Full wwPDB EM Validation Report

Nov 2, 2024 – 03:10 pm GMT

PDB ID	:	6TDA
EMDB ID	:	EMD-10465
Title	:	Structure of SWI/SNF chromatin remodeler RSC bound to a nucleosome
Authors	:	Wagner, F.R.; Dienemann, C.; Wang, H.; Stuetzer, A.; Tegunov, D.; Urlaub, H.; Cramer, P.
Deposited on	:	2019-11-08
Resolution	:	15.00 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:

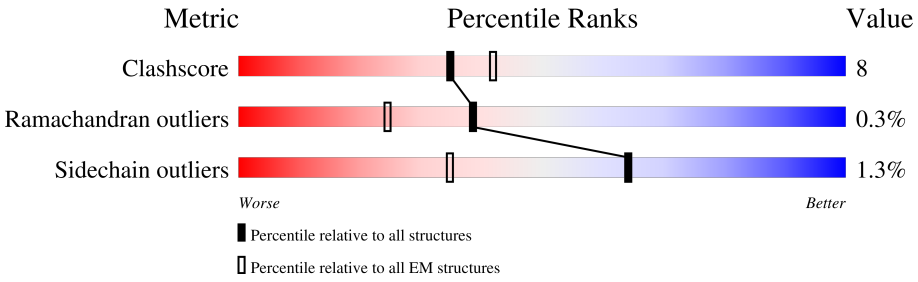
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 15.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	135	59% 12% 29%
1	E	135	59% 12% 30%
2	B	102	6% 70% 16% 15%
2	F	102	65% 16% 20%
3	C	129	65% 14% 21%
3	G	129	70% 9% 21%
4	D	122	70% 6% 25%
4	H	122	60% 16% 25%

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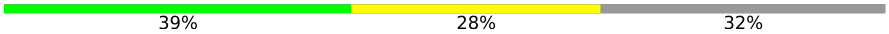
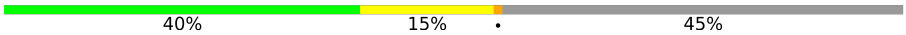
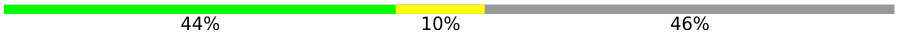
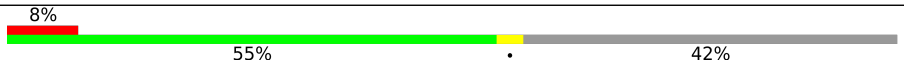
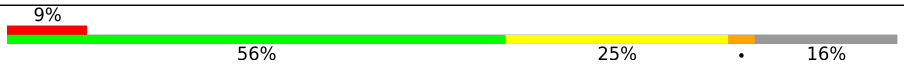
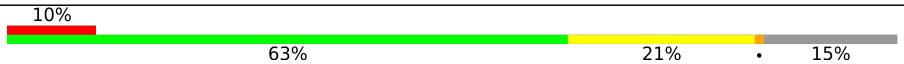
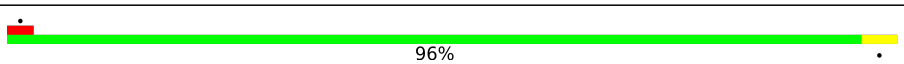
Mol	Chain	Length	Quality of chain
5	I	237	
6	J	237	
7	K	426	
8	L	1114	
9	M	435	
10	N	581	
11	O	483	
12	P	502	
13	Q	78	
14	R	625	
15	S	1359	
16	T	477	
17	U	467	
18	V	157	
19	X	383	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 42577 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	96	Total	C	N	O	S	0	0
			795	501	154	137	3		
1	E	95	Total	C	N	O	S	0	0
			785	495	151	136	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	conflict	UNP P84233
E	102	ALA	GLY	conflict	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	87	Total	C	N	O	S	0	0
			673	423	132	117	1		
2	F	82	Total	C	N	O	S	0	0
			652	412	127	112	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	102	Total	C	N	O	0	0
			788	496	154	138		
3	G	102	Total	C	N	O	0	0
			788	496	154	138		

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	92	Total	C	N	O	S	0	0
			719	453	129	135	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	92	Total	C	N	O	S	0	0
			719	453	129	135	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	conflict	UNP P02281
H	29	THR	SER	conflict	UNP P02281

- Molecule 5 is a DNA chain called DNA-I.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	160	Total	C	N	O	P	0	0
			3256	1547	583	966	160		

- Molecule 6 is a DNA chain called DNA-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	160	Total	C	N	O	P	0	0
			3301	1561	629	952	159		

- Molecule 7 is a protein called Chromatin structure-remodeling complex subunit SFH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	235	Total	C	N	O	S	0	0
			1893	1195	329	362	7		

- Molecule 8 is a protein called Chromatin structure-remodeling complex protein RSC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	596	Total	C	N	O	S	0	0
			4887	3118	818	929	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	108	Total	C	N	O	S	0	0
			879	547	151	179	2		

- Molecule 10 is a protein called Chromatin structure-remodeling complex subunit RSC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	367	Total	C	N	O	S	0	0
			2929	1888	474	551	16		

- Molecule 11 is a protein called Chromatin structure-remodeling complex protein RSC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	212	Total	C	N	O	S	0	0
			1693	1077	280	332	4		

- Molecule 12 is a protein called Chromatin structure-remodeling complex protein RSC58.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	347	Total	C	N	O	S	0	0
			2838	1831	480	519	8		

- Molecule 13 is a protein called High temperature lethal protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	58	Total	C	N	O	S	0	0
			473	290	87	92	4		

- Molecule 14 is a protein called Chromatin structure-remodeling complex subunit RSC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	131	Total	C	N	O	S	0	0
			1087	697	178	206	6		

- Molecule 15 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	783	Total	C	N	O	S	1	0
			4591	2798	883	908	2		

- Molecule 16 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	T	399	Total	C	N	O	S	Se	3	0
			3227	2081	528	603	4	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	MSE	-	initiating methionine	UNP Q12406

- Molecule 17 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	U	396	Total	C	N	O	S	Se	1	0
			3198	2053	523	615	4	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	1	MSE	-	initiating methionine	UNP Q05123

- Molecule 18 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	54	Total	C	N	O	Se	0	0
			490	313	84	92	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	1	MSE	-	initiating methionine	UNP P53330

- Molecule 19 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	383	Total	C	N	O	0	0
			1915	1149	383	383		

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

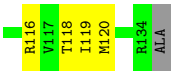
Mol	Chain	Residues	Atoms		AltConf
20	L	1	Total	Zn	0
			1	1	

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.

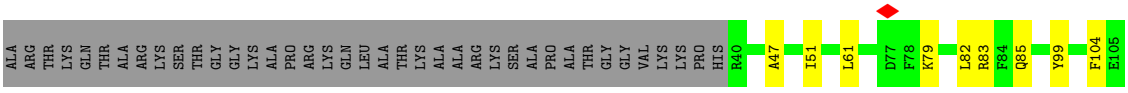
• Molecule 1: Histone H3.2

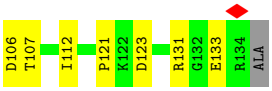
Chain A:



• Molecule 1: Histone H3.2

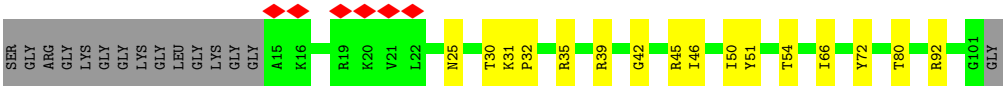
Chain E:





• Molecule 2: Histone H4

Chain B:

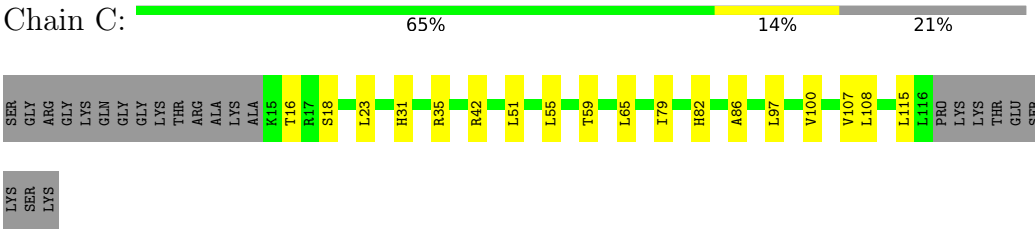


• Molecule 2: Histone H4

Chain F:

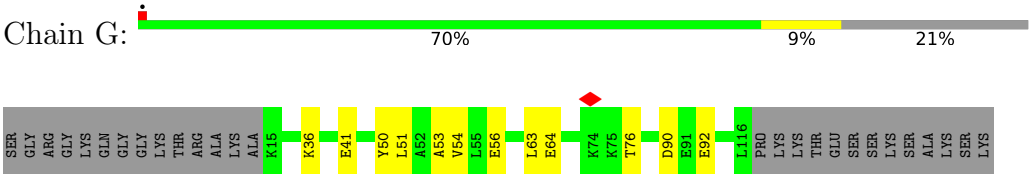
• Molecule 3: Histone H2A

Chain C:



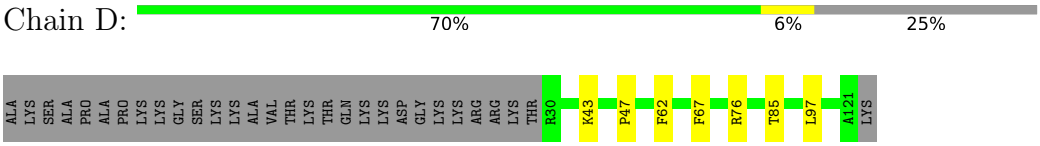
• Molecule 3: Histone H2A

Chain G:



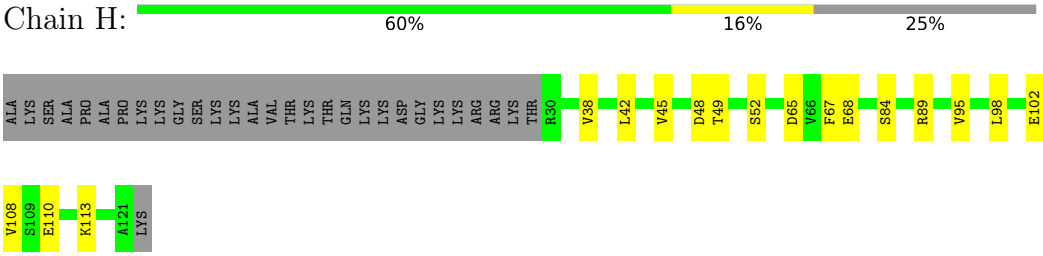
• Molecule 4: Histone H2B 1.1

Chain D:



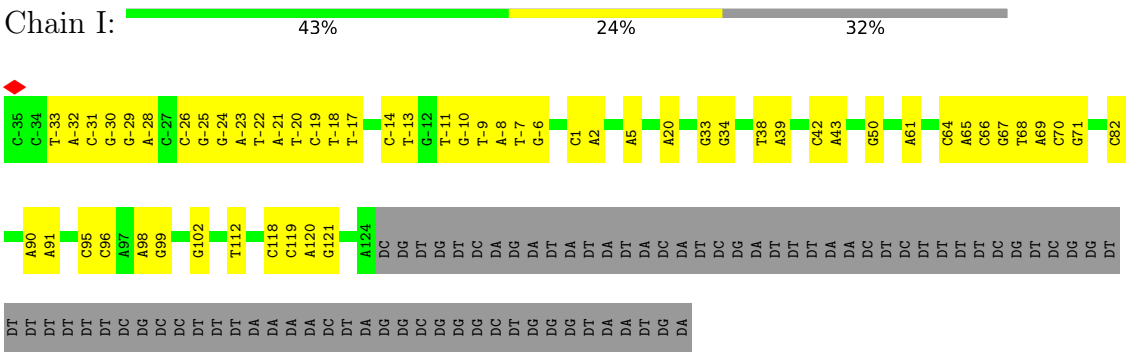
• Molecule 4: Histone H2B 1.1

Chain H:



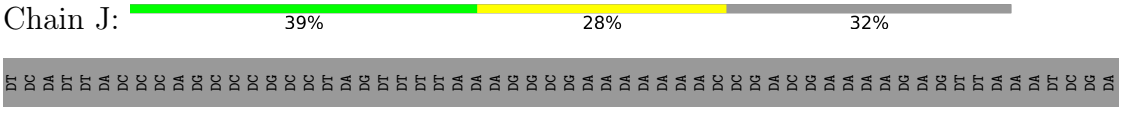
• Molecule 5: DNA-I

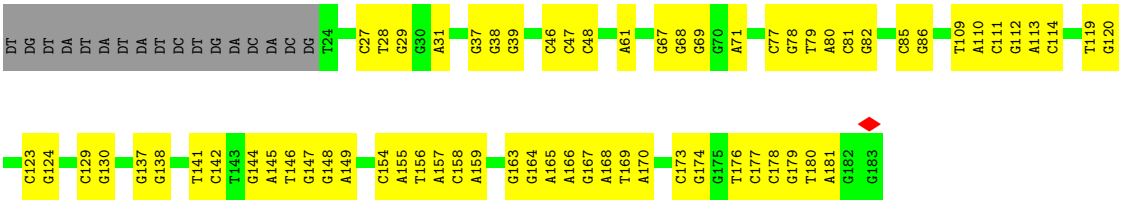
Chain I:



• Molecule 6: DNA-J

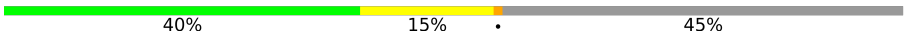
Chain J:

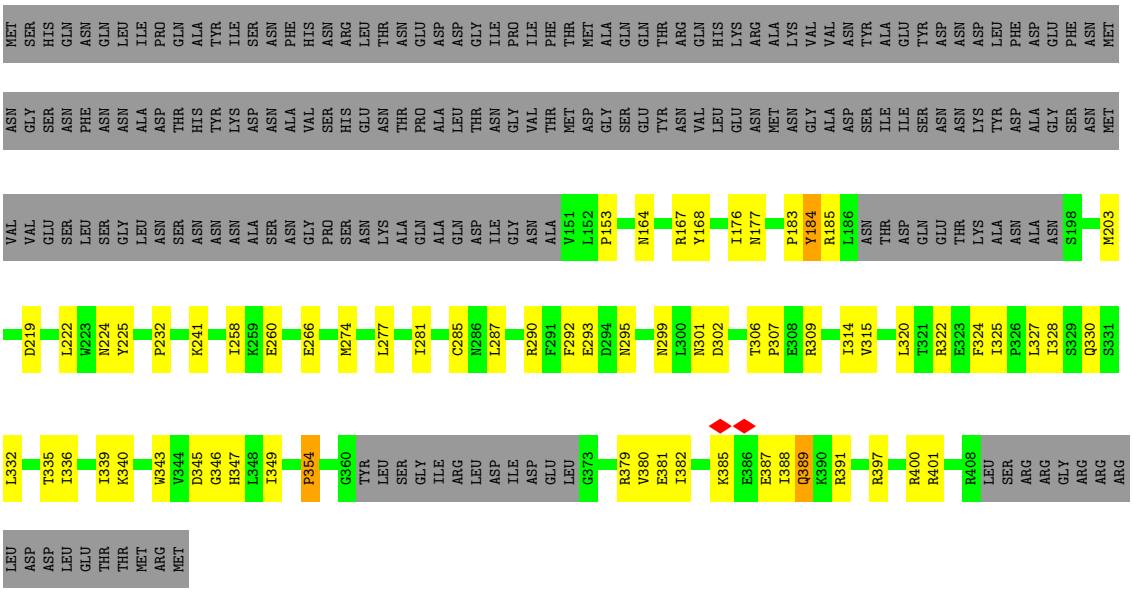




• Molecule 7: Chromatin structure-remodeling complex subunit SFH1

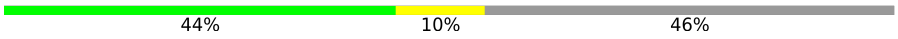
Chain K:

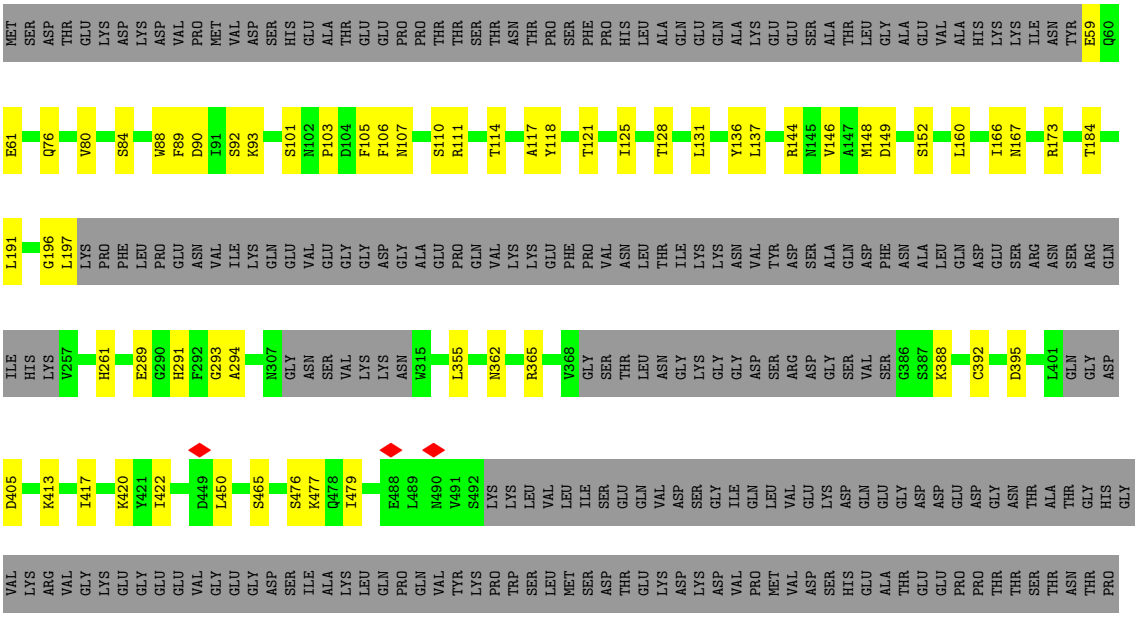


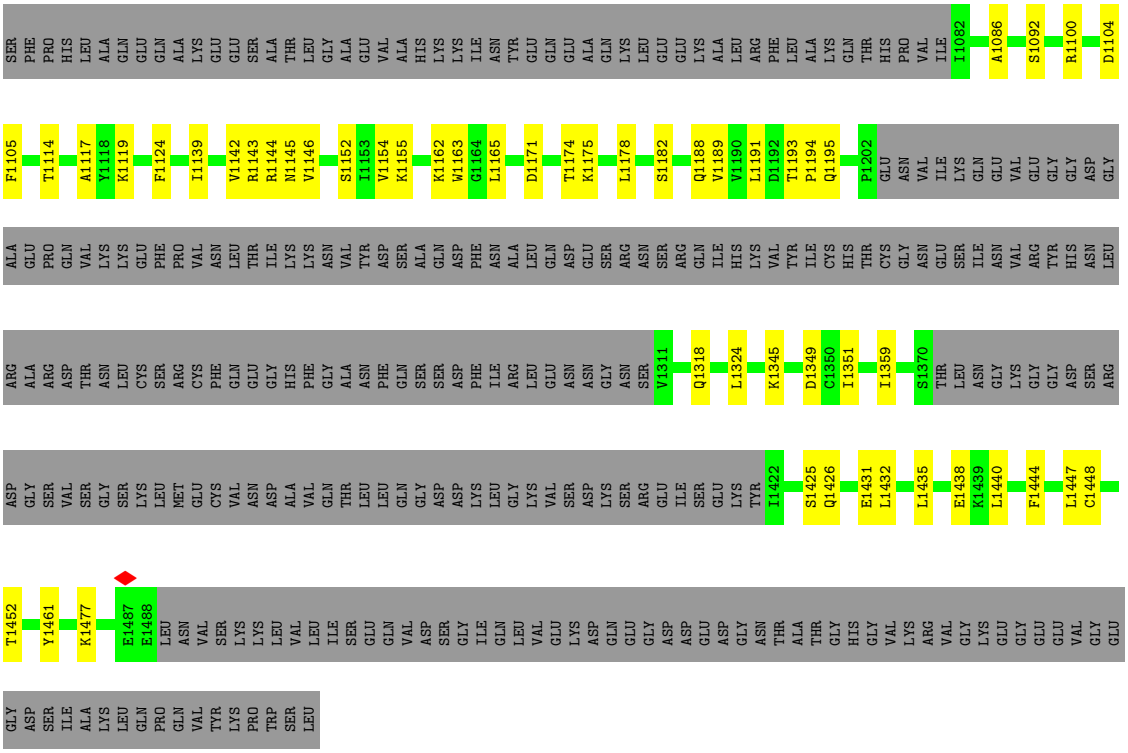


• Molecule 8: Chromatin structure-remodeling complex protein RSC8

Chain L:

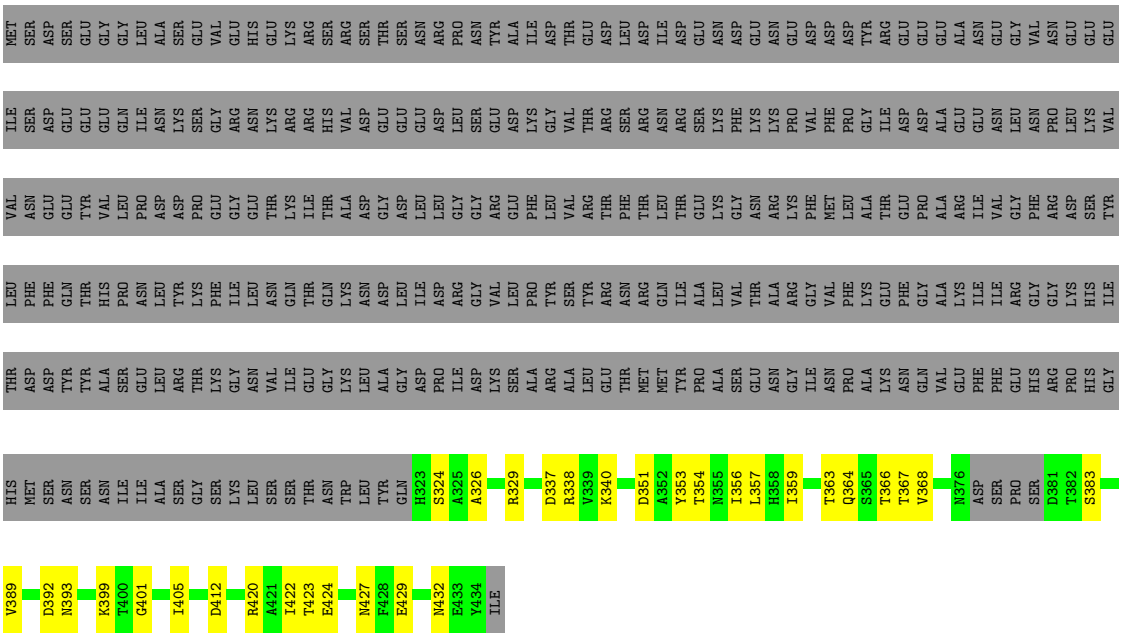






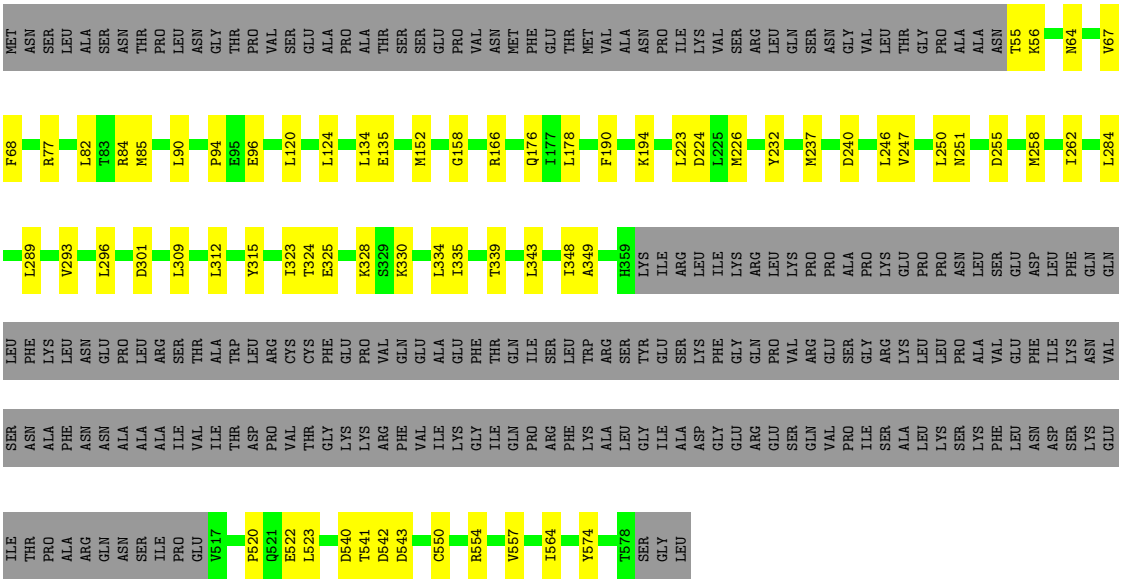
• Molecule 9: Chromatin structure-remodeling complex subunit RSC7

Chain M:



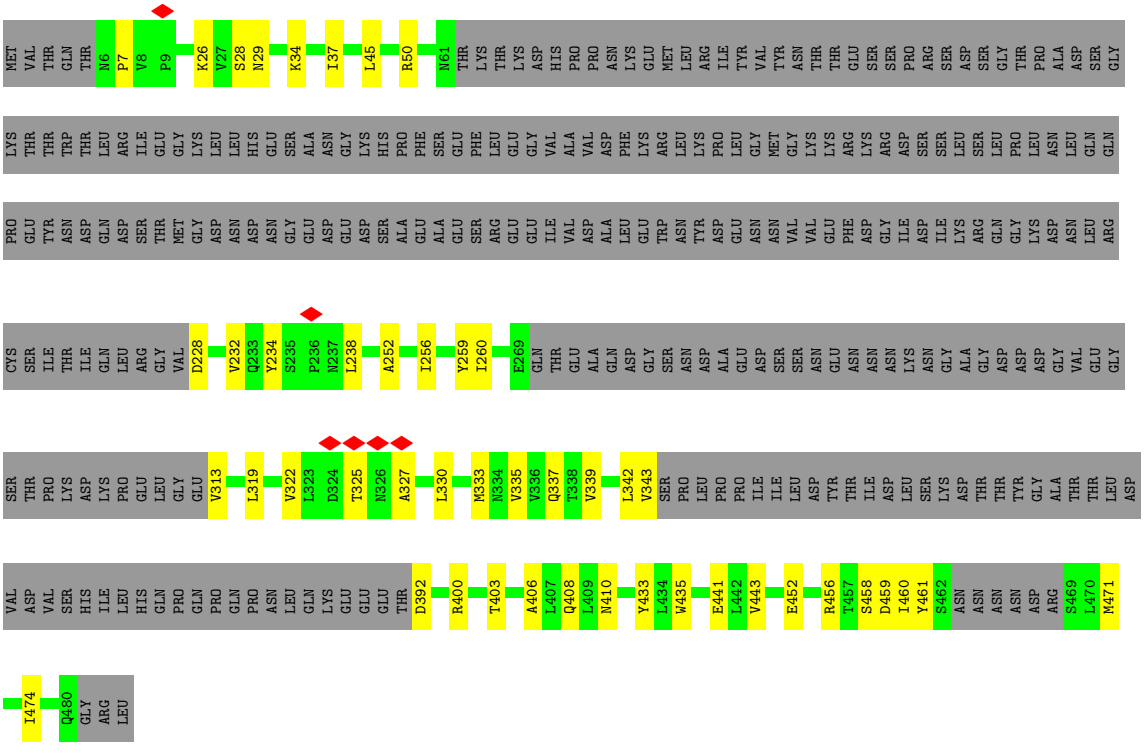
• Molecule 10: Chromatin structure-remodeling complex subunit RSC9

Chain N:



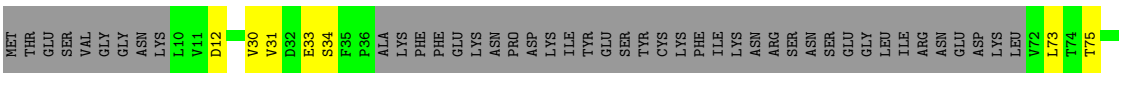
• Molecule 11: Chromatin structure-remodeling complex protein RSC6

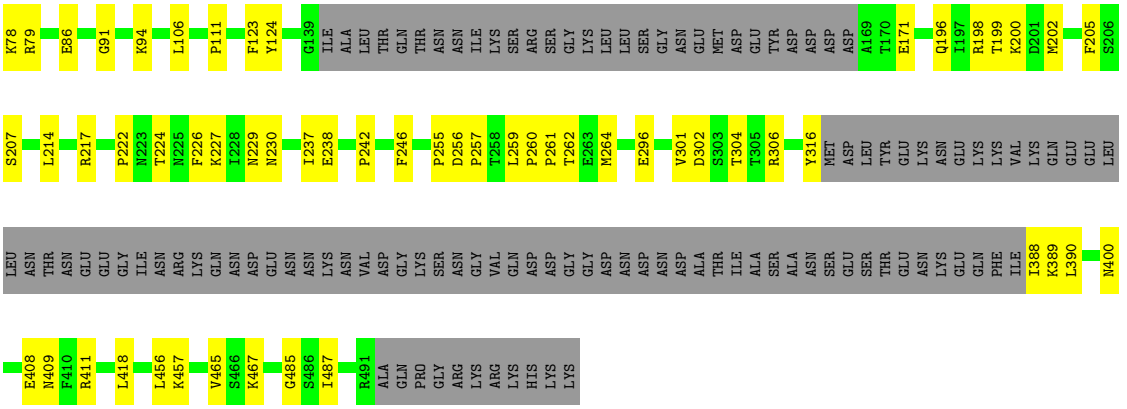
Chain O:



• Molecule 12: Chromatin structure-remodeling complex protein RSC58

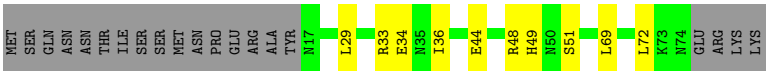
Chain P:





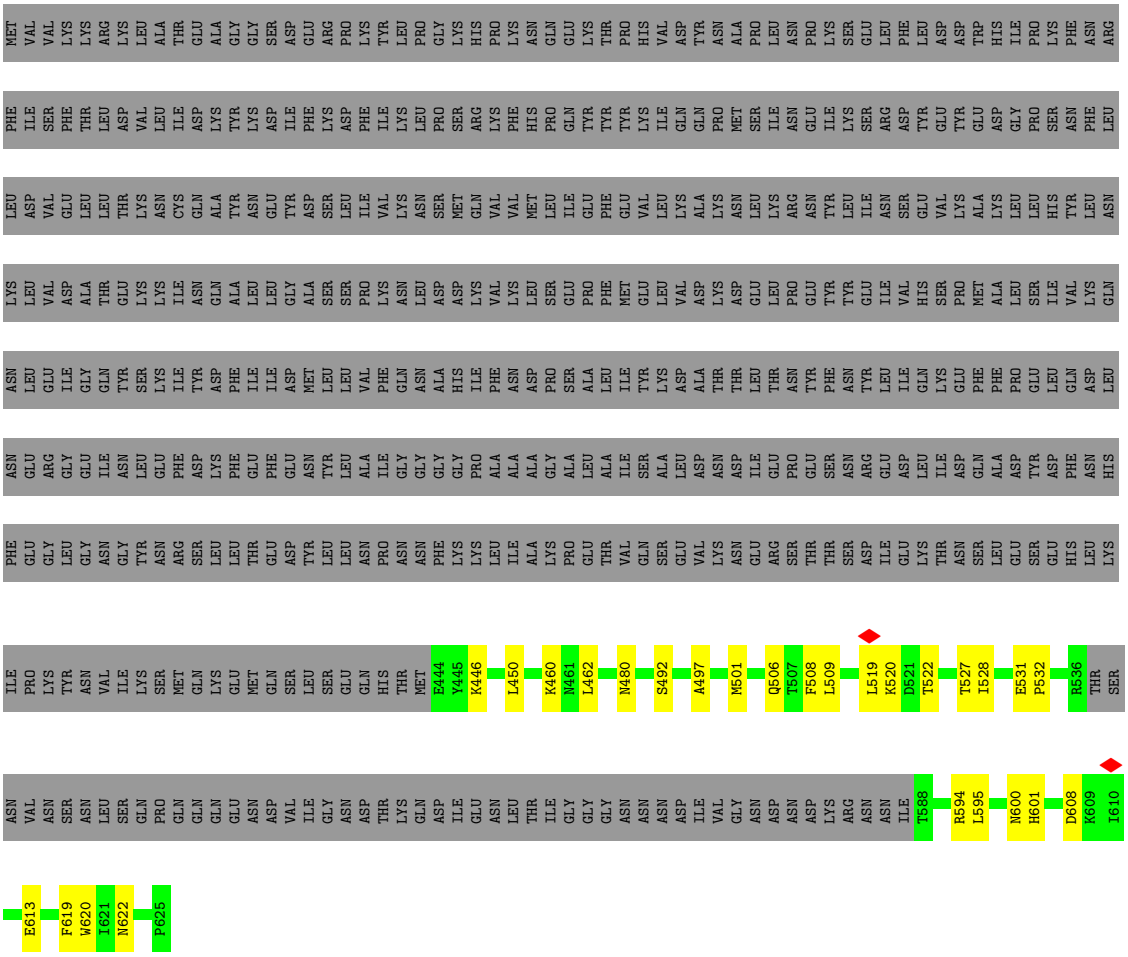
• Molecule 13: High temperature lethal protein 1

Chain Q: 62% 13% 26%



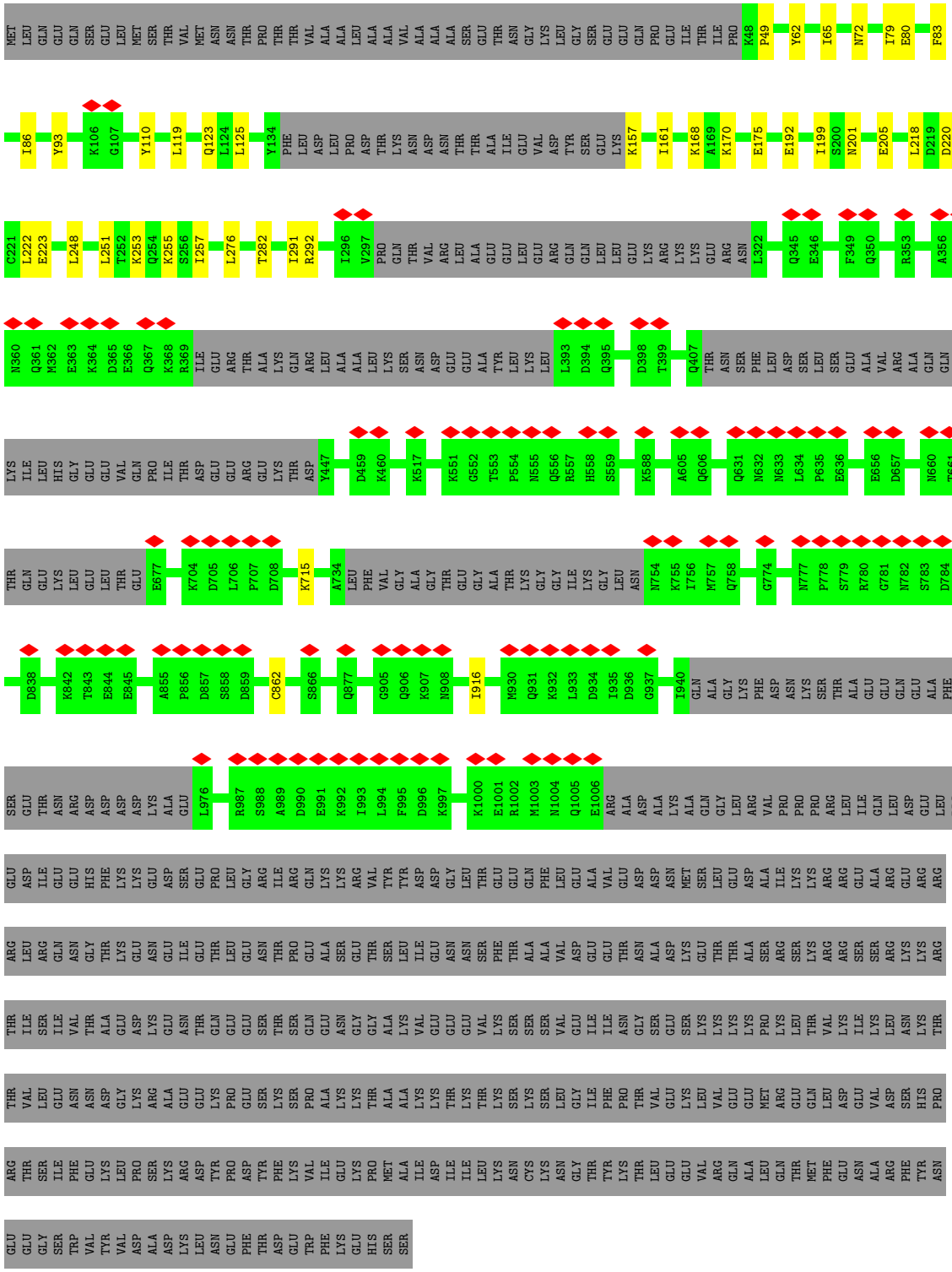
• Molecule 14: Chromatin structure-remodeling complex subunit RSC4

Chain R: 17% 79%



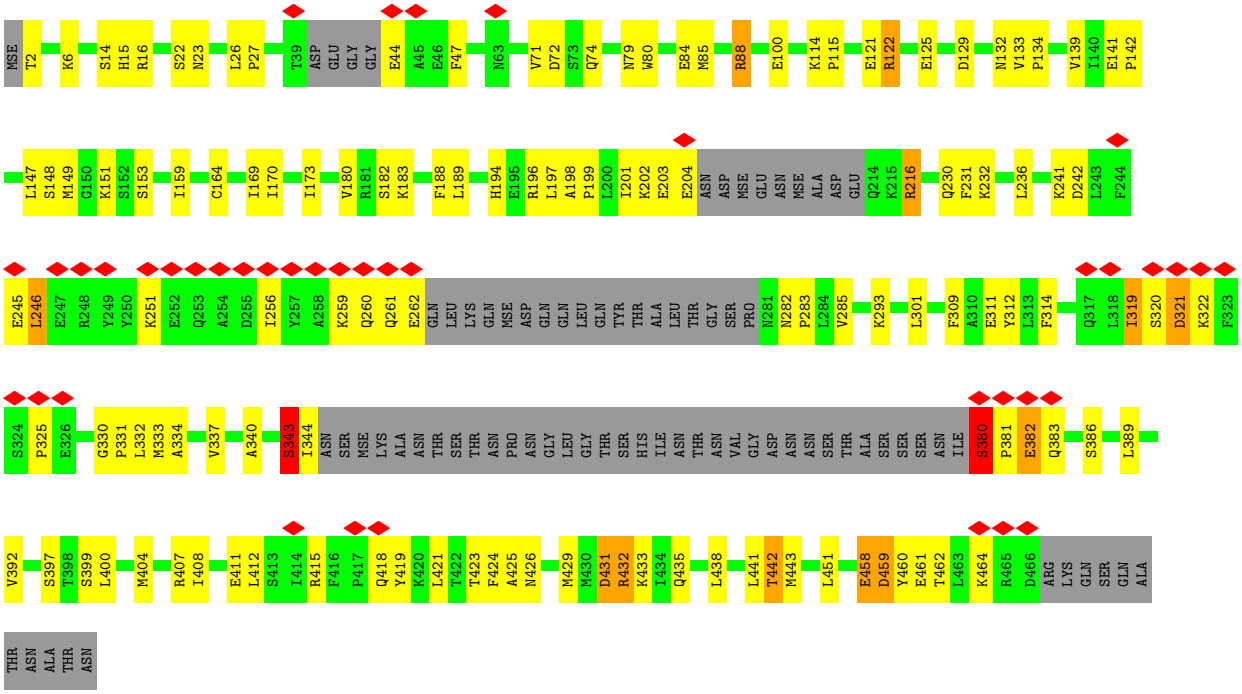
• Molecule 15: Nuclear protein STH1/NPS1

Chain S:



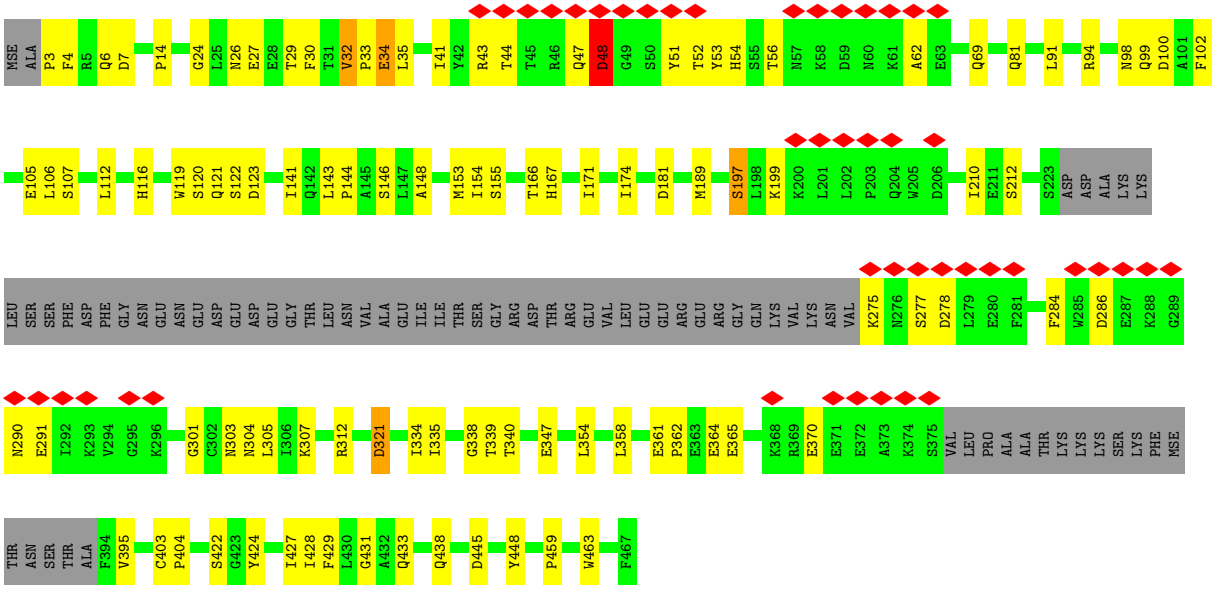
• Molecule 16: Actin-related protein 7

Chain T:



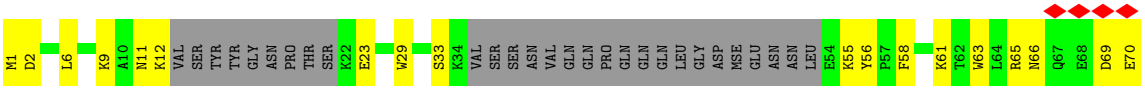
• Molecule 17: Actin-like protein ARP9

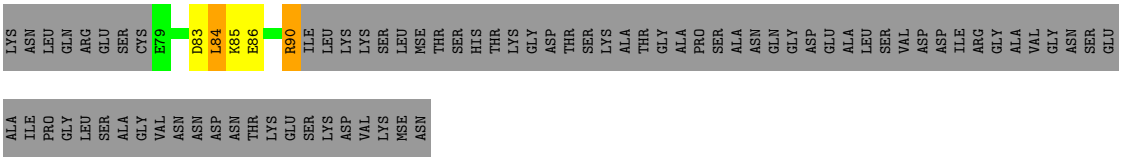
Chain U:



• Molecule 18: Regulator of Ty1 transposition protein 102

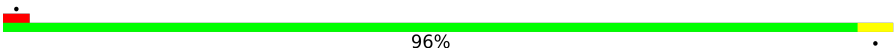
Chain V:

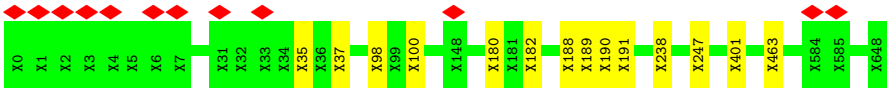




• Molecule 19: Unknown protein

Chain X:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	372442	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.043	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0115	Depositor
Map size (Å)	356.99997, 356.99997, 356.99997	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	A	0.24	0/806	0.36	0/1081
1	E	0.23	0/795	0.36	0/1066
2	B	0.23	0/680	0.39	0/913
2	F	0.23	0/659	0.40	0/883
3	C	0.23	0/797	0.39	0/1076
3	G	0.23	0/797	0.39	0/1076
4	D	0.23	0/730	0.35	0/983
4	H	0.23	0/730	0.36	0/983
5	I	0.48	0/3645	0.89	0/5618
6	J	0.48	0/3710	0.84	0/5730
7	K	0.28	0/1926	0.49	1/2606 (0.0%)
8	L	0.27	0/4977	0.42	0/6699
9	M	0.26	0/893	0.48	0/1210
10	N	0.28	0/2983	0.45	0/4040
11	O	0.27	0/1720	0.44	0/2336
12	P	0.28	0/2903	0.46	0/3940
13	Q	0.24	0/475	0.41	0/636
14	R	0.27	0/1112	0.48	0/1501
15	S	0.27	0/4609	0.43	0/6326
16	T	0.44	0/3292	0.61	1/4432 (0.0%)
17	U	0.45	0/3266	0.59	0/4423
18	V	0.41	0/501	0.57	0/669
All	All	0.34	0/42006	0.57	2/58227 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	354	PRO	N-CA-CB	6.16	110.69	103.30
16	T	380	SER	C-N-CD	5.96	140.91	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	795	0	833	14	0
1	E	785	0	826	11	0
2	B	673	0	692	14	0
2	F	652	0	696	14	0
3	C	788	0	839	13	0
3	G	788	0	839	15	0
4	D	719	0	740	6	0
4	H	719	0	740	15	0
5	I	3256	0	1798	34	0
6	J	3301	0	1793	43	0
7	K	1893	0	1849	54	0
8	L	4887	0	4889	85	0
9	M	879	0	846	28	0
10	N	2929	0	2998	40	0
11	O	1693	0	1696	35	0
12	P	2838	0	2872	48	0
13	Q	473	0	488	10	0
14	R	1087	0	1066	17	0
15	S	4591	0	3071	28	0
16	T	3227	0	3251	107	0
17	U	3198	0	3187	63	0
18	V	490	0	467	21	0
19	X	1915	0	468	9	0
20	L	1	0	0	0	0
All	All	42577	0	36944	613	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 8.

All (613) 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)
16:T:343:SER:CB	16:T:344:ILE:HA	1.81	1.11
16:T:343:SER:HB3	16:T:344:ILE:HA	1.09	1.09
16:T:216:ARG:HG2	16:T:216:ARG:HH11	1.17	1.04
8:L:289:GLU:HB3	8:L:291:HIS:NE2	1.72	1.03
16:T:122:ARG:HG2	16:T:122:ARG:HH11	1.25	1.01
16:T:114:LYS:HG3	16:T:115:PRO:HD3	1.37	1.01
7:K:299:ASN:ND2	7:K:302:ASP:OD2	1.95	0.99
16:T:343:SER:HB3	16:T:344:ILE:CA	1.95	0.96
7:K:387:GLU:HB2	7:K:389:GLN:HG3	1.49	0.95
3:G:64:GLU:CD	7:K:400:ARG:HD2	1.90	0.92
16:T:84:GLU:OE2	16:T:88:ARG:NH1	2.05	0.89
16:T:216:ARG:HG2	16:T:216:ARG:NH1	1.94	0.81
8:L:1171:ASP:OD1	8:L:1174:THR:OG1	2.00	0.80
17:U:459:PRO:HG2	18:V:63:TRP:CD2	2.18	0.79
8:L:1359:ILE:H	15:S:123:GLN:HE22	1.31	0.77
8:L:289:GLU:HB3	8:L:291:HIS:CD2	2.19	0.77
16:T:159:ILE:HD11	16:T:408:ILE:HD11	1.65	0.76
16:T:122:ARG:HH11	16:T:122:ARG:CG	1.99	0.76
16:T:100:GLU:HG2	16:T:132:ASN:HB3	1.68	0.75
14:R:450:LEU:HD21	14:R:613:GLU:HG3	1.67	0.75
16:T:114:LYS:HG3	16:T:115:PRO:CD	2.14	0.75
1:E:83:ARG:HB2	2:F:80:THR:HG22	1.69	0.73
3:G:90:ASP:CG	7:K:397:ARG:HH22	1.91	0.73
8:L:1182:SER:HA	9:M:364:GLN:HE21	1.53	0.72
10:N:250:LEU:HB2	10:N:262:ILE:HG21	1.70	0.72
18:V:84:LEU:O	18:V:85:LYS:HB2	1.89	0.72
8:L:289:GLU:CB	8:L:291:HIS:NE2	2.50	0.71
8:L:1194:PRO:HG3	10:N:84:ARG:HD3	1.72	0.71
16:T:344:ILE:HG23	16:T:344:ILE:O	1.92	0.70
16:T:183:LYS:O	16:T:183:LYS:HG2	1.91	0.70
7:K:183:PRO:HG2	7:K:185:ARG:HH12	1.57	0.69
18:V:1:MSE:HG2	18:V:2:ASP:N	2.06	0.69
16:T:14:SER:HA	16:T:71:VAL:HB	1.74	0.69
8:L:92:SER:HB3	9:M:367:THR:HA	1.76	0.68
11:O:441:GLU:OE2	13:Q:33:ARG:NH2	2.26	0.68
16:T:392:VAL:HB	16:T:423:THR:HG22	1.75	0.68
17:U:98:ASN:O	17:U:99:GLN:HG2	1.93	0.68
17:U:107:SER:O	18:V:11:ASN:HA	1.95	0.67
16:T:311:GLU:OE2	16:T:407:ARG:NH2	2.28	0.67
8:L:1100:ARG:NH1	9:M:412:ASP:OD2	2.27	0.67
16:T:139:VAL:HG11	16:T:443:MSE:HG3	1.76	0.67
14:R:480:ASN:O	14:R:506:GLN:NE2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:111:PRO:O	12:P:217:ARG:NH2	2.28	0.67
17:U:275:LYS:HB3	17:U:278:ASP:OD2	1.94	0.66
12:P:199:THR:HG23	12:P:200:LYS:H	1.60	0.66
5:I:33:DG:H2"	5:I:34:DG:H5"	1.77	0.65
7:K:184:TYR:HD2	7:K:241:LYS:HD3	1.61	0.65
16:T:458:GLU:HG2	16:T:459:ASP:N	2.10	0.65
15:S:222:LEU:HD21	19:X:247:UNK:CB	2.26	0.65
8:L:261:HIS:ND1	8:L:261:HIS:O	2.29	0.65
2:F:90:LEU:HB3	2:F:95:ARG:HG3	1.79	0.65
3:G:64:GLU:OE1	7:K:400:ARG:HB3	1.96	0.64
15:S:170:LYS:HA	15:S:175:GLU:HB3	1.78	0.64
16:T:180:VAL:HG11	16:T:332:LEU:HG	1.78	0.64
16:T:148:SER:HB2	16:T:442:THR:HG21	1.79	0.64
16:T:121:GLU:O	16:T:125:GLU:HG3	1.98	0.64
6:J:158:DC:H2"	6:J:159:DA:C8	2.33	0.64
8:L:1162:LYS:HD3	9:M:405:ILE:HG12	1.80	0.64
11:O:452:GLU:HG2	12:P:264:MET:HB3	1.79	0.64
3:G:64:GLU:OE2	7:K:400:ARG:HD2	1.97	0.63
8:L:1318:GLN:NE2	19:X:238:UNK:O	2.27	0.63
5:I:102:DG:N2	6:J:47:DC:O2	2.31	0.63
11:O:319:LEU:HA	11:O:322:VAL:HG12	1.81	0.63
12:P:255:PRO:HB3	12:P:259:LEU:HD12	1.80	0.63
15:S:62:TYR:HB2	15:S:79:ILE:HG21	1.81	0.63
9:M:366:THR:HG22	9:M:367:THR:HG23	1.80	0.62
8:L:1425:SER:OG	8:L:1426:GLN:NE2	2.33	0.62
12:P:465:VAL:HG12	15:S:110:TYR:HB3	1.80	0.62
16:T:153:SER:HA	16:T:169:ILE:O	1.99	0.62
6:J:167:DG:H2"	6:J:168:DA:C8	2.34	0.62
7:K:293:GLU:OE1	7:K:391:ARG:NH2	2.33	0.62
7:K:380:VAL:HA	8:L:1144:ARG:HH12	1.64	0.61
7:K:225:TYR:CZ	7:K:266:GLU:HG2	2.35	0.61
8:L:1175:LYS:O	9:M:338:ARG:NH1	2.33	0.61
17:U:189:MSE:HE2	17:U:305:LEU:HA	1.82	0.61
7:K:287:LEU:HB2	7:K:327:LEU:HD22	1.82	0.61
12:P:389:LYS:HD2	15:S:83:PHE:HB3	1.82	0.61
17:U:47:GLN:O	17:U:48:ASP:HB3	1.99	0.61
4:H:102:GLU:OE2	7:K:397:ARG:HG2	2.01	0.61
8:L:1435:LEU:HB3	13:Q:72:LEU:HD23	1.81	0.61
16:T:256:ILE:O	16:T:260:GLN:HB2	2.01	0.61
16:T:382:GLU:H	16:T:382:GLU:CD	2.03	0.61
16:T:203:GLU:O	16:T:204:GLU:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:330:GLY:HA2	16:T:333:MSE:HE2	1.83	0.60
17:U:53:TYR:CD1	17:U:81:GLN:HG3	2.37	0.60
9:M:363:THR:OG1	9:M:364:GLN:OE1	2.19	0.60
16:T:429:MSE:HE3	17:U:321:ASP:O	2.01	0.60
8:L:106:PHE:O	8:L:107:ASN:ND2	2.35	0.60
8:L:131:LEU:HD21	8:L:1182:SER:HB2	1.84	0.60
14:R:446:LYS:H	14:R:492:SER:HB2	1.65	0.60
8:L:289:GLU:CB	8:L:291:HIS:CE1	2.85	0.59
11:O:256:ILE:HD13	11:O:339:VAL:HG22	1.84	0.59
14:R:522:THR:HG23	14:R:608:ASP:HA	1.83	0.59
12:P:31:VAL:O	12:P:75:THR:OG1	2.20	0.59
17:U:44:THR:OG1	17:U:62:ALA:HB2	2.02	0.59
17:U:199:LYS:HD2	17:U:210:ILE:HD13	1.85	0.59
5:I:118:DC:H2"	5:I:119:DC:H5'	1.85	0.59
2:B:72:TYR:OH	4:D:76:ARG:NH2	2.35	0.59
7:K:277:LEU:HD12	7:K:349:ILE:CB	2.33	0.59
16:T:400:LEU:HD12	16:T:433:LYS:HE2	1.84	0.59
17:U:35:LEU:HD11	18:V:84:LEU:HD13	1.84	0.59
16:T:380:SER:O	16:T:383:GLN:HB2	2.03	0.58
16:T:334:ALA:HB2	16:T:415:ARG:HD3	1.85	0.58
16:T:389:LEU:HB3	16:T:421:LEU:HD23	1.84	0.58
18:V:29:TRP:CD2	18:V:61:LYS:HD3	2.38	0.58
7:K:314:ILE:HD11	8:L:1143:ARG:HH12	1.68	0.58
7:K:315:VAL:HG11	7:K:325:ILE:HG12	1.86	0.58
11:O:325:THR:HG22	11:O:327:ALA:H	1.68	0.58
5:I:-18:DT:H2"	5:I:-17:DT:C6	2.38	0.58
6:J:111:DC:H2"	6:J:112:DG:C8	2.39	0.58
16:T:159:ILE:HG23	16:T:164:CYS:SG	2.44	0.58
2:F:92:ARG:HH21	4:H:98:LEU:HA	1.68	0.58
16:T:381:PRO:HG2	16:T:382:GLU:OE2	2.04	0.58
7:K:335:THR:O	7:K:339:ILE:HG12	2.04	0.57
7:K:343:TRP:HA	7:K:347:HIS:CB	2.34	0.57
10:N:348:ILE:HD13	10:N:564:ILE:HD13	1.85	0.57
16:T:343:SER:CB	16:T:344:ILE:CA	2.66	0.57
17:U:141:ILE:HG12	17:U:448:TYR:HB3	1.85	0.57
3:C:42:ARG:HB2	4:D:85:THR:HG22	1.86	0.57
9:M:351:ASP:OD2	9:M:354:THR:N	2.33	0.57
16:T:241:LYS:NZ	16:T:245:GLU:HB3	2.19	0.57
1:A:69:ARG:HB3	2:B:25:ASN:HD21	1.70	0.57
10:N:335:ILE:HD11	11:O:45:LEU:HD21	1.87	0.57
6:J:67:DG:H2"	6:J:68:DG:N7	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:ARG:NH2	4:D:97:LEU:O	2.38	0.57
2:B:30:THR:HG21	6:J:61:DA:H5"	1.87	0.56
16:T:194:HIS:NE2	16:T:203:GLU:OE1	2.39	0.56
8:L:80:VAL:HG23	8:L:1189:VAL:HA	1.87	0.56
10:N:293:VAL:HG12	10:N:312:LEU:HD11	1.86	0.56
16:T:216:ARG:HH11	16:T:216:ARG:CG	2.04	0.56
16:T:418:GLN:HG3	16:T:418:GLN:O	2.03	0.56
3:G:64:GLU:OE2	7:K:400:ARG:CG	2.54	0.56
11:O:408:GLN:NE2	12:P:316:TYR:OH	2.39	0.56
16:T:72:ASP:OD1	16:T:74:GLN:HB2	2.05	0.56
5:I:-20:DT:H2"	5:I:-19:DC:C5	2.41	0.56
8:L:184:THR:OG1	9:M:383:SER:O	2.24	0.56
14:R:497:ALA:HB1	14:R:620:TRP:HZ3	1.71	0.56
7:K:332:LEU:O	7:K:335:THR:OG1	2.22	0.56
7:K:381:GLU:OE1	8:L:1144:ARG:NH2	2.39	0.56
11:O:410:ASN:ND2	12:P:304:THR:OG1	2.38	0.56
12:P:260:PRO:N	12:P:261:PRO:HD2	2.21	0.56
13:Q:34:GLU:OE2	13:Q:48:ARG:NH2	2.39	0.56
16:T:44:GLU:HG2	16:T:44:GLU:O	2.05	0.56
7:K:380:VAL:CG1	7:K:382:ILE:HG12	2.36	0.56
8:L:149:ASP:OD1	8:L:152:SER:OG	2.13	0.56
7:K:322:ARG:HH22	8:L:1178:LEU:HD21	1.70	0.56
8:L:1448:CYS:O	8:L:1452:THR:HG23	2.06	0.56
10:N:247:VAL:O	10:N:251:ASN:ND2	2.39	0.56
16:T:26:LEU:HB3	16:T:27:PRO:HD2	1.88	0.56
14:R:462:LEU:HD12	14:R:508:PHE:HD2	1.72	0.55
18:V:69:ASP:O	18:V:70:GLU:HG3	2.07	0.55
16:T:147:LEU:CD2	16:T:443:MSE:SE	3.04	0.55
16:T:196:ARG:NH2	16:T:312:TYR:OH	2.39	0.55
1:E:85:GLN:NE2	5:I:50:DG:OP1	2.39	0.55
16:T:216:ARG:NE	16:T:216:ARG:HA	2.20	0.55
8:L:1440:LEU:O	8:L:1444:PHE:HB2	2.06	0.55
10:N:301:ASP:HB3	11:O:7:PRO:HD3	1.89	0.55
11:O:28:SER:O	11:O:29:ASN:ND2	2.39	0.55
16:T:426:ASN:HB3	16:T:432:ARG:HG2	1.89	0.55
14:R:527:THR:HA	14:R:532:PRO:HA	1.89	0.55
12:P:34:SER:HB3	12:P:73:LEU:HB3	1.89	0.55
10:N:82:LEU:HD21	10:N:120:LEU:HD11	1.88	0.55
2:F:30:THR:HG21	5:I:61:DA:H5"	1.89	0.54
6:J:164:DG:H2"	6:J:165:DA:C8	2.42	0.54
7:K:232:PRO:HB3	7:K:258:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:388:ILE:HD12	7:K:391:ARG:HH22	1.72	0.54
10:N:67:VAL:HG23	10:N:68:PHE:HD1	1.72	0.54
11:O:238:LEU:HD22	11:O:342:LEU:HD22	1.89	0.54
12:P:301:VAL:HG21	12:P:306:ARG:HB2	1.89	0.54
5:I:98:DA:H2"	5:I:99:DG:C8	2.42	0.54
8:L:76:GLN:OE1	8:L:1188:GLN:N	2.39	0.54
16:T:333:MSE:HE3	16:T:412:LEU:HD13	1.87	0.54
5:I:-7:DT:H2"	5:I:-6:DG:C8	2.43	0.54
10:N:315:TYR:OH	10:N:325:GLU:OE1	2.25	0.54
17:U:43:ARG:HG3	17:U:53:TYR:CE2	2.42	0.54
17:U:275:LYS:HE3	17:U:277:SER:H	1.73	0.54
6:J:156:DT:H2"	6:J:157:DA:C8	2.43	0.54
8:L:105:PHE:HD2	8:L:118:TYR:HB2	1.73	0.54
7:K:307:PRO:HB3	7:K:332:LEU:HD22	1.88	0.54
15:S:253:LYS:HE3	15:S:257:ILE:HD11	1.91	0.53
7:K:292:PHE:HZ	7:K:328:ILE:HD12	1.74	0.53
8:L:101:SER:OG	8:L:103:PRO:HD2	2.08	0.53
10:N:330:LYS:HE2	10:N:334:LEU:HD21	1.91	0.53
16:T:216:ARG:NH1	16:T:216:ARG:CG	2.69	0.53
16:T:261:GLN:HB2	16:T:262:GLU:OE1	2.08	0.53
1:E:79:LYS:HB3	1:E:82:LEU:HD11	1.91	0.53
3:G:76:THR:HA	4:H:49:THR:HG22	1.91	0.53
14:R:508:PHE:HE1	14:R:594:ARG:HE	1.54	0.53
19:X:189:UNK:O	19:X:191:UNK:N	2.42	0.53
5:I:-22:DT:H2"	5:I:-21:DA:N7	2.24	0.53
8:L:294:ALA:HA	12:P:485:GLY:HA3	1.89	0.53
3:C:100:VAL:HG21	2:F:98:TYR:CZ	2.44	0.52
7:K:379:ARG:O	8:L:1144:ARG:NH1	2.43	0.52
8:L:422:ILE:HD13	11:O:26:LYS:HG2	1.91	0.52
9:M:424:GLU:HA	9:M:427:ASN:HD21	1.75	0.52
11:O:232:VAL:HG11	11:O:343:VAL:HB	1.91	0.52
16:T:147:LEU:HD22	16:T:443:MSE:SE	2.59	0.52
16:T:438:LEU:O	16:T:442:THR:HG23	2.08	0.52
1:A:83:ARG:HB2	2:B:80:THR:HG22	1.90	0.52
1:E:121:PRO:HB3	2:F:53:GLU:HG3	1.92	0.52
5:I:-26:DC:H2"	5:I:-25:DG:C8	2.44	0.52
3:G:64:GLU:OE2	7:K:400:ARG:CD	2.56	0.52
7:K:203:MET:SD	7:K:224:ASN:HB2	2.49	0.52
16:T:6:LYS:HE3	17:U:121:GLN:OE1	2.09	0.52
1:A:113:HIS:NE2	1:E:123:ASP:OD1	2.41	0.52
2:F:64:ASN:OD1	2:F:67:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:30:VAL:HG11	12:P:123:PHE:CE2	2.44	0.52
16:T:399:SER:OG	16:T:432:ARG:NH1	2.42	0.52
17:U:34:GLU:CD	17:U:34:GLU:H	2.13	0.52
17:U:43:ARG:HD3	17:U:51:TYR:CD1	2.44	0.52
6:J:129:DC:H2"	6:J:130:DG:C8	2.44	0.52
18:V:1:MSE:HG2	18:V:2:ASP:H	1.72	0.52
8:L:1162:LYS:HG3	9:M:401:GLY:HA3	1.91	0.52
8:L:1431:GLU:HG2	13:Q:69:LEU:HD11	1.92	0.52
11:O:392:ASP:OD1	11:O:392:ASP:N	2.40	0.52
16:T:381:PRO:C	16:T:383:GLN:H	2.11	0.52
10:N:296:LEU:HB3	10:N:339:THR:HG21	1.92	0.52
2:F:77:LYS:HG2	4:H:89:ARG:HH12	1.75	0.51
12:P:79:ARG:HH21	12:P:94:LYS:HD3	1.75	0.51
8:L:88:TRP:O	8:L:89:PHE:HB3	2.10	0.51
14:R:595:LEU:HB3	14:R:600:ASN:HD21	1.74	0.51
7:K:153:PRO:HB3	7:K:168:TYR:CE2	2.46	0.51
7:K:219:ASP:OD1	7:K:219:ASP:N	2.42	0.51
16:T:80:TRP:NE1	16:T:122:ARG:HD3	2.25	0.51
17:U:47:GLN:O	17:U:48:ASP:CB	2.59	0.51
17:U:335:ILE:HG22	17:U:340:THR:HG21	1.93	0.51
3:C:16:THR:HA	6:J:31:DA:H5"	1.93	0.51
12:P:256:ASP:OD1	12:P:256:ASP:N	2.40	0.51
8:L:392:CYS:HA	8:L:395:ASP:OD2	2.11	0.51
16:T:133:VAL:HG13	16:T:134:PRO:HD2	1.91	0.51
5:I:-29:DG:H2"	5:I:-28:DA:C8	2.46	0.51
6:J:28:DT:H2"	6:J:29:DG:C8	2.45	0.51
6:J:113:DA:H2"	6:J:114:DC:H5"	1.92	0.51
16:T:197:LEU:HD11	16:T:231:PHE:CZ	2.45	0.51
16:T:201:ILE:O	16:T:202:LYS:HB2	2.11	0.51
10:N:237:MET:HG3	10:N:240:ASP:HB2	1.92	0.51
11:O:313:VAL:N	11:O:330:LEU:O	2.44	0.51
16:T:399:SER:HA	16:T:404:MSE:HG2	1.92	0.51
17:U:32:VAL:HG23	17:U:33:PRO:HD2	1.92	0.51
17:U:116[B]:HIS:HD2	17:U:119:TRP:CZ2	2.29	0.51
18:V:85:LYS:O	18:V:90:ARG:NH1	2.44	0.50
10:N:550:CYS:HB3	10:N:574:TYR:HE1	1.75	0.50
6:J:27:DC:H2"	6:J:28:DT:C5	2.46	0.50
6:J:81:DC:H2"	6:J:82:DG:C8	2.45	0.50
6:J:173:DC:H2"	6:J:174:DG:C8	2.46	0.50
8:L:289:GLU:CB	8:L:291:HIS:CD2	2.94	0.50
1:E:47:ALA:O	1:E:51:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:78:DG:H2"	6:J:79:DT:C5	2.46	0.50
8:L:1104:ASP:OD2	8:L:1155:LYS:NZ	2.43	0.50
10:N:166:ARG:NH1	15:S:291:ILE:O	2.44	0.50
10:N:541:THR:HG22	10:N:542:ASP:N	2.27	0.50
16:T:141:GLU:HB3	16:T:142:PRO:HD3	1.94	0.50
8:L:1139:ILE:HD13	8:L:1154:VAL:HG22	1.92	0.50
3:C:100:VAL:HG23	2:F:96:THR:HB	1.93	0.50
17:U:102:PHE:HZ	18:V:6:LEU:CD2	2.25	0.50
17:U:189:MSE:HE2	17:U:305:LEU:CA	2.41	0.50
1:E:104:PHE:HA	1:E:107:THR:HG22	1.94	0.50
9:M:399:LYS:HE3	9:M:429:GLU:OE2	2.11	0.50
16:T:22:SER:HA	16:T:441:LEU:CD1	2.42	0.50
16:T:418:GLN:HG2	16:T:419:TYR:CE1	2.46	0.50
3:C:115:LEU:HD11	1:E:112:ILE:HG12	1.94	0.50
11:O:458:SER:O	11:O:458:SER:OG	2.27	0.50
15:S:161:ILE:HD12	15:S:168:LYS:HG3	1.94	0.50
17:U:171:ILE:HD13	17:U:312:ARG:CG	2.42	0.50
3:G:41:GLU:HG2	4:H:84:SER:HB2	1.93	0.50
6:J:180:DT:H2"	6:J:181:DA:C8	2.47	0.49
6:J:69:DG:H5'	6:J:69:DG:C8	2.47	0.49
8:L:90:ASP:OD1	8:L:93:LYS:N	2.41	0.49
16:T:407:ARG:O	16:T:411:GLU:HB2	2.12	0.49
8:L:1351:ILE:HD11	12:P:457:LYS:HG3	1.93	0.49
16:T:460:TYR:CZ	16:T:464:LYS:HE3	2.47	0.49
12:P:296:GLU:HB3	12:P:302:ASP:OD1	2.12	0.49
6:J:137:DG:H2"	6:J:138:DG:C8	2.48	0.49
14:R:528:ILE:O	14:R:531:GLU:HG2	2.13	0.49
1:A:104:PHE:HA	1:A:107:THR:HG22	1.94	0.49
8:L:1193:THR:HG22	8:L:1195:GLN:H	1.78	0.49
17:U:303:ASN:OD1	17:U:307:LYS:NZ	2.45	0.49
16:T:241:LYS:O	16:T:242:ASP:C	2.52	0.49
1:A:108:ASN:ND2	2:B:42:GLY:O	2.46	0.49
5:I:95:DC:H2'	5:I:96:DC:C6	2.48	0.48
11:O:333:MET:O	11:O:337:GLN:HG2	2.13	0.48
6:J:144:DG:H2"	6:J:145:DA:C8	2.47	0.48
10:N:166:ARG:NH2	10:N:224:ASP:OD2	2.36	0.48
12:P:389:LYS:NZ	15:S:80:GLU:OE2	2.40	0.48
16:T:170:ILE:O	16:T:173:ILE:HG22	2.13	0.48
1:E:99:TYR:OH	1:E:133:GLU:OE1	2.31	0.48
12:P:257:PRO:HB3	15:S:251:LEU:HD23	1.94	0.48
1:E:61:LEU:HD12	2:F:37:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:176:ILE:HG13	7:K:177:ASN:N	2.27	0.48
10:N:349:ALA:O	10:N:520:PRO:HG3	2.14	0.48
16:T:458:GLU:O	16:T:461:GLU:N	2.47	0.48
8:L:84:SER:HA	8:L:1191:LEU:HD22	1.96	0.48
8:L:362:ASN:OD1	8:L:365:ARG:NH2	2.45	0.48
8:L:450:LEU:HD21	11:O:50:ARG:HG3	1.96	0.48
12:P:86:GLU:H	12:P:91:GLY:HA3	1.78	0.48
12:P:409:ASN:HD22	12:P:418:LEU:HB2	1.78	0.48
3:G:64:GLU:OE2	7:K:400:ARG:HG2	2.13	0.48
7:K:336:ILE:HG22	7:K:340:LYS:HE2	1.96	0.48
17:U:286:ASP:HB3	17:U:290:ASN:H	1.79	0.48
6:J:77:DC:H2"	6:J:78:DG:C8	2.49	0.48
15:S:199:ILE:HG23	15:S:248:LEU:HD22	1.96	0.48
17:U:148:ALA:O	17:U:431:GLY:HA3	2.14	0.48
17:U:286:ASP:HB2	17:U:290:ASN:HB2	1.95	0.48
12:P:196:GLN:HB2	12:P:205:PHE:HD1	1.79	0.48
12:P:229:ASN:HA	14:R:497:ALA:HB3	1.95	0.47
15:S:65:ILE:HD12	15:S:72:ASN:HD21	1.79	0.47
16:T:188:PHE:HZ	16:T:319:ILE:HD13	1.79	0.47
16:T:389:LEU:O	16:T:421:LEU:HA	2.13	0.47
15:S:276:LEU:O	15:S:282:THR:HG21	2.14	0.47
17:U:364:GLU:HG2	17:U:365:GLU:N	2.29	0.47
5:I:1:DC:H2"	5:I:2:DA:N7	2.29	0.47
19:X:180:UNK:C	19:X:182:UNK:H	2.27	0.47
4:H:110:GLU:HA	4:H:113:LYS:HD3	1.95	0.47
8:L:1345:LYS:HD2	8:L:1349:ASP:HB2	1.97	0.47
9:M:326:ALA:HA	9:M:329:ARG:HB2	1.97	0.47
10:N:323:ILE:HD12	10:N:540:ASP:OD1	2.14	0.47
17:U:120:SER:HB2	17:U:123:ASP:H	1.79	0.47
3:C:65:LEU:HB3	3:C:86:ALA:HB1	1.96	0.47
3:G:50:TYR:O	3:G:54:VAL:HG23	2.15	0.47
6:J:178:DC:H2"	6:J:179:DG:C8	2.50	0.47
7:K:164:ASN:HB3	7:K:167:ARG:HH11	1.80	0.47
7:K:281:ILE:O	7:K:295:ASN:HA	2.15	0.47
10:N:284:LEU:HD13	10:N:289:LEU:HG	1.95	0.47
2:F:38:ALA:HB1	2:F:43:VAL:HB	1.95	0.47
14:R:519:LEU:O	14:R:520:LYS:HD2	2.13	0.47
17:U:26:ASN:O	17:U:27:GLU:HB2	2.15	0.47
1:A:51:ILE:HG13	2:B:39:ARG:HD2	1.96	0.47
3:G:54:VAL:HG21	4:H:95:VAL:HG11	1.96	0.47
6:J:165:DA:H2"	6:J:166:DA:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:169:DT:H2"	6:J:170:DA:C8	2.49	0.47
16:T:241:LYS:HZ2	16:T:245:GLU:HB3	1.80	0.47
16:T:337:VAL:O	16:T:340:ALA:HB3	2.15	0.47
17:U:30:PHE:HB3	17:U:433:GLN:OE1	2.14	0.47
17:U:153:MSE:HG3	17:U:334:ILE:HD13	1.97	0.47
17:U:403:CYS:HB2	17:U:404:PRO:HA	1.97	0.47
6:J:79:DT:H2"	6:J:80:DA:C8	2.50	0.47
10:N:94:PRO:C	10:N:96:GLU:H	2.18	0.47
13:Q:44:GLU:HB2	15:S:157:LYS:HG3	1.97	0.47
16:T:15:HIS:ND1	16:T:16[B]:ARG:HG2	2.29	0.47
17:U:370:GLU:HG3	17:U:395:VAL:HG21	1.97	0.47
18:V:9:LYS:HD2	18:V:12:LYS:HE2	1.97	0.47
2:B:35:ARG:HH22	5:I:82:DC:H2'	1.80	0.47
2:F:50:ILE:O	2:F:54:THR:HG23	2.15	0.47
10:N:554:ARG:HA	10:N:557:VAL:HG12	1.97	0.47
11:O:228:ASP:OD1	11:O:228:ASP:N	2.45	0.47
16:T:6:LYS:HD2	16:T:23:ASN:ND2	2.30	0.47
16:T:325:PRO:O	16:T:331:PRO:HG2	2.15	0.47
18:V:83:ASP:C	18:V:84:LEU:O	2.52	0.47
5:I:-9:DT:H2"	5:I:-8:DA:N7	2.31	0.46
8:L:1426:GLN:OE1	11:O:28:SER:OG	2.32	0.46
12:P:262:THR:HB	15:S:255:LYS:HZ1	1.80	0.46
8:L:1114:THR:HG23	8:L:1117:ALA:H	1.78	0.46
8:L:1477:LYS:HZ3	11:O:259:TYR:HH	1.58	0.46
9:M:424:GLU:HA	9:M:427:ASN:ND2	2.30	0.46
12:P:242:PRO:HB3	12:P:246:PHE:HB3	1.98	0.46
16:T:320:SER:OG	16:T:322:LYS:N	2.38	0.46
7:K:306:THR:HG23	7:K:309:ARG:H	1.80	0.46
8:L:191:LEU:HD22	9:M:368:VAL:HG22	1.98	0.46
13:Q:48:ARG:O	13:Q:51:SER:OG	2.29	0.46
4:H:42:LEU:HA	4:H:45:VAL:HG12	1.97	0.46
14:R:509:LEU:HD21	14:R:595:LEU:HD11	1.97	0.46
8:L:121:THR:O	8:L:125:ILE:HG12	2.16	0.46
16:T:183:LYS:O	16:T:183:LYS:CG	2.60	0.46
18:V:56:TYR:HB3	18:V:58:PHE:CE2	2.50	0.46
12:P:196:GLN:HE21	12:P:227:LYS:HB2	1.80	0.46
16:T:259:LYS:HD2	16:T:259:LYS:O	2.14	0.46
17:U:424:TYR:CD1	17:U:427:ILE:HD12	2.51	0.46
4:H:105:LYS:O	4:H:108:VAL:HG22	2.16	0.46
11:O:400:ARG:HA	11:O:403:THR:HG22	1.96	0.46
11:O:456:ARG:NH1	15:S:192:GLU:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:260:GLU:OE1	7:K:260:GLU:N	2.47	0.46
7:K:388:ILE:HB	7:K:391:ARG:HH12	1.81	0.46
10:N:541:THR:HG22	10:N:543:ASP:H	1.81	0.46
16:T:320:SER:OG	16:T:321:ASP:N	2.49	0.46
17:U:286:ASP:CB	17:U:290:ASN:H	2.29	0.46
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.51	0.46
5:I:-33:DT:H2"	5:I:-32:DA:C8	2.51	0.46
7:K:320:LEU:HG	7:K:324:PHE:HD2	1.80	0.46
8:L:1324:LEU:HB3	15:S:218:LEU:HD11	1.98	0.46
12:P:207:SER:OG	19:X:401:UNK:N	2.49	0.46
17:U:143:LEU:HD12	17:U:144:PRO:HD2	1.98	0.46
3:C:18:SER:OG	3:C:23:LEU:O	2.30	0.45
8:L:413:LYS:O	8:L:417:ILE:HG13	2.16	0.45
18:V:66:ASN:HB3	18:V:70:GLU:HB2	1.98	0.45
5:I:-31:DC:H2"	5:I:-30:DG:C8	2.50	0.45
8:L:1092:SER:O	8:L:1119:LYS:NZ	2.43	0.45
10:N:309:LEU:HD11	10:N:343:LEU:HD13	1.98	0.45
16:T:419:TYR:CD1	16:T:419:TYR:N	2.84	0.45
7:K:285:CYS:SG	7:K:328:ILE:HA	2.56	0.45
17:U:30:PHE:CD1	17:U:30:PHE:N	2.84	0.45
17:U:212:SER:HB3	17:U:284:PHE:HE2	1.81	0.45
18:V:33:SER:HB3	18:V:55:LYS:HD3	1.98	0.45
6:J:154:DC:H2"	6:J:155:DA:C8	2.51	0.45
7:K:345:ASP:N	7:K:345:ASP:OD1	2.49	0.45
17:U:354:LEU:HD22	17:U:358:LEU:HD22	1.99	0.45
16:T:246:LEU:HD23	16:T:246:LEU:HA	1.75	0.45
17:U:102:PHE:HZ	18:V:6:LEU:HD23	1.82	0.45
5:I:-11:DT:H2"	5:I:-10:DG:N7	2.30	0.45
8:L:114:THR:HG23	8:L:117:ALA:H	1.80	0.45
16:T:282:ASN:O	16:T:285:VAL:HG22	2.16	0.45
16:T:334:ALA:CB	16:T:415:ARG:HD3	2.46	0.45
16:T:426:ASN:O	16:T:432:ARG:NE	2.35	0.45
5:I:38:DT:H2"	5:I:39:DA:N7	2.31	0.45
8:L:1142:VAL:O	8:L:1146:VAL:HG12	2.17	0.45
3:G:51:LEU:HD21	4:H:67:PHE:HD1	1.82	0.45
3:G:92:GLU:HB2	7:K:397:ARG:HH12	1.81	0.45
6:J:146:DT:H2"	6:J:147:DG:C8	2.52	0.45
7:K:203:MET:HB3	7:K:222:LEU:HD12	1.99	0.45
8:L:355:LEU:HD21	15:S:257:ILE:HG22	1.98	0.45
8:L:1432:LEU:HD12	13:Q:69:LEU:HB2	1.98	0.45
8:L:1435:LEU:O	8:L:1438:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:224:THR:HG22	12:P:224:THR:O	2.17	0.45
17:U:121:GLN:HG2	17:U:463:TRP:CH2	2.52	0.45
18:V:33:SER:HB3	18:V:55:LYS:CD	2.46	0.45
16:T:236:LEU:HD22	16:T:309:PHE:CD2	2.51	0.45
9:M:359:ILE:HB	9:M:364:GLN:NE2	2.31	0.45
10:N:124:LEU:HD11	10:N:178:LEU:HD23	1.99	0.45
4:D:43:LYS:NZ	4:D:47:PRO:O	2.43	0.44
6:J:38:DG:H2"	6:J:39:DG:C8	2.51	0.44
6:J:47:DC:H2"	6:J:48:DC:C5	2.52	0.44
16:T:164:CYS:HB2	16:T:182:SER:HB3	1.98	0.44
3:C:51:LEU:HD21	4:D:67:PHE:HD1	1.82	0.44
5:I:-18:DT:O2	6:J:167:DG:N2	2.50	0.44
11:O:471:MET:O	11:O:474:ILE:HG22	2.18	0.44
18:V:23:GLU:OE2	18:V:65:ARG:HD3	2.16	0.44
7:K:295:ASN:N	7:K:295:ASN:OD1	2.49	0.44
12:P:171:GLU:HG2	14:R:460:LYS:HD2	2.00	0.44
15:S:715:LYS:HA	15:S:916:ILE:O	2.18	0.44
3:G:63:LEU:HD11	4:H:38:VAL:HG13	1.99	0.44
1:A:62:ILE:O	1:A:93:GLN:NE2	2.50	0.44
1:A:119:ILE:HD11	2:B:46:ILE:HG23	2.00	0.44
11:O:443:VAL:HG22	15:S:276:LEU:HD23	1.99	0.44
5:I:5:DA:H5'	5:I:5:DA:C8	2.53	0.44
7:K:320:LEU:HG	7:K:324:PHE:CD2	2.53	0.44
11:O:238:LEU:HD11	11:O:256:ILE:HD11	2.00	0.44
16:T:232:LYS:HA	16:T:236:LEU:HG	1.99	0.44
16:T:412:LEU:HD12	16:T:412:LEU:HA	1.76	0.44
19:X:98:UNK:C	19:X:100:UNK:H	2.31	0.44
7:K:388:ILE:HB	7:K:391:ARG:NH1	2.32	0.44
17:U:146:SER:HB2	17:U:174:ILE:HD11	1.99	0.44
17:U:197:SER:HB3	17:U:301:GLY:HA2	1.99	0.44
5:I:64:DC:H2"	5:I:65:DA:C8	2.53	0.44
5:I:64:DC:H2"	5:I:65:DA:H8	1.81	0.44
6:J:141:DT:H2"	6:J:142:DC:C5	2.52	0.44
7:K:380:VAL:HA	8:L:1144:ARG:NH1	2.31	0.44
16:T:151:LYS:HE3	16:T:424:PHE:CE1	2.53	0.44
16:T:282:ASN:HA	16:T:283:PRO:HD2	1.91	0.44
2:F:90:LEU:HD22	2:F:95:ARG:HD2	2.00	0.43
4:H:102:GLU:OE2	4:H:106:HIS:CE1	2.71	0.43
3:C:31:HIS:CE1	3:C:35:ARG:HE	2.36	0.43
6:J:46:DC:H2"	6:J:47:DC:C5	2.53	0.43
7:K:299:ASN:OD1	7:K:299:ASN:O	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:14:PRO:O	17:U:116[B]:HIS:NE2	2.48	0.43
10:N:324:THR:O	10:N:328:LYS:HG2	2.18	0.43
12:P:301:VAL:HG23	12:P:302:ASP:H	1.84	0.43
16:T:129:ASP:OD2	16:T:460:TYR:HE2	2.01	0.43
6:J:85:DC:H2"	6:J:86:DG:C8	2.53	0.43
6:J:123:DC:H2"	6:J:124:DG:C8	2.53	0.43
10:N:82:LEU:HA	10:N:85:MET:HE3	1.99	0.43
11:O:458:SER:HA	11:O:461:TYR:HD2	1.82	0.43
12:P:229:ASN:OD1	12:P:230:ASN:N	2.52	0.43
14:R:601:HIS:HB3	14:R:620:TRP:CD1	2.52	0.43
18:V:83:ASP:O	18:V:86:GLU:HG3	2.18	0.43
3:G:53:ALA:O	3:G:56:GLU:HG3	2.18	0.43
5:I:68:DT:H2"	5:I:69:DA:N7	2.33	0.43
8:L:1447:LEU:HD12	8:L:1447:LEU:HA	1.87	0.43
9:M:392:ASP:OD1	9:M:393:ASN:N	2.51	0.43
12:P:388:ILE:HG22	12:P:389:LYS:HG3	2.00	0.43
16:T:458:GLU:O	16:T:459:ASP:C	2.57	0.43
5:I:42:DC:H2"	5:I:43:DA:H8	1.84	0.43
8:L:1086:ALA:HB2	9:M:422:ILE:HD11	2.01	0.43
9:M:423:THR:O	9:M:427:ASN:ND2	2.52	0.43
10:N:90:LEU:HD23	10:N:90:LEU:H	1.84	0.43
12:P:408:GLU:OE2	12:P:411:ARG:NH2	2.36	0.43
16:T:47:PHE:CD2	16:T:85:MSE:HE1	2.54	0.43
6:J:163:DG:H2"	6:J:164:DG:C8	2.54	0.43
8:L:1124:PHE:CE1	9:M:324:SER:HB2	2.54	0.43
8:L:1163:TRP:C	8:L:1165:LEU:H	2.22	0.43
10:N:55:THR:OG1	10:N:56:LYS:N	2.46	0.43
16:T:80:TRP:CE2	16:T:122:ARG:HD3	2.54	0.43
17:U:361:GLU:HA	17:U:362:PRO:HD3	1.93	0.43
7:K:290:ARG:HG2	7:K:385:LYS:HE2	2.00	0.43
8:L:136:TYR:CE2	8:L:167:ASN:HB3	2.54	0.43
11:O:256:ILE:O	11:O:260:ILE:HG13	2.18	0.43
3:C:97:LEU:HD21	4:D:62:PHE:HE1	1.84	0.43
4:H:65:ASP:O	4:H:68:GLU:HG3	2.19	0.43
8:L:110:SER:OG	8:L:111:ARG:N	2.52	0.43
12:P:75:THR:HG23	12:P:78:LYS:H	1.84	0.43
15:S:220:ASP:O	15:S:223:GLU:HG2	2.19	0.43
17:U:286:ASP:HB2	17:U:290:ASN:O	2.18	0.43
12:P:259:LEU:HB3	12:P:261:PRO:HD2	2.00	0.43
1:E:106:ASP:OD2	1:E:131:ARG:NE	2.52	0.42
8:L:128:THR:HG23	9:M:356:ILE:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:351:ASP:HB3	9:M:354:THR:O	2.19	0.42
12:P:222:PRO:HG2	12:P:226:PHE:CE2	2.54	0.42
16:T:198:ALA:N	16:T:199:PRO:HD2	2.34	0.42
17:U:189:MSE:HG2	17:U:305:LEU:CD1	2.49	0.42
15:S:49:PRO:HD2	15:S:86:ILE:HD11	1.99	0.42
5:I:66:DC:H2"	5:I:67:DG:C8	2.54	0.42
16:T:381:PRO:C	16:T:383:GLN:N	2.72	0.42
17:U:189:MSE:HE1	17:U:304:ASN:OD1	2.18	0.42
16:T:314:PHE:CZ	16:T:407:ARG:HG3	2.54	0.42
17:U:91:LEU:CD2	17:U:106:LEU:HD22	2.50	0.42
16:T:197:LEU:HD11	16:T:231:PHE:CE1	2.55	0.42
17:U:445:ASP:HA	17:U:448:TYR:CE1	2.55	0.42
18:V:9:LYS:HD2	18:V:12:LYS:NZ	2.34	0.42
3:C:107:VAL:HG23	3:C:108:LEU:H	1.84	0.42
8:L:289:GLU:HB3	8:L:291:HIS:HE2	1.73	0.42
6:J:148:DG:H2"	6:J:149:DA:C8	2.55	0.42
7:K:292:PHE:CZ	7:K:328:ILE:HD12	2.54	0.42
8:L:1145:ASN:N	8:L:1145:ASN:OD1	2.52	0.42
16:T:431:ASP:O	16:T:435:GLN:HB2	2.19	0.42
5:I:90:DA:H2"	5:I:91:DA:C8	2.55	0.42
5:I:120:DA:H2"	5:I:121:DG:N7	2.34	0.42
8:L:388:LYS:H	8:L:388:LYS:HG2	1.71	0.42
10:N:226:MET:SD	10:N:246:LEU:HD11	2.60	0.42
17:U:6:GLN:O	17:U:24:GLY:HA2	2.19	0.42
17:U:429:PHE:HE1	17:U:433:GLN:HE21	1.68	0.42
4:H:48:ASP:OD1	4:H:48:ASP:N	2.46	0.42
5:I:112:DT:O2	6:J:37:DG:N2	2.52	0.42
7:K:274:MET:HA	7:K:301:ASN:HD21	1.85	0.42
8:L:476:SER:O	8:L:479:ILE:HG22	2.20	0.42
11:O:34:LYS:HA	11:O:37:ILE:HG22	2.02	0.42
11:O:234:TYR:CE1	11:O:252:ALA:HB2	2.55	0.42
12:P:124:TYR:CE2	12:P:214:LEU:HD11	2.54	0.42
6:J:109:DT:H6	6:J:109:DT:H2'	1.74	0.42
8:L:1105:PHE:HZ	8:L:1152:SER:HB2	1.84	0.42
11:O:459:ASP:OD1	11:O:460:ILE:HG23	2.20	0.42
16:T:381:PRO:HG2	16:T:382:GLU:CD	2.39	0.42
8:L:137:LEU:HD23	8:L:137:LEU:HA	1.89	0.41
10:N:134:LEU:HD11	10:N:158:GLY:HA3	2.02	0.41
16:T:381:PRO:O	16:T:383:GLN:N	2.53	0.41
1:A:71:VAL:HG13	2:B:66:ILE:HD11	2.02	0.41
5:I:-24:DG:H2"	5:I:-23:DA:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:37:DG:H2"	6:J:38:DG:C8	2.56	0.41
16:T:122:ARG:CG	16:T:122:ARG:NH1	2.66	0.41
4:H:52:SER:HA	5:I:20:DA:H5"	2.03	0.41
6:J:119:DT:H2"	6:J:120:DG:N7	2.35	0.41
8:L:420:LYS:HD2	13:Q:49:HIS:CE1	2.56	0.41
9:M:420:ARG:HA	9:M:423:THR:HG22	2.02	0.41
10:N:64:ASN:OD1	10:N:64:ASN:N	2.53	0.41
17:U:275:LYS:HA	17:U:275:LYS:HD2	1.91	0.41
1:A:118:THR:HG22	2:B:45:ARG:HB3	2.02	0.41
6:J:176:DT:H2"	6:J:177:DC:C6	2.55	0.41
8:L:88:TRP:O	8:L:88:TRP:CE3	2.73	0.41
16:T:149:MSE:HE1	16:T:425:ALA:CA	2.51	0.41
16:T:451:LEU:HD23	16:T:451:LEU:HA	1.81	0.41
8:L:146:VAL:HG12	8:L:148:MET:H	1.86	0.41
8:L:196:GLY:O	8:L:197:LEU:HD23	2.20	0.41
10:N:135:GLU:HG3	10:N:190:PHE:CD2	2.55	0.41
10:N:190:PHE:CE1	10:N:194:LYS:HE2	2.56	0.41
11:O:406:ALA:O	11:O:410:ASN:HB2	2.20	0.41
12:P:237:ILE:HG13	12:P:238:GLU:N	2.35	0.41
13:Q:29:LEU:HA	13:Q:29:LEU:HD23	1.87	0.41
16:T:418:GLN:HG2	16:T:419:TYR:CD1	2.56	0.41
17:U:154:ILE:HG22	17:U:154:ILE:O	2.21	0.41
12:P:390:LEU:HD12	12:P:390:LEU:HA	1.87	0.41
3:C:55:LEU:O	3:C:59:THR:HG23	2.21	0.41
8:L:465:SER:HB2	8:L:1461:TYR:HD1	1.86	0.41
10:N:522:GLU:HG3	10:N:523:LEU:H	1.85	0.41
11:O:433:TYR:CE1	13:Q:36:ILE:HG13	2.56	0.41
17:U:26:ASN:HB3	17:U:29:THR:O	2.21	0.41
17:U:166:THR:HG22	17:U:167:HIS:CE1	2.56	0.41
1:A:63:ARG:HA	1:A:63:ARG:HD3	1.83	0.41
2:F:77:LYS:HD3	2:F:77:LYS:HA	1.86	0.41
5:I:70:DC:H2"	5:I:71:DG:C8	2.55	0.41
6:J:109:DT:H2"	6:J:110:DA:N7	2.36	0.41
9:M:389:VAL:HG12	19:X:463:UNK:HA	2.02	0.41
12:P:198:ARG:HA	12:P:202:MET:O	2.21	0.41
16:T:189:LEU:HA	16:T:189:LEU:HD23	1.84	0.41
1:A:118:THR:OG1	6:J:71:DA:H5"	2.21	0.41
5:I:-14:DC:H2'	5:I:-13:DT:H71	2.02	0.41
8:L:160:LEU:HB3	8:L:166:ILE:HG12	2.03	0.41
9:M:357:LEU:HG	9:M:359:ILE:HD11	2.02	0.41
9:M:399:LYS:NZ	9:M:432:ASN:HD22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:152:MET:HG3	11:O:435:TRP:HH2	1.85	0.41
10:N:255:ASP:OD1	10:N:258:MET:HB2	2.21	0.41
12:P:301:VAL:HG23	12:P:302:ASP:N	2.36	0.41
12:P:456:LEU:HD13	15:S:119:LEU:HD23	2.03	0.41
14:R:501:MET:HG2	14:R:622:ASN:HB2	2.03	0.41
15:S:125:LEU:HA	15:S:125:LEU:HD23	1.85	0.41
15:S:201:ASN:O	15:S:205:GLU:HG3	2.21	0.41
15:S:810:VAL:O	15:S:862:CYS:HA	2.20	0.41
16:T:458:GLU:O	16:T:460:TYR:N	2.53	0.41
17:U:3:PRO:HA	17:U:4:PHE:HA	1.67	0.41
17:U:338:GLY:O	17:U:339:THR:C	2.59	0.41
17:U:459:PRO:HG2	18:V:63:TRP:CE2	2.56	0.41
19:X:35:UNK:C	19:X:37:UNK:H	2.32	0.41
1:A:116:ARG:NH1	1:A:120:MET:SD	2.94	0.41
2:B:30:THR:OG1	2:B:32:PRO:HD2	2.21	0.41
2:B:31:LYS:HG3	2:B:51:TYR:CZ	2.56	0.41
19:X:188:UNK:O	19:X:190:UNK:N	2.54	0.41
8:L:144:ARG:HG2	9:M:353:TYR:CZ	2.56	0.40
9:M:337:ASP:O	9:M:340:LYS:HB3	2.21	0.40
11:O:335:VAL:O	11:O:339:VAL:HG23	2.20	0.40
12:P:400:ASN:O	15:S:93:TYR:HB2	2.21	0.40
17:U:148:ALA:HB1	17:U:428:ILE:O	2.22	0.40
7:K:222:LEU:HB3	7:K:330:GLN:OE1	2.20	0.40
10:N:289:LEU:HD23	10:N:289:LEU:HA	1.92	0.40
12:P:12:ASP:OD1	12:P:12:ASP:N	2.52	0.40
12:P:33:GLU:HG3	12:P:106:LEU:HD11	2.03	0.40
12:P:467:LYS:HD3	12:P:467:LYS:HA	1.90	0.40
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.89	0.40
8:L:59:GLU:HB2	8:L:61:GLU:OE2	2.22	0.40
8:L:293:GLY:HA2	12:P:487:ILE:HG13	2.04	0.40
10:N:176:GLN:HG2	10:N:232:TYR:CE2	2.56	0.40
2:B:50:ILE:O	2:B:54:THR:HG22	2.21	0.40
16:T:256:ILE:O	16:T:260:GLN:CB	2.70	0.40
17:U:112:LEU:HD12	17:U:141:ILE:HD12	2.02	0.40
8:L:405:ASP:N	8:L:405:ASP:OD1	2.54	0.40
8:L:477:LYS:HE3	8:L:477:LYS:HB3	1.82	0.40
10:N:223:LEU:HG	10:N:258:MET:SD	2.62	0.40
14:R:601:HIS:HA	14:R:619:PHE:O	2.21	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	A	94/135 (70%)	94 (100%)	0	0	100	100
1	E	93/135 (69%)	93 (100%)	0	0	100	100
2	B	85/102 (83%)	83 (98%)	2 (2%)	0	100	100
2	F	80/102 (78%)	79 (99%)	1 (1%)	0	100	100
3	C	100/129 (78%)	97 (97%)	3 (3%)	0	100	100
3	G	100/129 (78%)	98 (98%)	2 (2%)	0	100	100
4	D	90/122 (74%)	90 (100%)	0	0	100	100
4	H	90/122 (74%)	89 (99%)	1 (1%)	0	100	100
7	K	229/426 (54%)	211 (92%)	15 (7%)	3 (1%)	10	43
8	L	580/1114 (52%)	559 (96%)	21 (4%)	0	100	100
9	M	104/435 (24%)	93 (89%)	11 (11%)	0	100	100
10	N	363/581 (62%)	337 (93%)	26 (7%)	0	100	100
11	O	202/483 (42%)	195 (96%)	7 (4%)	0	100	100
12	P	339/502 (68%)	310 (91%)	29 (9%)	0	100	100
13	Q	56/78 (72%)	52 (93%)	4 (7%)	0	100	100
14	R	127/625 (20%)	123 (97%)	4 (3%)	0	100	100
15	S	767/1359 (56%)	745 (97%)	21 (3%)	1 (0%)	48	83
16	T	392/477 (82%)	369 (94%)	18 (5%)	5 (1%)	10	43
17	U	391/467 (84%)	368 (94%)	21 (5%)	2 (0%)	25	64
18	V	46/157 (29%)	43 (94%)	2 (4%)	1 (2%)	5	29
All	All	4328/7680 (56%)	4128 (95%)	188 (4%)	12 (0%)	38	73

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	U	48	ASP

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Mol	Chain	Res	Type
7	K	346	GLY
7	K	389	GLN
16	T	343	SER
16	T	382	GLU
16	T	459	ASP
18	V	84	LEU
7	K	354	PRO
16	T	431	ASP
16	T	458	GLU
17	U	155	SER
15	S	292	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/110 (76%)	84 (100%)	0	100	100
1	E	83/110 (76%)	83 (100%)	0	100	100
2	B	65/78 (83%)	65 (100%)	0	100	100
2	F	67/78 (86%)	67 (100%)	0	100	100
3	C	81/101 (80%)	81 (100%)	0	100	100
3	G	81/101 (80%)	80 (99%)	1 (1%)	67	78
4	D	78/102 (76%)	78 (100%)	0	100	100
4	H	78/102 (76%)	78 (100%)	0	100	100
7	K	208/384 (54%)	206 (99%)	2 (1%)	73	82
8	L	554/1000 (55%)	553 (100%)	1 (0%)	92	94
9	M	101/388 (26%)	101 (100%)	0	100	100
10	N	335/521 (64%)	334 (100%)	1 (0%)	91	92
11	O	194/435 (45%)	194 (100%)	0	100	100
12	P	324/462 (70%)	324 (100%)	0	100	100
13	Q	56/75 (75%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	R	126/578 (22%)	126 (100%)	0	100	100
15	S	207/1228 (17%)	207 (100%)	0	100	100
16	T	357/404 (88%)	338 (95%)	19 (5%)	19	40
17	U	363/418 (87%)	343 (94%)	20 (6%)	18	39
18	V	53/136 (39%)	52 (98%)	1 (2%)	52	69
All	All	3495/6811 (51%)	3450 (99%)	45 (1%)	64	77

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	36	LYS
7	K	184	TYR
7	K	401	ARG
8	L	173	ARG
10	N	77	ARG
16	T	2	THR
16	T	79	ASN
16	T	88	ARG
16	T	122	ARG
16	T	216	ARG
16	T	230	GLN
16	T	246	LEU
16	T	251	LYS
16	T	293	LYS
16	T	301	LEU
16	T	319	ILE
16	T	321	ASP
16	T	343	SER
16	T	380	SER
16	T	386	SER
16	T	397	SER
16	T	432	ARG
16	T	442	THR
16	T	462	THR
17	U	7	ASP
17	U	32	VAL
17	U	34	GLU
17	U	41	ILE
17	U	48	ASP
17	U	52	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	U	54	HIS
17	U	56	THR
17	U	69	GLN
17	U	94	ARG
17	U	100	ASP
17	U	105	GLU
17	U	122	SER
17	U	181	ASP
17	U	197	SER
17	U	291	GLU
17	U	321	ASP
17	U	347	GLU
17	U	422	SER
17	U	438	GLN
18	V	90	ARG

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

Mol	Chain	Res	Type
4	H	106	HIS
7	K	160	HIS
7	K	301	ASN
8	L	188	GLN
8	L	291	HIS
8	L	1167	ASN
8	L	1426	GLN
9	M	323	HIS
9	M	346	GLN
9	M	432	ASN
10	N	170	GLN
10	N	196	GLN
10	N	251	ASN
11	O	29	ASN
11	O	410	ASN
11	O	445	GLN
12	P	112	GLN
12	P	196	GLN
12	P	223	ASN
12	P	239	ASN
12	P	253	ASN
12	P	392	ASN
12	P	409	ASN

Continued on next page...

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Mol	Chain	Res	Type
12	P	472	ASN
13	Q	49	HIS
14	R	600	ASN
15	S	90	GLN

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 oligosaccharides 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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
19	X	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	612:UNK	C	632:UNK	N	63.76
1	X	438:UNK	C	458:UNK	N	59.07
1	X	327:UNK	C	347:UNK	N	57.31
1	X	359:UNK	C	379:UNK	N	56.50
1	X	510:UNK	C	530:UNK	N	55.64
1	X	200:UNK	C	220:UNK	N	36.87
1	X	252:UNK	C	272:UNK	N	33.67
1	X	125:UNK	C	145:UNK	N	30.13
1	X	10:UNK	C	30:UNK	N	30.11
1	X	404:UNK	C	424:UNK	N	21.61
1	X	77:UNK	C	97:UNK	N	19.22
1	X	158:UNK	C	178:UNK	N	13.77
1	X	564:UNK	C	584:UNK	N	12.78
1	X	473:UNK	C	493:UNK	N	6.67

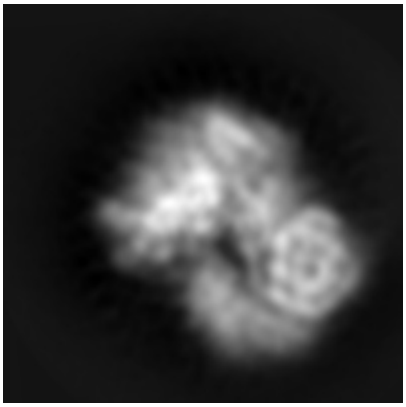
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10465. These allow visual inspection of the internal detail of the map and identification of artifacts.

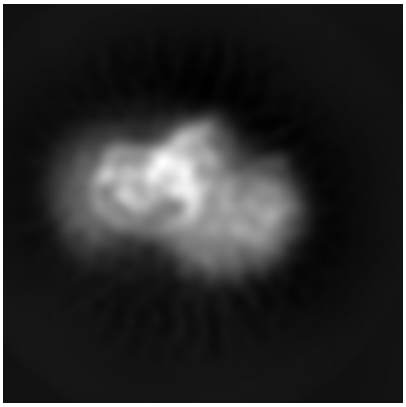
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

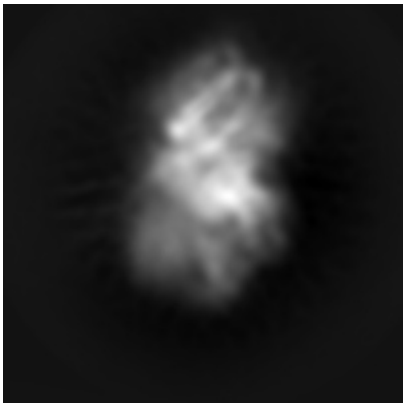
6.1.1 Primary map



X



Y

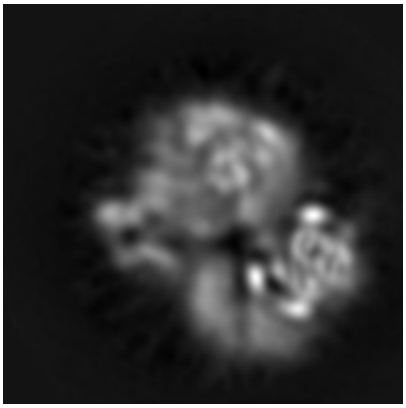


Z

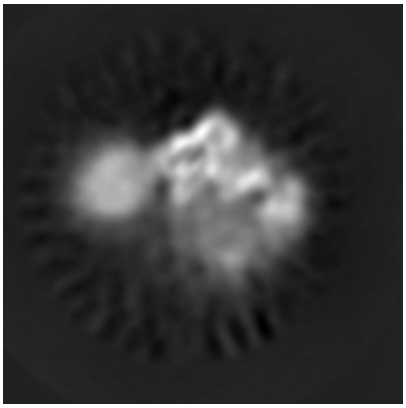
The images above show the map projected in three orthogonal directions.

6.2 Central slices

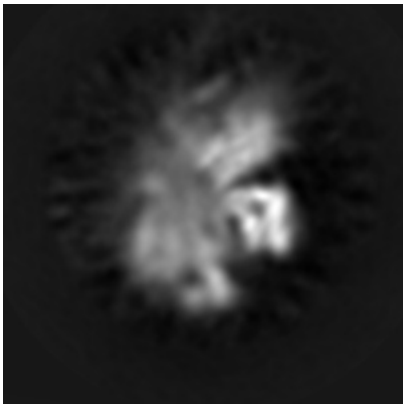
6.2.1 Primary map



X Index: 170



Y Index: 170

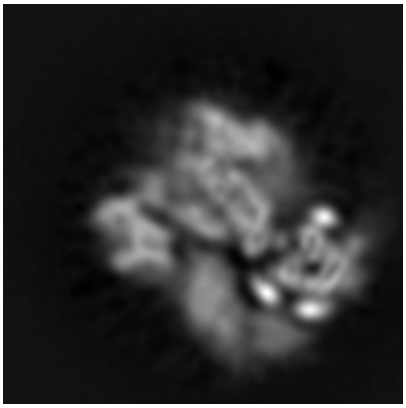


Z Index: 170

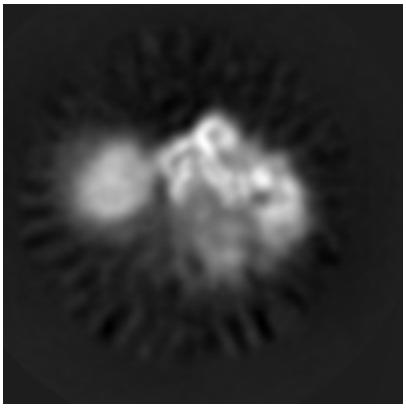
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

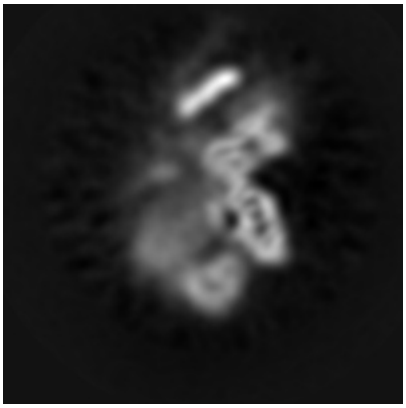
6.3.1 Primary map



X Index: 182



Y Index: 175

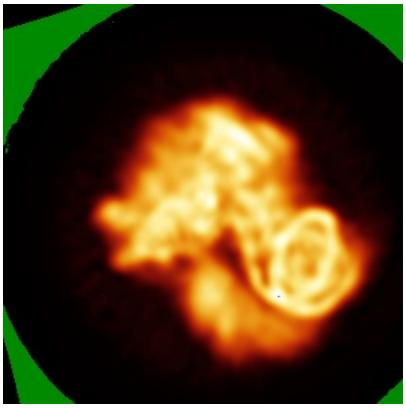


Z Index: 157

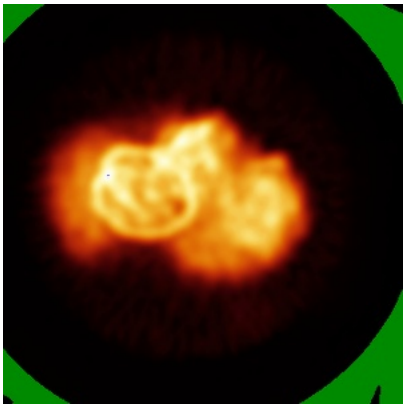
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

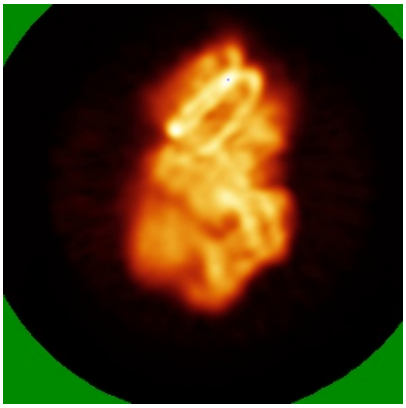
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0115. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

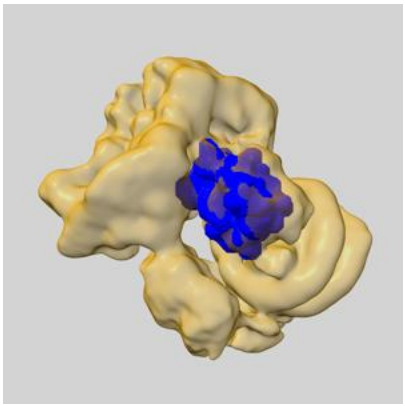
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

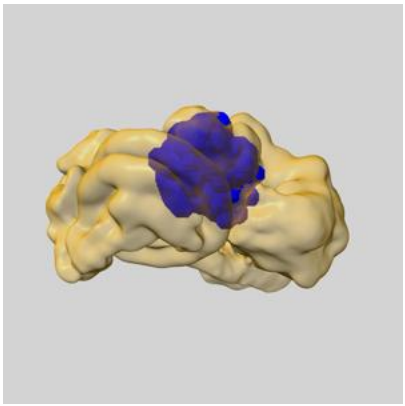
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

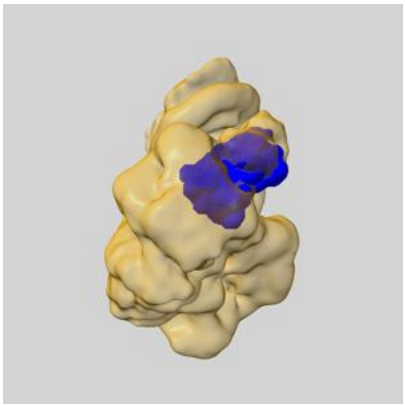
6.6.1 emd_10465_msk_4.map



X

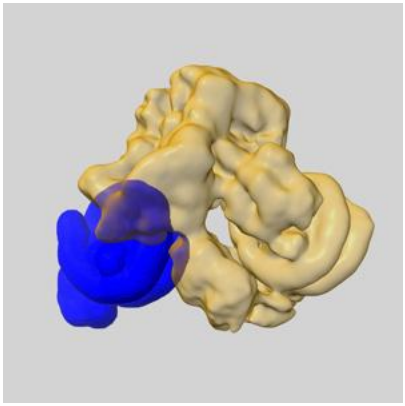


Y

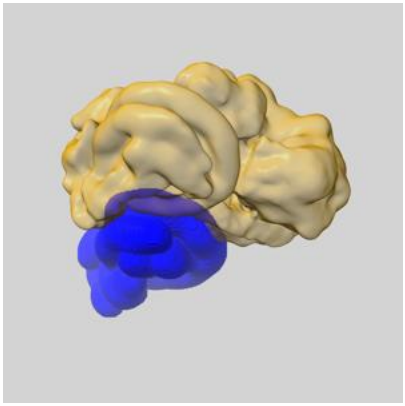


Z

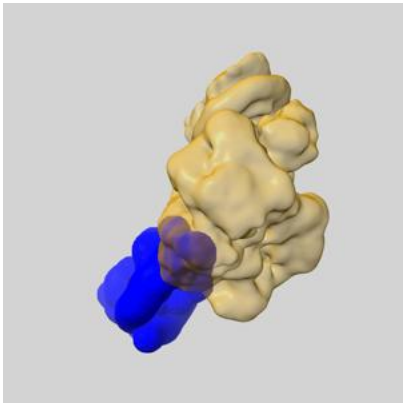
6.6.2 emd_10465_msk_5.map



X

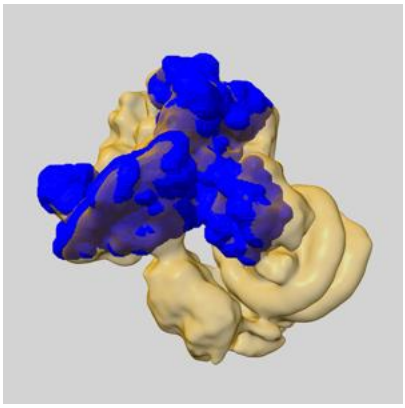


Y

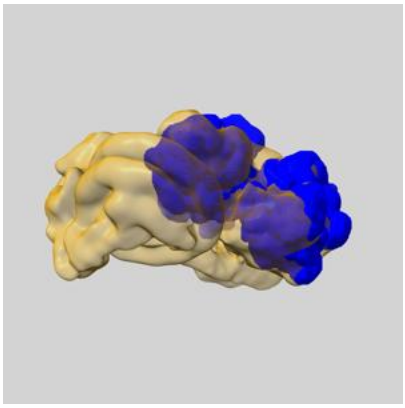


Z

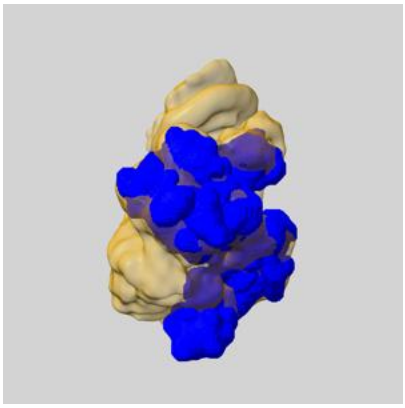
6.6.3 emd_10465_msk_1.map



X

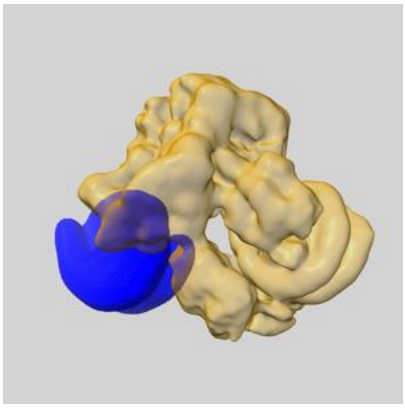


Y

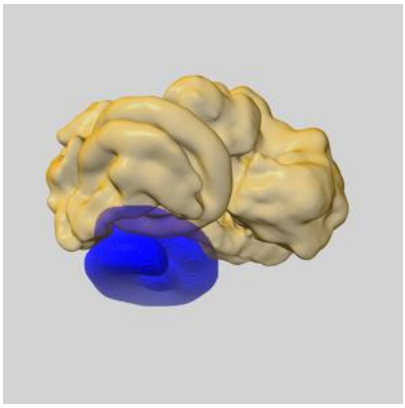


Z

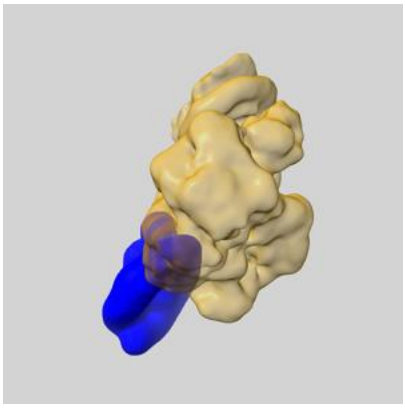
6.6.4 emd_10465_msk_6.map



X

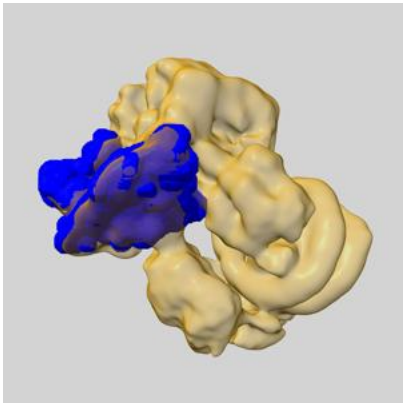


Y

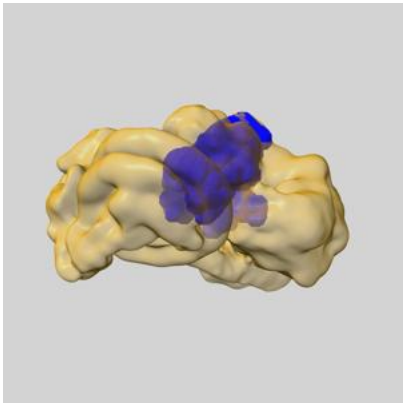


Z

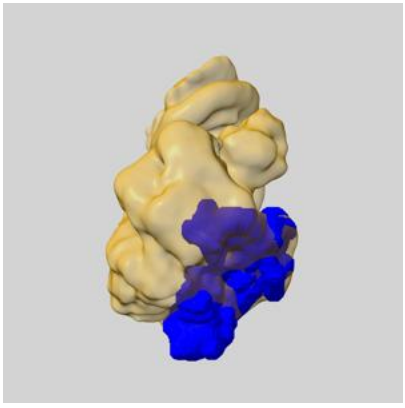
6.6.5 emd_10465_msk_2.map



X

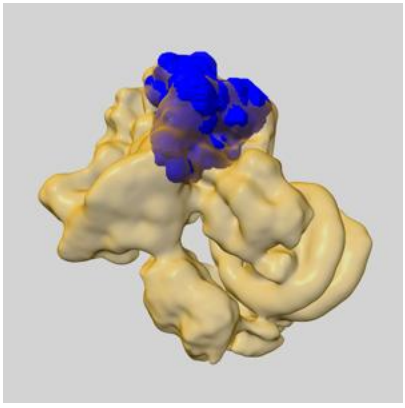


Y

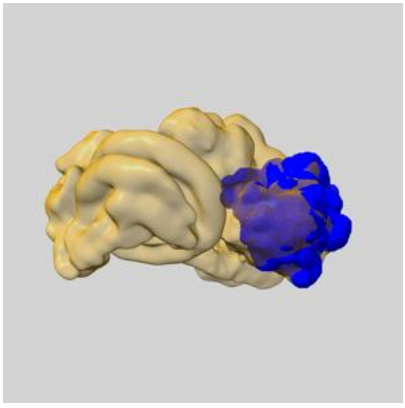


Z

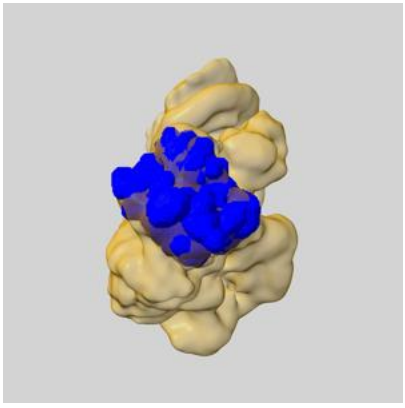
6.6.6 emd_10465_msk_3.map



X



Y

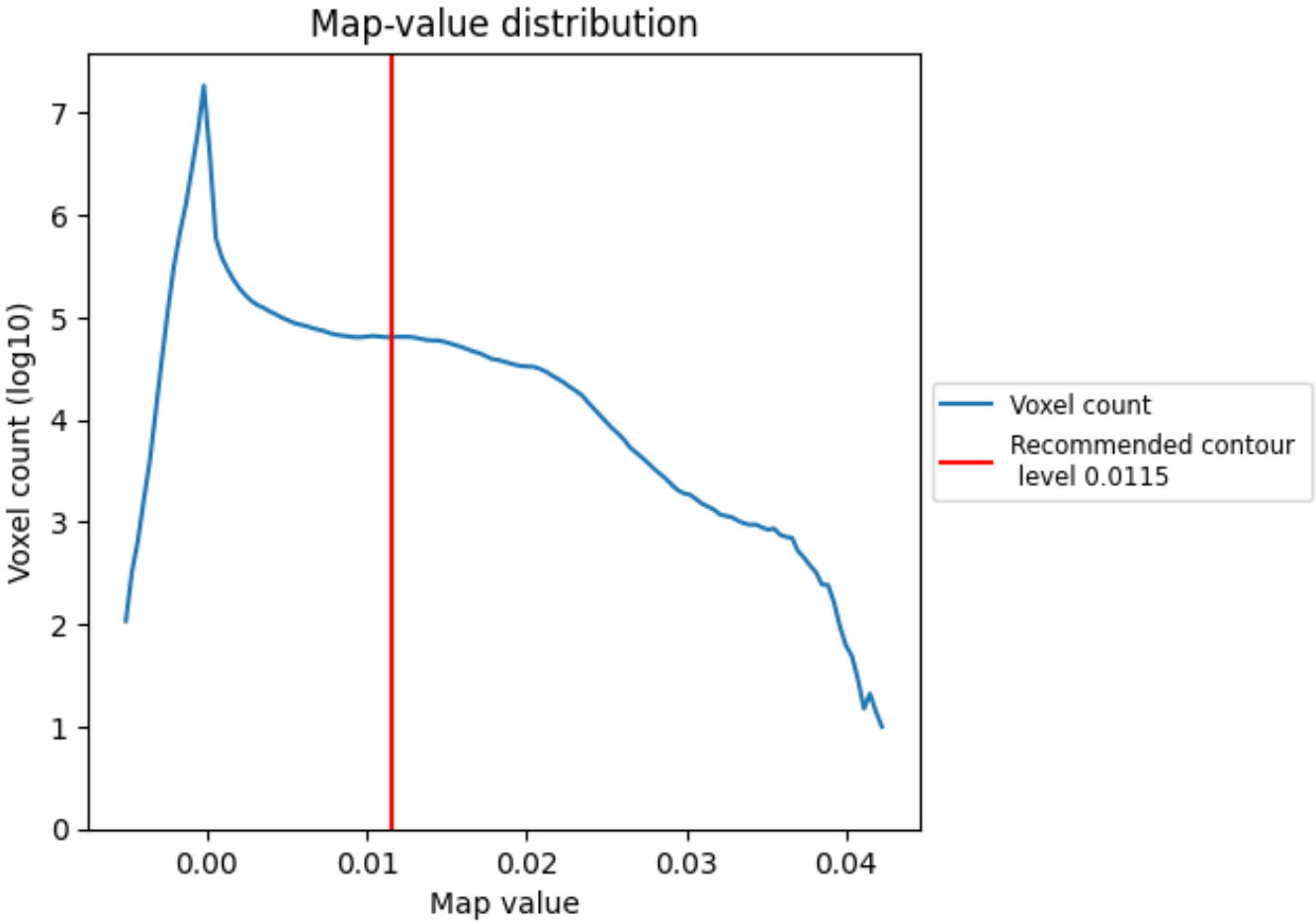


Z

7 Map analysis

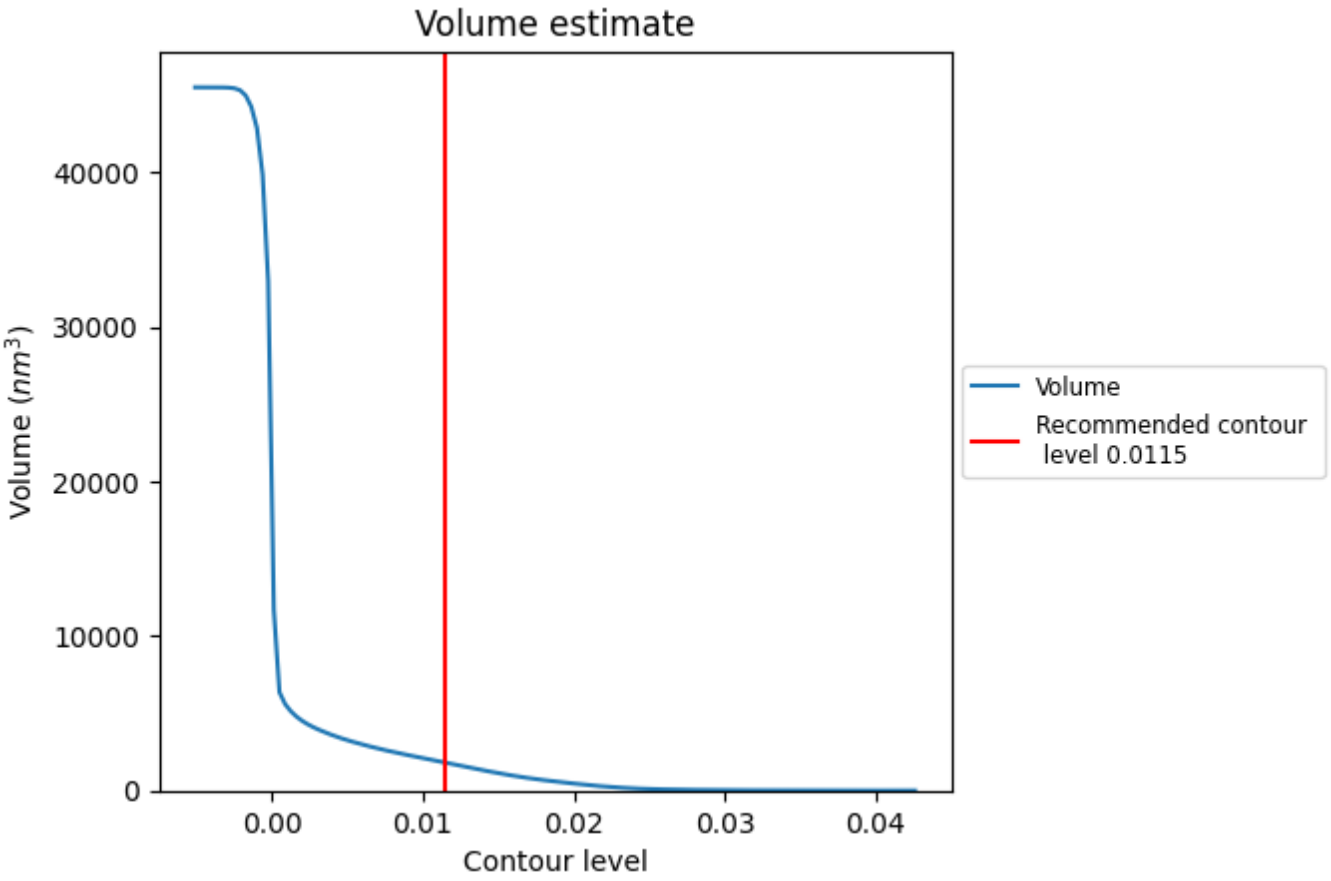
This section contains the results of statistical analysis of the map.

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.

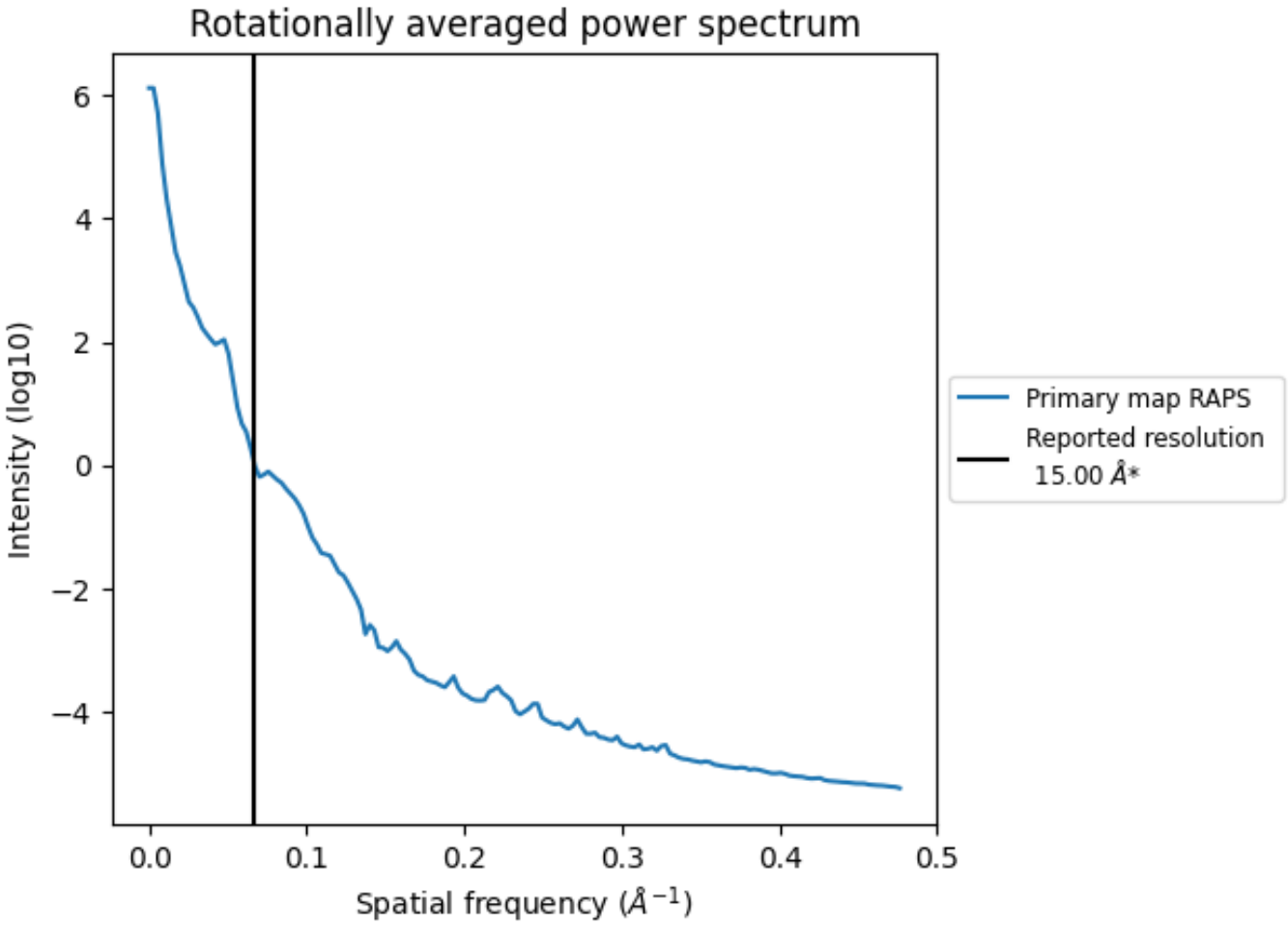
7.2 Volume estimate



The volume at the recommended contour level is 1801 nm^3; this corresponds to an approximate mass of 1627 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 0.067 Å^{-1}

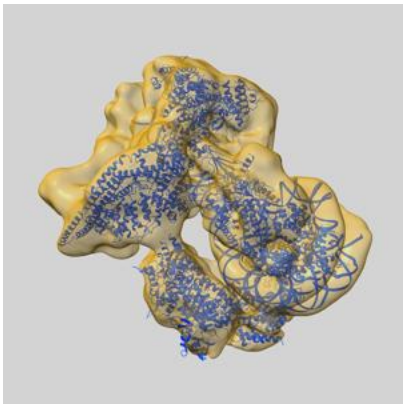
8 Fourier-Shell correlation

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

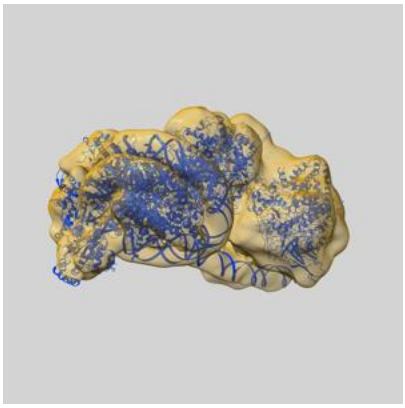
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10465 and PDB model 6TDA. Per-residue inclusion information can be found in section 3 on page 8.

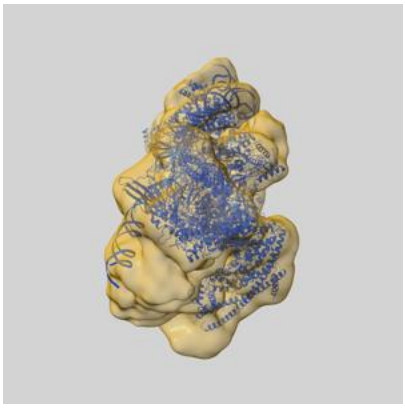
9.1 Map-model overlay



X



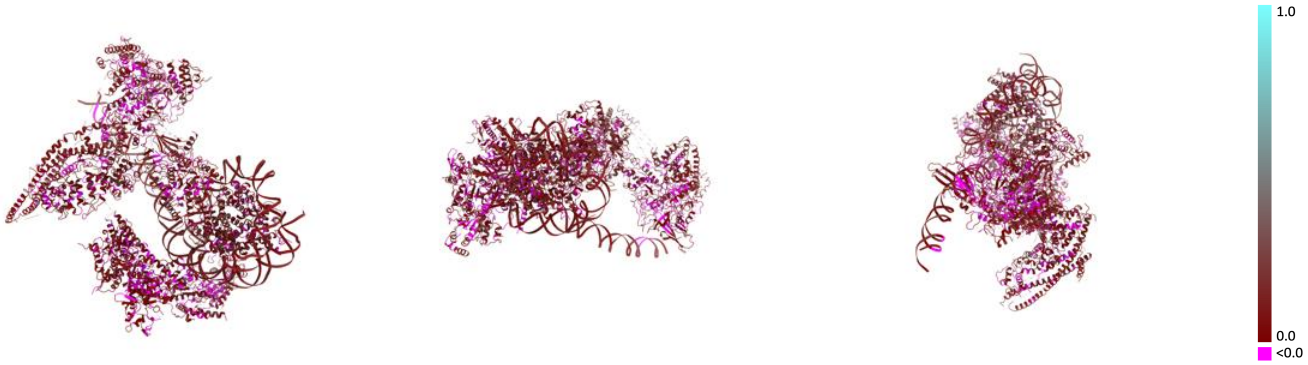
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0115 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.

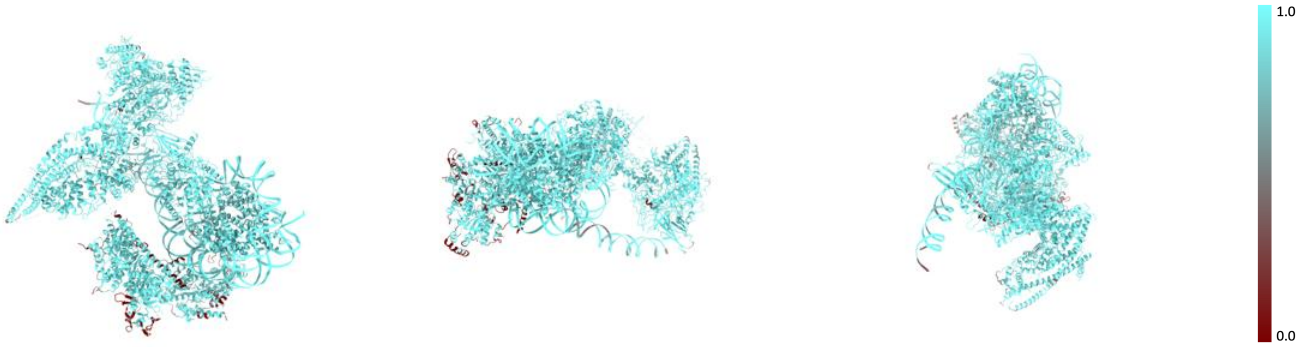
9.2 Q-score mapped to coordinate model (i)



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.

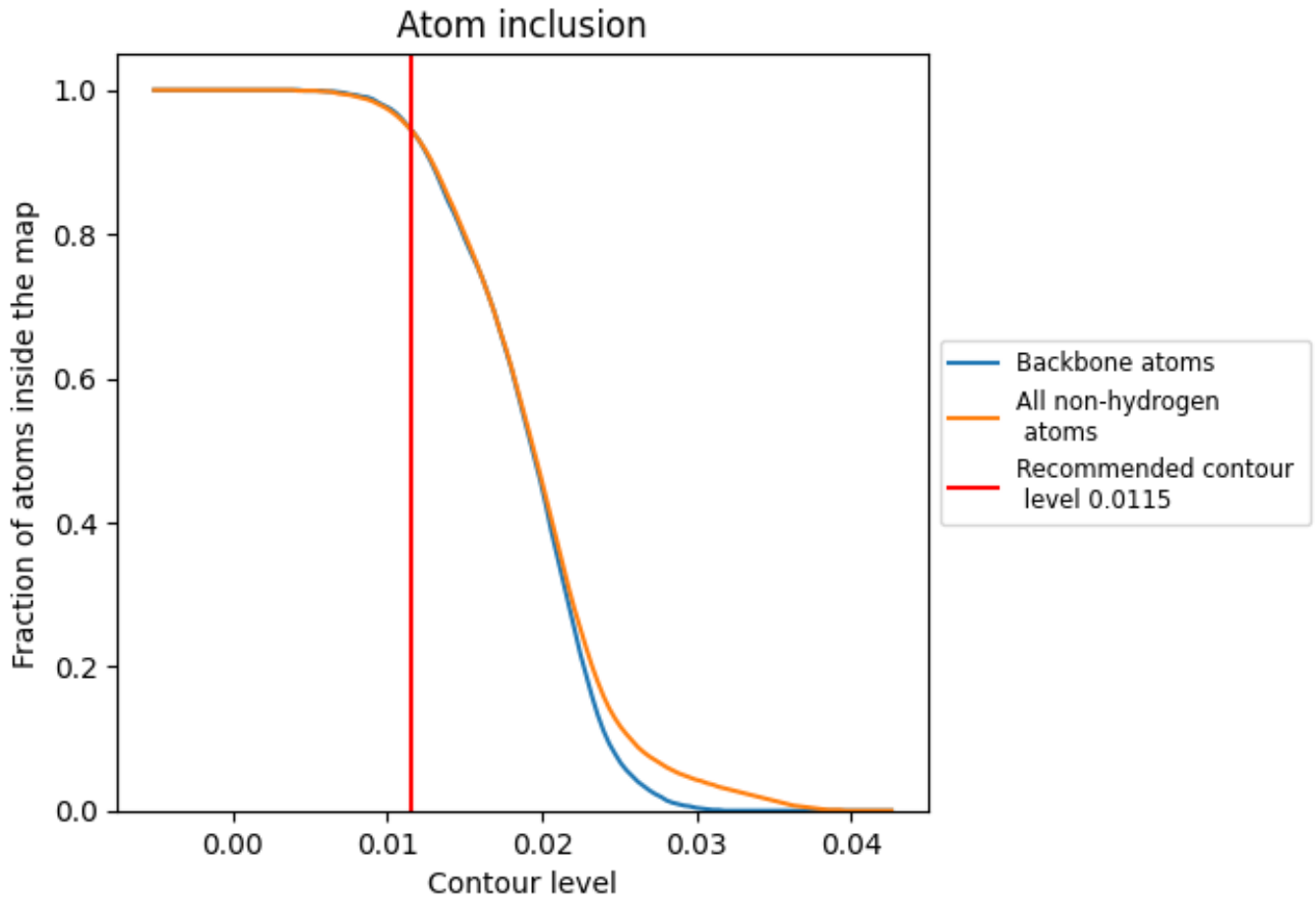
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0115).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.0115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9450	0.0810
A	0.9690	0.0920
B	0.9460	0.1020
C	0.9920	0.0970
D	0.9970	0.1230
E	0.9800	0.1000
F	0.9620	0.0960
G	0.9650	0.1020
H	0.9870	0.1060
I	0.9550	0.1190
J	0.9370	0.1040
K	0.9810	0.1050
L	0.9890	0.0840
M	0.9860	0.1110
N	0.9850	0.0840
O	0.9570	0.0730
P	0.9960	0.0780
Q	0.9740	0.0670
R	0.9710	0.0570
S	0.8750	0.0600
T	0.8750	0.0610
U	0.8560	0.0350
V	0.9010	0.0460
X	0.9680	0.0560