



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 5, 2020 – 06:34 PM EST

PDB ID : 6V8O
EMDB ID: : EMD-21107
Title : RSC core
Authors : Patel, A.B.; Moore, C.M.; Greber, B.J.; Nogales, E.
Deposited on : 2019-12-11
Resolution : 3.07 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 ⓘ 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

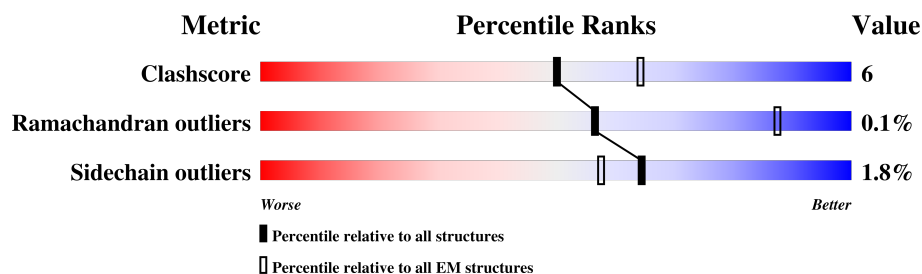
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.07 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	C	78	
2	D	180	
3	E	435	
4	F	889	
5	G	885	
6	H	625	
7	I	557	
7	J	557	
7	K	557	

Continued on next page...

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Mol	Chain	Length	Quality of chain
7	L	557	 44%9%46%
8	M	483	 51%13%36%
9	N	581	 57%13%29%
10	O	502	 63%13%24%
11	Q	426	 48%12%38%
12	R	1359	 16%81%
13	S	883	 96%
14	2	28	 96%
15	3	19	 100%
15	4	19	 95%5%
16	5	14	 100%
17	6	15	 100%
18	7	49	 96%

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 25103 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 High temperature lethal protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	60	Total	C	N	O	S	0	0
			493	301	92	96	4		

- Molecule 2 is a protein called Chromatin structure-remodeling complex protein RSC14.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	100	Total	C	N	O	S	0	0
			772	490	132	148	2		

- Molecule 3 is a protein called Chromatin structure-remodeling complex subunit RSC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	120	Total	C	N	O	S	0	0
			978	610	166	200	2		

- Molecule 4 is a protein called Chromatin structure-remodeling complex subunit RSC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	67	Total	C	N	O	S	0	0
			536	346	94	95	1		

- Molecule 5 is a protein called Chromatin structure-remodeling complex protein RSC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	53	Total	C	N	O	S	0	0
			422	270	71	79	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	767	SER	THR	conflict	UNP Q06639

- Molecule 6 is a protein called Chromatin structure-remodeling complex subunit RSC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	131	Total	C	N	O	S	0	0
			1083	696	175	205	7		

- Molecule 7 is a protein called Chromatin structure-remodeling complex protein RSC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	293	Total	C	N	O	S	0	0
			2416	1537	423	448	8		
7	J	115	Total	C	N	O	S	0	0
			924	579	149	190	6		
7	K	109	Total	C	N	O	S	0	0
			878	554	139	179	6		
7	L	298	Total	C	N	O	S	0	0
			2445	1557	428	452	8		

- Molecule 8 is a protein called Chromatin structure-remodeling complex protein RSC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	310	Total	C	N	O	S	0	0
			2474	1558	414	496	6		

- Molecule 9 is a protein called Chromatin structure-remodeling complex subunit RSC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	412	Total	C	N	O	S	0	0
			3275	2105	540	612	18		

- Molecule 10 is a protein called Chromatin structure-remodeling complex protein RSC58.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	384	Total	C	N	O	S	0	0
			3145	2025	529	581	10		

- Molecule 11 is a protein called Chromatin structure-remodeling complex subunit SFH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	264	Total	C	N	O	S	0	0
			2137	1349	362	418	8		

- Molecule 12 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	262	Total	C	N	O	S	0	0
			2126	1339	378	407	2		

- Molecule 13 is a protein called Chromatin structure-remodeling complex protein RSC30.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	34	Total	C	N	O	S	0	0
			278	182	41	54	1		

- Molecule 14 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	2	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 15 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	3	19	Total	C	N	O	0	0
			95	57	19	19		
15	4	19	Total	C	N	O	0	0
			95	57	19	19		

- Molecule 16 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	5	14	Total	C	N	O	0	0
			70	42	14	14		

- Molecule 17 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	6	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 18 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	7	49	Total	C	N	O	0	0
			245	147	49	49		

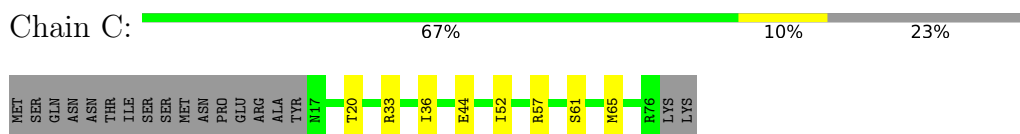
- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

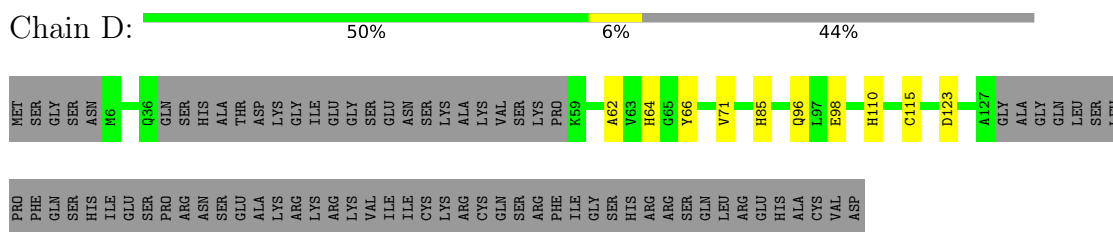
3 Residue-property plots

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.

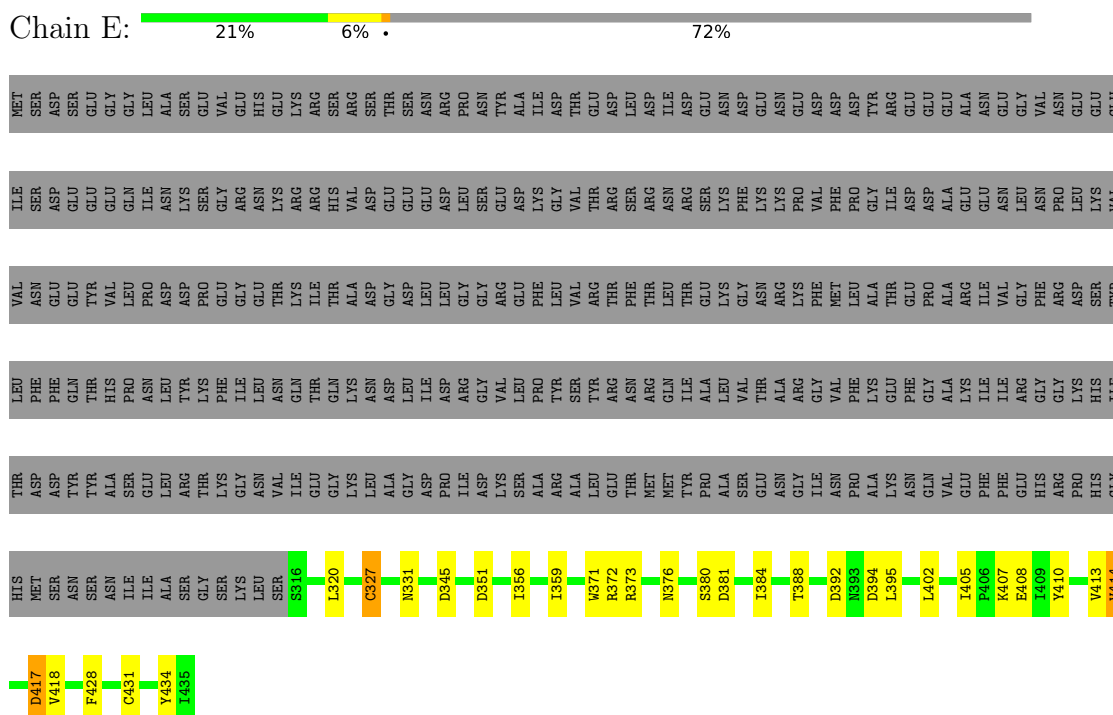
- Molecule 1: High temperature lethal protein 1



- Molecule 2: Chromatin structure-remodeling complex protein RSC14

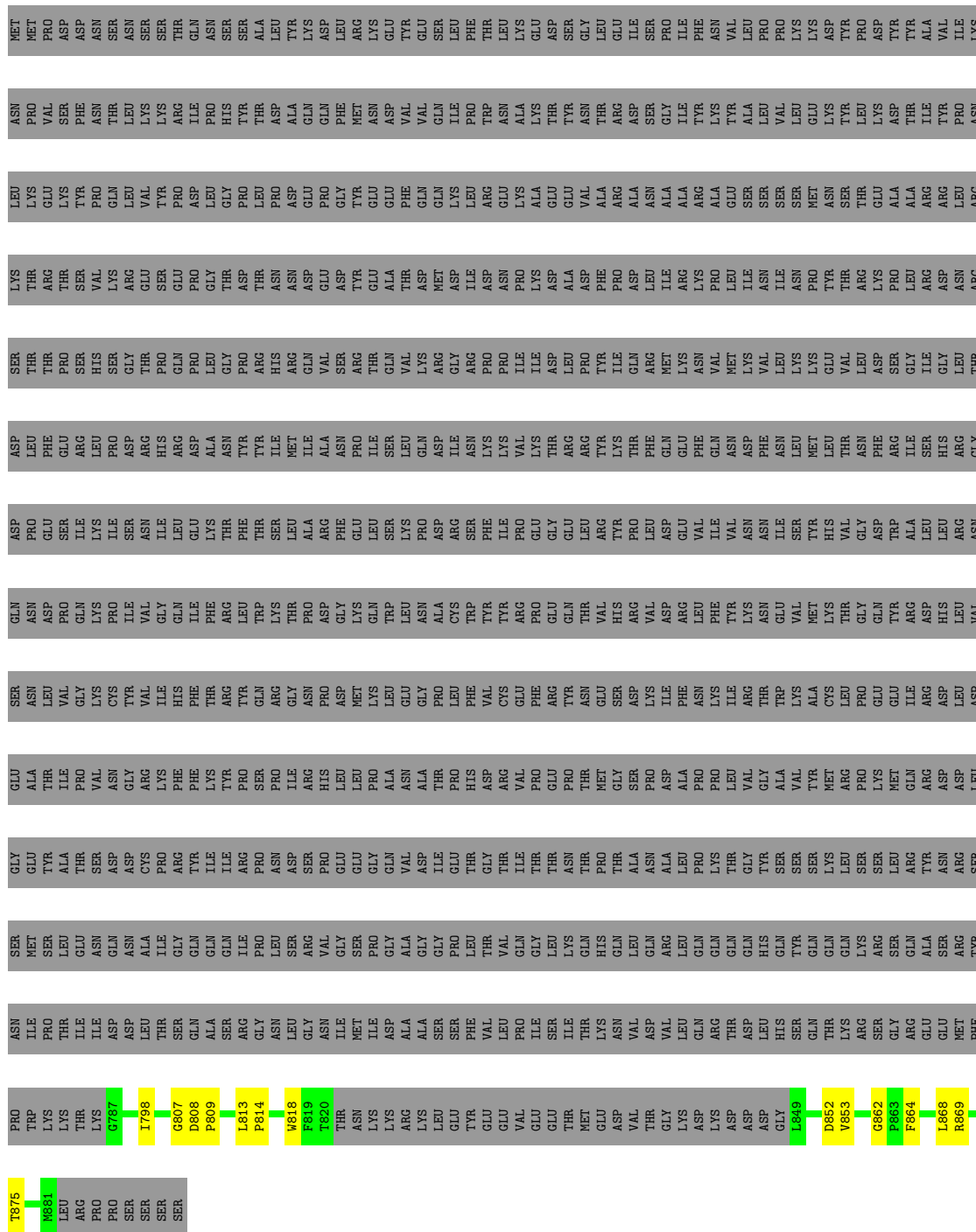


- Molecule 3: Chromatin structure-remodeling complex subunit RSC7



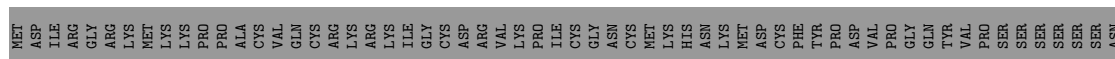
- Molecule 4: Chromatin structure-remodeling complex subunit RSC2

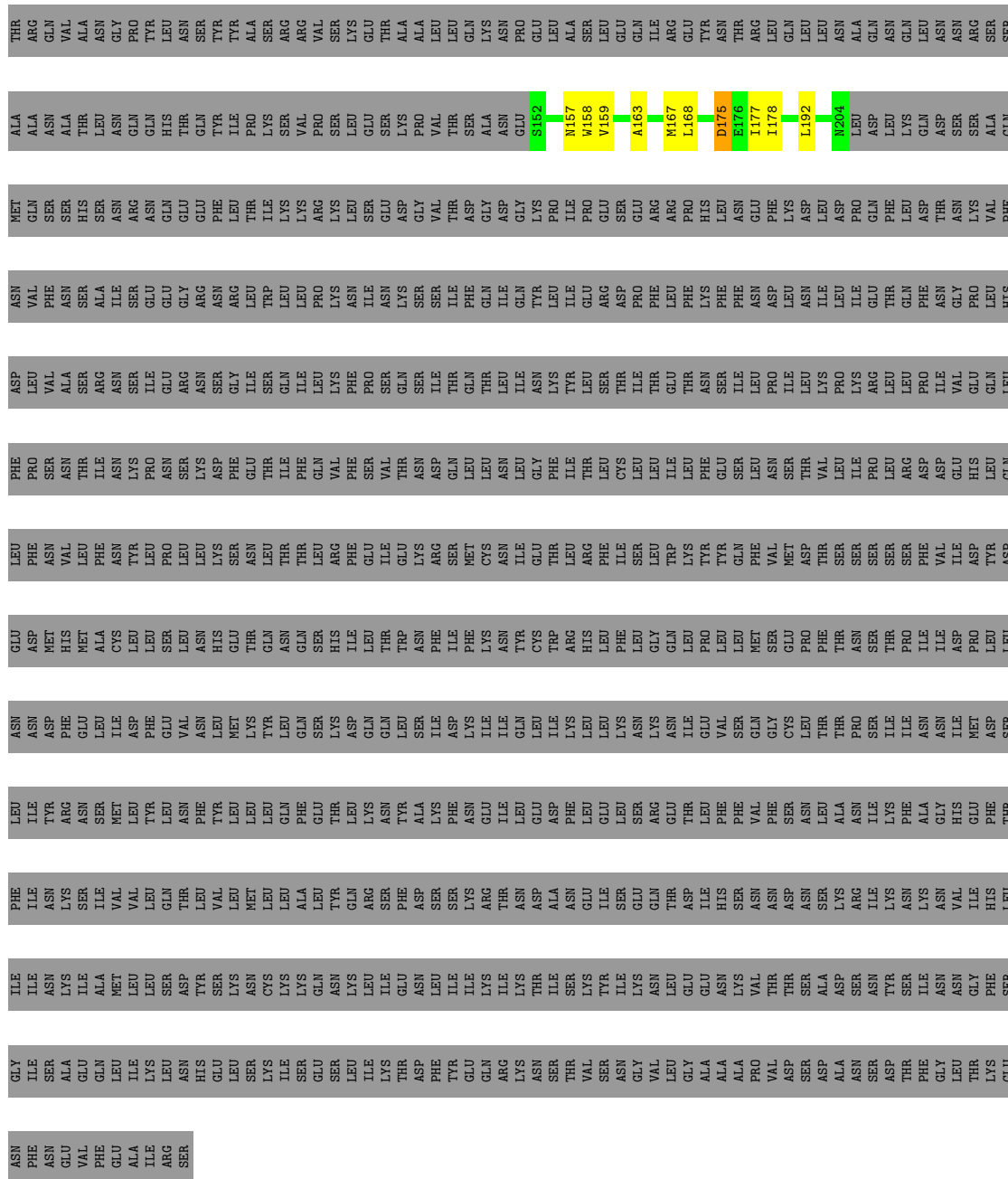
Chain F: 6% . 92%



- Molecule 5: Chromatin structure-remodeling complex protein RSC3

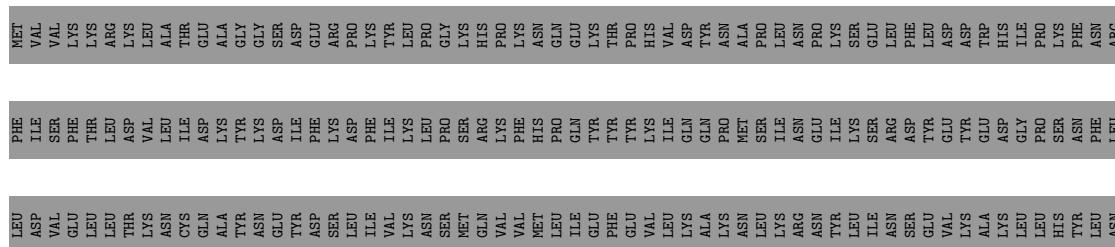
Chain G: 5% . 94%

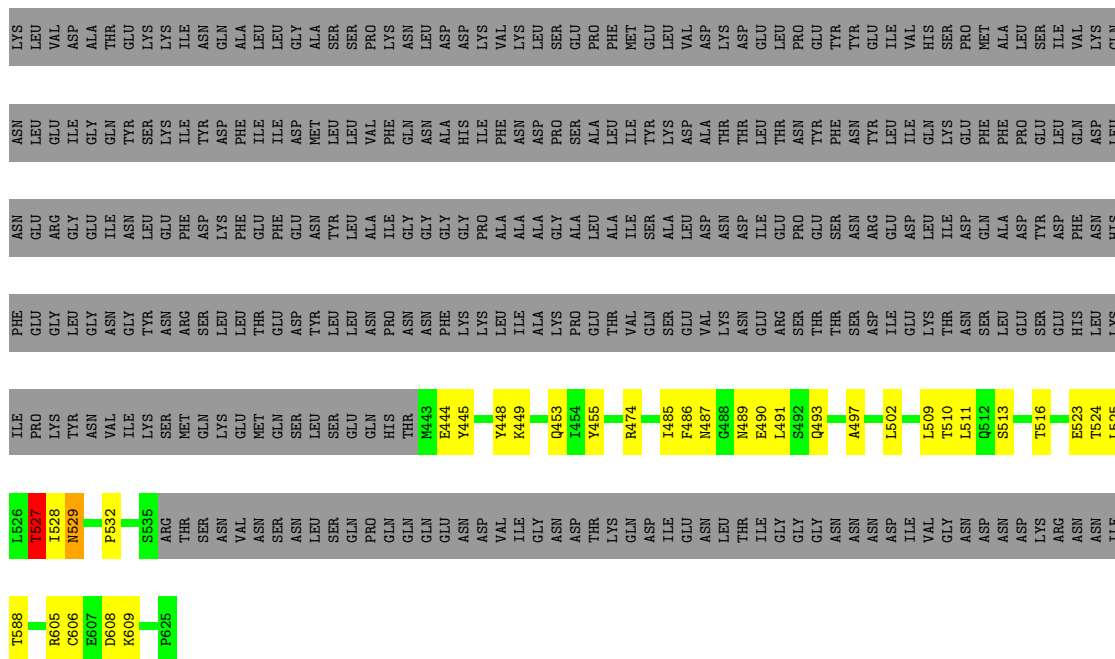




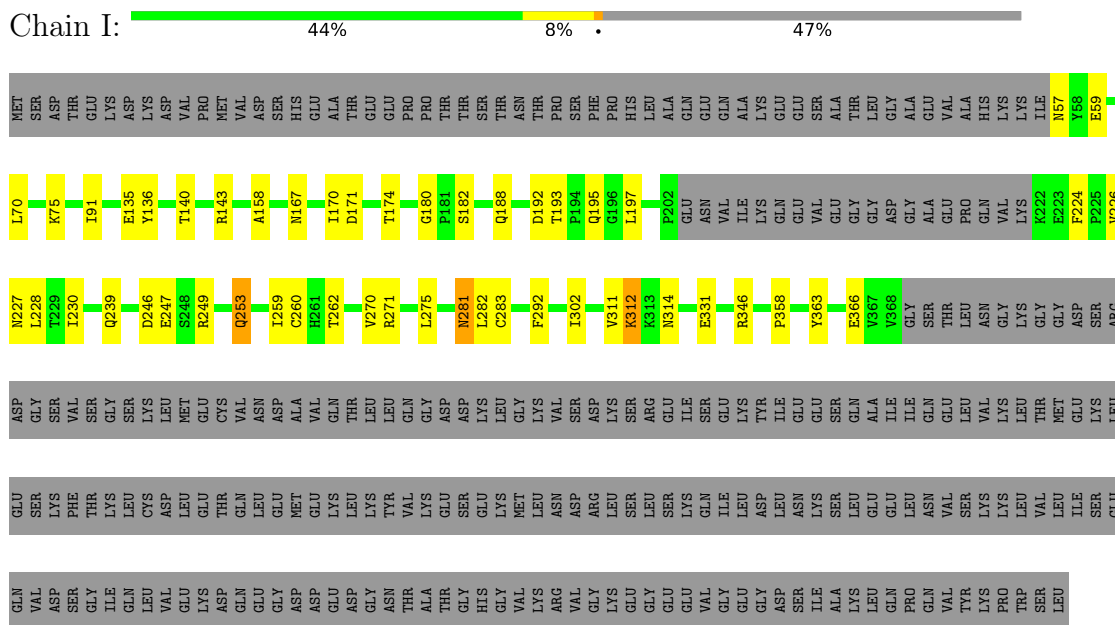
- Molecule 6: Chromatin structure-remodeling complex subunit RSC4

Chain H: 16% 5% 79%

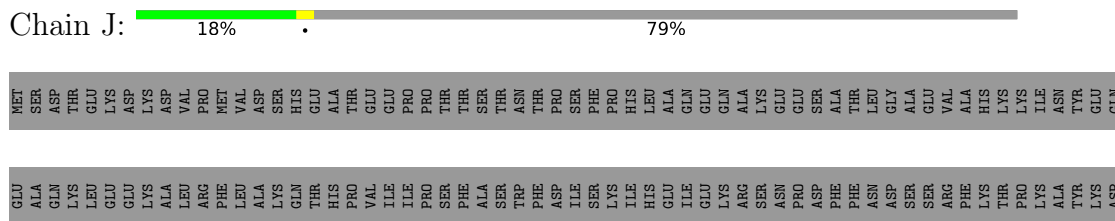


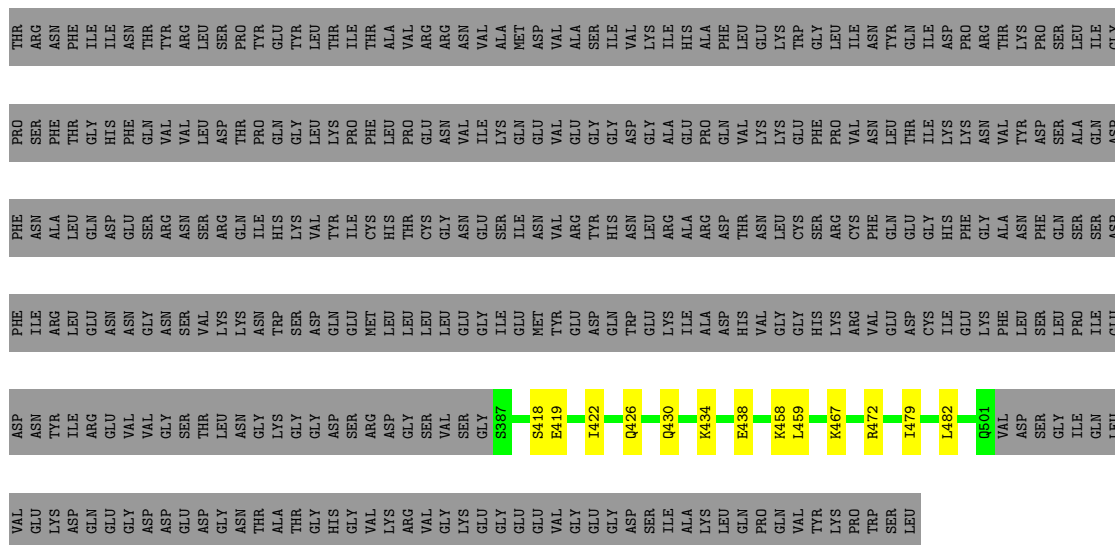


- Molecule 7: Chromatin structure-remodeling complex protein RSC8



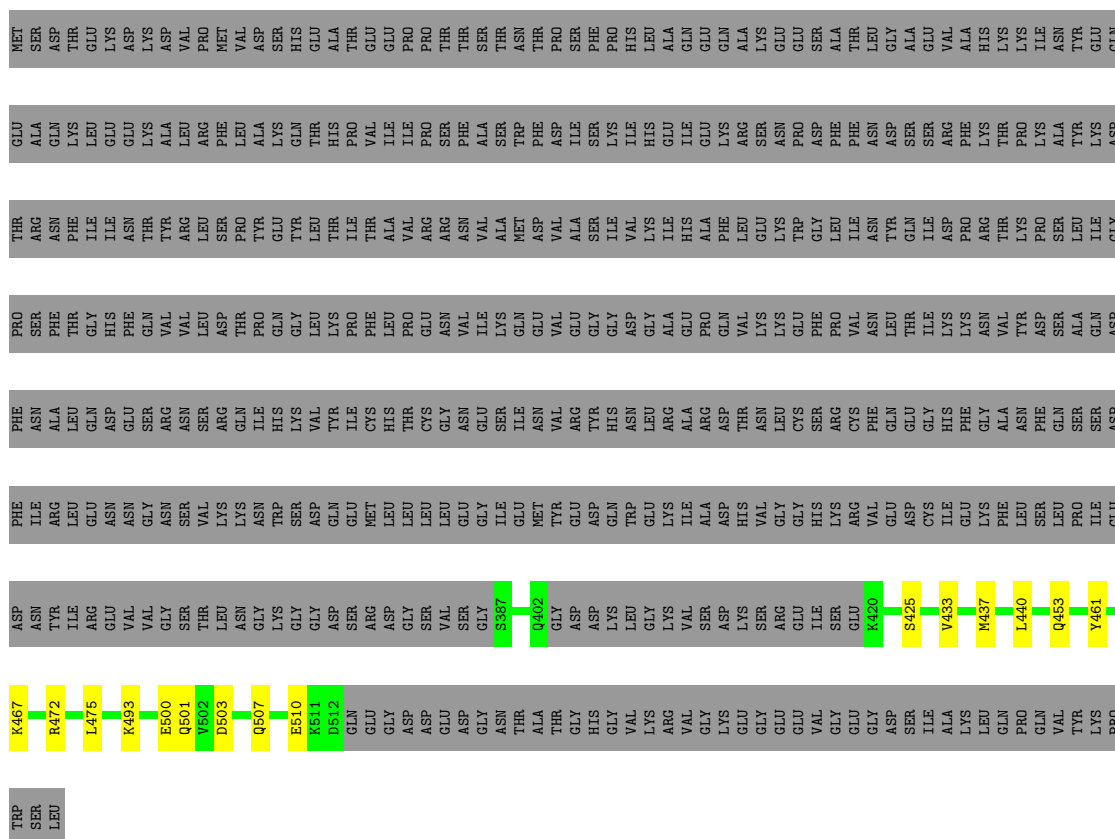
- Molecule 7: Chromatin structure-remodeling complex protein RSC8





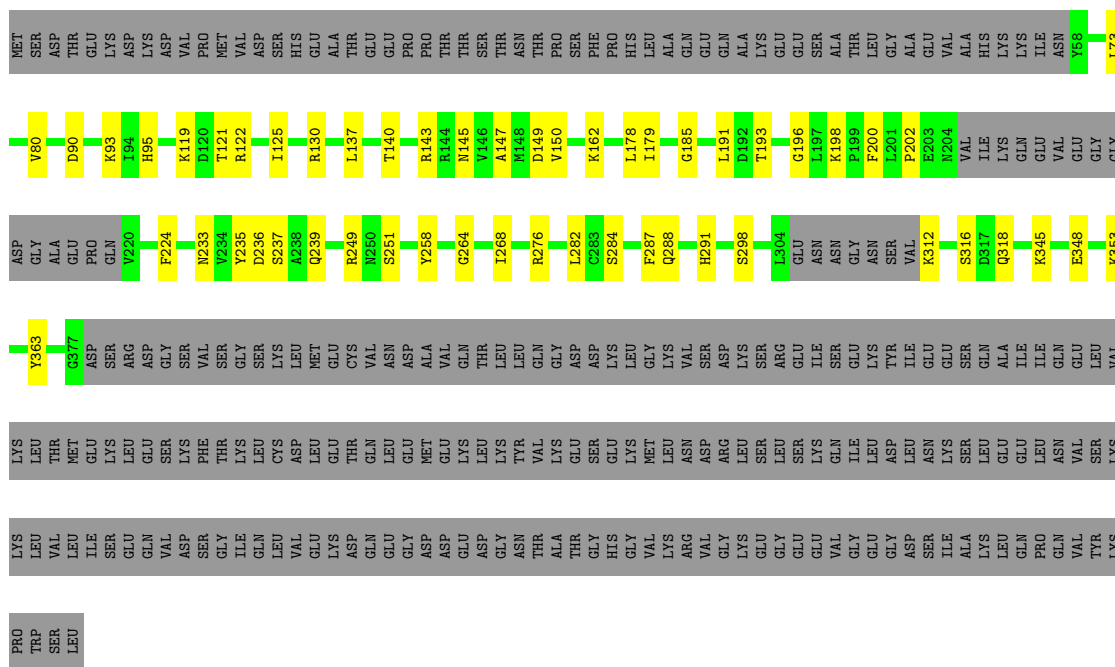
- Molecule 7: Chromatin structure-remodeling complex protein RSC8

Chain K: 17% 80%



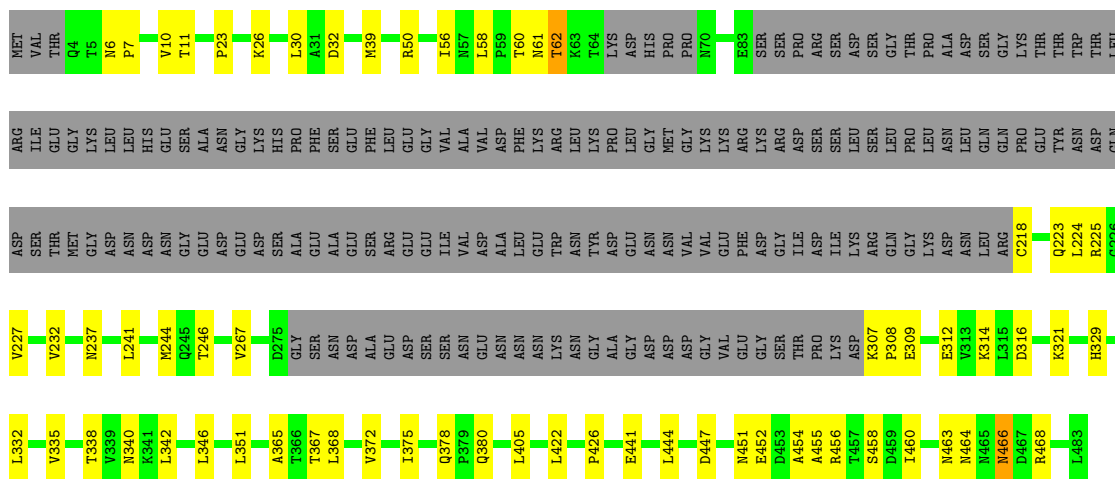
- Molecule 7: Chromatin structure-remodeling complex protein RSC8

Chain L: 44% 9% 46%



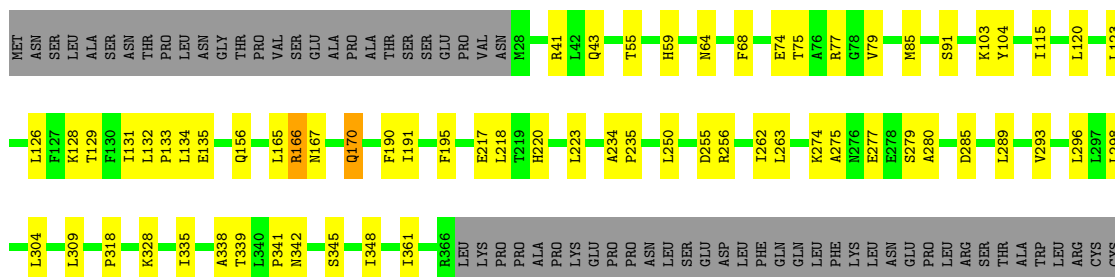
- Molecule 8: Chromatin structure-remodeling complex protein RSC6

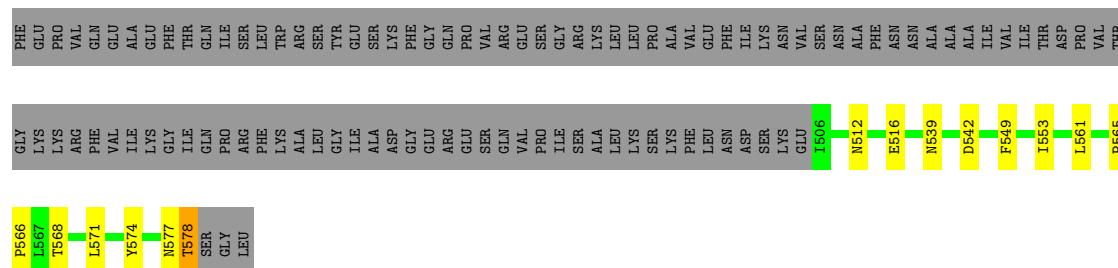
Chain M:  51% 13% 36%



- Molecule 9: Chromatin structure-remodeling complex subunit RSC9

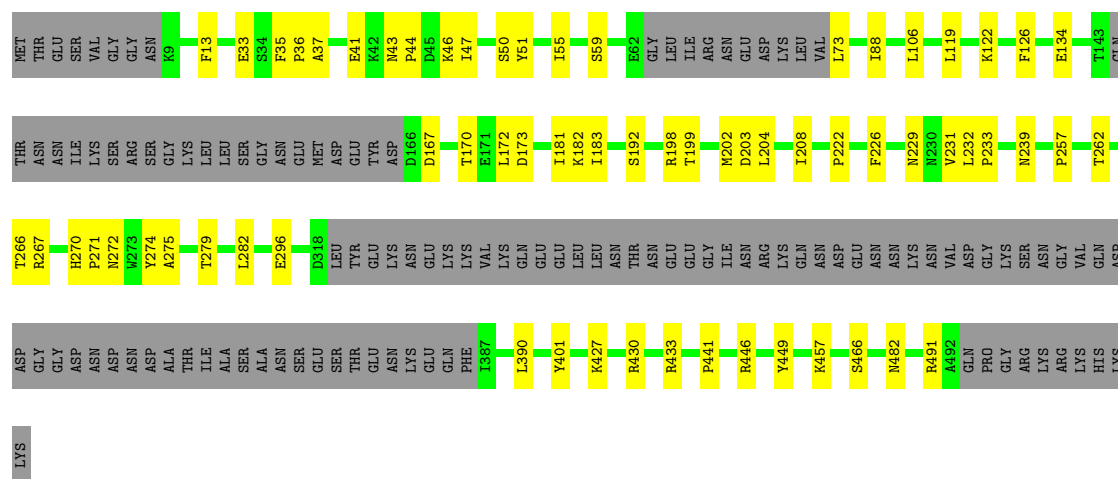
Chain N:  57% 13% . 29%





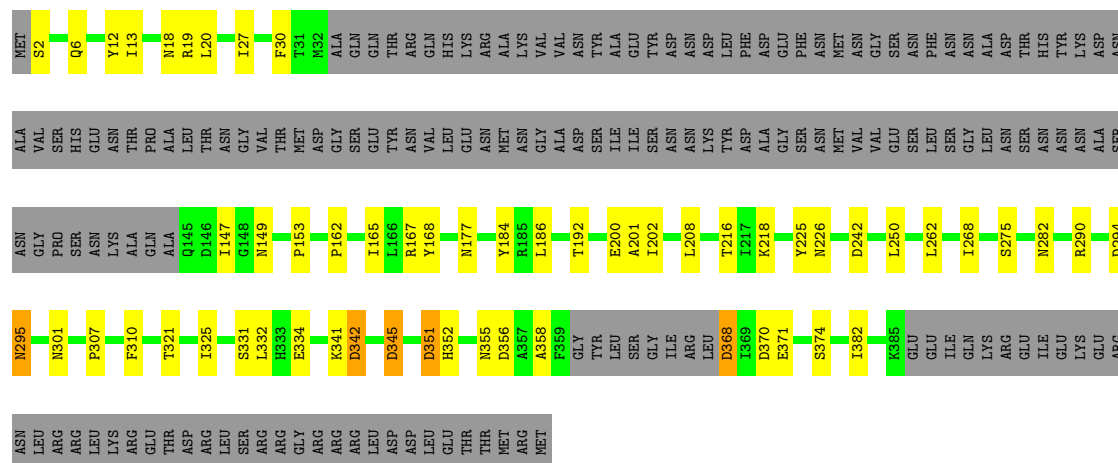
• Molecule 10: Chromatin structure-remodeling complex protein RSC58

Chain O: 63% 13% 24%



• Molecule 11: Chromatin structure-remodeling complex subunit SFH1

Chain Q: 48% 12% 38%



• Molecule 12: Nuclear protein STH1/NPS1

Chain R: 16% 81%

[illegible]

GLU	VAL	ASP	SER	HIS	PRO	ARG	THR	SER	ILE	PHE	GLU	LYS	LEU	PRO	SER	LYS	ARG	ASP	TYR	PRO	ASP	TYR	LYS	VAL	ILE	GLU	LYS	PRO	MET	ALA	ALA	ILE	ILE	ILE	LEU	LYS	ASN	CYS	CYS	LYS	ASN	GLY	THR	TYR	LYS	THR	THR	LEU	GLU	GLU	VAL	VAL	ARG	GLN	GLN	ALA	ALA	LEU	GLN	THR	MET	PHE	GLN
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ASN ALA ARG PHE TYR ASN GLU GLU GLY SER TRP VAL TYR VAL ASP ALA ASP LYS LEU ASN GLU PHE THR ASP GLU TRP PHE LYS GLU HIS SER SER

- Molecule 13: Chromatin structure-remodeling complex protein RSC30

Chain S: .. 96%

MET	MET	ASP	MET	GLN	VAL	ARG	LYS	VAL	ARG	ARG	LYS	PRO	PRO	ALA	ALA	CYS	THR	GLN	CYS	ARG	LYS	ARG	ALA	ALA	LYS	LYS	ILE	GLY	CYS	ASP	ARG	ASN	VAL	VAL	LYS	TYR	TYR	ASN	LYS	PRO	ASP	CYS	PHE	PRO	PRO	GLY	LYS	VAL	VAL	ALA	ALA	LYS	GLY	PRO	PRO	SER	SER	TYR
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MET	THR	GLY	ASN	GLN	GLY	SER	ASN	HIS	PHE	SER	GLN	GLY	ASN	VAL	ASN	GLN	LYS	ASN	VAL	MET	ILE	GLN	THR	THR	TYR	PRO	ILE	MET	GLN	THR	SER	ILE	GLU	ALA	PHE	ASN	PHE	SER	PHE	ASN	PRO	SER	VAL	ASP	ALA	THR	ALA	MET	GLN	TRP	THR	LYS	ALA	ALA	ALA	SER	THR
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[illegible][illegible]

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

ILE	LEU	HIS	ASP	ILE	CYS	HIS	ILE	ASN	GLN	PHE	LYS	VAL	SER	PRO	PRO	ASN	ASN	ASN	LYS	HIS	GLN	GLN	TYR	MET	GLU	GLU	CYS	LYS	VAL	ASN	ASN	PHE	PRO	PRO	PRO	LYS	ILE	ALA	ILE	ILE	ILE	THR	GLU	LEU	ASN	SER	GLU	SER	SER	LEU	LEU	ASN	ASN	ASN	ILE	ILE	ILE	GLU	PHE	PRO	PRO	ILE	PHE	SER
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[illegible]

SER	LEU	ALA	LEU	ASN	ASN	LEU	ARG	GLN	SER	THR	LEU	ASN	LEU	GLU	TYR	ASP	GLN	GLU	THR	ILE	LYS	PHE	ILE	ALA	ILE	THR	LYS	PHE	TYR	GLU	SER	LEU	LEU	TYR	MET	HIS	ASP	ASP	HIS	LYS	SER	SER	LEU	GLU	ASP	LEU	LEU	SER	PHE	TYR	GLN
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ILE	LYS	ASP	PHE	LYS	LEU	PHE	HIS	LYS	LYS	LYS	MET	TYR	TYR	SER	SER	ARG	HIS	SER	LEU	LEU	GLY	GLN	SER	SER	PHE	MET	VAL	PRO	PRO	ALA	ALA	GLU	ASN	LEU	LEU	SER	PRO	PRO	ILE	ILE	ALA	ALA	ASP	ASP	ASP	ILE	ILE	PRO	LEU	LEU	ILE	ALA	ALA	ASN	ASN	LYS	LEU	LEU	GLU	THR	THR	GLN	ALA
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LYS LEU LEU ASN ASN PHE TYR LEU LEU VAL VAL ASN ASN TYR LYS LYS ILE GLU GLU THR LEU LEU THR MET MET GLY VAL SER ASN THR THR VAL ASP LEU LEU PHE TYR HIS ASP ASN GLU VAL VAL ARG ARG LYS LYS GLU TRP TRP LYS ASP THR ASP LEU LEU ASN ASN PHE ILE ILE THR THR VAL VAL

THR	ASN	PHE	PHE	LEU	PHE	VAL	GLN	GLU	ASN	SER	SER	LEU	SER	MET	ALA	ALA	GLN	HIS	SER	SER	ASN	ASN	ASN	LYS	THR	THR	ASN	ASN	GLU	ARG	CYS	ALA	LYS	ASP	LEU	MET	LYS	ILE	ILE	ILE	SER	SER	ASN	MET	HIS	PHE	PHE	ASN	PHE	ILE	THR	TYR	SER	ILE	ILE	PHE	THR	PHE	ASN	PRO	PHE	PHE	ILE	ILE	LYS	SER	ILE
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LYS	SER	PHE	SER	SER	GLY	ASN	ASN	PHE	HIS	SER	ASN	GLY	LYS	PHE	LEU	LEU	GLN	ASN	PHE	ILE	GLU	ILE	LEU	LEU	GLN	GLN	PHE	ILE	ALA	ALA	PHE	ALA	ALA	PHE	GLN	ARG	CYS	GLU	VAL	ILE	ILE	LEU	TYR	ASP	GLU	PHE	TYR	LYS	ASN	ASN	SER	LEU	LEU	ILE	ILE	GLU	GLU	ASN	ASN	VAL
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GLN LEU LEU LEU LEU HIS ASP LYS ILE ILE LEU LEU LEU LEU ILE ILE LEU LYS LYS ILE ILE LEU GLU GLU ILE ILE ILE VAL SER SER PHE ARG ARG ASP GLU MET MET ASN ASN SER SER SER GLY GLY SER SER PHE LYS LYS LYS LYS VAL LEU ASN ASN ILE ILE ILE TYR TYR MET MET LEU LEU ARG ARG PHE PHE SER SER LYS LYS LYS LYS GLN ASN GLN PHE PHE ILE

ARG	ASN	SER	ASP	ASN	ASN	ASN	ASN	ASN	VAL	THR	ASP	SER	GLN	SER	ALA	LYS	ASN	LYS	ASN	VAL	VAL	LEU	LEU	LYS	PHE	PRO	VAL	SER	SER	GLU	LEU	LEU	ASN	ARG	ARG	ILE	TYR	ILE	LEU	LEU	LYS	LYS	PHE	GLU	GLU	ILE	ILE	SER	SER	ASP	PHE	LEU	MET	GLU	GLU	ARG	ARG	GLU	VAL	VAL	GLN	ARG	SER	ILE	ILE	ILE	ILE	ASP	LYS	ASP	LEU	LEU
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SER
ASP
ASN
LEU
GLY
ILE
THR
THR
ALA
ASN
PHE
ASN
ASP
PHE
TYR
ASP
ALA
PHE
TYR
ASN

- Molecule 14: Unknown protein

Chain 2:  96%



- Molecule 15: Unknown Protein

Chain 3:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: Unknown Protein

Chain 4:  95%



- Molecule 16: Unknown protein

Chain 5:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: Unknown Protein

Chain 6:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: Unknown Protein

Chain 7:  96%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1920066	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
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:
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	C	0.24	0/495	0.36	0/662
10	O	0.30	0/3216	0.42	1/4358 (0.0%)
11	Q	0.27	0/2181	0.45	0/2964
12	R	0.27	0/2154	0.40	0/2897
13	S	0.26	0/281	0.35	0/378
2	D	0.27	0/786	0.38	0/1062
3	E	0.28	0/997	0.44	0/1356
4	F	0.27	0/551	0.41	0/748
5	G	0.26	0/431	0.43	0/584
6	H	0.29	0/1108	0.48	0/1497
7	I	0.32	0/2474	0.41	0/3343
7	J	0.30	0/926	0.40	0/1233
7	K	0.27	0/879	0.39	0/1172
7	L	0.29	0/2502	0.40	0/3376
8	M	0.28	0/2515	0.42	0/3423
9	N	0.30	0/3334	0.42	0/4515
All	All	0.29	0/24830	0.42	1/33568 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	O	231	VAL	C-N-CA	5.36	135.09	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	C	493	0	507	6	0
2	D	772	0	754	11	0
3	E	978	0	935	24	0
4	F	536	0	533	14	0
5	G	422	0	423	10	0
6	H	1083	0	1062	22	0
7	I	2416	0	2358	35	0
7	J	924	0	976	10	0
7	K	878	0	930	14	0
7	L	2445	0	2402	47	0
8	M	2474	0	2465	51	0
9	N	3275	0	3373	51	0
10	O	3145	0	3168	50	0
11	Q	2137	0	2069	39	0
12	R	2126	0	2205	34	0
13	S	278	0	287	6	0
14	2	140	0	34	1	0
15	3	95	0	21	0	0
15	4	95	0	21	1	0
16	5	70	0	16	0	0
17	6	75	0	17	0	0
18	7	245	0	63	2	0
19	I	1	0	0	0	0
All	All	25103	0	24619	323	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 6.

The worst 5 of 323 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:Q:282:ASN:OD1	11:Q:295:ASN:ND2	2.20	0.75
9:N:217:GLU:OE1	12:R:287:ARG:NH1	2.21	0.74
2:D:96:GLN:NE2	15:4:15:UNK:O	2.22	0.72
4:F:813:LEU:HD11	10:O:183:ILE:HD12	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:268:ILE:HD11	10:O:232:LEU:HD22	1.73	0.70

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	C	58/78 (74%)	56 (97%)	2 (3%)	0	100	100
2	D	96/180 (53%)	90 (94%)	6 (6%)	0	100	100
3	E	118/435 (27%)	108 (92%)	10 (8%)	0	100	100
4	F	63/889 (7%)	56 (89%)	7 (11%)	0	100	100
5	G	51/885 (6%)	49 (96%)	2 (4%)	0	100	100
6	H	127/625 (20%)	114 (90%)	10 (8%)	3 (2%)	6	29
7	I	289/557 (52%)	274 (95%)	15 (5%)	0	100	100
7	J	113/557 (20%)	109 (96%)	4 (4%)	0	100	100
7	K	105/557 (19%)	101 (96%)	4 (4%)	0	100	100
7	L	292/557 (52%)	278 (95%)	14 (5%)	0	100	100
8	M	302/483 (62%)	281 (93%)	21 (7%)	0	100	100
9	N	408/581 (70%)	380 (93%)	28 (7%)	0	100	100
10	O	376/502 (75%)	352 (94%)	24 (6%)	0	100	100
11	Q	258/426 (61%)	224 (87%)	34 (13%)	0	100	100
12	R	258/1359 (19%)	236 (92%)	22 (8%)	0	100	100
13	S	32/883 (4%)	32 (100%)	0	0	100	100
All	All	2946/9554 (31%)	2740 (93%)	203 (7%)	3 (0%)	56	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	H	528	ILE
6	H	529	ASN
6	H	527	THR

5.3.2 Protein sidechains ⓘ

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	C	58/75 (77%)	58 (100%)	0	100	100
2	D	82/151 (54%)	82 (100%)	0	100	100
3	E	113/388 (29%)	105 (93%)	8 (7%)	16	48
4	F	60/810 (7%)	60 (100%)	0	100	100
5	G	48/832 (6%)	47 (98%)	1 (2%)	56	81
6	H	126/578 (22%)	124 (98%)	2 (2%)	65	86
7	I	268/500 (54%)	261 (97%)	7 (3%)	49	77
7	J	111/500 (22%)	110 (99%)	1 (1%)	81	91
7	K	106/500 (21%)	106 (100%)	0	100	100
7	L	270/500 (54%)	270 (100%)	0	100	100
8	M	286/435 (66%)	281 (98%)	5 (2%)	63	85
9	N	374/521 (72%)	366 (98%)	8 (2%)	56	81
10	O	358/462 (78%)	354 (99%)	4 (1%)	76	89
11	Q	243/384 (63%)	233 (96%)	10 (4%)	33	68
12	R	240/1228 (20%)	237 (99%)	3 (1%)	71	88
13	S	33/824 (4%)	32 (97%)	1 (3%)	44	74
All	All	2776/8688 (32%)	2726 (98%)	50 (2%)	64	84

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	M	241	LEU
9	N	123	LEU
12	R	215	THR

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Mol	Chain	Res	Type
8	M	466	ASN
9	N	91	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
8	M	233	GLN
9	N	512	ASN
12	R	116	ASN
8	M	340	ASN
8	M	380	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	7	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	57:UNK	C	60:UNK	N	4.98