



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 07:04 PM UTC

PDB ID : 3IYF / pdb_00003iyf
EMDB ID : EMD-5140
Title : Atomic Model of the Lidless Mm-cpn in the Open State
Authors : Zhang, J.; Baker, M.L.; Schroeder, G.; Douglas, N.R.; Reissmann, S.; Jakana, J.; Dougherty, M.; Fu, C.J.; Levitt, M.; Ludtke, S.J.; Frydman, J.; Chiu, W.
Deposited on : 2009-10-23
Resolution : 8.00 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:

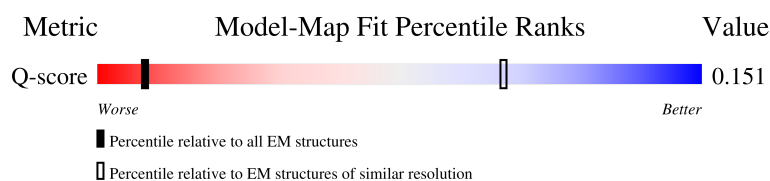
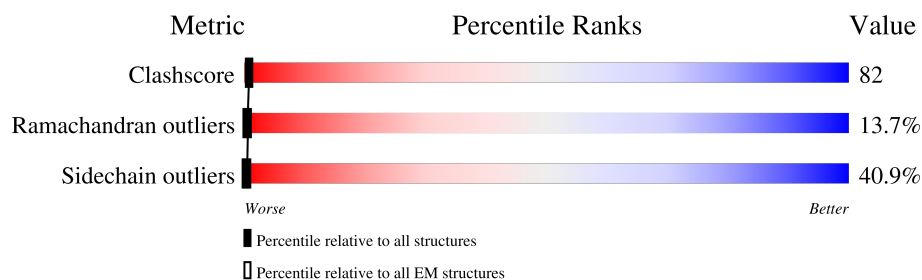
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 8.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	361 (7.50 - 8.50)

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	521	
1	B	521	
1	C	521	
1	D	521	

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Mol	Chain	Length	Quality of chain
1	E	521	
1	F	521	
1	G	521	
1	H	521	
1	I	521	
1	J	521	
1	K	521	
1	L	521	
1	M	521	
1	N	521	
1	O	521	
1	P	521	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 58624 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 Chaperonin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	491	Total	C	N	O	S	0	0
			3664	2272	635	733	24		
1	B	491	Total	C	N	O	S	0	0
			3664	2272	635	733	24		
1	C	491	Total	C	N	O	S	0	0
			3664	2272	635	733	24		
1	D	491	Total	C	N	O	S	0	0
			3664	2272	635	733	24		
1	E	491	Total	C	N	O	S	0	0
			3664	2272	635	733	24		
1	F	491	Total	C	N	O	S	0	0
			3664	2272	635	733	24		
1	G	491	Total	C	N	O	S	0	0
			3664	2272	635	733	24		
1	H	491	Total	C	N	O	S	0	0
			3664	2272	635	733	24		
1	I	491	Total	C	N	O	S	0	0
			3664	2272	635	733	24		
1	J	491	Total	C	N	O	S	0	0
			3664	2272	635	733	24		
1	K	491	Total	C	N	O	S	0	0
			3664	2272	635	733	24		
1	L	491	Total	C	N	O	S	0	0
			3664	2272	635	733	24		
1	M	491	Total	C	N	O	S	0	0
			3664	2272	635	733	24		
1	N	491	Total	C	N	O	S	0	0
			3664	2272	635	733	24		
1	O	491	Total	C	N	O	S	0	0
			3664	2272	635	733	24		
1	P	491	Total	C	N	O	S	0	0
			3664	2272	635	733	24		

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	-	linker	UNP Q877G8
A	242	THR	-	linker	UNP Q877G8
A	243	ALA	-	linker	UNP Q877G8
A	244	SER	-	linker	UNP Q877G8
A	245	GLU	-	linker	UNP Q877G8
B	241	GLU	-	linker	UNP Q877G8
B	242	THR	-	linker	UNP Q877G8
B	243	ALA	-	linker	UNP Q877G8
B	244	SER	-	linker	UNP Q877G8
B	245	GLU	-	linker	UNP Q877G8
C	241	GLU	-	linker	UNP Q877G8
C	242	THR	-	linker	UNP Q877G8
C	243	ALA	-	linker	UNP Q877G8
C	244	SER	-	linker	UNP Q877G8
C	245	GLU	-	linker	UNP Q877G8
D	241	GLU	-	linker	UNP Q877G8
D	242	THR	-	linker	UNP Q877G8
D	243	ALA	-	linker	UNP Q877G8
D	244	SER	-	linker	UNP Q877G8
D	245	GLU	-	linker	UNP Q877G8
E	241	GLU	-	linker	UNP Q877G8
E	242	THR	-	linker	UNP Q877G8
E	243	ALA	-	linker	UNP Q877G8
E	244	SER	-	linker	UNP Q877G8
E	245	GLU	-	linker	UNP Q877G8
F	241	GLU	-	linker	UNP Q877G8
F	242	THR	-	linker	UNP Q877G8
F	243	ALA	-	linker	UNP Q877G8
F	244	SER	-	linker	UNP Q877G8
F	245	GLU	-	linker	UNP Q877G8
G	241	GLU	-	linker	UNP Q877G8
G	242	THR	-	linker	UNP Q877G8
G	243	ALA	-	linker	UNP Q877G8
G	244	SER	-	linker	UNP Q877G8
G	245	GLU	-	linker	UNP Q877G8
H	241	GLU	-	linker	UNP Q877G8
H	242	THR	-	linker	UNP Q877G8
H	243	ALA	-	linker	UNP Q877G8
H	244	SER	-	linker	UNP Q877G8
H	245	GLU	-	linker	UNP Q877G8
I	241	GLU	-	linker	UNP Q877G8
I	242	THR	-	linker	UNP Q877G8
I	243	ALA	-	linker	UNP Q877G8

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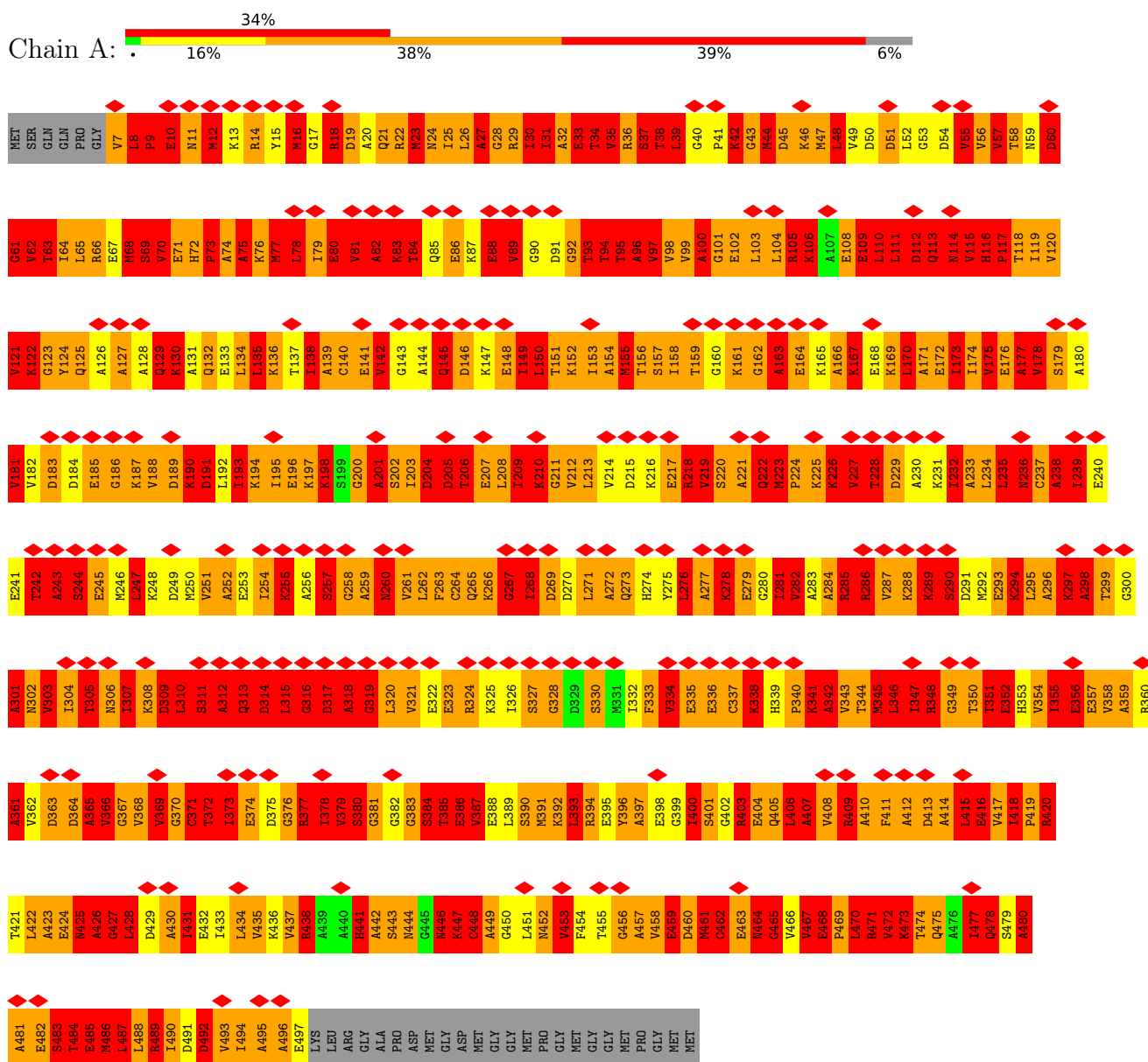
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Chain	Residue	Modelled	Actual	Comment	Reference
I	244	SER	-	linker	UNP Q877G8
I	245	GLU	-	linker	UNP Q877G8
J	241	GLU	-	linker	UNP Q877G8
J	242	THR	-	linker	UNP Q877G8
J	243	ALA	-	linker	UNP Q877G8
J	244	SER	-	linker	UNP Q877G8
J	245	GLU	-	linker	UNP Q877G8
K	241	GLU	-	linker	UNP Q877G8
K	242	THR	-	linker	UNP Q877G8
K	243	ALA	-	linker	UNP Q877G8
K	244	SER	-	linker	UNP Q877G8
K	245	GLU	-	linker	UNP Q877G8
L	241	GLU	-	linker	UNP Q877G8
L	242	THR	-	linker	UNP Q877G8
L	243	ALA	-	linker	UNP Q877G8
L	244	SER	-	linker	UNP Q877G8
L	245	GLU	-	linker	UNP Q877G8
M	241	GLU	-	linker	UNP Q877G8
M	242	THR	-	linker	UNP Q877G8
M	243	ALA	-	linker	UNP Q877G8
M	244	SER	-	linker	UNP Q877G8
M	245	GLU	-	linker	UNP Q877G8
N	241	GLU	-	linker	UNP Q877G8
N	242	THR	-	linker	UNP Q877G8
N	243	ALA	-	linker	UNP Q877G8
N	244	SER	-	linker	UNP Q877G8
N	245	GLU	-	linker	UNP Q877G8
O	241	GLU	-	linker	UNP Q877G8
O	242	THR	-	linker	UNP Q877G8
O	243	ALA	-	linker	UNP Q877G8
O	244	SER	-	linker	UNP Q877G8
O	245	GLU	-	linker	UNP Q877G8
P	241	GLU	-	linker	UNP Q877G8
P	242	THR	-	linker	UNP Q877G8
P	243	ALA	-	linker	UNP Q877G8
P	244	SER	-	linker	UNP Q877G8
P	245	GLU	-	linker	UNP Q877G8

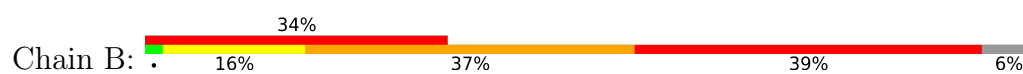
3 Residue-property plots

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: Chaperonin

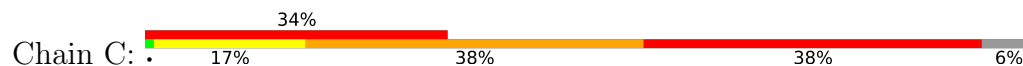


• Molecule 1: Chaperonin



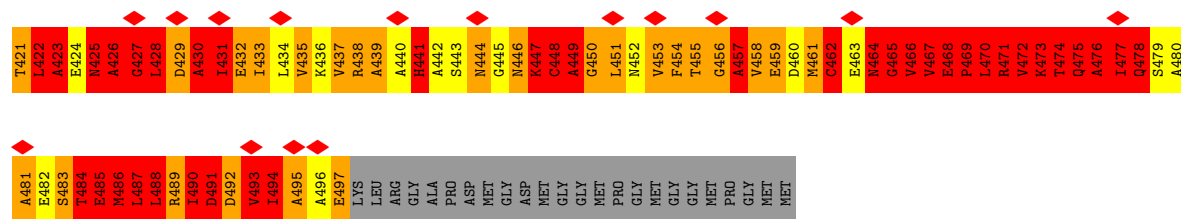
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G61	V62	T63	I64	L65	R66	E67	M68	S69	V70	E71	H72	P73	A74	K75	M76	M77	L78	I79	E80	V81	A82	K83	T84	Q85	E86	K87	E88	V89	G90	D91	T92	T93	T94	T95	A96	V97	V98	V99	A100	G101	E102	L103	L104	R105	K106	A107	E108	E109	L110	L111	D112	Q113	N114	V115	H116	P117	T118	I119	V120
V121	K122	G123	Y124	Q125	A126	A127	A128	Q129	K130	A131	Q132	E133	L134	L135	K136	T137	I138	A139	C140	E141	V142	G143	A144	Q145	D146	K147	E148	I149	L150	T151	K152	I153	A154	M155	T156	A157	I158	T159	G160	K161	G162	A163	E164	K165	A166	K167	E168	K169	L170	A171	I172	I173	L174	V175	E176	A177	V178	S179	A180
V181	V182	D183	D184	E185	G186	K187	V188	D189	K190	D191	L192	I193	K194	I195	E196	K197	K198	S199	G200	A201	S202	L203	D204	D205	T206	E207	L208	I209	G210	G211	V212	L213	V214	D215	K216	E217	R218	V219	S220	A221	Q222	M223	P224	K225	K226	V227	T228	D229	A230	K231	T232	A233	L234	L235	N236	C237	A238	I239	E240
E241	T242	A243	S244	E245	M246	L247	K248	D249	V250	E251	A252	E253	T254	K255	A256	S257	G258	A259	N260	V261	L262	F263	C264	Q265	K266	G267	I268	D269	D270	L271	A272	Q273	H274	V275	L276	A277	K278	E279	G280	T281	V282	A283	A284	K285	K286	V287	K288	K289	S290	D291	N292	E293	K294	L295	A296	K297	T298	G300	
A301	K302	V303	T304	T305	K306	L307	K308	D309	L310	S311	A312	Q313	D314	L315	G316	D317	A318	G319	L320	V321	E322	E323	R324	K325	I326	S327	G328	D329	S330	K331	F332	V333	V334	E335	E336	C337	K338	H339	P340	K341	V342	V343	T344	K345	L346	T347	D413	G349	T350	T351	E352	K353	V354	I355	E356	E357	V358	A359	P360
A361	V362	D363	D364	A365	V366	G367	V368	V369	G370	C371	T372	L373	E374	D375	K376	R377	L378	V379	S380	G381	G382	G383	S384	T385	E386	V387	E388	L389	S390	K391	K392	L393	R394	E395	V396	A397	E398	G399	L400	S401	G402	R403	E404	Q405	L406	A407	V408	A409	A410	F411	A412	D413	A414	L415	V416	A417	A418	A419	R420
T421	L422	A423	E424	N425	A426	C427	L428	D429	A430	L431	E432	L433	L434	V435	K436	V437	R438	A439	A440	H441	A442	S443	N444	G445	N446	K447	C448	A449	G450	L451	N452	V453	F454	T455	G456	A457	V458	E459	A460	A461	C462	E463	P469	L470	R471	V472	K473	T474	Q475	A476	L477	Q478	S479	A480					
A481	E482	S483	T484	E485	M486	L487	L488	R489	I490	D491	G492	V493	I494	A495	A496	E497	LYS	LEU	ARG	GLY	ALA	PRO	ASP	MET	GLY	ASP	MET	C448	GLY	GLY	GLY	MET	PRD	GLY	E459	A461	C462	E463	P469	L470	R471	V472	K473	T474	Q475	A476	L477	Q478	S479	A480									

• Molecule 1: Chaperonin

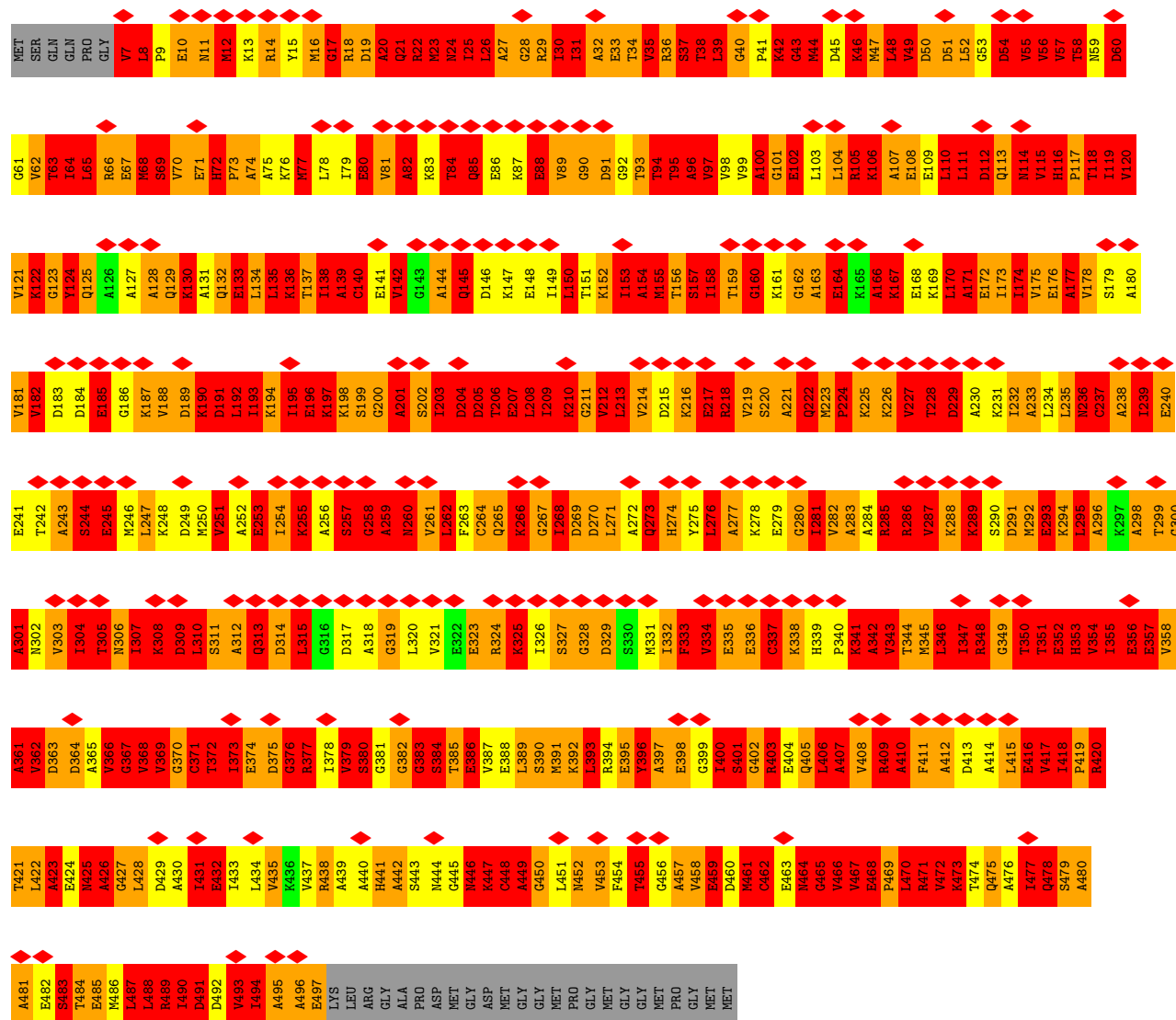


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G61	V62	T63	I64	L65	R66	E67	M68	S69	V70	E71	H72	P73	A74	K75	M76	M77	L78	I79	E80	V81	A82	K83	T84	Q85	E86	K87	E88	V89	G90	D91	T92	T93	T94	N95	A96	V97	V98	V99	A100	G101	E102	L103	L104	R105	K106	A107	E108	E109	L110	L111	D112	Q113	N114	V115	H116	P117	T118	I119	V120
V121	K122	G123	Y124	Q125	A126	A127	A128	Q129	K130	A131	Q132	E133	L134	L135	K136	T137	I138	A139	C140	E141	V142	G143	A144	Q145	D146	K147	E148	I149	L150	T151	K152	I153	A154	M155	T156	S157	I158	T159	G160	K161	G162	A163	E164	K165	A166	K167	E168	K169	L170	A171	E172	I173	I174	V175	E176	A177	V178	S179	A180

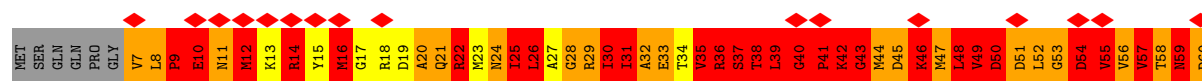


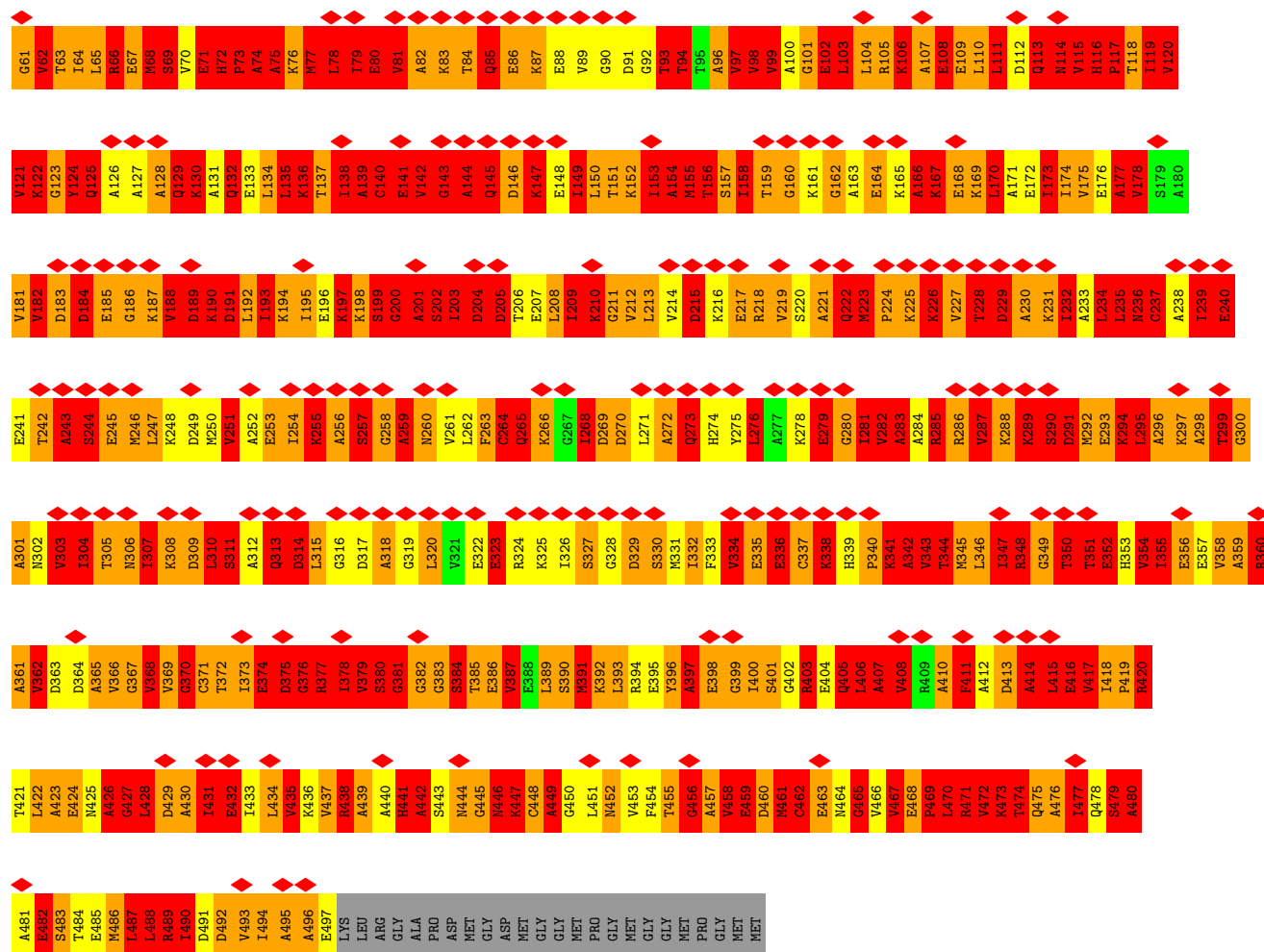


• Molecule 1: Chaperonin

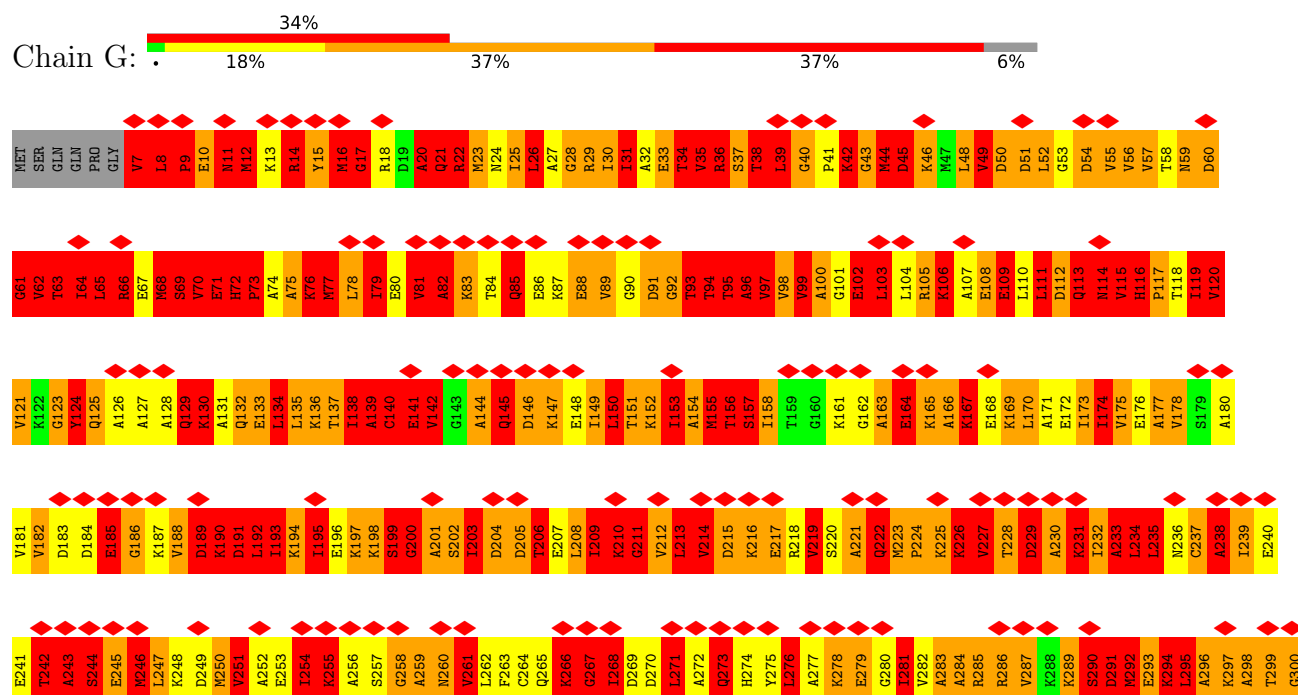


• Molecule 1: Chaperonin

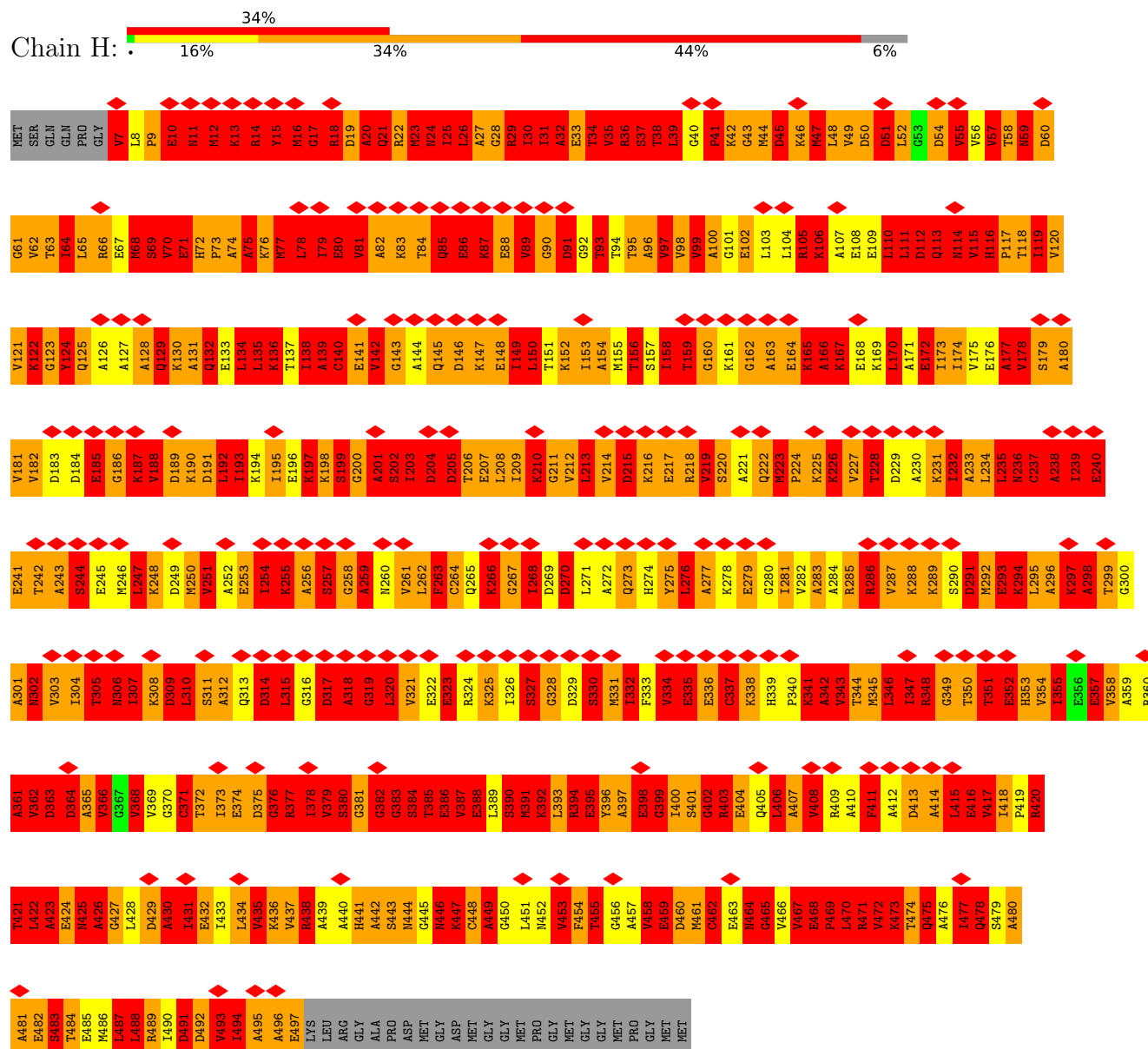




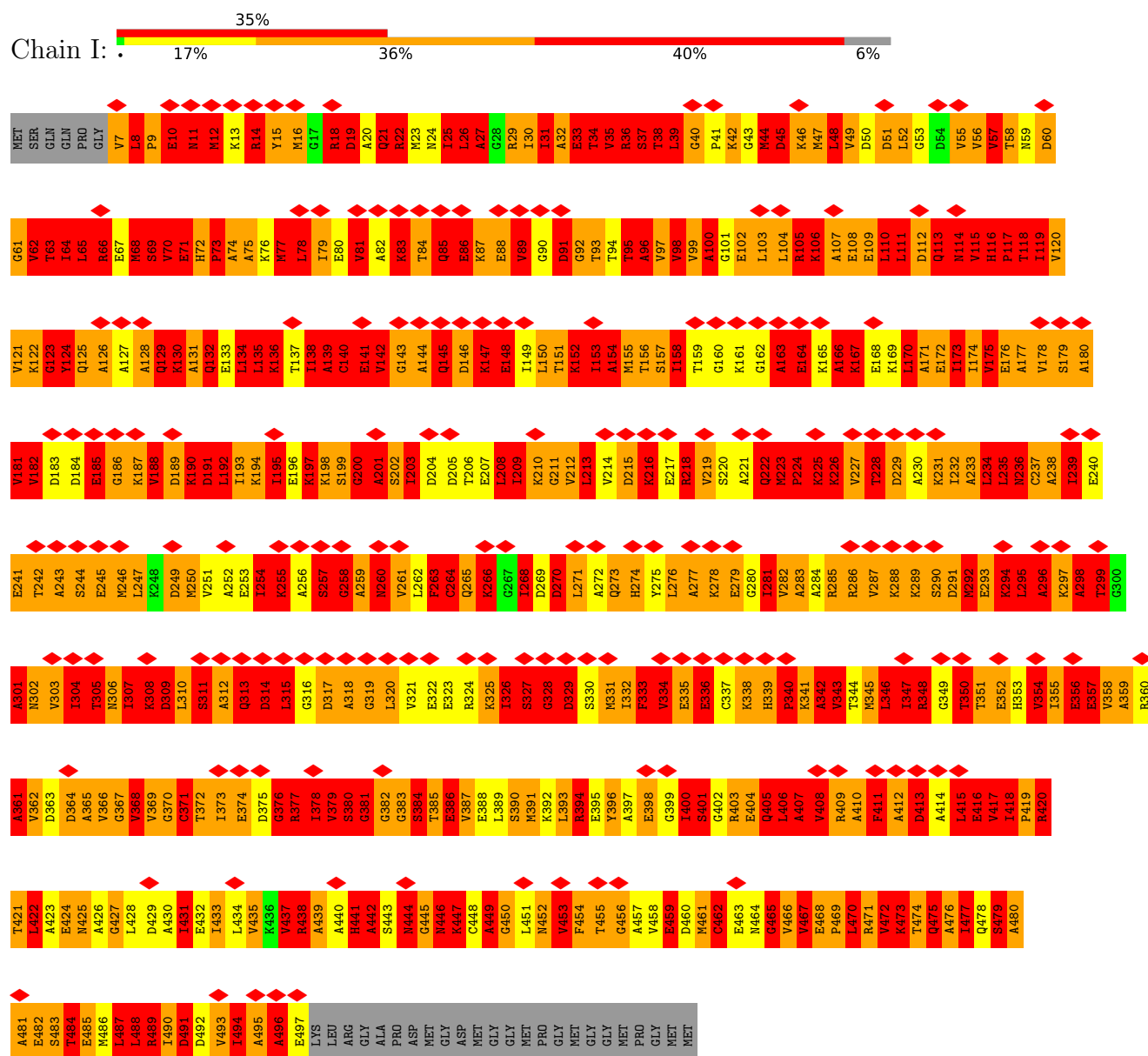
• Molecule 1: Chaperonin



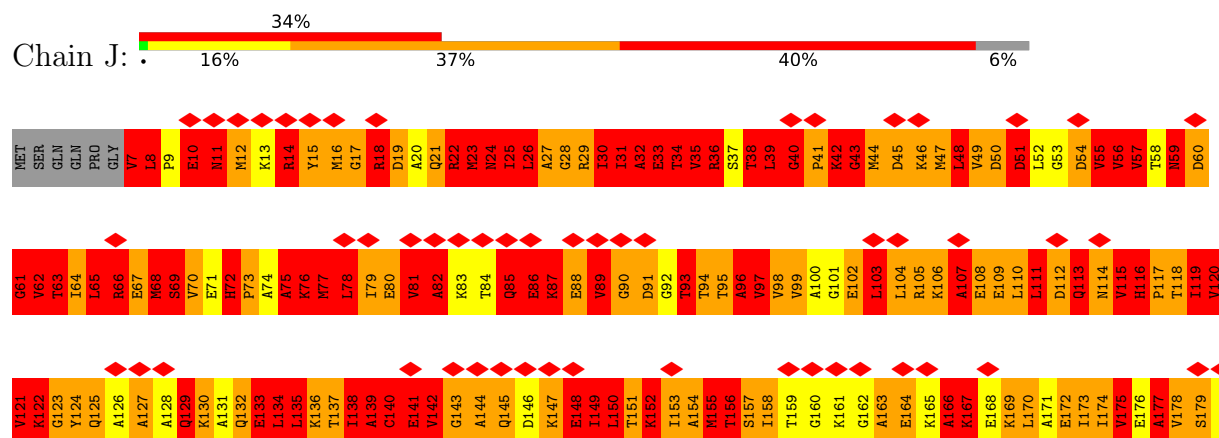
- Molecule 1: Chaperonin

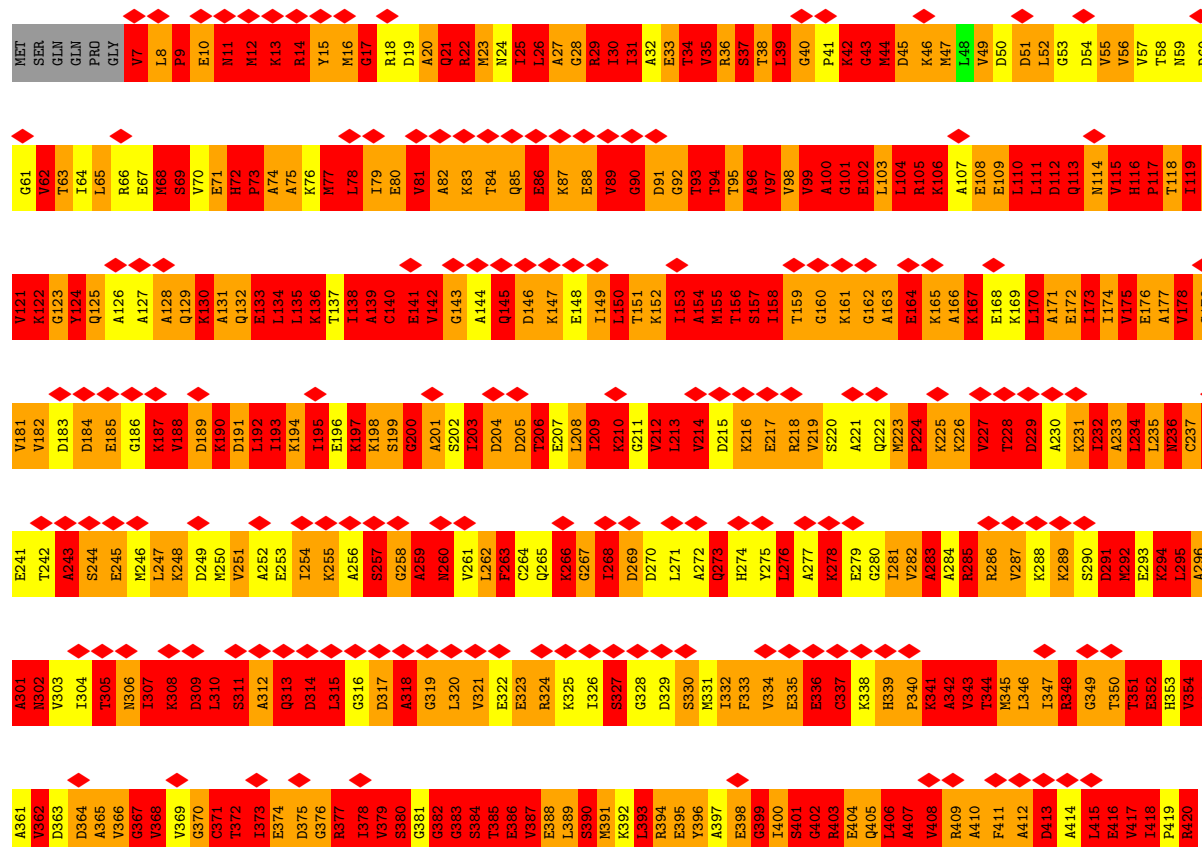


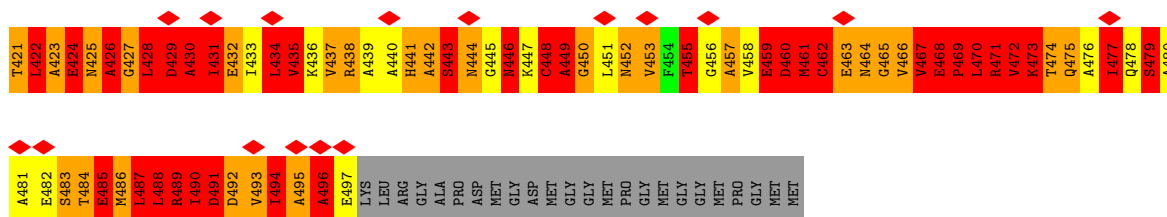
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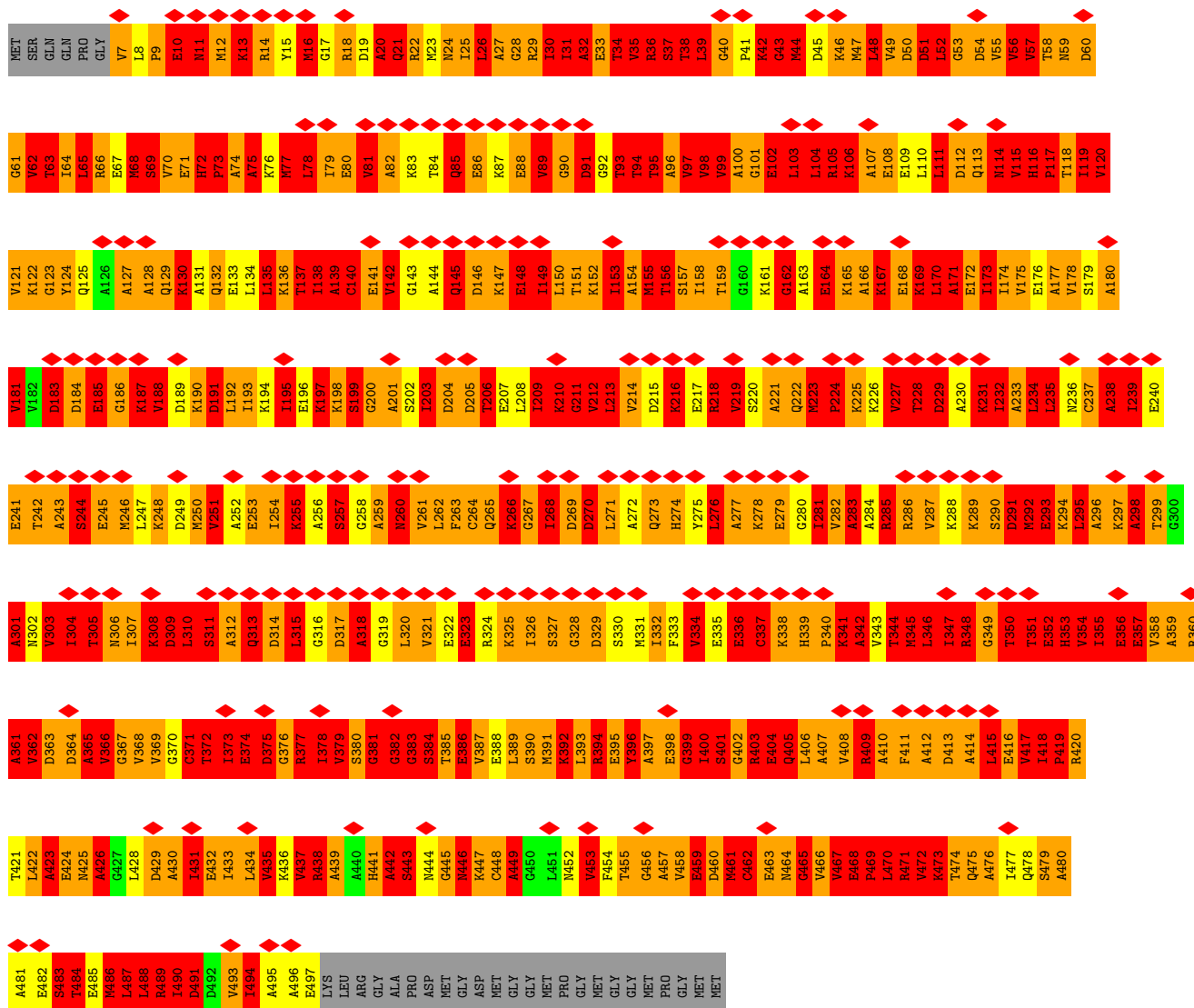
• Molecule 1: Chaperonin





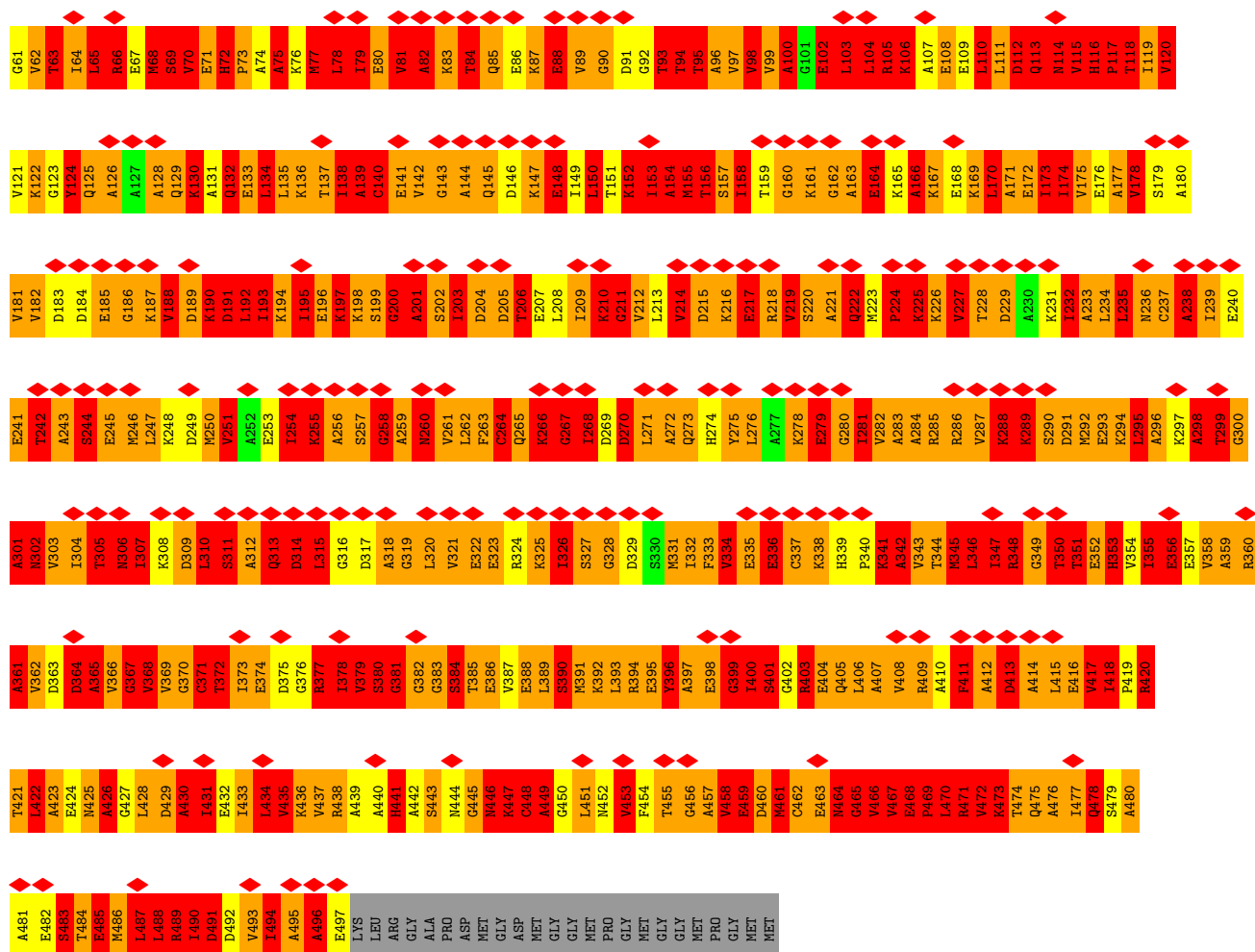


• Molecule 1: Chaperonin

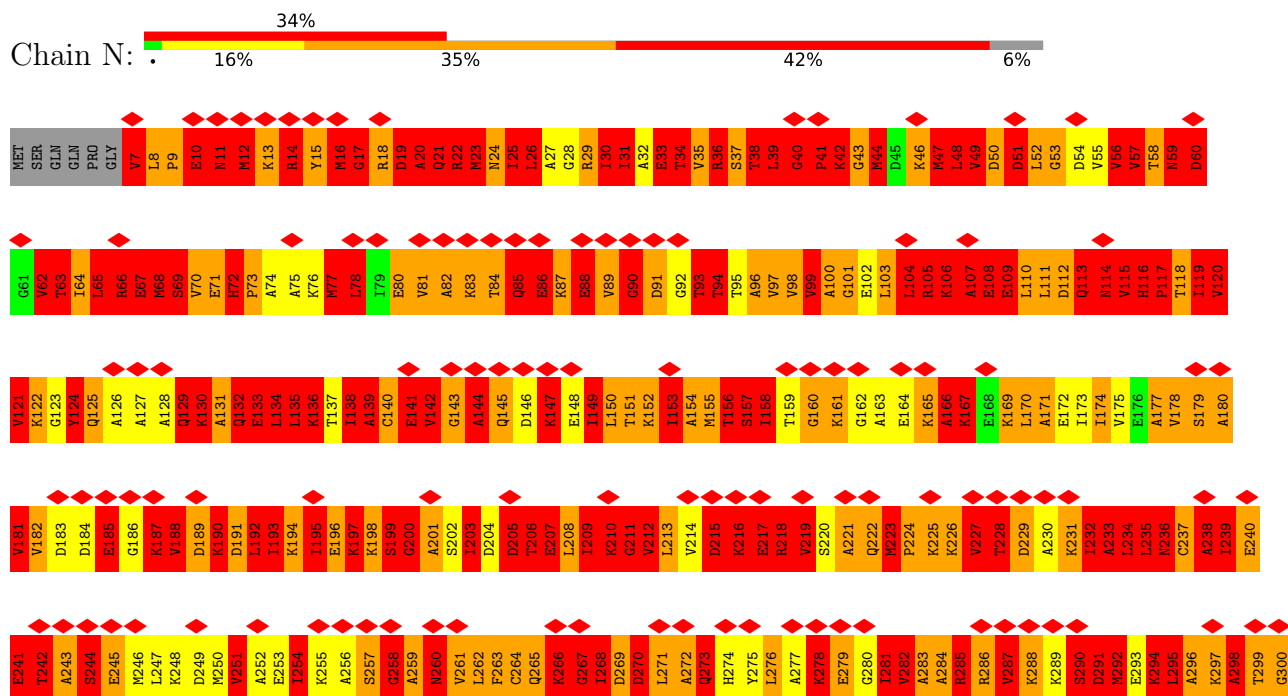


• Molecule 1: Chaperonin

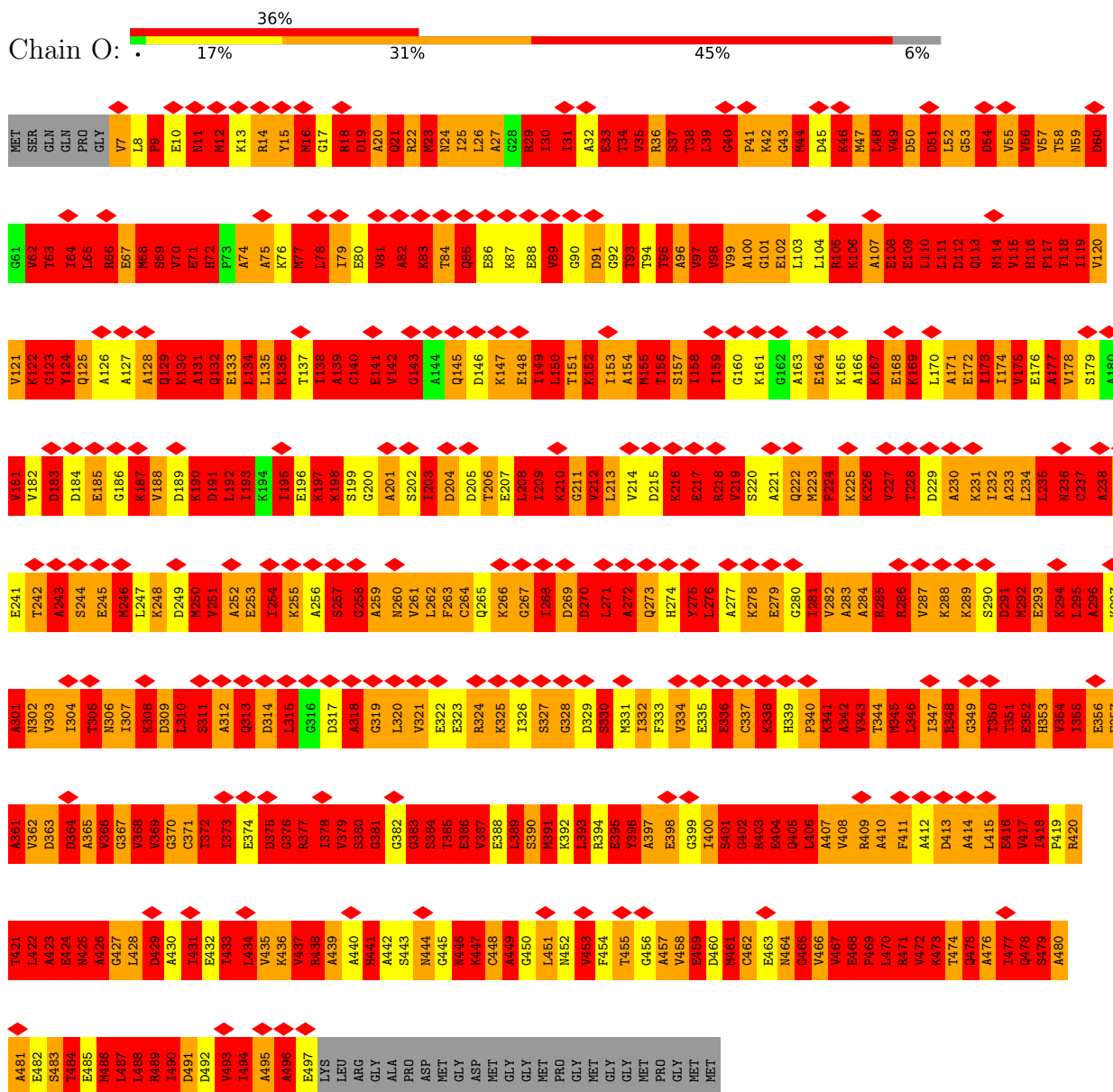




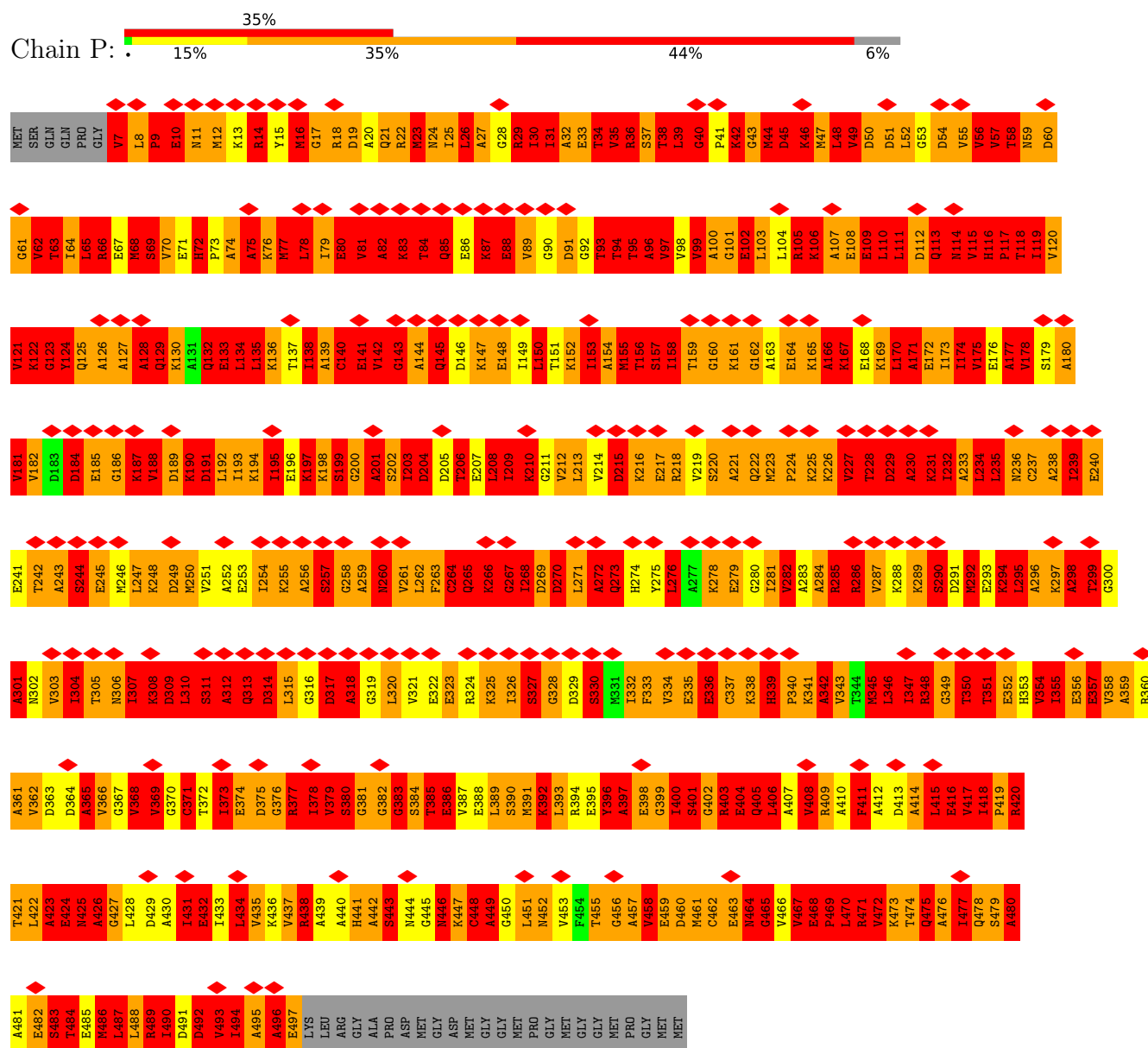
• Molecule 1: Chaperonin



- Molecule 1: Chaperonin



● Molecule 1: Chaperonin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D8	Depositor
Number of particles used	Not provided	
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	112000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	2.477	Depositor
Minimum map value	-1.784	Depositor
Average map value	0.034	Depositor
Map value standard deviation	0.191	Depositor
Recommended contour level	0.95	Depositor
Map size ($\text{\AA}$)	319.2, 319.2, 319.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing ($\text{\AA}$)	1.33, 1.33, 1.33	Depositor

5 Model quality

5.1 Standard geometry

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	2.82	321/3685 (8.7%)	4.35	1139/4961 (23.0%)
1	B	2.85	333/3685 (9.0%)	4.31	1111/4961 (22.4%)
1	C	2.81	304/3685 (8.2%)	4.31	1078/4961 (21.7%)
1	D	2.80	310/3685 (8.4%)	4.30	1078/4961 (21.7%)
1	E	2.82	309/3685 (8.4%)	4.20	1045/4961 (21.1%)
1	F	2.85	325/3685 (8.8%)	4.35	1137/4961 (22.9%)
1	G	2.79	298/3685 (8.1%)	4.35	1102/4961 (22.2%)
1	H	2.84	325/3685 (8.8%)	4.28	1086/4961 (21.9%)
1	I	2.85	337/3685 (9.1%)	4.38	1164/4961 (23.5%)
1	J	2.84	339/3685 (9.2%)	4.32	1111/4961 (22.4%)
1	K	2.84	320/3685 (8.7%)	4.35	1114/4961 (22.5%)
1	L	2.80	305/3685 (8.3%)	4.31	1102/4961 (22.2%)
1	M	2.90	331/3685 (9.0%)	4.30	1102/4961 (22.2%)
1	N	2.81	299/3685 (8.1%)	4.28	1069/4961 (21.5%)
1	O	2.77	306/3685 (8.3%)	4.35	1124/4961 (22.7%)
1	P	2.87	321/3685 (8.7%)	4.43	1185/4961 (23.9%)
All	All	2.83	5083/58960 (8.6%)	4.32	17747/79376 (22.4%)

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	A	71	243
1	B	55	257
1	C	57	264
1	D	60	284
1	E	51	259
1	F	58	270
1	G	63	258
1	H	61	282
1	I	60	252

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	53	260
1	K	57	267
1	L	44	284
1	M	54	279
1	N	50	292
1	O	63	275
1	P	67	288
All	All	924	4314

The worst 5 of 5083 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	450	GLY	N-CA	15.10	1.56	1.44
1	N	200	GLY	CA-C	13.10	1.61	1.52
1	M	195	ILE	CA-C	12.10	1.63	1.53
1	P	193	ILE	CA-CB	11.62	1.66	1.53
1	J	59	ASN	CA-C	10.63	1.60	1.52

The worst 5 of 17747 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	14	ARG	CD-NE-CZ	37.50	176.90	124.40
1	P	249	ASP	CA-CB-CG	30.42	143.02	112.60
1	O	18	ARG	CD-NE-CZ	30.14	166.59	124.40
1	I	218	ARG	CD-NE-CZ	28.48	164.27	124.40
1	B	186	GLY	CA-C-N	25.51	160.14	122.39

5 of 924 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	7	VAL	CA
1	A	8	LEU	CA
1	A	10	GLU	CA
1	A	15	TYR	CA
1	A	30	ILE	CB

5 of 4314 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	GLU	Mainchain
1	A	11	ASN	Mainchain
1	A	12	MET	Peptide

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Mol	Chain	Res	Type	Group
1	A	8	LEU	Peptide
1	A	9	PRO	Peptide

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	3664	0	3799	725	0
1	B	3664	0	3800	632	0
1	C	3664	0	3798	623	0
1	D	3664	0	3801	634	0
1	E	3664	0	3801	694	0
1	F	3664	0	3800	533	0
1	G	3664	0	3800	579	0
1	H	3664	0	3801	578	0
1	I	3664	0	3799	614	0
1	J	3664	0	3801	651	0
1	K	3664	0	3798	619	0
1	L	3664	0	3801	621	0
1	M	3664	0	3799	631	0
1	N	3664	0	3799	661	0
1	O	3664	0	3800	583	0
1	P	3664	0	3800	642	0
All	All	58624	0	60797	9630	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 82.

The worst 5 of 9630 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:N:403:ARG:HH11	1:N:403:ARG:CG	1.06	1.44
1:M:420:ARG:HH11	1:M:420:ARG:CB	1.31	1.41
1:B:488:LEU:CD2	1:B:488:LEU:O	1.68	1.40
1:E:488:LEU:HD12	1:E:488:LEU:O	1.11	1.29
1:E:391:MET:CE	1:E:438:ARG:HB3	1.65	1.26

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	489/521 (94%)	345 (71%)	78 (16%)	66 (14%)	0	4
1	B	489/521 (94%)	343 (70%)	85 (17%)	61 (12%)	0	4
1	C	489/521 (94%)	346 (71%)	68 (14%)	75 (15%)	0	3
1	D	489/521 (94%)	339 (69%)	80 (16%)	70 (14%)	0	3
1	E	489/521 (94%)	339 (69%)	80 (16%)	70 (14%)	0	3
1	F	489/521 (94%)	345 (71%)	74 (15%)	70 (14%)	0	3
1	G	489/521 (94%)	347 (71%)	77 (16%)	65 (13%)	0	4
1	H	489/521 (94%)	334 (68%)	84 (17%)	71 (14%)	0	3
1	I	489/521 (94%)	343 (70%)	78 (16%)	68 (14%)	0	3
1	J	489/521 (94%)	350 (72%)	71 (14%)	68 (14%)	0	3
1	K	489/521 (94%)	353 (72%)	81 (17%)	55 (11%)	0	5
1	L	489/521 (94%)	337 (69%)	89 (18%)	63 (13%)	0	4
1	M	489/521 (94%)	352 (72%)	76 (16%)	61 (12%)	0	4
1	N	489/521 (94%)	348 (71%)	72 (15%)	69 (14%)	0	3
1	O	489/521 (94%)	343 (70%)	73 (15%)	73 (15%)	0	3
1	P	489/521 (94%)	339 (69%)	80 (16%)	70 (14%)	0	3
All	All	7824/8336 (94%)	5503 (70%)	1246 (16%)	1075 (14%)	0	4

5 of 1075 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	9	PRO
1	A	10	GLU
1	A	16	MET

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Mol	Chain	Res	Type
1	A	62	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	393/413 (95%)	243 (62%)	150 (38%)	0	1
1	B	393/413 (95%)	229 (58%)	164 (42%)	0	0
1	C	393/413 (95%)	246 (63%)	147 (37%)	0	1
1	D	393/413 (95%)	228 (58%)	165 (42%)	0	0
1	E	393/413 (95%)	231 (59%)	162 (41%)	0	0
1	F	393/413 (95%)	222 (56%)	171 (44%)	0	0
1	G	393/413 (95%)	245 (62%)	148 (38%)	0	1
1	H	393/413 (95%)	221 (56%)	172 (44%)	0	0
1	I	393/413 (95%)	234 (60%)	159 (40%)	0	0
1	J	393/413 (95%)	236 (60%)	157 (40%)	0	1
1	K	393/413 (95%)	239 (61%)	154 (39%)	0	1
1	L	393/413 (95%)	241 (61%)	152 (39%)	0	1
1	M	393/413 (95%)	229 (58%)	164 (42%)	0	0
1	N	393/413 (95%)	237 (60%)	156 (40%)	0	1
1	O	393/413 (95%)	221 (56%)	172 (44%)	0	0
1	P	393/413 (95%)	216 (55%)	177 (45%)	0	0
All	All	6288/6608 (95%)	3718 (59%)	2570 (41%)	0	0

5 of 2570 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	323	GLU
1	O	218	ARG
1	M	16	MET
1	L	315	LEU

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Mol	Chain	Res	Type
1	N	39	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 204 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	24	ASN
1	L	59	ASN
1	P	339	HIS
1	J	125	GLN
1	K	24	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

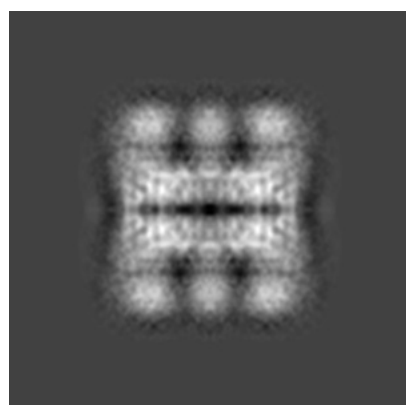
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5140. These allow visual inspection of the internal detail of the map and identification of artifacts.

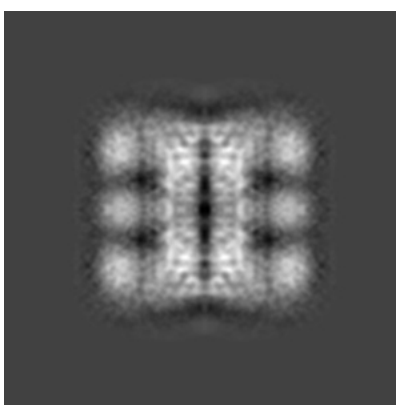
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

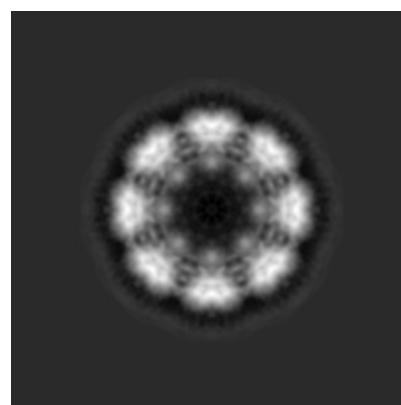
6.1.1 Primary map



X



Y

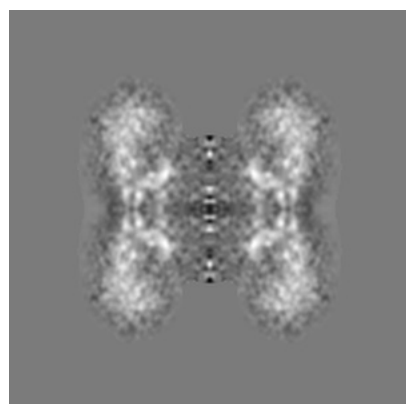


Z

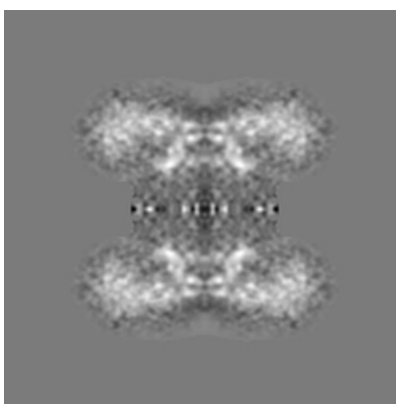
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

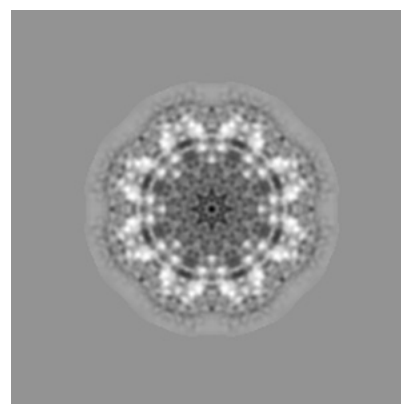
6.2.1 Primary map



X Index: 120



Y Index: 120

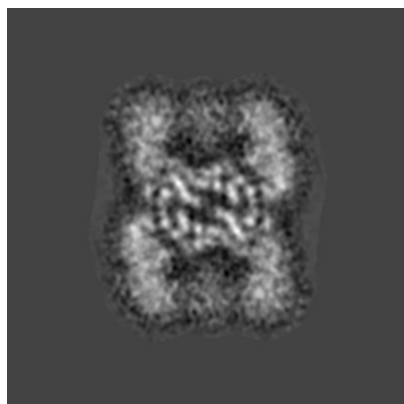


Z Index: 120

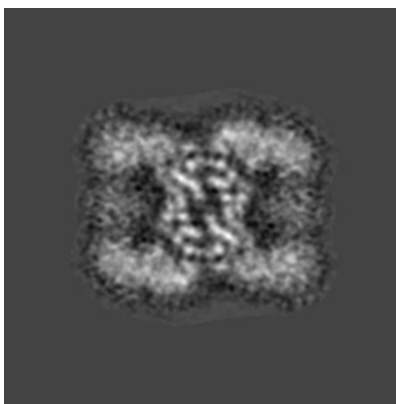
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

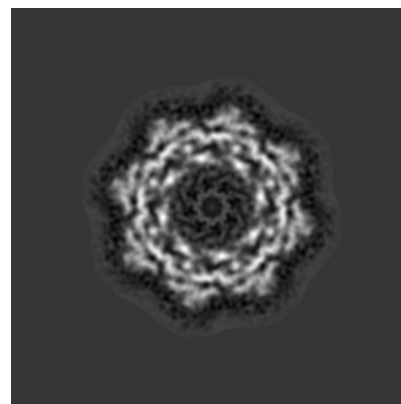
6.3.1 Primary map



X Index: 85



Y Index: 155

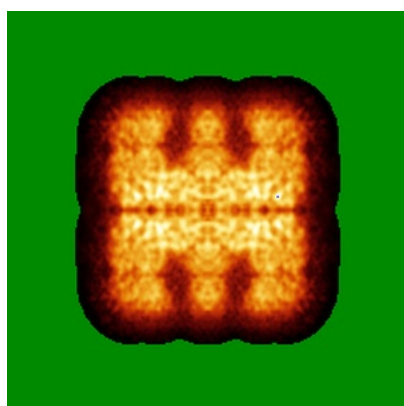


Z Index: 129

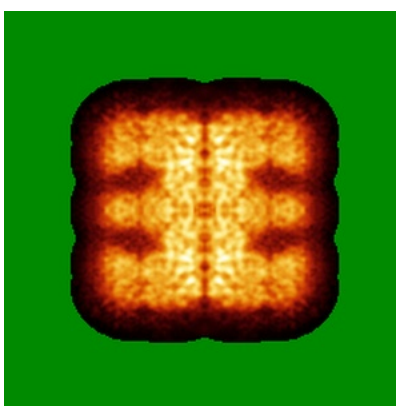
The images above show the largest variance slices of the map in three orthogonal directions.

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

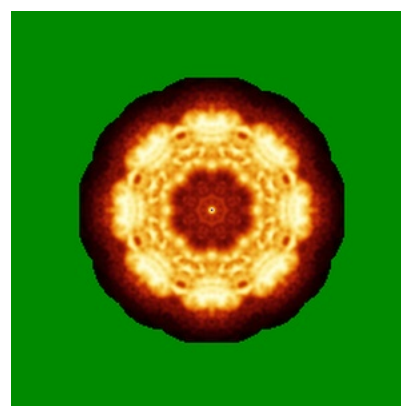
6.4.1 Primary map



X



Y

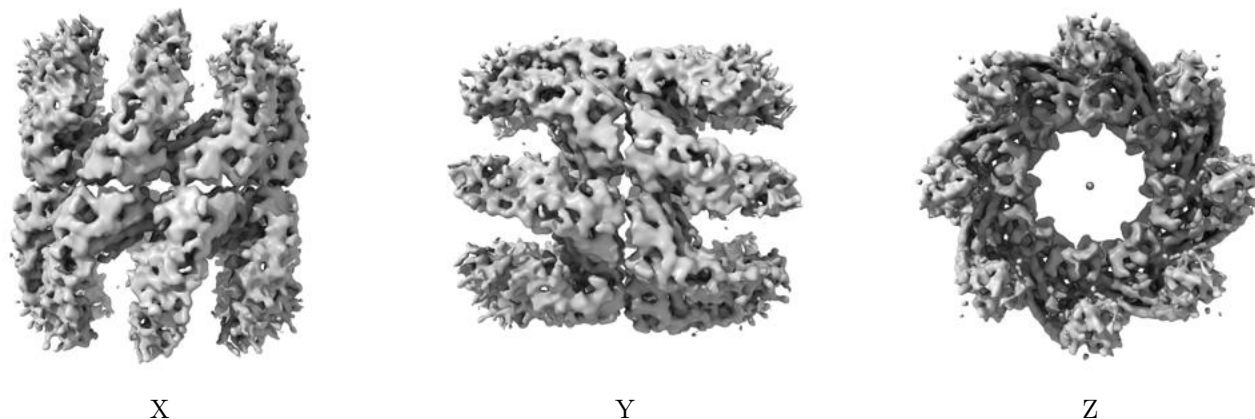


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.95. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

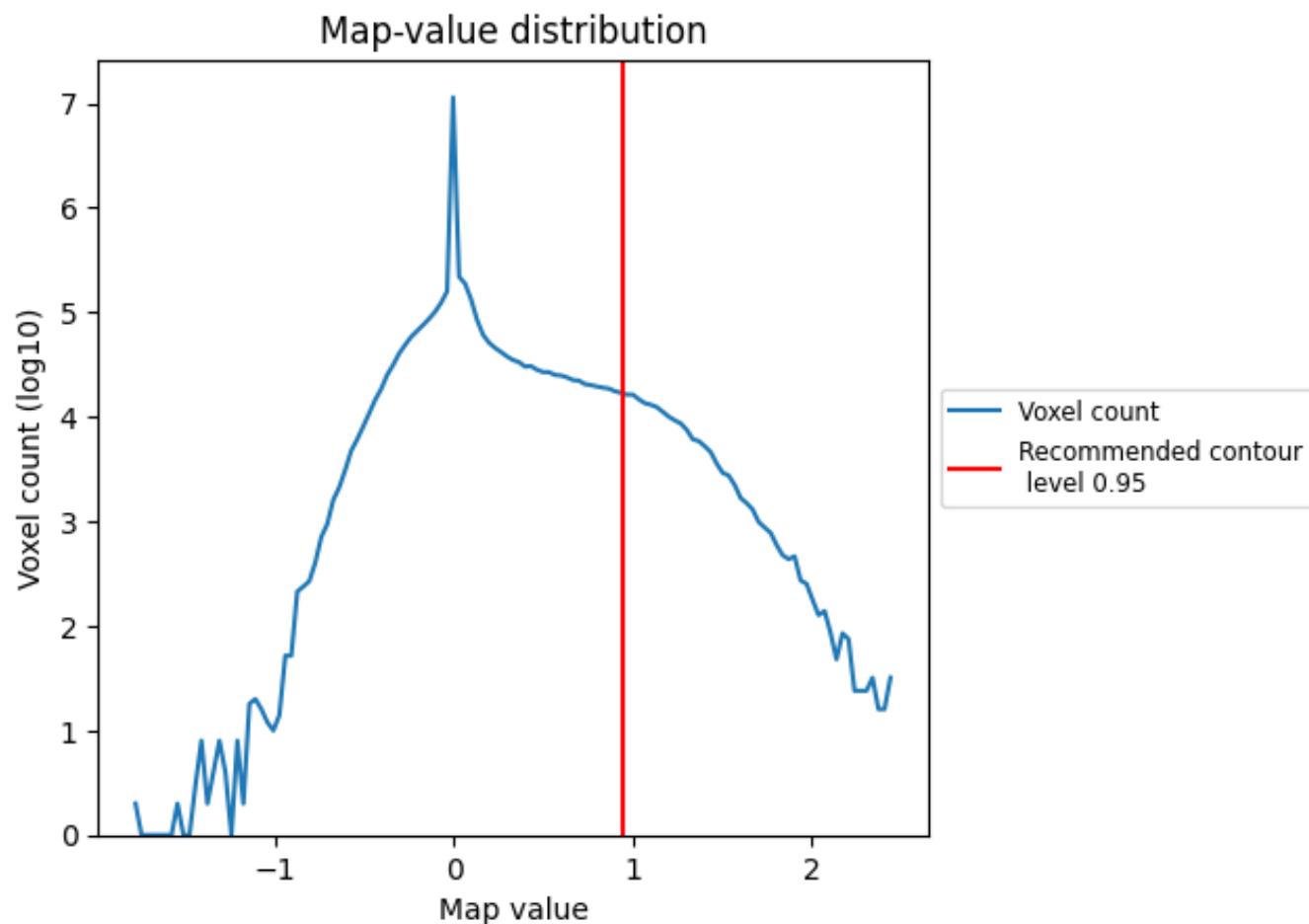
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

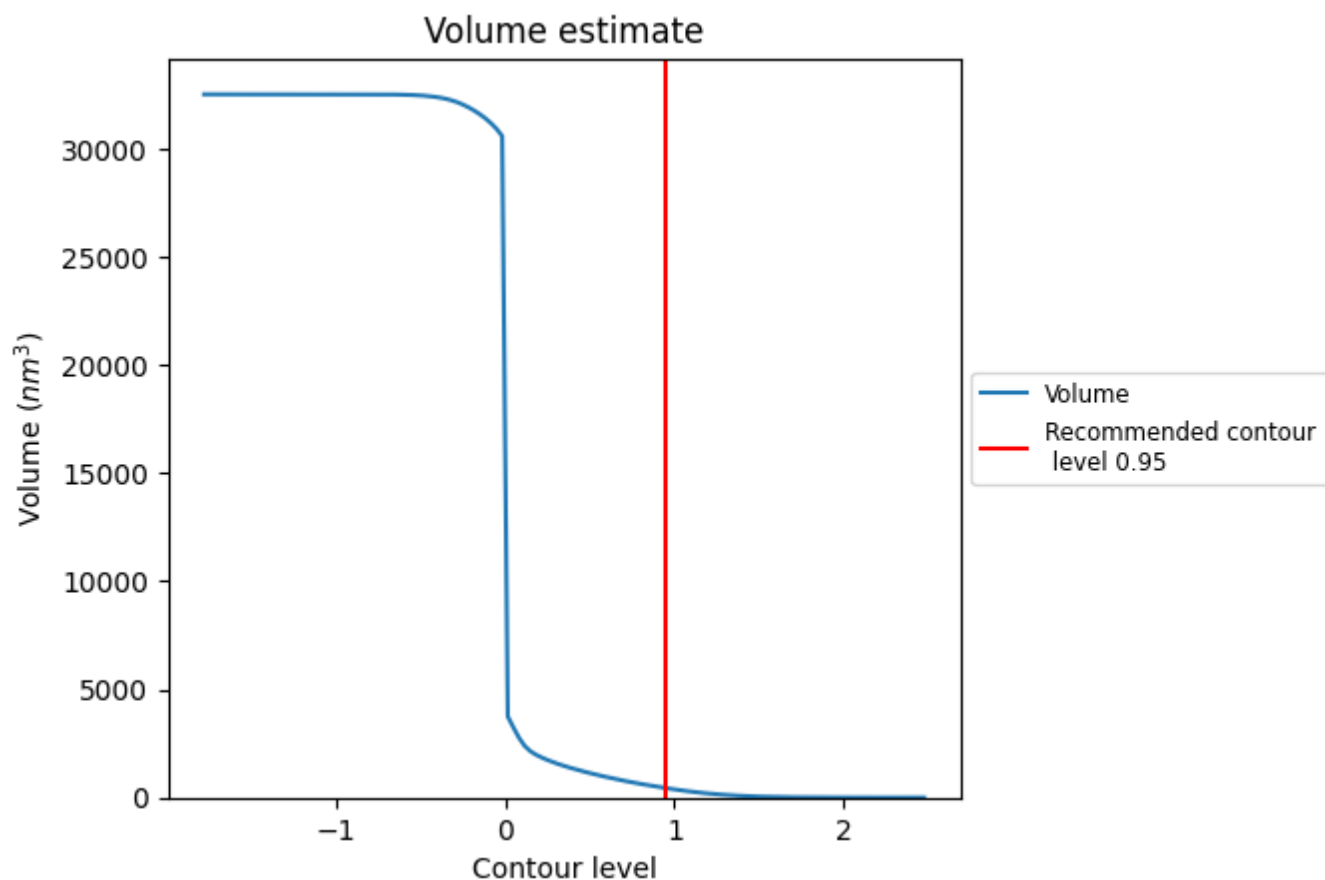
This section contains the results of statistical analysis of the map.

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.

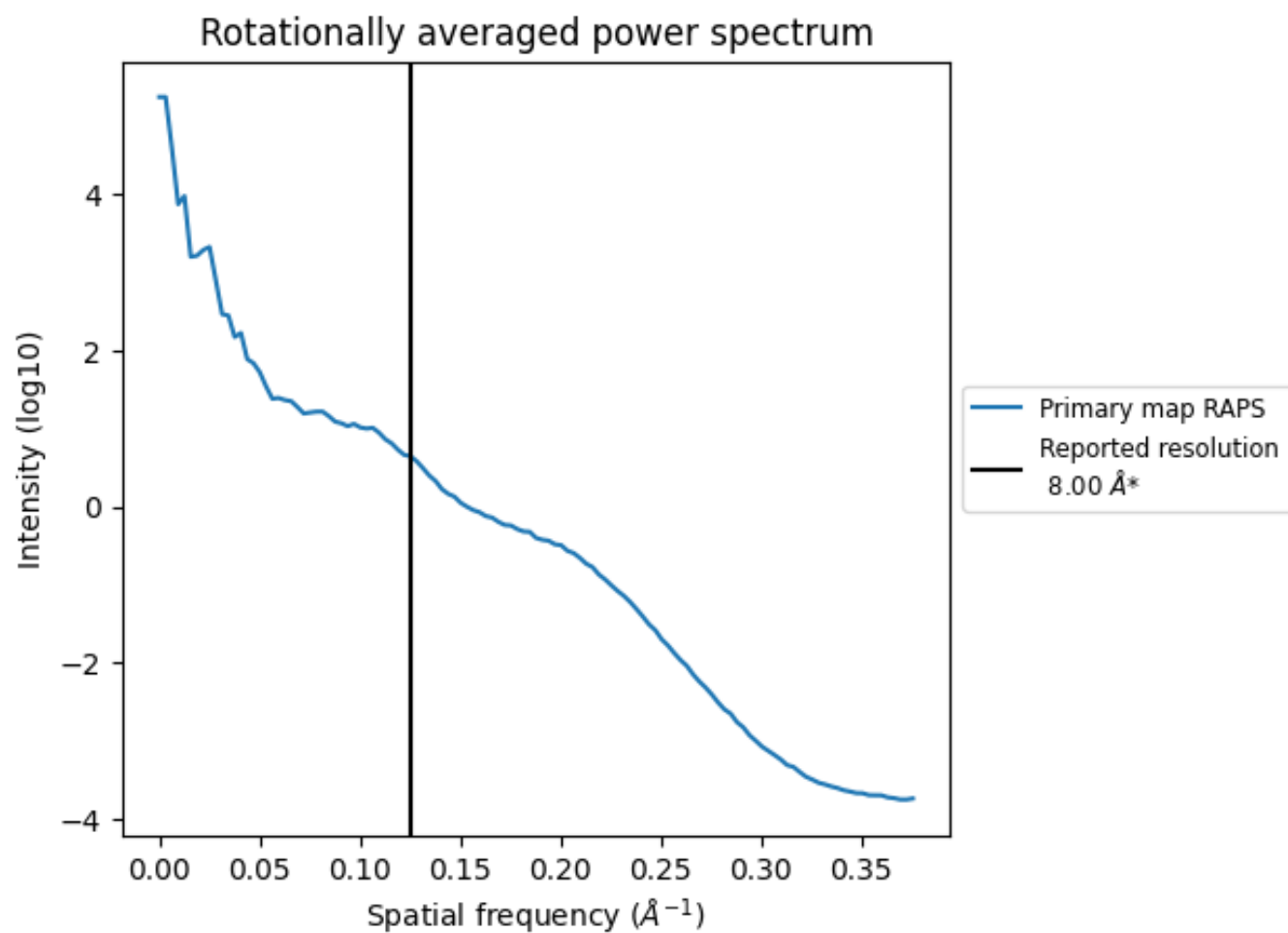
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 437 nm³; this corresponds to an approximate mass of 395 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 0.125 Å⁻¹

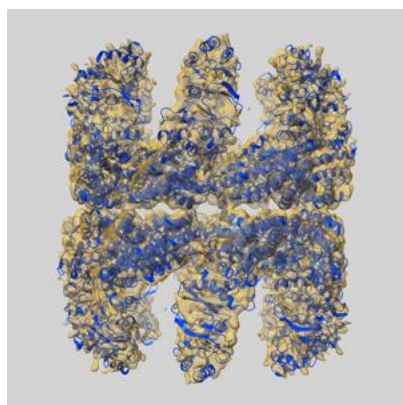
8 Fourier-Shell correlation

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

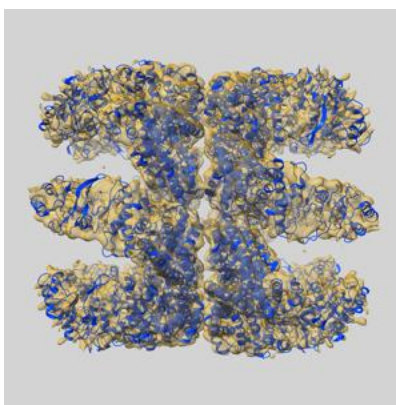
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5140 and PDB model 3IYF. Per-residue inclusion information can be found in section [3](#) on page [7](#).

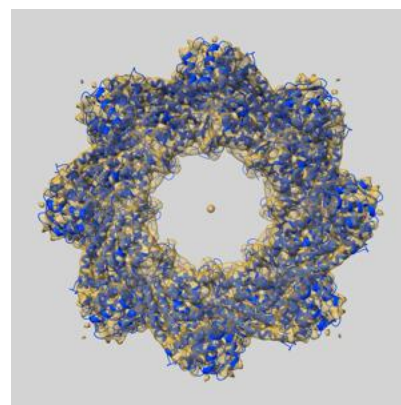
9.1 Map-model overlay [i](#)



X



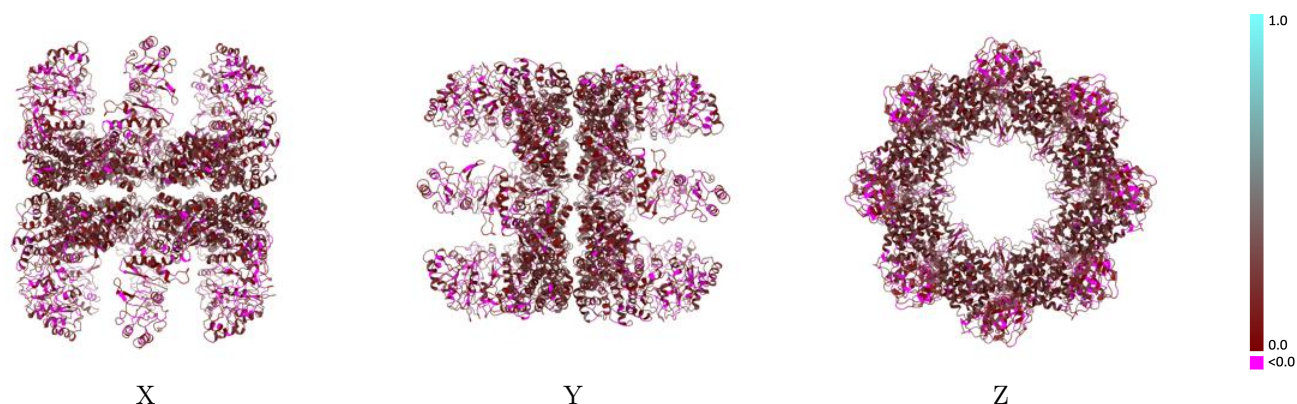
Y



Z

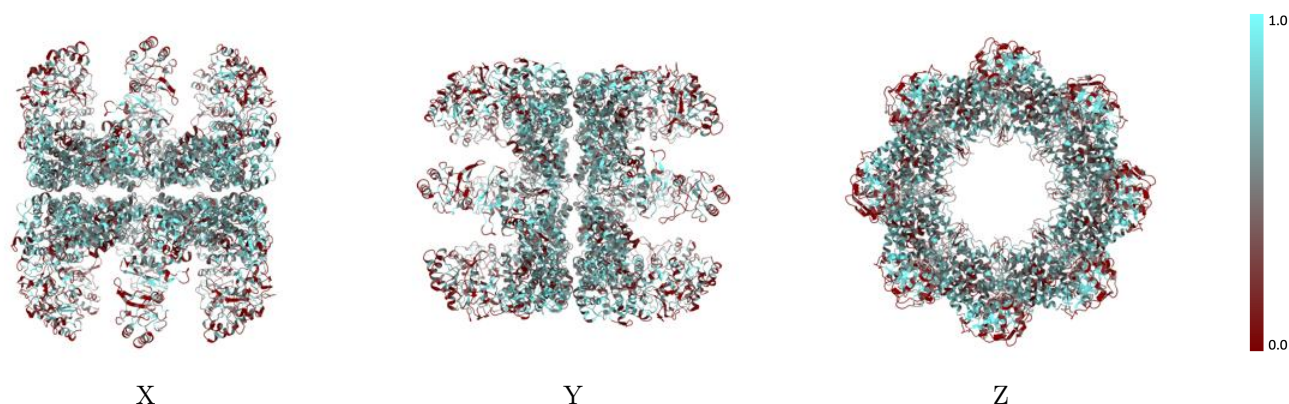
The images above show the 3D surface view of the map at the recommended contour level 0.95 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



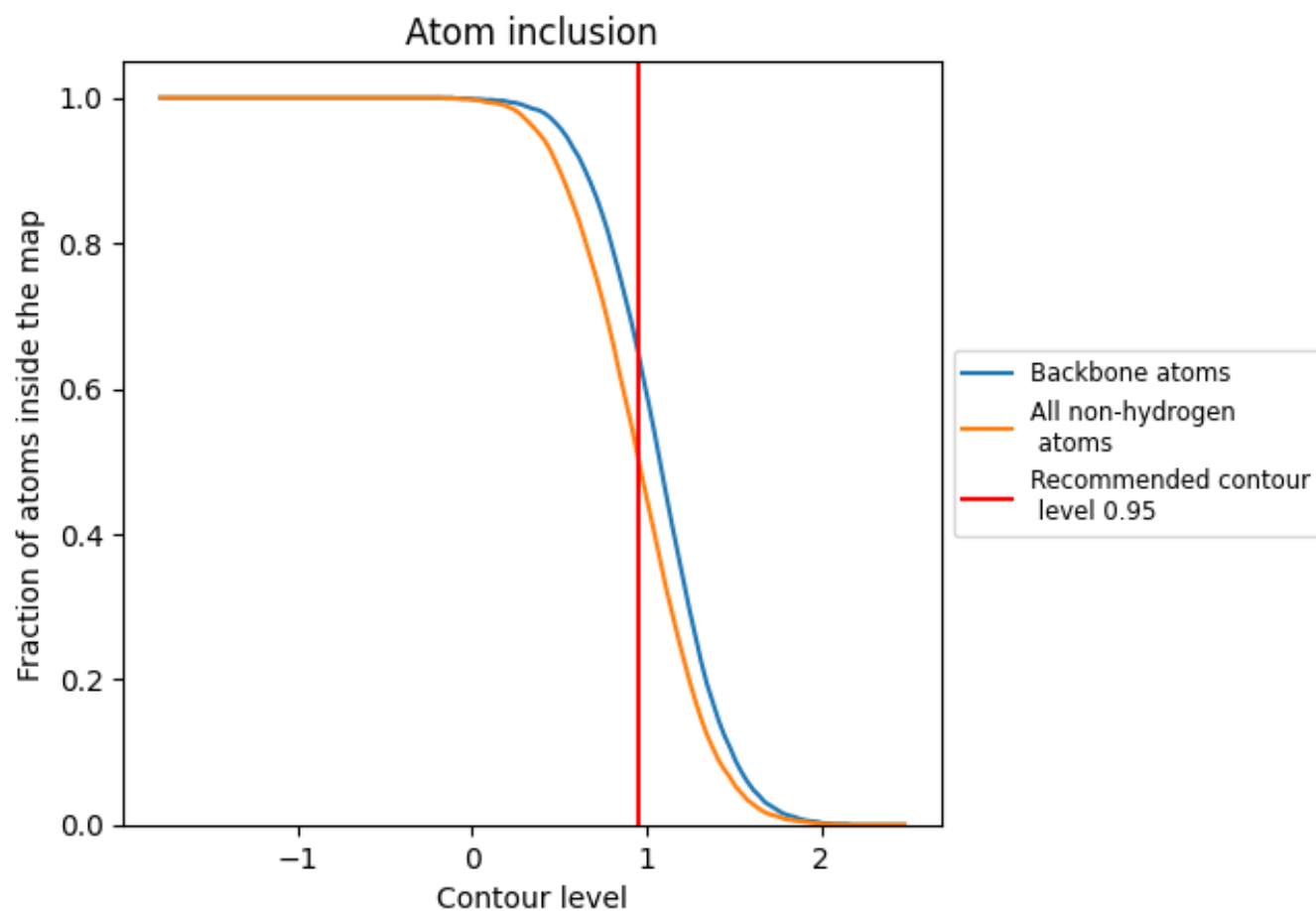
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.95).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 51% 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 (0.95) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5070	0.1510
A	0.5090	0.1500
B	0.5100	0.1480
C	0.5120	0.1510
D	0.5080	0.1520
E	0.5070	0.1550
F	0.5030	0.1500
G	0.4980	0.1500
H	0.5090	0.1520
I	0.5030	0.1510
J	0.5070	0.1510
K	0.5060	0.1510
L	0.5090	0.1490
M	0.5100	0.1540
N	0.5040	0.1530
O	0.5080	0.1490
P	0.5080	0.1530

1.0

0.0

<0.0