Full wwPDB EM Validation Report

Dec 16, 2020 – 08:50 AM JST

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

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

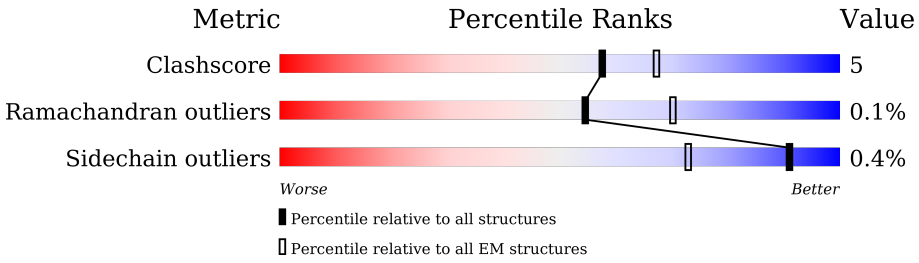
EMDB validation analysis	:	0.0.0.dev61
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.15.1

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 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	F	435	6% 25% · 73%
2	D	557	12% 48% 7% 45%
2	H	557	10% 62% 9% 29%
3	M	581	7% 62% · 34%
4	I	483	14% 46% 5% 49%
5	G	426	10% 47% 11% 42%
6	A	502	18% 62% 11% 27%
7	J	1359	6% 15% · 83%

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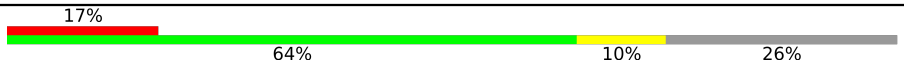
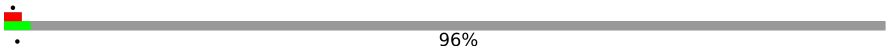
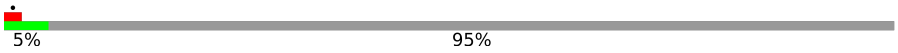
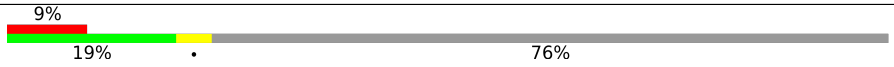
Mol	Chain	Length	Quality of chain
8	E	78	
9	C	883	
10	K	885	
11	X	625	
12	L	889	

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 21486 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chromatin structure-remodeling complex subunit RSC7.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

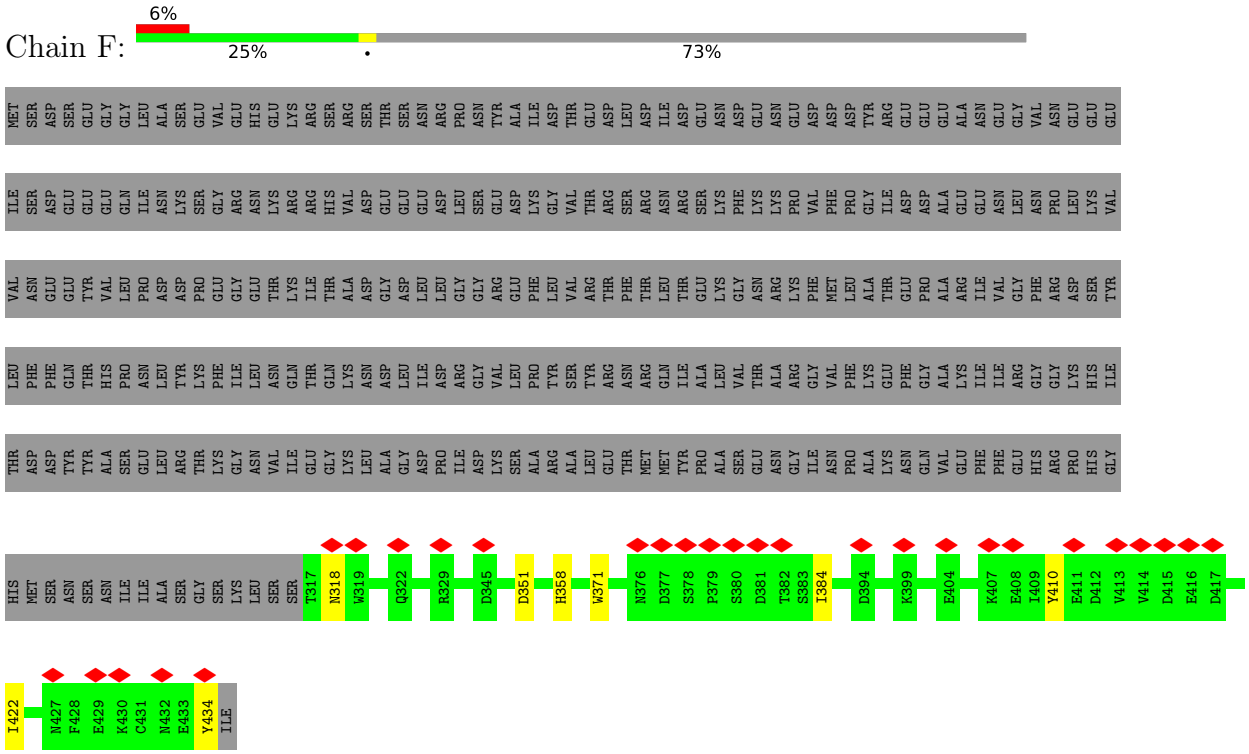
- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

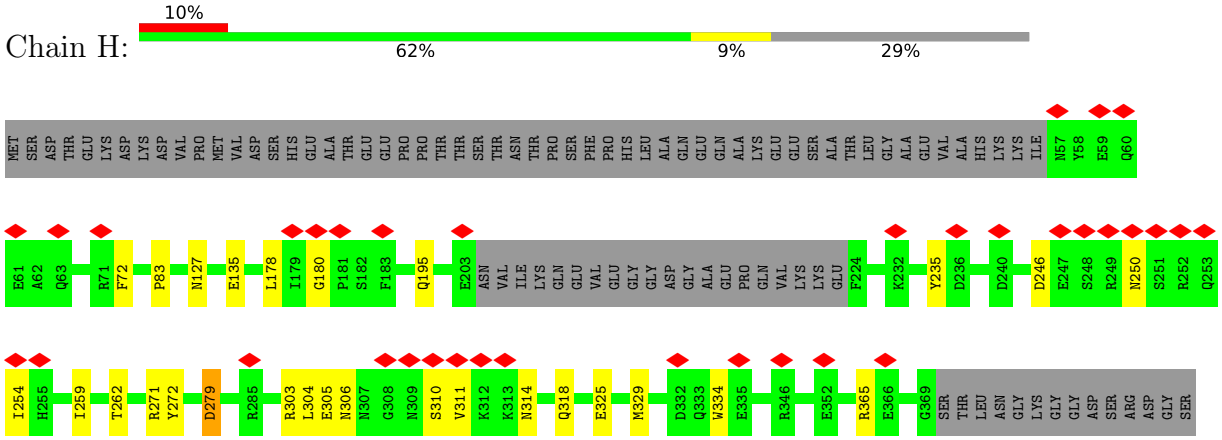
3 Residue-property plots (i)

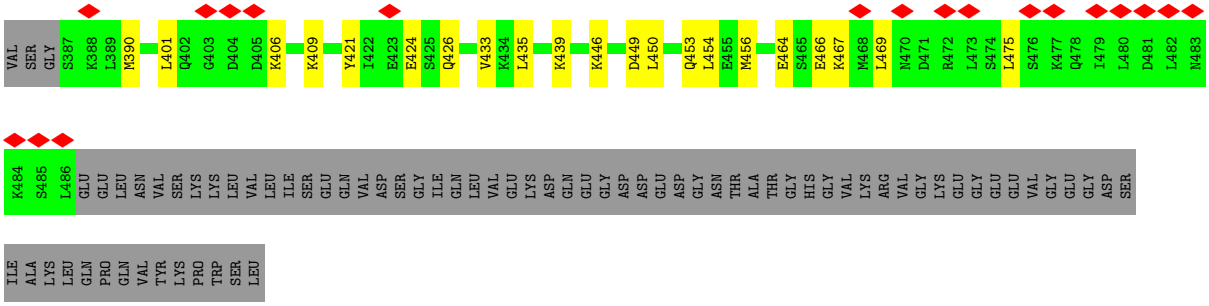
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Chromatin structure-remodeling complex subunit RSC7



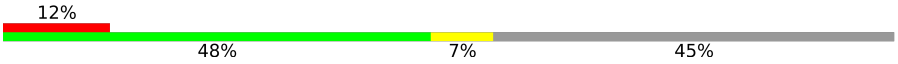
• Molecule 2: Chromatin structure-remodeling complex protein RSC8

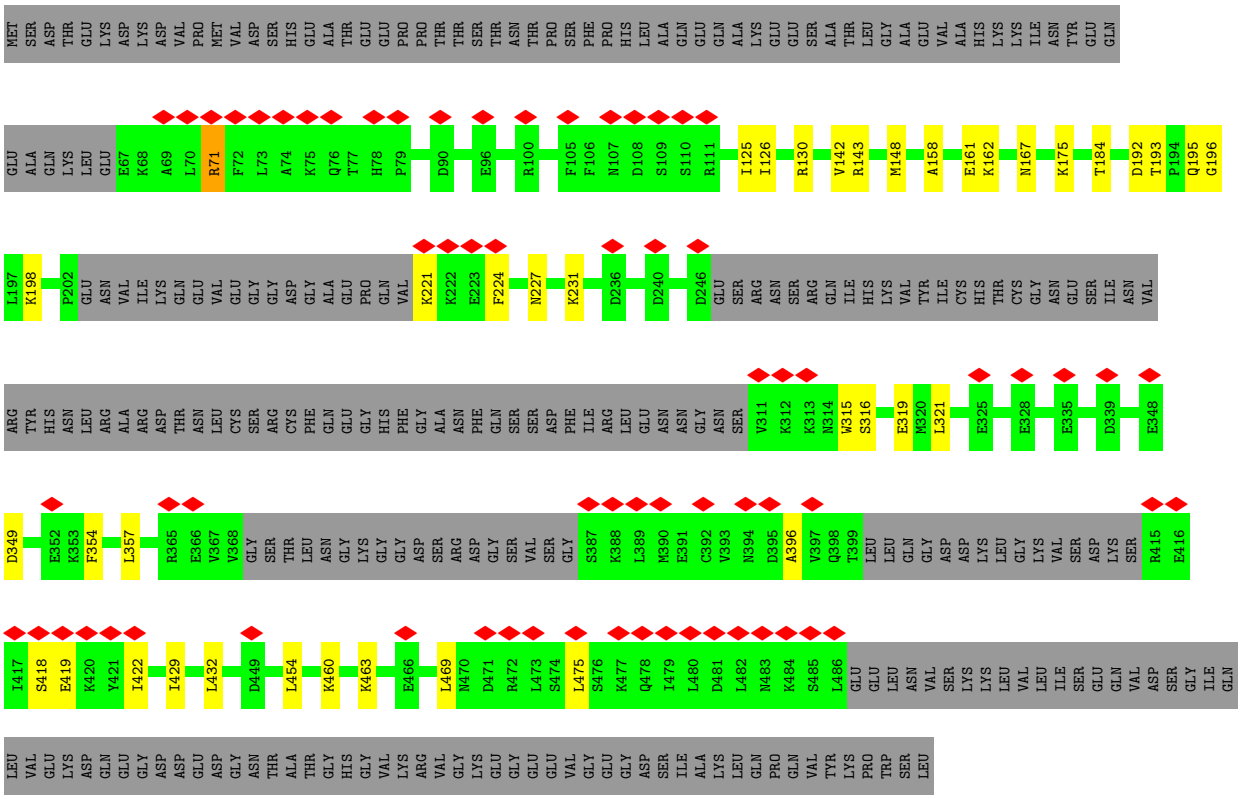




• Molecule 2: Chromatin structure-remodeling complex protein RSC8

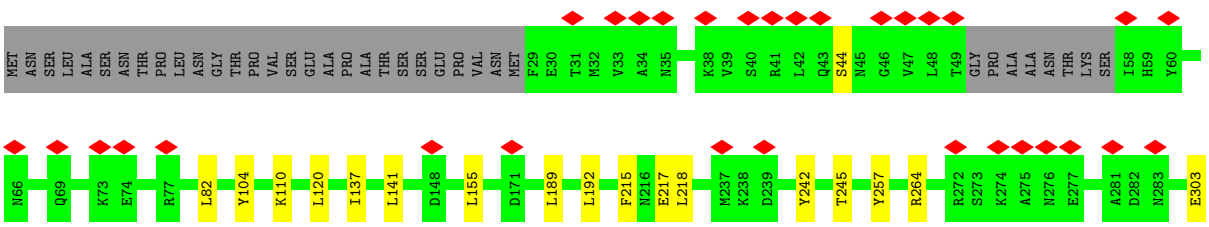
Chain D:

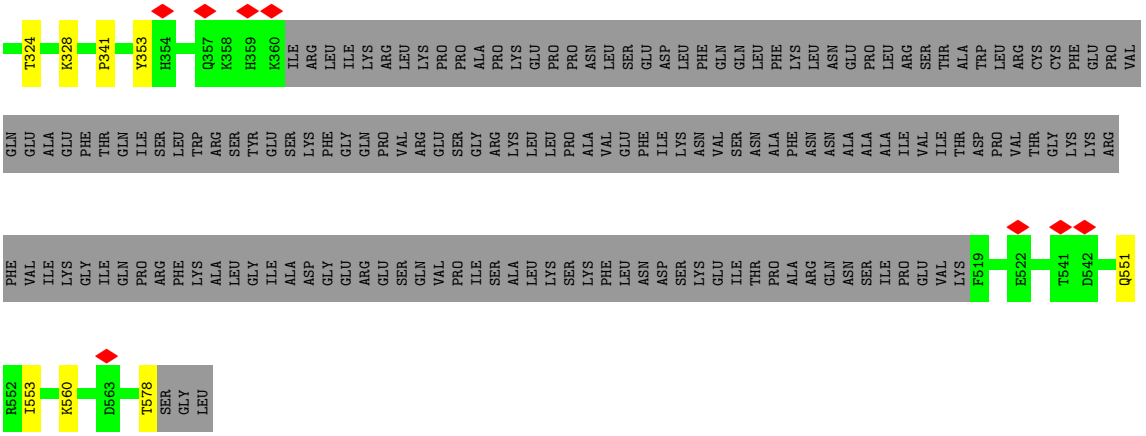




• Molecule 3: Chromatin structure-remodeling complex subunit RSC9

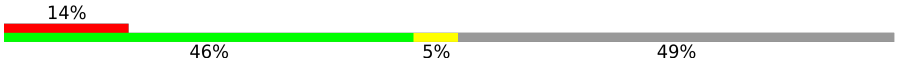
Chain M:

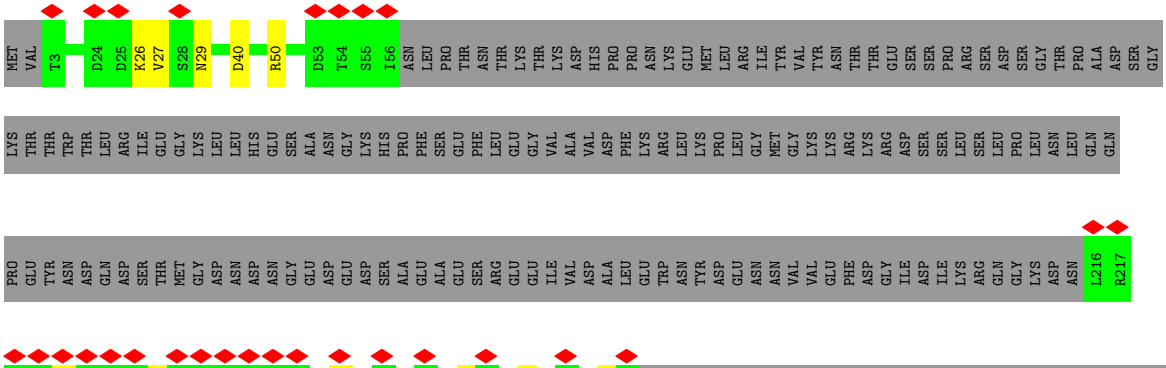




• Molecule 4: Chromatin structure-remodeling complex protein RSC6

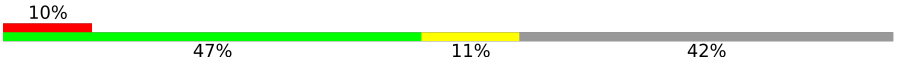
Chain I:

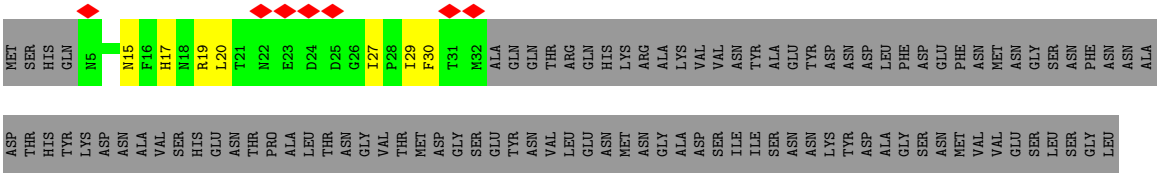


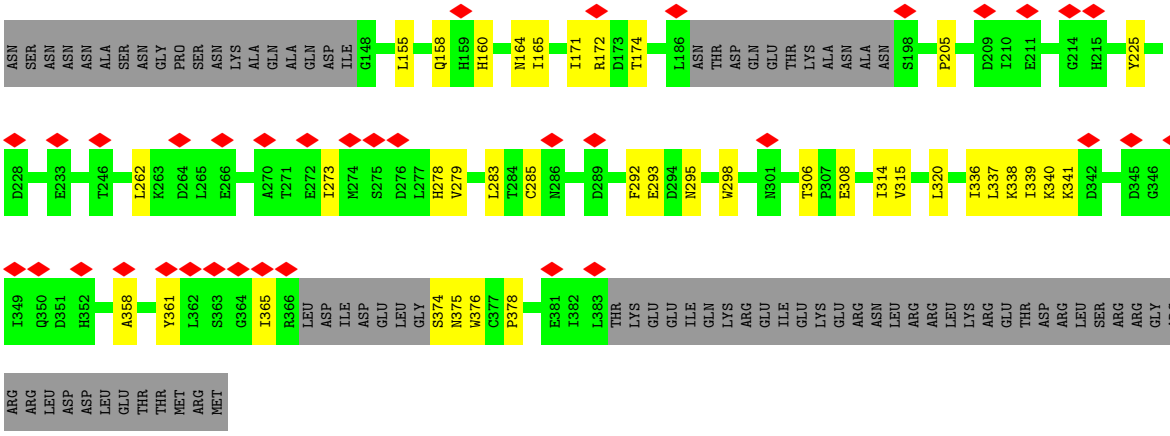


• Molecule 5: Chromatin structure-remodeling complex subunit SFH1

Chain G:

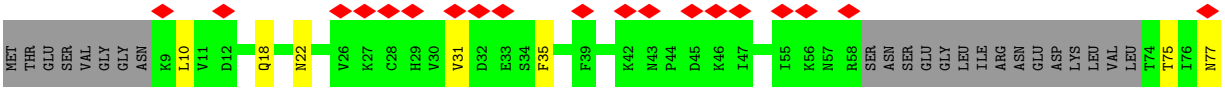


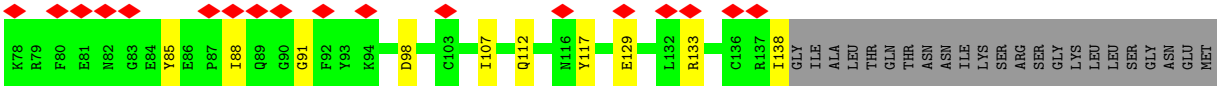


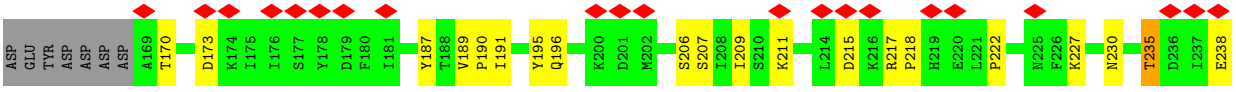


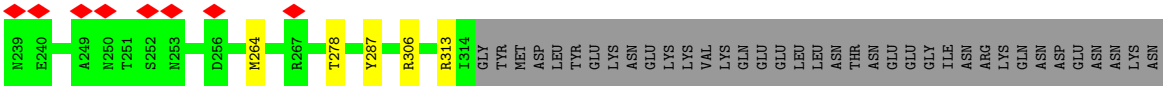
• Molecule 6: Chromatin structure-remodeling complex protein RSC58

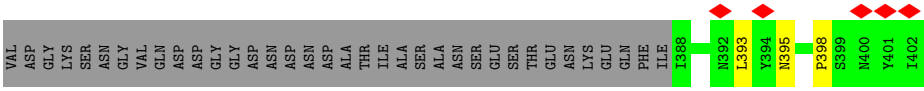
Chain A:

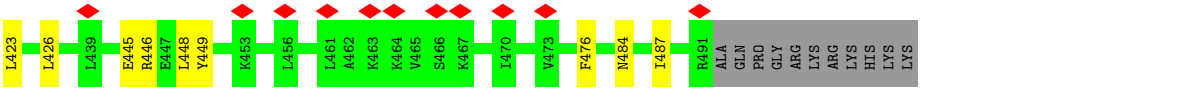






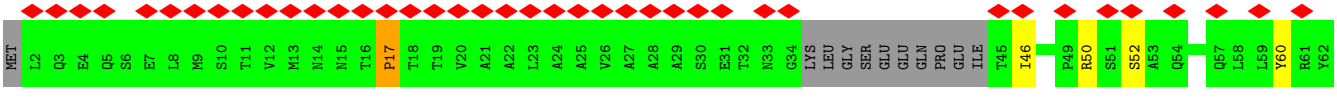


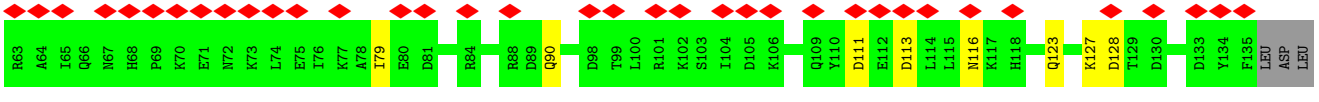


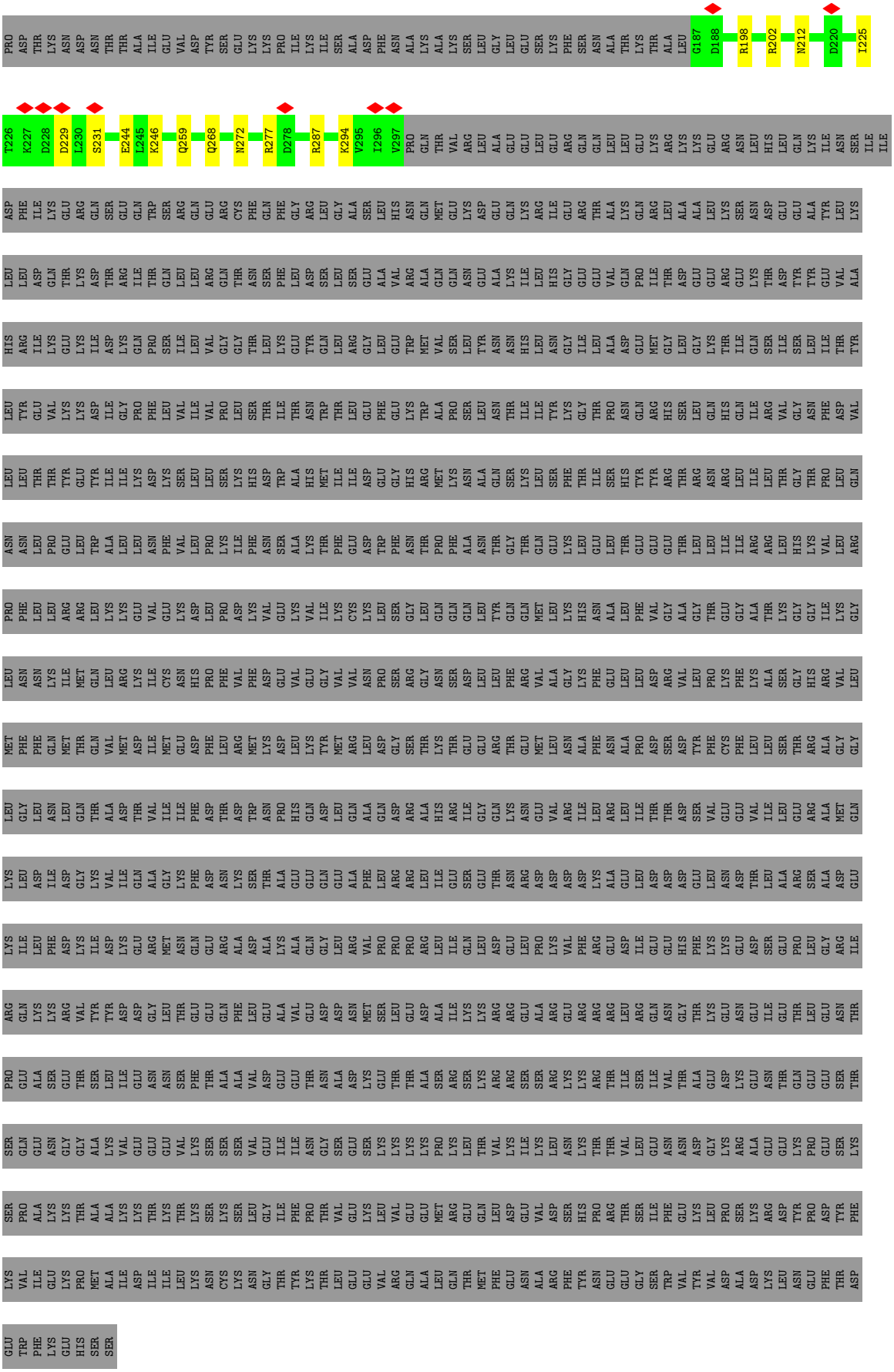


• Molecule 7: Nuclear protein STH1/NPS1

Chain J:

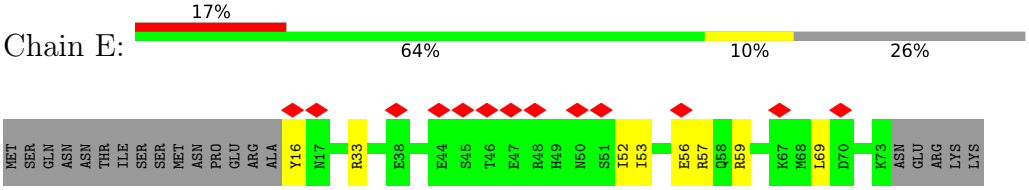





PRO ASP THR LYS ASN ASP ASN THR THR ALA ILE GLU VAL ASP TYR SER GLU LYS LYS PRO ILE LYS ILE SER ALA ASP PHE ASN ALA LYS ALA LYS SER LEU GLY LEU GLU SER LYS PHE SER ASN ALA THR LYS THR ALA LEU G187 D188 R198 R202 N212 D220 I225
T226 K227 D228 D229 L230 S231 E244 L245 K246 Q259 Q268 N272 R277 D278 R287 K294 V295 I296 V297 PRO GLN THR VAL ARG LEU GLU ALA GLU GLN GLU GLU LEU GLU GLU ARG GLN GLN LEU LEU GLU GLU LYS LYS ARG LYS VAL ALA
ASP 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 ARG ILE GLU ARG THR ALA LYS GLN ARG LEU ALA LEU LYS SER ASN ASP GLU LEU ASP GLN ASP THR ARG ILE THR GLN LEU LEU ARG GLN THR ASN SER PHE LEU ASP SER LEU SER GLU GLN GLU ALA LYS ILE LEU HIS GLY GLU GLU VAL GLN PRO ILE THR ASP GLU LEU ASP GLN ASP THR LYS ASP THR ARG ILE THR GLN LEU LEU ARG GLN THR ASN SER PHE LEU ASP SER LEU SER GLU GLN GLU VAL GLN PRO ILE THR ASP GLU GLU ARG GLN ARG LEU SER GLU ALA VAL ARG GLN ASN GLU ALA LYS ILE LEU HIS GLY GLU

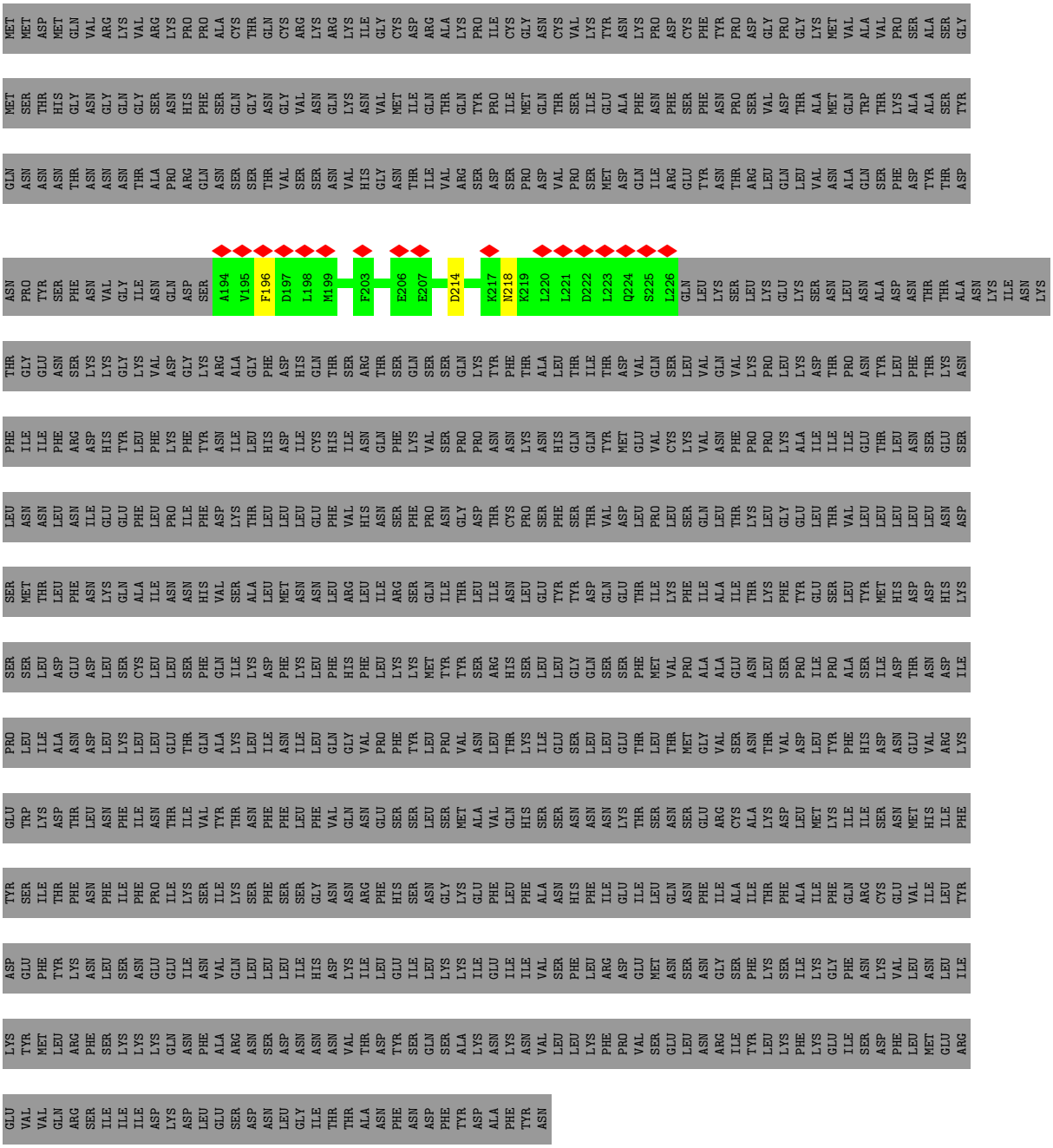
• Molecule 8: High temperature lethal protein 1

Chain E:



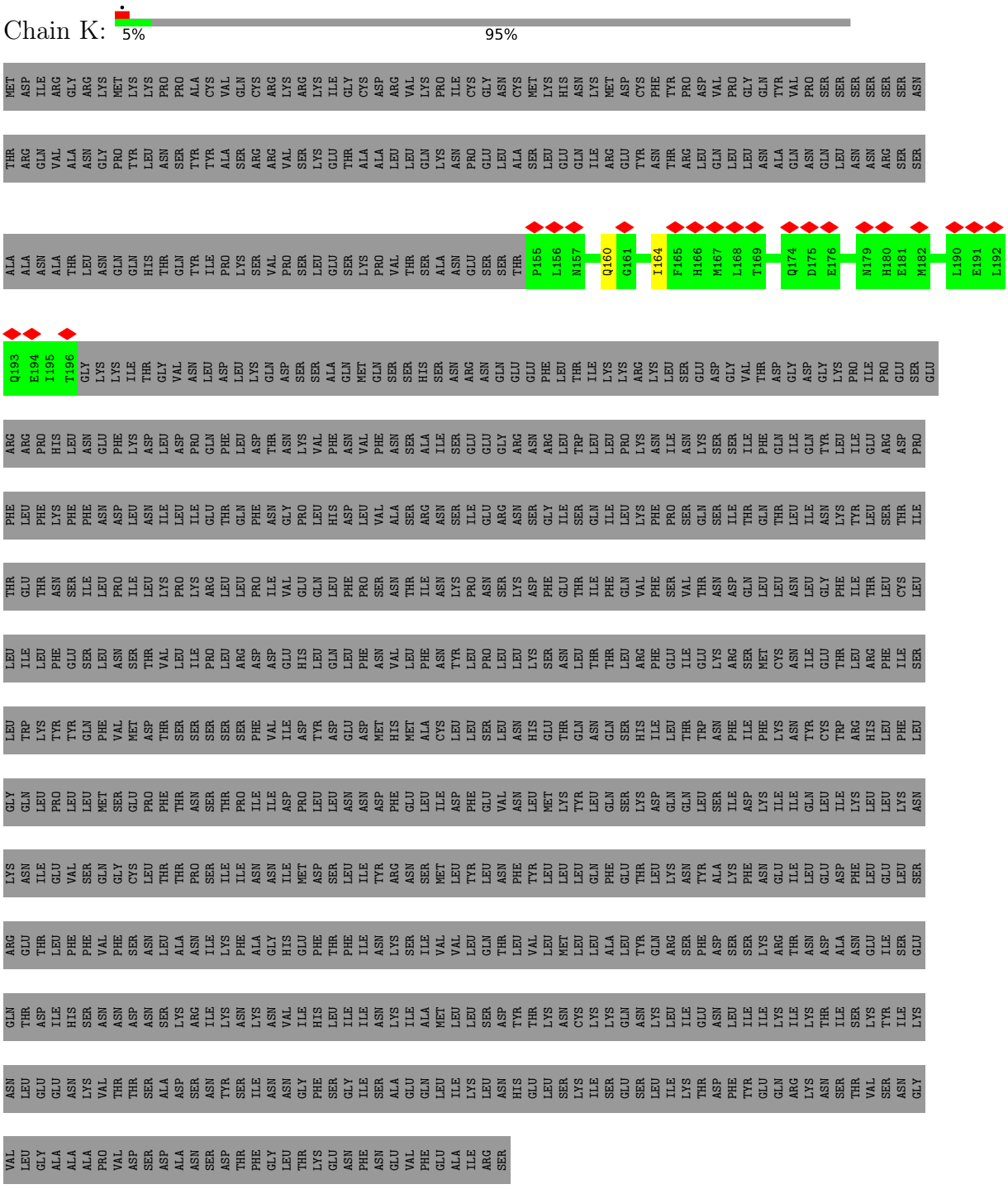
• Molecule 9: Chromatin structure-remodeling complex protein RSC30

Chain C:



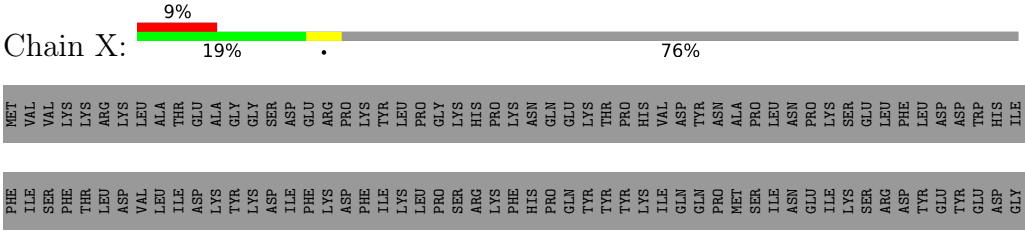
• Molecule 10: Chromatin structure-remodeling complex protein RSC3

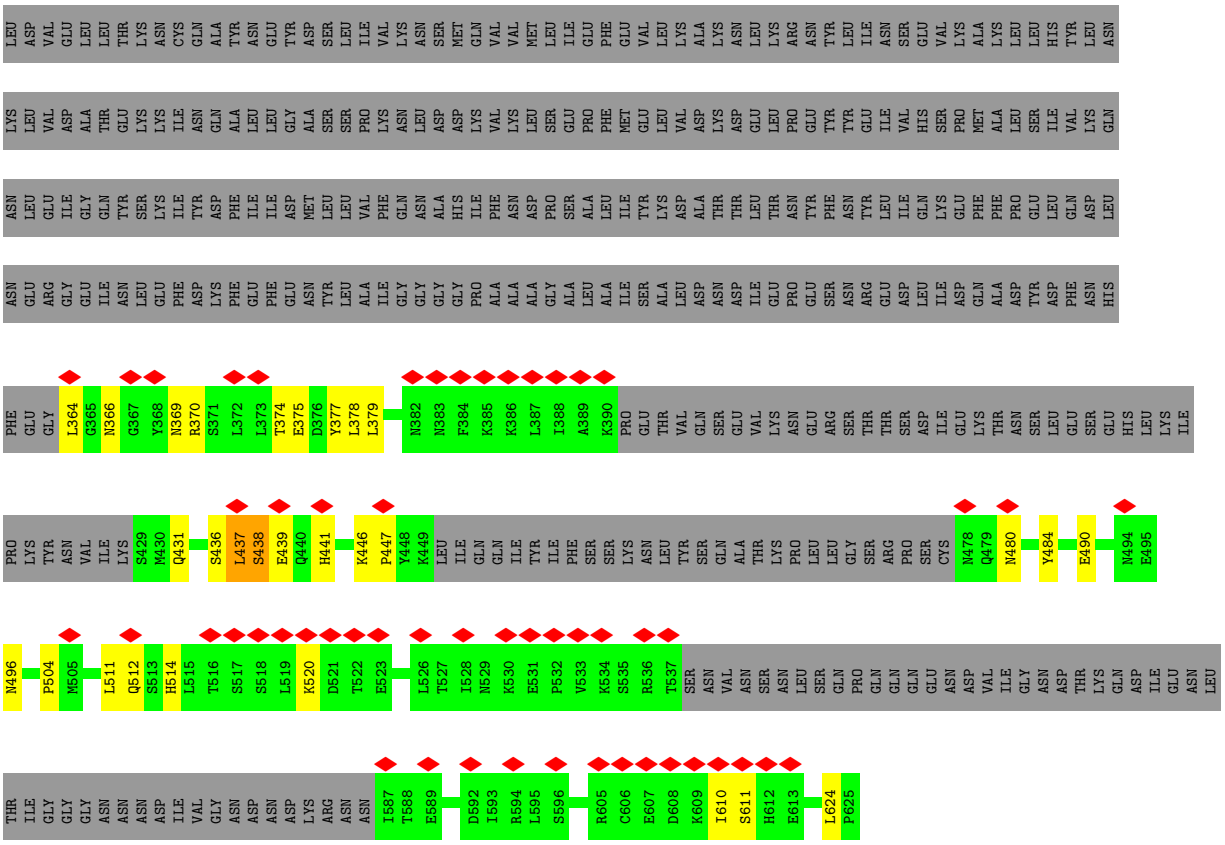
Chain K:



• Molecule 11: Chromatin structure-remodeling complex subunit RSC4

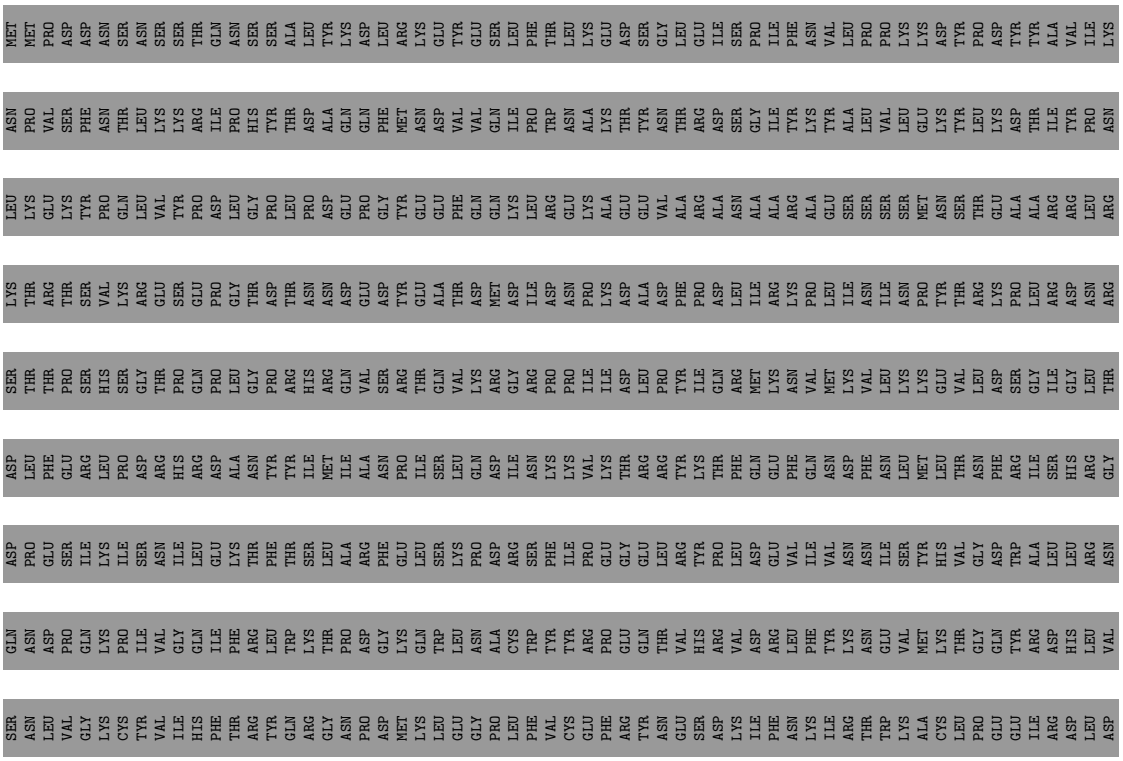
Chain X:

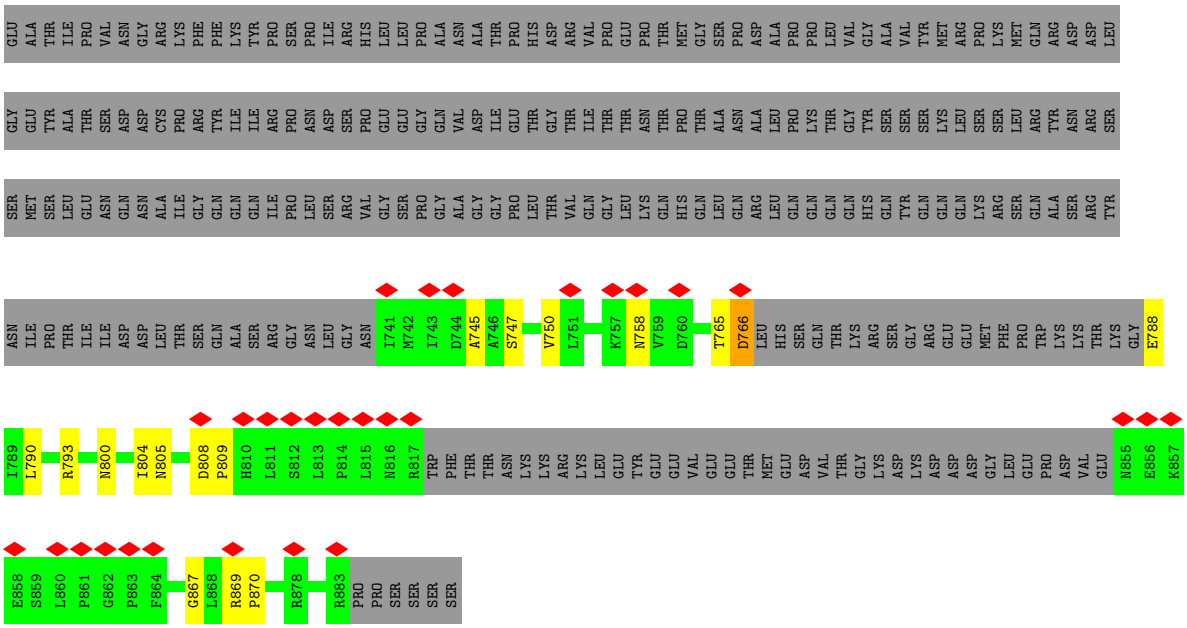




• Molecule 12: Chromatin structure-remodeling complex subunit RSC2

Chain L:




GLU ALA THR ILE PRO VAL ASN GLY ARG LYS PHE PHE LYS TYR PRO SER PRO ILE ARG HIS LEU LEU PRO ALA ASN ALA THR PRO HIS ASP ARG VAL PRO GLU PRO THR MET GLY SER PRO ASP ALA PRO PRO LEU VAL GLY ALA VAL TYR MET ARG PRO LYS MET GLN ARG ASP ASP LEU
GLY GLU TYR ALA THR SER ASP ASP CYS PRO ARG TYR ILE ILE ARG PRO ASN ASP SER PRO GLU GLU GLY GLN VAL ASP ILE GLU THR GLY THR ILE THR THR ASN THR PRO THR ALA ASN ALA LEU PRO LYS THR GLY TYR SER SER SER LYS LEU SER SER LEU ARG TYR ASN ARG SER
SER MET SER LEU GLU ASN GLN ASN ALA ILE GLY GLN GLN GLN ILE PRO LEU SER ARG VAL GLY SER PRO GLY ALA GLY GLY PRO LEU THR VAL GLN GLY LEU LYS GLN HIS GLN LEU GLN ARG LEU GLN GLN GLN GLN HIS GLN GLN TYR GLN GLN GLN GLN LYS ARG SER GLN ALA SER ARG TYR
ASN ILE PRO THR ILE ILE ASP ASP LEU THR SER GLN ALA SER ARG GLY ASN LEU GLY ASN I741 M742 I743 D744 A745 A746 S747 V750 L751 K757 N758 V759 D760 T765 D766 LEU HIS SER GLN THR LYS ARG SER GLY ARG GLU GLU MET PHE PRO TRP LYS LYS THR LYS GLY E788
I789 L790 R793 N800 I804 N805 D808 P809 H810 L811 S812 L813 P814 L815 N816 R817 TRP PHE THR THR ASN LYS LYS ARG LYS LEU GLU TYR GLU GLU VAL GLU GLU THR MET GLU ASP VAL THR GLY LYS ASP LYS ASP ASP ASP GLY LEU LEU GLU PRO ASP VAL GLU N855 E856 K857
E858 S859 L860 P861 G862 P863 F864 G867 L868 R869 P870 R878 R883 PRO PRO SER SER SER SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	280000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.092	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	F	0.28	0/983	0.57	0/1337
2	D	0.29	0/2557	0.50	0/3442
2	H	0.30	0/3275	0.53	1/4409 (0.0%)
3	M	0.31	0/3113	0.58	0/4215
4	I	0.28	0/1976	0.56	0/2685
5	G	0.29	0/2033	0.57	0/2761
6	A	0.30	0/3077	0.54	0/4169
7	J	0.29	0/1836	0.55	1/2480 (0.0%)
8	E	0.27	0/480	0.56	0/643
9	C	0.28	0/272	0.44	0/366
10	K	0.27	0/356	0.50	0/483
11	X	0.31	0/1243	0.57	0/1672
12	L	0.28	0/681	0.62	1/921 (0.1%)
All	All	0.29	0/21882	0.55	3/29583 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:439:GLU:OE1	11:X:490:GLU:CG	1.64	1.46
6:A:238:GLU:OE2	7:J:212:ASN:ND2	1.71	1.21
12:L:765:THR:HG22	12:L:790:LEU:HD21	1.23	1.16
11:X:439:GLU:OE1	11:X:490:GLU:HG2	0.91	1.07
6:A:187:TYR:OH	6:A:235:THR:HG21	1.56	1.04
12:L:750:VAL:HG11	12:L:788:GLU:OE1	1.59	1.02
6:A:190:PRO:HB3	11:X:437:LEU:CD2	1.91	1.00
6:A:190:PRO:HB3	11:X:437:LEU:HD22	1.43	0.98
12:L:765:THR:HG22	12:L:790:LEU:CD2	1.94	0.97
6:A:238:GLU:CD	7:J:212:ASN:ND2	2.18	0.95
11:X:439:GLU:OE1	11:X:490:GLU:CD	2.09	0.90
5:G:279:VAL:HG21	5:G:339:ILE:HD13	1.57	0.86
12:L:765:THR:CG2	12:L:790:LEU:HD21	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:476:LEU:HD21	4:I:480:GLN:NE2	1.94	0.82
6:A:218:PRO:HA	11:X:364:LEU:HD23	1.62	0.81
4:I:476:LEU:CD2	4:I:480:GLN:NE2	2.45	0.80
5:G:273:ILE:HD11	5:G:340:LYS:HG2	1.65	0.79
2:H:254:ILE:O	2:H:254:ILE:HG22	1.84	0.77
11:X:377:TYR:O	11:X:511:LEU:HA	1.84	0.77
12:L:765:THR:CG2	12:L:790:LEU:CD2	2.63	0.76
11:X:366:ASN:O	11:X:369:ASN:CG	2.28	0.72
6:A:238:GLU:OE1	7:J:212:ASN:ND2	2.23	0.71
4:I:476:LEU:HD21	4:I:480:GLN:HE22	1.53	0.70
5:G:15:ASN:HD22	5:G:174:THR:HA	1.56	0.69
6:A:187:TYR:HH	6:A:235:THR:HG21	1.57	0.68
6:A:218:PRO:HA	11:X:364:LEU:CD2	2.24	0.68
6:A:190:PRO:HB3	11:X:437:LEU:HD23	1.76	0.66
2:H:304:LEU:HD22	2:H:318:GLN:HG3	1.78	0.66
5:G:273:ILE:CD1	5:G:340:LYS:HG2	2.26	0.65
6:A:170:THR:HG23	11:X:379:LEU:HD22	1.80	0.64
6:A:264:MET:HA	7:J:259:GLN:HE21	1.63	0.62
2:H:439:LYS:NZ	4:I:40:ASP:OD2	2.32	0.62
6:A:238:GLU:CD	7:J:212:ASN:HD22	2.00	0.61
11:X:437:LEU:HD23	11:X:437:LEU:O	2.01	0.61
2:H:83:PRO:HA	2:D:192:ASP:HB3	1.82	0.60
6:A:238:GLU:O	6:A:238:GLU:HG3	1.99	0.60
6:A:222:PRO:HG3	12:L:758:ASN:HB2	1.84	0.60
6:A:88:ILE:HG13	6:A:91:GLY:H	1.66	0.60
4:I:237:ASN:HB3	4:I:322:VAL:HG12	1.83	0.60
6:A:189:VAL:O	11:X:437:LEU:N	2.27	0.59
11:X:375:GLU:HB2	11:X:514:HIS:HB2	1.85	0.59
2:H:279:ASP:OD1	2:H:329:MET:CE	2.51	0.58
11:X:438:SER:HB3	11:X:441:HIS:HE1	1.68	0.58
2:H:311:VAL:O	2:H:314:ASN:ND2	2.38	0.57
5:G:338:LYS:O	5:G:341:LYS:HB3	2.05	0.57
6:A:395:ASN:O	7:J:90:GLN:NE2	2.38	0.56
2:H:310:SER:OG	2:H:314:ASN:ND2	2.38	0.56
2:H:464:GLU:O	2:H:467:LYS:HB3	2.04	0.56
6:A:195:TYR:H	6:A:206:SER:HB3	1.70	0.56
2:H:435:LEU:O	4:I:398:LYS:NZ	2.38	0.56
6:A:209:ILE:HG22	6:A:211:LYS:H	1.71	0.56
2:H:246:ASP:OD2	5:G:160:HIS:NE2	2.39	0.56
2:H:325:GLU:OE2	7:J:246:LYS:NZ	2.34	0.56
2:H:446:LYS:NZ	6:A:287:TYR:OH	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:805:ASN:ND2	12:L:808:ASP:OD2	2.39	0.55
2:H:406:LYS:NZ	2:D:396:ALA:O	2.38	0.55
3:M:257:TYR:OH	7:J:294:LYS:NZ	2.40	0.55
2:H:127:ASN:ND2	2:D:184:THR:OG1	2.40	0.55
5:G:273:ILE:HD12	5:G:340:LYS:HE2	1.87	0.55
5:G:279:VAL:HG21	5:G:339:ILE:CD1	2.35	0.55
6:A:484:ASN:HD22	11:X:624:LEU:HD13	1.72	0.55
7:J:128:ASP:OD2	7:J:198:ARG:NH2	2.39	0.55
2:H:279:ASP:OD1	2:H:329:MET:HE1	2.06	0.54
4:I:267:VAL:HG21	4:I:309:GLU:HB2	1.87	0.54
6:A:238:GLU:HB3	12:L:804:ILE:HD11	1.89	0.54
11:X:366:ASN:O	11:X:369:ASN:ND2	2.41	0.54
2:H:178:LEU:HD11	2:D:195:GLN:HG3	1.89	0.54
2:H:446:LYS:O	2:H:449:ASP:HB2	2.08	0.54
2:H:272:TYR:OH	2:H:303:ARG:NH1	2.41	0.54
11:X:520:LYS:NZ	11:X:611:SER:OG	2.39	0.53
2:H:271:ARG:NH1	2:H:305:GLU:O	2.42	0.53
2:D:125:ILE:HG12	2:D:142:VAL:HG21	1.90	0.53
5:G:158:GLN:O	5:G:164:ASN:ND2	2.42	0.53
12:L:765:THR:O	12:L:766:ASP:HB2	2.09	0.53
3:M:551:GLN:NE2	3:M:578:THR:O	2.42	0.53
6:A:313:ARG:NH1	8:E:16:TYR:O	2.41	0.52
2:H:421:TYR:O	2:H:424:GLU:HB3	2.08	0.52
2:D:227:ASN:ND2	7:J:244:GLU:OE2	2.38	0.52
11:X:366:ASN:O	11:X:369:ASN:OD1	2.26	0.52
11:X:431:GLN:HG2	11:X:446:LYS:HB3	1.91	0.52
2:H:475:LEU:HD21	2:D:475:LEU:HD11	1.91	0.52
2:D:469:LEU:HD22	4:I:258:LYS:HD3	1.92	0.52
4:I:476:LEU:HD23	4:I:480:GLN:NE2	2.21	0.52
4:I:482:ARG:O	4:I:483:LEU:CB	2.56	0.52
7:J:268:GLN:OE1	7:J:272:ASN:ND2	2.42	0.52
2:D:158:ALA:O	2:D:162:LYS:HB2	2.10	0.51
2:H:453:GLN:O	2:H:456:MET:HB3	2.10	0.51
6:A:129:GLU:OE2	12:L:869:ARG:NE	2.42	0.51
3:M:264:ARG:NH2	3:M:303:GLU:OE2	2.40	0.51
2:H:426:GLN:HB2	2:D:422:ILE:HD11	1.93	0.51
6:A:398:PRO:HD3	7:J:52:SER:HA	1.93	0.51
2:H:254:ILE:CG2	2:H:254:ILE:O	2.57	0.51
6:A:18:GLN:OE1	6:A:22:ASN:ND2	2.44	0.50
4:I:220:ILE:HD12	4:I:351:LEU:HD22	1.92	0.50
12:L:765:THR:HG22	12:L:790:LEU:CG	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:438:SER:HB3	11:X:441:HIS:CE1	2.46	0.50
9:C:196:PHE:HB3	10:K:160:GLN:HE21	1.77	0.50
6:A:445:GLU:O	6:A:449:TYR:N	2.44	0.50
2:D:143:ARG:HH12	5:G:314:ILE:HD11	1.75	0.50
6:A:112:GLN:HE21	6:A:217:ARG:HD2	1.77	0.50
11:X:447:PRO:HB3	11:X:480:ASN:HD22	1.77	0.50
3:M:82:LEU:HD21	3:M:120:LEU:HD21	1.93	0.49
11:X:377:TYR:HB2	11:X:512:GLN:HB3	1.94	0.49
2:H:454:LEU:HB3	2:D:454:LEU:HD11	1.94	0.49
5:G:285:CYS:HB2	5:G:292:PHE:HB3	1.95	0.49
7:J:46:ILE:HD13	7:J:79:ILE:HG12	1.95	0.49
3:M:341:PRO:HG3	3:M:553:ILE:HG23	1.95	0.49
1:F:351:ASP:HB2	1:F:358:HIS:CD2	2.47	0.48
2:H:433:VAL:HG11	2:D:429:ILE:HG23	1.95	0.48
2:D:231:LYS:HG2	7:J:202:ARG:HH22	1.79	0.48
2:D:460:LYS:HA	2:D:463:LYS:HG2	1.96	0.48
1:F:371:TRP:O	1:F:434:TYR:OH	2.32	0.48
7:J:123:GLN:OE1	7:J:127:LYS:NZ	2.44	0.48
5:G:374:SER:OG	5:G:375:ASN:N	2.46	0.48
5:G:315:VAL:HG13	5:G:320:LEU:HB2	1.95	0.48
3:M:324:THR:O	3:M:328:LYS:HB2	2.14	0.47
2:H:259:ILE:HB	3:M:44:SER:HA	1.95	0.47
6:A:393:LEU:O	7:J:60:TYR:OH	2.32	0.47
3:M:192:LEU:HB3	3:M:245:THR:HG21	1.95	0.47
7:J:225:ILE:HG23	7:J:229:ASP:HB3	1.95	0.47
6:A:487:ILE:HD13	12:L:747:SER:HB2	1.96	0.47
2:H:450:LEU:HD13	4:I:50:ARG:HG2	1.95	0.47
11:X:374:THR:OG1	11:X:514:HIS:O	2.30	0.47
1:F:384:ILE:HB	2:H:235:TYR:HB2	1.97	0.47
2:H:279:ASP:OD1	2:H:329:MET:HE2	2.14	0.47
2:H:401:LEU:HD22	4:I:427:ARG:HD2	1.97	0.47
3:M:341:PRO:O	3:M:560:LYS:NZ	2.47	0.46
2:H:271:ARG:NH1	2:H:306:ASN:OD1	2.40	0.46
6:A:278:THR:OG1	6:A:306:ARG:NH2	2.48	0.46
2:D:418:SER:O	2:D:422:ILE:HB	2.15	0.46
1:F:410:TYR:CE2	1:F:422:ILE:HG21	2.50	0.46
1:F:318:ASN:OD1	2:D:71:ARG:NH2	2.48	0.46
2:H:195:GLN:HE22	2:D:175:LYS:HD3	1.81	0.46
6:A:190:PRO:CB	11:X:437:LEU:HD22	2.30	0.45
2:D:316:SER:OG	2:D:319:GLU:OE1	2.22	0.45
5:G:165:ILE:HG12	5:G:171:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:27:ILE:HG22	5:G:29:ILE:H	1.81	0.45
12:L:750:VAL:HG11	12:L:788:GLU:CD	2.32	0.45
6:A:112:GLN:NE2	6:A:215:ASP:OD2	2.50	0.45
5:G:205:PRO:HD2	5:G:337:LEU:HD21	1.98	0.45
3:M:215:PHE:O	3:M:218:LEU:HB3	2.17	0.45
11:X:520:LYS:HZ3	11:X:610:ILE:HB	1.81	0.45
2:D:315:TRP:NE1	2:D:349:ASP:OD2	2.45	0.45
5:G:358:ALA:HB1	5:G:365:ILE:H	1.81	0.45
6:A:206:SER:OG	6:A:207:SER:N	2.50	0.45
2:H:135:GLU:OE2	5:G:19:ARG:NH2	2.50	0.45
3:M:217:GLU:OE2	7:J:287:ARG:NH2	2.43	0.45
3:M:137:ILE:HG21	3:M:155:LEU:HD13	1.99	0.45
2:D:321:LEU:HD23	6:A:476:PHE:HE1	1.83	0.44
12:L:867:GLY:O	12:L:869:ARG:NH1	2.49	0.44
4:I:27:VAL:HG12	4:I:29:ASN:H	1.82	0.44
2:H:454:LEU:HD11	4:I:50:ARG:HD3	1.99	0.44
2:D:143:ARG:HH21	5:G:378:PRO:HD3	1.83	0.44
6:A:235:THR:O	6:A:235:THR:HG22	2.18	0.44
7:J:113:ASP:HA	7:J:116:ASN:HD22	1.82	0.44
6:A:31:VAL:HG12	6:A:77:ASN:HB2	2.00	0.44
5:G:306:THR:HG22	5:G:308:GLU:H	1.83	0.44
6:A:235:THR:OG1	12:L:800:ASN:ND2	2.48	0.44
5:G:17:HIS:HA	5:G:20:LEU:HD12	1.98	0.44
2:H:334:TRP:HE1	4:I:483:LEU:HD21	1.82	0.44
12:L:745:ALA:HB1	12:L:793:ARG:HH22	1.82	0.44
2:D:432:LEU:HD13	8:E:69:LEU:HD22	2.00	0.43
5:G:20:LEU:HB3	5:G:30:PHE:HD2	1.83	0.43
8:E:52:ILE:O	8:E:57:ARG:NH2	2.52	0.43
2:H:365:ARG:HH22	2:D:221:LYS:NZ	2.17	0.43
2:H:72:PHE:HA	5:G:155:LEU:HD22	2.00	0.43
2:H:178:LEU:HG	2:D:196:GLY:HA3	2.00	0.43
8:E:56:GLU:HA	8:E:59:ARG:HG2	2.01	0.43
6:A:191:ILE:HD12	6:A:230:ASN:HB3	2.00	0.43
6:A:196:GLN:HB3	6:A:227:LYS:HB2	2.01	0.43
6:A:445:GLU:HA	6:A:448:LEU:HB3	2.00	0.43
9:C:214:ASP:O	9:C:218:ASN:ND2	2.52	0.42
3:M:110:LYS:HG3	10:K:164:ILE:HG23	2.01	0.42
4:I:224:LEU:HD21	4:I:349:ILE:HD12	2.01	0.42
11:X:370:ARG:NH2	11:X:496:ASN:OD1	2.40	0.42
6:A:10:LEU:HD21	6:A:138:ILE:HG21	2.01	0.42
6:A:446:ARG:HH12	7:J:50:ARG:HH21	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:GLU:HG3	2:D:167:ASN:HB2	2.01	0.42
5:G:295:ASN:HB2	5:G:376:TRP:HB2	2.01	0.42
2:H:426:GLN:NE2	4:I:26:LYS:O	2.52	0.42
6:A:133:ARG:NH2	12:L:870:PRO:O	2.53	0.42
6:A:107:ILE:HG23	6:A:117:TYR:HE1	1.85	0.42
3:M:137:ILE:O	3:M:141:LEU:HB2	2.18	0.42
2:D:193:THR:HG22	2:D:195:GLN:H	1.85	0.42
5:G:336:ILE:O	5:G:340:LYS:HG3	2.19	0.42
2:H:466:GLU:HA	2:H:469:LEU:HD12	2.02	0.42
11:X:439:GLU:CD	11:X:490:GLU:CD	2.78	0.42
2:D:354:PHE:HA	2:D:357:LEU:HD13	2.02	0.41
2:D:419:GLU:HA	2:D:422:ILE:HG22	2.02	0.41
3:M:189:LEU:HB2	3:M:242:TYR:HE1	1.84	0.41
2:H:424:GLU:HA	8:E:53:ILE:HD11	2.03	0.41
4:I:422:LEU:HA	4:I:429:THR:HG21	2.02	0.41
2:D:224:PHE:HZ	7:J:244:GLU:HG2	1.85	0.41
2:H:390:MET:HG3	8:E:33:ARG:HD2	2.02	0.41
6:A:423:LEU:HD23	6:A:426:LEU:HD12	2.02	0.41
7:J:225:ILE:HG12	7:J:231:SER:HB3	2.02	0.41
2:H:180:GLY:HA3	2:D:198:LYS:HE2	2.02	0.41
4:I:319:LEU:HA	4:I:322:VAL:HG22	2.03	0.41
7:J:111:ASP:N	7:J:111:ASP:OD1	2.54	0.41
6:A:191:ILE:HG23	11:X:436:SER:HB3	2.03	0.41
2:D:126:ILE:O	2:D:130:ARG:HG2	2.20	0.41
5:G:283:LEU:O	5:G:293:GLU:HA	2.21	0.41
6:A:35:PHE:H	6:A:75:THR:HG22	1.86	0.40
4:I:482:ARG:O	4:I:483:LEU:HB3	2.20	0.40
3:M:353:TYR:CZ	4:I:250:ASN:HB3	2.56	0.40
2:H:406:LYS:HD2	2:H:409:LYS:HD2	2.03	0.40
11:X:504:PRO:HD3	11:X:624:LEU:HB2	2.02	0.40
6:A:85:TYR:OH	6:A:98:ASP:OD2	2.37	0.40
2:D:148:MET:HG3	5:G:361:TYR:CE1	2.57	0.40
5:G:278:HIS:HA	5:G:298:TRP:O	2.20	0.40
6:A:170:THR:HG22	6:A:173:ASP:H	1.86	0.40
5:G:225:TYR:HD1	5:G:262:LEU:HD12	1.85	0.40
11:X:378:LEU:HB2	11:X:484:TYR:HB2	2.02	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	F	116/435 (27%)	102 (88%)	14 (12%)	0	100	100
2	D	295/557 (53%)	280 (95%)	15 (5%)	0	100	100
2	H	387/557 (70%)	356 (92%)	31 (8%)	0	100	100
3	M	378/581 (65%)	349 (92%)	29 (8%)	0	100	100
4	I	236/483 (49%)	218 (92%)	18 (8%)	0	100	100
5	G	238/426 (56%)	213 (90%)	25 (10%)	0	100	100
6	A	357/502 (71%)	321 (90%)	36 (10%)	0	100	100
7	J	229/1359 (17%)	201 (88%)	27 (12%)	1 (0%)	34	67
8	E	56/78 (72%)	53 (95%)	3 (5%)	0	100	100
9	C	31/883 (4%)	31 (100%)	0	0	100	100
10	K	40/885 (4%)	38 (95%)	2 (5%)	0	100	100
11	X	139/625 (22%)	126 (91%)	13 (9%)	0	100	100
12	L	79/889 (9%)	69 (87%)	9 (11%)	1 (1%)	12	39
All	All	2581/8260 (31%)	2357 (91%)	222 (9%)	2 (0%)	54	82

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	111/388 (29%)	111 (100%)	0	100 100
2	D	285/500 (57%)	284 (100%)	1 (0%)	91 95
2	H	363/500 (73%)	361 (99%)	2 (1%)	86 94
3	M	349/521 (67%)	348 (100%)	1 (0%)	92 97
4	I	223/435 (51%)	223 (100%)	0	100 100
5	G	225/384 (59%)	224 (100%)	1 (0%)	91 95
6	A	343/462 (74%)	342 (100%)	1 (0%)	92 97
7	J	187/1228 (15%)	186 (100%)	1 (0%)	88 94
8	E	56/75 (75%)	56 (100%)	0	100 100
9	C	32/824 (4%)	32 (100%)	0	100 100
10	K	39/832 (5%)	39 (100%)	0	100 100
11	X	141/578 (24%)	139 (99%)	2 (1%)	67 83
12	L	77/810 (10%)	77 (100%)	0	100 100
All	All	2431/7537 (32%)	2422 (100%)	9 (0%)	91 95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	250	ASN
2	H	262	THR
2	D	71	ARG
3	M	104	TYR
5	G	172	ARG
6	A	235	THR
7	J	277	ARG
11	X	437	LEU
11	X	438	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	127	ASN
2	H	167	ASN
2	H	195	GLN
2	H	250	ASN
2	H	314	ASN
2	D	145	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	242	ASN
3	M	203	ASN
3	M	359	HIS
3	M	551	GLN
4	I	337	GLN
4	I	432	HIS
4	I	463	ASN
4	I	480	GLN
5	G	352	HIS
6	A	112	GLN
6	A	484	ASN
7	J	90	GLN
7	J	259	GLN
9	C	218	ASN
10	K	160	GLN
11	X	369	ASN
11	X	380	ASN
11	X	480	ASN
11	X	494	ASN
12	L	800	ASN
12	L	810	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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.

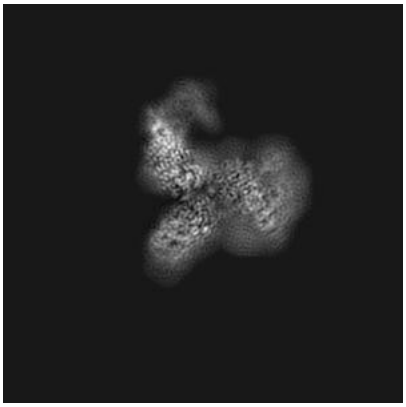
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9905. These allow visual inspection of the internal detail of the map and identification of artifacts.

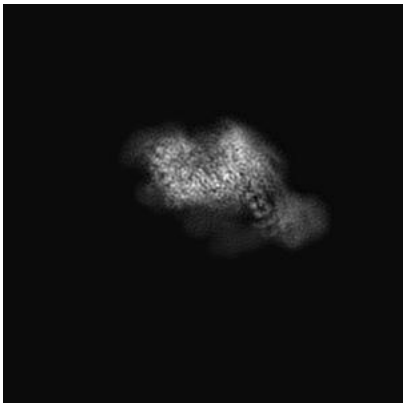
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

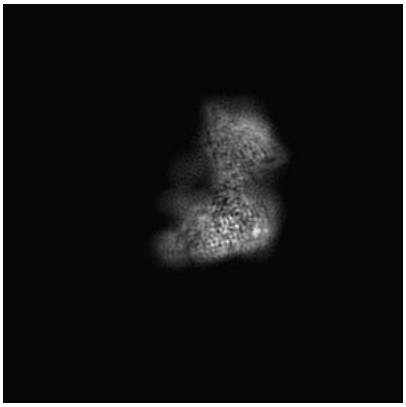
6.1.1 Primary map



X



Y



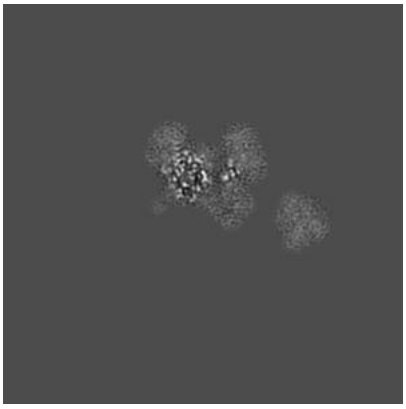
Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 180



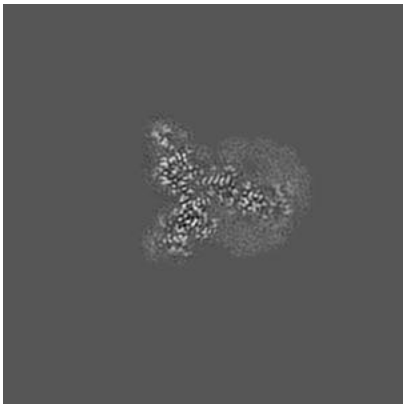
Y Index: 180

Z Index: 180

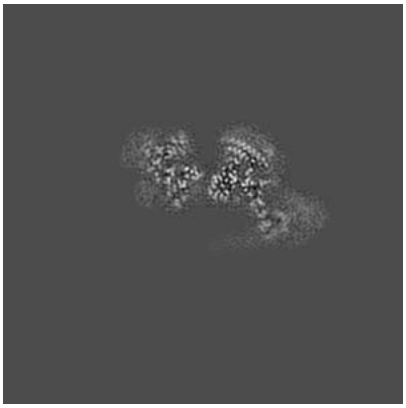
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

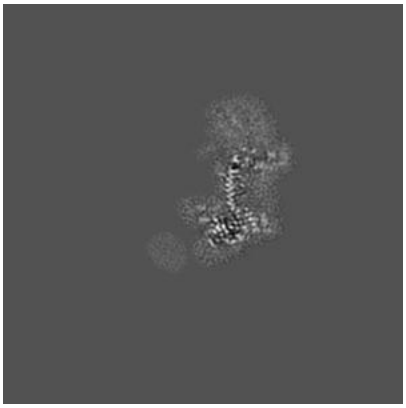
6.3.1 Primary map



X Index: 202



Y Index: 154

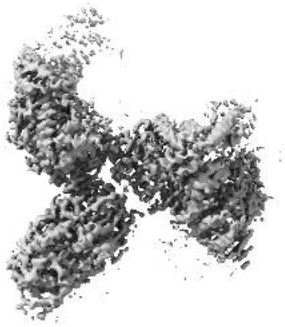


Z Index: 201

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

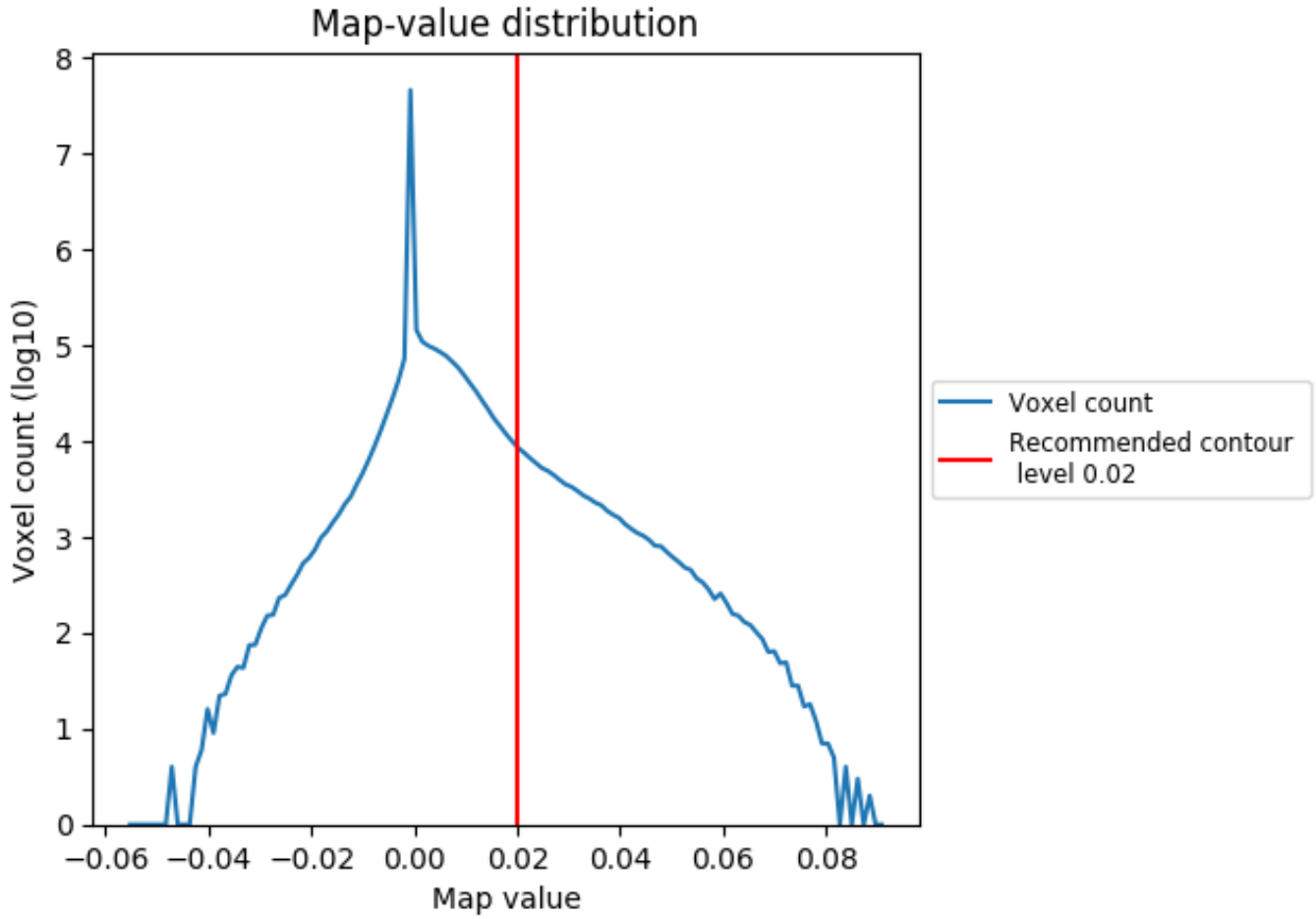
6.5 Mask visualisation (i)

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

7 Map analysis

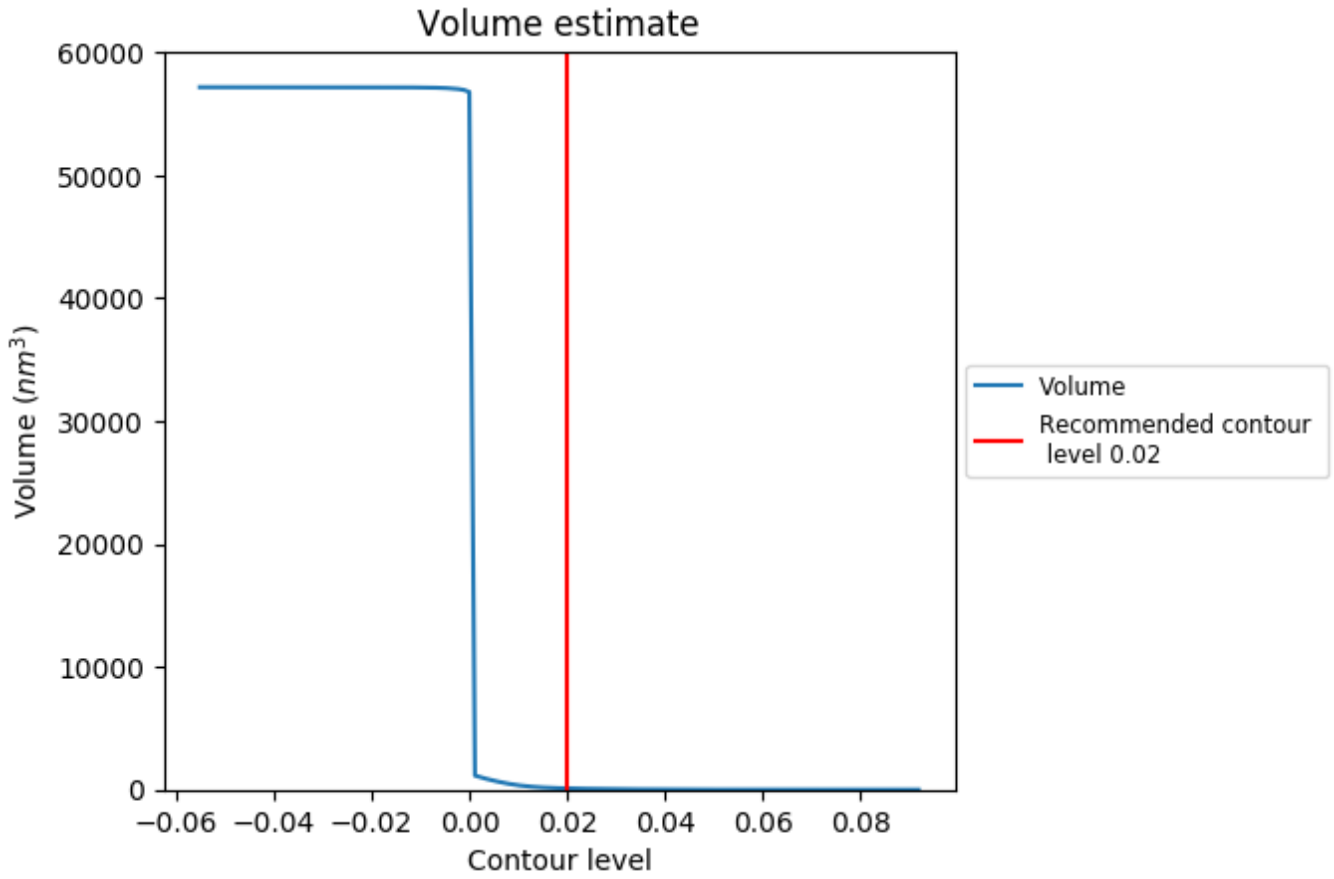
This section contains the results of statistical analysis of the map.

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.

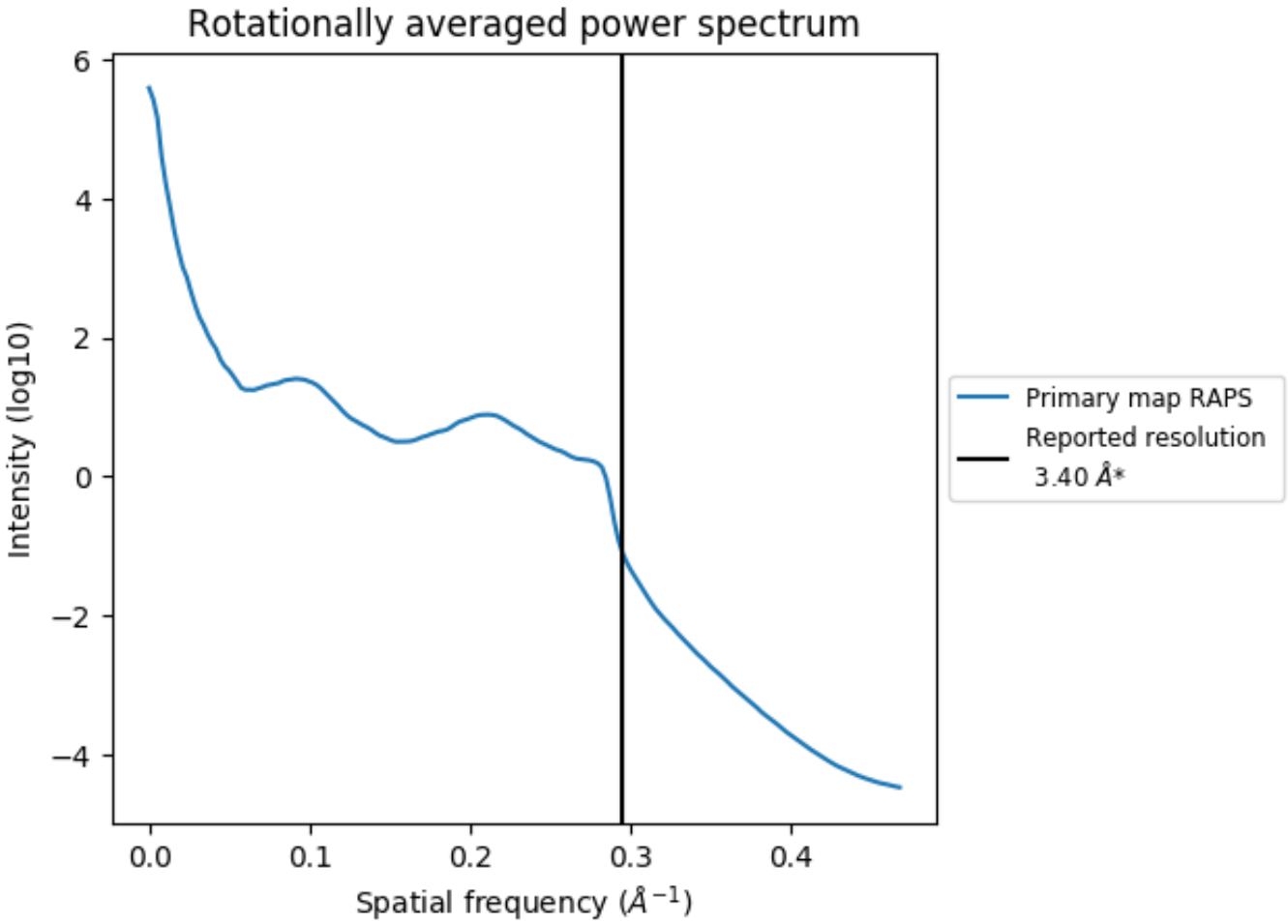
7.2 Volume estimate



The volume at the recommended contour level is 105 nm^3; this corresponds to an approximate mass of 95 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 0.294 $Å^{-1}$

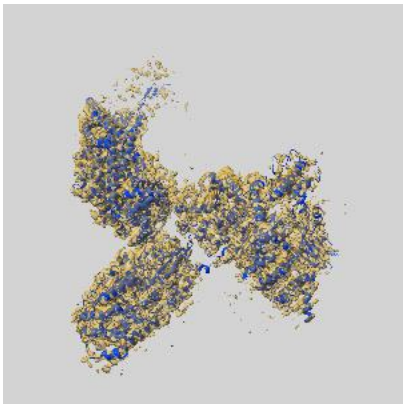
8 Fourier-Shell correlation (i)

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

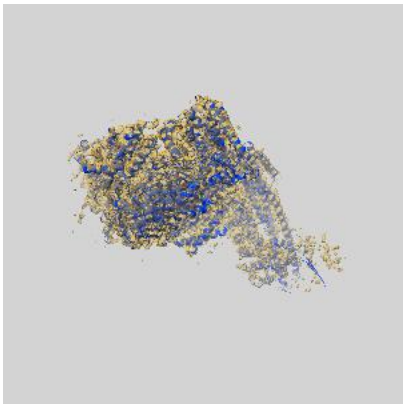
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9905 and PDB model 6K15. Per-residue inclusion information can be found in section 3 on page 7.

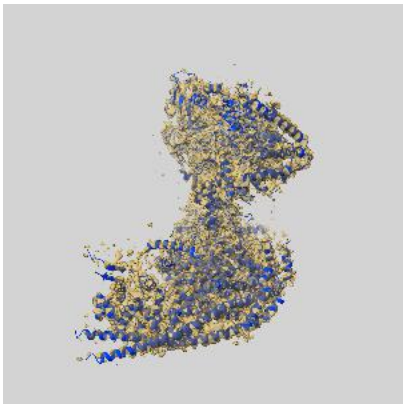
9.1 Map-model overlay



X



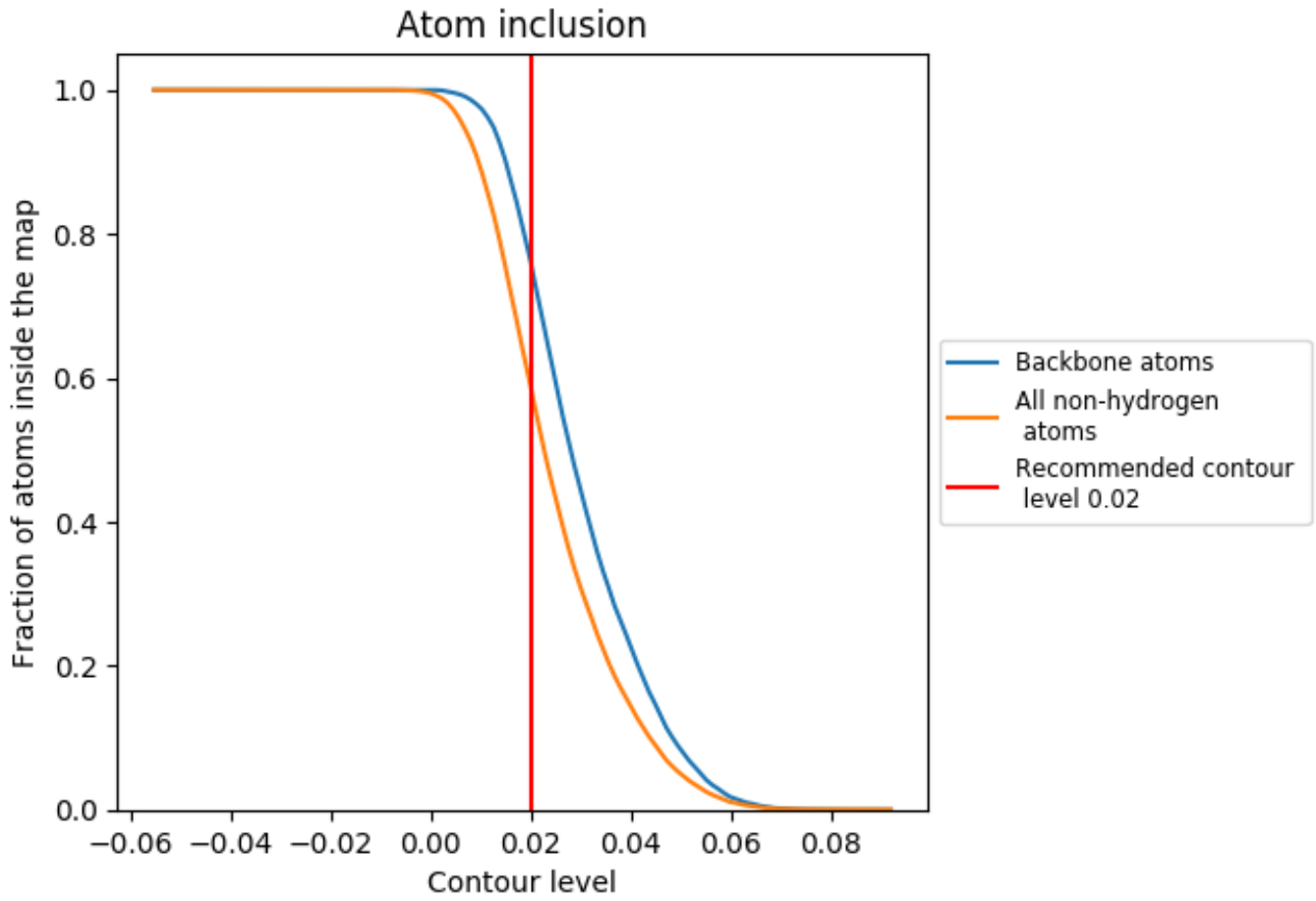
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.