Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 11:10 AM JST

PDB ID	:	6KW3
EMDB ID	:	EMD-0777
Title	:	The ClassA RSC-Nucleosome Complex
Authors	:	Ye, Y.P.; Wu, H.; Chen, K.J.; Verma, N.; Cairns, B.; Gao, N.; Chen, Z.C.
Deposited on	:	2019-09-05
Resolution	:	7.13 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 ⓘ 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:

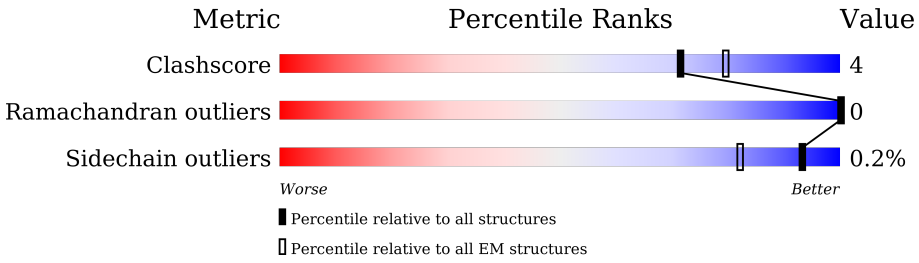
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 7.13 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% 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	B	103	71% 9% 20%
1	R	103	9% 71% 14% 16%
2	N	136	64% 8% 28%
2	Q	136	61% 9% 30%
3	O	130	8% 73% 9% 18%
3	S	130	72% 10% 18%
4	U	167	77% 10% 13%
5	V	167	79% 8% 13%

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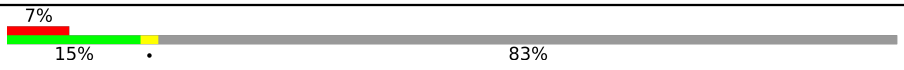
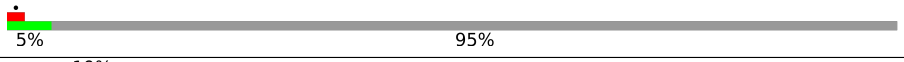
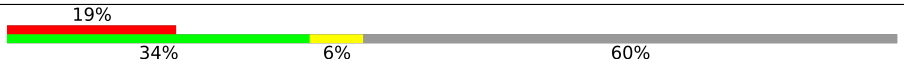
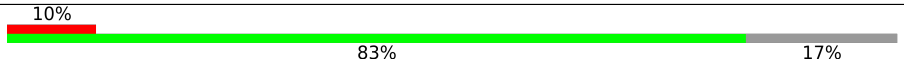
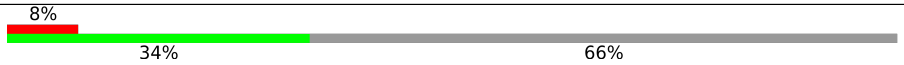
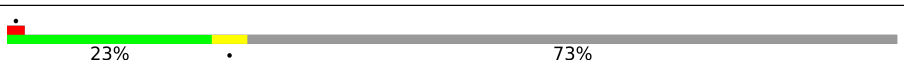
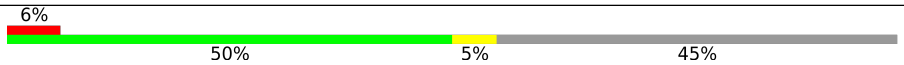
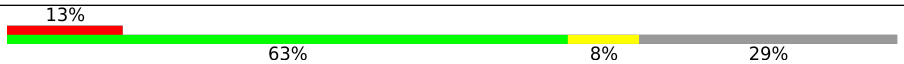
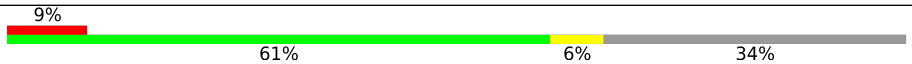
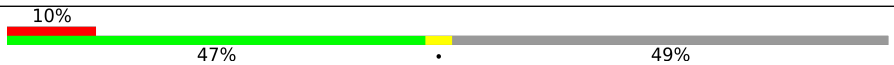
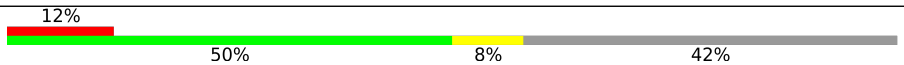
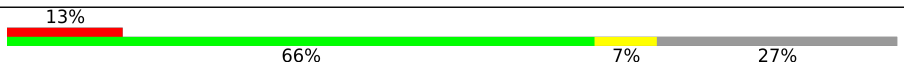
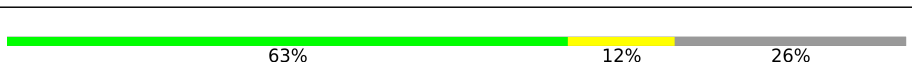
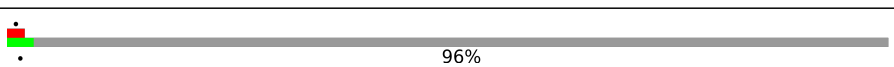
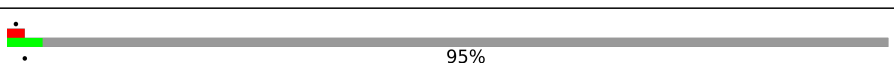
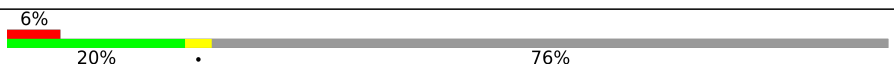
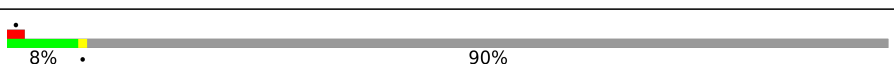
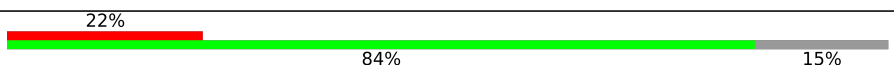
Mol	Chain	Length	Quality of chain
6	J	1359	
6	W	1359	
6	Y	1359	
7	f	477	
8	h	157	
9	F	435	
10	D	557	
10	H	557	
11	M	581	
12	I	483	
13	G	426	
14	A	502	
15	E	78	
16	C	883	
17	K	885	
18	X	625	
19	L	889	
20	P	126	
20	T	126	
21	g	467	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 45514 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 H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	82	Total 657	C 416	N 128	O 112	S 1	0	0
1	R	87	Total 703	C 443	N 142	O 117	S 1	0	0

- Molecule 2 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	98	Total 810	C 511	N 157	O 139	S 3	0	0
2	Q	95	Total 784	C 494	N 151	O 136	S 3	0	0

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	107	Total 823	C 519	N 161	O 143	0	0
3	S	107	Total 823	C 519	N 161	O 143	0	0

- Molecule 4 is a DNA chain called DNA 167.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	146	Total 2977	C 1414	N 542	O 875	P 146	0	0

- Molecule 5 is a DNA chain called DNA 167.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	146	Total 3009	C 1425	N 561	O 877	P 146	0	0

- Molecule 6 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	W	69	Total	C	N	O	S	0	0
			592	364	121	105	2		
6	J	235	Total	C	N	O	S	0	0
			1814	1136	327	349	2		
6	Y	548	Total	C	N	O	S	0	0
			4503	2873	780	832	18		

- Molecule 7 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	398	Total	C	N	O	S	3	0
			3219	2075	527	602	15		

- Molecule 8 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	54	Total	C	N	O	S	0	0
			490	313	84	92	1		

- Molecule 9 is a protein called Chromatin structure-remodeling complex subunit RSC7.

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

- Molecule 10 is a protein called Chromatin structure-remodeling complex protein RSC8.

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

- Molecule 11 is a protein called Chromatin structure-remodeling complex subunit RSC9.

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

- Molecule 12 is a protein called Chromatin structure-remodeling complex protein RSC6.

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

- Molecule 13 is a protein called Chromatin structure-remodeling complex subunit SFH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	246	Total	C	N	O	S	0	0
			1996	1271	337	380	8		

- Molecule 14 is a protein called Chromatin structure-remodeling complex protein RSC58.

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

- Molecule 15 is a protein called High temperature lethal protein 1.

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

- Molecule 16 is a protein called Chromatin structure-remodeling complex protein RSC30.

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

- Molecule 17 is a protein called Chromatin structure-remodeling complex protein RSC3.

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

- Molecule 18 is a protein called Chromatin structure-remodeling complex subunit RSC4.

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

- Molecule 19 is a protein called Chromatin structure-remodeling complex subunit RSC2.

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

- Molecule 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	93	Total	C	N	O	S	0	0
			725	456	130	137	2		
20	P	93	Total	C	N	O	S	0	0
			717	450	128	137	2		

- Molecule 21 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	395	Total	C	N	O	S	1	0
			3191	2048	522	614	7		

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

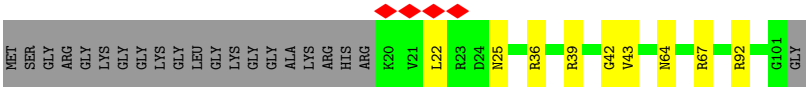
Mol	Chain	Residues	Atoms		AltConf
22	H	1	Total	Zn	0
			1	1	

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.

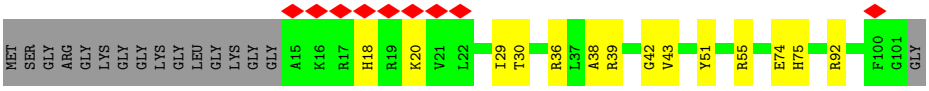
• Molecule 1: Histone H4

Chain B:



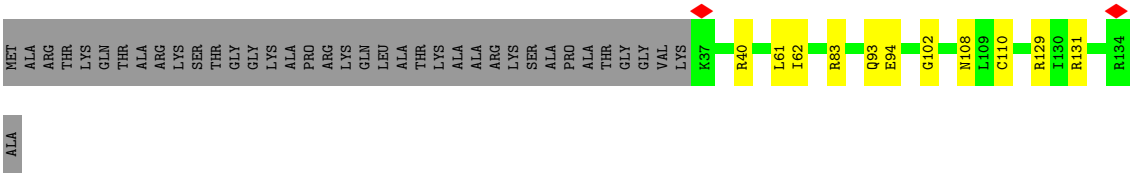
• Molecule 1: Histone H4

Chain R:



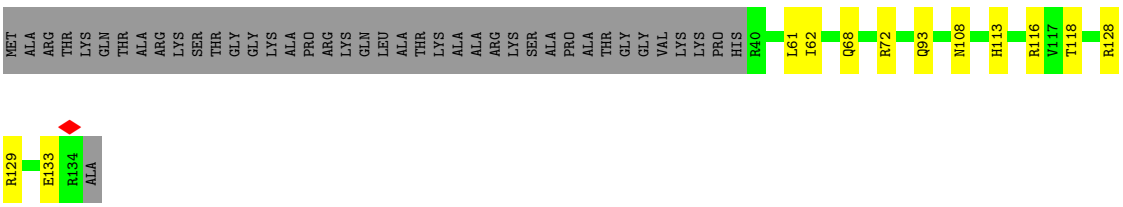
• Molecule 2: Histone H3.2

Chain N:



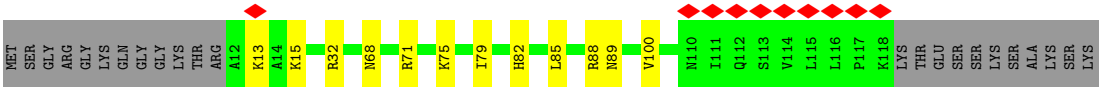
• Molecule 2: Histone H3.2

Chain Q:



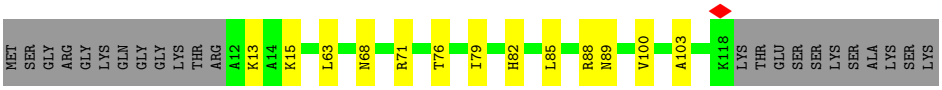
• Molecule 3: Histone H2A

Chain O:



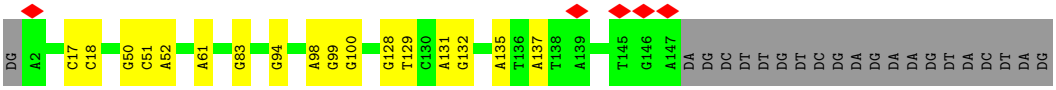
• Molecule 3: Histone H2A

Chain S:



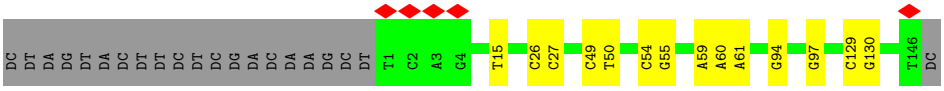
• Molecule 4: DNA 167

Chain U:



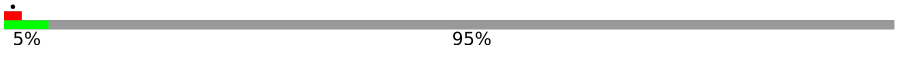
• Molecule 5: DNA 167

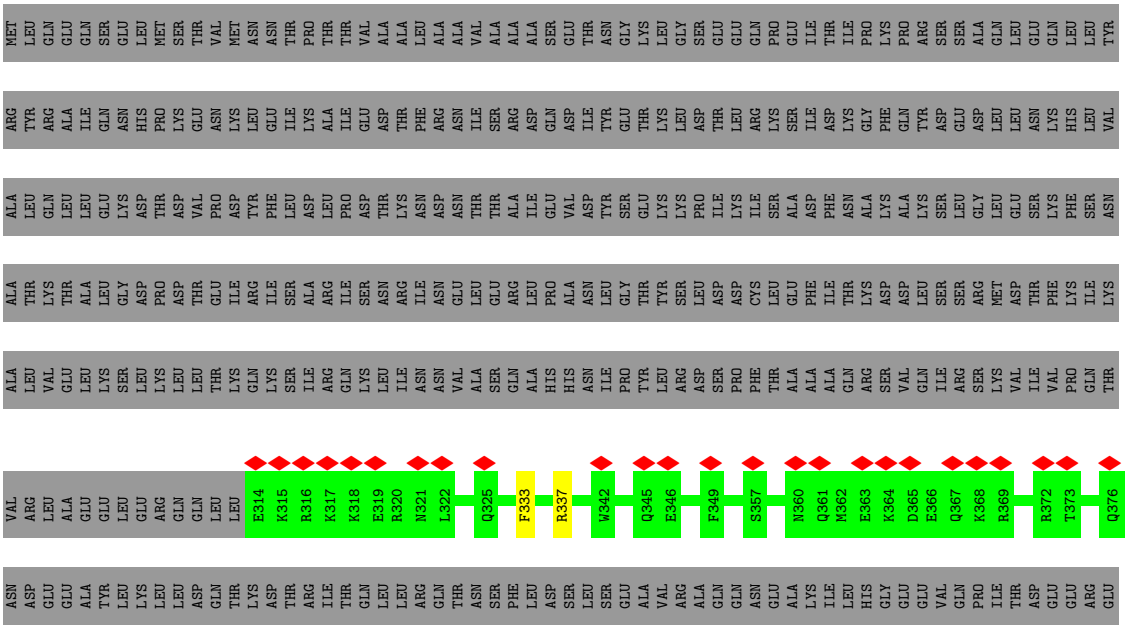
Chain V:

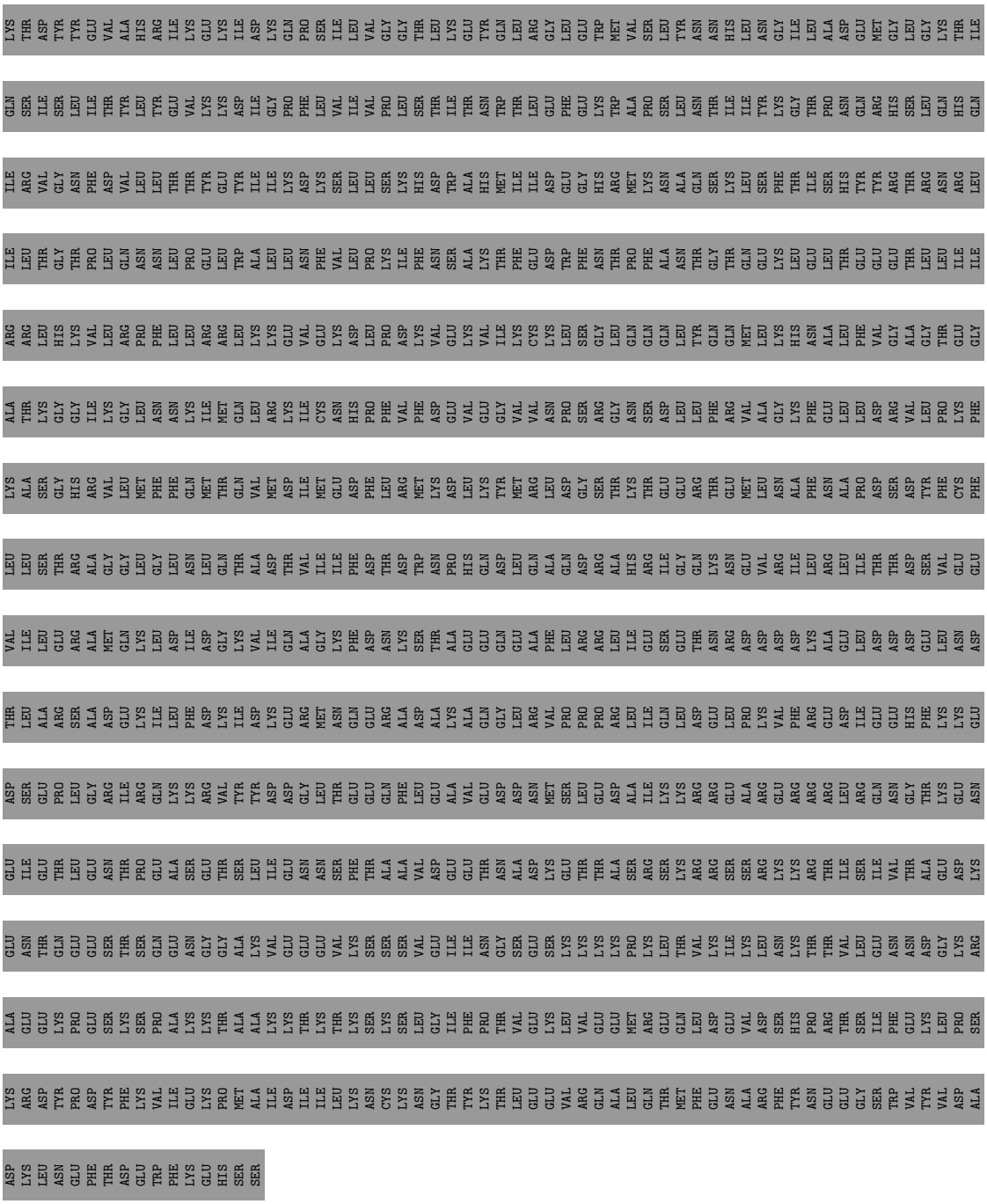


• Molecule 6: Nuclear protein STH1/NPS1

Chain W:

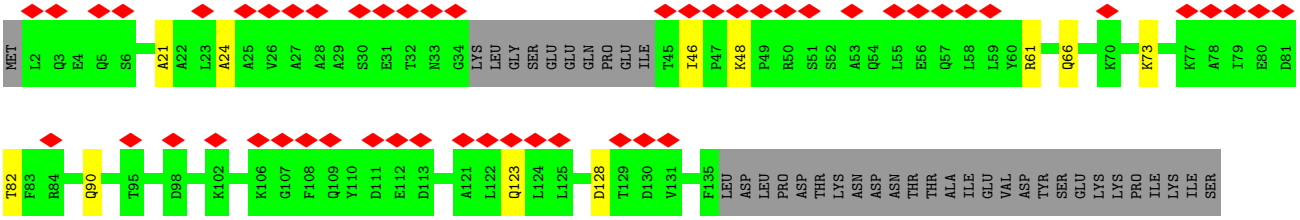


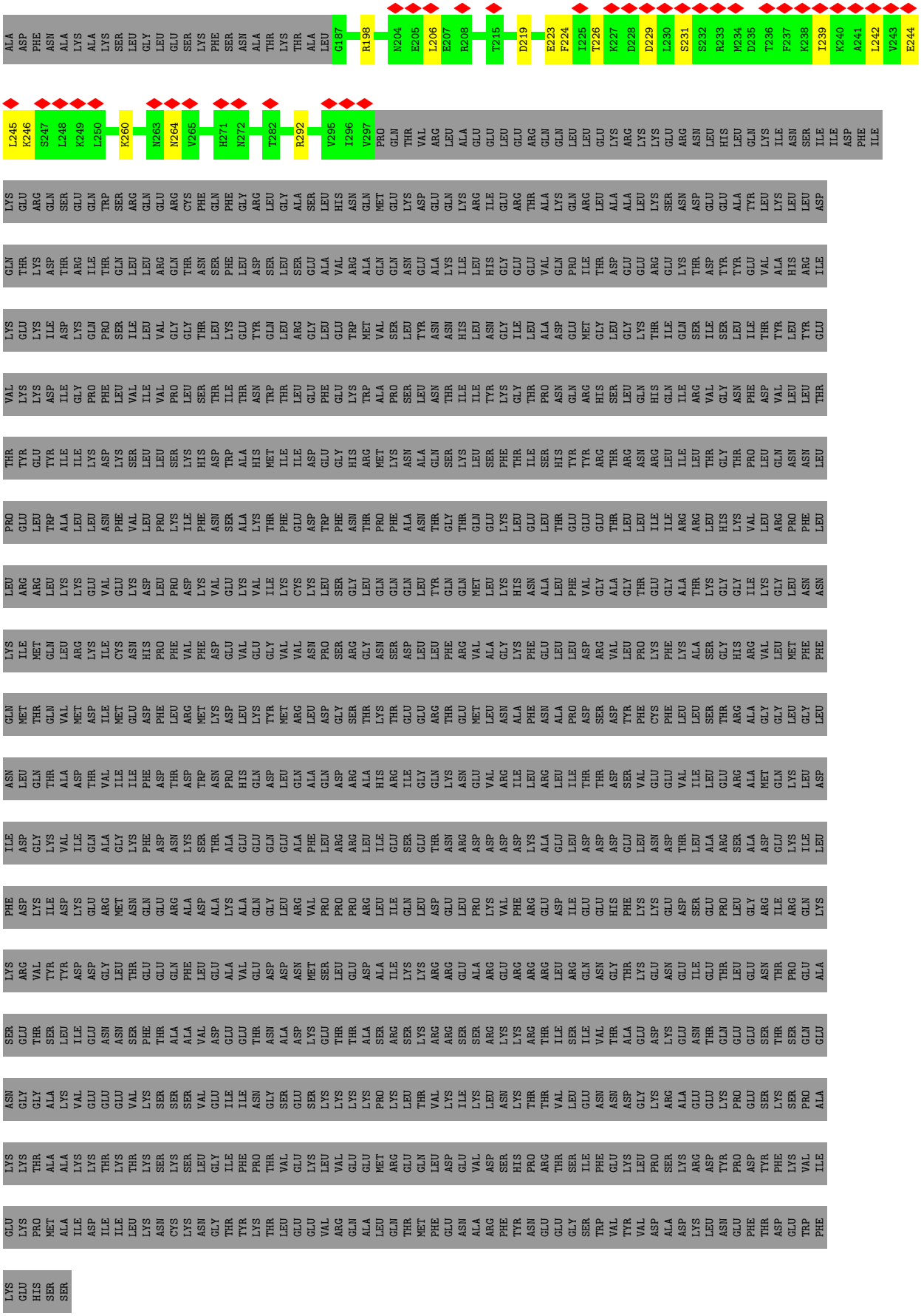




• Molecule 6: Nuclear protein STH1/NPS1

Chain J:

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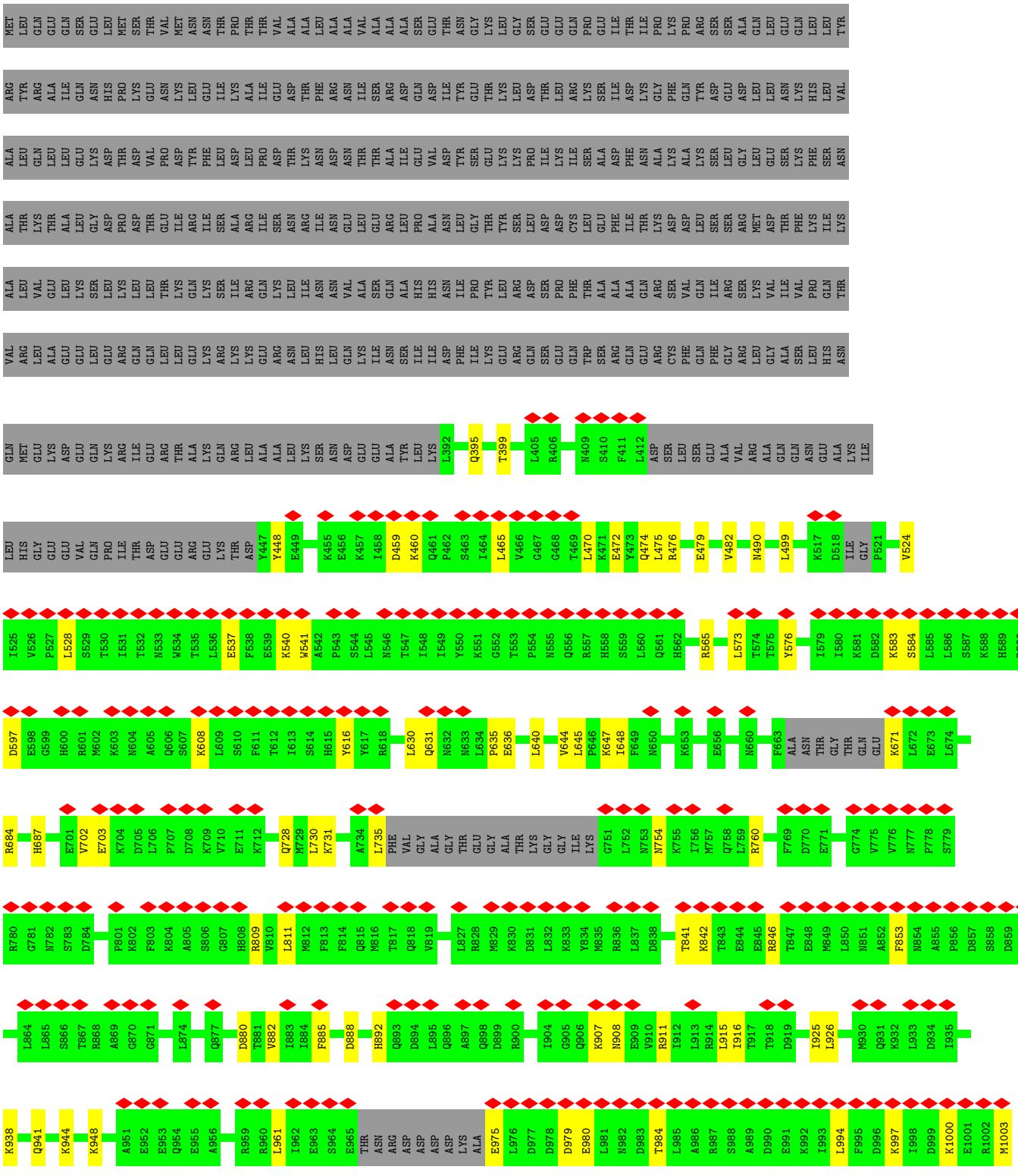
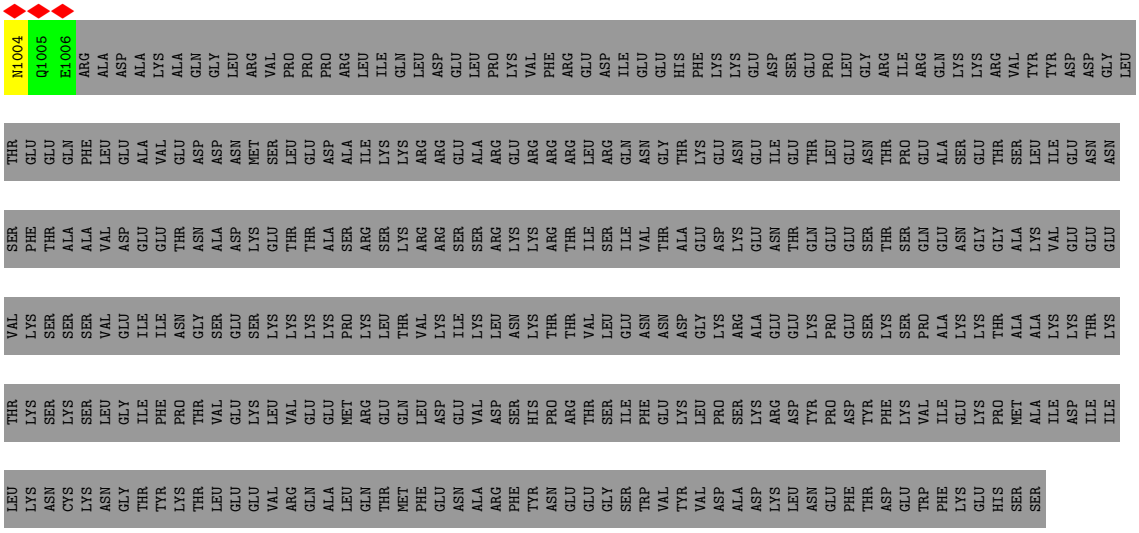
G187 R198 N204 E205 L206 E207 R208 T215 D219 E223 F224 I225 T226 K227 D228 D229 L230 S231 S232 R233 M234 D235 T236 F237 K238 I239 K240 A241 L242 V243 E244
L245 K246 S247 L248 K249 L250 K260 N263 N264 V265 H271 N272 T282 R292 V295 I296 V297
PRO GLN THR VAL ARG LEU ALA GLU GLU LEU ARG GLN LEU LEU LYS ARG LEU ALA LYS SER LEU LEU ARG ASN LEU HIS LEU GLN LYS ILE LEU ILE ASN SER ILE LEU PHE ILE
LYS GLU ARG GLN SER GLU GLN TRP SER ARG GLN GLU ARG CYS PHE GLN PHE GLY ARG LEU GLY ALA SER LEU HIS ASN GLN MET GLU LYS ASP GLU GLN LYS ASP ARG ILE GLU ARG THR ALA LYS GLN ARG LEU ALA LEU LYS SER ASN ASP GLU GLU ALA TYR LEU LYS LEU ASP
GLN THR LYS ASP THR ARG ILE THR GLN LEU LEU ARG GLN THR ASN SER PHE LEU ASP SER LEU SER GLU ALA VAL ARG ALA GLN GLN ASN GLU ALA LYS ILE LEU HIS GLY GLU GLU VAL GLN PRO ILE THR ASP GLU GLU ARG GLU LYS THR ASP GLU GLU ARG GLU LYS THR ILE GLU
LYS GLU LYS ILE ASP LYS GLN PRO SER ILE LEU VAL GLY GLY THR LEU LYS GLU TYR GLN LEU ARG GLY GLU TRP MET VAL SER LEU TYR ASN ASN HIS LEU ASN GLY ILE LEU ALA ASP GLU MET GLY LEU GLY GLY LYS THR ILE GLN SER ILE SER LEU ILE THR TYR LEU TYR GLU
VAL LYS LYS ASP ILE GLY PRO PHE LEU VAL ILE VAL PRO LEU SER THR ILE THR ASN TRP THR LEU GLU GLU PHE GLU LYS TRP ALA PRO SER LEU ASN THR ILE ILE TYR LYS GLY THR PRO ASN GLN ARG HIS SER LEU GLN HIS GLN ILE ARG VAL GLY GLY ASN PHE ASP VAL LEU LEU THR
THR TYR GLU TYR ILE ILE LYS ASP LYS SER LEU LEU LEU SER LYS HIS ASP TRP ALA HIS MET ILE ILE ASP GLU GLY HIS ARG MET LYS ASN ALA GLN SER LYS LEU SER PHE THR ILE SER HIS TYR TYR ARG THR ARG ASN ARG LEU ILE LEU THR GLY THR PRO LEU GLN ASN ASN LEU
PRO GLU LEU TRP ALA LEU LEU ASN PHE VAL LEU LEU PRO LYS ILE PHE ASN SER ALA LYS THR PHE GLU ASP TRP PHE ASN THR PRO PHE ALA ASN THR GLY THR GLN GLU LYS LEU GLU LEU THR GLU GLU GLU THR LEU LEU GLU LEU LEU ILE ILE ARG ARG LEU HIS LYS VAL LEU ARG PRO PHE LEU
LEU ARG ARG LEU LYS LYS GLU VAL GLU LYS ASP LEU PRO ASP LYS VAL GLU LYS VAL ILE ILE LYS CYS LYS LEU SER GLY LEU GLN GLN GLN LEU TYR GLN GLN MET LEU LYS HIS ASN ALA LEU LEU PHE VAL GLY ALA GLY THR GLU GLY ALA THR LYS GLY GLY ILE LYS GLY LEU ASN ASN
LYS ILE MET GLN LEU ARG LYS ILE CYS ASN HIS PRO PHE VAL PHE ASP GLU VAL GLY VAL VAL ASN PRO SER ARG GLY ASN SER ASP LEU LEU PHE ARG VAL ALA GLY LYS PHE GLU LEU LEU ASP ARG VAL LEU PRO LYS PHE LYS ALA SER GLY HIS ARG VAL LEU MET PHE PHE
GLN MET THR GLN VAL MET ILE MET GLU ASP PHE LEU ARG MET LYS ASP LEU LYS TYR MET ARG LEU ASP GLY SER THR LYS THR GLU GLU ARG THR GLU MET LEU ASN ALA PHE ASN ALA PRO ASP SER ASP TYR PHE CYS PHE LEU LEU LEU SER THR ARG GLY GLY LEU GLY LEU
ASN LEU GLN THR ALA ASP THR VAL ILE ILE PHE ASP THR ASP TRP ASN PRO HIS GLN ASP LEU GLN ALA GLN ASP ARG ALA HIS ARG ILE GLY GLN LYS ASN GLU VAL ARG ILE ILE LEU ARG LEU ILE THR THR ASP SER VAL GLU GLU VAL ILE LEU LEU GLU ARG ALA MET GLN LYS LEU ASP
ILE ASP GLY LYS VAL ILE GLN ILE GLU SER GLU THR ASN ARG ASP ASP ASP LYS ALA GLU LEU ASP ASP ASP GLU LEU ASN VAL ASP THR LEU ALA ARG ASP SER ALA ILE GLU ASP ASN ILE LYS
PHE ASP LYS ILE ASP LYS GLU ARG MET ASN GLN GLU ARG ALA ASP ALA LYS ALA GLY LEU ARG VAL PRO PRO PRO ARG LEU ILE GLN LEU ASP GLU LEU PRO LYS VAL PHE ARG GLU ASP ILE GLU GLU HIS PHE LYS LYS GLU ASP SER GLU PHE PRO LEU GLY ARG ILE ARG GLN LYS
LYS ARG VAL TYR TYR ASP ASP GLY LEU THR GLU GLU GLN PHE LEU GLU ALA VAL GLU ASP ASP ASN MET SER LEU GLU ASP ALA ILE LYS LYS ARG GLU ARG ARG GLU ALA ARG GLU ASP ARG ARG ARG LEU ARG GLN ASN GLY THR LYS GLU ASN GLY GLU ILE GLU THR THR LEU GLU GLU ASN THR PRO GLU ALA
SER GLU THR SER LEU ILE GLU ASN SER PHE THR ALA ALA VAL ASP GLU GLU GLU THR THR ALA SER ARG SER LYS ARG ARG ARG SER GLU SER SER ARG LYS LYS ARG THR ILE SER ILE VAL THR ALA GLU GLU ASP LYS GLU GLY GLN THR GLN GLU GLU SER THR GLN GLU
ASN GLY GLY ALA LYS VAL GLU GLU ILE ILE ASN GLY SER GLU SER SER VAL GLU ILE LYS LYS LYS LYS PRO LYS LEU THR VAL LYS ILE LYS LEU GLU ASN LYS THR THR VAL LEU GLU ASN ASN LYS GLY GLY LYS ARG ALA GLU GLU LYS PRO GLU SER LYS SER PRO ALA
LYS LYS THR LYS THR LYS SER SER LEU GLY ILE PHE PRO THR VAL GLU GLU LEU ASP GLU VAL ASP SER HIS PRO ARG THR SER ILE PHE GLU LYS LEU PRO GLU ASP TYR PHE LYS VAL ILE
GLU LYS PRO MET ALA ILE ASP ILE ILE LEU LYS ASN CYS LYS ASN GLY THR TYR LYS THR LEU GLU GLU VAL ARG GLN ALA LEU GLN THR MET PHE GLU ASN ALA ARG PHE TYR ASN GLU GLU GLY SER TRP VAL TYR VAL ASP ALA ASP LYS ASN GLU PHE THR ASP GLU TRP PHE
LYS GLU HIS SER SER

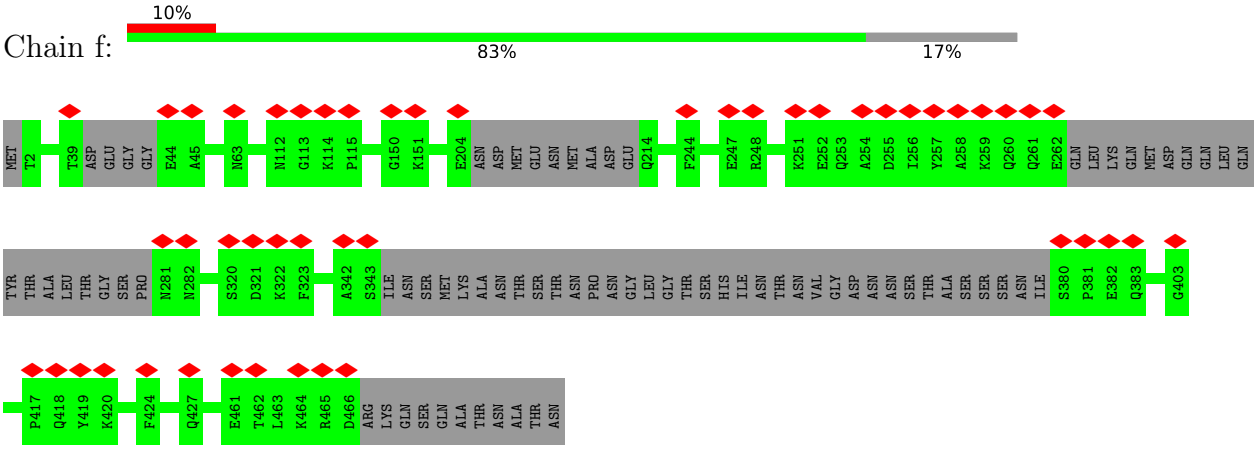
• Molecule 6: Nuclear protein STH1/NPS1

Chain Y:

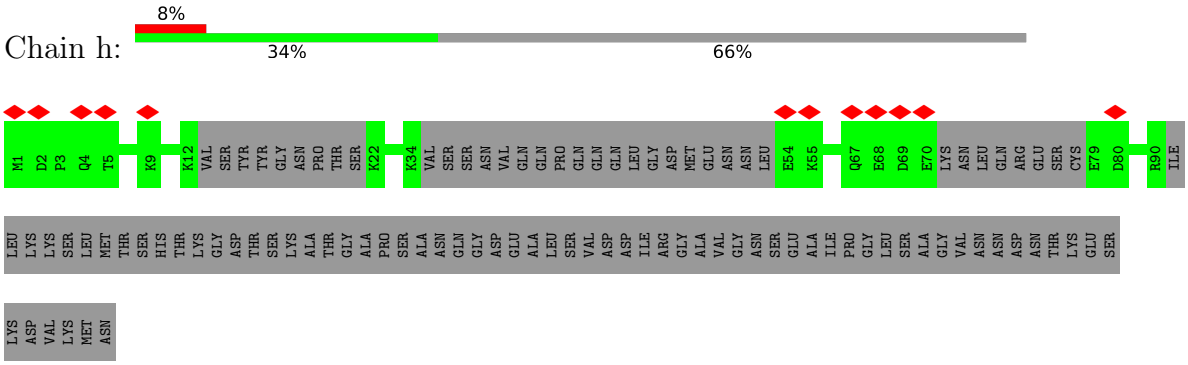




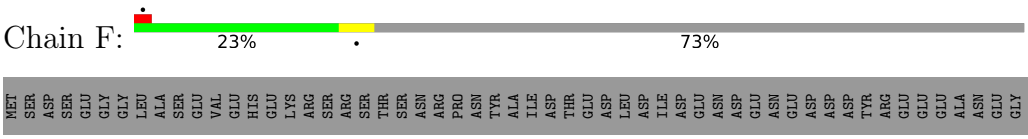
• Molecule 7: Actin-related protein 7

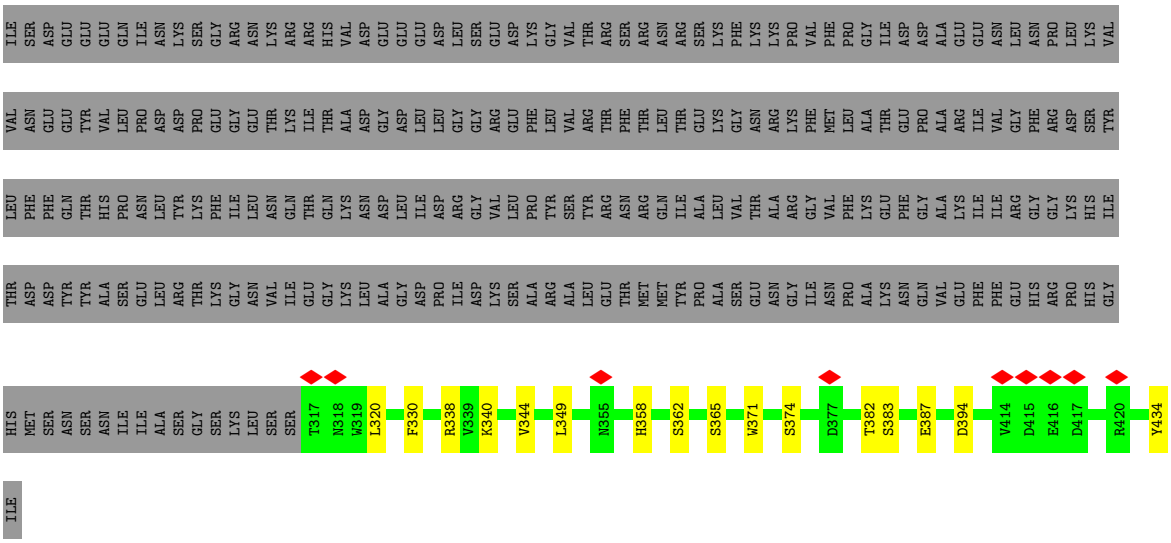


• Molecule 8: Regulator of Ty1 transposition protein 102



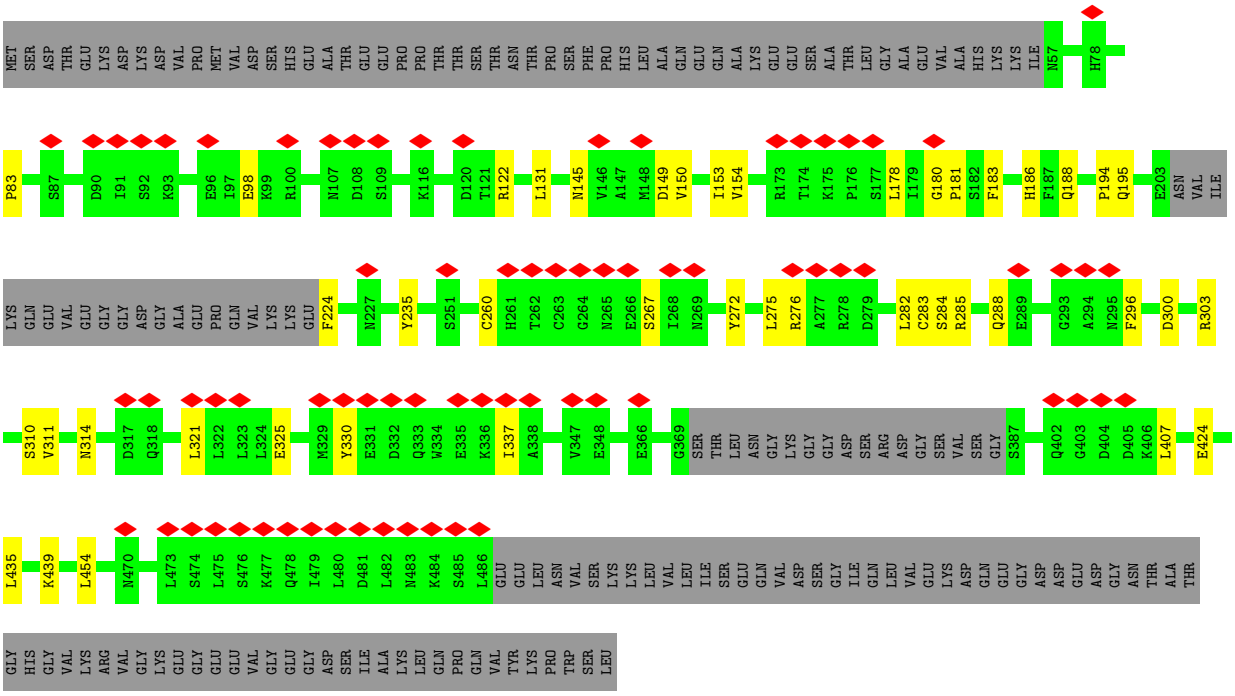
• Molecule 9: Chromatin structure-remodeling complex subunit RSC7





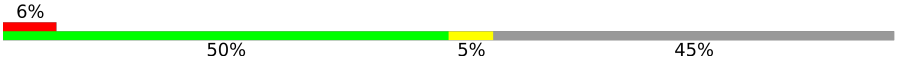
• Molecule 10: Chromatin structure-remodeling complex protein RSC8

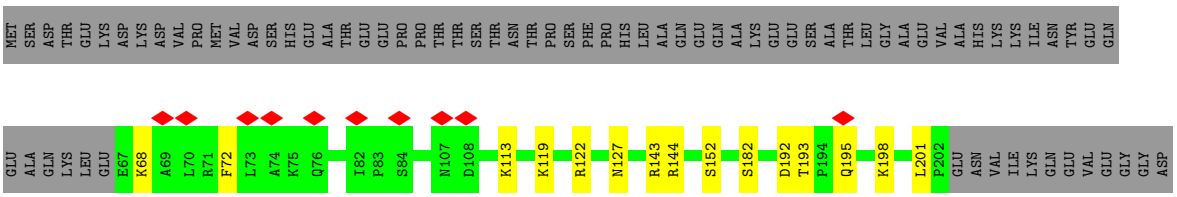
Chain H:

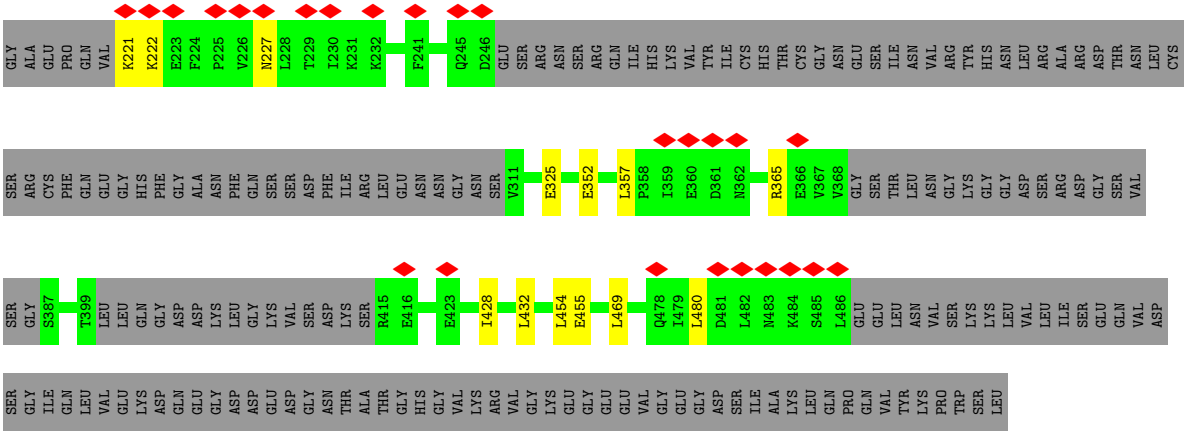


• Molecule 10: Chromatin structure-remodeling complex protein RSC8

Chain D:

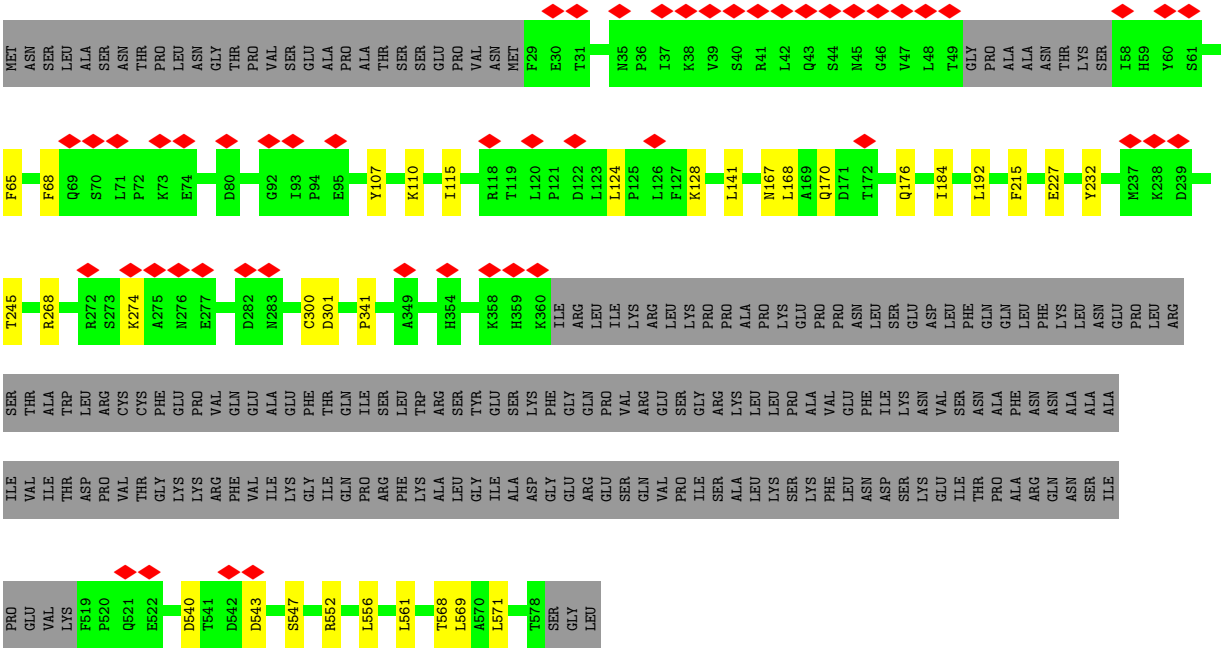






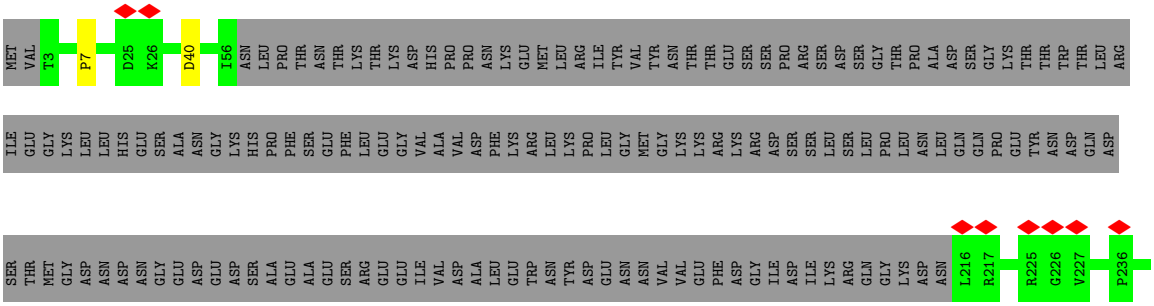
• Molecule 11: Chromatin structure-remodeling complex subunit RSC9

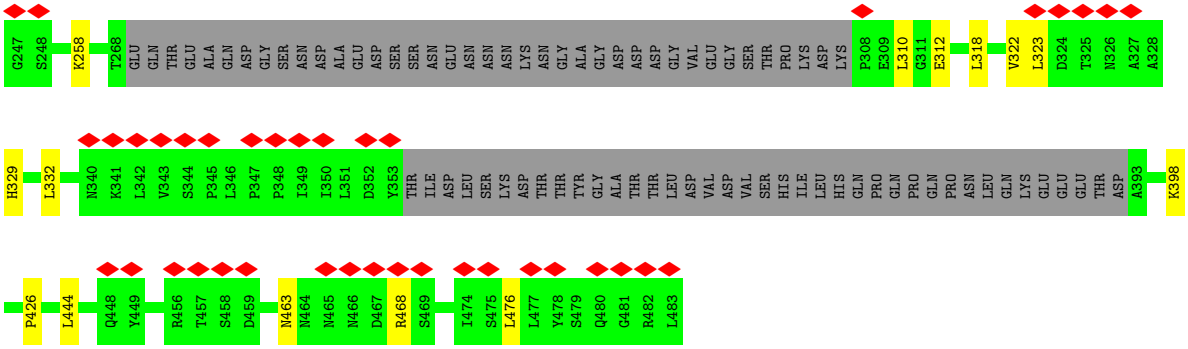
Chain M:



• Molecule 12: Chromatin structure-remodeling complex protein RSC6

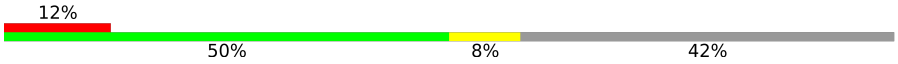
Chain I:

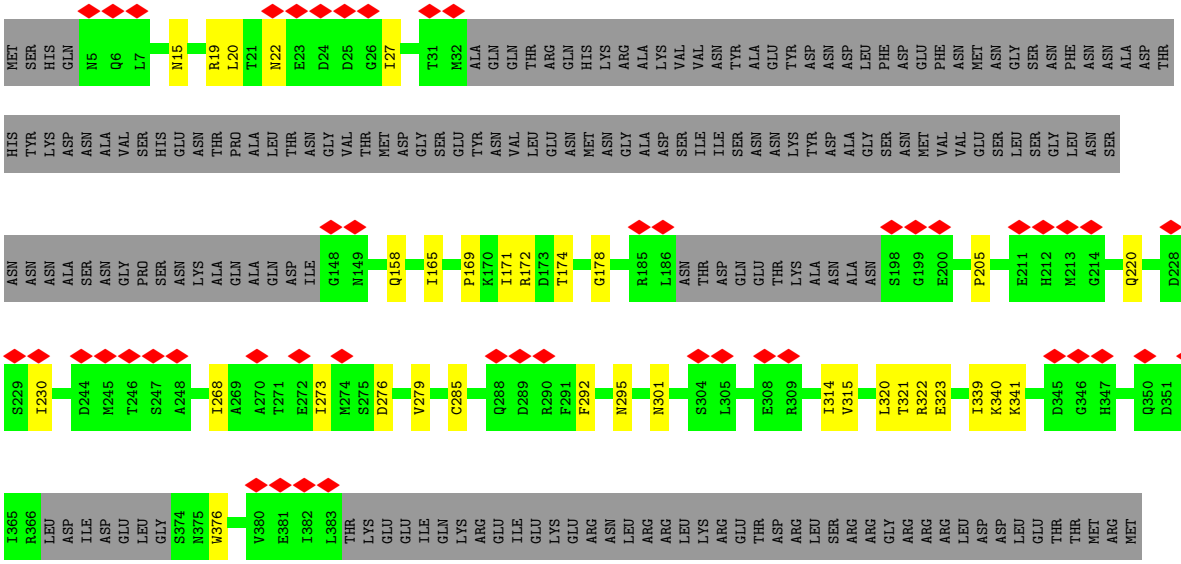




• Molecule 13: Chromatin structure-remodeling complex subunit SFH1

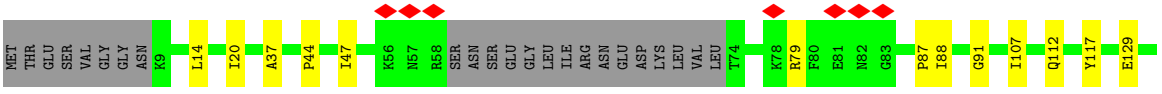
Chain G:

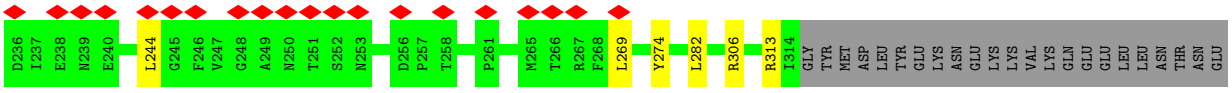


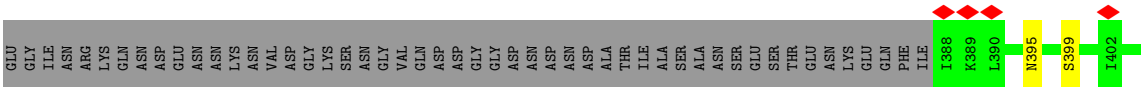


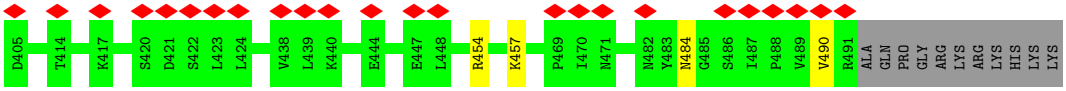
• Molecule 14: Chromatin structure-remodeling complex protein RSC58

Chain A:



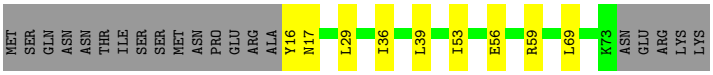






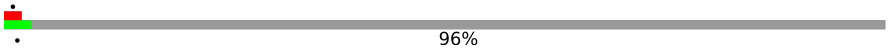
• Molecule 15: High temperature lethal protein 1

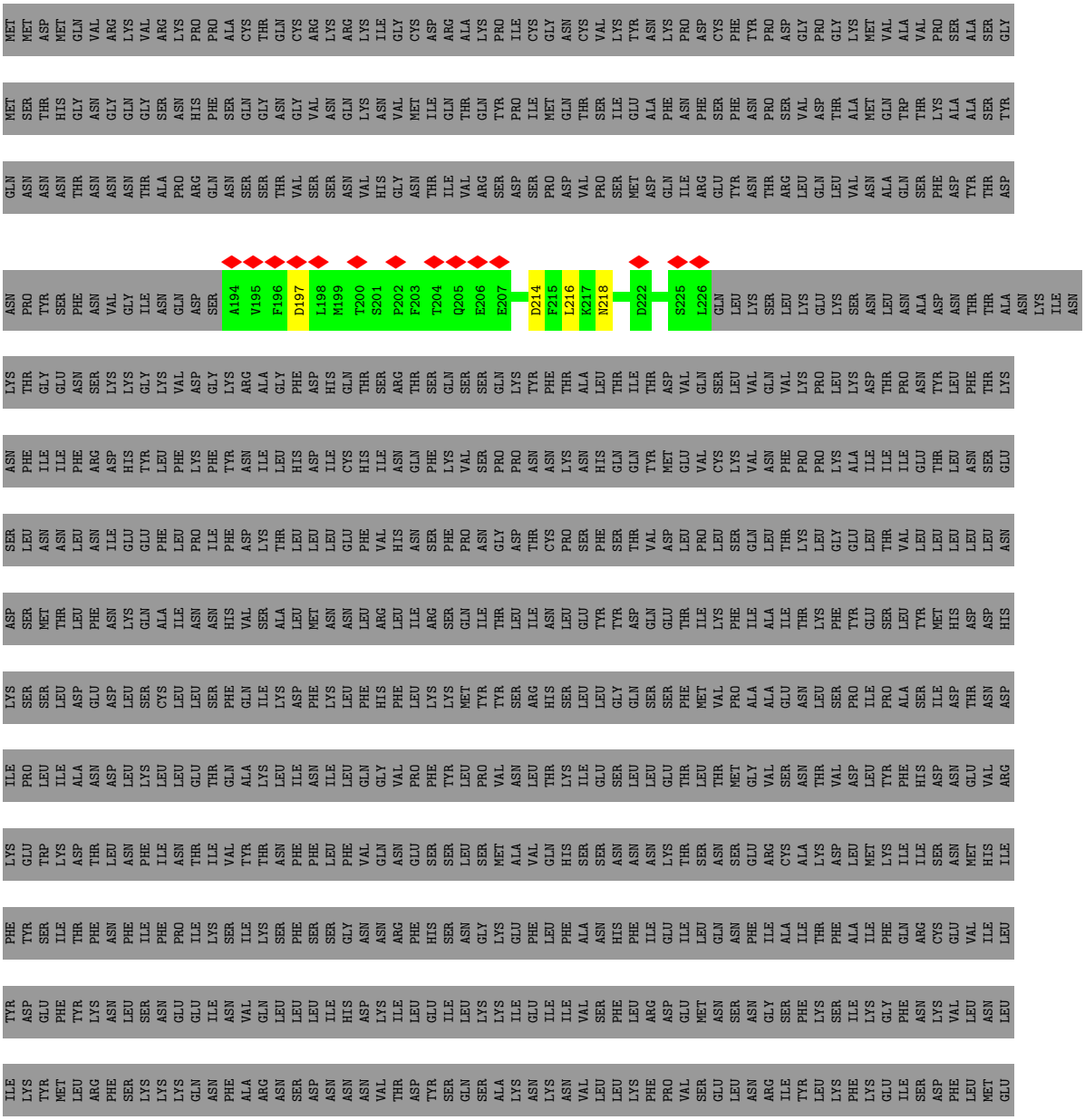
Chain E:

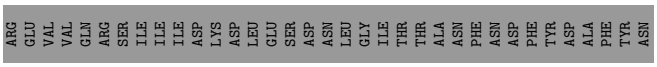


• Molecule 16: Chromatin structure-remodeling complex protein RSC30

Chain C:

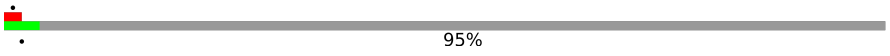


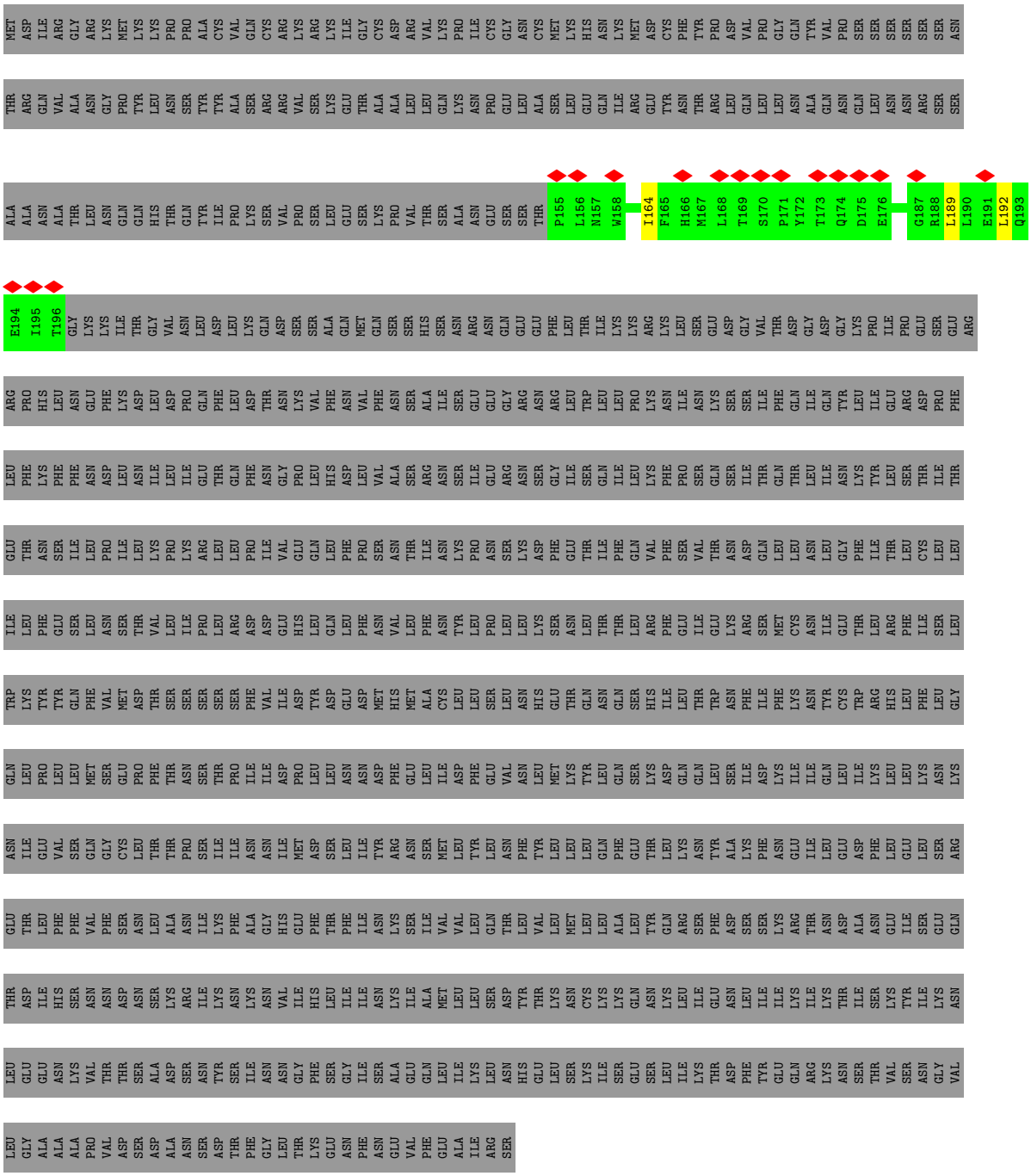




• Molecule 17: Chromatin structure-remodeling complex protein RSC3

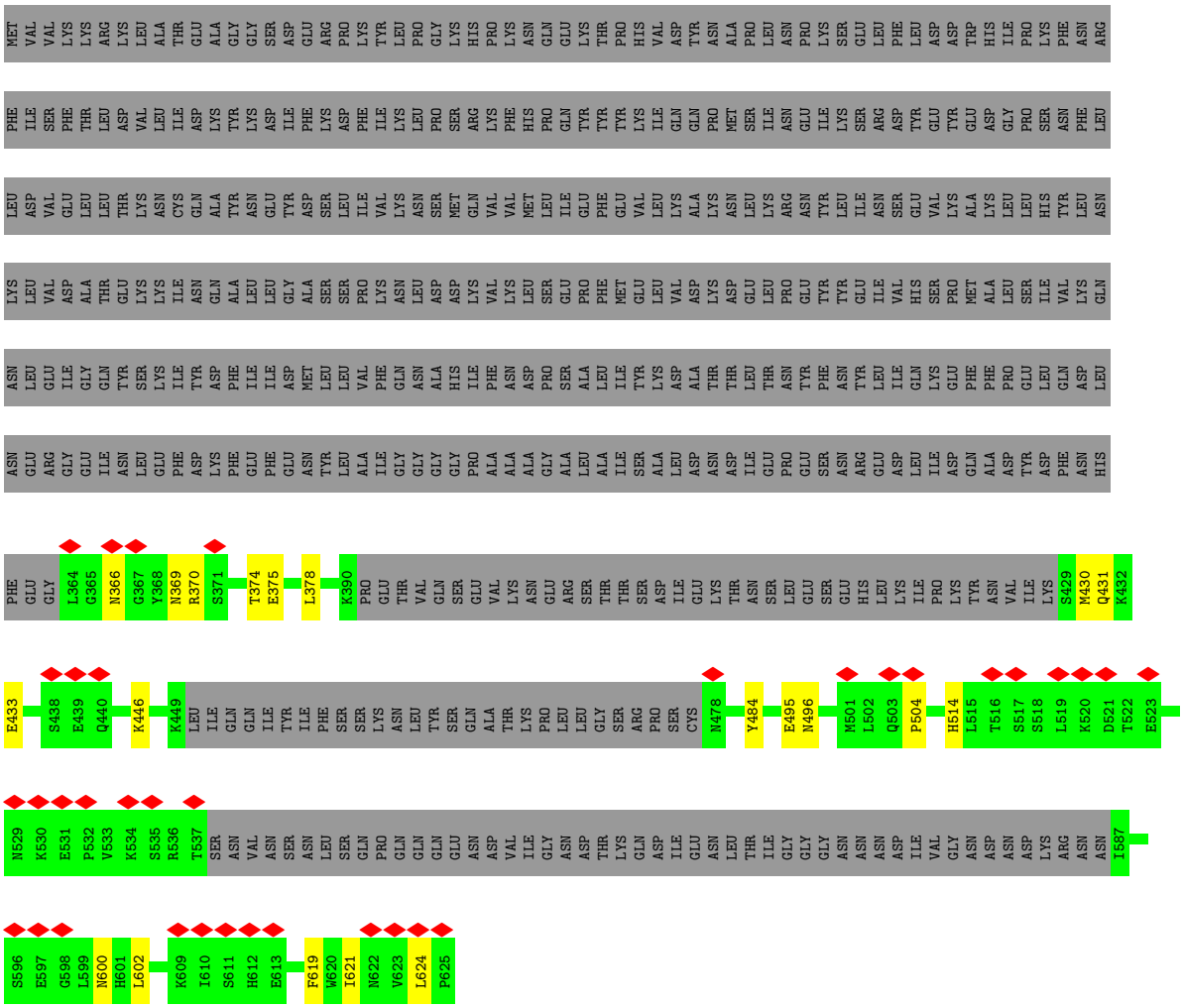
Chain K:





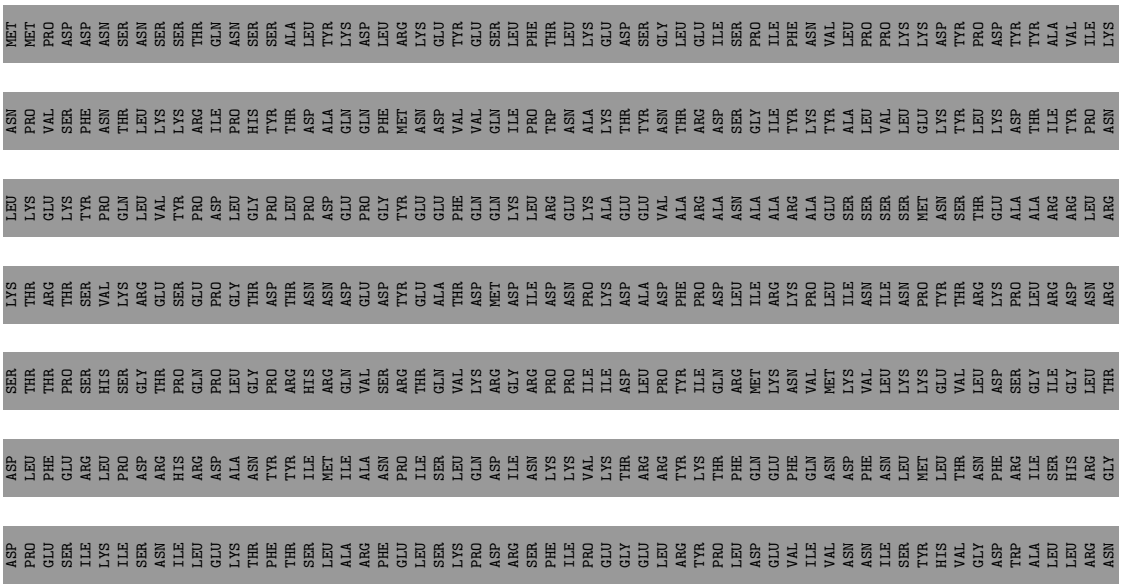
• Molecule 18: Chromatin structure-remodeling complex subunit RSC4

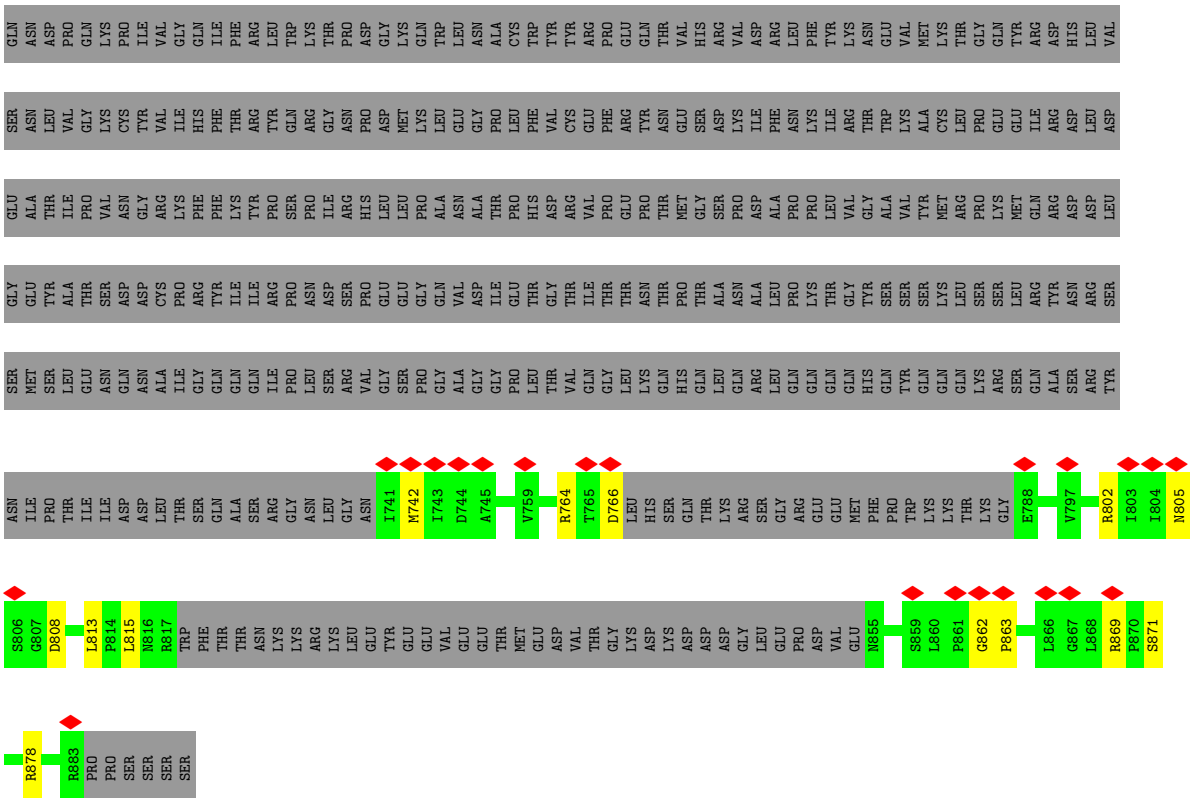
Chain X:



• Molecule 19: Chromatin structure-remodeling complex subunit RSC2

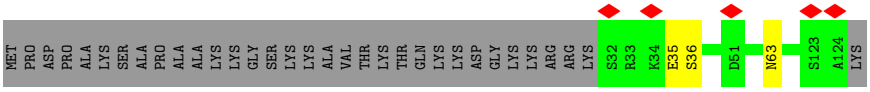
Chain L:





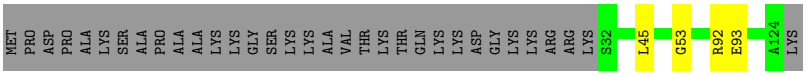
• Molecule 20: Histone H4

Chain T:



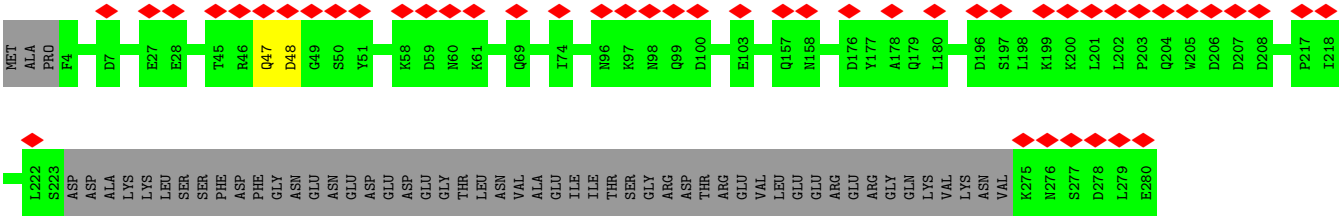
• Molecule 20: Histone H4

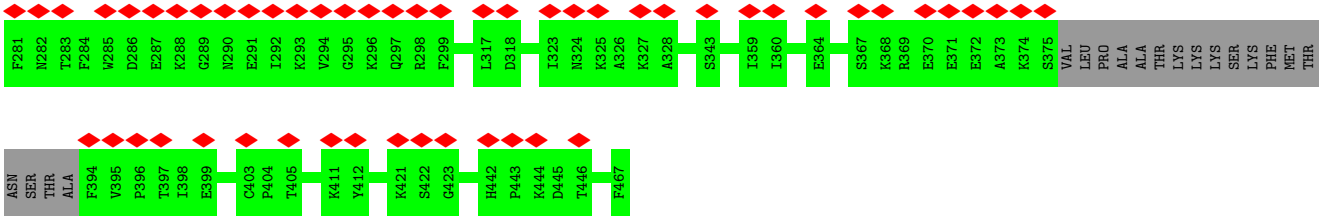
Chain P:



• Molecule 21: Actin-like protein ARP9

Chain g:




F281 N282 T283 F284 W285 D286 E287 K288 G289 N290 E291 I292 K293 V294 G295 K296 Q297 R298 F299 L317 D318 I323 N324 K325 A326 K327 A328 S343 I359 I360 E364 S367 K368 R369 E370 E371 E372 A373 K374 S375 VAL LEU PRO ALA ALA THR LYS LYS LYS SER LYS PHE MET THR
ASN SER THR ALA F394 V395 P396 T397 I398 E399 C403 P404 T405 K411 Y412 K421 S422 G423 H442 P443 K444 D445 T446 F467

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45077	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	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.14, 2.14, 2.14	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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	B	0.24	0/664	0.45	0/889
1	R	0.24	0/711	0.48	0/950
2	N	0.25	0/822	0.40	0/1102
2	Q	0.25	0/794	0.40	0/1064
3	O	0.24	0/833	0.42	0/1124
3	S	0.24	0/833	0.43	0/1124
4	U	0.56	0/3336	0.95	0/5142
5	V	0.54	0/3378	0.93	1/5216 (0.0%)
6	J	0.25	0/1836	0.49	0/2480
6	W	0.26	0/598	0.39	0/789
6	Y	0.25	0/4580	0.50	1/6167 (0.0%)
7	f	0.26	0/3295	0.47	0/4454
8	h	0.24	0/501	0.45	0/669
9	F	0.25	0/983	0.51	0/1337
10	D	0.25	0/2557	0.46	0/3442
10	H	0.25	0/3275	0.45	0/4409
11	M	0.27	0/3113	0.51	1/4215 (0.0%)
12	I	0.24	0/1976	0.48	0/2685
13	G	0.27	0/2039	0.51	0/2769
14	A	0.26	0/3077	0.45	0/4169
15	E	0.25	0/480	0.51	0/643
16	C	0.25	0/272	0.43	0/366
17	K	0.24	0/356	0.47	0/483
18	X	0.25	0/1243	0.50	0/1672
19	L	0.26	0/681	0.49	0/921
20	P	0.23	0/728	0.40	0/983
20	T	0.24	0/736	0.41	0/991
21	g	0.26	0/3261	0.48	2/4421 (0.0%)
All	All	0.31	0/46958	0.57	5/64676 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	g	48	ASP	CB-CG-OD1	7.21	124.79	118.30
21	g	47	GLN	C-N-CA	6.00	136.69	121.70
11	M	124	LEU	CA-CB-CG	5.98	129.05	115.30
6	Y	888	ASP	CB-CG-OD1	5.66	123.39	118.30
5	V	15	DT	P-O3'-C3'	5.06	125.77	119.70

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	B	657	0	706	6	0
1	R	703	0	757	11	0
2	N	810	0	851	8	0
2	Q	784	0	824	7	0
3	O	823	0	882	7	0
3	S	823	0	882	8	0
4	U	2977	0	1639	13	0
5	V	3009	0	1640	10	0
6	J	1814	0	1777	20	0
6	W	592	0	610	1	0
6	Y	4503	0	4573	43	0
7	f	3219	0	3240	0	0
8	h	490	0	467	0	0
9	F	964	0	919	12	0
10	D	2510	0	2542	23	0
10	H	3215	0	3196	36	0
11	M	3058	0	3127	19	0
12	I	1944	0	1964	14	0
13	G	1996	0	1948	19	0
14	A	3007	0	3045	23	0
15	E	477	0	491	8	0
16	C	269	0	279	3	0
17	K	347	0	342	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	X	1220	0	1192	13	0
19	L	669	0	693	10	0
20	P	717	0	723	4	0
20	T	725	0	745	2	0
21	g	3191	0	3179	0	0
22	H	1	0	0	0	0
All	All	45514	0	43233	241	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 4.

All (241) 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)
18:X:375:GLU:HB2	18:X:514:HIS:HB2	1.79	0.64
6:Y:760:ARG:HH21	6:Y:925:ILE:HD13	1.62	0.63
10:D:193:THR:HG22	10:D:195:GLN:H	1.64	0.62
13:G:285:CYS:HB2	13:G:292:PHE:HB3	1.80	0.62
14:A:484:ASN:HD22	18:X:624:LEU:HD13	1.64	0.61
9:F:349:LEU:HB2	9:F:358:HIS:HB2	1.83	0.61
1:R:29:ILE:O	1:R:55:ARG:NH2	2.36	0.59
6:Y:490:ASN:H	6:Y:645:LEU:HD21	1.69	0.58
1:B:42:GLY:O	2:N:108:ASN:ND2	2.36	0.57
6:Y:702:VAL:HG23	6:Y:703:GLU:HG3	1.86	0.57
3:S:88:ARG:NH2	3:S:100:VAL:O	2.38	0.56
11:M:227:GLU:OE2	11:M:268:ARG:NH1	2.37	0.56
18:X:378:LEU:HB2	18:X:484:TYR:HB2	1.88	0.56
1:R:38:ALA:HB1	1:R:43:VAL:HB	1.88	0.56
3:O:88:ARG:NH2	3:O:100:VAL:O	2.39	0.56
6:Y:728:GLN:HE21	6:Y:730:LEU:HD12	1.70	0.55
9:F:365:SER:H	10:H:194:PRO:HB3	1.71	0.55
10:D:357:LEU:O	6:J:123:GLN:NE2	2.39	0.55
2:Q:108:ASN:ND2	1:R:42:GLY:O	2.40	0.55
1:R:18:HIS:HD2	1:R:20:LYS:HB3	1.72	0.55
2:Q:116:ARG:NH1	2:Q:118:THR:O	2.41	0.54
6:Y:811:LEU:HB2	6:Y:882:VAL:HG13	1.89	0.54
10:D:119:LYS:HD2	10:D:122:ARG:HD3	1.90	0.54
13:G:20:LEU:HD23	13:G:27:ILE:HD13	1.90	0.54
14:A:14:LEU:HD11	14:A:87:PRO:HG3	1.90	0.54
4:U:100:DG:N2	5:V:49:DC:O2	2.40	0.53
11:M:115:ILE:HG13	11:M:168:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:97:DG:OP1	6:Y:631:GLN:NE2	2.41	0.53
13:G:15:ASN:HD22	13:G:174:THR:HA	1.73	0.53
14:A:399:SER:O	14:A:454:ARG:NH2	2.42	0.53
6:Y:635:PRO:HG2	6:Y:636:GLU:HG3	1.89	0.53
11:M:170:GLN:HB2	6:J:292:ARG:HH12	1.73	0.53
10:H:272:TYR:HB2	10:H:282:LEU:HB2	1.91	0.53
6:Y:644:VAL:HG12	6:Y:645:LEU:HG	1.91	0.53
10:H:180:GLY:O	12:I:468:ARG:NH1	2.41	0.53
18:X:504:PRO:HD3	18:X:624:LEU:HB2	1.91	0.53
1:R:39:ARG:NH1	1:R:43:VAL:O	2.41	0.53
4:U:52:DA:H5'	6:Y:754:ASN:HD22	1.74	0.52
11:M:110:LYS:HG3	17:K:164:ILE:HG23	1.91	0.52
10:H:311:VAL:O	10:H:314:ASN:ND2	2.41	0.52
6:J:260:LYS:O	6:J:264:ASN:ND2	2.42	0.52
14:A:88:ILE:HG13	14:A:91:GLY:H	1.74	0.52
10:H:285:ARG:NH2	14:A:208:ILE:O	2.42	0.52
10:H:131:LEU:HD11	10:D:182:SER:H	1.75	0.52
10:H:83:PRO:HA	10:D:192:ASP:HB3	1.91	0.52
14:A:37:ALA:O	14:A:79:ARG:NH2	2.44	0.51
2:N:62:ILE:O	2:N:93:GLN:NE2	2.44	0.51
1:B:22:LEU:HD12	1:B:25:ASN:HD21	1.74	0.51
10:H:454:LEU:HB3	10:D:454:LEU:HD11	1.92	0.51
14:A:176:ILE:HD13	18:X:446:LYS:HD2	1.93	0.51
6:Y:1000:LYS:HA	6:Y:1004:ASN:HD22	1.76	0.51
1:R:75:HIS:HE1	20:P:93:GLU:HG3	1.76	0.51
6:J:46:ILE:HD11	6:J:82:THR:HG21	1.93	0.51
10:H:154:VAL:HG11	13:G:230:ILE:HD12	1.93	0.51
10:H:272:TYR:OH	10:H:303:ARG:NH1	2.44	0.50
14:A:112:GLN:NE2	14:A:215:ASP:OD2	2.44	0.50
9:F:362:SER:OG	10:H:195:GLN:O	2.29	0.50
6:Y:395:GLN:O	6:Y:399:THR:OG1	2.29	0.50
1:B:36:ARG:NH1	5:V:61:DA:OP2	2.38	0.50
10:D:480:LEU:HD11	12:I:318:LEU:HD11	1.93	0.50
6:Y:880:ASP:HB3	6:Y:908:ASN:HB3	1.94	0.50
2:N:94:GLU:HG2	3:S:103:ALA:HA	1.93	0.50
3:S:85:LEU:O	3:S:89:ASN:ND2	2.45	0.50
10:H:325:GLU:OE2	6:J:246:LYS:NZ	2.39	0.50
16:C:214:ASP:O	16:C:218:ASN:ND2	2.44	0.50
18:X:370:ARG:NH2	18:X:496:ASN:OD1	2.41	0.50
10:H:424:GLU:HA	15:E:53:ILE:HD11	1.92	0.50
18:X:600:ASN:HB2	18:X:621:ILE:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:85:LEU:O	3:O:89:ASN:ND2	2.45	0.50
2:N:83:ARG:HB3	5:V:50:DT:H4'	1.94	0.49
6:Y:941:GLN:HA	6:Y:944:LYS:HE3	1.93	0.49
19:L:764:ARG:NH2	19:L:766:ASP:OD1	2.46	0.49
10:H:439:LYS:NZ	12:I:40:ASP:OD2	2.44	0.49
6:J:219:ASP:OD1	19:L:878:ARG:NH1	2.42	0.49
16:C:216:LEU:HB3	17:K:189:LEU:HD11	1.94	0.49
6:Y:528:LEU:O	6:Y:846:ARG:NH1	2.44	0.49
14:A:107:ILE:HG23	14:A:117:TYR:HE1	1.77	0.49
10:H:275:LEU:HB2	10:H:300:ASP:HB2	1.93	0.49
13:G:315:VAL:HG13	13:G:320:LEU:HB2	1.95	0.49
14:A:193:GLN:NE2	18:X:495:GLU:OE2	2.45	0.49
6:Y:630:LEU:HD11	6:Y:640:LEU:HD12	1.94	0.49
10:D:469:LEU:HD22	12:I:258:LYS:HD3	1.94	0.49
2:Q:61:LEU:HD13	1:R:36:ARG:HB3	1.95	0.49
10:D:143:ARG:HH12	13:G:314:ILE:HD11	1.78	0.49
10:H:407:LEU:HD22	12:I:426:PRO:HB2	1.94	0.49
13:G:268:ILE:HD11	13:G:341:LYS:HB2	1.94	0.49
2:Q:62:ILE:O	2:Q:93:GLN:NE2	2.46	0.48
10:D:227:ASN:ND2	6:J:244:GLU:OE2	2.43	0.48
11:M:128:LYS:HG2	11:M:184:ILE:HD11	1.95	0.48
1:B:39:ARG:NH1	1:B:43:VAL:O	2.46	0.48
9:F:374:SER:HB2	10:H:186:HIS:HB2	1.94	0.48
10:H:180:GLY:HA3	10:D:198:LYS:HE2	1.94	0.48
10:D:455:GLU:OE2	11:M:552:ARG:NH1	2.46	0.48
18:X:430:MET:HB2	19:L:813:LEU:HD11	1.96	0.48
3:O:79:ILE:HG13	3:O:82:HIS:H	1.79	0.48
10:H:321:LEU:HD22	6:J:239:ILE:HG23	1.95	0.48
6:Y:911:ARG:NH1	6:Y:984:THR:O	2.46	0.48
10:H:98:GLU:OE1	10:H:122:ARG:NH1	2.47	0.48
11:M:65:PHE:HB2	11:M:68:PHE:HD2	1.78	0.48
14:A:490:VAL:HG23	19:L:742:MET:HB2	1.96	0.48
10:H:288:GLN:HA	19:L:802:ARG:HH22	1.78	0.48
13:G:321:THR:HG23	13:G:323:GLU:H	1.77	0.48
9:F:383:SER:HA	10:H:235:TYR:O	2.14	0.47
4:U:128:DG:H1'	4:U:129:DT:H5'	1.96	0.47
13:G:276:ASP:OD1	13:G:301:ASN:ND2	2.46	0.47
1:R:74:GLU:O	20:P:92:ARG:NH2	2.47	0.47
11:M:176:GLN:NE2	11:M:232:TYR:OH	2.46	0.47
2:Q:68:GLN:HE21	2:Q:72:ARG:HH21	1.63	0.47
6:Y:647:LYS:HG2	6:Y:648:ILE:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ASN:OD1	1:B:67:ARG:NH1	2.47	0.47
11:M:540:ASP:O	11:M:547:SER:OG	2.32	0.47
6:Y:916:ILE:HG13	6:Y:926:LEU:HD22	1.96	0.47
6:J:128:ASP:OD2	6:J:198:ARG:NH2	2.48	0.47
9:F:387:GLU:O	10:H:188:GLN:HA	2.15	0.47
6:Y:576:TYR:OH	6:Y:597:ASP:O	2.33	0.47
4:U:50:DG:H1'	4:U:51:DC:H5'	1.97	0.47
10:D:113:LYS:NZ	10:D:152:SER:OG	2.48	0.47
9:F:394:ASP:O	10:H:224:PHE:N	2.48	0.46
12:I:444:LEU:HD12	15:E:29:LEU:HD13	1.97	0.46
11:M:300:CYS:SG	11:M:301:ASP:N	2.88	0.46
6:J:21:ALA:HB1	6:J:66:GLN:HE21	1.80	0.46
6:Y:731:LYS:HA	6:Y:735:LEU:HD12	1.98	0.46
14:A:44:PRO:HA	14:A:47:ILE:HB	1.98	0.46
3:S:79:ILE:HG13	3:S:82:HIS:H	1.80	0.46
2:N:102:GLY:O	2:N:131:ARG:NH2	2.49	0.46
13:G:205:PRO:HB2	13:G:220:GLN:HE21	1.80	0.46
2:Q:128:ARG:HB3	2:Q:133:GLU:HB2	1.97	0.46
14:A:129:GLU:OE2	19:L:869:ARG:NE	2.44	0.46
10:D:428:ILE:HG23	15:E:69:LEU:HD11	1.98	0.46
10:D:222:LYS:HG3	12:I:463:ASN:HD21	1.81	0.46
1:R:30:THR:HG21	4:U:61:DA:H5"	1.98	0.46
11:M:167:ASN:O	6:J:292:ARG:NH1	2.43	0.46
11:M:543:ASP:HA	11:M:547:SER:HB2	1.99	0.46
13:G:273:ILE:HD11	13:G:340:LYS:HG2	1.97	0.46
13:G:279:VAL:HG21	13:G:339:ILE:HD13	1.98	0.45
6:J:61:ARG:HD2	19:L:815:LEU:HD13	1.98	0.45
17:K:189:LEU:HA	17:K:192:LEU:HG	1.97	0.45
4:U:137:DA:OP2	6:Y:565:ARG:NH1	2.49	0.45
10:D:221:LYS:O	10:D:365:ARG:NH2	2.49	0.45
11:M:569:LEU:HD13	12:I:310:LEU:HB2	1.99	0.45
13:G:295:ASN:HB2	13:G:376:TRP:HB2	1.98	0.45
14:A:244:LEU:HD22	6:J:242:LEU:HD21	1.98	0.45
18:X:366:ASN:O	18:X:369:ASN:ND2	2.48	0.45
9:F:382:THR:HA	10:H:183:PHE:HB3	1.97	0.45
10:H:260:CYS:SG	10:H:267:SER:OG	2.74	0.45
10:D:432:LEU:HD13	15:E:69:LEU:HD23	1.97	0.45
15:E:36:ILE:HD12	15:E:39:LEU:HD12	1.99	0.45
6:Y:474:GLN:NE2	6:Y:499:LEU:O	2.50	0.45
11:M:568:THR:HG21	12:I:332:LEU:HD13	1.98	0.45
13:G:15:ASN:HB2	13:G:178:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:206:LEU:HB3	6:J:245:LEU:HD12	1.98	0.45
6:J:226:THR:H	6:J:229:ASP:HB2	1.83	0.45
18:X:431:GLN:HE22	18:X:433:GLU:HB2	1.81	0.45
5:V:59:DA:H2"	5:V:60:DA:C8	2.52	0.44
10:H:150:VAL:HA	10:H:153:ILE:HG22	1.99	0.44
10:H:181:PRO:HG3	10:D:201:LEU:HB2	1.99	0.44
18:X:374:THR:OG1	18:X:514:HIS:O	2.31	0.44
6:Y:809:ARG:HH22	6:Y:853:PHE:HA	1.83	0.44
4:U:94:DG:H1	5:V:54:DC:H42	1.65	0.44
9:F:371:TRP:O	9:F:434:TYR:OH	2.35	0.44
6:J:223:GLU:OE1	6:J:231:SER:OG	2.32	0.44
3:S:63:LEU:HD13	20:P:45:LEU:HB2	2.00	0.44
6:Y:537:GLU:HG2	6:Y:540:LYS:HE2	1.99	0.44
10:H:145:ASN:HB3	13:G:322:ARG:HE	1.83	0.44
10:H:149:ASP:OD1	10:H:149:ASP:N	2.50	0.44
6:Y:841:THR:OG1	6:Y:842:LYS:N	2.51	0.44
4:U:98:DA:H2"	4:U:99:DG:C8	2.53	0.44
19:L:805:ASN:ND2	19:L:808:ASP:OD2	2.51	0.43
10:D:325:GLU:OE2	19:L:871:SER:OG	2.31	0.43
13:G:165:ILE:HG12	13:G:171:ILE:HG21	1.99	0.43
11:M:341:PRO:HG2	11:M:556:LEU:HD23	1.99	0.43
2:N:40:ARG:HH12	4:U:83:DG:H21	1.66	0.43
13:G:169:PRO:HA	13:G:172:ARG:HG2	2.00	0.43
3:O:75:LYS:HB2	3:O:82:HIS:HE1	1.83	0.43
14:A:20:ILE:HG23	6:J:224:PHE:HE1	1.82	0.43
5:V:94:DG:H3'	6:Y:608:LYS:HD2	2.00	0.43
6:Y:459:ASP:HB3	6:Y:475:LEU:HD13	2.00	0.43
6:Y:994:LEU:O	6:Y:997:LYS:NZ	2.51	0.43
9:F:340:LYS:HA	9:F:344:VAL:HB	2.00	0.43
6:Y:537:GLU:HA	6:Y:540:LYS:HG2	2.00	0.43
12:I:312:GLU:HB3	12:I:329:HIS:HB3	2.01	0.43
1:R:36:ARG:NH1	4:U:61:DA:OP2	2.39	0.42
10:H:283:CYS:SG	10:H:284:SER:N	2.92	0.42
10:H:310:SER:OG	10:H:314:ASN:ND2	2.52	0.42
14:A:177:SER:OG	14:A:182:LYS:NZ	2.50	0.42
6:Y:465:LEU:HD22	6:Y:541:TRP:HE3	1.84	0.42
4:U:17:DC:H2"	4:U:18:DC:C5	2.54	0.42
3:O:68:ASN:OD1	3:O:71:ARG:NH2	2.53	0.42
1:R:51:TYR:O	1:R:55:ARG:NH1	2.52	0.42
6:Y:479:GLU:HA	6:Y:482:VAL:HB	2.01	0.42
6:Y:524:VAL:HB	6:Y:573:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:76:THR:O	20:P:53:GLY:N	2.47	0.42
4:U:135:DA:H4'	6:Y:584:SER:HB3	2.02	0.42
14:A:209:ILE:HG22	14:A:211:LYS:H	1.85	0.42
14:A:313:ARG:HD3	15:E:16:TYR:HB3	2.00	0.42
5:V:54:DC:N4	5:V:55:DG:O6	2.52	0.42
10:H:435:LEU:O	12:I:398:LYS:NZ	2.44	0.42
11:M:107:TYR:OH	16:C:197:ASP:OD2	2.38	0.42
3:O:13:LYS:HG3	3:O:15:LYS:HG3	2.02	0.42
5:V:129:DC:H2"	5:V:130:DG:C8	2.54	0.42
10:H:330:TYR:HB2	10:H:337:ILE:HD11	2.01	0.42
13:G:158:GLN:HE22	13:G:165:ILE:HG13	1.83	0.42
5:V:26:DC:H4'	5:V:27:DC:H5'	2.02	0.41
10:D:352:GLU:OE2	14:A:457:LYS:NZ	2.44	0.41
6:Y:630:LEU:O	6:Y:892:HIS:NE2	2.53	0.41
14:A:306:ARG:NH1	15:E:17:ASN:O	2.53	0.41
19:L:862:GLY:HA2	19:L:863:PRO:HD3	1.94	0.41
11:M:141:LEU:HD21	11:M:215:PHE:HB2	2.01	0.41
15:E:56:GLU:HA	15:E:59:ARG:HG2	2.01	0.41
6:Y:583:LYS:HG2	6:Y:616:TYR:HE1	1.86	0.41
6:Y:885:PHE:HE1	6:Y:915:LEU:HB2	1.86	0.41
3:S:13:LYS:HG3	3:S:15:LYS:HG3	2.01	0.41
6:Y:684:ARG:HA	6:Y:687:HIS:HD2	1.85	0.41
4:U:131:DA:H2"	4:U:132:DG:H5"	2.02	0.41
6:W:333:PHE:HB3	6:W:337:ARG:HH12	1.85	0.41
20:T:36:SER:OG	20:T:63:ASN:ND2	2.54	0.41
6:Y:448:TYR:OH	6:Y:948:LYS:O	2.38	0.41
10:H:276:ARG:HB2	10:H:296:PHE:HE1	1.85	0.41
6:Y:938:LYS:HG2	6:Y:961:LEU:HD21	2.03	0.41
6:Y:975:GLU:HG2	6:Y:980:GLU:HB3	2.02	0.41
6:Y:979:ASP:OD1	6:Y:979:ASP:N	2.54	0.41
2:N:110:CYS:SG	2:Q:113:HIS:NE2	2.94	0.41
14:A:269:LEU:HG	14:A:274:TYR:HE1	1.86	0.41
6:Y:472:GLU:OE2	6:Y:476:ARG:NE	2.54	0.41
9:F:320:LEU:HB2	10:D:68:LYS:HE3	2.01	0.41
10:H:178:LEU:HD21	12:I:476:LEU:HB2	2.01	0.41
11:M:192:LEU:HB3	11:M:245:THR:HG21	2.02	0.41
11:M:561:LEU:HD11	11:M:571:LEU:HD12	2.03	0.41
6:J:48:LYS:HE2	6:J:82:THR:HG23	2.03	0.41
1:B:36:ARG:HB3	2:N:61:LEU:HD13	2.03	0.41
12:I:7:PRO:HB2	14:A:282:LEU:HB3	2.01	0.41
3:O:32:ARG:NH2	20:T:35:GLU:OE2	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:395:ASN:O	6:J:90:GLN:NE2	2.54	0.40
9:F:330:PHE:HB2	10:D:144:ARG:HH11	1.87	0.40
13:G:19:ARG:HA	13:G:22:ASN:HB2	2.02	0.40
6:Y:470:LEU:HD13	6:Y:475:LEU:HD21	2.02	0.40
10:D:72:PHE:HE2	10:D:127:ASN:HB3	1.84	0.40
18:X:602:LEU:HD23	18:X:619:PHE:HB2	2.02	0.40
12:I:322:VAL:HG23	12:I:323:LEU:HG	2.03	0.40
6:J:24:ALA:HB3	6:J:73:LYS:HD2	2.03	0.40
3:S:68:ASN:OD1	3:S:71:ARG:NH2	2.55	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	B	80/103 (78%)	78 (98%)	2 (2%)	0	100	100
1	R	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	N	96/136 (71%)	94 (98%)	2 (2%)	0	100	100
2	Q	93/136 (68%)	93 (100%)	0	0	100	100
3	O	105/130 (81%)	105 (100%)	0	0	100	100
3	S	105/130 (81%)	105 (100%)	0	0	100	100
6	J	229/1359 (17%)	210 (92%)	19 (8%)	0	100	100
6	W	67/1359 (5%)	67 (100%)	0	0	100	100
6	Y	536/1359 (39%)	497 (93%)	39 (7%)	0	100	100
7	f	391/477 (82%)	383 (98%)	8 (2%)	0	100	100
8	h	46/157 (29%)	44 (96%)	2 (4%)	0	100	100
9	F	116/435 (27%)	108 (93%)	8 (7%)	0	100	100
10	D	295/557 (53%)	283 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	H	387/557 (70%)	369 (95%)	18 (5%)	0	100	100
11	M	378/581 (65%)	362 (96%)	16 (4%)	0	100	100
12	I	236/483 (49%)	223 (94%)	13 (6%)	0	100	100
13	G	238/426 (56%)	221 (93%)	17 (7%)	0	100	100
14	A	357/502 (71%)	331 (93%)	26 (7%)	0	100	100
15	E	56/78 (72%)	55 (98%)	1 (2%)	0	100	100
16	C	31/883 (4%)	31 (100%)	0	0	100	100
17	K	40/885 (4%)	40 (100%)	0	0	100	100
18	X	139/625 (22%)	127 (91%)	12 (9%)	0	100	100
19	L	79/889 (9%)	70 (89%)	9 (11%)	0	100	100
20	P	91/126 (72%)	91 (100%)	0	0	100	100
20	T	91/126 (72%)	91 (100%)	0	0	100	100
21	g	390/467 (84%)	381 (98%)	9 (2%)	0	100	100
All	All	4757/13069 (36%)	4542 (96%)	215 (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	B	68/79 (86%)	67 (98%)	1 (2%)	65	80
1	R	72/79 (91%)	71 (99%)	1 (1%)	67	80
2	N	86/111 (78%)	85 (99%)	1 (1%)	71	83
2	Q	83/111 (75%)	82 (99%)	1 (1%)	71	83
3	O	84/102 (82%)	84 (100%)	0	100	100
3	S	84/102 (82%)	84 (100%)	0	100	100
6	J	187/1228 (15%)	187 (100%)	0	100	100
6	W	63/1228 (5%)	63 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	Y	502/1228 (41%)	498 (99%)	4 (1%)	81 89
7	f	356/420 (85%)	356 (100%)	0	100 100
8	h	53/140 (38%)	53 (100%)	0	100 100
9	F	111/388 (29%)	110 (99%)	1 (1%)	78 87
10	D	285/500 (57%)	285 (100%)	0	100 100
10	H	363/500 (73%)	363 (100%)	0	100 100
11	M	349/521 (67%)	348 (100%)	1 (0%)	92 95
12	I	223/435 (51%)	223 (100%)	0	100 100
13	G	226/384 (59%)	226 (100%)	0	100 100
14	A	343/462 (74%)	343 (100%)	0	100 100
15	E	56/75 (75%)	56 (100%)	0	100 100
16	C	32/824 (4%)	32 (100%)	0	100 100
17	K	39/832 (5%)	39 (100%)	0	100 100
18	X	141/578 (24%)	141 (100%)	0	100 100
19	L	77/810 (10%)	77 (100%)	0	100 100
20	P	77/105 (73%)	77 (100%)	0	100 100
20	T	79/105 (75%)	79 (100%)	0	100 100
21	g	362/423 (86%)	362 (100%)	0	100 100
All	All	4401/11770 (37%)	4391 (100%)	10 (0%)	93 96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	92	ARG
2	N	129	ARG
2	Q	129	ARG
1	R	92	ARG
9	F	338	ARG
11	M	274	LYS
6	Y	460	LYS
6	Y	671	LYS
6	Y	907	LYS
6	Y	1003	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	25	ASN
3	O	73	ASN
3	O	82	HIS
2	Q	68	GLN
1	R	18	HIS
3	S	31	HIS
3	S	73	ASN
3	S	82	HIS
7	f	79	ASN
7	f	86	GLN
9	F	376	ASN
10	H	107	ASN
10	H	127	ASN
10	H	145	ASN
10	H	186	HIS
10	H	242	ASN
10	H	314	ASN
10	D	145	ASN
10	D	242	ASN
11	M	521	GLN
11	M	559	HIS
12	I	463	ASN
13	G	10	GLN
13	G	220	GLN
14	A	484	ASN
6	J	66	GLN
6	J	90	GLN
6	J	123	GLN
6	J	254	GLN
15	E	23	ASN
17	K	160	GLN
18	X	431	GLN
18	X	487	ASN
18	X	489	ASN
20	T	63	ASN
20	P	49	HIS
20	P	63	ASN
21	g	81	GLN
6	Y	488	HIS
6	Y	533	ASN
6	Y	558	HIS
6	Y	604	ASN
6	Y	615	HIS

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Mol	Chain	Res	Type
6	Y	621	ASN
6	Y	632	ASN
6	Y	687	HIS
6	Y	728	GLN
6	Y	754	ASN
6	Y	808	HIS
6	Y	890	ASN
6	Y	1004	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 monosaccharides 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.

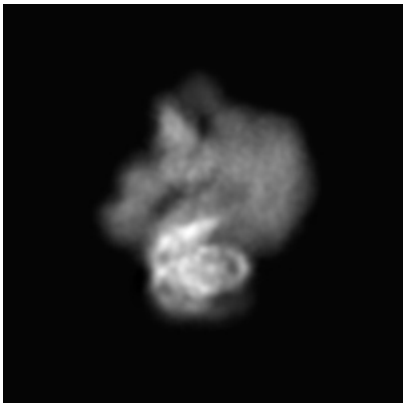
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0777. These allow visual inspection of the internal detail of the map and identification of artifacts.

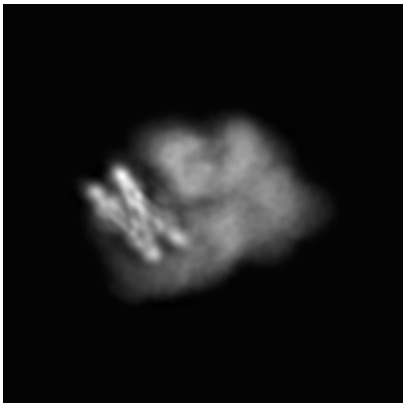
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

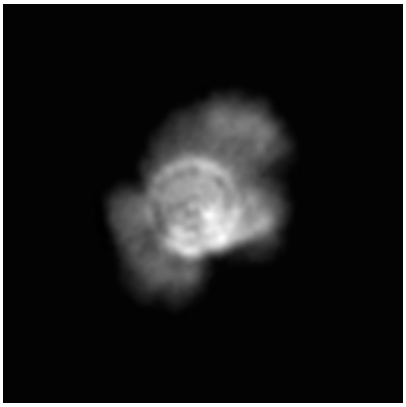
6.1.1 Primary map



X



Y

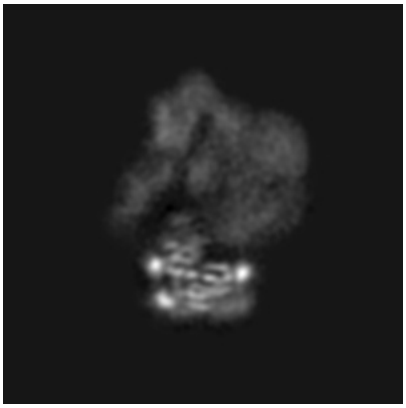


Z

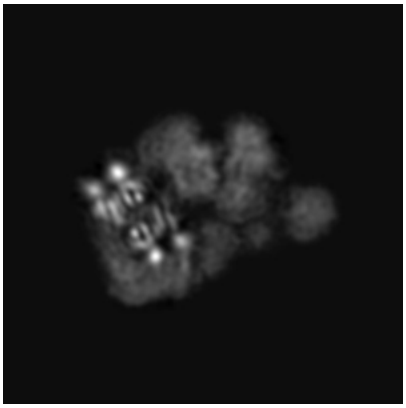
The images above show the map projected in three orthogonal directions.

6.2 Central slices

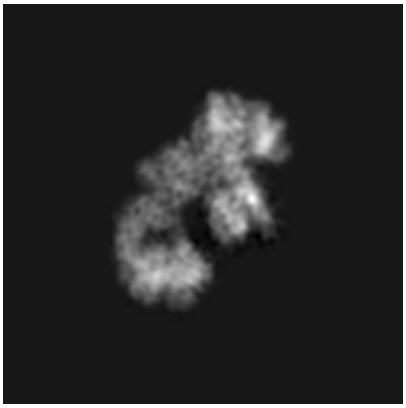
6.2.1 Primary map



X Index: 90



Y Index: 90

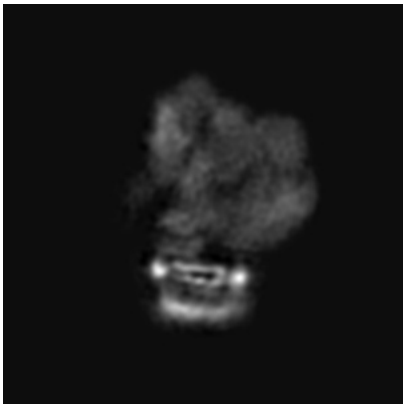


Z Index: 90

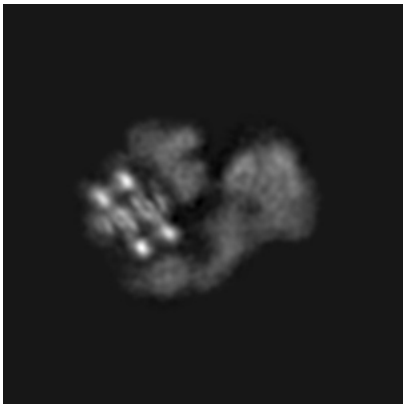
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

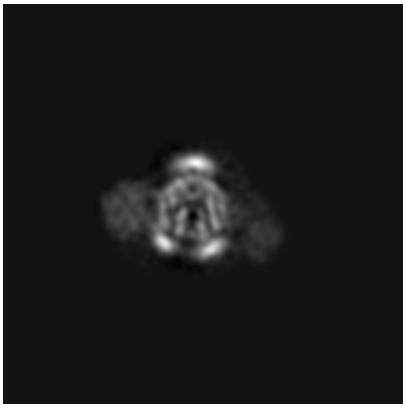
6.3.1 Primary map



X Index: 94



Y Index: 75

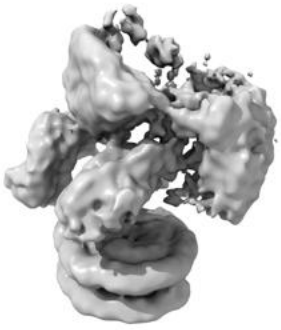


Z Index: 60

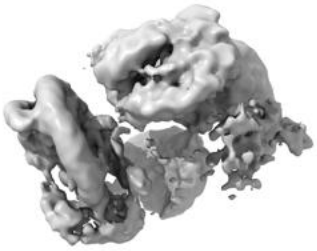
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

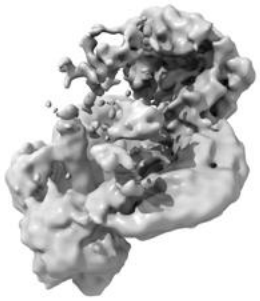
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

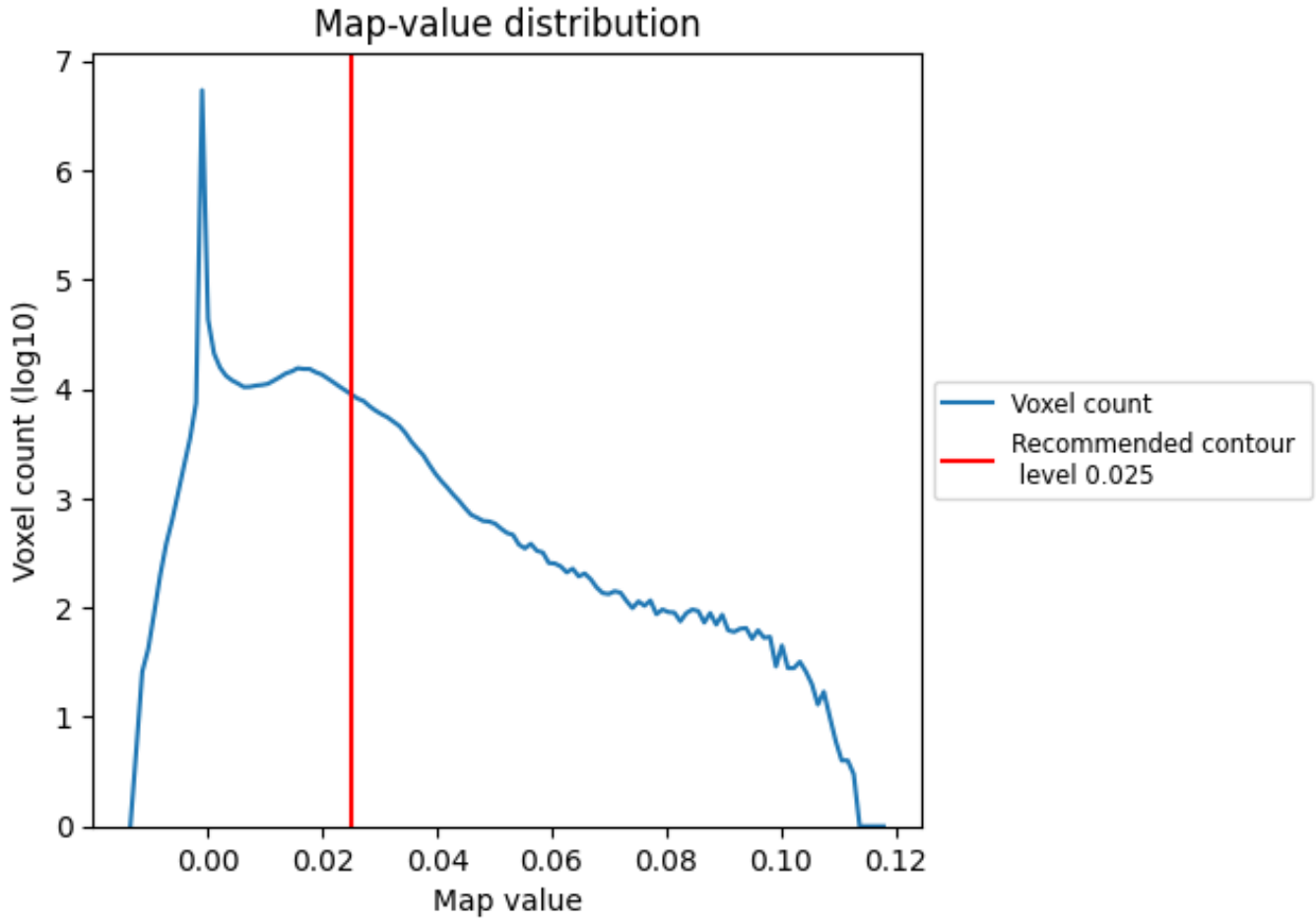
6.5 Mask visualisation (i)

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

7 Map analysis

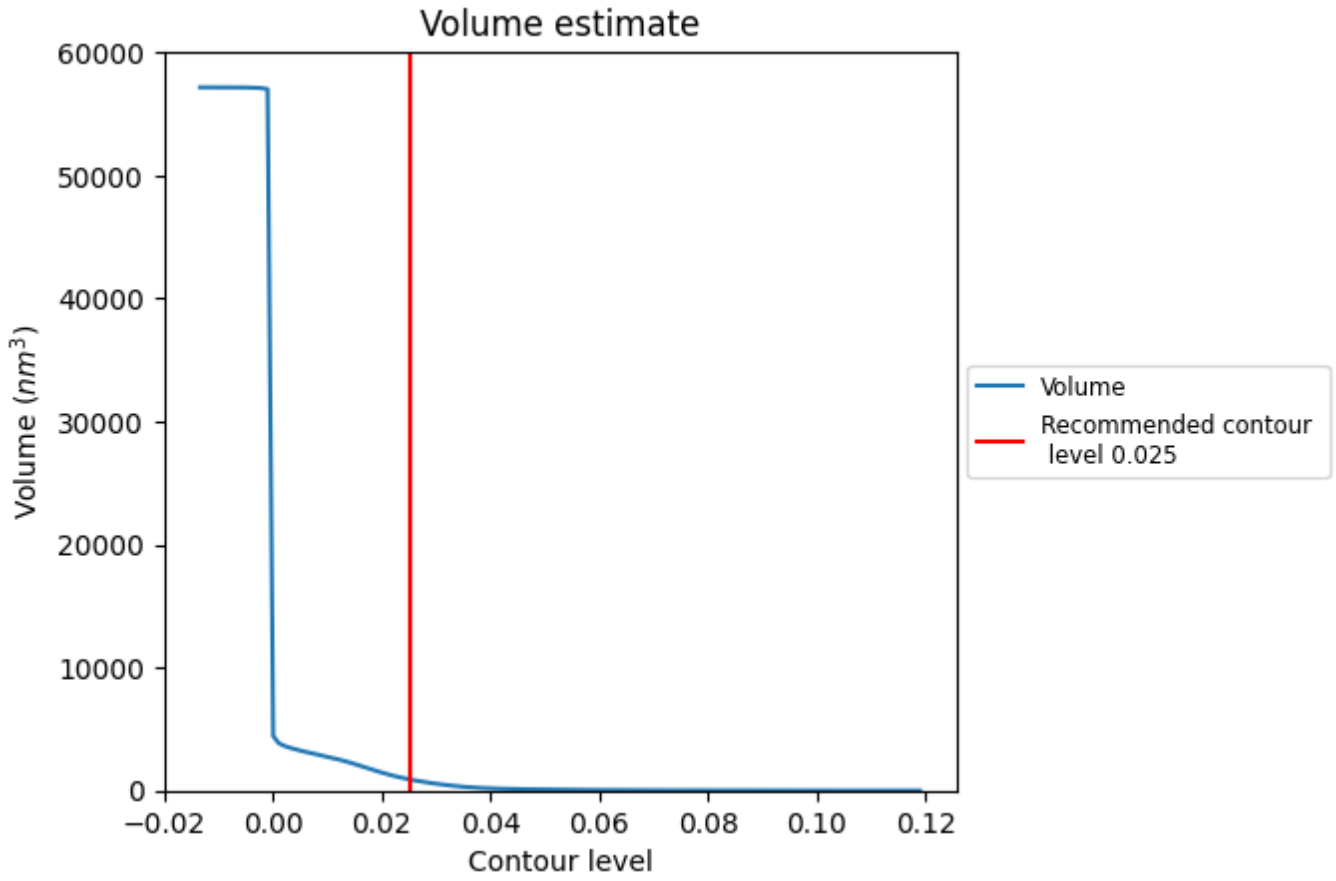
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

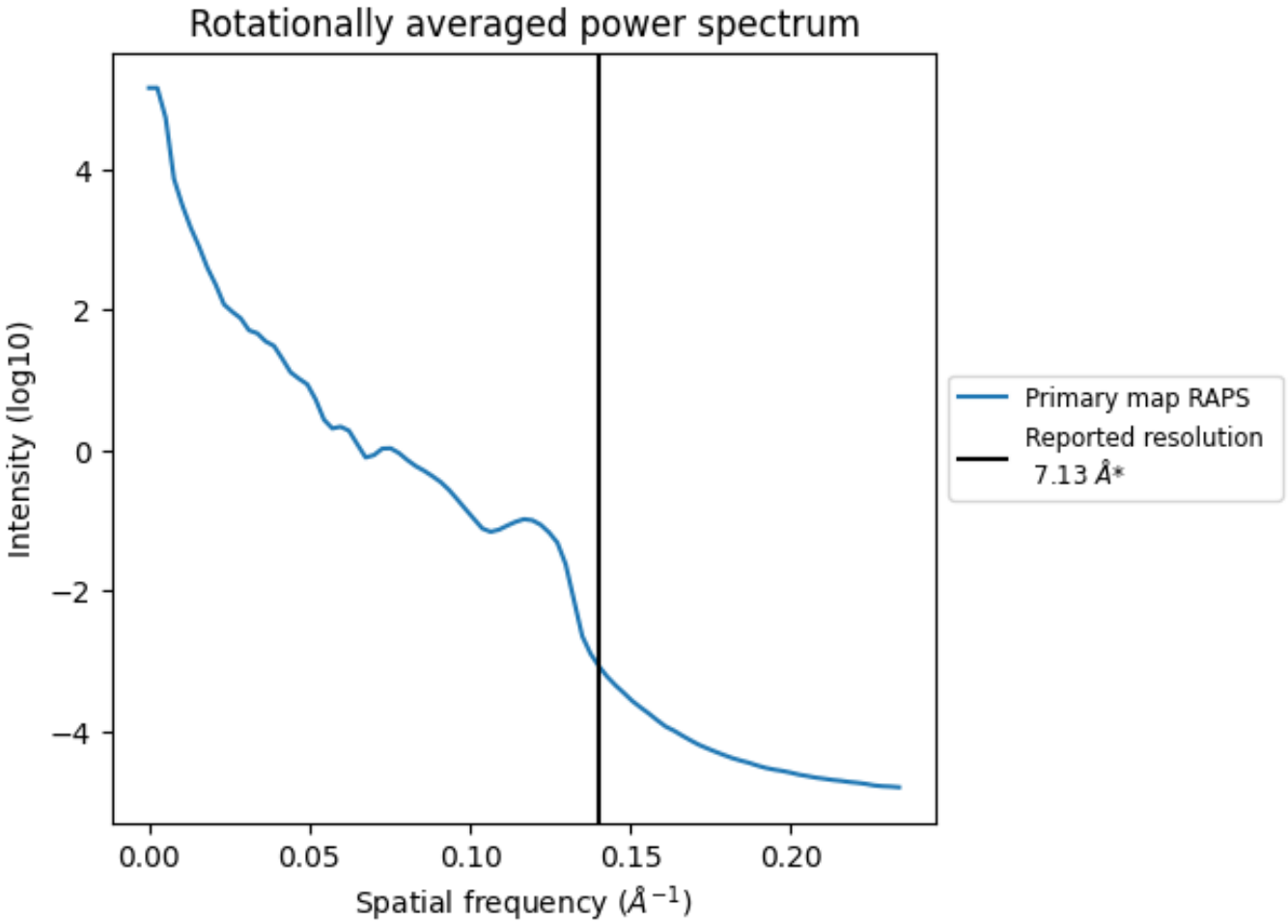
7.2 Volume estimate



The volume at the recommended contour level is 915 nm^3; this corresponds to an approximate mass of 827 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 0.140 Å^{-1}

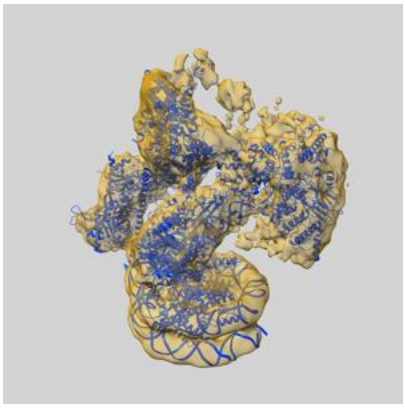
8 Fourier-Shell correlation (i)

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

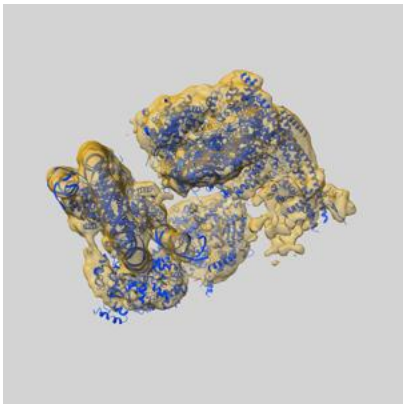
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0777 and PDB model 6KW3. Per-residue inclusion information can be found in section 3 on page 8.

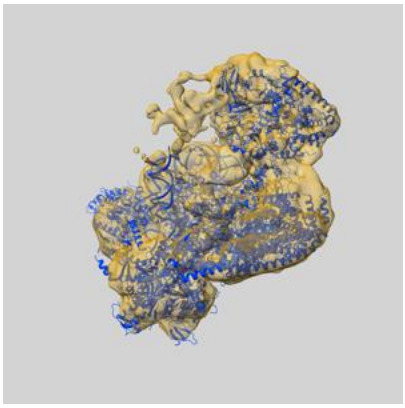
9.1 Map-model overlay



X



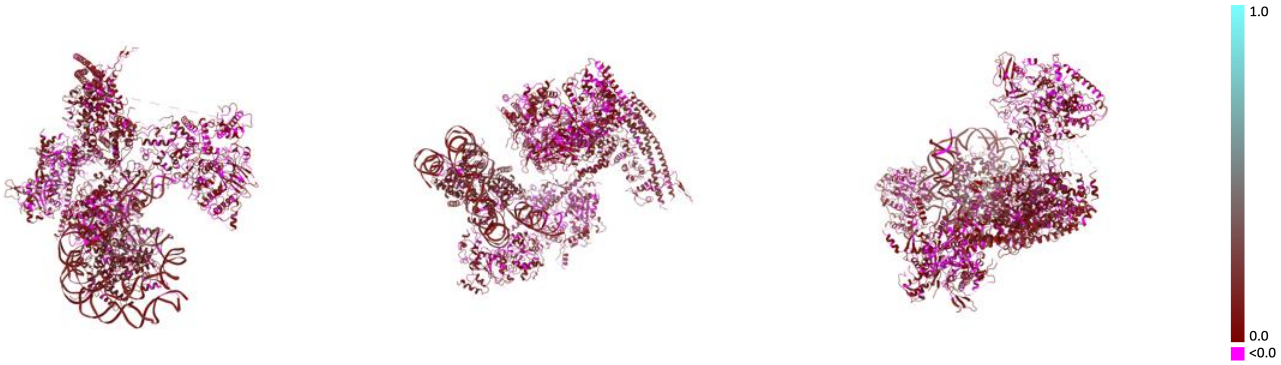
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

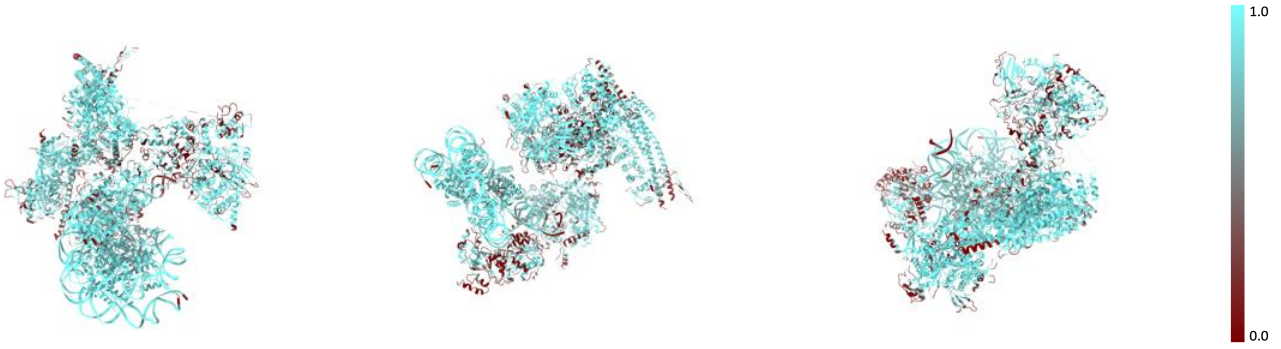
9.2 Q-score mapped to coordinate model (i)



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.

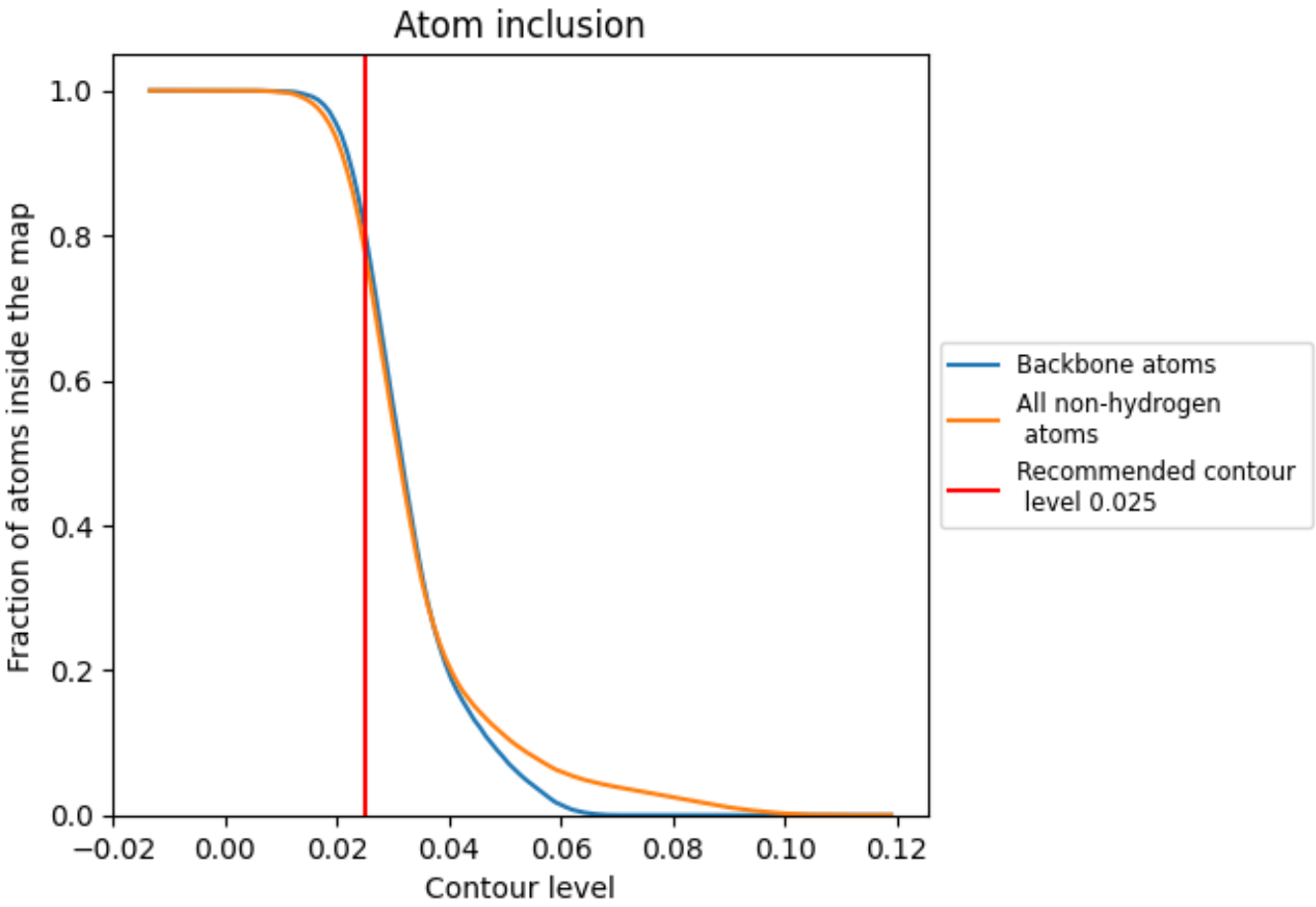
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7743	0.0860
A	0.7841	0.0650
B	0.9097	0.1200
C	0.5167	0.0940
D	0.8261	0.0890
E	0.9274	0.0990
F	0.8739	0.0960
G	0.7561	0.0770
H	0.7561	0.0820
I	0.7625	0.0840
J	0.5729	0.0520
K	0.5015	0.1200
L	0.6911	0.0260
M	0.8138	0.0970
N	0.9332	0.1350
O	0.8208	0.1220
P	0.9529	0.1470
Q	0.9336	0.1330
R	0.8366	0.1170
S	0.9624	0.1380
T	0.8842	0.1460
U	0.9167	0.1190
V	0.9236	0.1220
W	0.5009	0.0830
X	0.7311	0.0530
Y	0.5038	0.0690
f	0.8535	0.0540
g	0.7068	0.0420
h	0.7378	0.0900