wwPDB EM Validation Summary Report

Oct 23, 2022 – 12:22 AM JST

PDB ID	:	7VVY
EMDB ID	:	EMD-32149
Title	:	TRA module of NuA4
Authors	:	Chen, Z.; Qu, K.
Deposited on	:	2021-11-09
Resolution	:	3.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

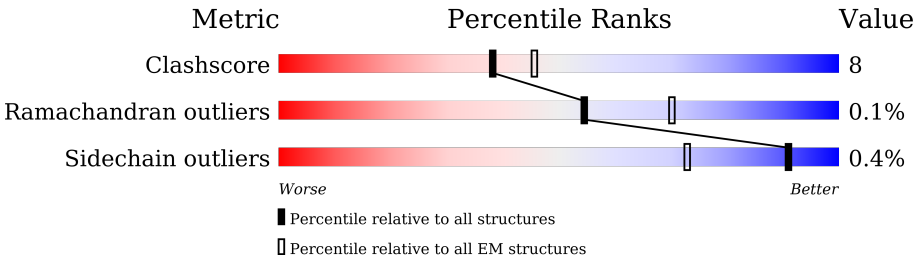
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	E	1168	5% 27% 8% 64%
2	F	489	12% 73% 11% 15%
3	G	375	54% 84% 11% 5%
4	K	476	9% 42% 8% 50%
5	H	832	11% 27% 6% 68%
6	L	3744	24% 76% 18% 6%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 42546 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 modification-related protein EAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	415	3448	2193	619	622	14	0	0

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	983	ARG	-	expression tag	UNP Q06337
E	984	THR	-	expression tag	UNP Q06337
E	985	LEU	-	expression tag	UNP Q06337
E	986	GLN	-	expression tag	UNP Q06337
E	987	VAL	-	expression tag	UNP Q06337
E	988	ASP	-	expression tag	UNP Q06337
E	989	TRP	-	expression tag	UNP Q06337
E	990	SER	-	expression tag	UNP Q06337
E	991	HIS	-	expression tag	UNP Q06337
E	992	PRO	-	expression tag	UNP Q06337
E	993	GLN	-	expression tag	UNP Q06337
E	994	PHE	-	expression tag	UNP Q06337
E	995	GLU	-	expression tag	UNP Q06337
E	996	LYS	-	expression tag	UNP Q06337
E	997	HIS	-	expression tag	UNP Q06337
E	998	HIS	-	expression tag	UNP Q06337
E	999	HIS	-	expression tag	UNP Q06337
E	1000	HIS	-	expression tag	UNP Q06337
E	1001	HIS	-	expression tag	UNP Q06337
E	1002	HIS	-	expression tag	UNP Q06337
E	1003	HIS	-	expression tag	UNP Q06337
E	1004	HIS	-	expression tag	UNP Q06337
E	1005	HIS	-	expression tag	UNP Q06337
E	1006	HIS	-	expression tag	UNP Q06337
E	1007	HIS	-	expression tag	UNP Q06337
E	1008	HIS	-	expression tag	UNP Q06337
E	1009	ASP	-	expression tag	UNP Q06337
E	1010	TYR	-	expression tag	UNP Q06337

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1011	ASP	-	expression tag	UNP Q06337
E	1012	ILE	-	expression tag	UNP Q06337
E	1013	PRO	-	expression tag	UNP Q06337
E	1014	THR	-	expression tag	UNP Q06337
E	1015	THR	-	expression tag	UNP Q06337
E	1016	ALA	-	expression tag	UNP Q06337
E	1017	SER	-	expression tag	UNP Q06337
E	1018	VAL	-	expression tag	UNP Q06337
E	1019	ASP	-	expression tag	UNP Q06337
E	1020	GLY	-	expression tag	UNP Q06337
E	1021	SER	-	expression tag	UNP Q06337
E	1022	GLU	-	expression tag	UNP Q06337
E	1023	ASN	-	expression tag	UNP Q06337
E	1024	LEU	-	expression tag	UNP Q06337
E	1025	TYR	-	expression tag	UNP Q06337
E	1026	PHE	-	expression tag	UNP Q06337
E	1027	GLN	-	expression tag	UNP Q06337
E	1028	GLY	-	expression tag	UNP Q06337
E	1029	SER	-	expression tag	UNP Q06337
E	1030	PRO	-	expression tag	UNP Q06337
E	1031	GLN	-	expression tag	UNP Q06337
E	1032	GLN	-	expression tag	UNP Q06337
E	1033	ASN	-	expression tag	UNP Q06337
E	1034	LYS	-	expression tag	UNP Q06337
E	1035	THR	-	expression tag	UNP Q06337
E	1036	ALA	-	expression tag	UNP Q06337
E	1037	ALA	-	expression tag	UNP Q06337
E	1038	LEU	-	expression tag	UNP Q06337
E	1039	ALA	-	expression tag	UNP Q06337
E	1040	GLN	-	expression tag	UNP Q06337
E	1041	HIS	-	expression tag	UNP Q06337
E	1042	ASP	-	expression tag	UNP Q06337
E	1043	GLU	-	expression tag	UNP Q06337
E	1044	ALA	-	expression tag	UNP Q06337
E	1045	VAL	-	expression tag	UNP Q06337
E	1046	ASP	-	expression tag	UNP Q06337
E	1047	ASN	-	expression tag	UNP Q06337
E	1048	LYS	-	expression tag	UNP Q06337
E	1049	PHE	-	expression tag	UNP Q06337
E	1050	ASN	-	expression tag	UNP Q06337
E	1051	LYS	-	expression tag	UNP Q06337
E	1052	GLU	-	expression tag	UNP Q06337

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1053	GLN	-	expression tag	UNP Q06337
E	1054	GLN	-	expression tag	UNP Q06337
E	1055	ASN	-	expression tag	UNP Q06337
E	1056	ALA	-	expression tag	UNP Q06337
E	1057	PHE	-	expression tag	UNP Q06337
E	1058	TYR	-	expression tag	UNP Q06337
E	1059	GLU	-	expression tag	UNP Q06337
E	1060	ILE	-	expression tag	UNP Q06337
E	1061	LEU	-	expression tag	UNP Q06337
E	1062	HIS	-	expression tag	UNP Q06337
E	1063	LEU	-	expression tag	UNP Q06337
E	1064	PRO	-	expression tag	UNP Q06337
E	1065	ASN	-	expression tag	UNP Q06337
E	1066	LEU	-	expression tag	UNP Q06337
E	1067	ASN	-	expression tag	UNP Q06337
E	1068	GLU	-	expression tag	UNP Q06337
E	1069	GLU	-	expression tag	UNP Q06337
E	1070	GLN	-	expression tag	UNP Q06337
E	1071	ARG	-	expression tag	UNP Q06337
E	1072	ASN	-	expression tag	UNP Q06337
E	1073	ALA	-	expression tag	UNP Q06337
E	1074	PHE	-	expression tag	UNP Q06337
E	1075	ILE	-	expression tag	UNP Q06337
E	1076	GLN	-	expression tag	UNP Q06337
E	1077	SER	-	expression tag	UNP Q06337
E	1078	LEU	-	expression tag	UNP Q06337
E	1079	LYS	-	expression tag	UNP Q06337
E	1080	ASP	-	expression tag	UNP Q06337
E	1081	ASP	-	expression tag	UNP Q06337
E	1082	PRO	-	expression tag	UNP Q06337
E	1083	SER	-	expression tag	UNP Q06337
E	1084	GLN	-	expression tag	UNP Q06337
E	1085	SER	-	expression tag	UNP Q06337
E	1086	ALA	-	expression tag	UNP Q06337
E	1087	ASN	-	expression tag	UNP Q06337
E	1088	LEU	-	expression tag	UNP Q06337
E	1089	LEU	-	expression tag	UNP Q06337
E	1090	ALA	-	expression tag	UNP Q06337
E	1091	GLU	-	expression tag	UNP Q06337
E	1092	ALA	-	expression tag	UNP Q06337
E	1093	LYS	-	expression tag	UNP Q06337
E	1094	LYS	-	expression tag	UNP Q06337

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1095	LEU	-	expression tag	UNP Q06337
E	1096	ASN	-	expression tag	UNP Q06337
E	1097	ASP	-	expression tag	UNP Q06337
E	1098	ALA	-	expression tag	UNP Q06337
E	1099	GLN	-	expression tag	UNP Q06337
E	1100	ALA	-	expression tag	UNP Q06337
E	1101	PRO	-	expression tag	UNP Q06337
E	1102	LYS	-	expression tag	UNP Q06337
E	1103	VAL	-	expression tag	UNP Q06337
E	1104	ASP	-	expression tag	UNP Q06337
E	1105	ASN	-	expression tag	UNP Q06337
E	1106	LYS	-	expression tag	UNP Q06337
E	1107	PHE	-	expression tag	UNP Q06337
E	1108	ASN	-	expression tag	UNP Q06337
E	1109	LYS	-	expression tag	UNP Q06337
E	1110	GLU	-	expression tag	UNP Q06337
E	1111	GLN	-	expression tag	UNP Q06337
E	1112	GLN	-	expression tag	UNP Q06337
E	1113	ASN	-	expression tag	UNP Q06337
E	1114	ALA	-	expression tag	UNP Q06337
E	1115	PHE	-	expression tag	UNP Q06337
E	1116	TYR	-	expression tag	UNP Q06337
E	1117	GLU	-	expression tag	UNP Q06337
E	1118	ILE	-	expression tag	UNP Q06337
E	1119	LEU	-	expression tag	UNP Q06337
E	1120	HIS	-	expression tag	UNP Q06337
E	1121	LEU	-	expression tag	UNP Q06337
E	1122	PRO	-	expression tag	UNP Q06337
E	1123	ASN	-	expression tag	UNP Q06337
E	1124	LEU	-	expression tag	UNP Q06337
E	1125	ASN	-	expression tag	UNP Q06337
E	1126	GLU	-	expression tag	UNP Q06337
E	1127	GLU	-	expression tag	UNP Q06337
E	1128	GLN	-	expression tag	UNP Q06337
E	1129	ARG	-	expression tag	UNP Q06337
E	1130	ASN	-	expression tag	UNP Q06337
E	1131	ALA	-	expression tag	UNP Q06337
E	1132	PHE	-	expression tag	UNP Q06337
E	1133	ILE	-	expression tag	UNP Q06337
E	1134	GLN	-	expression tag	UNP Q06337
E	1135	SER	-	expression tag	UNP Q06337
E	1136	LEU	-	expression tag	UNP Q06337

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1137	LYS	-	expression tag	UNP Q06337
E	1138	ASP	-	expression tag	UNP Q06337
E	1139	ASP	-	expression tag	UNP Q06337
E	1140	PRO	-	expression tag	UNP Q06337
E	1141	SER	-	expression tag	UNP Q06337
E	1142	GLN	-	expression tag	UNP Q06337
E	1143	SER	-	expression tag	UNP Q06337
E	1144	ALA	-	expression tag	UNP Q06337
E	1145	ASN	-	expression tag	UNP Q06337
E	1146	LEU	-	expression tag	UNP Q06337
E	1147	LEU	-	expression tag	UNP Q06337
E	1148	ALA	-	expression tag	UNP Q06337
E	1149	GLU	-	expression tag	UNP Q06337
E	1150	ALA	-	expression tag	UNP Q06337
E	1151	LYS	-	expression tag	UNP Q06337
E	1152	LYS	-	expression tag	UNP Q06337
E	1153	LEU	-	expression tag	UNP Q06337
E	1154	ASN	-	expression tag	UNP Q06337
E	1155	ASP	-	expression tag	UNP Q06337
E	1156	ALA	-	expression tag	UNP Q06337
E	1157	GLN	-	expression tag	UNP Q06337
E	1158	ALA	-	expression tag	UNP Q06337
E	1159	PRO	-	expression tag	UNP Q06337
E	1160	LYS	-	expression tag	UNP Q06337
E	1161	VAL	-	expression tag	UNP Q06337
E	1162	ASP	-	expression tag	UNP Q06337
E	1163	ALA	-	expression tag	UNP Q06337
E	1164	ASN	-	expression tag	UNP Q06337
E	1165	SER	-	expression tag	UNP Q06337
E	1166	ALA	-	expression tag	UNP Q06337
E	1167	ALA	-	expression tag	UNP Q06337
E	1168	LEU	-	expression tag	UNP Q06337

- Molecule 2 is a protein called Actin-related protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	414	Total	C	N	O	S	0	0
			3278	2088	541	638	11		

- Molecule 3 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	357	Total	C	N	O	S	0	0
			2788	1772	468	531	17		

- Molecule 4 is a protein called SWR1-complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	237	Total	C	N	O	S	0	0
			1989	1275	337	370	7		

- Molecule 5 is a protein called Enhancer of polycomb-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	269	Total	C	N	O	S	0	0
			2250	1427	380	438	5		

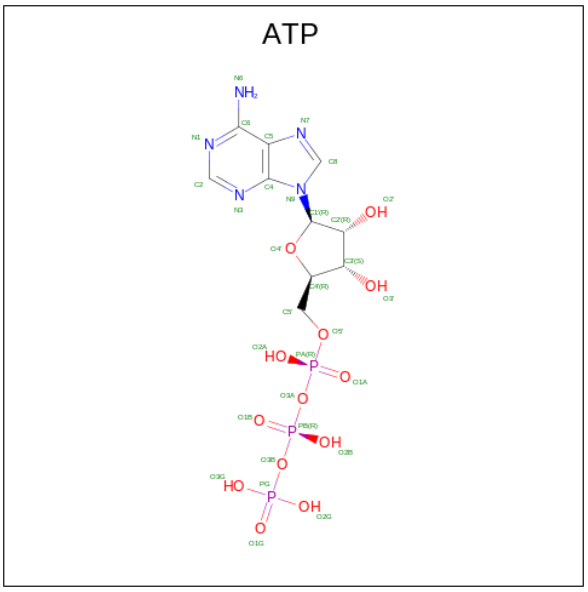
- Molecule 6 is a protein called Transcription-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	3513	Total	C	N	O	S	0	0
			28729	18596	4776	5237	120		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	F	1	Total	Mg	0
			1	1	
7	G	1	Total	Mg	0
			1	1	

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



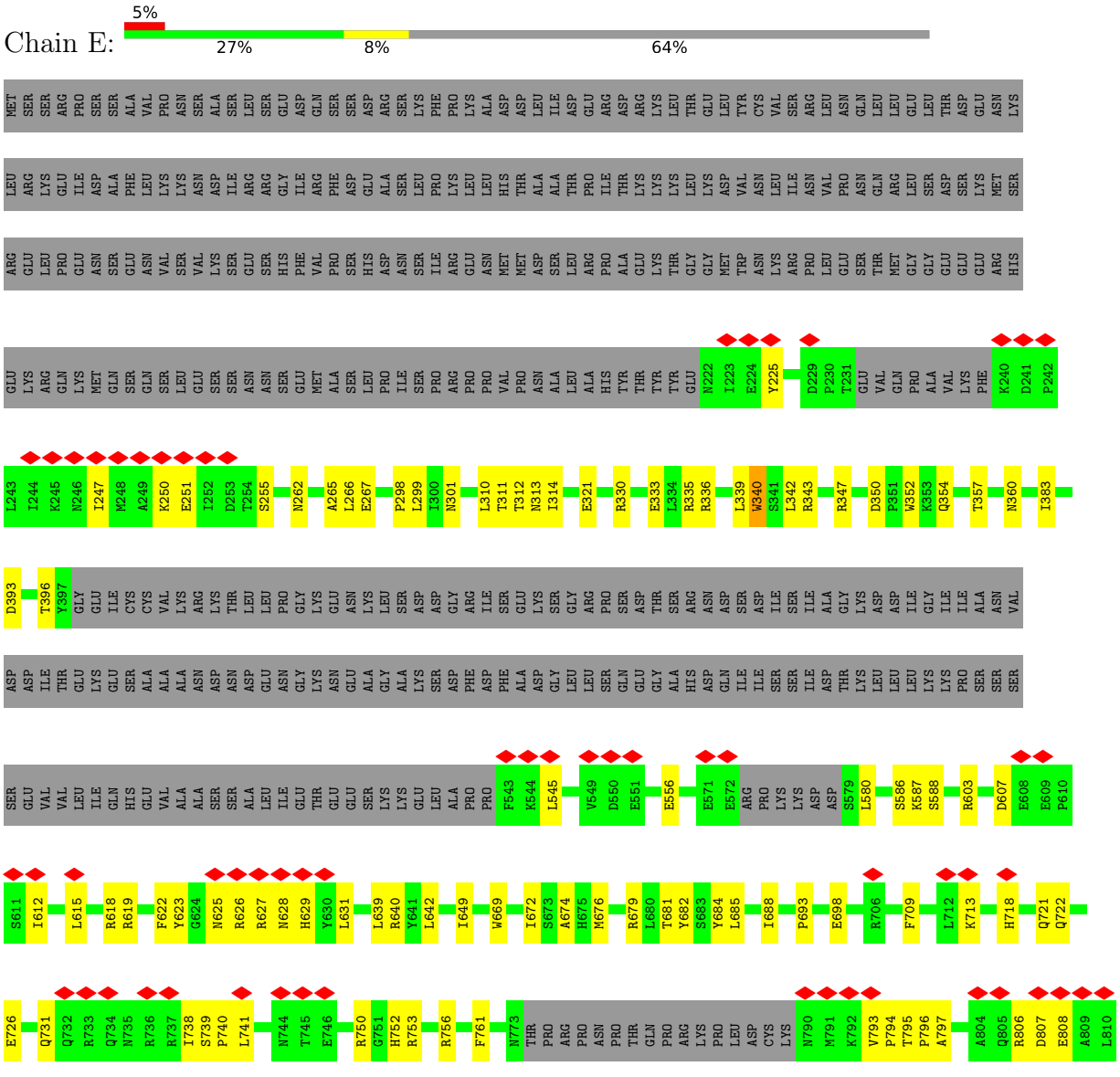
Mol	Chain	Residues	Atoms					AltConf
8	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

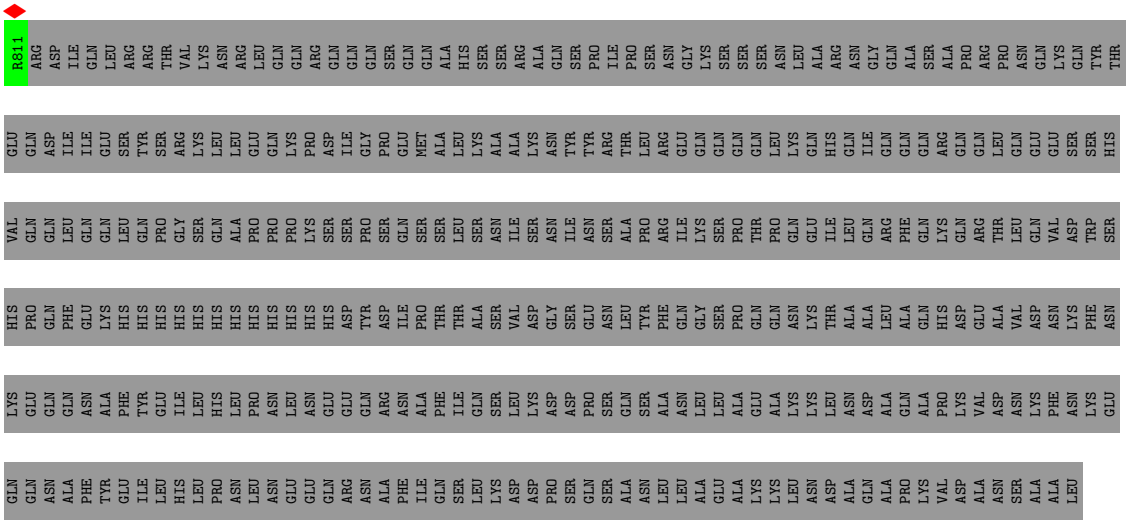
3 Residue-property plots (i)

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 modification-related protein EAF1

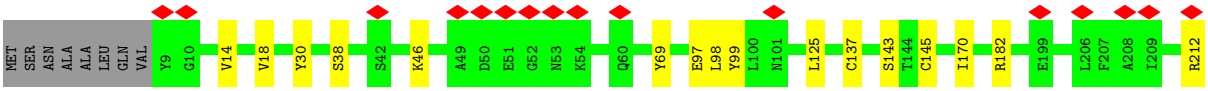
Chain E:

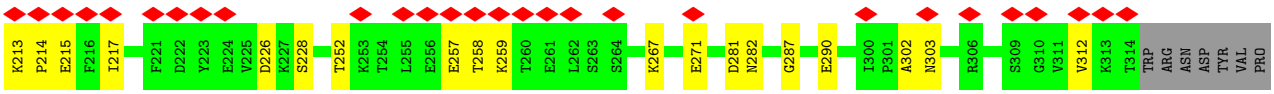


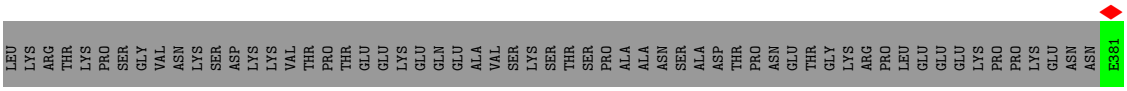


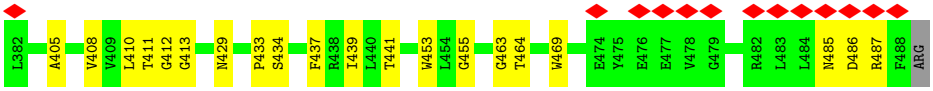
• Molecule 2: Actin-related protein 4

Chain F:



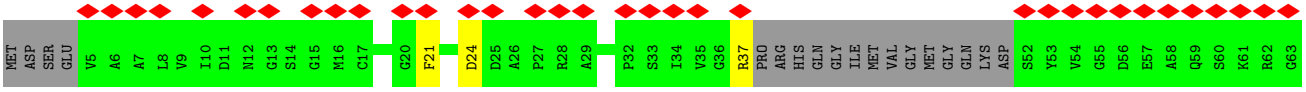


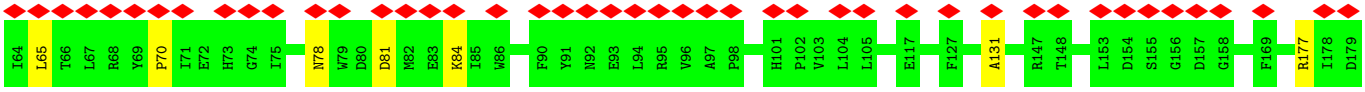


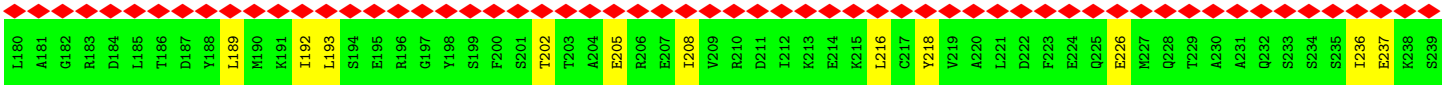


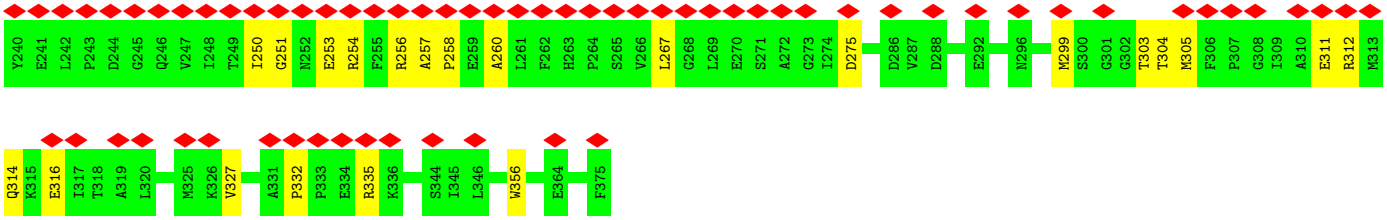
• Molecule 3: Actin

Chain G:



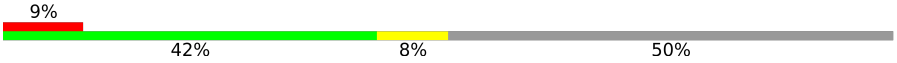


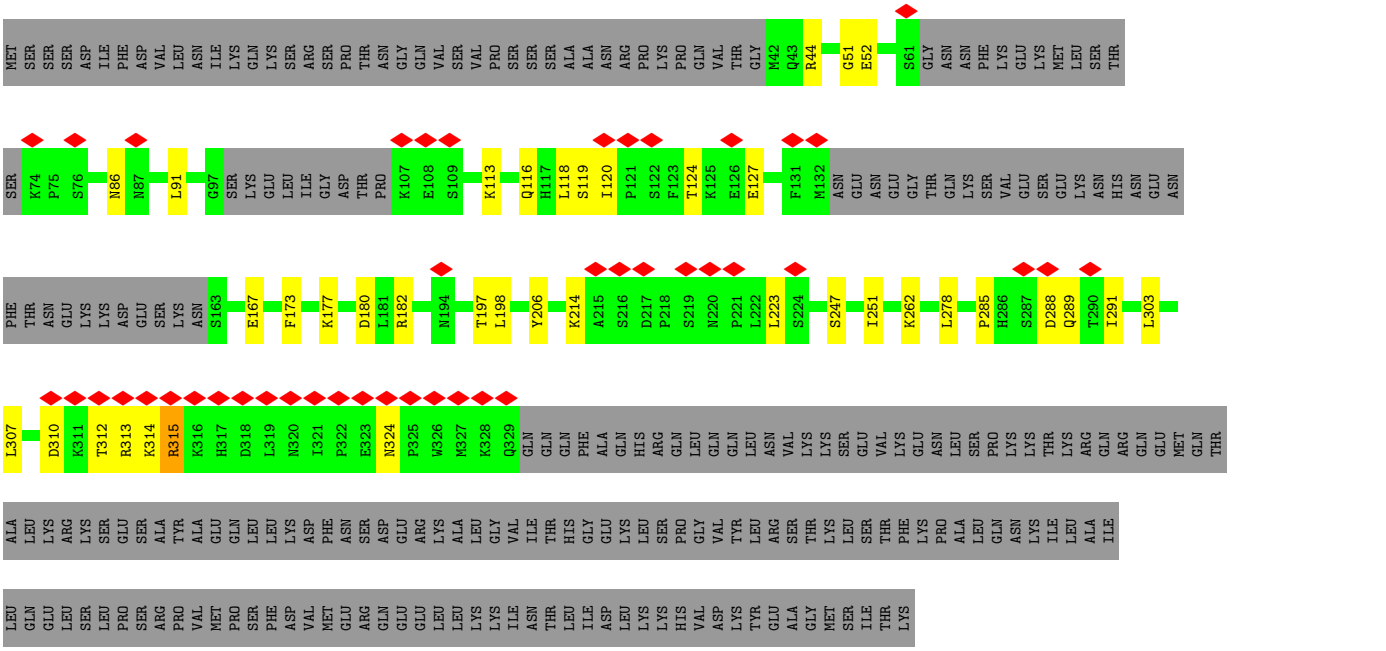




• Molecule 4: SWR1-complex protein 4

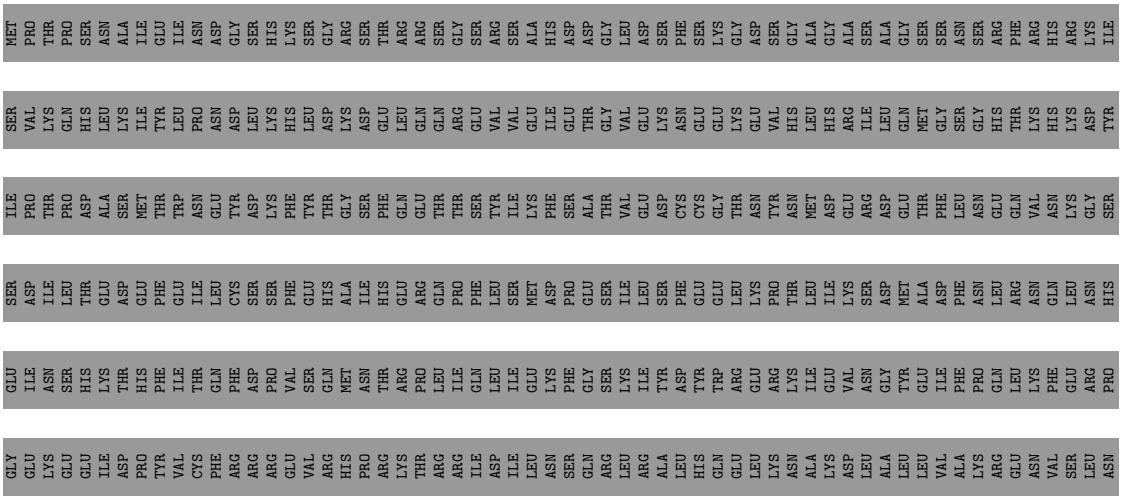
Chain K:

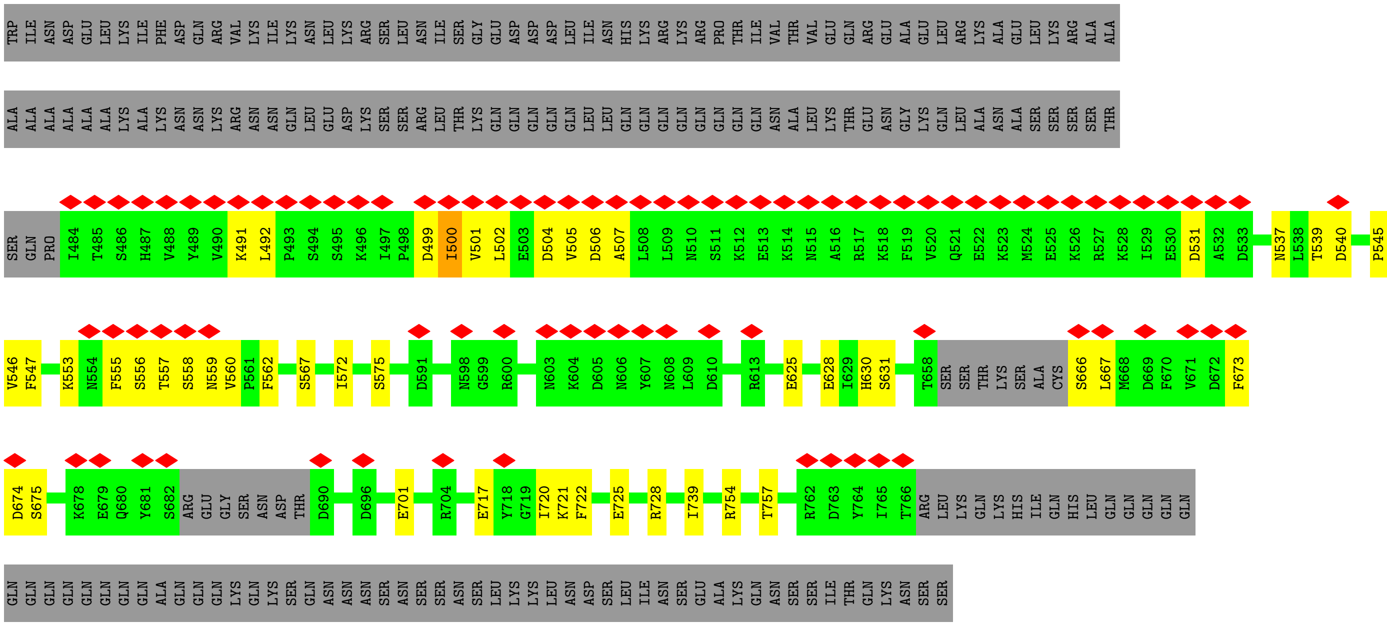




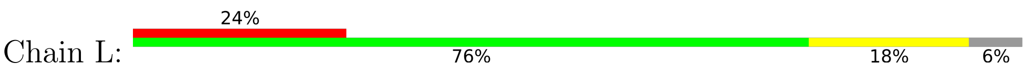
• Molecule 5: Enhancer of polycomb-like protein 1

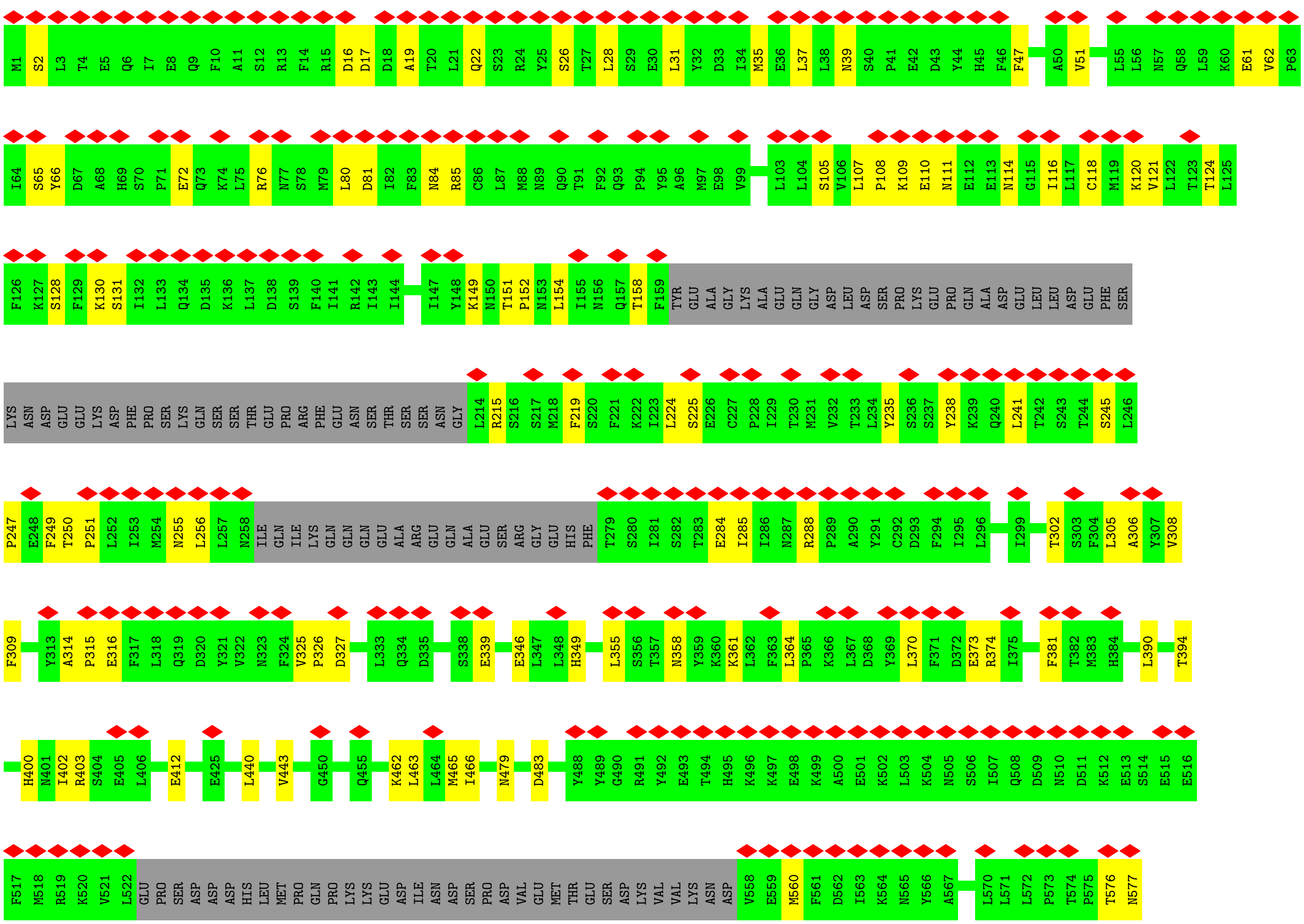
Chain H:

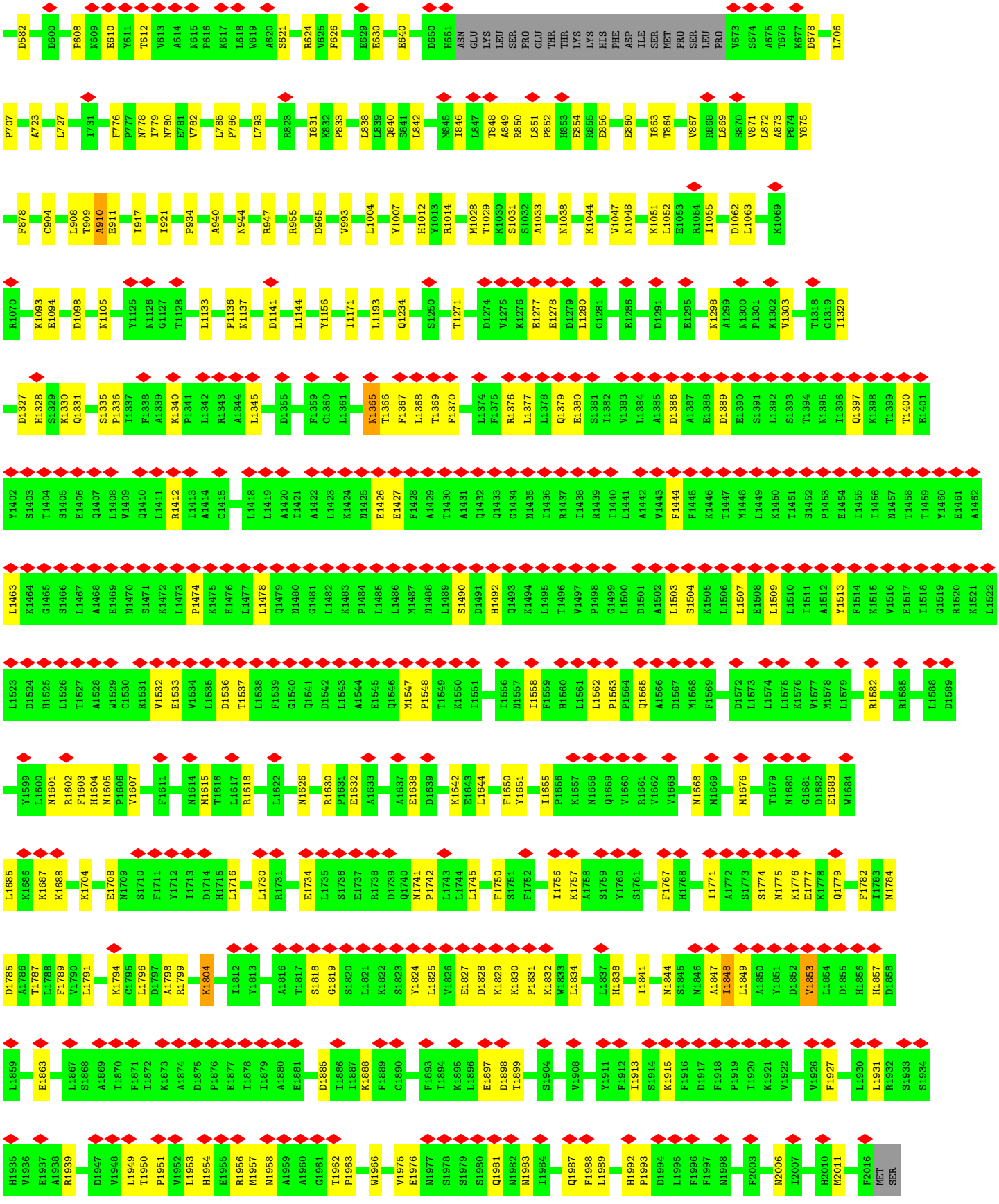




• Molecule 6: Transcription-associated protein 1



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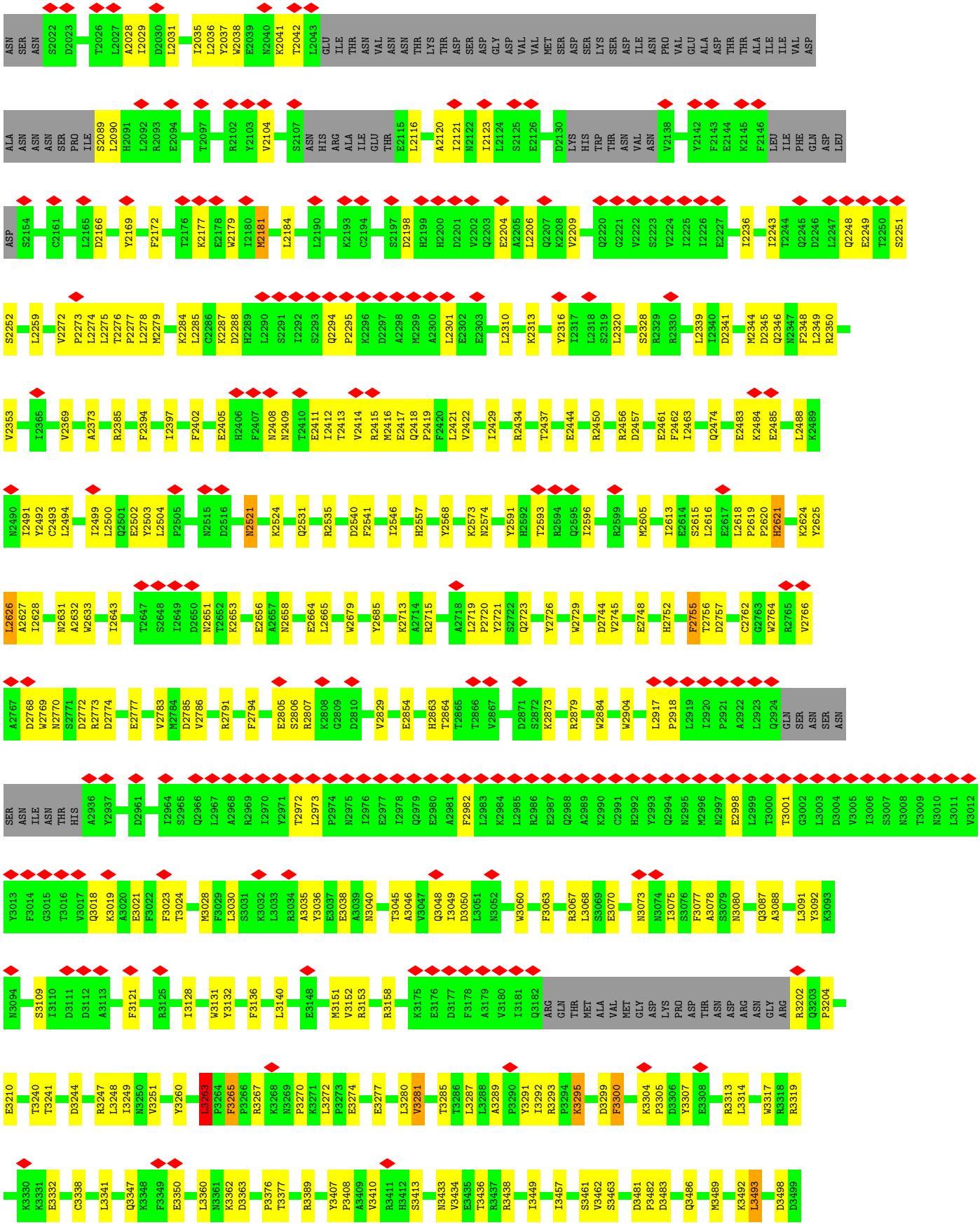
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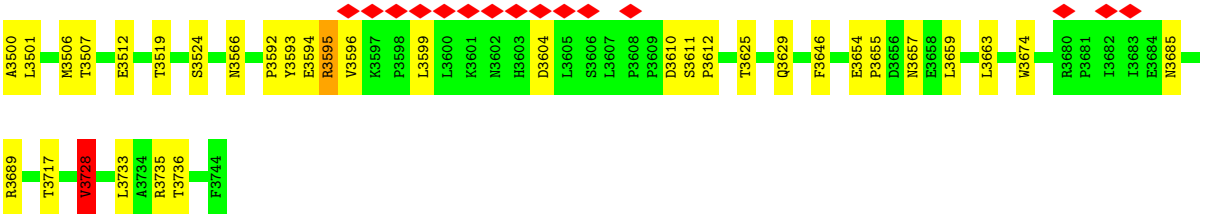
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E3684
N3685
R3689
T3717
V3728
L3733
A3734
R3735
T3736
F3744

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69770	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	407.02, 407.02, 407.02	wwPDB
Map dimensions	376, 376, 376	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP

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	E	0.67	0/3527	0.62	0/4769
2	F	0.69	0/3350	0.57	0/4544
3	G	0.57	0/2849	0.54	0/3859
4	K	0.70	0/2036	0.57	0/2739
5	H	0.71	0/2298	0.63	0/3093
6	L	0.58	3/29358 (0.0%)	0.58	2/39779 (0.0%)
All	All	0.61	3/43418 (0.0%)	0.58	2/58783 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	L	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	2755	PHE	CB-CG	-5.68	1.41	1.51
6	L	3728	VAL	CB-CG2	-5.29	1.41	1.52
6	L	3512	GLU	CB-CG	-5.13	1.42	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	2626	LEU	CB-CG-CD2	-6.71	99.60	111.00
6	L	3263	LEU	CA-CB-CG	5.96	129.01	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	L	2621	HIS	Peptide

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	E	3448	0	3448	102	0
2	F	3278	0	3238	31	0
3	G	2788	0	2760	29	0
4	K	1989	0	1961	37	0
5	H	2250	0	2192	53	0
6	L	28729	0	29144	499	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
8	F	31	0	12	1	0
8	G	31	0	12	1	0
All	All	42546	0	42767	686	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.

The worst 5 of 686 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)
1:E:640:ARG:NH2	1:E:726:GLU:OE1	1.98	0.97
6:L:944:ASN:OD1	6:L:947:ARG:NH2	2.01	0.92
1:E:312:THR:OG1	6:L:3728:VAL:O	1.88	0.88
6:L:3244:ASP:OD1	6:L:3247:ARG:NH1	2.13	0.81
4:K:262:LYS:NZ	5:H:545:PRO:O	2.14	0.80

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	E	405/1168 (35%)	363 (90%)	41 (10%)	1 (0%)	47	79
2	F	410/489 (84%)	384 (94%)	26 (6%)	0	100	100
3	G	353/375 (94%)	343 (97%)	10 (3%)	0	100	100
4	K	229/476 (48%)	211 (92%)	17 (7%)	1 (0%)	34	69
5	H	263/832 (32%)	232 (88%)	30 (11%)	1 (0%)	34	69
6	L	3489/3744 (93%)	3204 (92%)	283 (8%)	2 (0%)	51	83
All	All	5149/7084 (73%)	4737 (92%)	407 (8%)	5 (0%)	54	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	K	315	ARG
5	H	500	ILE
6	L	1848	ILE
1	E	340	TRP
6	L	910	ALA

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	E	379/1054 (36%)	379 (100%)	0	100	100
2	F	367/434 (85%)	367 (100%)	0	100	100
3	G	305/320 (95%)	305 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	K	221/441 (50%)	221 (100%)	0	100 100
5	H	256/769 (33%)	256 (100%)	0	100 100
6	L	3238/3452 (94%)	3218 (99%)	20 (1%)	86 94
All	All	4766/6470 (74%)	4746 (100%)	20 (0%)	91 96

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	L	3486	GLN
6	L	3506	MET
6	L	3728	VAL
6	L	3595	ARG
6	L	3263	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
6	L	1605	ASN
6	L	2907	HIS
6	L	2913	ASN
6	L	2941	HIS
6	L	2992	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	ATP	G	502	7	26,33,33	0.69	0	31,52,52	0.82	1 (3%)
8	ATP	F	1002	7	26,33,33	0.74	0	31,52,52	0.75	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ATP	G	502	7	-	0/18/38/38	0/3/3/3
8	ATP	F	1002	7	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	G	502	ATP	C5-C6-N6	2.26	123.79	120.35
8	F	1002	ATP	C5-C6-N6	2.26	123.78	120.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	1002	ATP	C5'-O5'-PA-O3A
8	F	1002	ATP	PG-O3B-PB-O2B
8	F	1002	ATP	C5'-O5'-PA-O2A
8	F	1002	ATP	O4'-C4'-C5'-O5'

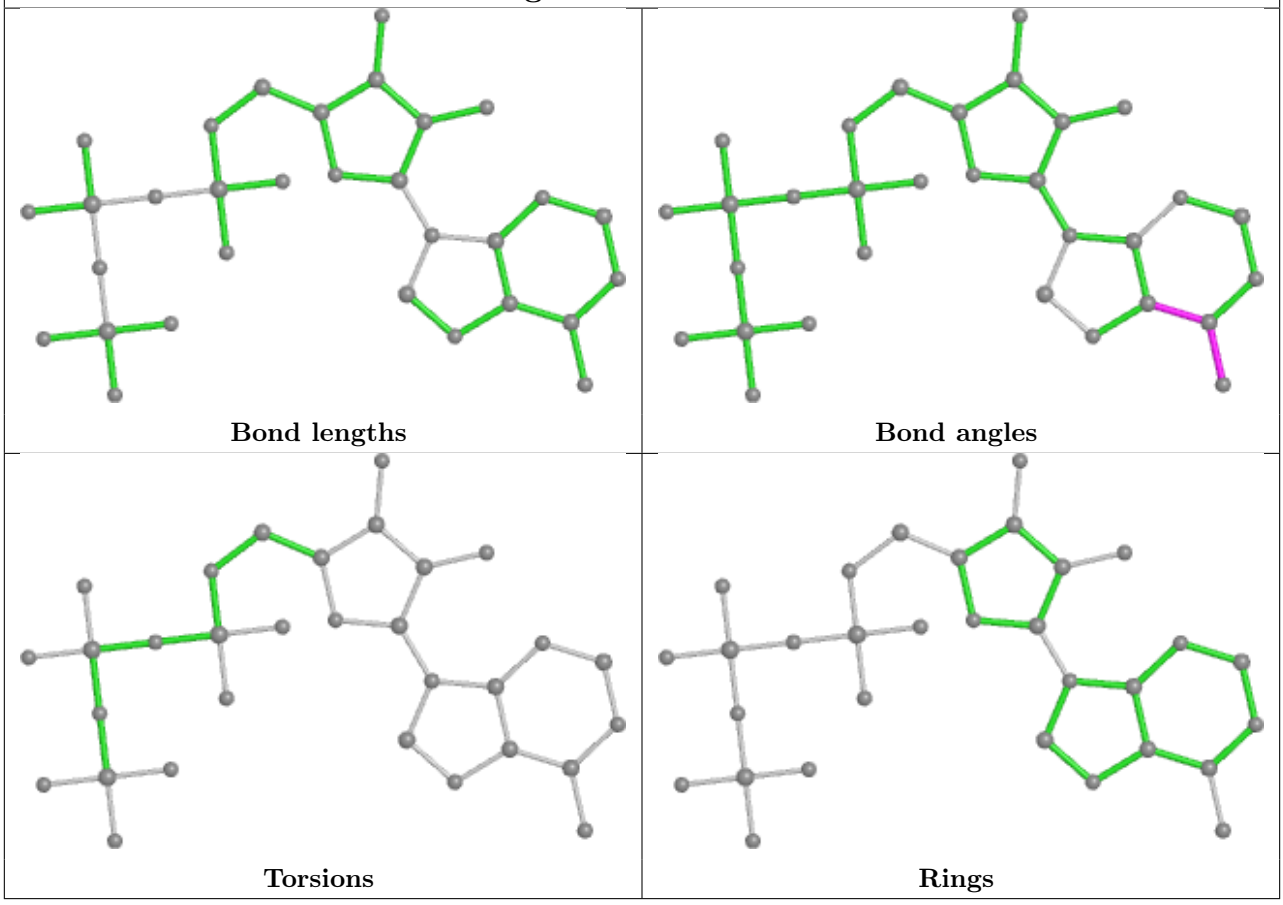
There are no ring outliers.

2 monomers are involved in 2 short contacts:

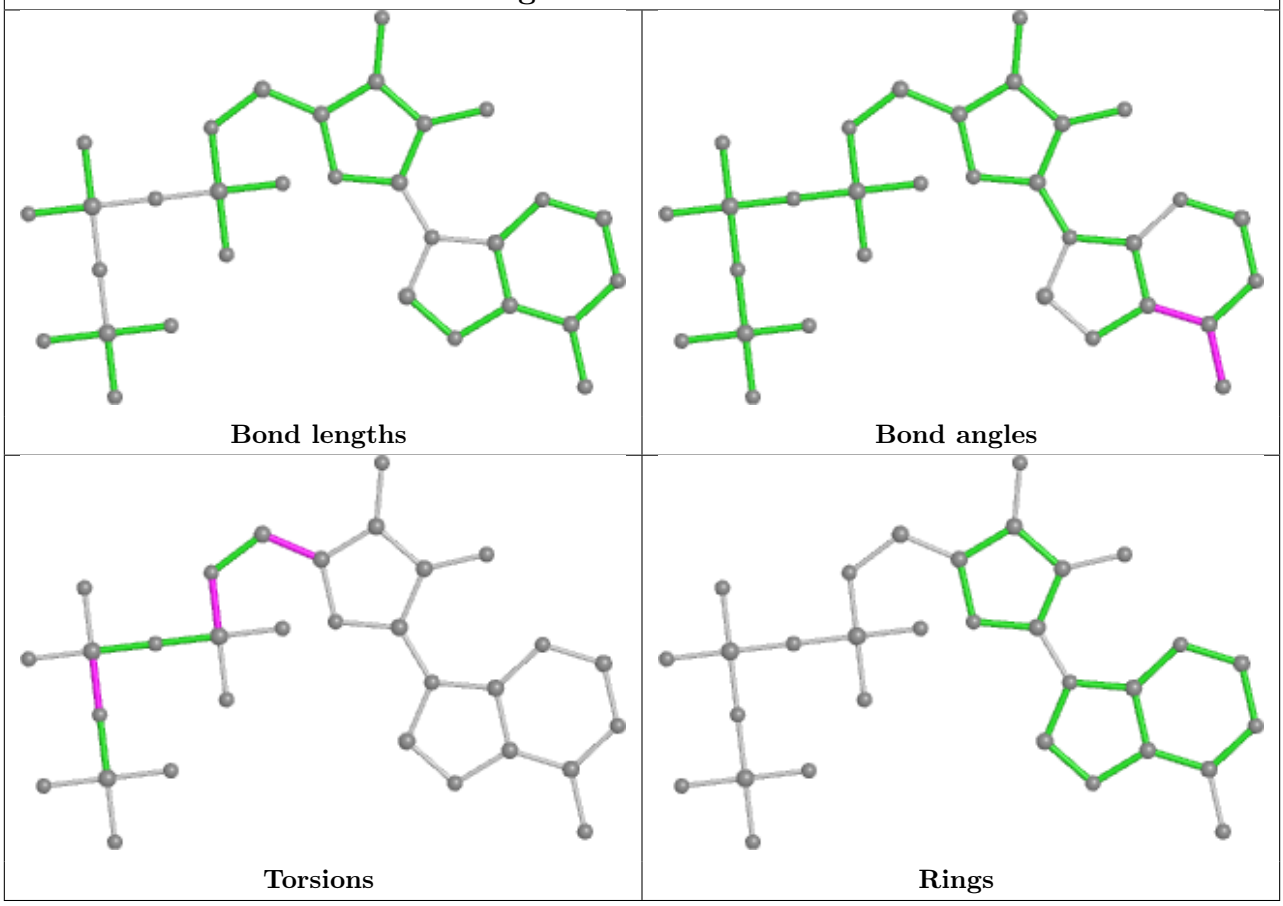
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	502	ATP	1	0
8	F	1002	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP G 502



Ligand ATP F 1002



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.

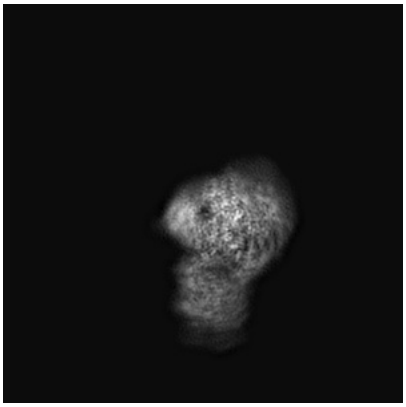
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32149. These allow visual inspection of the internal detail of the map and identification of artifacts.

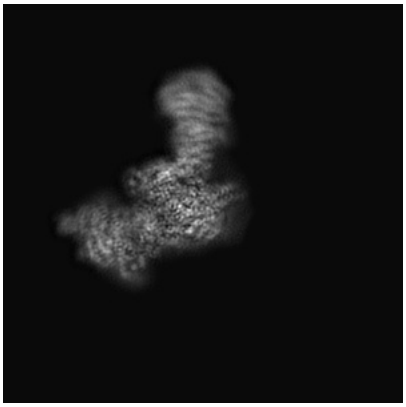
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

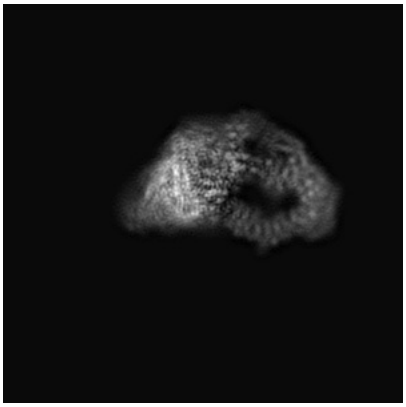
6.1.1 Primary map



X



Y

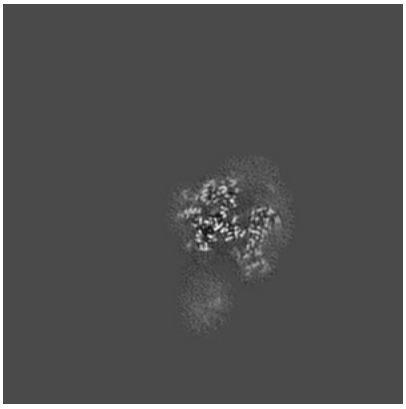


Z

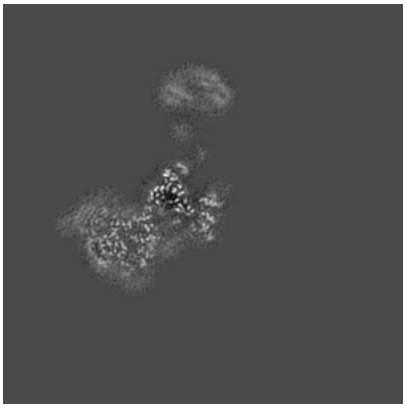
The images above show the map projected in three orthogonal directions.

6.2 Central slices

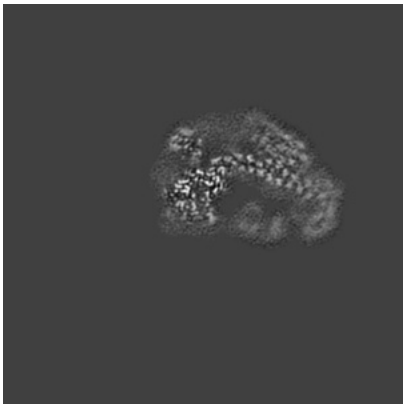
6.2.1 Primary map



X Index: 188



Y Index: 188

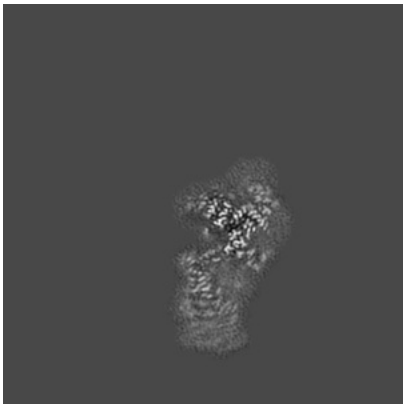


Z Index: 188

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

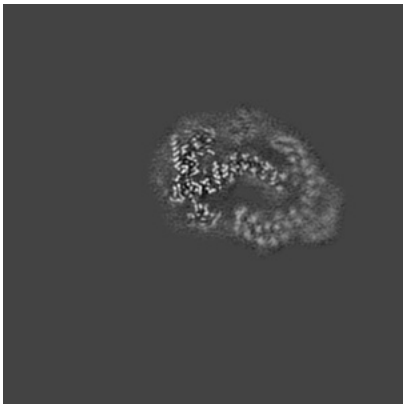
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 169

Y Index: 198



Z Index: 176

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

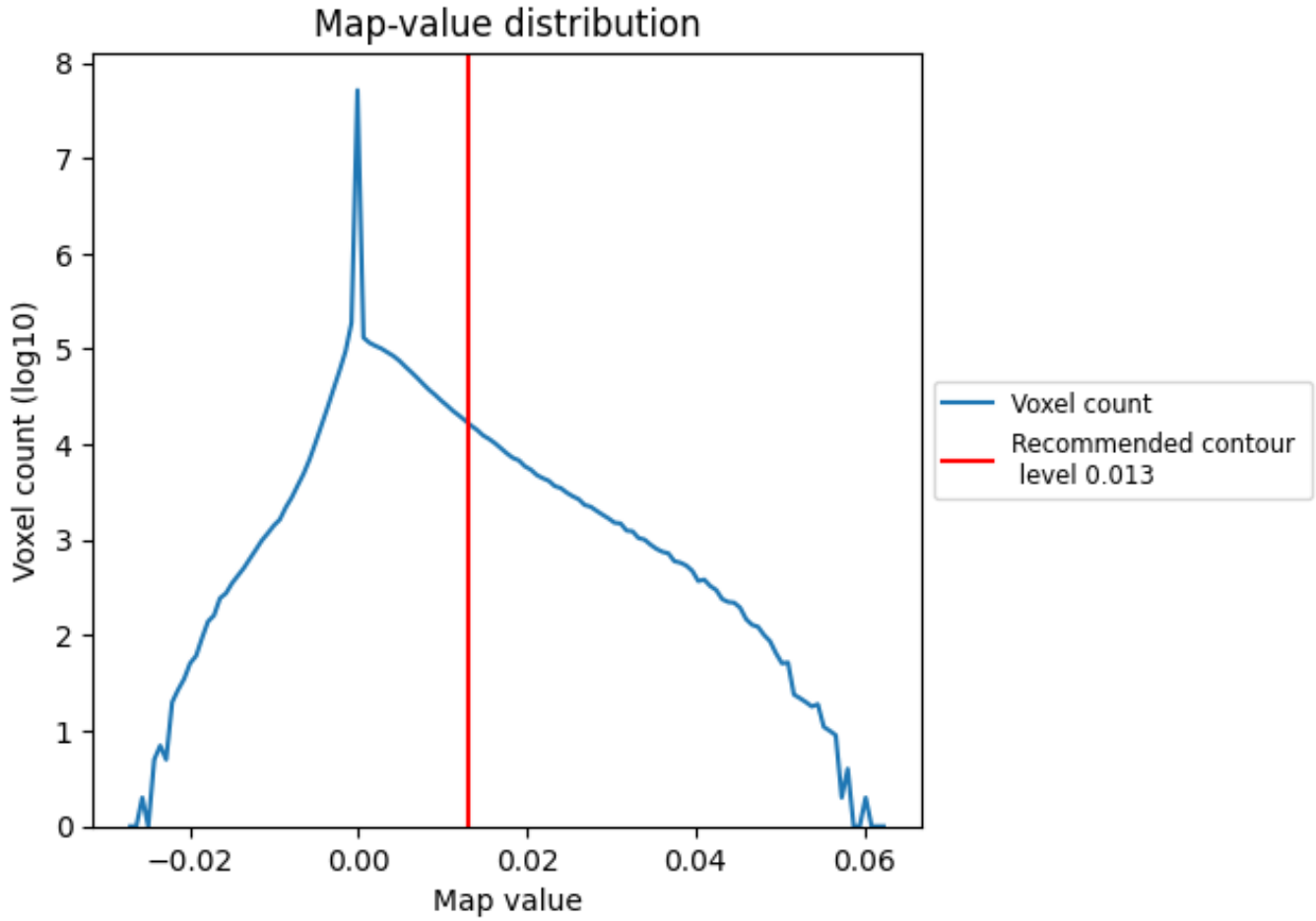
6.5 Mask visualisation (i)

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

7 Map analysis

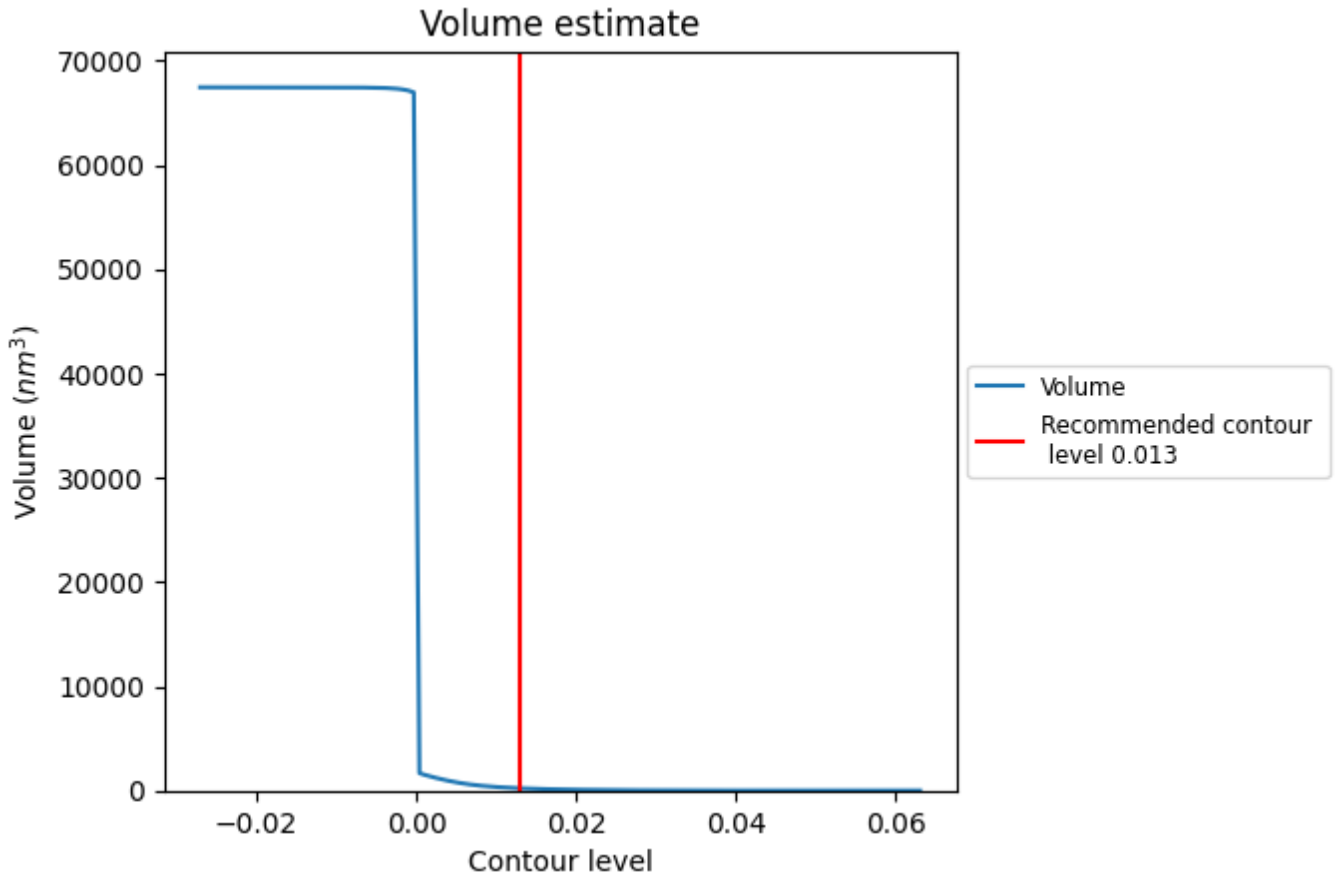
This section contains the results of statistical analysis of the map.

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.

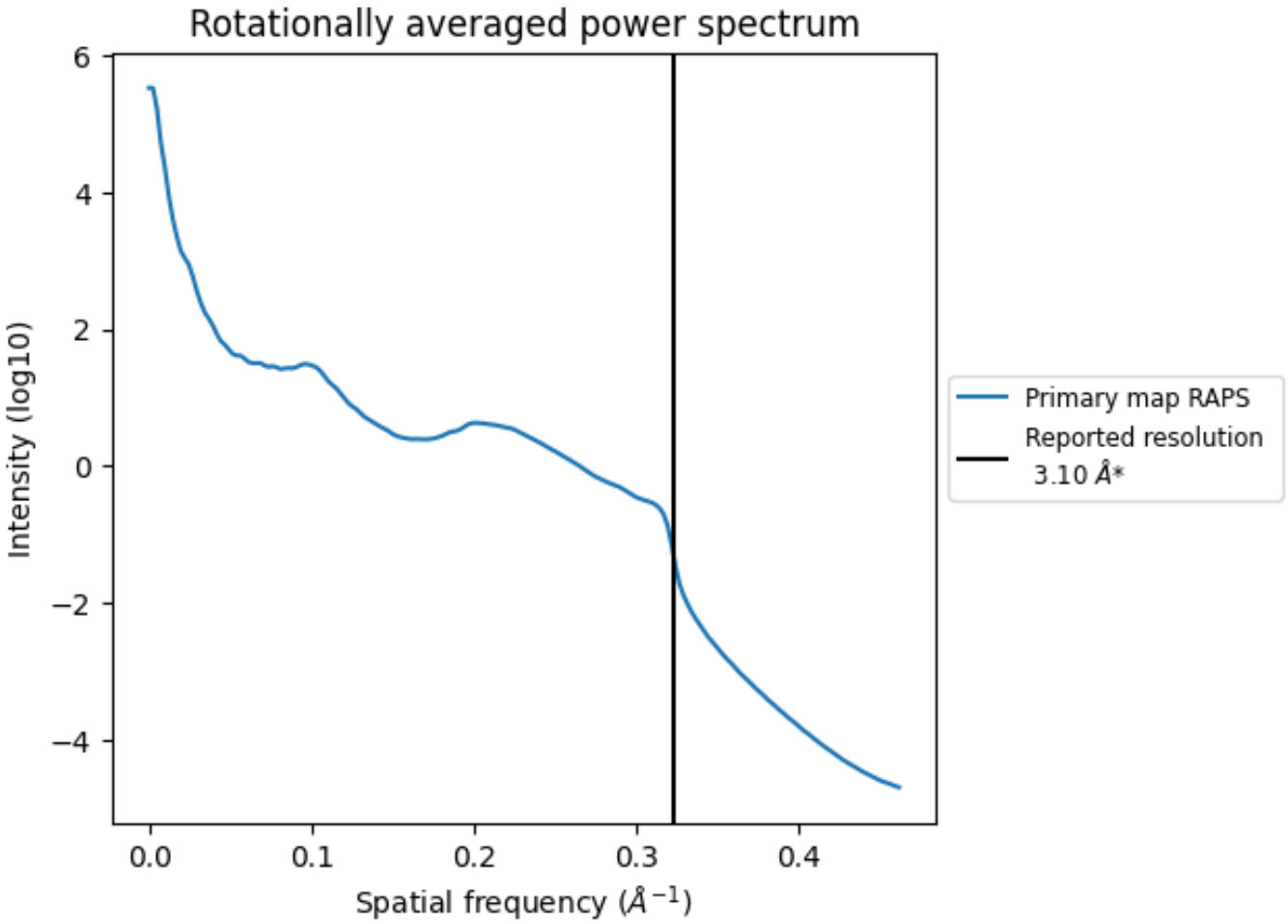
7.2 Volume estimate (i)



The volume at the recommended contour level is 217 nm^3; this corresponds to an approximate mass of 196 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)

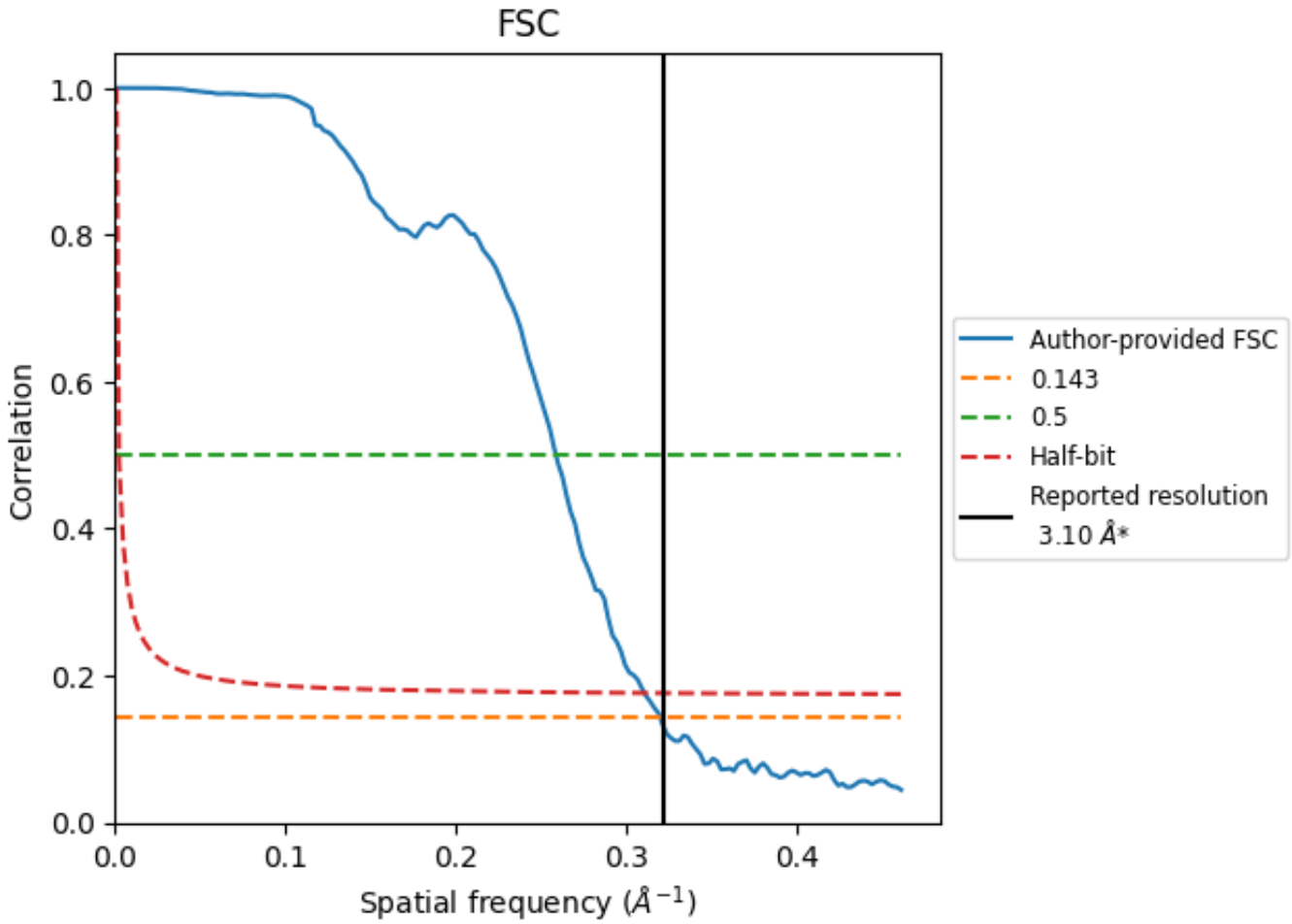


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

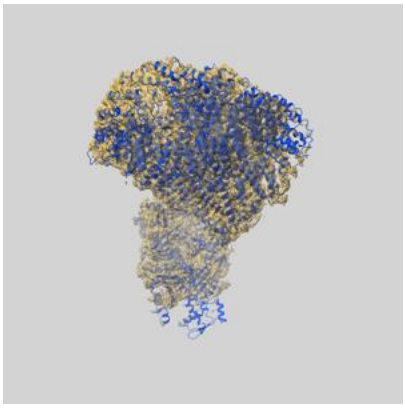
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.12	3.86	3.21
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

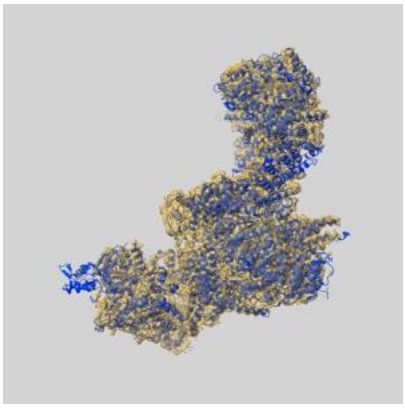
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32149 and PDB model 7VVY. Per-residue inclusion information can be found in section 3 on page 10.

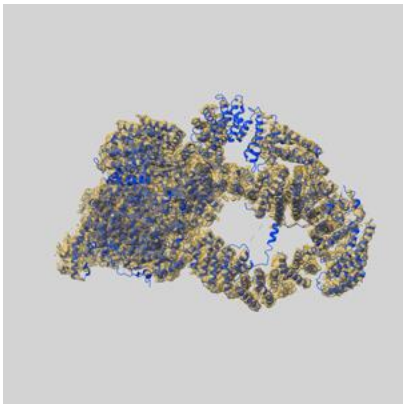
9.1 Map-model overlay



X



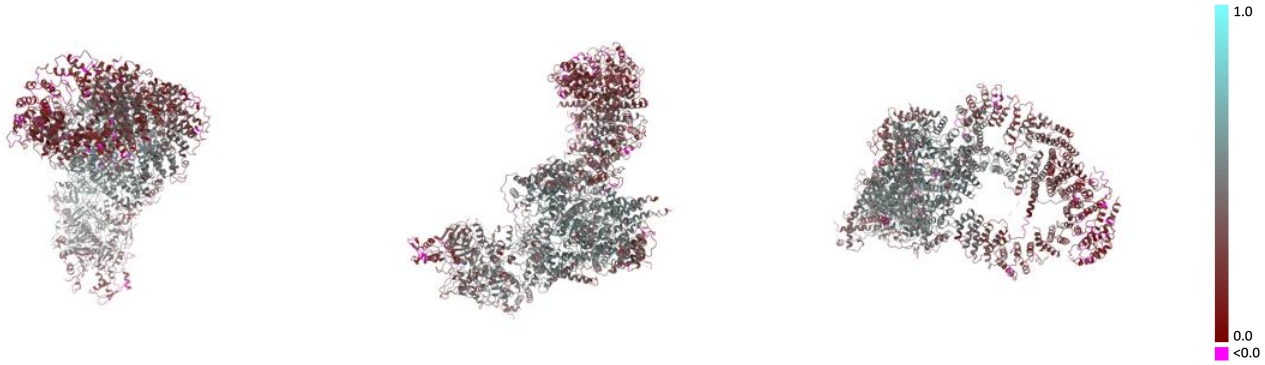
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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.

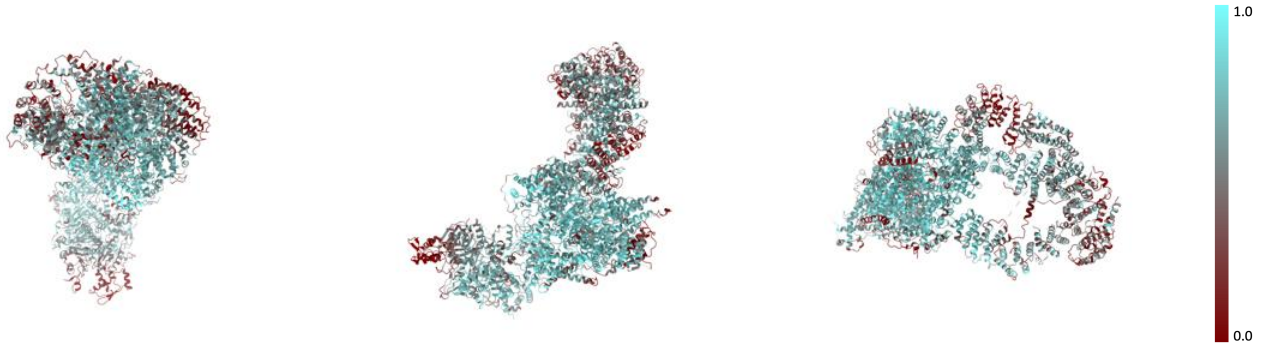
9.2 Q-score mapped to coordinate model



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.

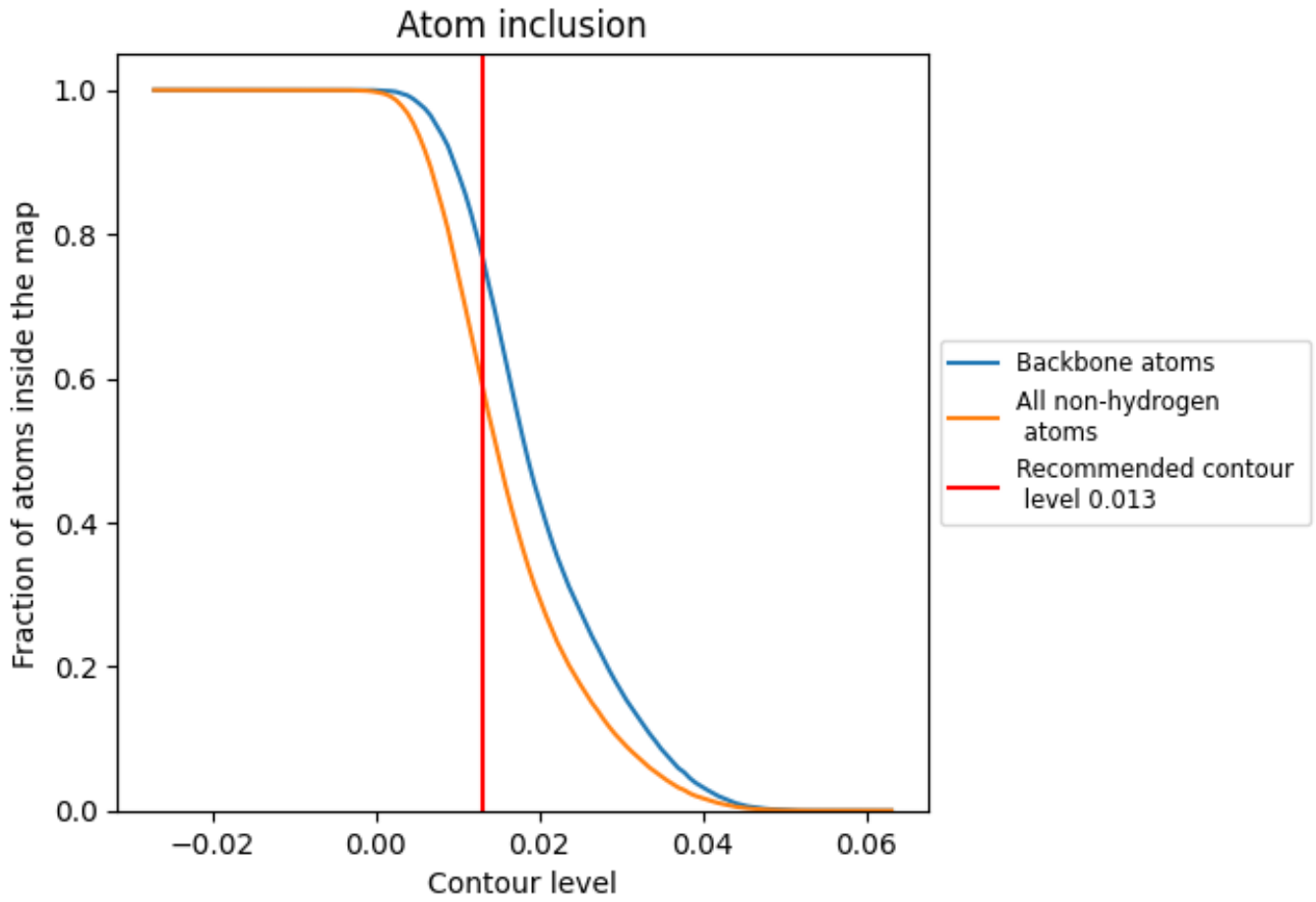
9.3 Atom inclusion mapped to coordinate model



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 (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 59% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5923	0.3840
E	0.6692	0.4670
F	0.6648	0.4250
G	0.3241	0.3010
H	0.5742	0.4230
K	0.6163	0.4160
L	0.6009	0.3730