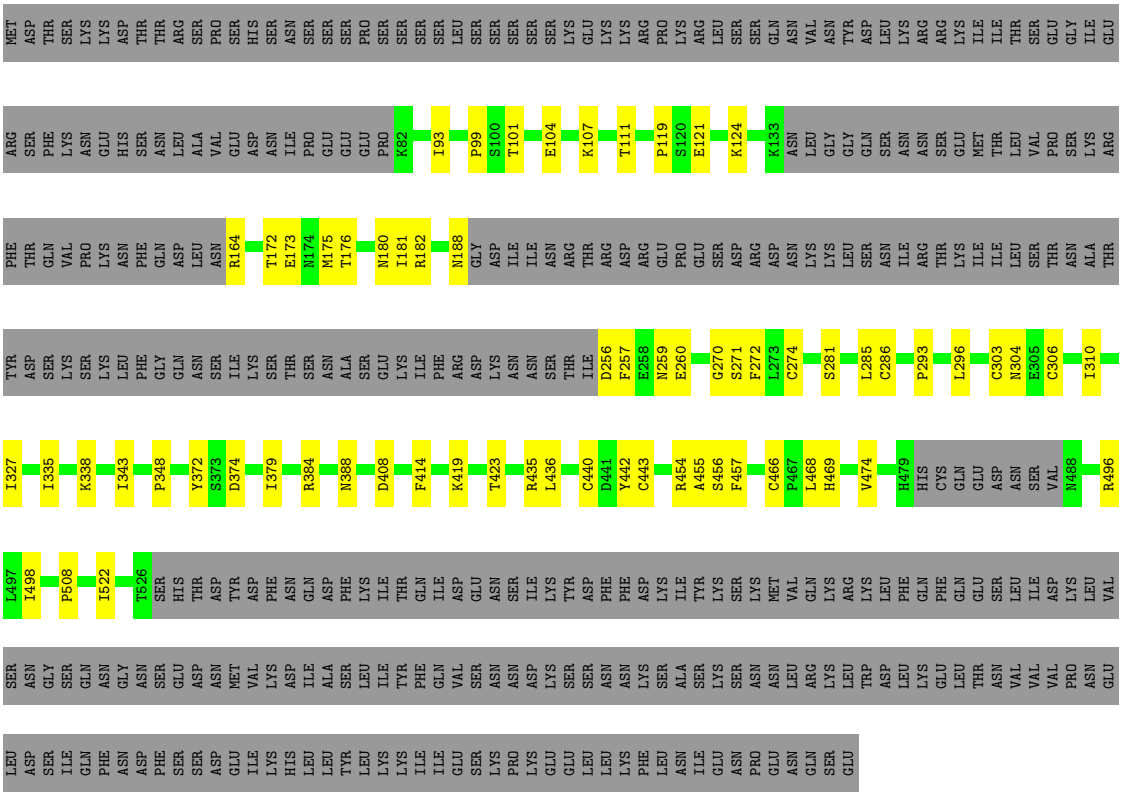
• Molecule 9: Chromatin modification-related protein EAF3

Chain M:



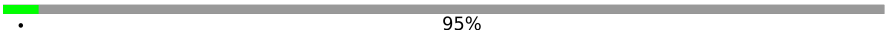
• Molecule 10: Transcriptional regulatory protein RCO1

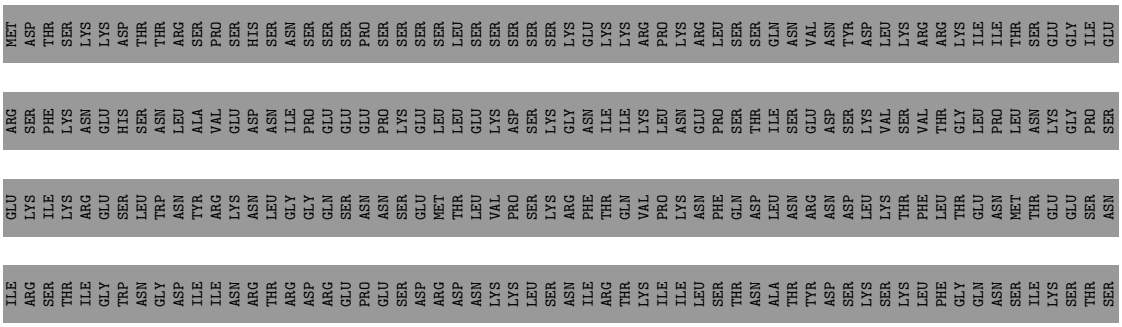
Chain N:

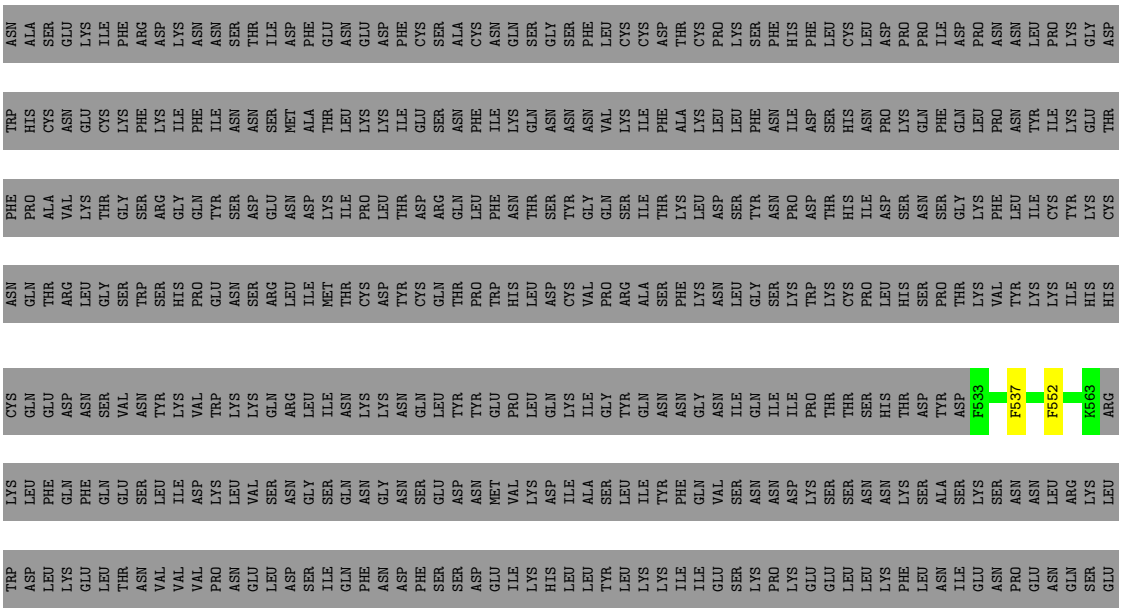


• Molecule 10: Transcriptional regulatory protein RCO1

Chain P:






F533
F537
F552
R563

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145512	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 ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k 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: ML3, 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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.50	0/836	0.64	0/1120
1	E	0.48	0/957	0.65	0/1279
2	B	0.61	0/648	0.70	0/868
2	F	0.58	0/634	0.76	0/848
3	C	0.48	0/853	0.61	0/1149
3	G	0.51	0/828	0.65	0/1117
4	D	0.56	0/768	0.68	0/1032
4	H	0.47	0/747	0.54	0/1004
5	I	0.55	0/3882	0.94	0/5985
6	J	0.50	0/3936	0.89	0/6077
7	K	0.32	0/4699	0.54	1/6334 (0.0%)
8	L	0.34	0/3127	0.51	0/4231
9	M	0.31	0/2446	0.57	3/3292 (0.1%)
10	N	0.32	0/2835	0.55	3/3826 (0.1%)
10	P	0.29	0/277	0.48	0/367
All	All	0.44	0/27473	0.70	7/38529 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	1288	LEU	CA-CB-CG	8.38	134.58	115.30
10	N	374	ASP	CB-CG-OD1	6.61	124.25	118.30
10	N	408	ASP	CB-CG-OD1	6.59	124.23	118.30
9	M	348	ASP	CB-CG-OD1	6.39	124.05	118.30
10	N	508	PRO	CA-N-CD	-5.86	103.30	111.50

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	837	0	885	87	0
1	E	945	0	1004	96	0
2	B	641	0	684	85	0
2	F	627	0	663	45	0
3	C	843	0	908	54	0
3	G	818	0	877	49	0
4	D	757	0	786	54	0
4	H	736	0	760	35	0
5	I	3466	0	1912	26	0
6	J	3504	0	1907	31	0
7	K	4597	0	4560	83	0
8	L	3048	0	2932	53	0
9	M	2398	0	2429	57	0
10	N	2769	0	2716	60	0
10	P	272	0	268	3	0
11	L	1	0	0	0	0
11	N	4	0	0	0	0
All	All	26263	0	23291	628	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 13.

The worst 5 of 628 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)
2:B:91:LYS:HD3	2:B:96:THR:HG22	1.39	1.04
2:B:65:VAL:HG22	2:B:93:GLN:HE22	1.18	1.03
2:B:91:LYS:HD3	2:B:96:THR:CG2	1.90	1.01
7:K:937:GLN:CB	7:K:940:LYS:HE2	1.90	1.00
3:C:79:ILE:HG23	3:C:80:PRO:HD2	1.43	0.98

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	99/135 (73%)	90 (91%)	9 (9%)	0	100	100
1	E	112/135 (83%)	108 (96%)	4 (4%)	0	100	100
2	B	78/102 (76%)	72 (92%)	6 (8%)	0	100	100
2	F	77/102 (76%)	74 (96%)	3 (4%)	0	100	100
3	C	107/129 (83%)	103 (96%)	4 (4%)	0	100	100
3	G	104/129 (81%)	97 (93%)	7 (7%)	0	100	100
4	D	94/122 (77%)	88 (94%)	6 (6%)	0	100	100
4	H	92/122 (75%)	81 (88%)	11 (12%)	0	100	100
7	K	543/1536 (35%)	525 (97%)	18 (3%)	0	100	100
8	L	382/433 (88%)	369 (97%)	13 (3%)	0	100	100
9	M	288/401 (72%)	284 (99%)	4 (1%)	0	100	100
10	N	332/684 (48%)	316 (95%)	16 (5%)	0	100	100
10	P	29/684 (4%)	28 (97%)	1 (3%)	0	100	100
All	All	2337/4714 (50%)	2235 (96%)	102 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	86/108 (80%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	98/108 (91%)	98 (100%)	0	100 100
2	B	66/78 (85%)	66 (100%)	0	100 100
2	F	64/78 (82%)	64 (100%)	0	100 100
3	C	86/101 (85%)	86 (100%)	0	100 100
3	G	84/101 (83%)	84 (100%)	0	100 100
4	D	82/102 (80%)	82 (100%)	0	100 100
4	H	80/102 (78%)	80 (100%)	0	100 100
7	K	510/1391 (37%)	509 (100%)	1 (0%)	93 97
8	L	326/367 (89%)	324 (99%)	2 (1%)	86 94
9	M	268/359 (75%)	267 (100%)	1 (0%)	91 96
10	N	321/653 (49%)	320 (100%)	1 (0%)	92 96
10	P	31/653 (5%)	31 (100%)	0	100 100
All	All	2102/4201 (50%)	2097 (100%)	5 (0%)	93 97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	K	1190	GLN
8	L	150	HIS
8	L	259	MET
9	M	292	CYS
10	N	260	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	81	ASN
7	K	1311	HIS
7	K	937	GLN
9	M	389	ASN
4	D	92	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$
1	ML3	A	36	1	10,11,12	0.77	0	10,14,16	0.82	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
1	ML3	A	36	1	-	5/8/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	36	ML3	SG-CD-CE-NZ
1	A	36	ML3	CD-CE-NZ-CM1
1	A	36	ML3	CD-CE-NZ-CM2
1	A	36	ML3	CD-CE-NZ-CM3
1	A	36	ML3	CA-CB-SG-CD

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	36	ML3	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are 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.