



wwPDB EM Validation Summary Report ⓘ

Jun 9, 2024 – 07:25 PM EDT

PDB ID : 8FNW
EMDB ID : EMD-29328
Title : Structure of RdrA-RdrB complex from Escherichia coli RADAR defense system
Authors : Duncan-Lowey, B.; Johnson, A.G.; Rawson, S.; Mayer, M.L.; Kranzusch, P.J.
Deposited on : 2022-12-28
Resolution : 6.73 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.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

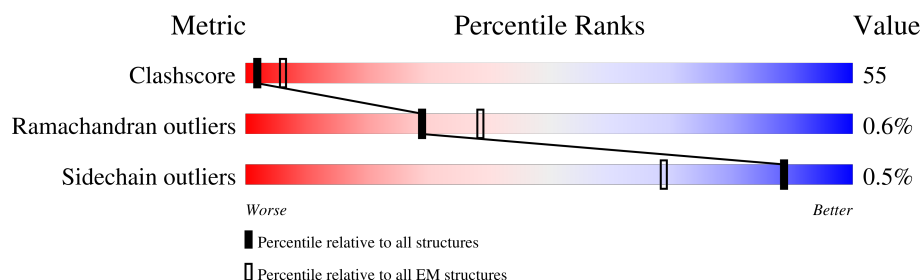
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.73 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 $\leq 5\%$. 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	799	<div> <div>62%</div> <div> <div>56%</div> <div>39%</div> <div>..</div> </div> </div>
1	B	799	<div> <div>58%</div> <div> <div>55%</div> <div>40%</div> <div>..</div> </div> </div>
1	C	799	<div> <div>21%</div> <div> <div>52%</div> <div>43%</div> <div>..</div> </div> </div>
1	D	799	<div> <div>22%</div> <div> <div>48%</div> <div>46%</div> <div>..</div> </div> </div>
1	E	799	<div> <div>48%</div> <div> <div>52%</div> <div>42%</div> <div>..</div> </div> </div>
1	F	799	<div> <div>44%</div> <div> <div>55%</div> <div>40%</div> <div>..</div> </div> </div>
1	G	799	<div> <div>45%</div> <div> <div>53%</div> <div>42%</div> <div>..</div> </div> </div>
1	H	799	<div> <div>37%</div> <div> <div>55%</div> <div>40%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	I	799	
1	J	799	
1	K	799	
1	L	799	
2	M	947	
2	N	947	
2	O	947	
2	P	947	
2	Q	947	
2	R	947	
2	S	947	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 118867 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 Adenosine deaminase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	B	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	C	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	D	767	Total	C	N	O	S	0	0
			6221	3989	1078	1120	34		
1	E	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	F	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	G	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	H	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	I	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	J	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	K	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	L	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	THR	ILE	conflict	UNP A0A8E2SFD7
B	274	THR	ILE	conflict	UNP A0A8E2SFD7
C	274	THR	ILE	conflict	UNP A0A8E2SFD7
D	274	THR	ILE	conflict	UNP A0A8E2SFD7
E	274	THR	ILE	conflict	UNP A0A8E2SFD7
F	274	THR	ILE	conflict	UNP A0A8E2SFD7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	274	THR	ILE	conflict	UNP A0A8E2SFD7
H	274	THR	ILE	conflict	UNP A0A8E2SFD7
I	274	THR	ILE	conflict	UNP A0A8E2SFD7
J	274	THR	ILE	conflict	UNP A0A8E2SFD7
K	274	THR	ILE	conflict	UNP A0A8E2SFD7
L	274	THR	ILE	conflict	UNP A0A8E2SFD7

- Molecule 2 is a protein called Archaeal ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	786	Total	C	N	O	S	0	0
			6277	3985	1085	1176	31		
2	N	786	Total	C	N	O	S	0	0
			6277	3985	1085	1176	31		
2	O	786	Total	C	N	O	S	0	0
			6277	3985	1085	1176	31		
2	P	786	Total	C	N	O	S	0	0
			6277	3985	1085	1176	31		
2	Q	786	Total	C	N	O	S	0	0
			6277	3985	1085	1176	31		
2	R	786	Total	C	N	O	S	0	0
			6277	3985	1085	1176	31		
2	S	786	Total	C	N	O	S	0	0
			6277	3985	1085	1176	31		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	11	LYS	GLU	conflict	UNP A0A8H9B1T2
M	24	SER	PRO	conflict	UNP A0A8H9B1T2
M	67	PRO	SER	conflict	UNP A0A8H9B1T2
M	335	SER	GLY	conflict	UNP A0A8H9B1T2
M	409	ASP	ASN	conflict	UNP A0A8H9B1T2
M	428	ASN	SER	conflict	UNP A0A8H9B1T2
M	583	ASN	HIS	conflict	UNP A0A8H9B1T2
M	586	GLU	GLY	conflict	UNP A0A8H9B1T2
M	636	ARG	LEU	conflict	UNP A0A8H9B1T2
M	858	ILE	VAL	conflict	UNP A0A8H9B1T2
N	11	LYS	GLU	conflict	UNP A0A8H9B1T2
N	24	SER	PRO	conflict	UNP A0A8H9B1T2
N	67	PRO	SER	conflict	UNP A0A8H9B1T2
N	335	SER	GLY	conflict	UNP A0A8H9B1T2

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Chain	Residue	Modelled	Actual	Comment	Reference
N	409	ASP	ASN	conflict	UNP A0A8H9B1T2
N	428	ASN	SER	conflict	UNP A0A8H9B1T2
N	583	ASN	HIS	conflict	UNP A0A8H9B1T2
N	586	GLU	GLY	conflict	UNP A0A8H9B1T2
N	636	ARG	LEU	conflict	UNP A0A8H9B1T2
N	858	ILE	VAL	conflict	UNP A0A8H9B1T2
O	11	LYS	GLU	conflict	UNP A0A8H9B1T2
O	24	SER	PRO	conflict	UNP A0A8H9B1T2
O	67	PRO	SER	conflict	UNP A0A8H9B1T2
O	335	SER	GLY	conflict	UNP A0A8H9B1T2
O	409	ASP	ASN	conflict	UNP A0A8H9B1T2
O	428	ASN	SER	conflict	UNP A0A8H9B1T2
O	583	ASN	HIS	conflict	UNP A0A8H9B1T2
O	586	GLU	GLY	conflict	UNP A0A8H9B1T2
O	636	ARG	LEU	conflict	UNP A0A8H9B1T2
O	858	ILE	VAL	conflict	UNP A0A8H9B1T2
P	11	LYS	GLU	conflict	UNP A0A8H9B1T2
P	24	SER	PRO	conflict	UNP A0A8H9B1T2
P	67	PRO	SER	conflict	UNP A0A8H9B1T2
P	335	SER	GLY	conflict	UNP A0A8H9B1T2
P	409	ASP	ASN	conflict	UNP A0A8H9B1T2
P	428	ASN	SER	conflict	UNP A0A8H9B1T2
P	583	ASN	HIS	conflict	UNP A0A8H9B1T2
P	586	GLU	GLY	conflict	UNP A0A8H9B1T2
P	636	ARG	LEU	conflict	UNP A0A8H9B1T2
P	858	ILE	VAL	conflict	UNP A0A8H9B1T2
Q	11	LYS	GLU	conflict	UNP A0A8H9B1T2
Q	24	SER	PRO	conflict	UNP A0A8H9B1T2
Q	67	PRO	SER	conflict	UNP A0A8H9B1T2
Q	335	SER	GLY	conflict	UNP A0A8H9B1T2
Q	409	ASP	ASN	conflict	UNP A0A8H9B1T2
Q	428	ASN	SER	conflict	UNP A0A8H9B1T2
Q	583	ASN	HIS	conflict	UNP A0A8H9B1T2
Q	586	GLU	GLY	conflict	UNP A0A8H9B1T2
Q	636	ARG	LEU	conflict	UNP A0A8H9B1T2
Q	858	ILE	VAL	conflict	UNP A0A8H9B1T2
R	11	LYS	GLU	conflict	UNP A0A8H9B1T2
R	24	SER	PRO	conflict	UNP A0A8H9B1T2
R	67	PRO	SER	conflict	UNP A0A8H9B1T2
R	335	SER	GLY	conflict	UNP A0A8H9B1T2
R	409	ASP	ASN	conflict	UNP A0A8H9B1T2
R	428	ASN	SER	conflict	UNP A0A8H9B1T2

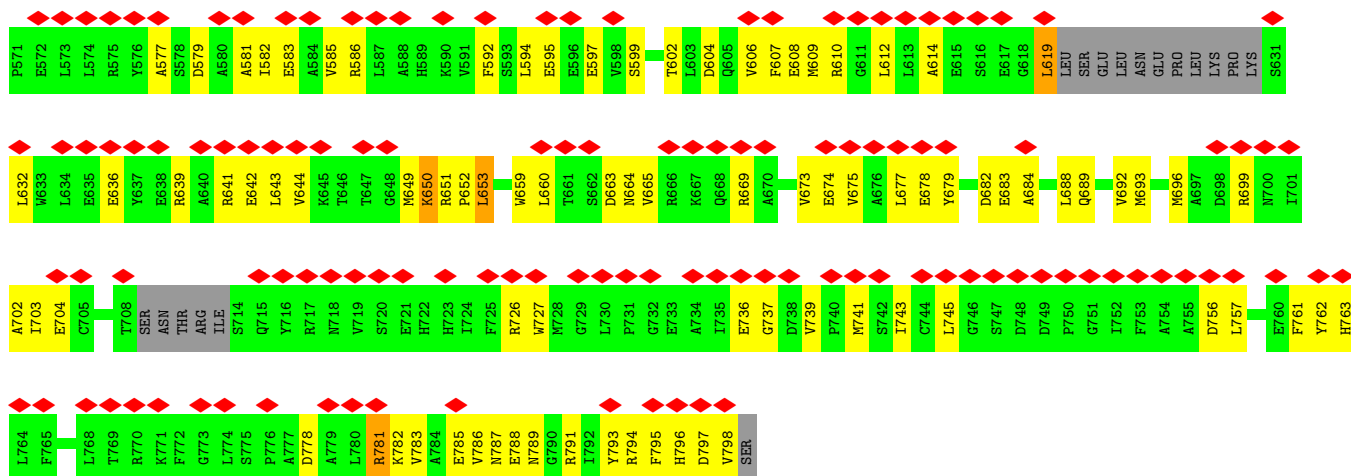
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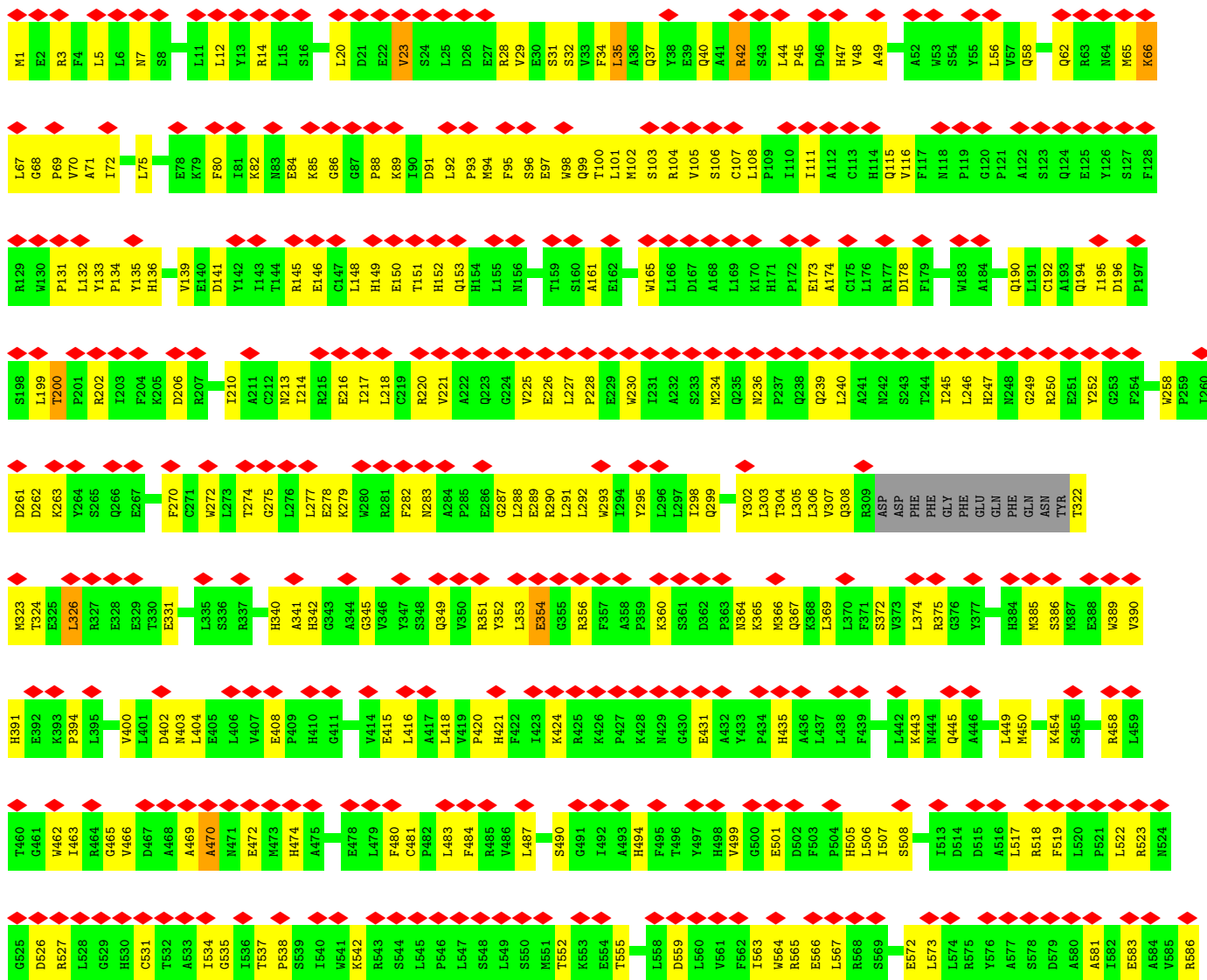
Chain	Residue	Modelled	Actual	Comment	Reference
R	583	ASN	HIS	conflict	UNP A0A8H9B1T2
R	586	GLU	GLY	conflict	UNP A0A8H9B1T2
R	636	ARG	LEU	conflict	UNP A0A8H9B1T2
R	858	ILE	VAL	conflict	UNP A0A8H9B1T2
S	11	LYS	GLU	conflict	UNP A0A8H9B1T2
S	24	SER	PRO	conflict	UNP A0A8H9B1T2
S	67	PRO	SER	conflict	UNP A0A8H9B1T2
S	335	SER	GLY	conflict	UNP A0A8H9B1T2
S	409	ASP	ASN	conflict	UNP A0A8H9B1T2
S	428	ASN	SER	conflict	UNP A0A8H9B1T2
S	583	ASN	HIS	conflict	UNP A0A8H9B1T2
S	586	GLU	GLY	conflict	UNP A0A8H9B1T2
S	636	ARG	LEU	conflict	UNP A0A8H9B1T2
S	858	ILE	VAL	conflict	UNP A0A8H9B1T2

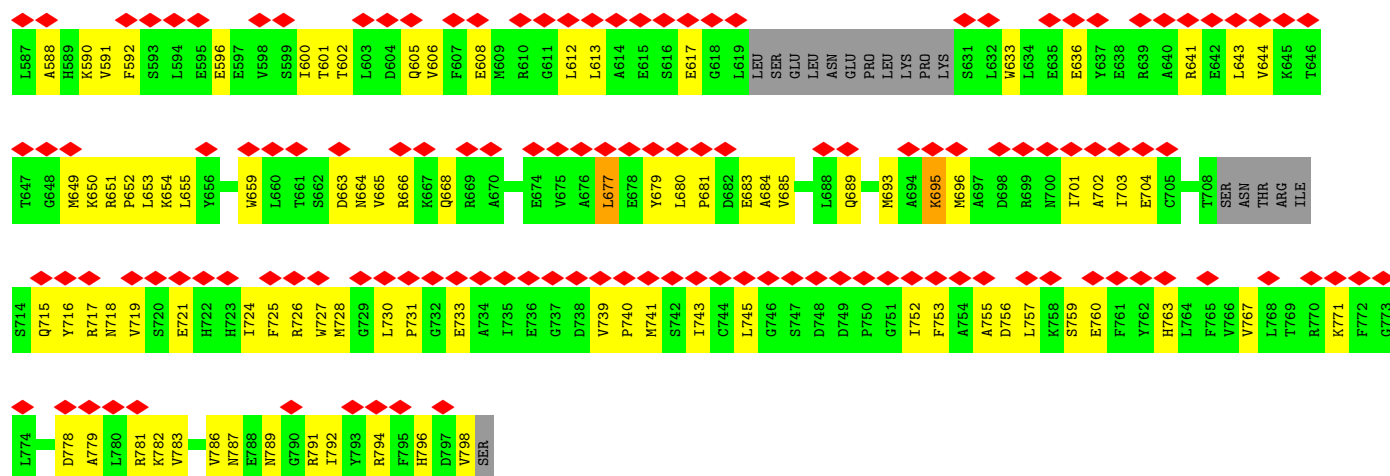
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Zn 1 1	0
3	B	1	Total Zn 1 1	0
3	C	1	Total Zn 1 1	0
3	D	1	Total Zn 1 1	0
3	E	1	Total Zn 1 1	0
3	F	1	Total Zn 1 1	0
3	G	1	Total Zn 1 1	0
3	H	1	Total Zn 1 1	0
3	I	1	Total Zn 1 1	0
3	J	1	Total Zn 1 1	0
3	K	1	Total Zn 1 1	0
3	L	1	Total Zn 1 1	0

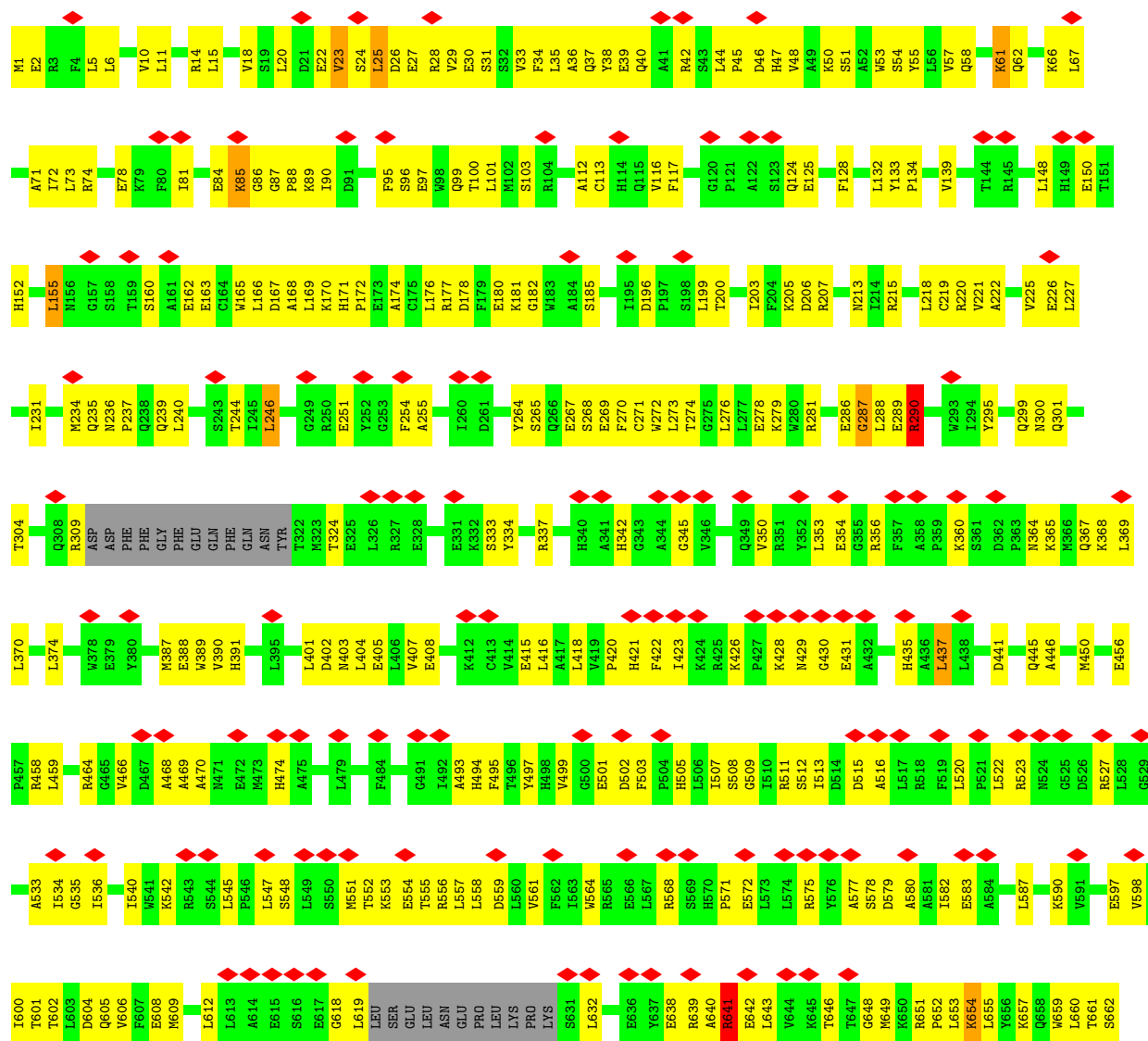


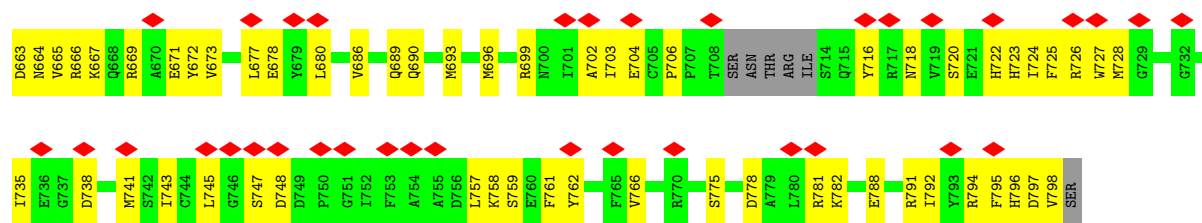
• Molecule 1: Adenosine deaminase





• Molecule 1: Adenosine deaminase





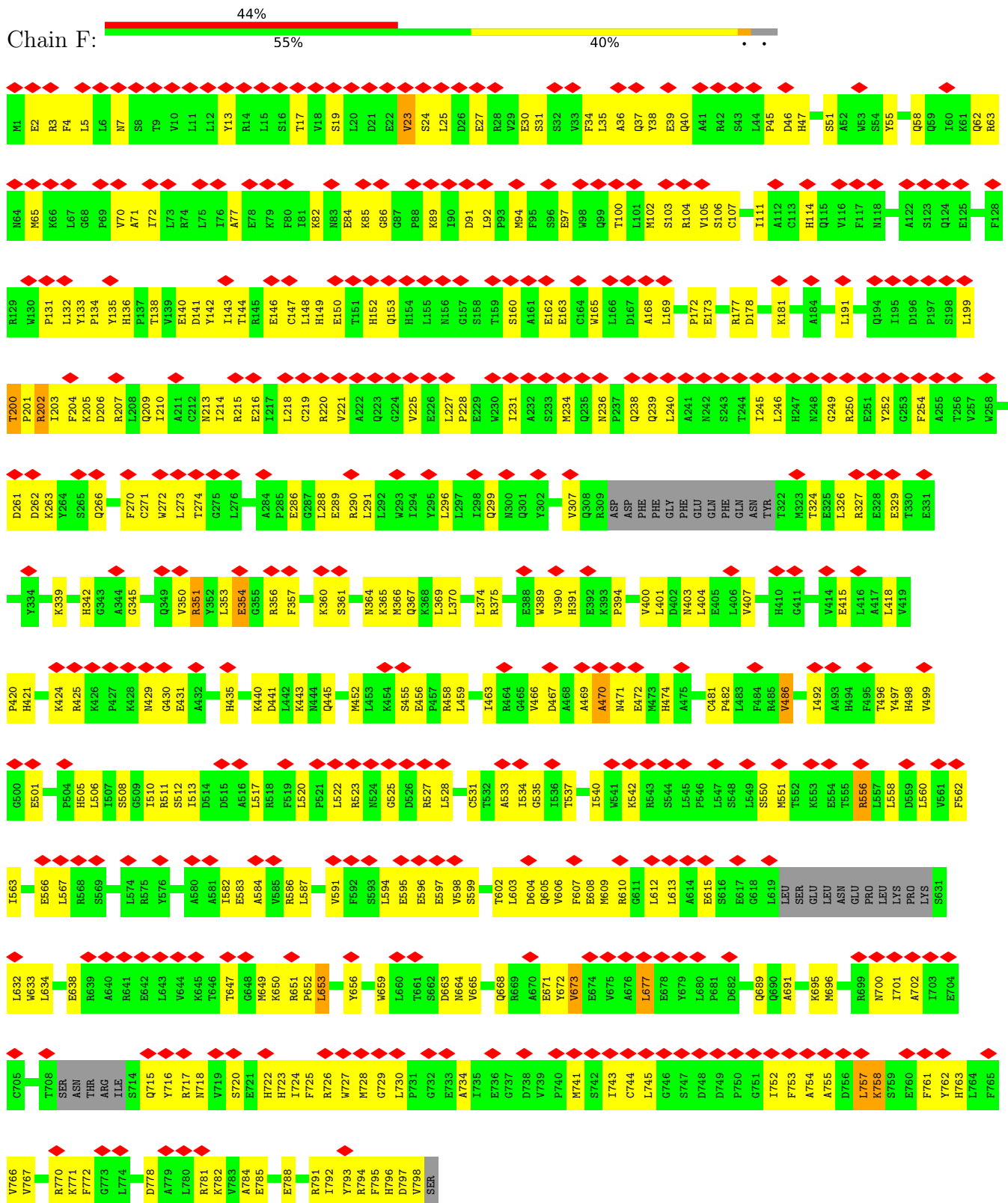
• Molecule 1: Adenosine deaminase





- Molecule 1: Adenosine deaminase

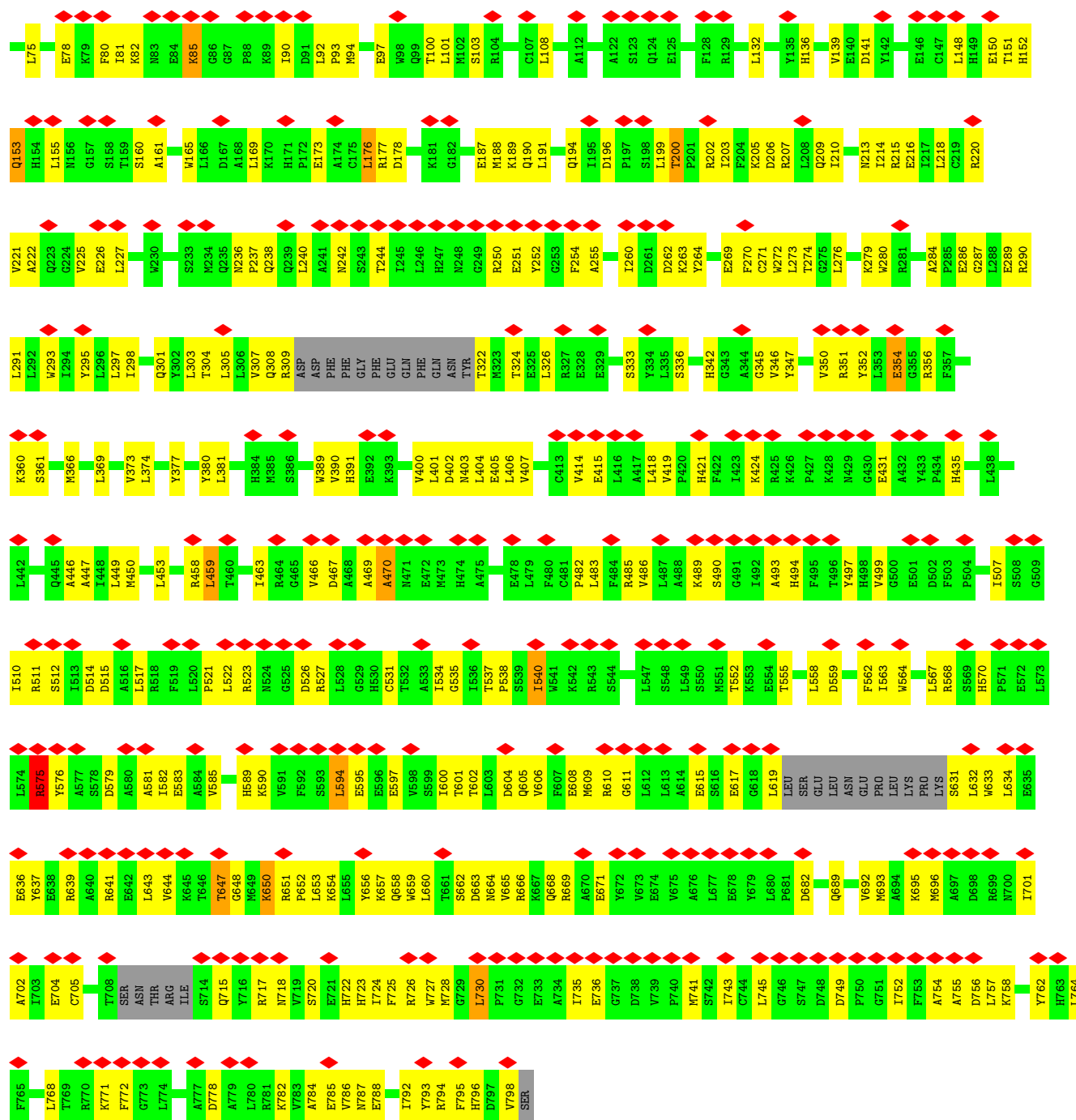
Chain F:

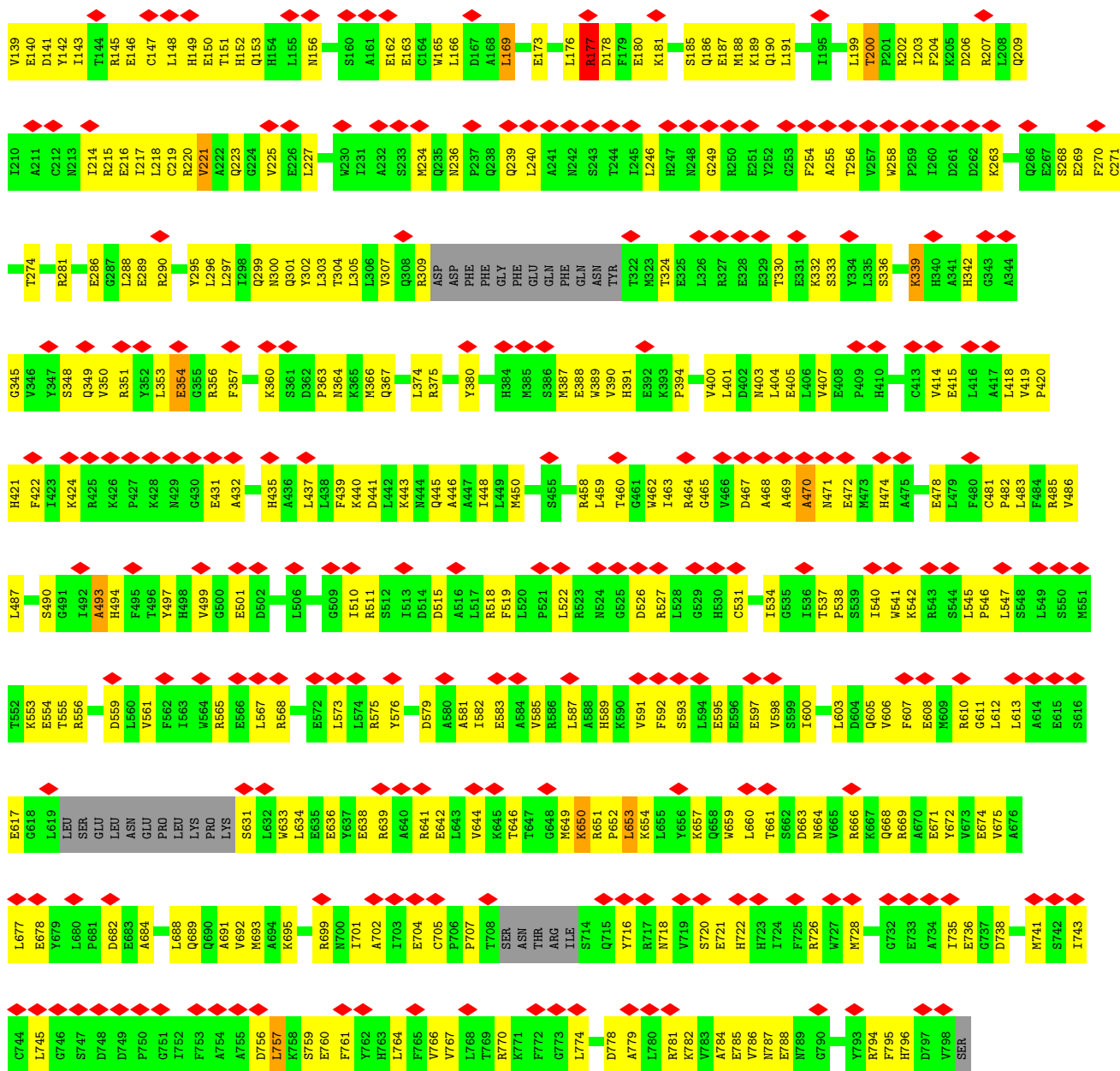


- Molecule 1: Adenosine deaminase

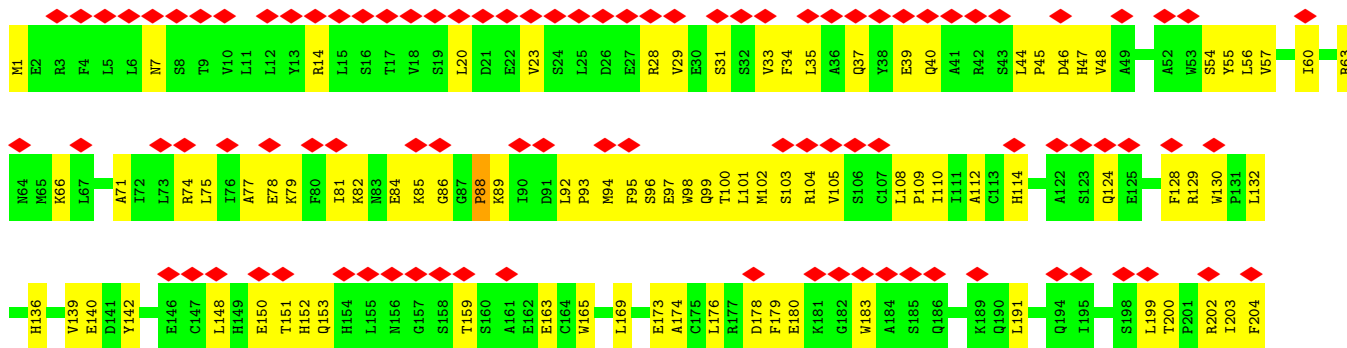
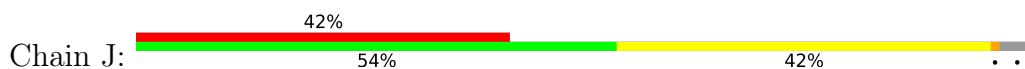
Chain G:

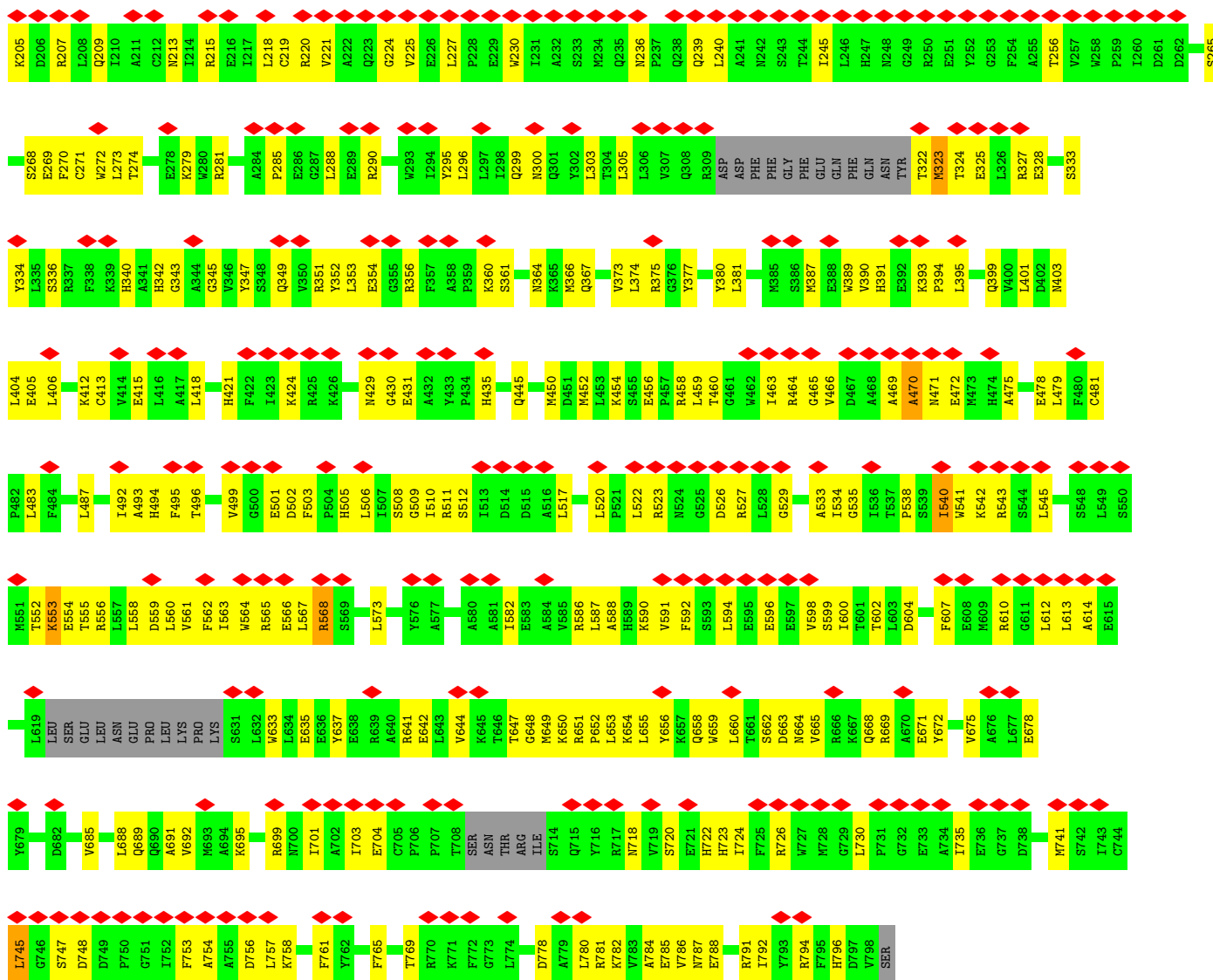




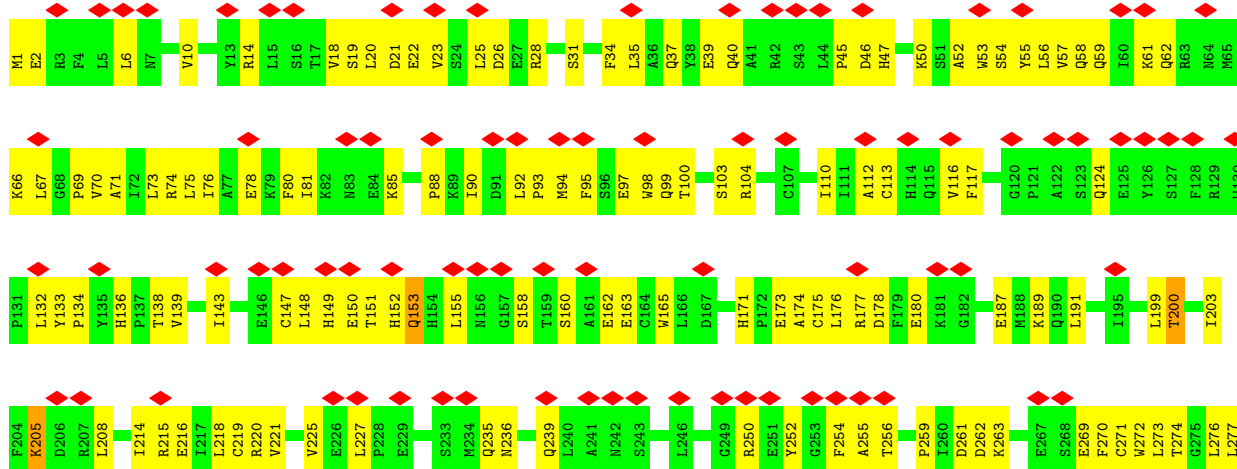


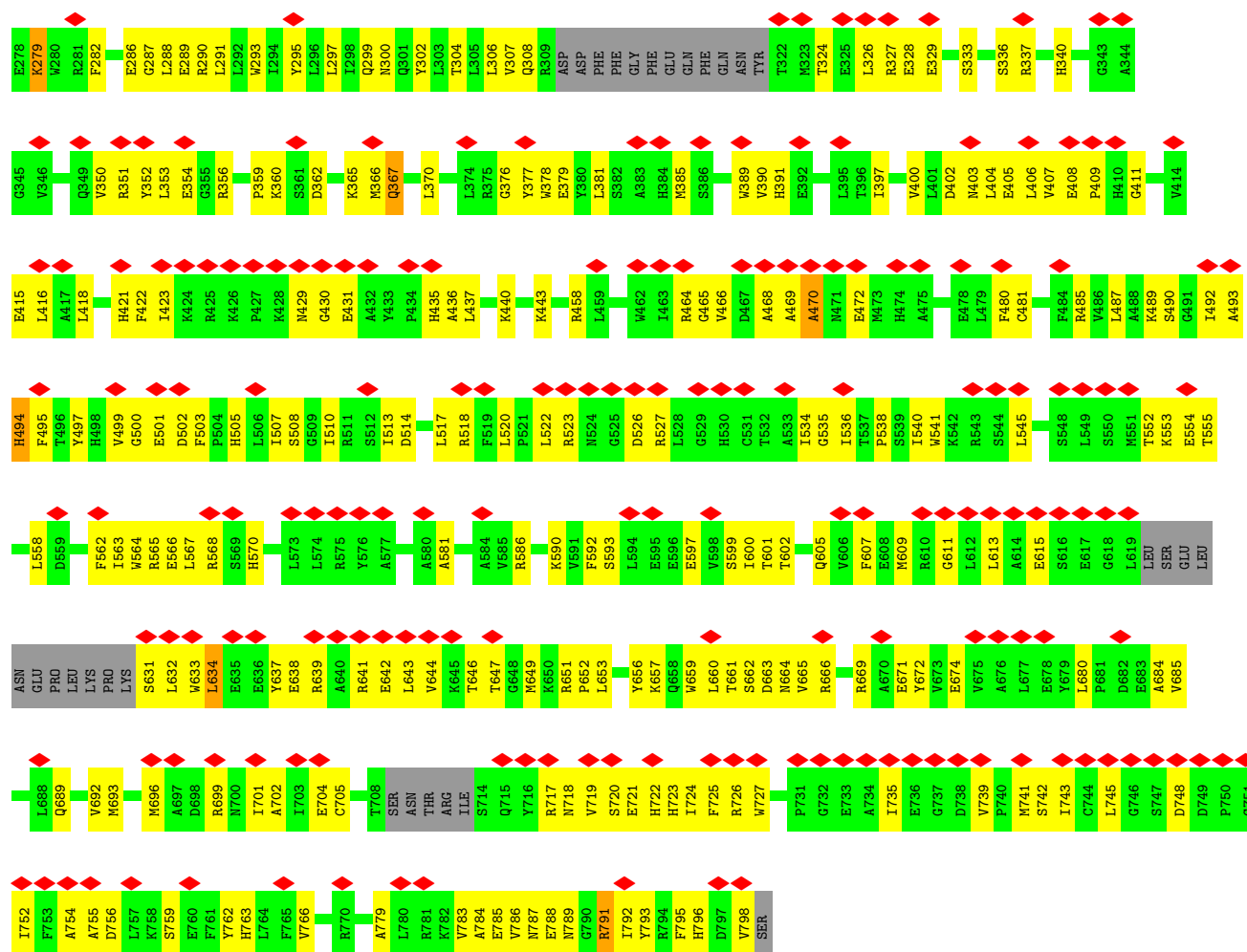
● Molecule 1: Adenosine deaminase



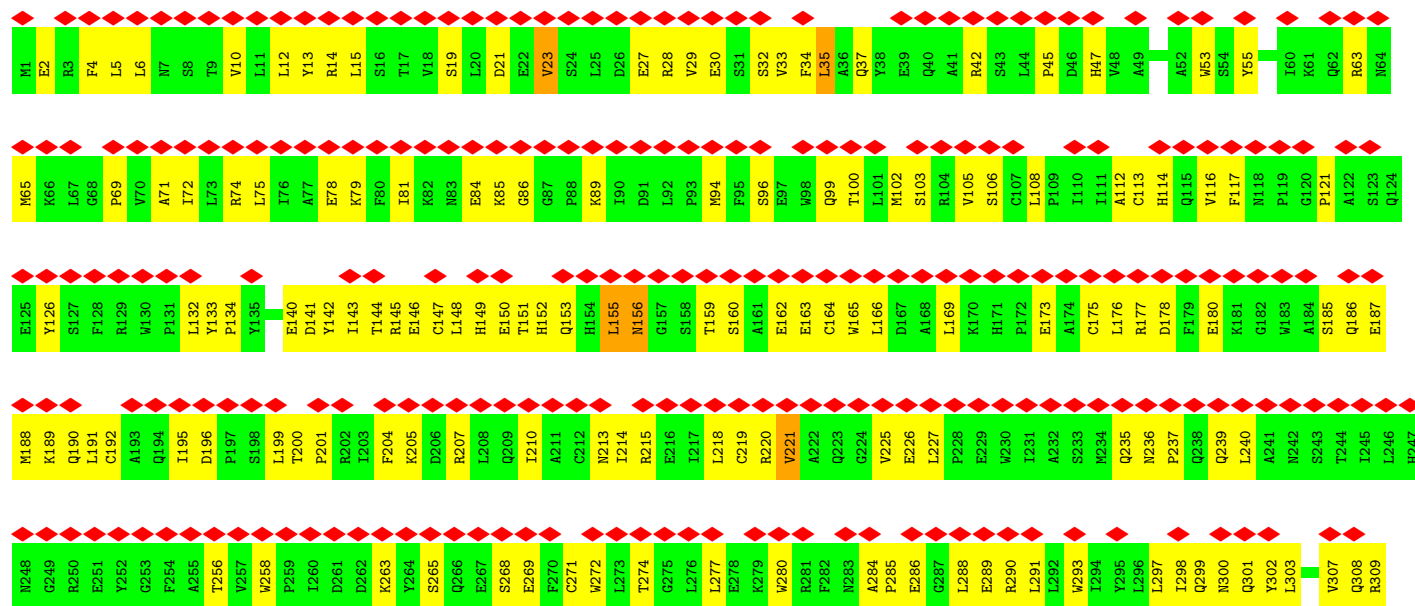


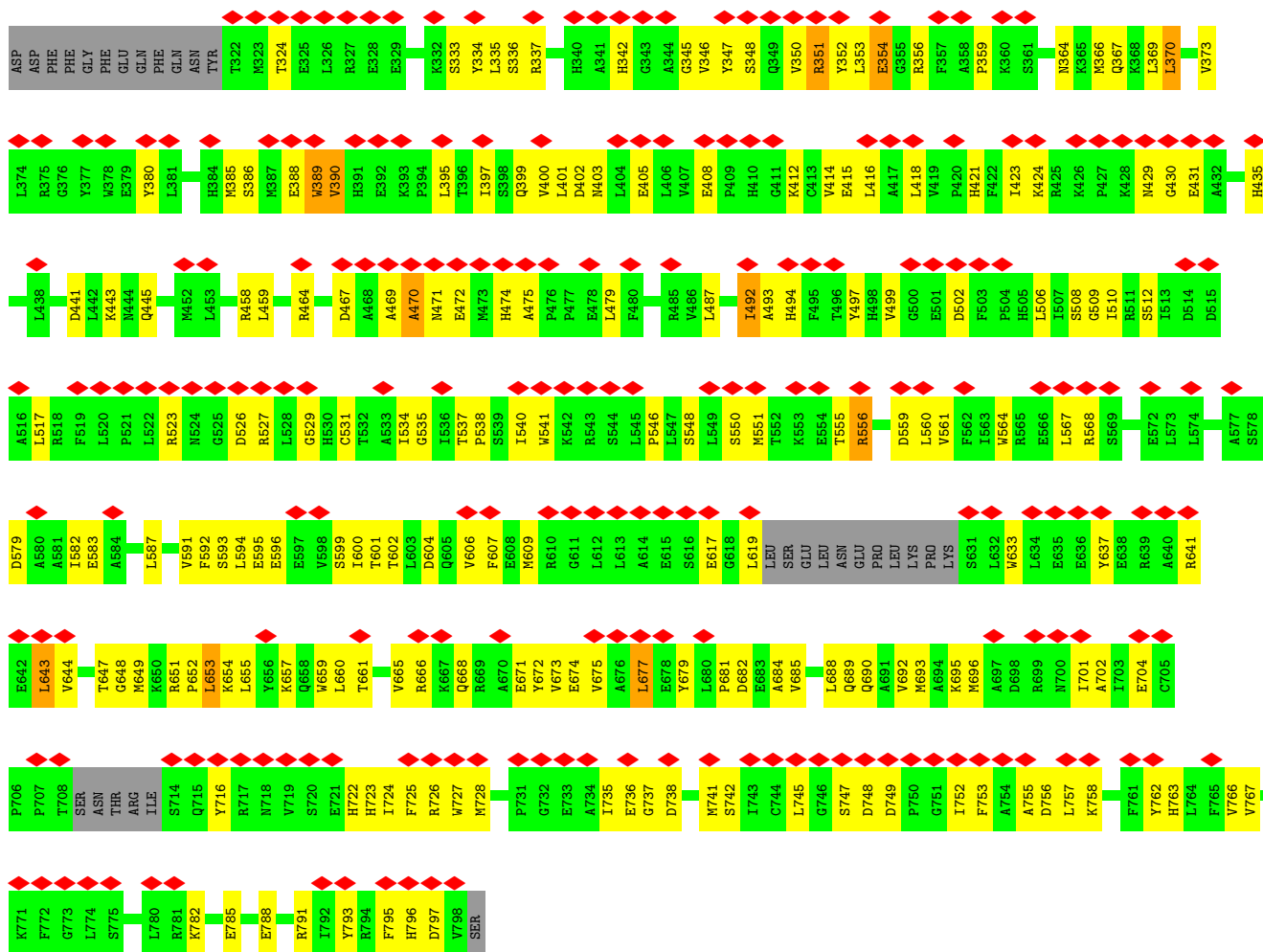
● Molecule 1: Adenosine deaminase



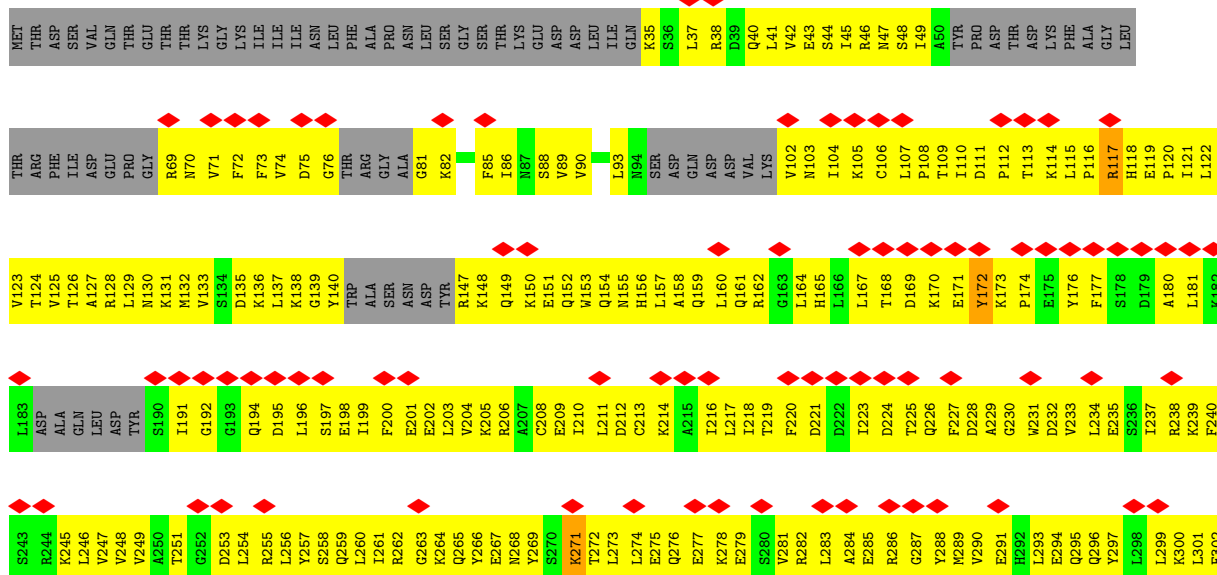
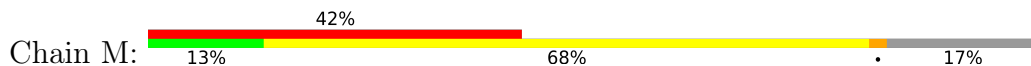


• Molecule 1: Adenosine deaminase



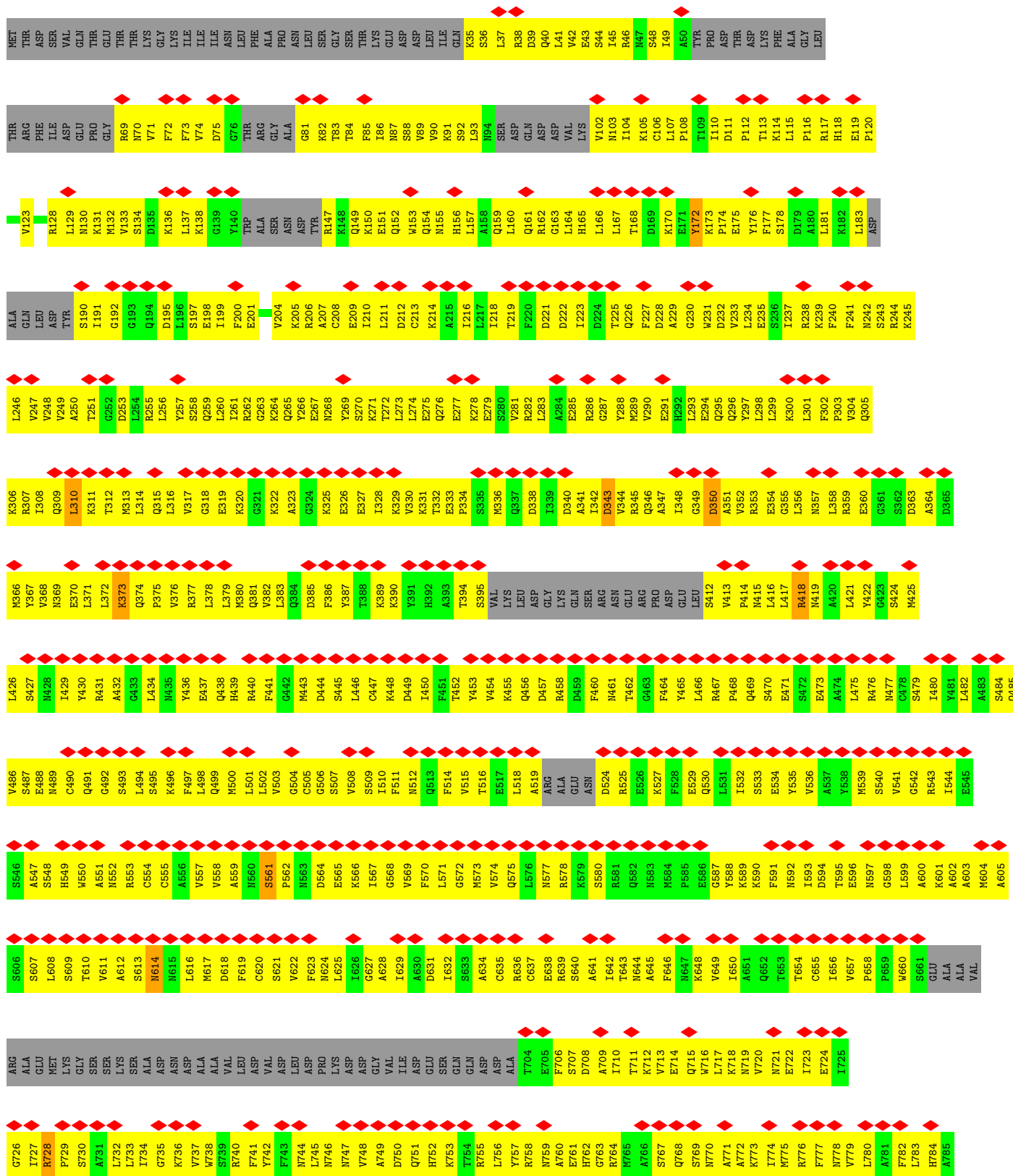


- Molecule 2: Archaeal ATPase



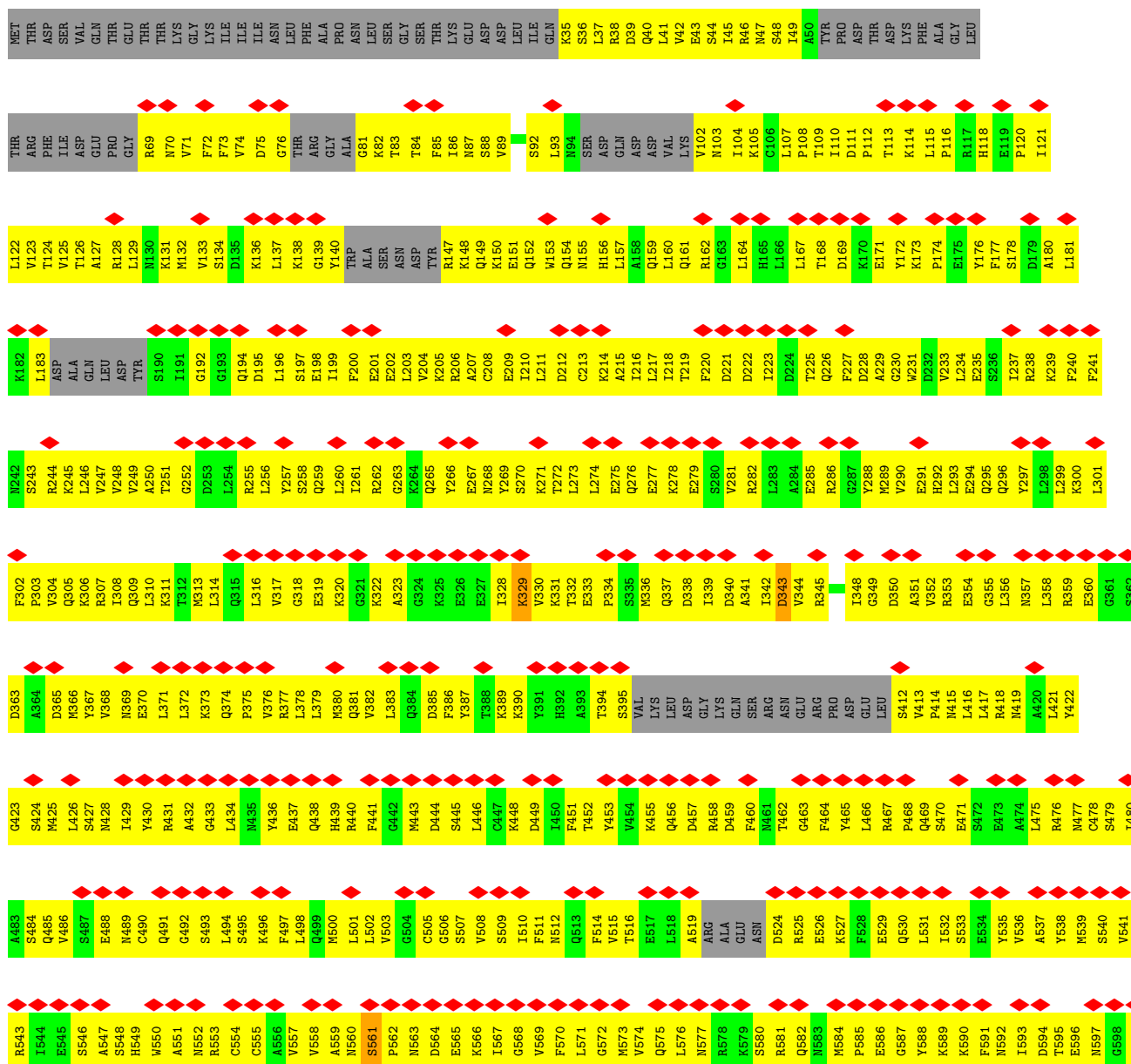
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GLN	C848	V786	G726	A605	E545	S484	S424	A364	V304	R244	K182	L122
I909	P849	L787	I727	S606	S546	Q485	M426	D365	Q305	K245	L183	V123
Q911	I850	V788	R728	S607	S547	V486	L426	M366	K306	L246	ASP	T124
N912	L851	E789	P729	S608	S548	S487	S427	Y367	R307	V247	ALA	V125
T913	H852	E790	H549	L608	H549	S487	M428	V368	I308	G247	GLN	T126
L914	P853	S791	H550	L609	H550	S487	M429	N369	Q309	V249	LEU	A127
T915	L855	L792	H551	T610	H551	S487	Y430	E370	L310	A250	ASP	R128
T916	L856	L793	H552	H611	H552	S487	Y431	L371	K311	T251	TYR	L129
S916	L857	H794	H553	A612	H553	S487	R431	L372	T312	G252	ASP	M130
L917	L858	S795	H554	S613	H554	S487	A432	L373	M313	D253	ASP	K131
N918	V796	V736	C554	H614	C555	S487	G433	Q374	L314	L254	ASP	M132
C859	S797	V737	A556	H615	A557	S487	L434	P375	L316	R255	ASP	V133
G860	S798	V738	V557	L616	V558	S487	M435	V376	V317	L256	ASP	S134
I861	S799	V739	V558	L617	V559	S487	Y436	R377	G318	Y257	ASP	D135
R862	E800	V740	V559	D618	V560	S487	E437	L378	E319	S258	ASP	K136
C863	V741	V742	H561	F619	H561	S487	Q438	L379	K320	L260	ASP	L137
S864	F743	F743	S562	C620	S562	S487	H439	M380	G321	I261	ASP	K138
V865	N744	N744	P562	S621	P563	S487	R440	Q381	K322	R262	ASP	G139
S926	L745	L745	D564	S622	D564	S487	F441	V382	A323	E267	ASP	Y140
L868	L746	L746	G504	V622	G505	S487	G442	Q384	G324	K264	ASP	TRP
H869	N746	N746	S507	F623	S507	S487	M443	D385	K325	E268	ASP	ALA
L806	N747	N747	S508	L624	S508	S487	D444	F386	G326	Y269	ASP	SER
L807	V748	V748	S509	L625	S509	S487	S445	E387	E327	N268	ASP	ASN
L808	A749	A749	F510	L626	F510	S487	L446	Y388	E328	K148	ASP	TYR
N809	D750	D750	F511	L629	F511	S487	C447	L388	I328	Q149	ASP	R147
P810	H751	H751	N512	A630	N512	S487	K448	K389	K329	K271	ASP	K150
V811	G752	G752	Q513	L631	Q513	S487	D449	Y390	V330	E151	ASP	E151
S812	K753	K753	F514	D631	F514	S487	L450	Y391	K331	Q152	ASP	Q152
D815	T754	T754	V515	S633	V515	S487	F451	H392	T332	L273	ASP	M153
E816	R755	R755	T516	L634	T516	S487	T452	A393	E333	L274	ASP	Q154
F817	L756	L756	E517	A634	E517	S487	Y453	T394	P334	E275	ASP	M155
V818	V757	V757	L518	C635	L518	S487	V454	S395	S335	E277	ASP	H156
K819	R758	R758	A519	R636	A519	S487	K455	VAL	M336	K278	ASP	L157
K820	H759	H759	ALA	C637	ALA	S487	Q456	ARG	Q337	E279	ASP	A158
I821	A760	A760	GLU	E638	GLU	S487	D457	ASP	D338	S280	ASP	Q159
K822	S761	S761	ASN	R639	ASN	S487	R458	GLY	I339	L281	ASP	L160
L823	H762	H762	D524	A641	D524	S487	D459	LYS	D340	R282	ASP	Q161
I824	G763	G763	R525	L642	R525	S487	F460	GLN	A341	L283	ASP	R162
G825	E826	E826	E526	T643	E526	S487	M461	ARG	I342	A284	ASP	G163
K827	R827	R827	E527	N644	E527	S487	T462	ASN	D343	E285	ASP	L164
L828	V827	V827	K527	F646	K527	S487	G463	GLU	V344	R286	ASP	H165
K829	H829	H829	F528	L647	F528	S487	Y465	ARG	Q346	G287	ASP	L166
S833	T834	T834	E529	K648	E529	S487	G464	PRO	A347	M289	ASP	L167
V835	V835	V835	Q530	V649	Q530	S487	L466	ASP	G349	E291	ASP	T168
K836	L717	L717	L531	T650	L531	S487	R467	GLU	D350	V290	ASP	D169
K837	H718	H718	I532	A651	I532	S487	P468	GLU	V352	E294	ASP	K170
T838	N719	N719	S533	D652	S533	S487	Q469	GLU	R353	Q295	ASP	E171
H839	T720	T720	E534	T653	E534	S487	S470	ARG	E354	Q296	ASP	K173
ASP	L774	L774	Y535	T654	Y535	S487	E471	GLU	E355	L298	ASP	P174
ASN	R775	R775	I593	C655	I593	S487	S472	GLU	L356	E297	ASP	E172
GLN	F776	F776	D594	T656	D594	S487	E473	GLU	L357	L299	ASP	K174
GLN	V777	V777	T595	V657	T595	S487	A474	GLU	R358	Q300	ASP	P175
LYS	K839	K839	E596	P658	E596	S487	L475	GLU	E360	L301	ASP	E176
ASP	L841	L841	N597	F659	N597	S487	R476	GLU	G361	F302	ASP	F177
ASP	F842	F842	G542	L660	G542	S487	M477	GLU	S362	L302	ASP	S178
GLN	L844	L844	L599	S661	L599	S487	C478	GLU	S363	L303	ASP	D179
THR	L845	L845	A600	L601	A600	S487	S479	GLU	S364	L304	ASP	A180
ASN	L846	L846	K601	A602	K601	S487	I480	GLU	S365	L305	ASP	
THR			A602		A602	S487	Y481	GLU	S366	L306	ASP	
ARG			A603		A603	S487	L482	GLU	S367	L307	ASP	

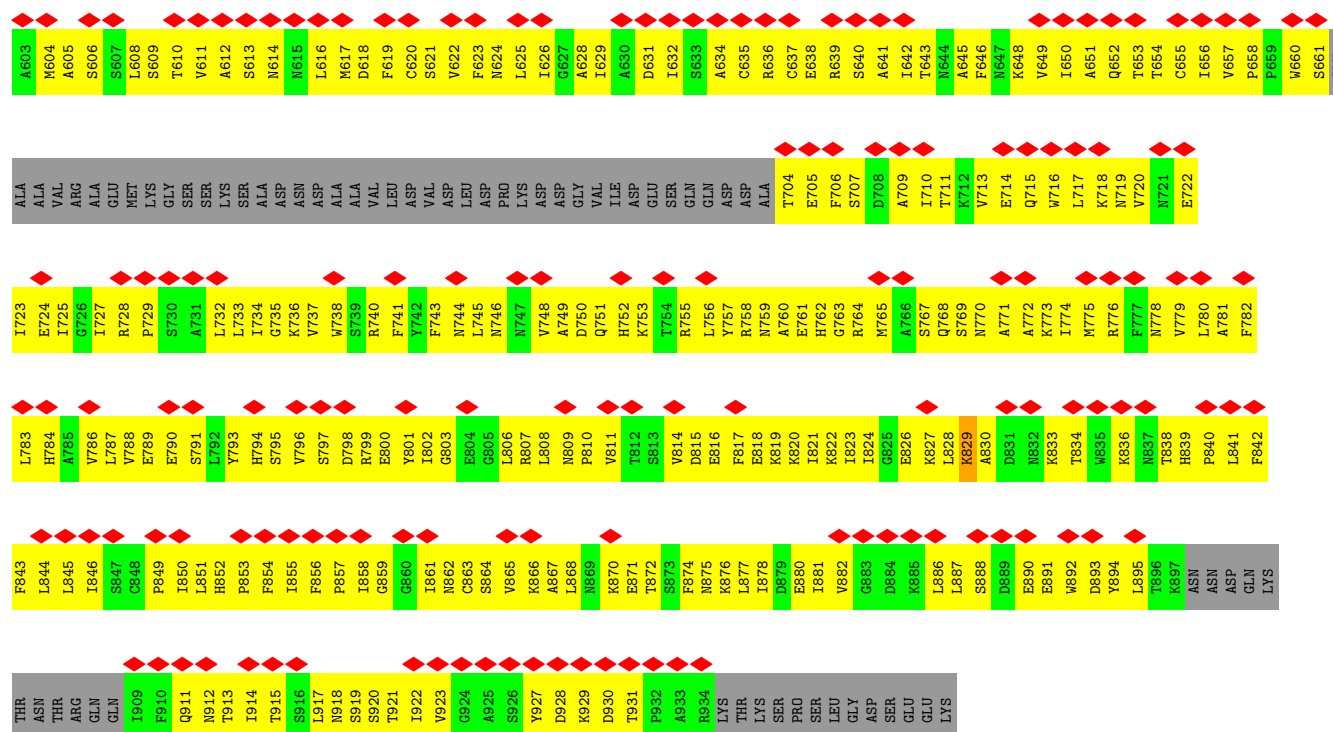
● Molecule 2: Archaeal ATPase



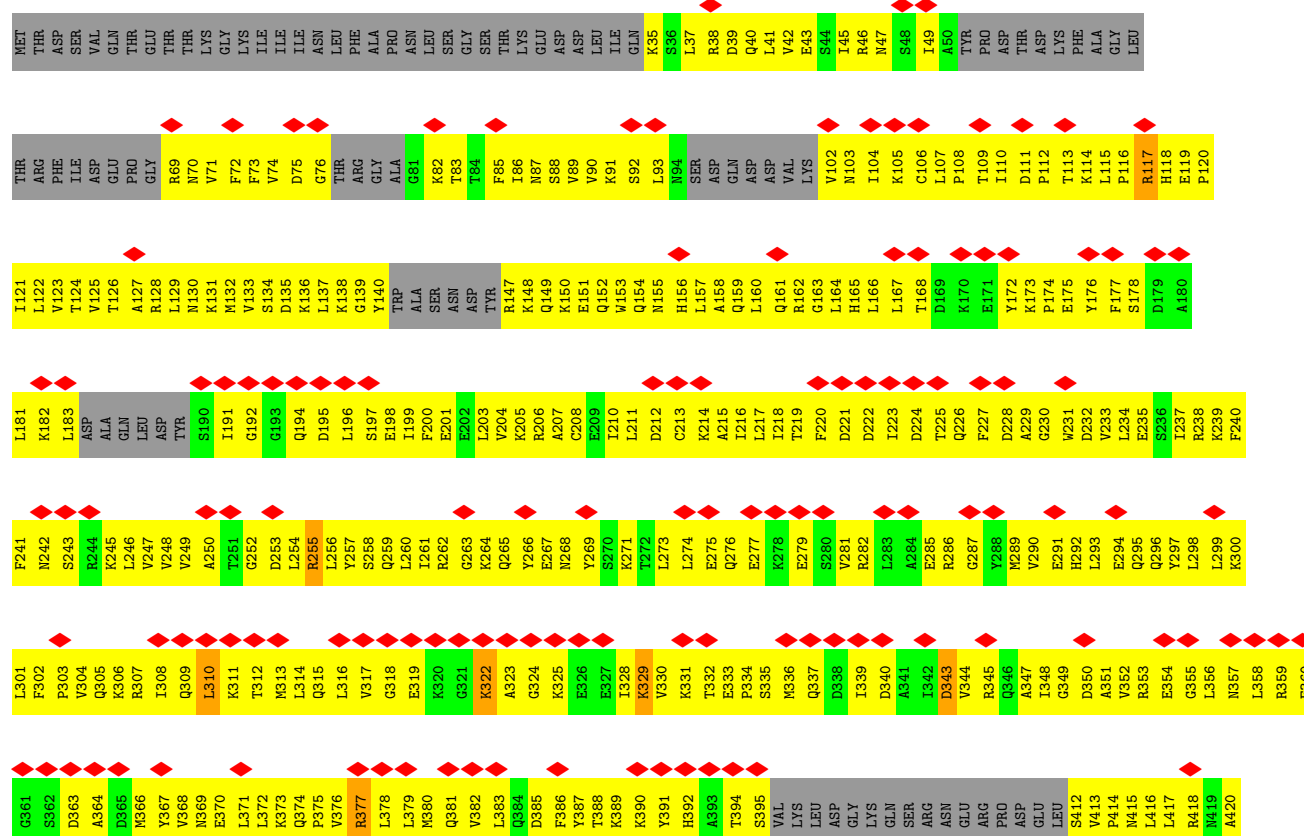


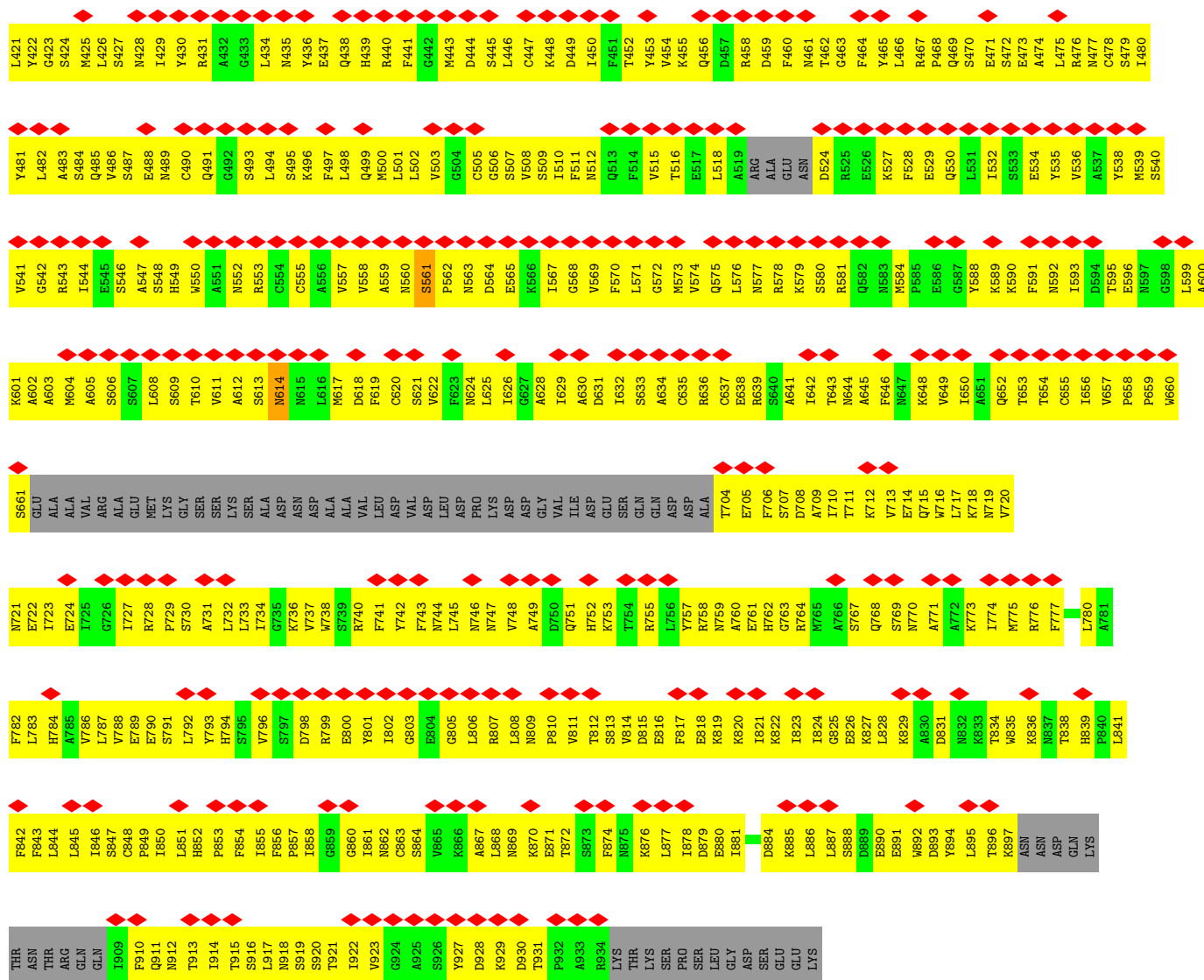
• Molecule 2: Archaeal ATPase



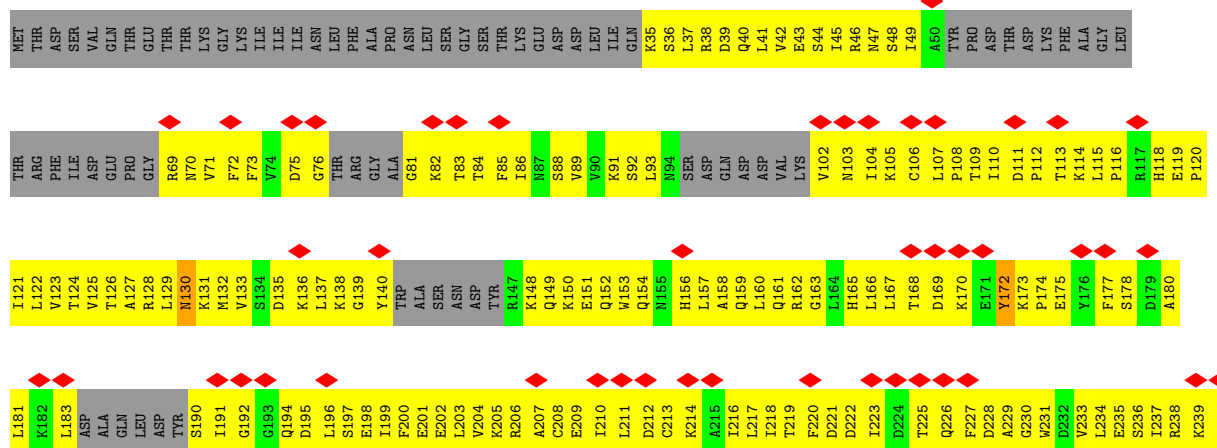


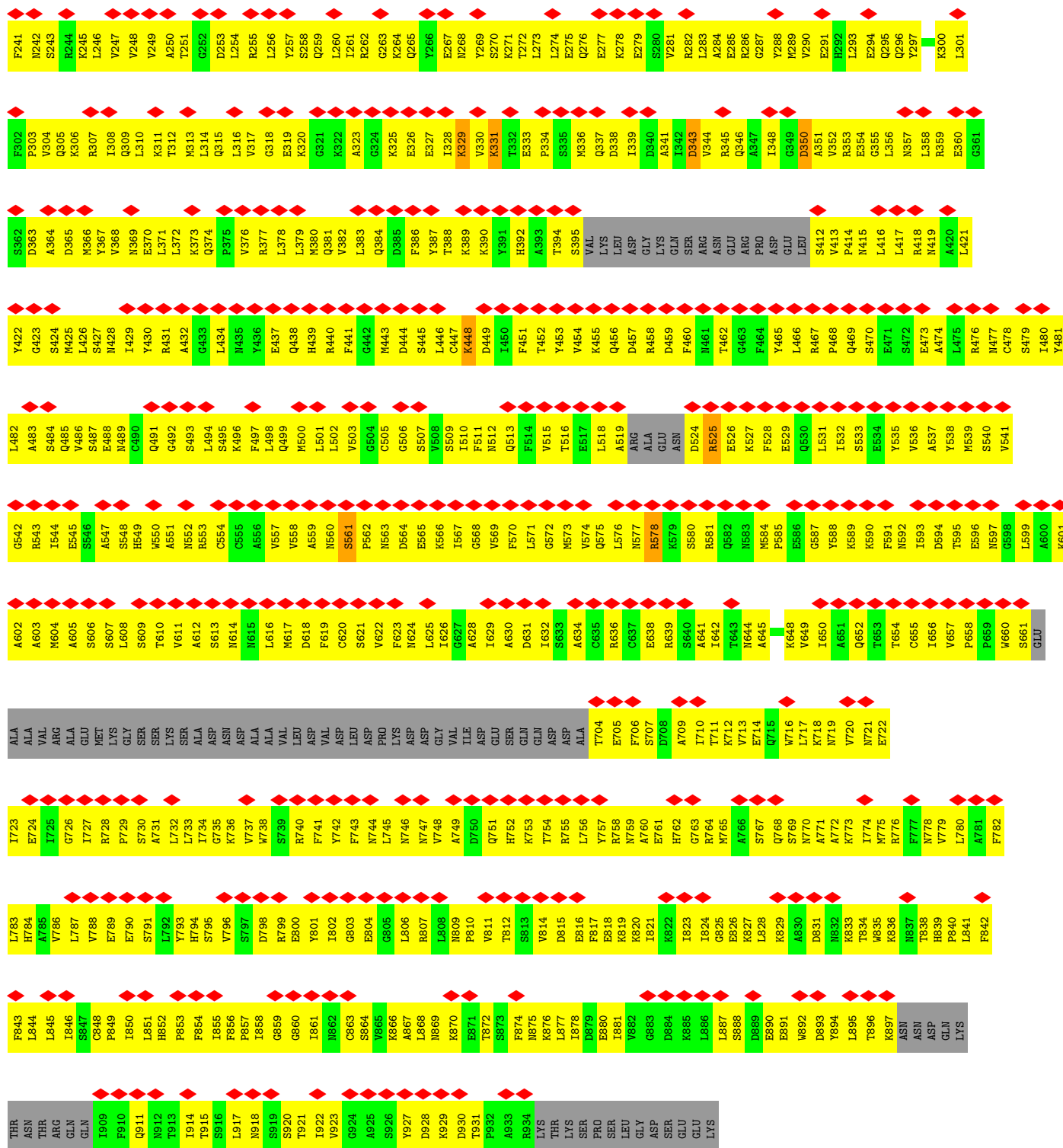
• Molecule 2: Archaeal ATPase



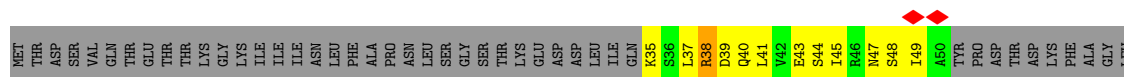


• Molecule 2: Archaeal ATPase





• Molecule 2: Archaeal ATPase





LYS	THR	ASN	THR	ARG	GLN	GLN	P909	P910	Q911	P912	T913	T914	T915	P916	T917	N918	S919	S920	T921	T922	T923	G924	A925	S926	T927	D928	K929	D930	T931	P932	A933	R934	LYS	THR	LYS	SER	PRO	SER	SER	LEU	GLY	ASP	SER	GLU	GLU	LYS
-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9236	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.256	Depositor
Minimum map value	-3.896	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.303	Depositor
Recommended contour level	1.9	Depositor
Map size (\AA)	659.9987, 659.9987, 659.9987	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.57812, 2.57812, 2.57812	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	0.30	0/6400	0.64	18/8672 (0.2%)
1	B	0.30	0/6400	0.62	17/8672 (0.2%)
1	C	0.33	0/6400	0.63	13/8672 (0.1%)
1	D	0.34	1/6375 (0.0%)	0.62	10/8637 (0.1%)
1	E	0.32	0/6400	0.63	14/8672 (0.2%)
1	F	0.32	0/6400	0.63	16/8672 (0.2%)
1	G	0.31	0/6400	0.59	13/8672 (0.1%)
1	H	0.31	0/6400	0.65	21/8672 (0.2%)
1	I	0.32	0/6400	0.63	14/8672 (0.2%)
1	J	0.31	0/6400	0.61	13/8672 (0.1%)
1	K	0.33	0/6400	0.63	11/8672 (0.1%)
1	L	0.31	0/6400	0.65	22/8672 (0.3%)
2	M	0.28	0/6379	0.50	2/8592 (0.0%)
2	N	0.29	0/6379	0.51	1/8592 (0.0%)
2	O	0.28	0/6379	0.49	2/8592 (0.0%)
2	P	0.28	0/6379	0.51	1/8592 (0.0%)
2	Q	0.28	0/6379	0.50	1/8592 (0.0%)
2	R	0.28	0/6379	0.50	2/8592 (0.0%)
2	S	0.29	0/6379	0.51	2/8592 (0.0%)
All	All	0.31	1/121428 (0.0%)	0.58	193/164173 (0.1%)

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
1	C	0	1
1	E	0	1
1	H	0	2
1	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
1	K	0	1
1	L	0	1
2	N	0	1
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	45	PRO	CG-CD	-5.40	1.32	1.50

The worst 5 of 193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	647	THR	C-N-CA	14.53	152.82	122.30
1	A	650	LYS	CD-CE-NZ	12.84	141.23	111.70
1	B	695	LYS	CD-CE-NZ	12.51	140.46	111.70
1	K	205	LYS	CD-CE-NZ	12.12	139.58	111.70
1	J	553	LYS	CD-CE-NZ	11.97	139.23	111.70

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	290	ARG	Sidechain
1	E	568	ARG	Sidechain
1	H	540	ILE	Peptide
1	H	575	ARG	Sidechain
1	I	177	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6245	0	6229	262	0
1	B	6245	0	6229	268	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6245	0	6229	316	0
1	D	6221	0	6209	329	0
1	E	6245	0	6229	331	0
1	F	6245	0	6229	284	0
1	G	6245	0	6229	311	0
1	H	6245	0	6228	275	0
1	I	6245	0	6229	318	0
1	J	6245	0	6229	273	0
1	K	6245	0	6229	328	0
1	L	6245	0	6229	311	0
2	M	6277	0	6328	1412	0
2	N	6277	0	6328	1517	0
2	O	6277	0	6328	1413	0
2	P	6277	0	6328	1428	0
2	Q	6277	0	6328	1431	0
2	R	6277	0	6328	1441	0
2	S	6277	0	6328	1433	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
All	All	118867	0	119023	13162	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 55.

The worst 5 of 13162 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)
2:S:173:LYS:NZ	2:S:175:GLU:HG3	1.07	1.40
2:P:751:GLN:OE1	2:P:811:VAL:CG1	1.70	1.38
2:M:751:GLN:OE1	2:M:811:VAL:CG1	1.69	1.38
2:R:751:GLN:OE1	2:R:811:VAL:CG1	1.76	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:751:GLN:OE1	2:O:811:VAL:CG1	1.73	1.33

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	762/799 (95%)	697 (92%)	61 (8%)	4 (0%)	29	69
1	B	762/799 (95%)	706 (93%)	51 (7%)	5 (1%)	22	63
1	C	762/799 (95%)	697 (92%)	60 (8%)	5 (1%)	22	63
1	D	757/799 (95%)	688 (91%)	64 (8%)	5 (1%)	22	63
1	E	762/799 (95%)	693 (91%)	65 (8%)	4 (0%)	29	69
1	F	762/799 (95%)	693 (91%)	64 (8%)	5 (1%)	22	63
1	G	762/799 (95%)	690 (91%)	67 (9%)	5 (1%)	22	63
1	H	762/799 (95%)	692 (91%)	65 (8%)	5 (1%)	22	63
1	I	762/799 (95%)	704 (92%)	53 (7%)	5 (1%)	22	63
1	J	762/799 (95%)	696 (91%)	61 (8%)	5 (1%)	22	63
1	K	762/799 (95%)	690 (91%)	66 (9%)	6 (1%)	19	60
1	L	762/799 (95%)	697 (92%)	60 (8%)	5 (1%)	22	63
2	M	766/947 (81%)	704 (92%)	58 (8%)	4 (0%)	29	69
2	N	766/947 (81%)	695 (91%)	66 (9%)	5 (1%)	22	63
2	O	766/947 (81%)	704 (92%)	58 (8%)	4 (0%)	29	69
2	P	766/947 (81%)	680 (89%)	82 (11%)	4 (0%)	29	69
2	Q	766/947 (81%)	698 (91%)	63 (8%)	5 (1%)	22	63
2	R	766/947 (81%)	706 (92%)	56 (7%)	4 (0%)	29	69
2	S	766/947 (81%)	700 (91%)	61 (8%)	5 (1%)	22	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	14501/16217 (89%)	13230 (91%)	1181 (8%)	90 (1%)	29 66

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	B	23	VAL
1	C	23	VAL
1	D	23	VAL
1	E	23	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	678/706 (96%)	673 (99%)	5 (1%)	84 90
1	B	678/706 (96%)	677 (100%)	1 (0%)	93 96
1	C	678/706 (96%)	673 (99%)	5 (1%)	84 90
1	D	675/706 (96%)	671 (99%)	4 (1%)	86 92
1	E	678/706 (96%)	673 (99%)	5 (1%)	84 90
1	F	678/706 (96%)	675 (100%)	3 (0%)	91 94
1	G	678/706 (96%)	677 (100%)	1 (0%)	93 96
1	H	678/706 (96%)	676 (100%)	2 (0%)	92 94
1	I	678/706 (96%)	675 (100%)	3 (0%)	91 94
1	J	678/706 (96%)	676 (100%)	2 (0%)	92 94
1	K	678/706 (96%)	676 (100%)	2 (0%)	92 94
1	L	678/706 (96%)	676 (100%)	2 (0%)	92 94
2	M	696/837 (83%)	687 (99%)	9 (1%)	69 82
2	N	696/837 (83%)	691 (99%)	5 (1%)	84 90
2	O	696/837 (83%)	692 (99%)	4 (1%)	86 92
2	P	696/837 (83%)	695 (100%)	1 (0%)	93 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q	696/837 (83%)	692 (99%)	4 (1%)	86	92
2	R	696/837 (83%)	691 (99%)	5 (1%)	84	90
2	S	696/837 (83%)	691 (99%)	5 (1%)	84	90
All	All	13005/14331 (91%)	12937 (100%)	68 (0%)	89	93

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Q	377	ARG
2	R	331	LYS
2	S	579	LYS
1	H	309	ARG
1	G	556	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	875	ASN
2	S	435	ASN
2	Q	276	GLN
2	Q	778	ASN
1	I	723	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are 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

There are no chain breaks in this entry.

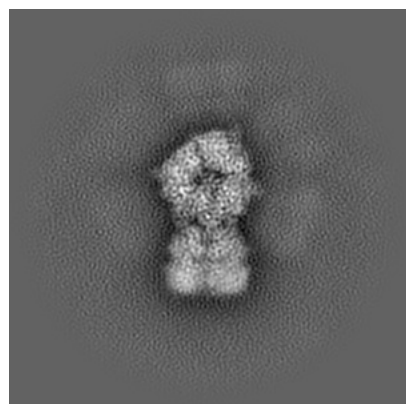
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29328. These allow visual inspection of the internal detail of the map and identification of artifacts.

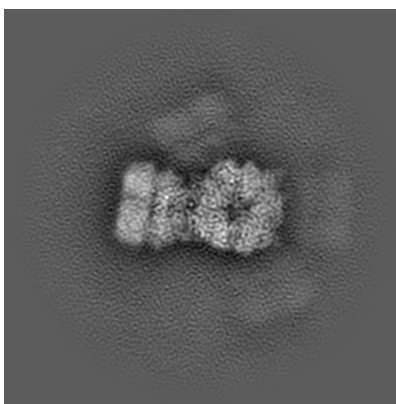
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

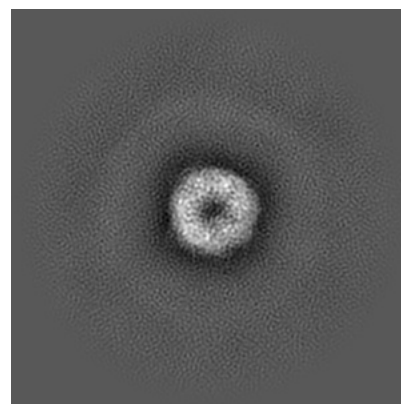
6.1.1 Primary map



X

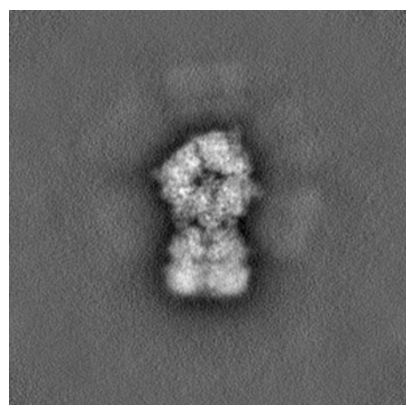


Y

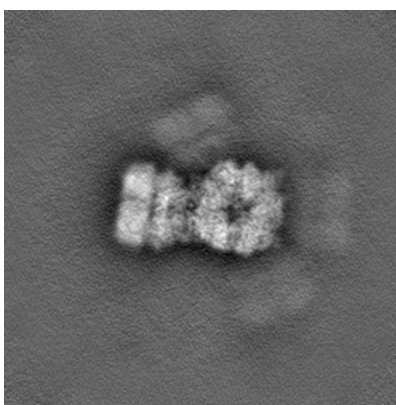


Z

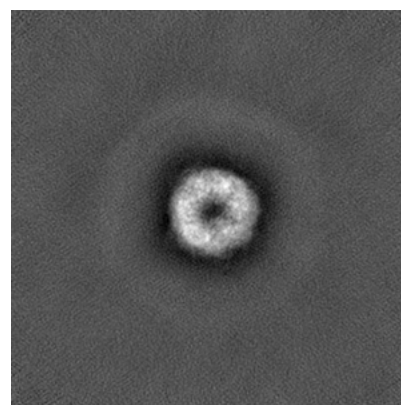
6.1.2 Raw map



X



Y

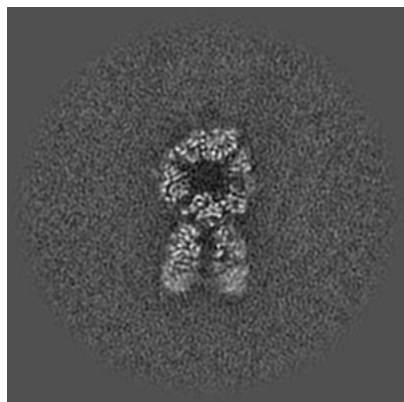


Z

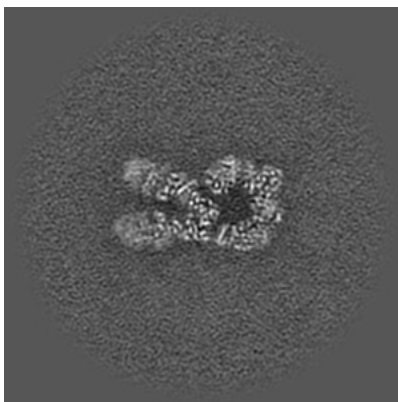
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

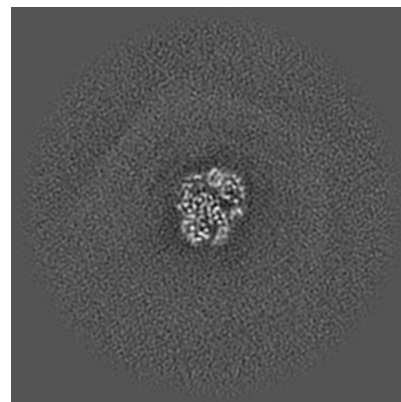
6.2.1 Primary map



X Index: 128

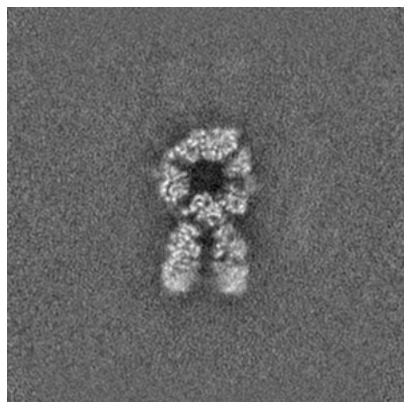


Y Index: 128

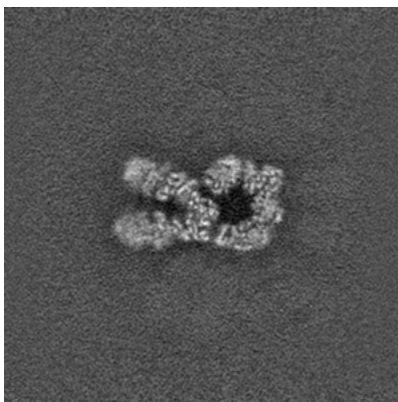


Z Index: 128

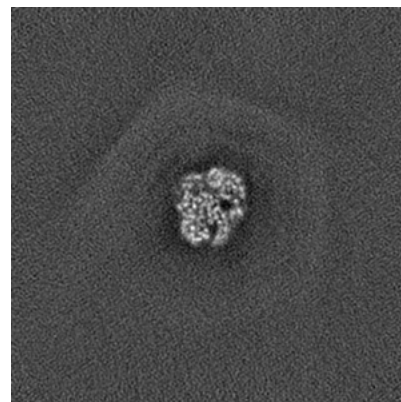
6.2.2 Raw map



X Index: 128



Y Index: 128

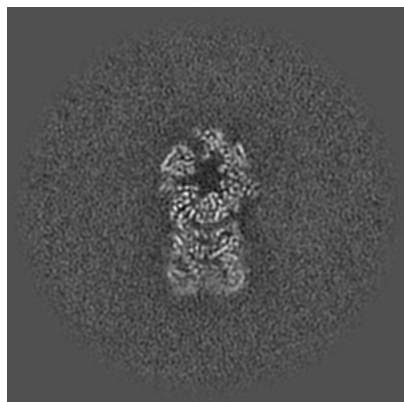


Z Index: 128

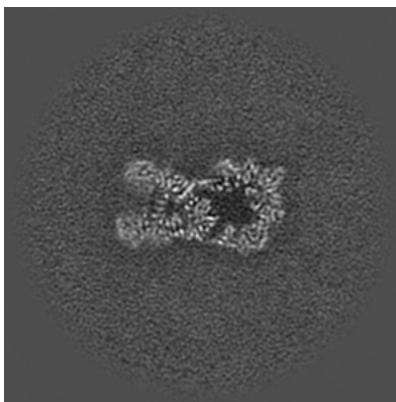
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

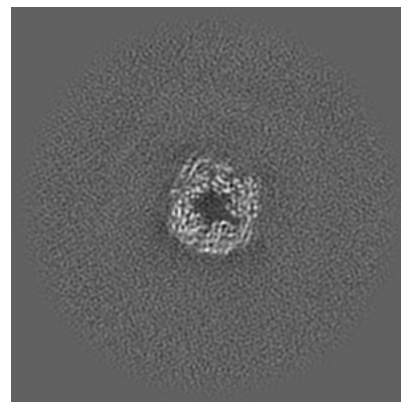
6.3.1 Primary map



X Index: 121

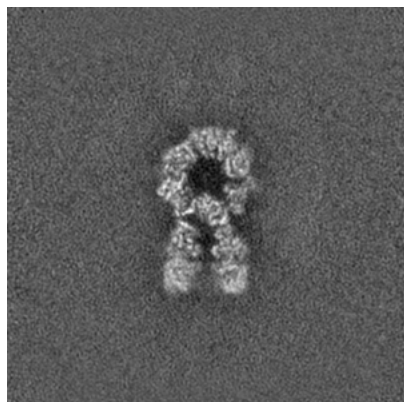


Y Index: 131

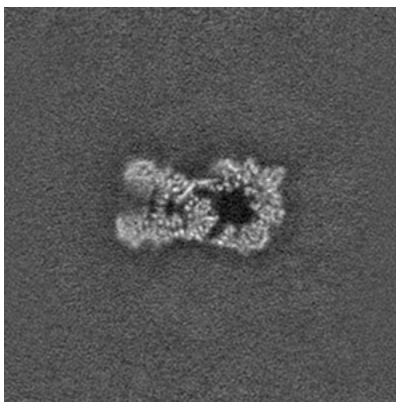


Z Index: 141

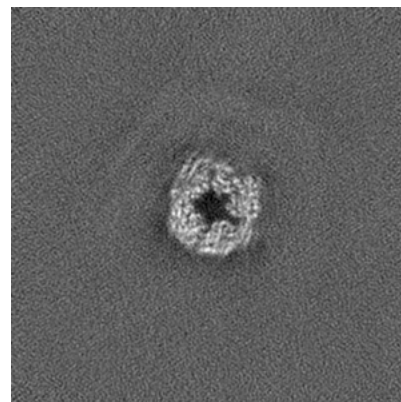
6.3.2 Raw map



X Index: 126



Y Index: 131

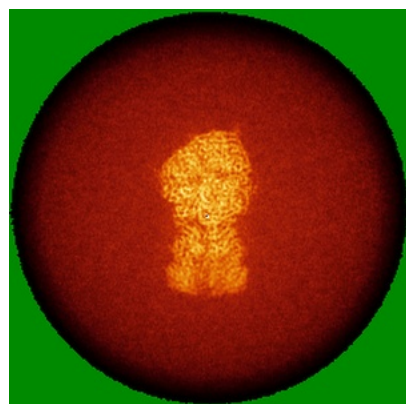


Z Index: 141

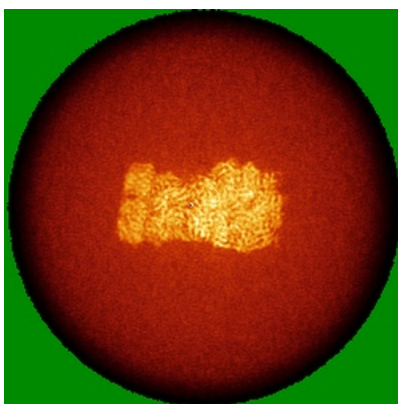
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

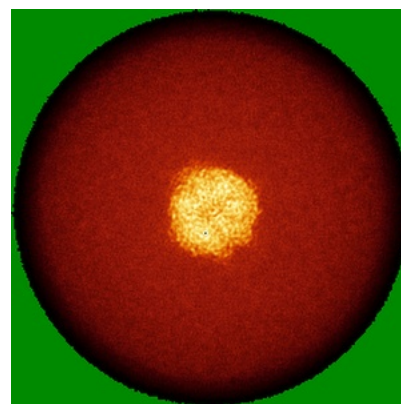
6.4.1 Primary map



X

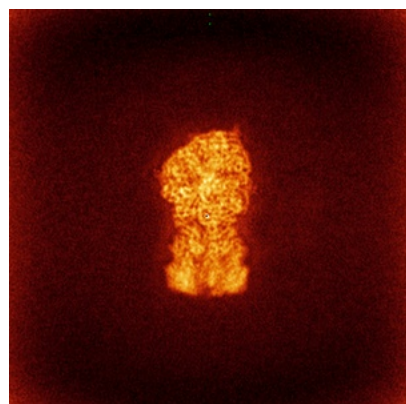


Y

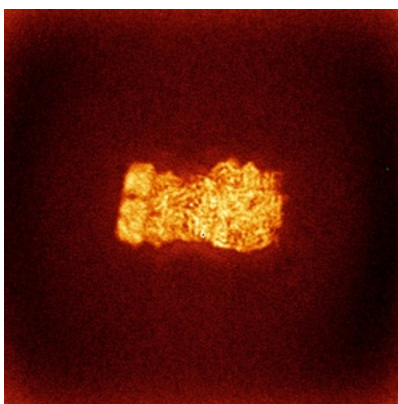


Z

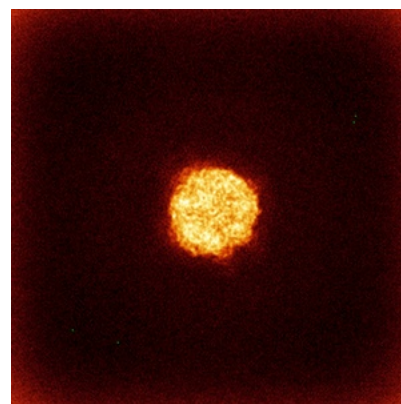
6.4.2 Raw map



X



Y

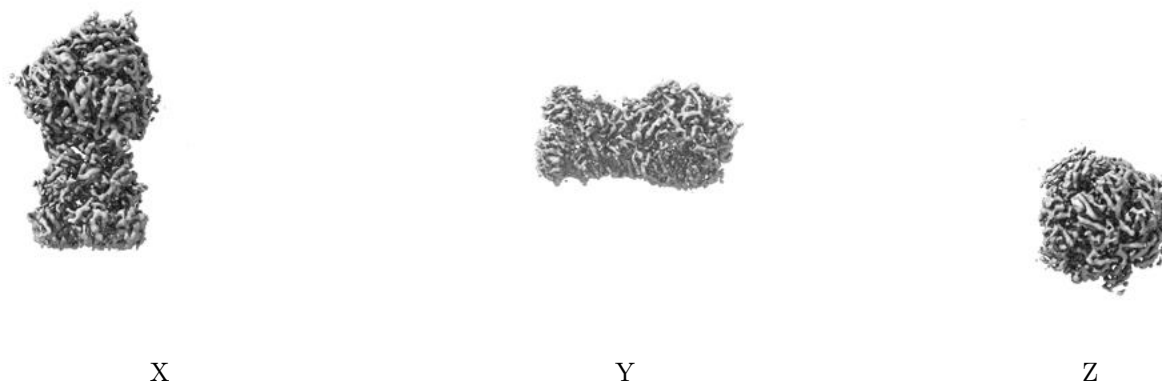


Z

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.

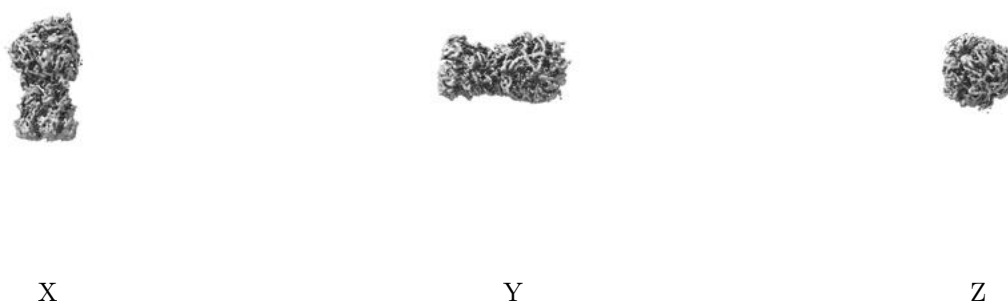
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

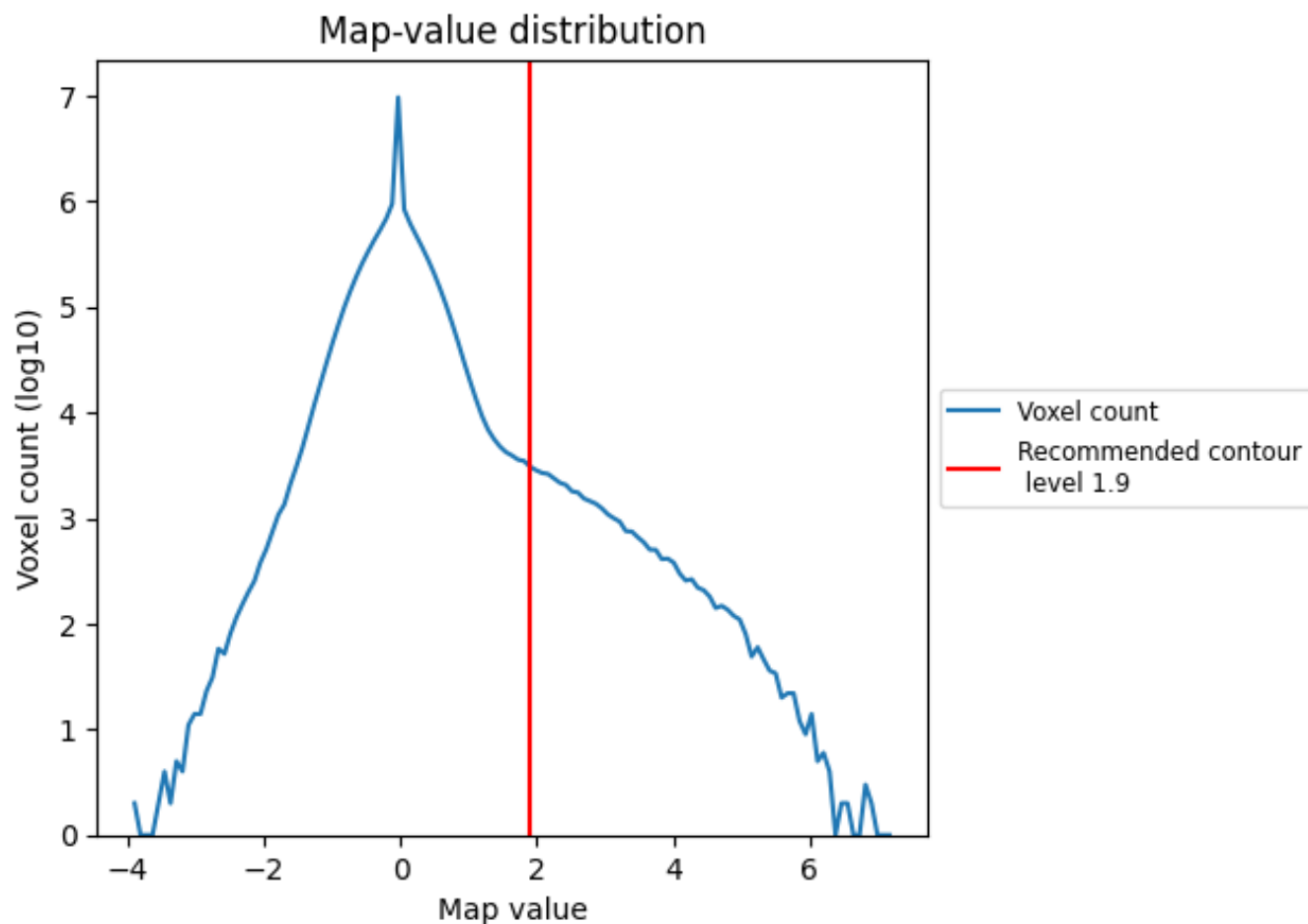
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

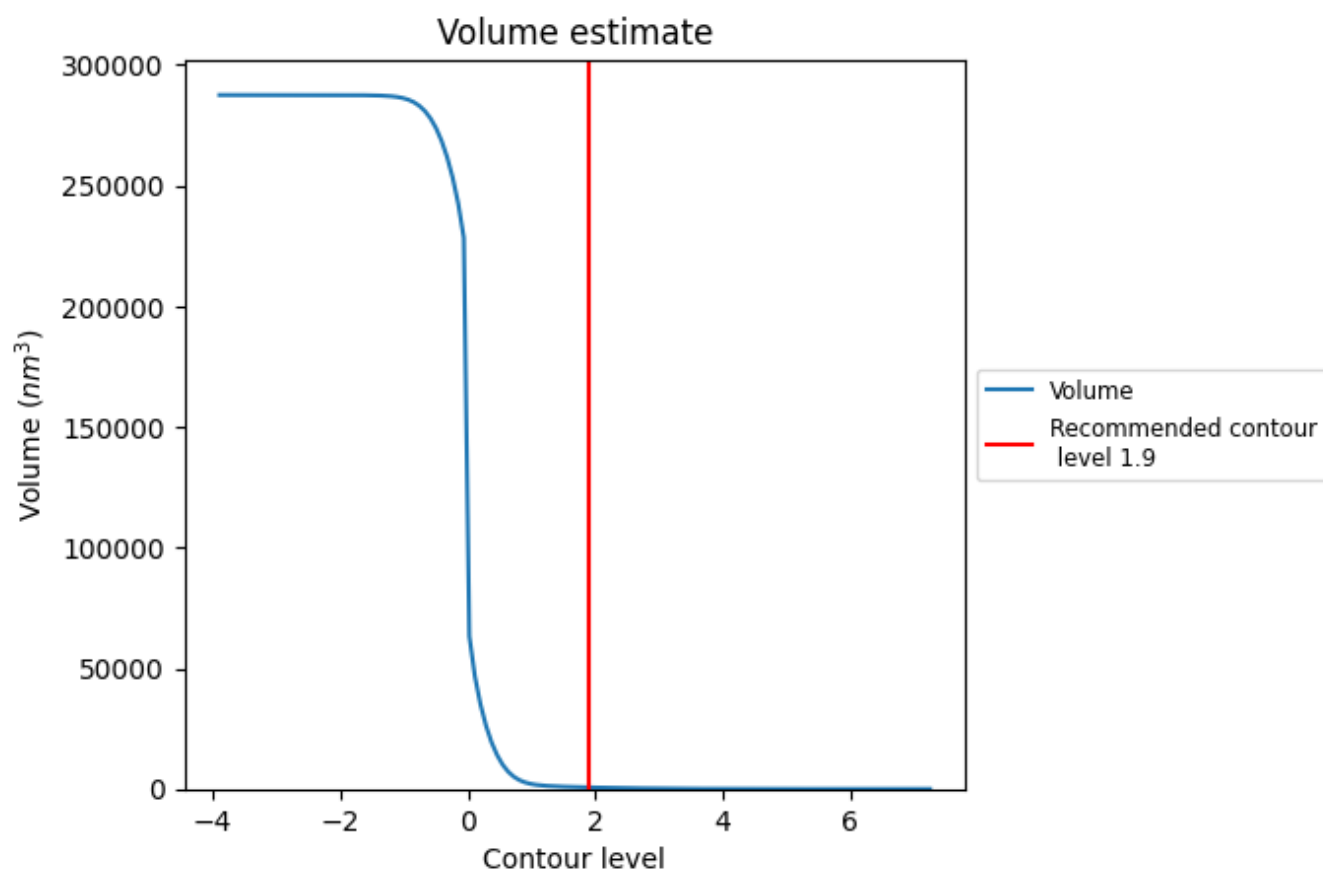
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

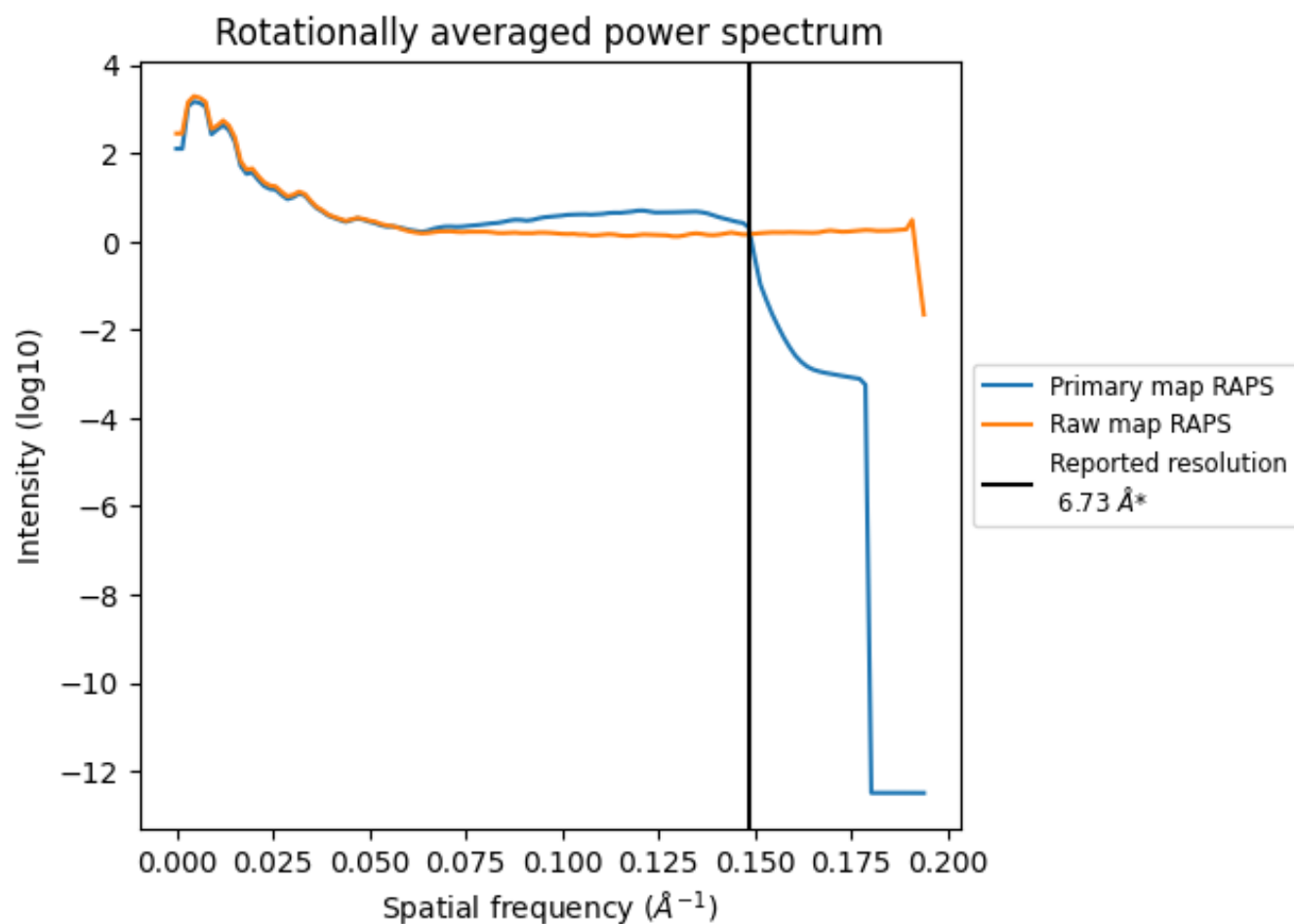
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 643 nm^3 ; this corresponds to an approximate mass of 581 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 ⓘ

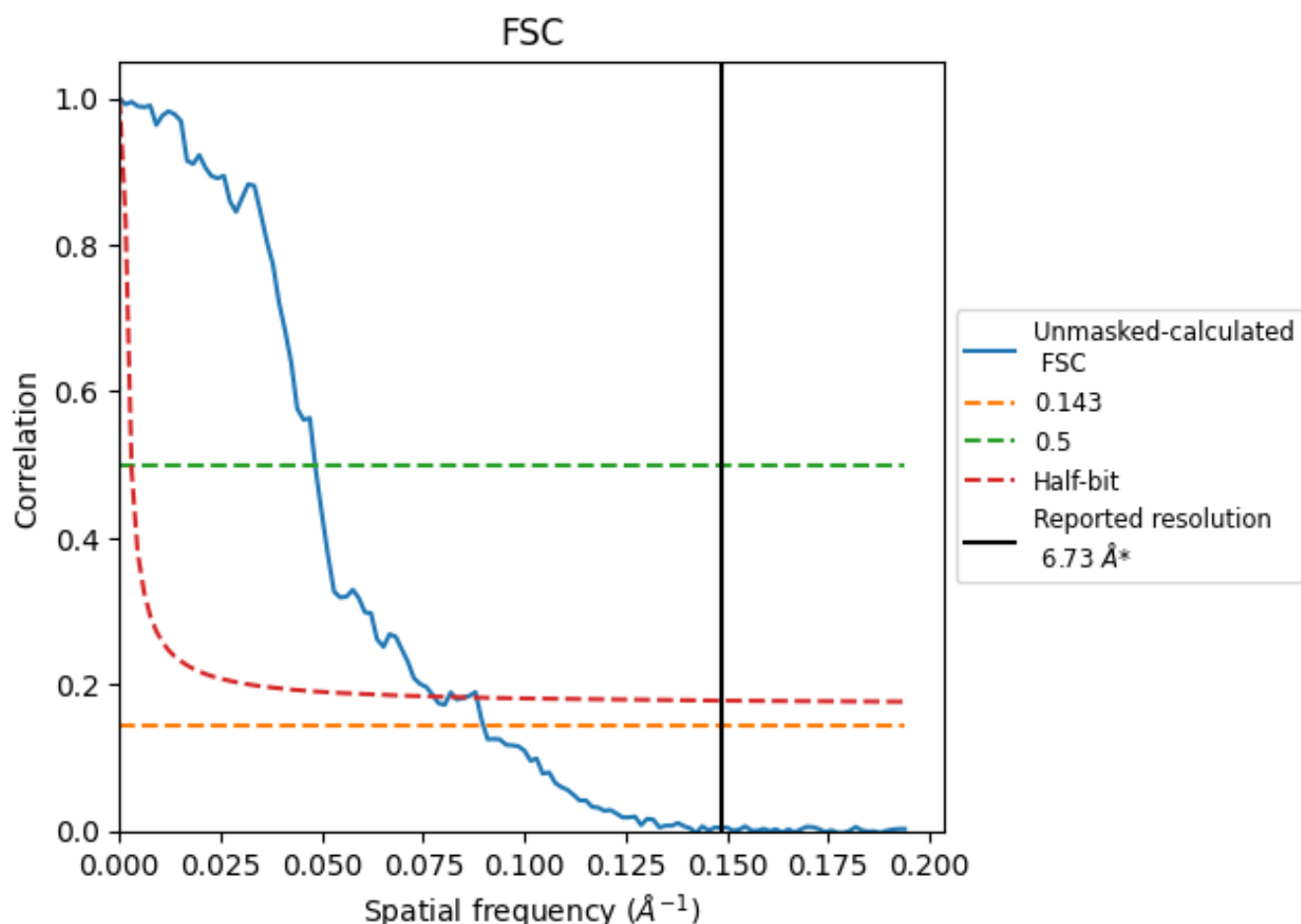


*Reported resolution corresponds to spatial frequency of 0.149 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.149 Å⁻¹

8.2 Resolution estimates [i](#)

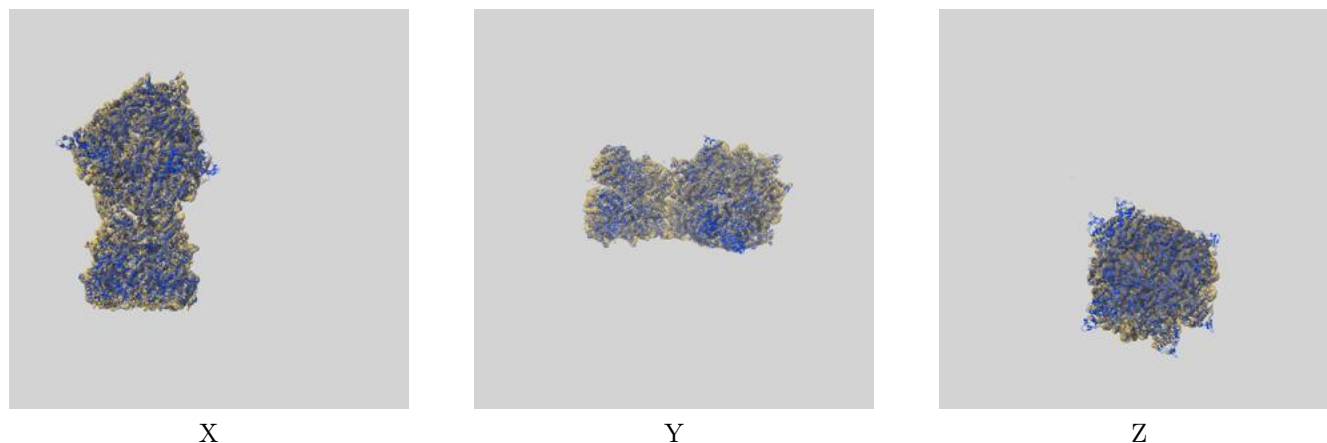
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	11.12	20.70	12.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 11.12 differs from the reported value 6.73 by more than 10 %

9 Map-model fit [i](#)

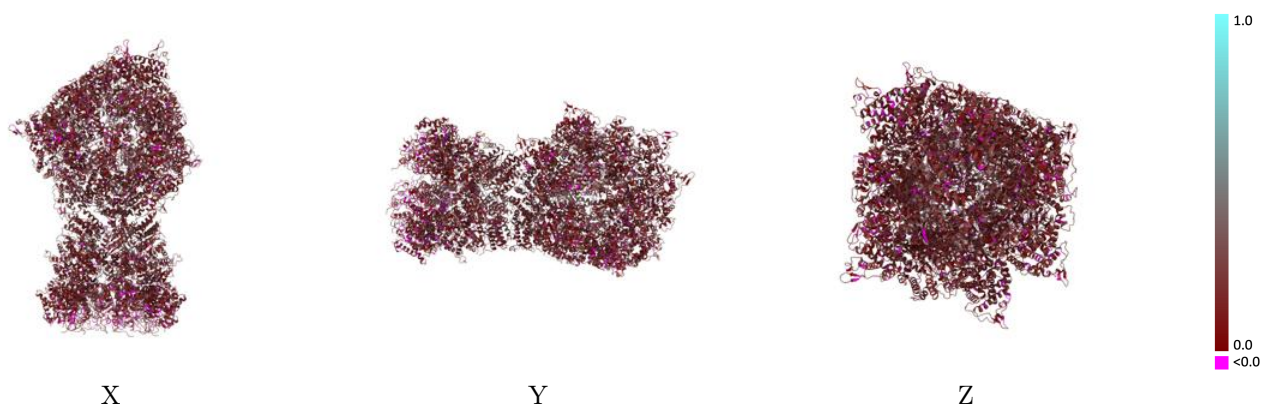
This section contains information regarding the fit between EMDB map EMD-29328 and PDB model 8FNW. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



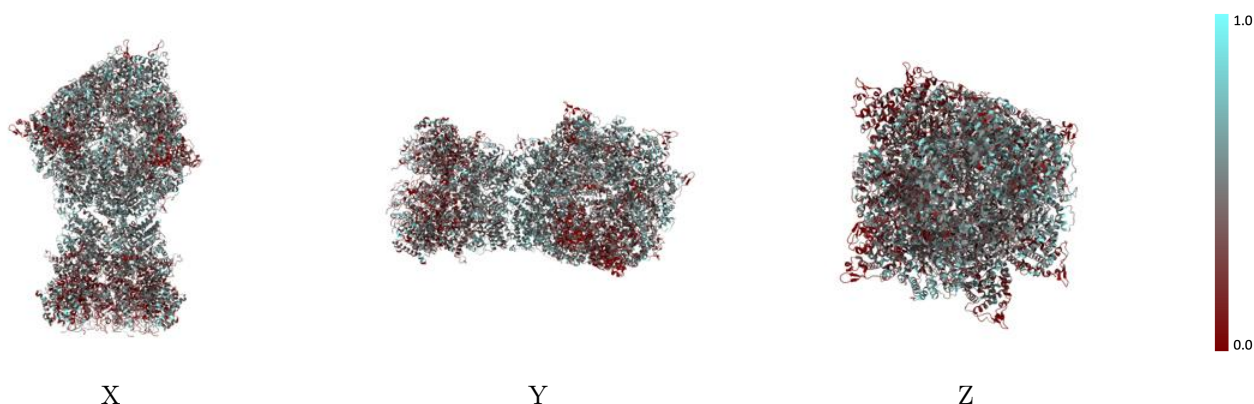
The images above show the 3D surface view of the map at the recommended contour level 1.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



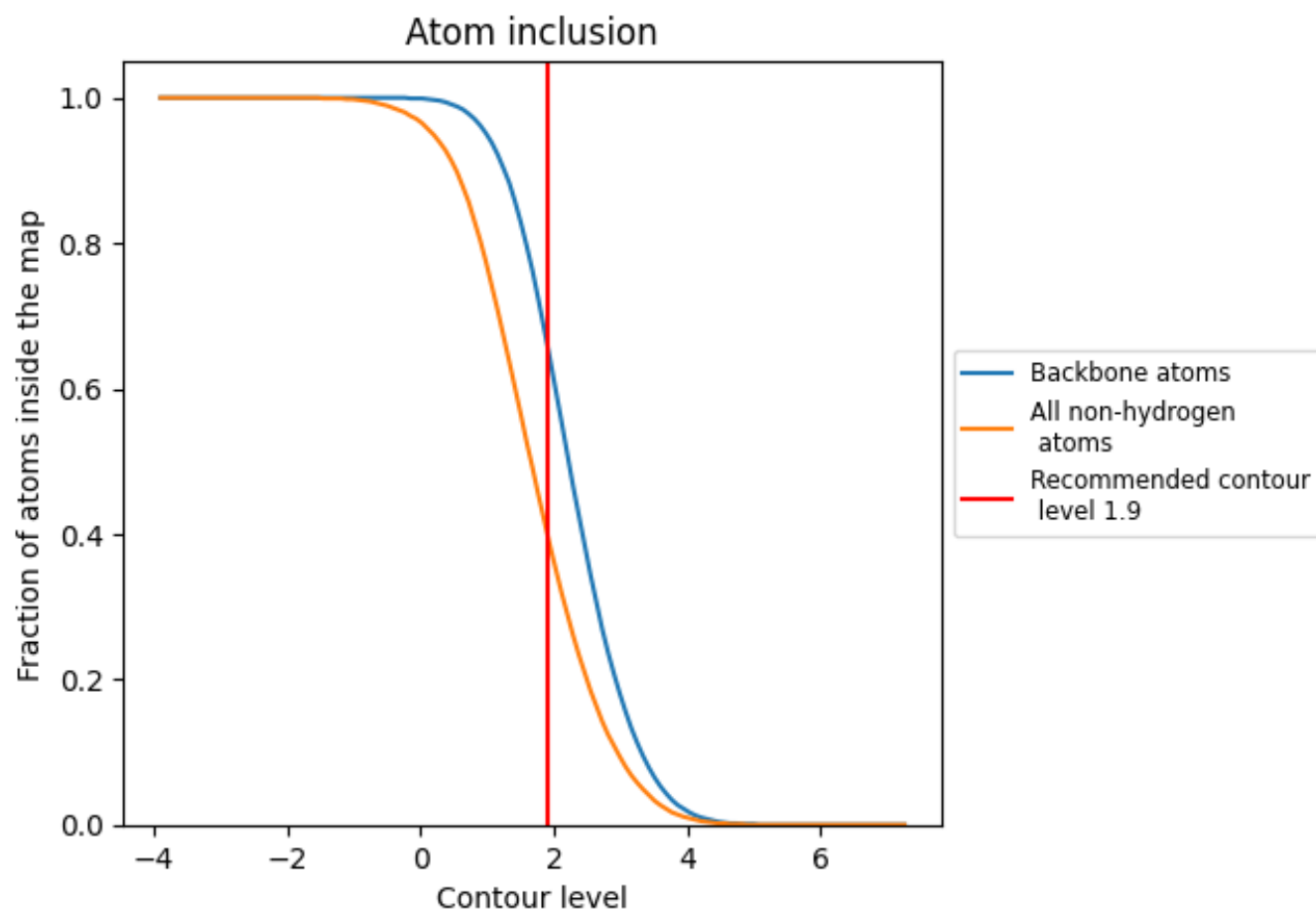
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (1.9).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 40% 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 (1.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4000	 0.1870
A	 0.3030	 0.1790
B	 0.3440	 0.1840
C	 0.5370	 0.1950
D	 0.5220	 0.2000
E	 0.3900	 0.1880
F	 0.4130	 0.1900
G	 0.4080	 0.1880
H	 0.4500	 0.1930
I	 0.4540	 0.1920
J	 0.4250	 0.1920
K	 0.4540	 0.1920
L	 0.3170	 0.1890
M	 0.3820	 0.1870
N	 0.3940	 0.1850
O	 0.3420	 0.1760
P	 0.3700	 0.1820
Q	 0.3830	 0.1820
R	 0.3470	 0.1820
S	 0.3680	 0.1830

