



wwPDB EM Validation Summary Report i

Mar 18, 2023 – 02:56 PM EDT

PDB ID : 8E2K
EMDB ID : EMD-27841
Title : Cryo-EM structure of BIRC6/HtrA2-S306A
Authors : Hunkeler, M.; Fischer, E.S.
Deposited on : 2022-08-15
Resolution : 3.21 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 i 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](#) ①) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
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) : 2.32.1

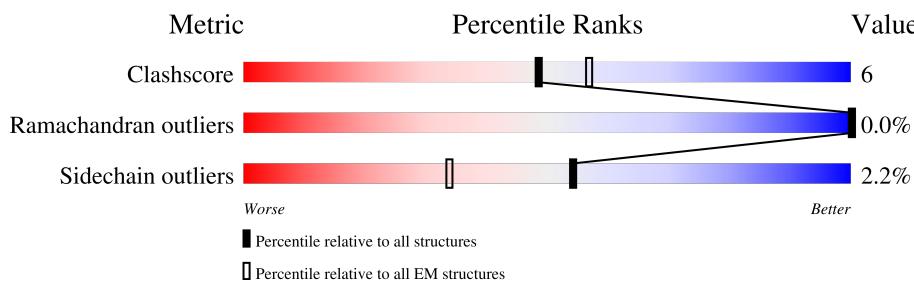
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

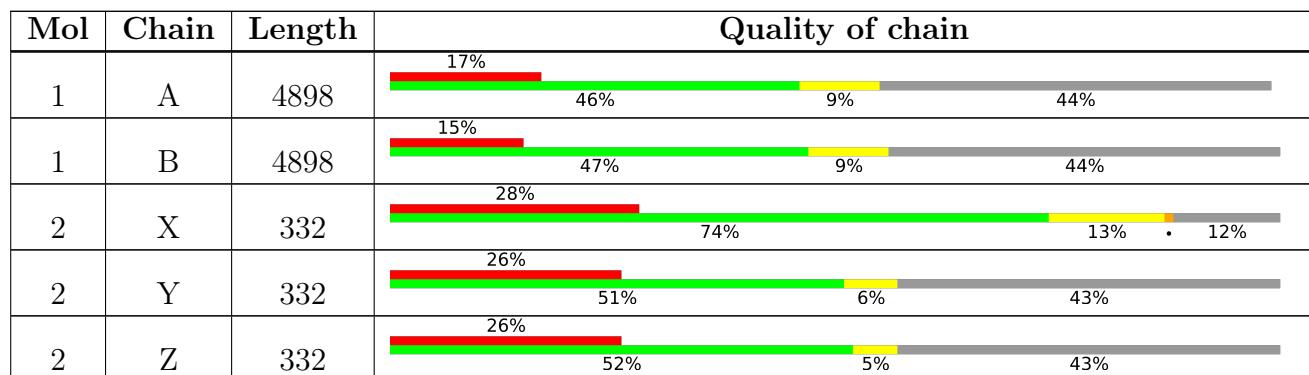
The reported resolution of this entry is 3.21 Å.

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.



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 96785 atoms, of which 48882 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 Baculoviral IAP repeat-containing protein 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	2745	43316	13710	21895	3643	3918	150	21	0
1	B	2745	43316	13710	21895	3643	3918	150	21	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	expression tag	UNP Q9NR09
A	-39	GLY	-	expression tag	UNP Q9NR09
A	-38	ASP	-	expression tag	UNP Q9NR09
A	-37	TYR	-	expression tag	UNP Q9NR09
A	-36	LYS	-	expression tag	UNP Q9NR09
A	-35	ASP	-	expression tag	UNP Q9NR09
A	-34	HIS	-	expression tag	UNP Q9NR09
A	-33	ASP	-	expression tag	UNP Q9NR09
A	-32	GLY	-	expression tag	UNP Q9NR09
A	-31	ASP	-	expression tag	UNP Q9NR09
A	-30	TYR	-	expression tag	UNP Q9NR09
A	-29	LYS	-	expression tag	UNP Q9NR09
A	-28	ASP	-	expression tag	UNP Q9NR09
A	-27	HIS	-	expression tag	UNP Q9NR09
A	-26	ASP	-	expression tag	UNP Q9NR09
A	-25	ILE	-	expression tag	UNP Q9NR09
A	-24	ASP	-	expression tag	UNP Q9NR09
A	-23	TYR	-	expression tag	UNP Q9NR09
A	-22	LYS	-	expression tag	UNP Q9NR09
A	-21	ASP	-	expression tag	UNP Q9NR09
A	-20	ASP	-	expression tag	UNP Q9NR09
A	-19	ASP	-	expression tag	UNP Q9NR09
A	-18	ASP	-	expression tag	UNP Q9NR09
A	-17	LYS	-	expression tag	UNP Q9NR09
A	-16	GLY	-	expression tag	UNP Q9NR09
A	-15	GLY	-	expression tag	UNP Q9NR09

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	GLY	-	expression tag	UNP Q9NR09
A	-13	SER	-	expression tag	UNP Q9NR09
A	-12	GLY	-	expression tag	UNP Q9NR09
A	-11	GLY	-	expression tag	UNP Q9NR09
A	-10	LEU	-	expression tag	UNP Q9NR09
A	-9	GLU	-	expression tag	UNP Q9NR09
A	-8	VAL	-	expression tag	UNP Q9NR09
A	-7	LEU	-	expression tag	UNP Q9NR09
A	-6	PHE	-	expression tag	UNP Q9NR09
A	-5	GLN	-	expression tag	UNP Q9NR09
A	-4	GLY	-	expression tag	UNP Q9NR09
A	-3	PRO	-	expression tag	UNP Q9NR09
A	-2	SER	-	expression tag	UNP Q9NR09
A	-1	ARG	-	expression tag	UNP Q9NR09
A	0	THR	-	expression tag	UNP Q9NR09
A	1332	VAL	LEU	conflict	UNP Q9NR09
B	-40	MET	-	expression tag	UNP Q9NR09
B	-39	GLY	-	expression tag	UNP Q9NR09
B	-38	ASP	-	expression tag	UNP Q9NR09
B	-37	TYR	-	expression tag	UNP Q9NR09
B	-36	LYS	-	expression tag	UNP Q9NR09
B	-35	ASP	-	expression tag	UNP Q9NR09
B	-34	HIS	-	expression tag	UNP Q9NR09
B	-33	ASP	-	expression tag	UNP Q9NR09
B	-32	GLY	-	expression tag	UNP Q9NR09
B	-31	ASP	-	expression tag	UNP Q9NR09
B	-30	TYR	-	expression tag	UNP Q9NR09
B	-29	LYS	-	expression tag	UNP Q9NR09
B	-28	ASP	-	expression tag	UNP Q9NR09
B	-27	HIS	-	expression tag	UNP Q9NR09
B	-26	ASP	-	expression tag	UNP Q9NR09
B	-25	ILE	-	expression tag	UNP Q9NR09
B	-24	ASP	-	expression tag	UNP Q9NR09
B	-23	TYR	-	expression tag	UNP Q9NR09
B	-22	LYS	-	expression tag	UNP Q9NR09
B	-21	ASP	-	expression tag	UNP Q9NR09
B	-20	ASP	-	expression tag	UNP Q9NR09
B	-19	ASP	-	expression tag	UNP Q9NR09
B	-18	ASP	-	expression tag	UNP Q9NR09
B	-17	LYS	-	expression tag	UNP Q9NR09
B	-16	GLY	-	expression tag	UNP Q9NR09
B	-15	GLY	-	expression tag	UNP Q9NR09

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	GLY	-	expression tag	UNP Q9NR09
B	-13	SER	-	expression tag	UNP Q9NR09
B	-12	GLY	-	expression tag	UNP Q9NR09
B	-11	GLY	-	expression tag	UNP Q9NR09
B	-10	LEU	-	expression tag	UNP Q9NR09
B	-9	GLU	-	expression tag	UNP Q9NR09
B	-8	VAL	-	expression tag	UNP Q9NR09
B	-7	LEU	-	expression tag	UNP Q9NR09
B	-6	PHE	-	expression tag	UNP Q9NR09
B	-5	GLN	-	expression tag	UNP Q9NR09
B	-4	GLY	-	expression tag	UNP Q9NR09
B	-3	PRO	-	expression tag	UNP Q9NR09
B	-2	SER	-	expression tag	UNP Q9NR09
B	-1	ARG	-	expression tag	UNP Q9NR09
B	0	THR	-	expression tag	UNP Q9NR09
B	1332	VAL	LEU	conflict	UNP Q9NR09

- Molecule 2 is a protein called Serine protease HTRA2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	X	292	Total	C	H	N	O	S	0	0
			4473	1405	2248	397	418	5		
2	Y	189	Total	C	H	N	O	S	0	0
			2840	897	1422	247	272	2		
2	Z	189	Total	C	H	N	O	S	0	0
			2840	897	1422	247	272	2		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	133	MET	-	initiating methionine	UNP O43464
X	306	ALA	SER	conflict	UNP O43464
X	459	HIS	-	expression tag	UNP O43464
X	460	HIS	-	expression tag	UNP O43464
X	461	HIS	-	expression tag	UNP O43464
X	462	HIS	-	expression tag	UNP O43464
X	463	HIS	-	expression tag	UNP O43464
X	464	HIS	-	expression tag	UNP O43464
Y	133	MET	-	initiating methionine	UNP O43464
Y	306	ALA	SER	conflict	UNP O43464
Y	459	HIS	-	expression tag	UNP O43464
Y	460	HIS	-	expression tag	UNP O43464

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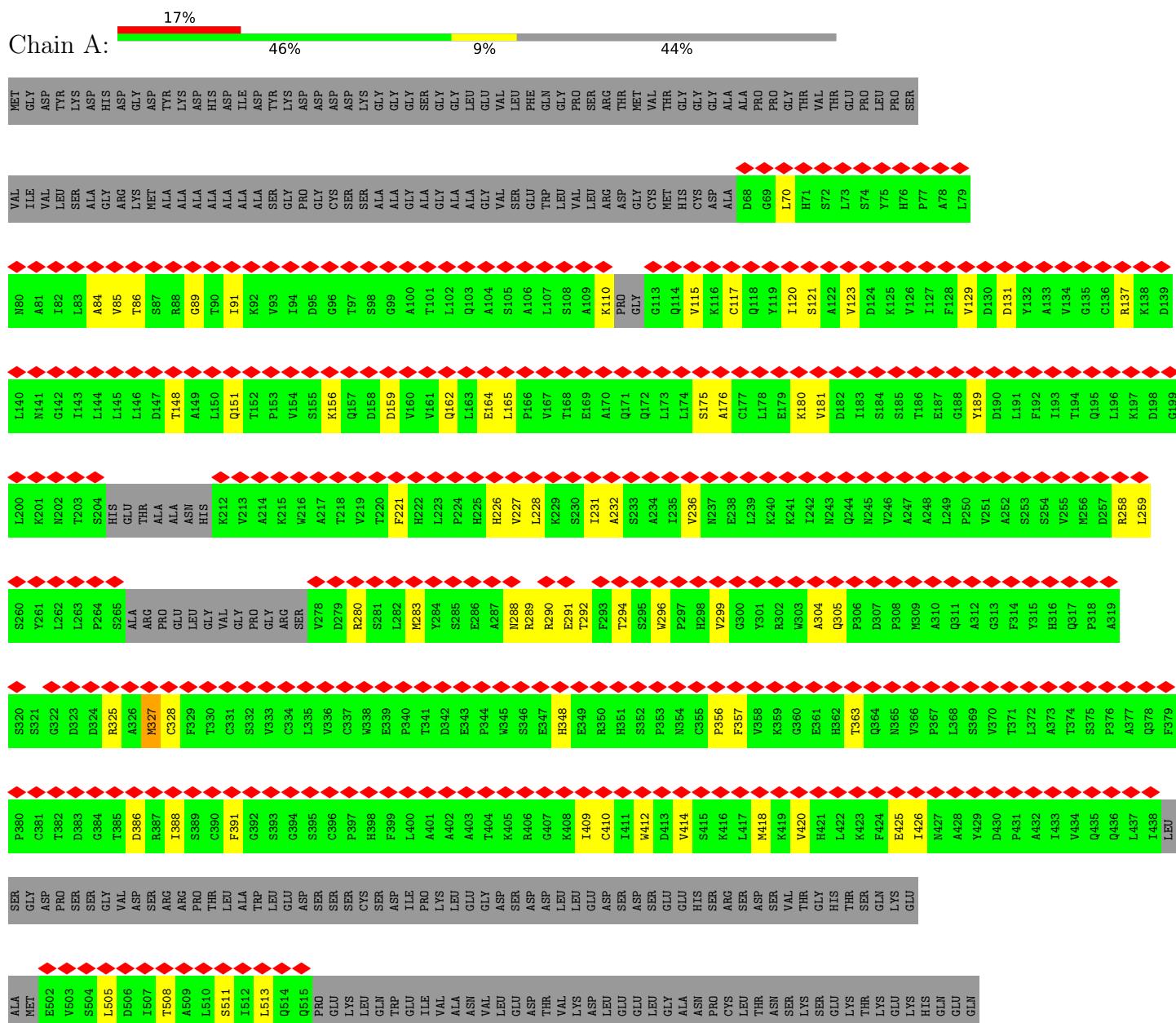
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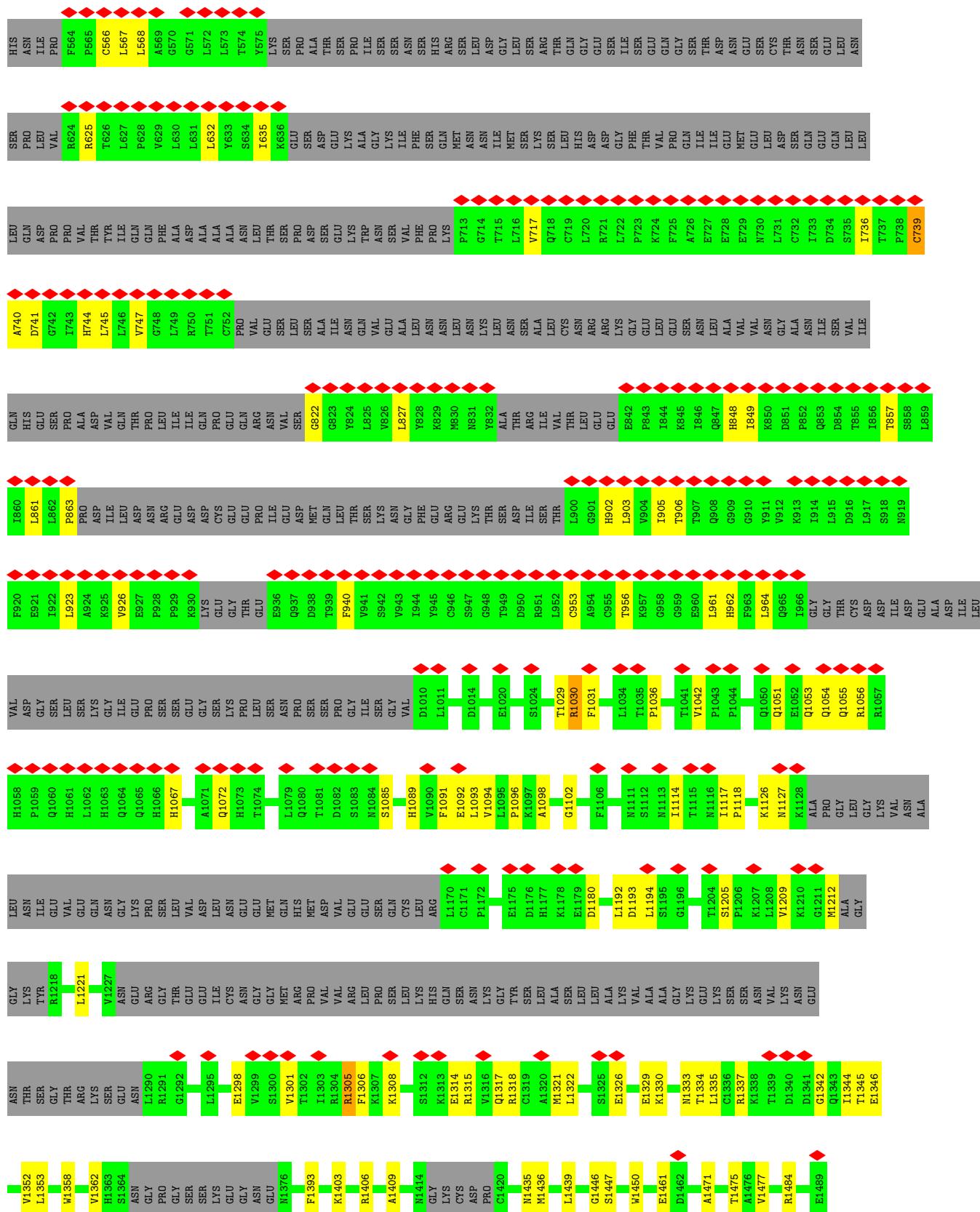
Chain	Residue	Modelled	Actual	Comment	Reference
Y	461	HIS	-	expression tag	UNP O43464
Y	462	HIS	-	expression tag	UNP O43464
Y	463	HIS	-	expression tag	UNP O43464
Y	464	HIS	-	expression tag	UNP O43464
Z	133	MET	-	initiating methionine	UNP O43464
Z	306	ALA	SER	conflict	UNP O43464
Z	459	HIS	-	expression tag	UNP O43464
Z	460	HIS	-	expression tag	UNP O43464
Z	461	HIS	-	expression tag	UNP O43464
Z	462	HIS	-	expression tag	UNP O43464
Z	463	HIS	-	expression tag	UNP O43464
Z	464	HIS	-	expression tag	UNP O43464

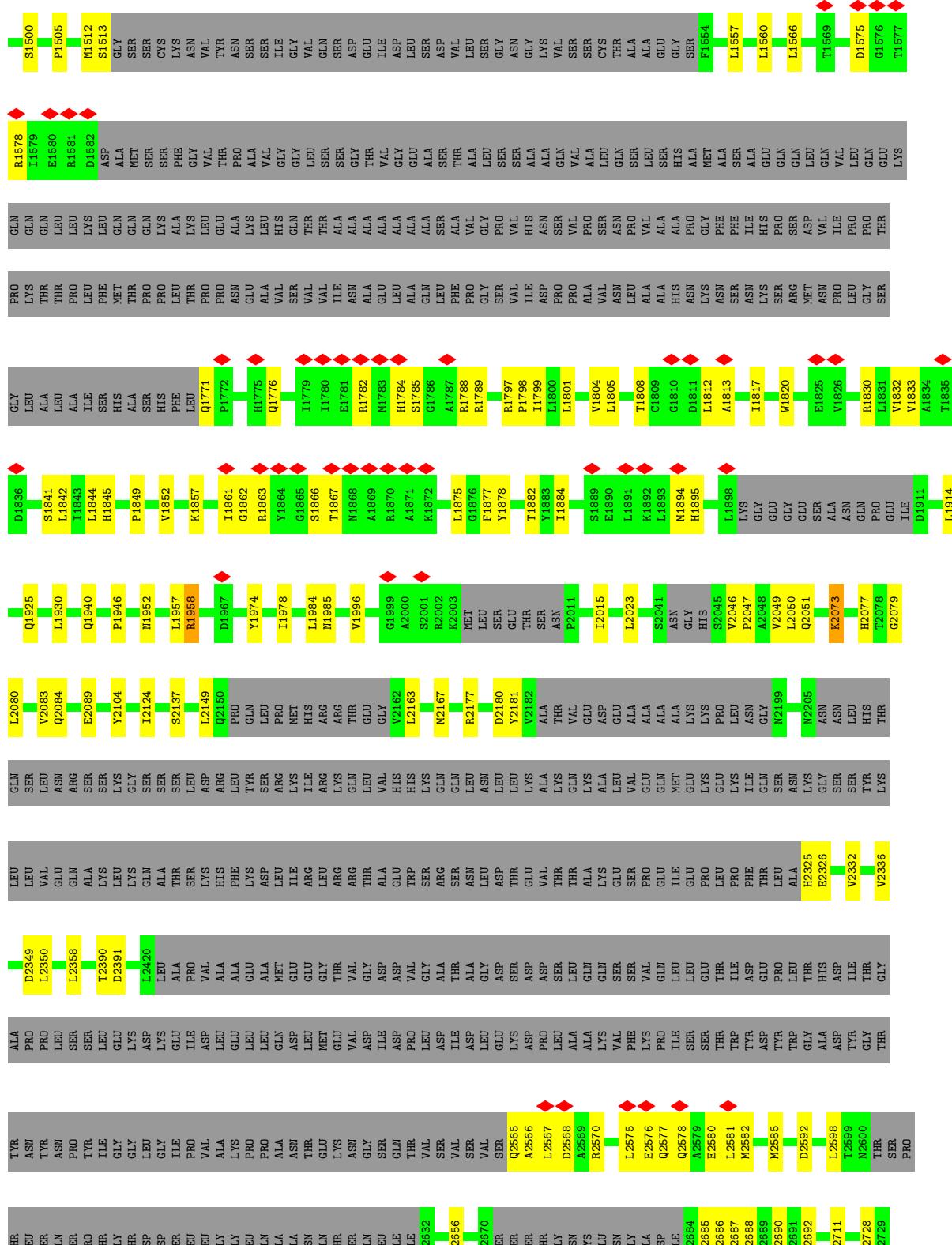
3 Residue-property plots

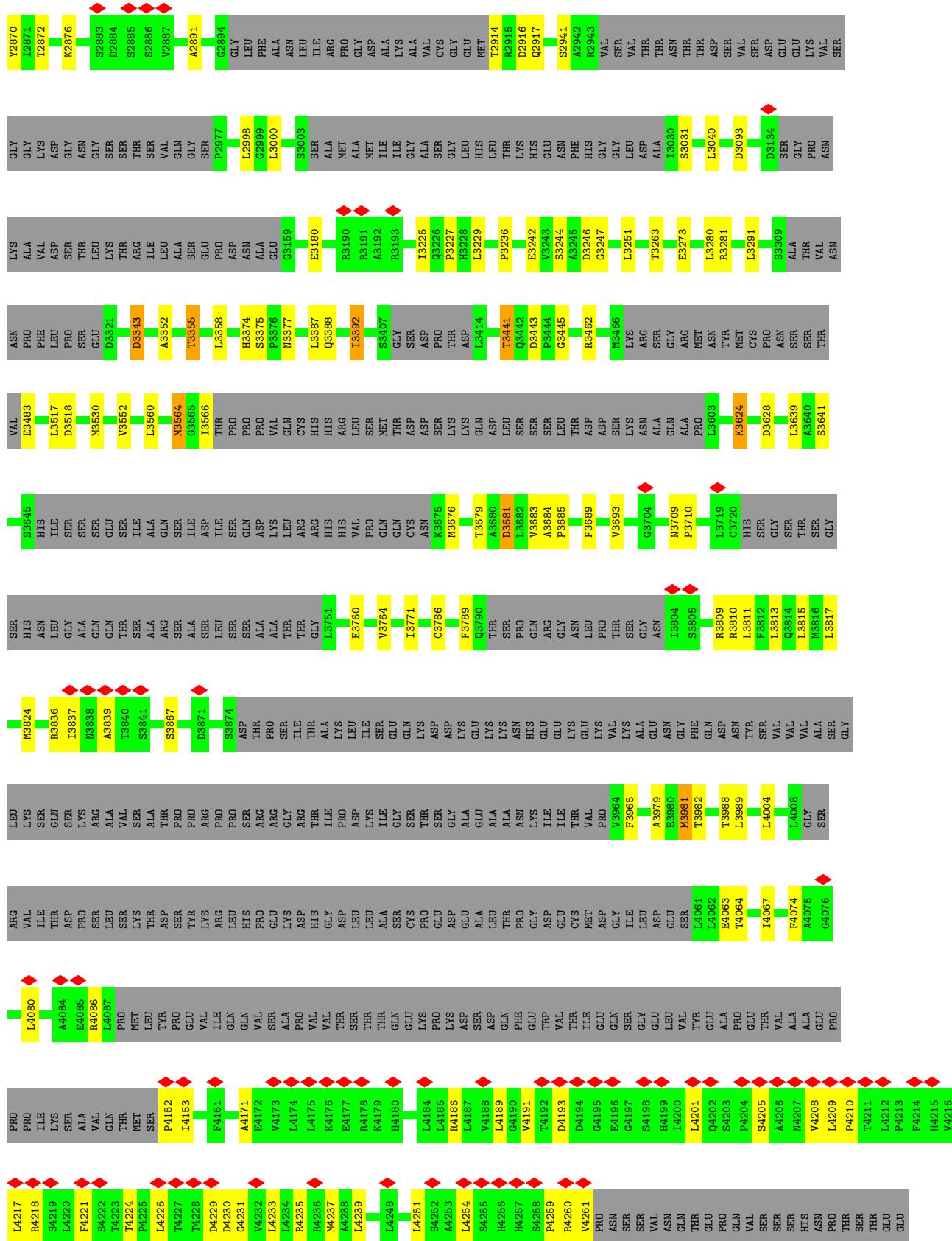
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

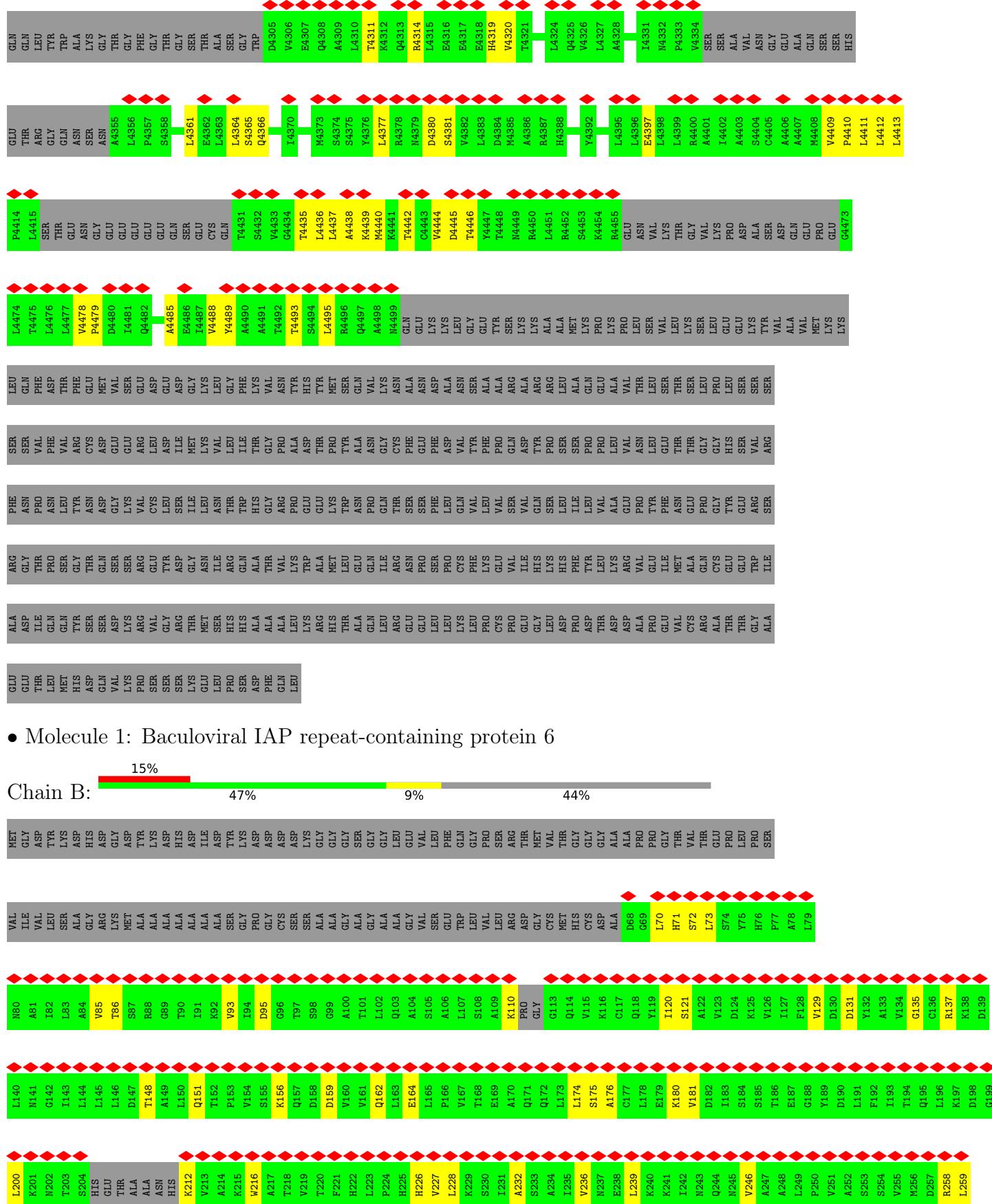
- Molecule 1: Baculoviral IAP repeat-containing protein 6

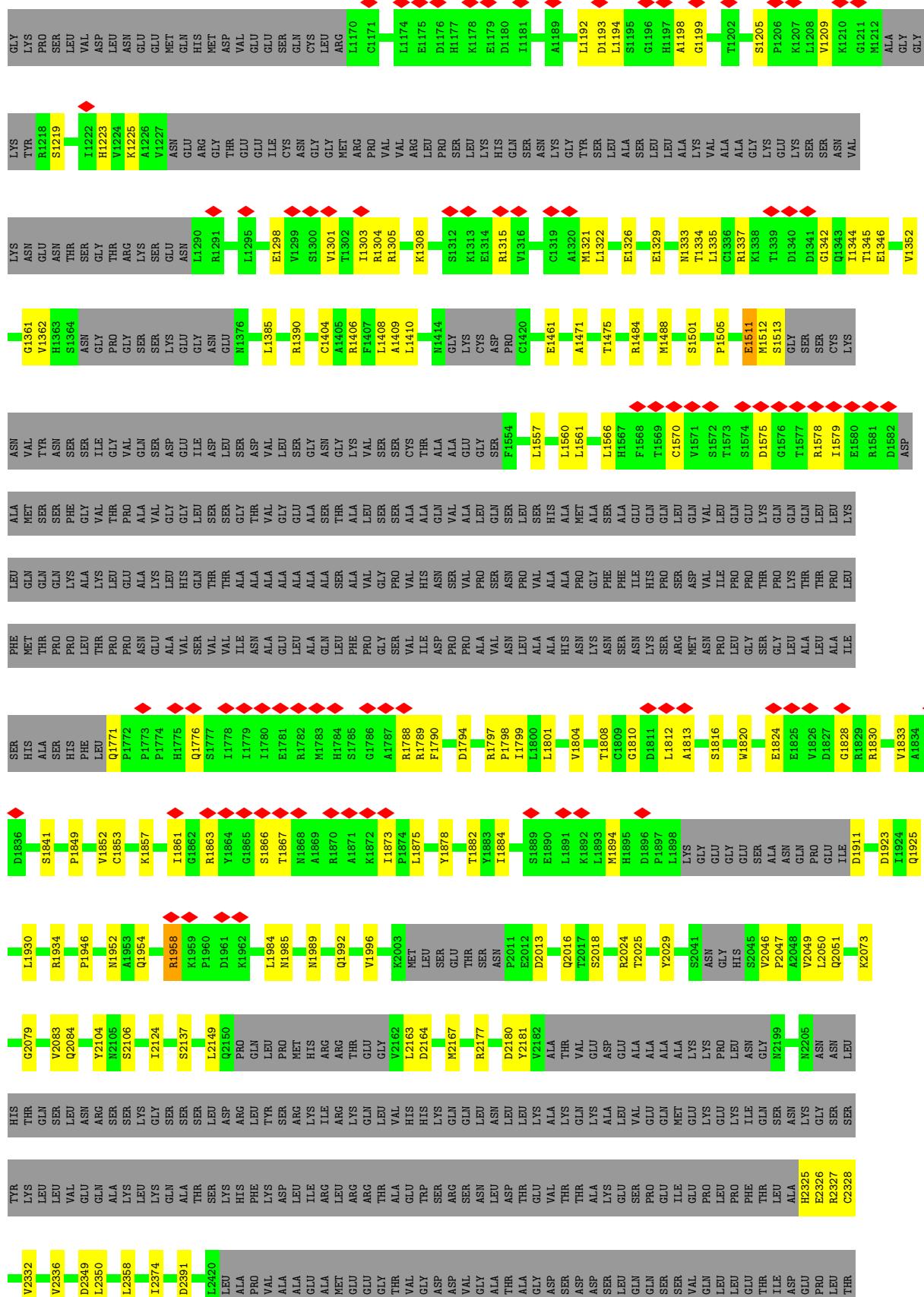


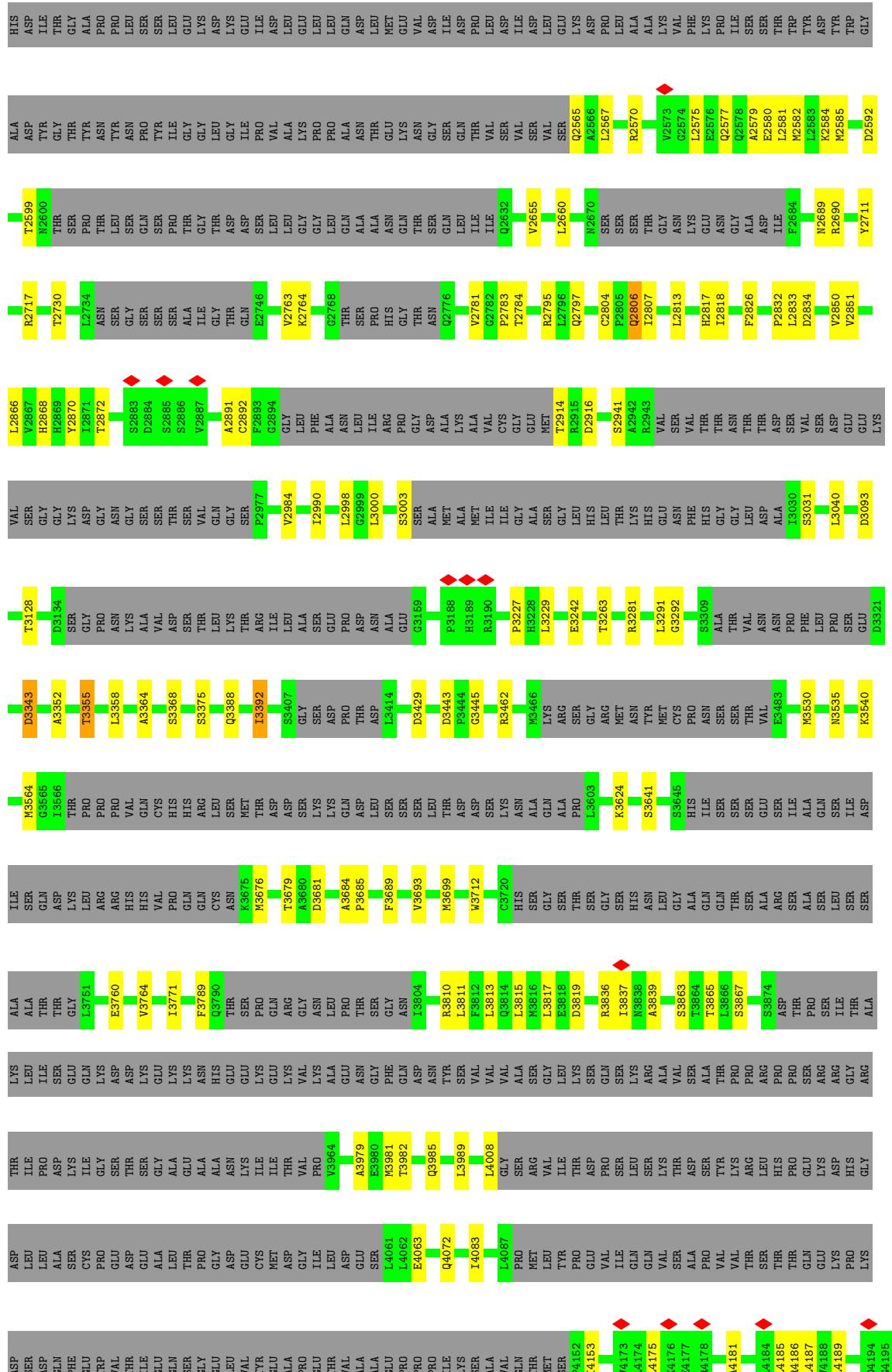


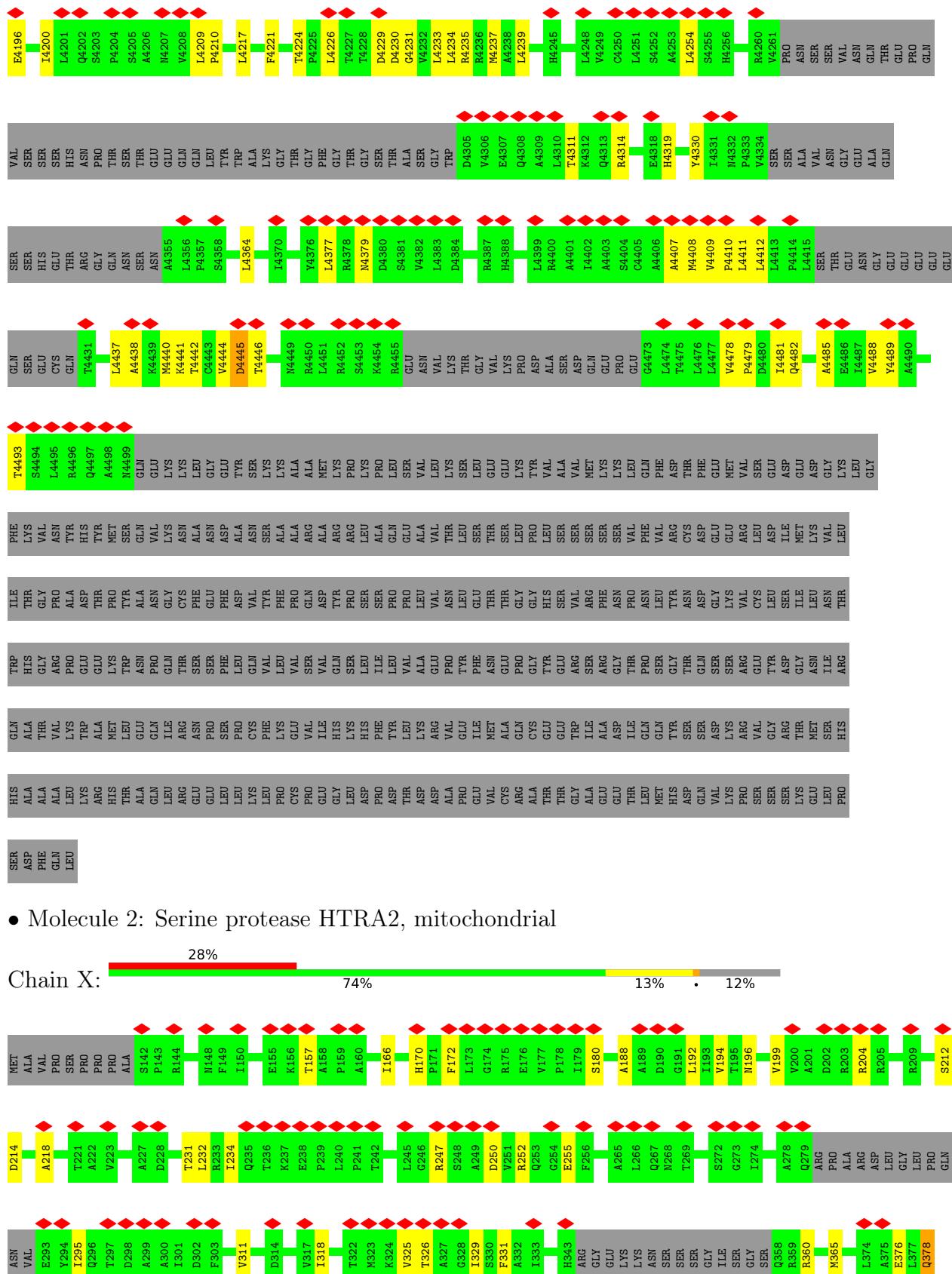


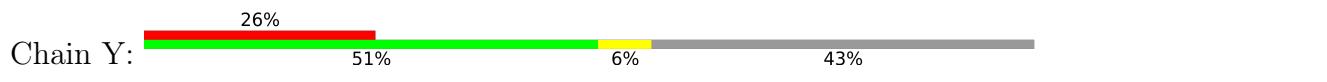






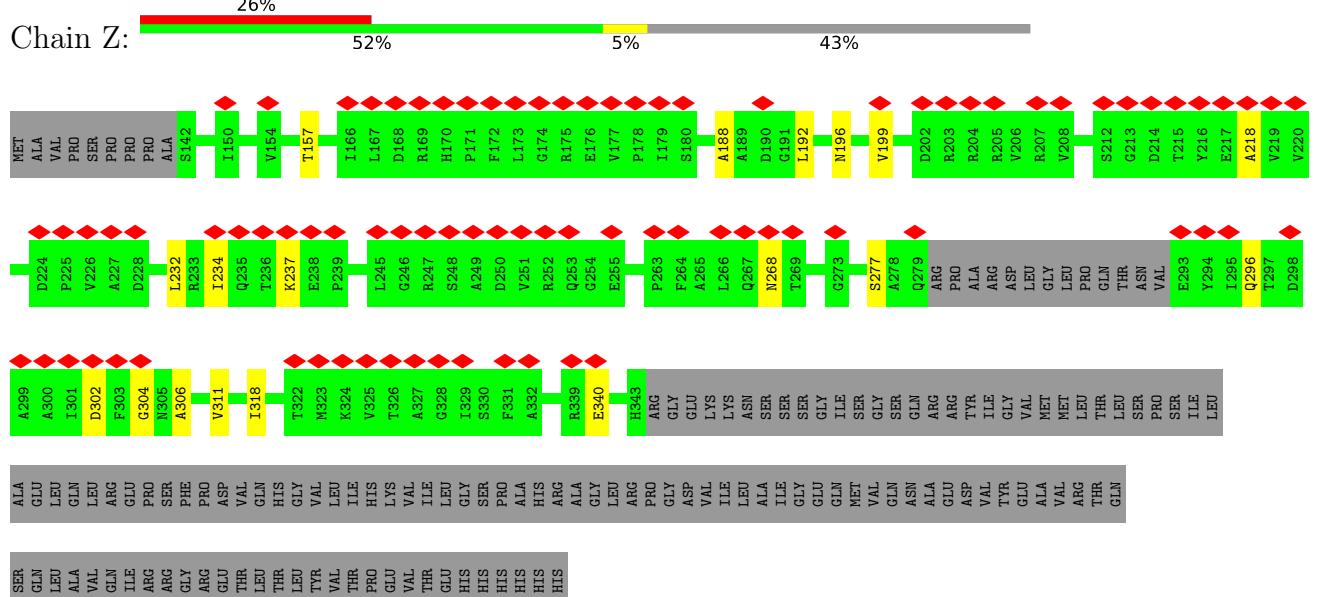






	VAL	D214	MET
THR	LEU	E293	ALA
GLU	ALA	T215	VAL
SER	Y294	Y216	PRO
VAL	PRO	E217	SER
VAL	I295	A218	PRO
ARG	E217	A218	PRO
THR	ILE	A227	P144
GLN	LEU	D228	I150
GLN	SER	T221	I150
GLN	ALA	A222	ALA
GLU	GLU	L232	S142
LEU	LEU	R233	P143
ALA	GLN	A227	P144
ALA	ALA	D228	I150
VAL	VAL	I229	ALA
GLN	GLN	L232	V154
ARG	PRO	R233	E155
ARG	SER	A227	V154
GLY	PHE	D228	E155
PHE	PRO	I229	K156
GLU	ASP	L232	K156
ASP	THR	R233	T157
GLU	VAL	K324	Q235
GLU	GLN	V325	T236
LEU	HTS	T326	K237
THR	HTS	T326	P159
GLY	TYR	V327	K156
TYR	VAL	A327	T166
VAL	LEU	G328	I167
VAL	THR	H329	D168
ILE	PRO	S330	D168
HTS	HTS	P241	R169
GLU	LYS	T242	H170
LYS	VAL	E238	P171
VAL	VAL	P239	F172
ILE	ILE	L240	L173
HTS	HTS	K237	G174
VAL	VAL	E238	D175
ILE	ILE	P239	E176
HTS	HTS	L240	F177
GLU	GLY	K237	P178
GLY	SER	E238	I179
SER	PRO	T247	N180
HTS	HTS	S248	N181
HTS	HTS	A249	V187
VAL	VAL	D250	A188
ILE	ILE	V251	A189
HTS	HTS	R252	D190
HTS	HTS	F253	G191
GLY	GLY	E340	L192
GLY	ALA	F256	V275
ALA	ALA	F256	S276
GLY	GLY	F254	V200
ASP	ASP	A295	A201
GLU	VAL	L266	D202
LYS	LYS	Q267	R203
ILE	ILE	N268	R204
ASN	ASN	T269	R205
ALA	ALA	I270	V206
ARG	ARG	T269	R207
GLU	GLU	I270	V208
GLN	GLN	S276	R209
GLY	GLY	V275	G210
ILE	ILE	S276	L211
VAL	VAL	V275	S212
SER	SER	S276	C213
GLN	GLN	V275	
ASN	ASN	S276	
ALA	ALA	V275	
ARG	ARG	S276	
GLU	GLU	V275	
TYR	TYR	S276	
ASP	ASP	V275	
GLU	GLU	S276	
GLN	GLN	V275	
THR	THR	S276	
ASN	ASN	V275	

- Molecule 2: Serine protease HTRA2, mitochondrial



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	73712	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.659	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.384	Depositor
Minimum map value	-0.530	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.215	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality [\(i\)](#)

5.1 Standard geometry [\(i\)](#)

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	0.28	0/21893	0.49	0/29721
1	B	0.28	0/21893	0.50	0/29721
2	X	0.28	0/2263	0.56	0/3082
2	Y	0.27	0/1442	0.56	0/1967
2	Z	0.27	0/1442	0.56	0/1967
All	All	0.28	0/48933	0.50	0/66458

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	21421	21895	21819	301	0
1	B	21421	21895	21819	268	0
2	X	2225	2248	2250	28	0
2	Y	1418	1422	1424	13	0
2	Z	1418	1422	1424	12	0
All	All	47903	48882	48736	603	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 6.

The worst 5 of 603 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:A:3817:LEU:HD11	1:A:4189:LEU:HD12	1.35	1.05
1:B:1194:LEU:HD13	1:B:2565:GLN:N	1.83	0.93
1:A:3813:LEU:HD23	1:A:3817:LEU:HD12	1.52	0.92
1:A:3374:HIS:N	2:X:381:GLU:OE2	2.04	0.90
1:A:3374:HIS:ND1	2:X:381:GLU:OE1	2.05	0.89

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	2668/4898 (54%)	2615 (98%)	53 (2%)	0	100 100
1	B	2668/4898 (54%)	2616 (98%)	52 (2%)	0	100 100
2	X	286/332 (86%)	270 (94%)	15 (5%)	1 (0%)	41 74
2	Y	185/332 (56%)	178 (96%)	7 (4%)	0	100 100
2	Z	185/332 (56%)	178 (96%)	7 (4%)	0	100 100
All	All	5992/10792 (56%)	5857 (98%)	134 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	X	381	GLU

5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2440/4249 (57%)	2382 (98%)	58 (2%)	49	76
1	B	2440/4249 (57%)	2386 (98%)	54 (2%)	52	78
2	X	241/276 (87%)	234 (97%)	7 (3%)	42	72
2	Y	153/276 (55%)	152 (99%)	1 (1%)	84	93
2	Z	153/276 (55%)	151 (99%)	2 (1%)	69	86
All	All	5427/9326 (58%)	5305 (98%)	122 (2%)	54	78

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4445	ASP
1	B	4379	ASN
1	B	1315	ARG
1	B	4239	LEU
2	X	387	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1895	HIS
1	B	2565	GLN
2	X	378	GLN
1	A	1845	HIS
1	A	1840	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 [\(i\)](#)

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.

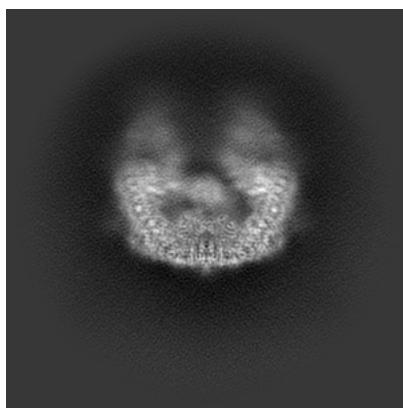
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-27841. These allow visual inspection of the internal detail of the map and identification of artifacts.

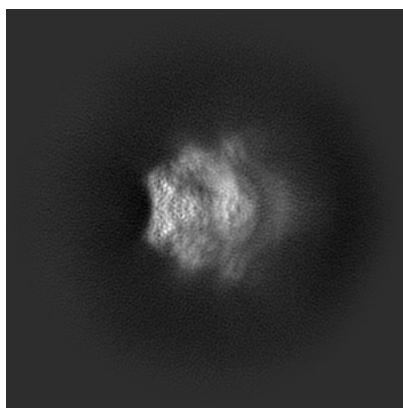
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

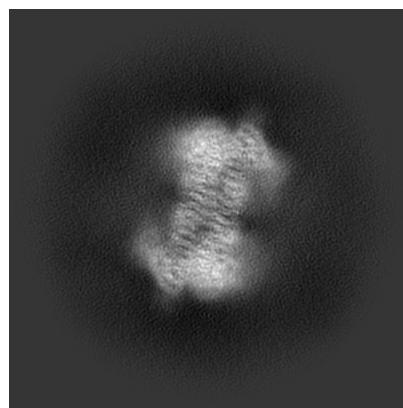
6.1.1 Primary map



X

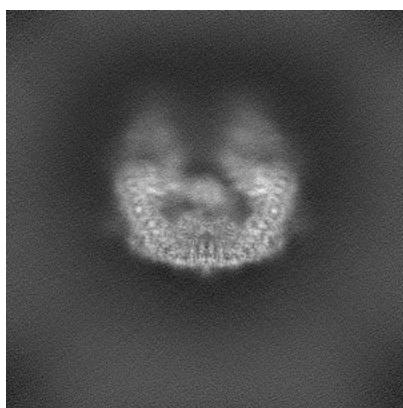


Y

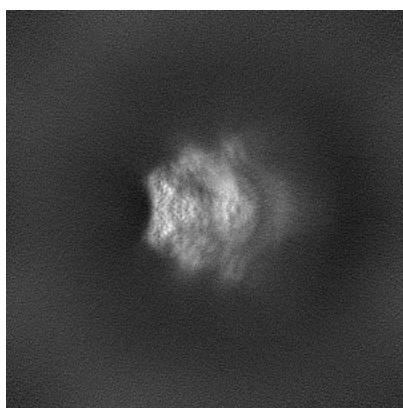


Z

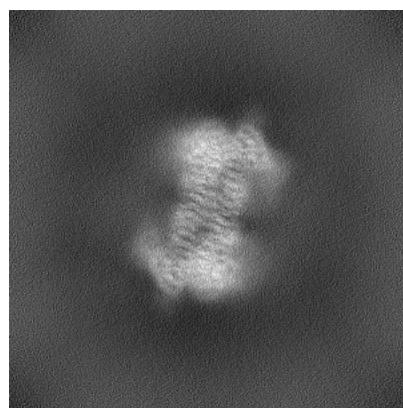
6.1.2 Raw map



X



Y

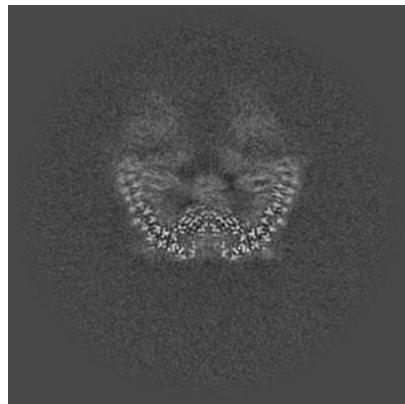


Z

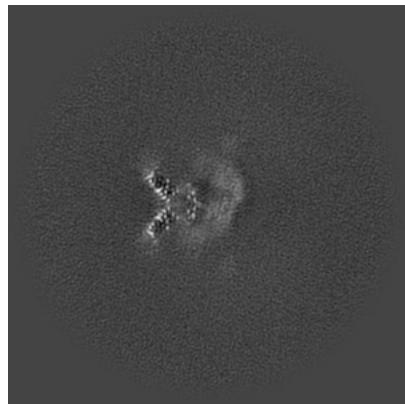
The images above show the map projected in three orthogonal directions.

6.2 Central slices [\(i\)](#)

6.2.1 Primary map



X Index: 176

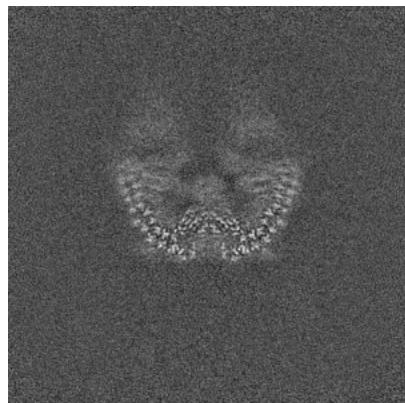


Y Index: 176

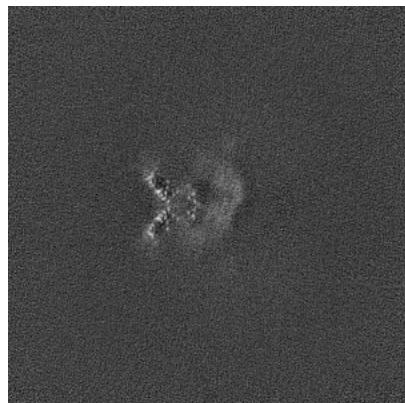


Z Index: 176

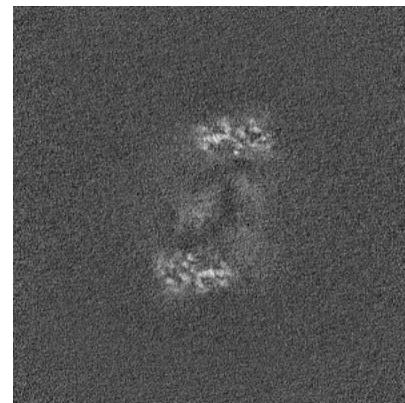
6.2.2 Raw map



X Index: 176



Y Index: 176

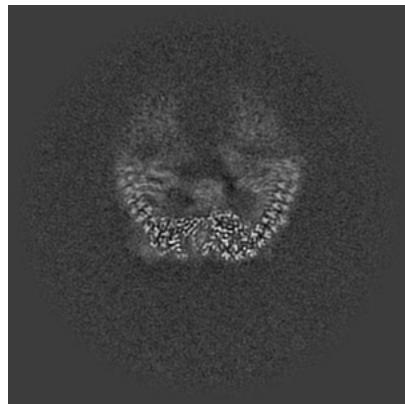


Z Index: 176

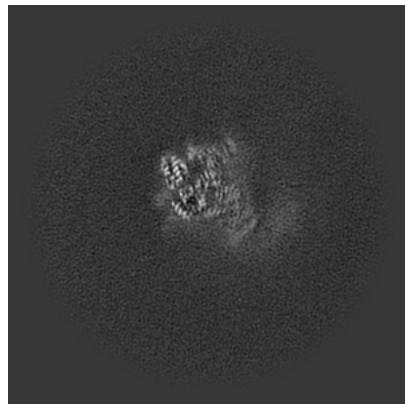
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

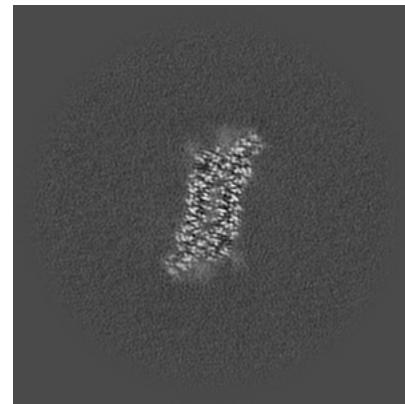
6.3.1 Primary map



X Index: 172

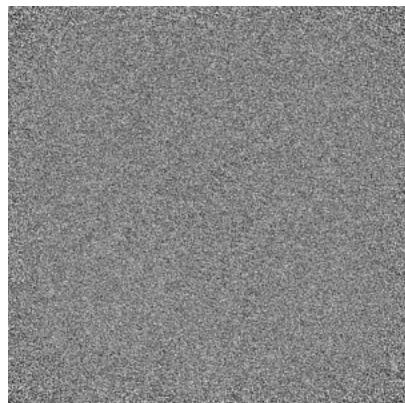


Y Index: 229

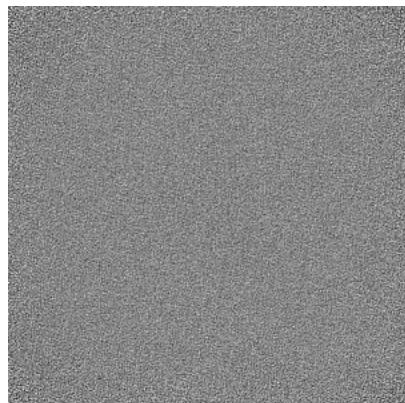


Z Index: 139

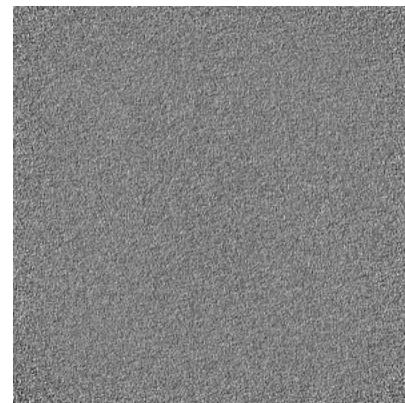
6.3.2 Raw map



X Index: 0



Y Index: 0

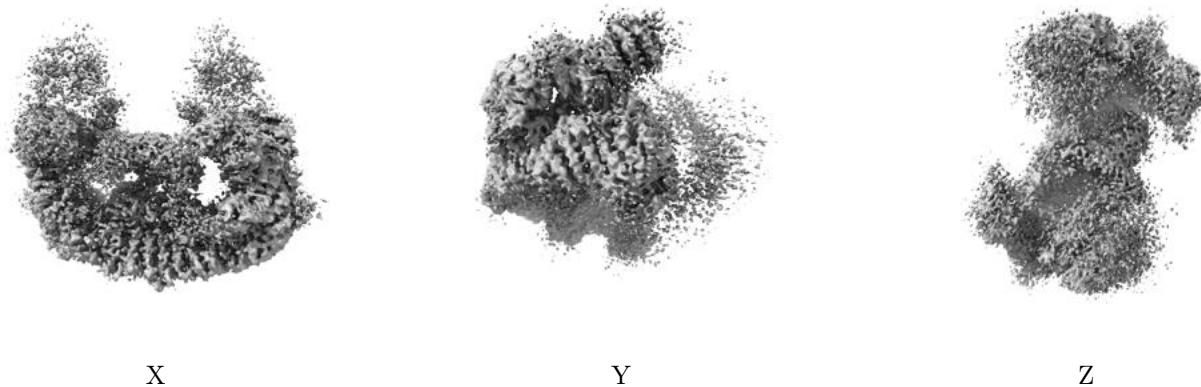


Z Index: 0

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

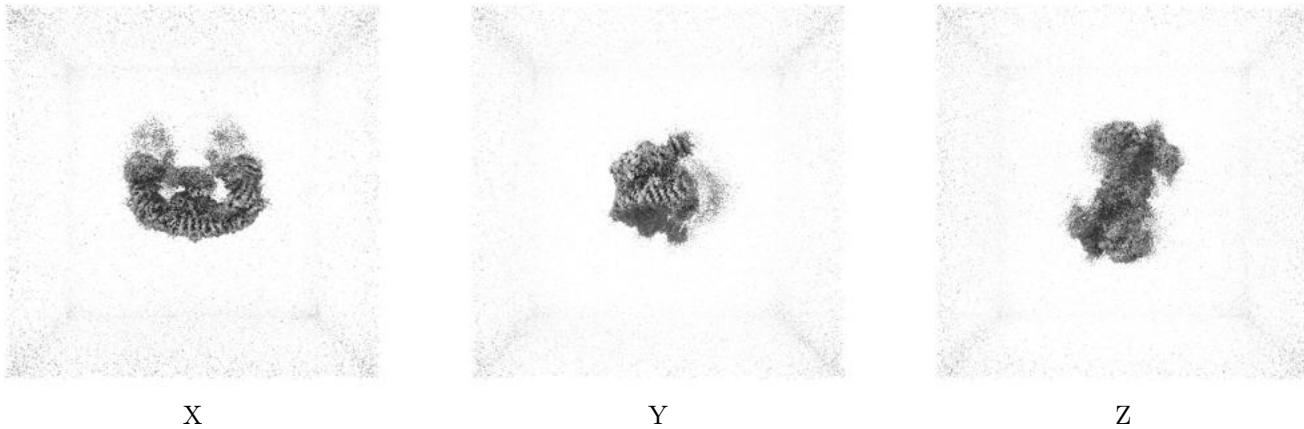
6.4 Orthogonal surface views [\(i\)](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.215. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

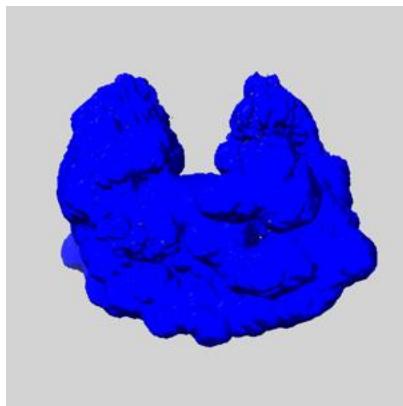
6.5 Mask visualisation [\(i\)](#)

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

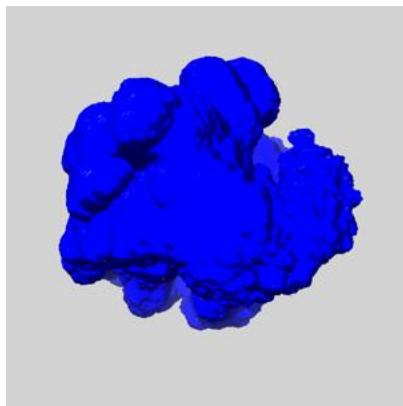
A mask typically either:

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

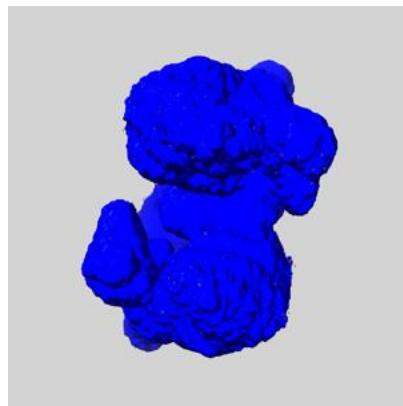
6.5.1 emd_27841_msk_1.map [\(i\)](#)



X

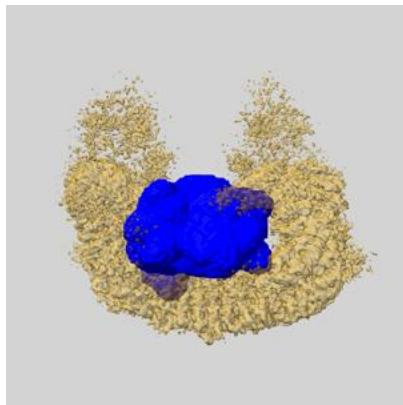


Y

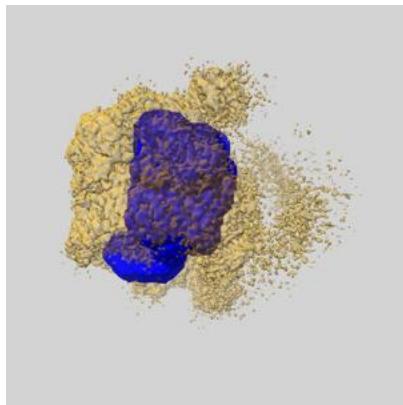


Z

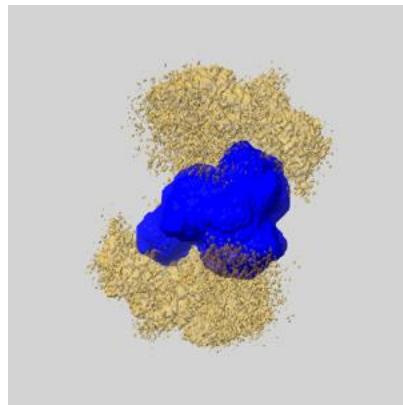
6.5.2 emd_27841_msk_2.map [\(i\)](#)



X



Y

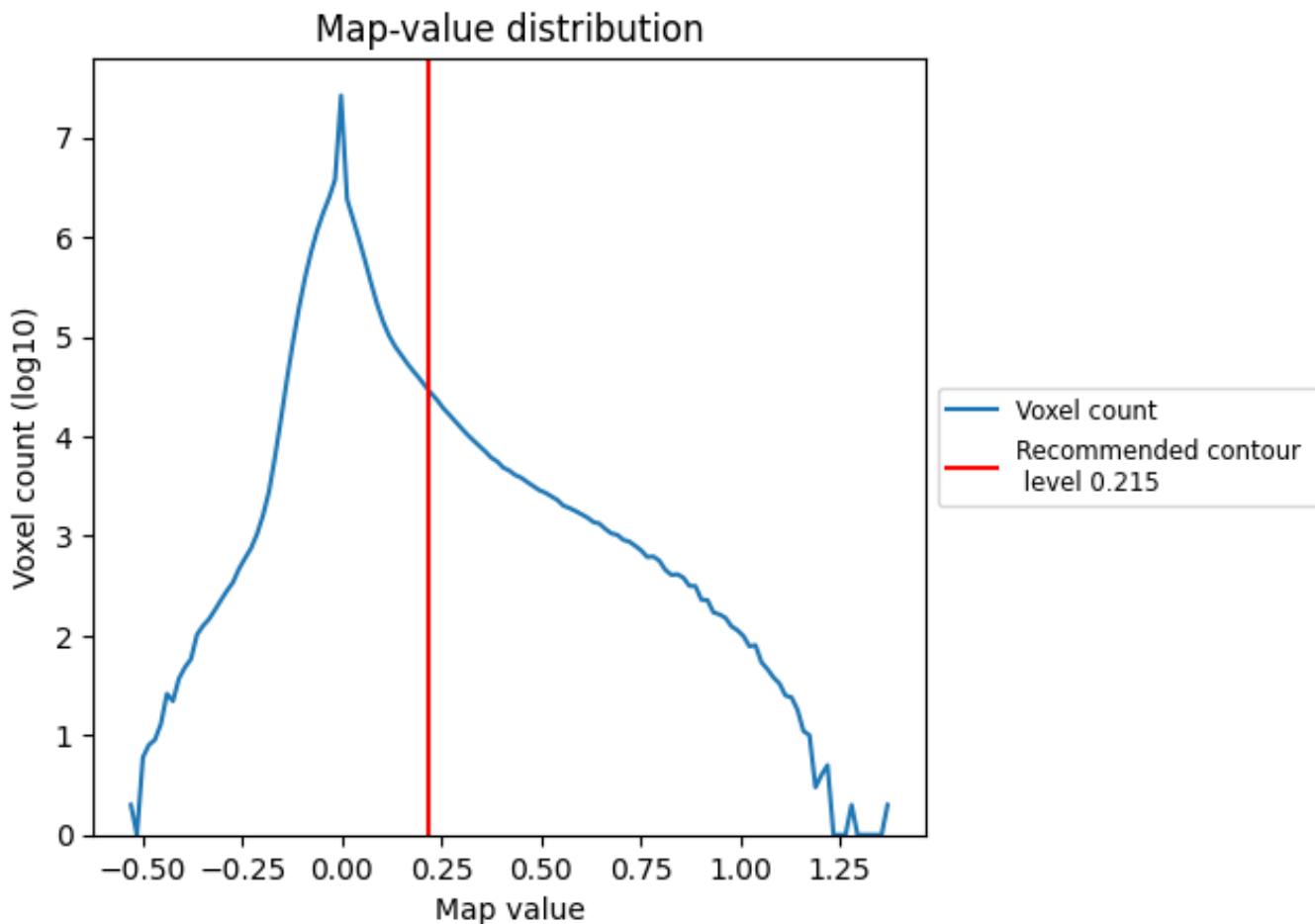


Z

7 Map analysis (i)

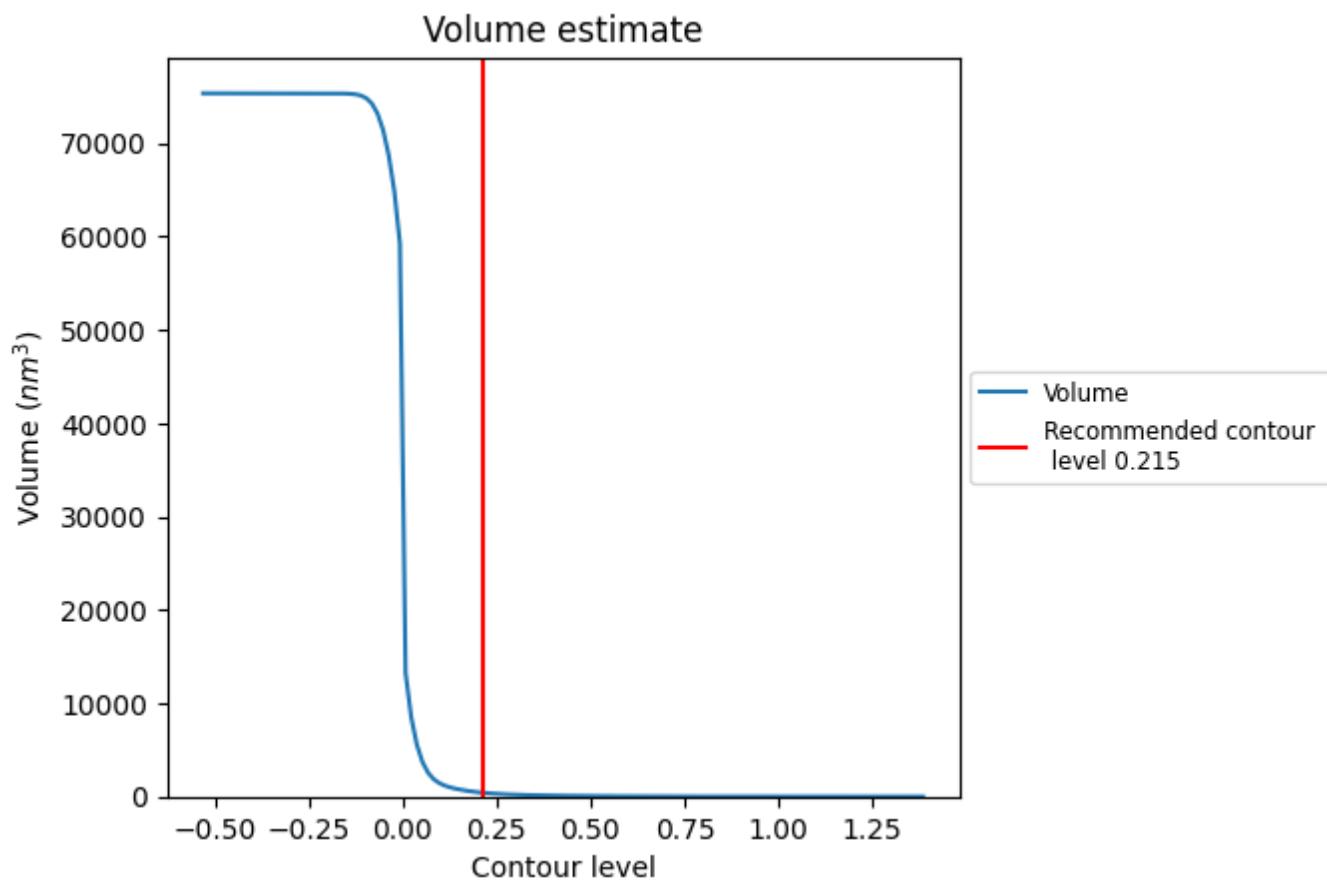
This section contains the results of statistical analysis of the map.

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.

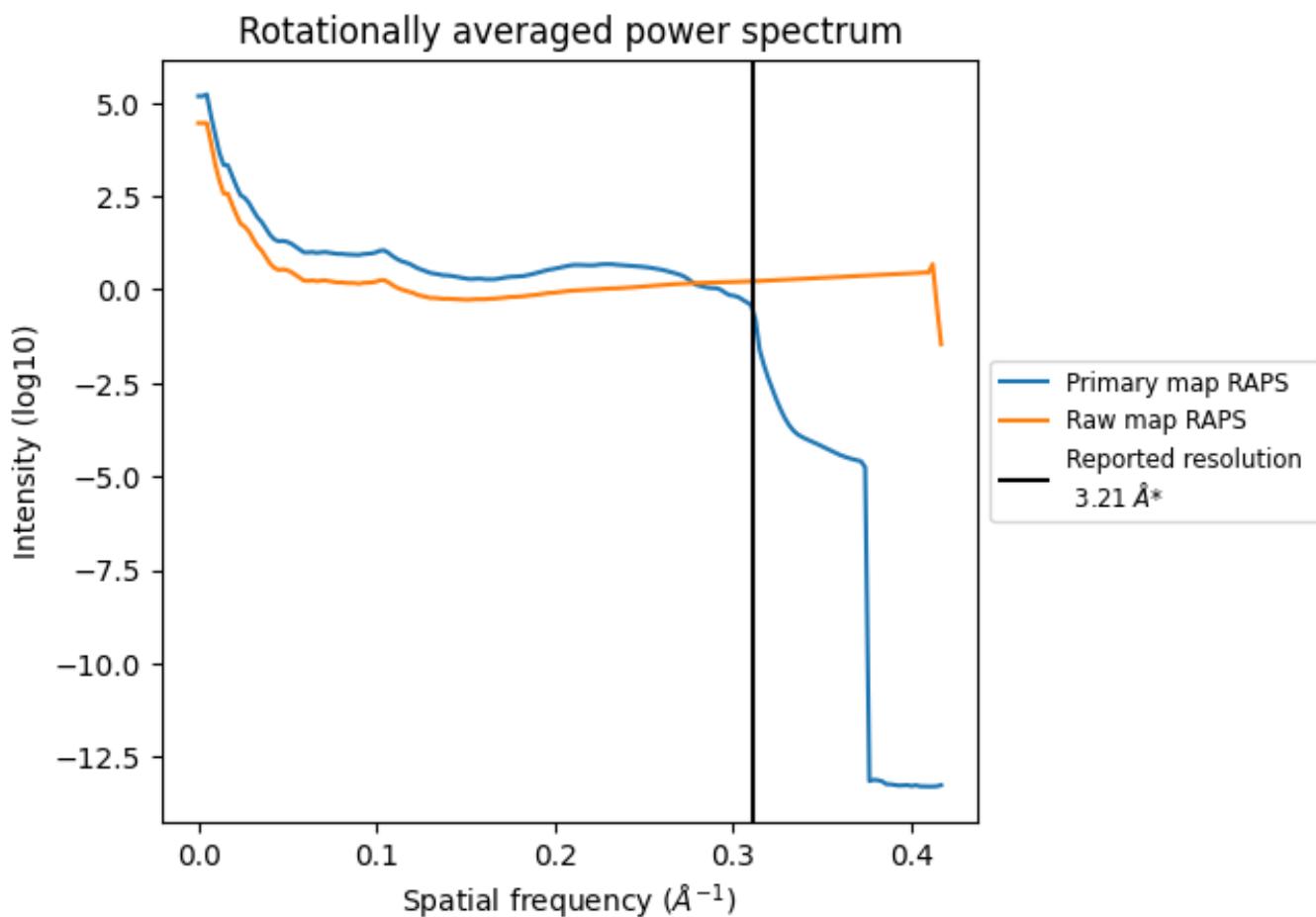
7.2 Volume estimate (i)



The volume at the recommended contour level is 405 nm^3 ; this corresponds to an approximate mass of 366 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 [\(i\)](#)

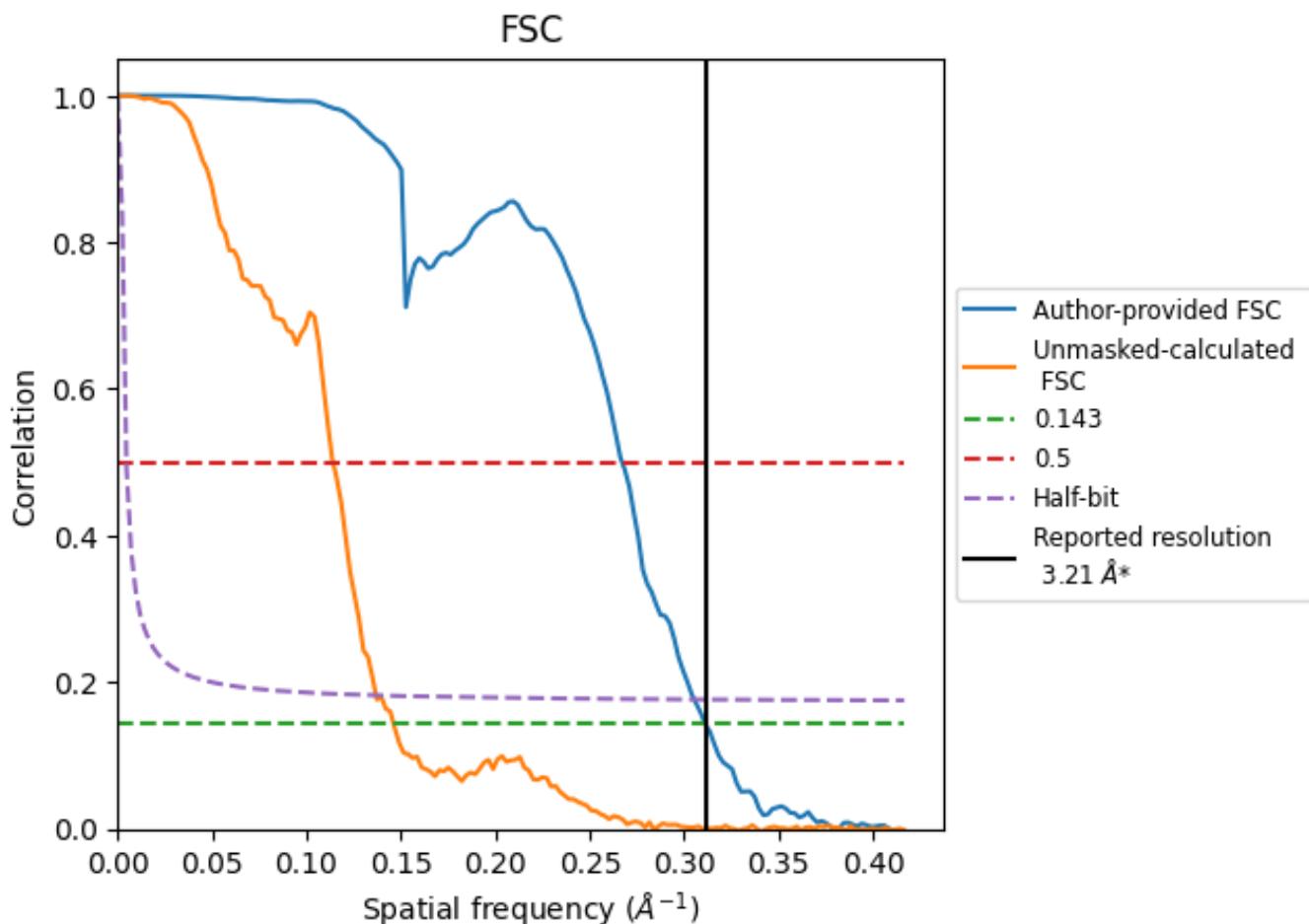


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

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 0.312 \AA^{-1}

8.2 Resolution estimates [\(i\)](#)

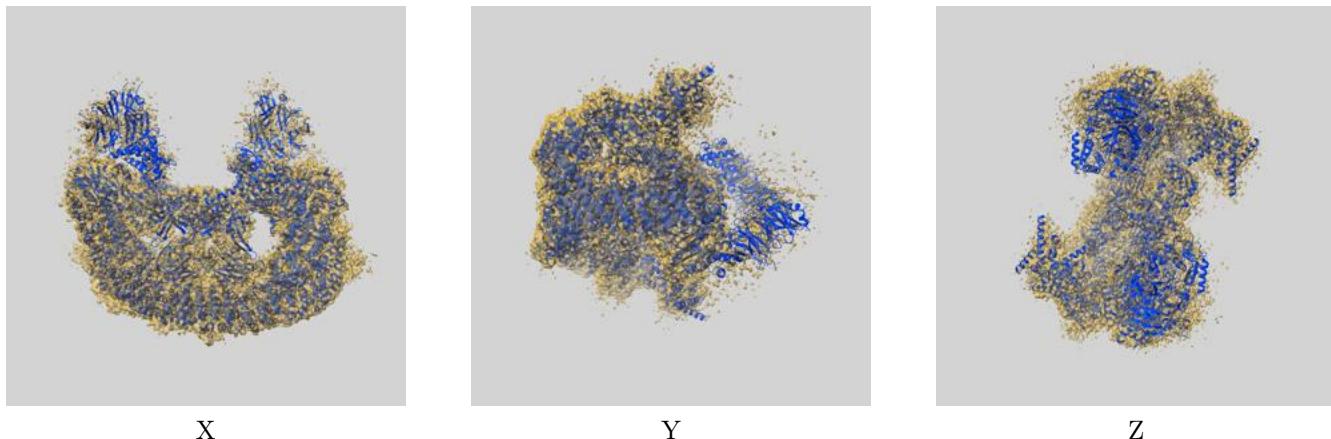
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	3.21	3.74	3.27
Unmasked-calculated*	6.84	8.76	7.30

*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 6.84 differs from the reported value 3.21 by more than 10 %

9 Map-model fit (i)

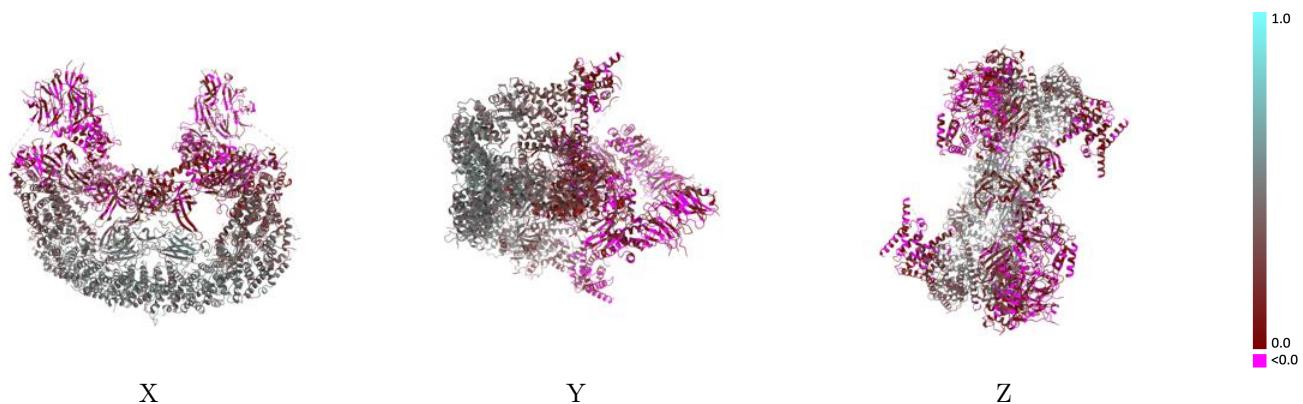
This section contains information regarding the fit between EMDB map EMD-27841 and PDB model 8E2K. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay (i)



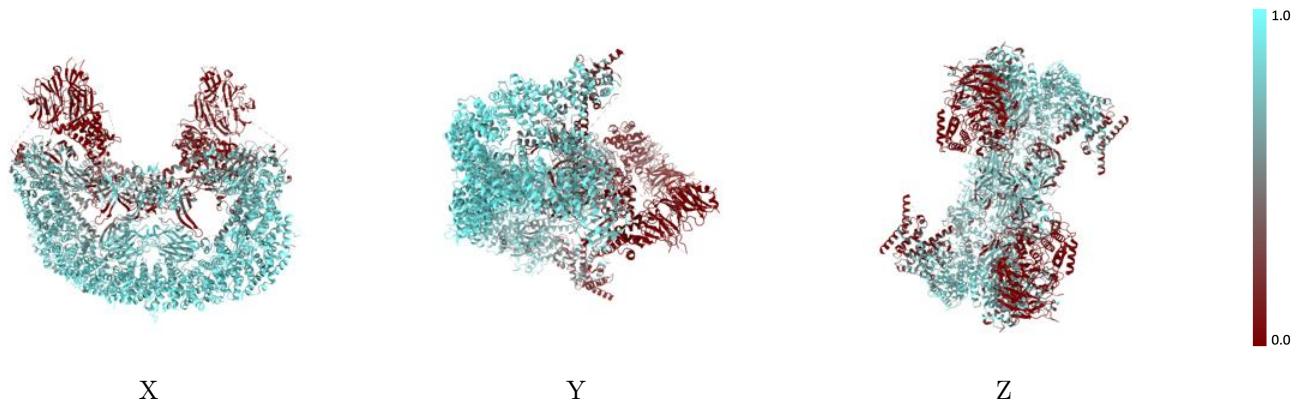
The images above show the 3D surface view of the map at the recommended contour level 0.215 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



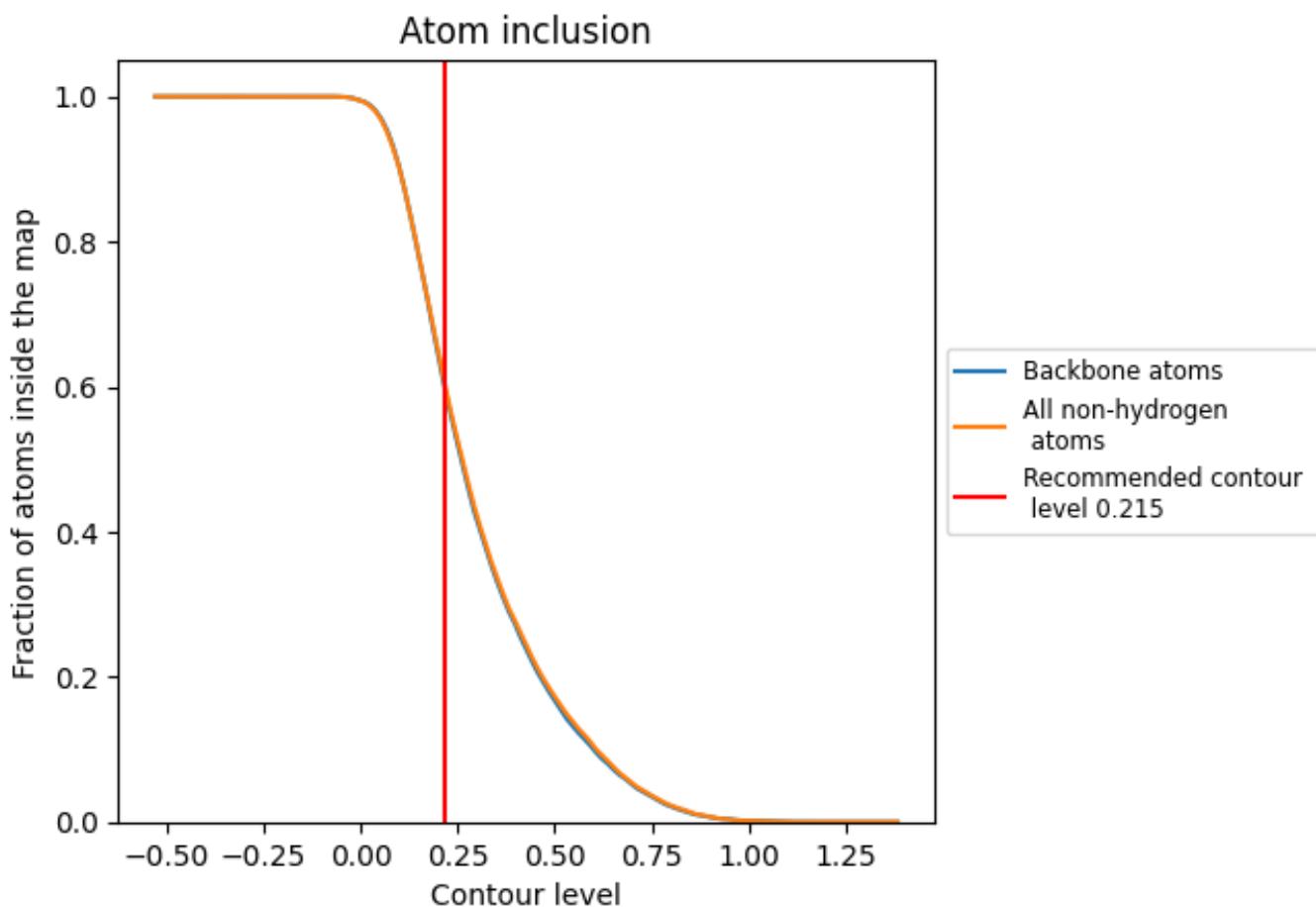
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.215).

9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 60% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [\(i\)](#)

The table lists the average atom inclusion at the recommended contour level (0.215) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6076	0.2770
A	0.6220	0.2830
B	0.6387	0.2890
X	0.5487	0.2640
Y	0.4590	0.1440
Z	0.4612	0.1690

