



wwPDB EM Validation Summary Report i

Apr 23, 2024 – 01:17 am BST

PDB ID : 6ZXK
EMDB ID : EMD-11523
Title : Fully-loaded anthrax lethal toxin in its heptameric pre-pore state and PA7LF(2+1B) arrangement
Authors : Quentin, D.; Antoni, C.; Gatsogiannis, C.; Raunser, S.
Deposited on : 2020-07-29
Resolution : 3.80 Å(reported)
Based on initial model : 6ZXJ

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:

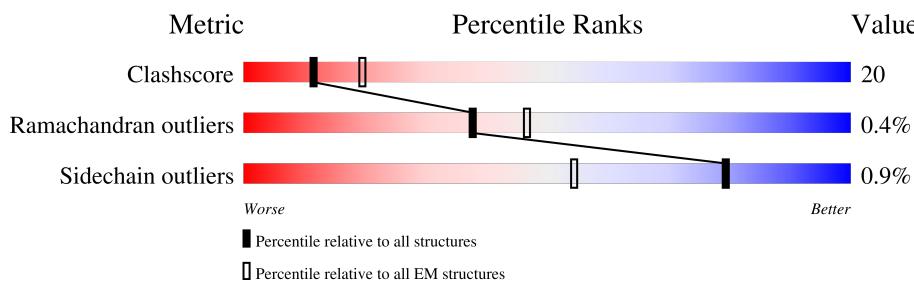
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance

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

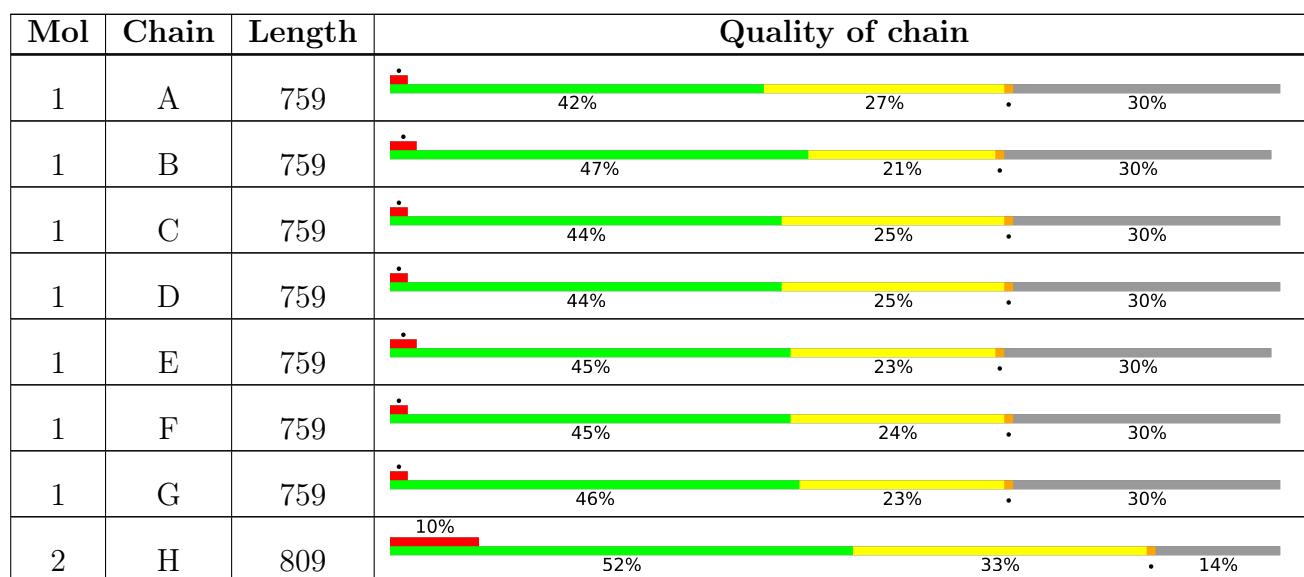
The reported resolution of this entry is 3.80 Å.

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.



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Mol	Chain	Length	Quality of chain				
2	I	809	37%	69%	18%	•	12%
2	J	809	50%	65%	16%	•	18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 42292 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 Protective antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	529	Total	C	N	O	S	0	0
			3984	2495	694	791	4		
1	B	529	Total	C	N	O	S	0	0
			3977	2488	692	793	4		
1	C	529	Total	C	N	O	S	0	0
			3977	2488	692	793	4		
1	D	528	Total	C	N	O	S	0	0
			3970	2483	691	792	4		
1	E	529	Total	C	N	O	S	0	0
			3977	2488	692	793	4		
1	F	529	Total	C	N	O	S	0	0
			3977	2488	692	793	4		
1	G	529	Total	C	N	O	S	0	0
			3977	2488	692	793	4		

There are 161 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP Q68GS1
A	-22	GLY	-	expression tag	UNP Q68GS1
A	-21	HIS	-	expression tag	UNP Q68GS1
A	-20	HIS	-	expression tag	UNP Q68GS1
A	-19	HIS	-	expression tag	UNP Q68GS1
A	-18	HIS	-	expression tag	UNP Q68GS1
A	-17	HIS	-	expression tag	UNP Q68GS1
A	-16	HIS	-	expression tag	UNP Q68GS1
A	-15	HIS	-	expression tag	UNP Q68GS1
A	-14	HIS	-	expression tag	UNP Q68GS1
A	-13	HIS	-	expression tag	UNP Q68GS1
A	-12	HIS	-	expression tag	UNP Q68GS1
A	-11	SER	-	expression tag	UNP Q68GS1
A	-10	SER	-	expression tag	UNP Q68GS1
A	-9	GLY	-	expression tag	UNP Q68GS1
A	-8	HIS	-	expression tag	UNP Q68GS1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ILE	-	expression tag	UNP Q68GS1
A	-6	ASP	-	expression tag	UNP Q68GS1
A	-5	ASP	-	expression tag	UNP Q68GS1
A	-4	ASP	-	expression tag	UNP Q68GS1
A	-3	ASP	-	expression tag	UNP Q68GS1
A	-2	LYS	-	expression tag	UNP Q68GS1
A	-1	HIS	-	expression tag	UNP Q68GS1
B	-23	MET	-	initiating methionine	UNP Q68GS1
B	-22	GLY	-	expression tag	UNP Q68GS1
B	-21	HIS	-	expression tag	UNP Q68GS1
B	-20	HIS	-	expression tag	UNP Q68GS1
B	-19	HIS	-	expression tag	UNP Q68GS1
B	-18	HIS	-	expression tag	UNP Q68GS1
B	-17	HIS	-	expression tag	UNP Q68GS1
B	-16	HIS	-	expression tag	UNP Q68GS1
B	-15	HIS	-	expression tag	UNP Q68GS1
B	-14	HIS	-	expression tag	UNP Q68GS1
B	-13	HIS	-	expression tag	UNP Q68GS1
B	-12	HIS	-	expression tag	UNP Q68GS1
B	-11	SER	-	expression tag	UNP Q68GS1
B	-10	SER	-	expression tag	UNP Q68GS1
B	-9	GLY	-	expression tag	UNP Q68GS1
B	-8	HIS	-	expression tag	UNP Q68GS1
B	-7	ILE	-	expression tag	UNP Q68GS1
B	-6	ASP	-	expression tag	UNP Q68GS1
B	-5	ASP	-	expression tag	UNP Q68GS1
B	-4	ASP	-	expression tag	UNP Q68GS1
B	-3	ASP	-	expression tag	UNP Q68GS1
B	-2	LYS	-	expression tag	UNP Q68GS1
B	-1	HIS	-	expression tag	UNP Q68GS1
C	-23	MET	-	initiating methionine	UNP Q68GS1
C	-22	GLY	-	expression tag	UNP Q68GS1
C	-21	HIS	-	expression tag	UNP Q68GS1
C	-20	HIS	-	expression tag	UNP Q68GS1
C	-19	HIS	-	expression tag	UNP Q68GS1
C	-18	HIS	-	expression tag	UNP Q68GS1
C	-17	HIS	-	expression tag	UNP Q68GS1
C	-16	HIS	-	expression tag	UNP Q68GS1
C	-15	HIS	-	expression tag	UNP Q68GS1
C	-14	HIS	-	expression tag	UNP Q68GS1
C	-13	HIS	-	expression tag	UNP Q68GS1
C	-12	HIS	-	expression tag	UNP Q68GS1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	SER	-	expression tag	UNP Q68GS1
C	-10	SER	-	expression tag	UNP Q68GS1
C	-9	GLY	-	expression tag	UNP Q68GS1
C	-8	HIS	-	expression tag	UNP Q68GS1
C	-7	ILE	-	expression tag	UNP Q68GS1
C	-6	ASP	-	expression tag	UNP Q68GS1
C	-5	ASP	-	expression tag	UNP Q68GS1
C	-4	ASP	-	expression tag	UNP Q68GS1
C	-3	ASP	-	expression tag	UNP Q68GS1
C	-2	LYS	-	expression tag	UNP Q68GS1
C	-1	HIS	-	expression tag	UNP Q68GS1
D	-23	MET	-	initiating methionine	UNP Q68GS1
D	-22	GLY	-	expression tag	UNP Q68GS1
D	-21	HIS	-	expression tag	UNP Q68GS1
D	-20	HIS	-	expression tag	UNP Q68GS1
D	-19	HIS	-	expression tag	UNP Q68GS1
D	-18	HIS	-	expression tag	UNP Q68GS1
D	-17	HIS	-	expression tag	UNP Q68GS1
D	-16	HIS	-	expression tag	UNP Q68GS1
D	-15	HIS	-	expression tag	UNP Q68GS1
D	-14	HIS	-	expression tag	UNP Q68GS1
D	-13	HIS	-	expression tag	UNP Q68GS1
D	-12	HIS	-	expression tag	UNP Q68GS1
D	-11	SER	-	expression tag	UNP Q68GS1
D	-10	SER	-	expression tag	UNP Q68GS1
D	-9	GLY	-	expression tag	UNP Q68GS1
D	-8	HIS	-	expression tag	UNP Q68GS1
D	-7	ILE	-	expression tag	UNP Q68GS1
D	-6	ASP	-	expression tag	UNP Q68GS1
D	-5	ASP	-	expression tag	UNP Q68GS1
D	-4	ASP	-	expression tag	UNP Q68GS1
D	-3	ASP	-	expression tag	UNP Q68GS1
D	-2	LYS	-	expression tag	UNP Q68GS1
D	-1	HIS	-	expression tag	UNP Q68GS1
E	-23	MET	-	initiating methionine	UNP Q68GS1
E	-22	GLY	-	expression tag	UNP Q68GS1
E	-21	HIS	-	expression tag	UNP Q68GS1
E	-20	HIS	-	expression tag	UNP Q68GS1
E	-19	HIS	-	expression tag	UNP Q68GS1
E	-18	HIS	-	expression tag	UNP Q68GS1
E	-17	HIS	-	expression tag	UNP Q68GS1
E	-16	HIS	-	expression tag	UNP Q68GS1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	HIS	-	expression tag	UNP Q68GS1
E	-14	HIS	-	expression tag	UNP Q68GS1
E	-13	HIS	-	expression tag	UNP Q68GS1
E	-12	HIS	-	expression tag	UNP Q68GS1
E	-11	SER	-	expression tag	UNP Q68GS1
E	-10	SER	-	expression tag	UNP Q68GS1
E	-9	GLY	-	expression tag	UNP Q68GS1
E	-8	HIS	-	expression tag	UNP Q68GS1
E	-7	ILE	-	expression tag	UNP Q68GS1
E	-6	ASP	-	expression tag	UNP Q68GS1
E	-5	ASP	-	expression tag	UNP Q68GS1
E	-4	ASP	-	expression tag	UNP Q68GS1
E	-3	ASP	-	expression tag	UNP Q68GS1
E	-2	LYS	-	expression tag	UNP Q68GS1
E	-1	HIS	-	expression tag	UNP Q68GS1
F	-23	MET	-	initiating methionine	UNP Q68GS1
F	-22	GLY	-	expression tag	UNP Q68GS1
F	-21	HIS	-	expression tag	UNP Q68GS1
F	-20	HIS	-	expression tag	UNP Q68GS1
F	-19	HIS	-	expression tag	UNP Q68GS1
F	-18	HIS	-	expression tag	UNP Q68GS1
F	-17	HIS	-	expression tag	UNP Q68GS1
F	-16	HIS	-	expression tag	UNP Q68GS1
F	-15	HIS	-	expression tag	UNP Q68GS1
F	-14	HIS	-	expression tag	UNP Q68GS1
F	-13	HIS	-	expression tag	UNP Q68GS1
F	-12	HIS	-	expression tag	UNP Q68GS1
F	-11	SER	-	expression tag	UNP Q68GS1
F	-10	SER	-	expression tag	UNP Q68GS1
F	-9	GLY	-	expression tag	UNP Q68GS1
F	-8	HIS	-	expression tag	UNP Q68GS1
F	-7	ILE	-	expression tag	UNP Q68GS1
F	-6	ASP	-	expression tag	UNP Q68GS1
F	-5	ASP	-	expression tag	UNP Q68GS1
F	-4	ASP	-	expression tag	UNP Q68GS1
F	-3	ASP	-	expression tag	UNP Q68GS1
F	-2	LYS	-	expression tag	UNP Q68GS1
F	-1	HIS	-	expression tag	UNP Q68GS1
G	-23	MET	-	initiating methionine	UNP Q68GS1
G	-22	GLY	-	expression tag	UNP Q68GS1
G	-21	HIS	-	expression tag	UNP Q68GS1
G	-20	HIS	-	expression tag	UNP Q68GS1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-19	HIS	-	expression tag	UNP Q68GS1
G	-18	HIS	-	expression tag	UNP Q68GS1
G	-17	HIS	-	expression tag	UNP Q68GS1
G	-16	HIS	-	expression tag	UNP Q68GS1
G	-15	HIS	-	expression tag	UNP Q68GS1
G	-14	HIS	-	expression tag	UNP Q68GS1
G	-13	HIS	-	expression tag	UNP Q68GS1
G	-12	HIS	-	expression tag	UNP Q68GS1
G	-11	SER	-	expression tag	UNP Q68GS1
G	-10	SER	-	expression tag	UNP Q68GS1
G	-9	GLY	-	expression tag	UNP Q68GS1
G	-8	HIS	-	expression tag	UNP Q68GS1
G	-7	ILE	-	expression tag	UNP Q68GS1
G	-6	ASP	-	expression tag	UNP Q68GS1
G	-5	ASP	-	expression tag	UNP Q68GS1
G	-4	ASP	-	expression tag	UNP Q68GS1
G	-3	ASP	-	expression tag	UNP Q68GS1
G	-2	LYS	-	expression tag	UNP Q68GS1
G	-1	HIS	-	expression tag	UNP Q68GS1

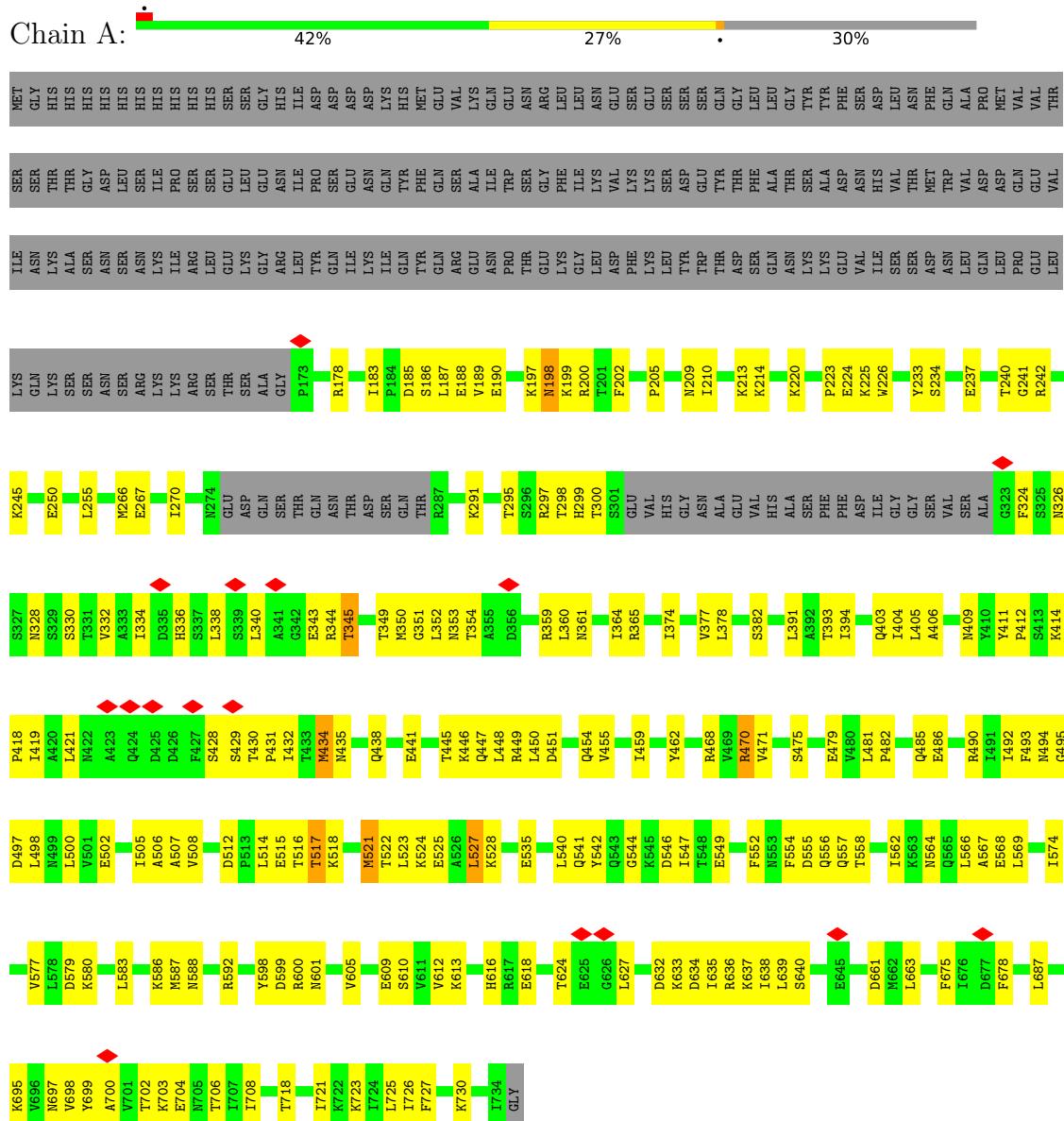
- Molecule 2 is a protein called Lethal factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	699	Total	C	N	O	S	0	0
			5401	3417	913	1065	6		
2	I	710	Total	C	N	O	S	0	0
			4734	2978	841	911	4		
2	J	661	Total	C	N	O	S	0	0
			4318	2717	758	841	2		

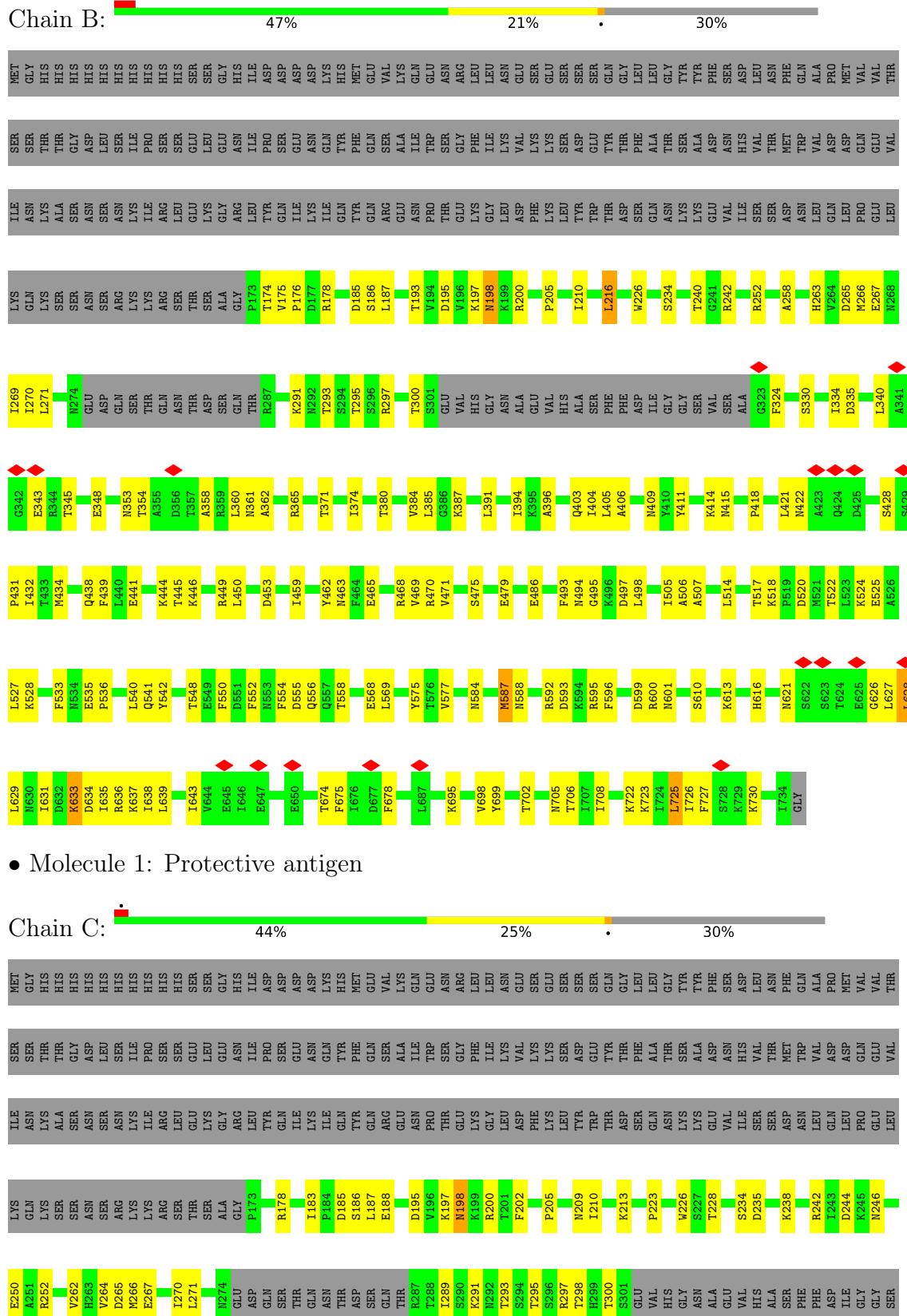
3 Residue-property plots [\(i\)](#)

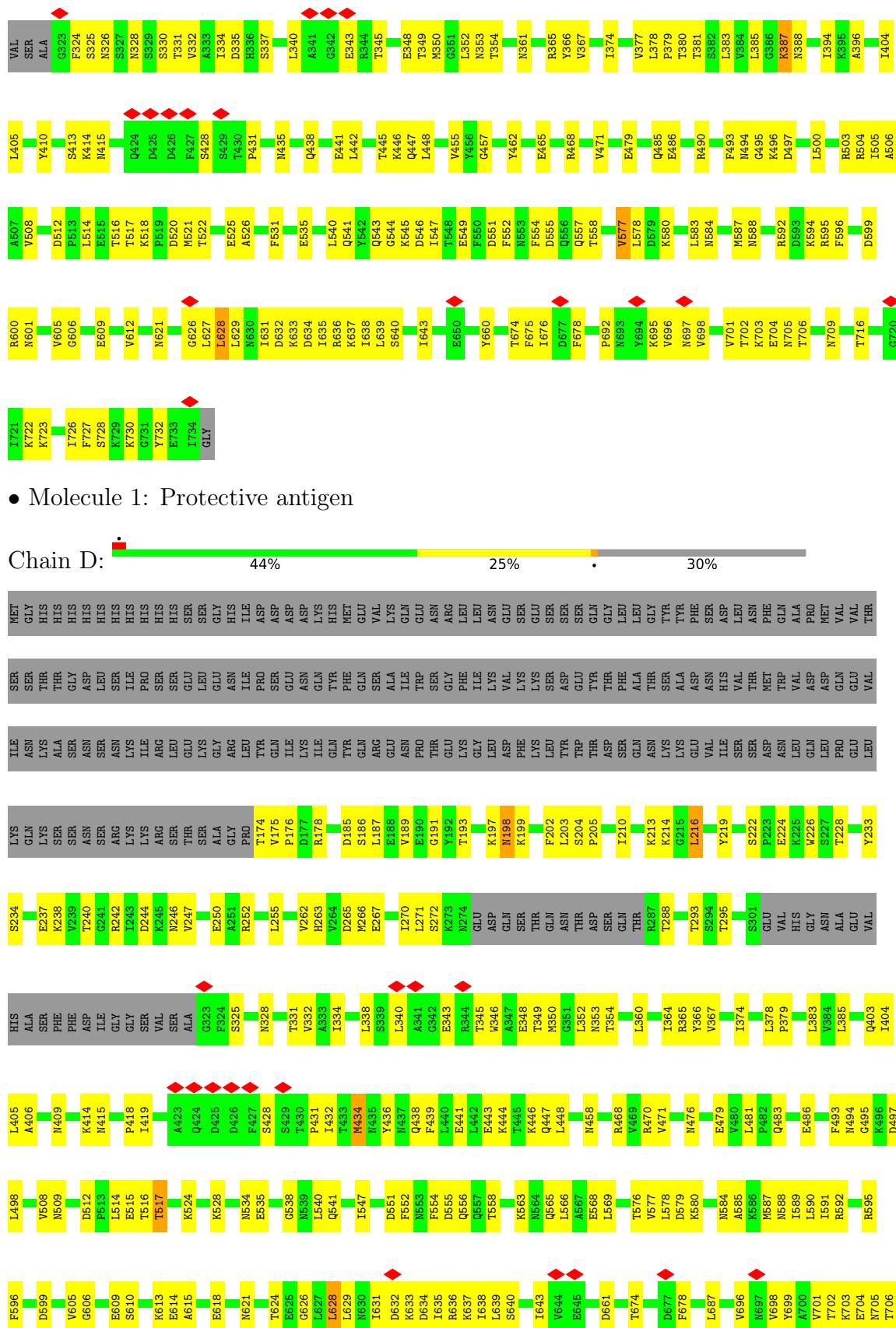
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Protective antigen

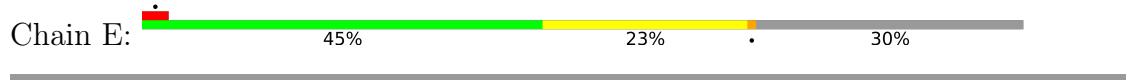


- Molecule 1: Protective antigen





- Molecule 1: Protective antigen

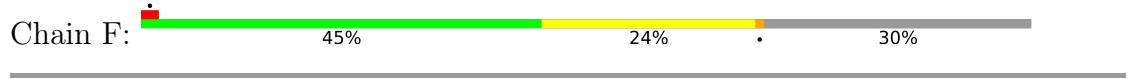


I261	ASP	R287	ASP	T300	GLU	G323
M266	GLN	T288	GLN	S301	GLU	F324
I270	SER	S289	K291	VAL	HIS	S325
L271	THR	S290	K292	VAL	GLY	N326
S272	GLN	T293	T293	ALA	ASN	S327
K273	ASN	S294	S294	ALA	ALA	
M274	THR	T295	T300	PHE	PHE	
				ASP	ASP	
				TLE	GLY	
				VAL	GLY	
				SER	SER	
				VAL	VAL	
				SER	SER	
				ALA	ALA	

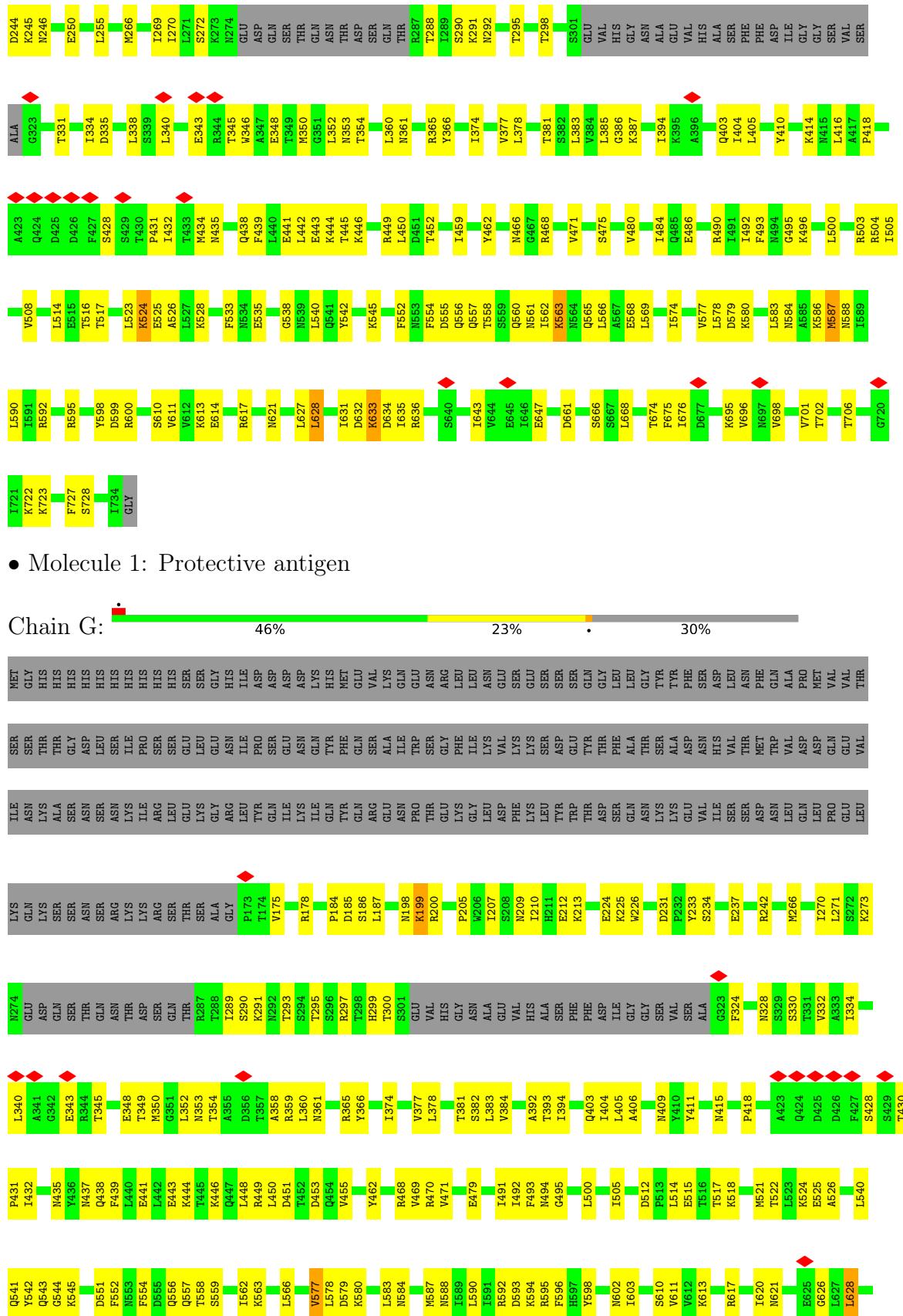
32828 3332 3333 3334 3335 3336 3337 3338 3441 3442 3443 3444 3445 3446 3447 3448 3449 3450 3451 3452 3453 3454 3455 3456 3457 3458 3459 3460 3461 3462 3463 3464 3465 3466 3467 3468 3469 3470 3471 3472 3473 3474 3475 3476 3477 3478 3479 3480 3481 3482 3483 3484 3485 3486 3487 3488 3489 3490 3491 3492 3493 3494 3495 3496 3497 3498 3499 3500 3501 3502 3503 3504 3505 3506 3507 3508 3509 3510 3511 3512 3513 3514 3515 3516 3517 3518 3519 3520 3521

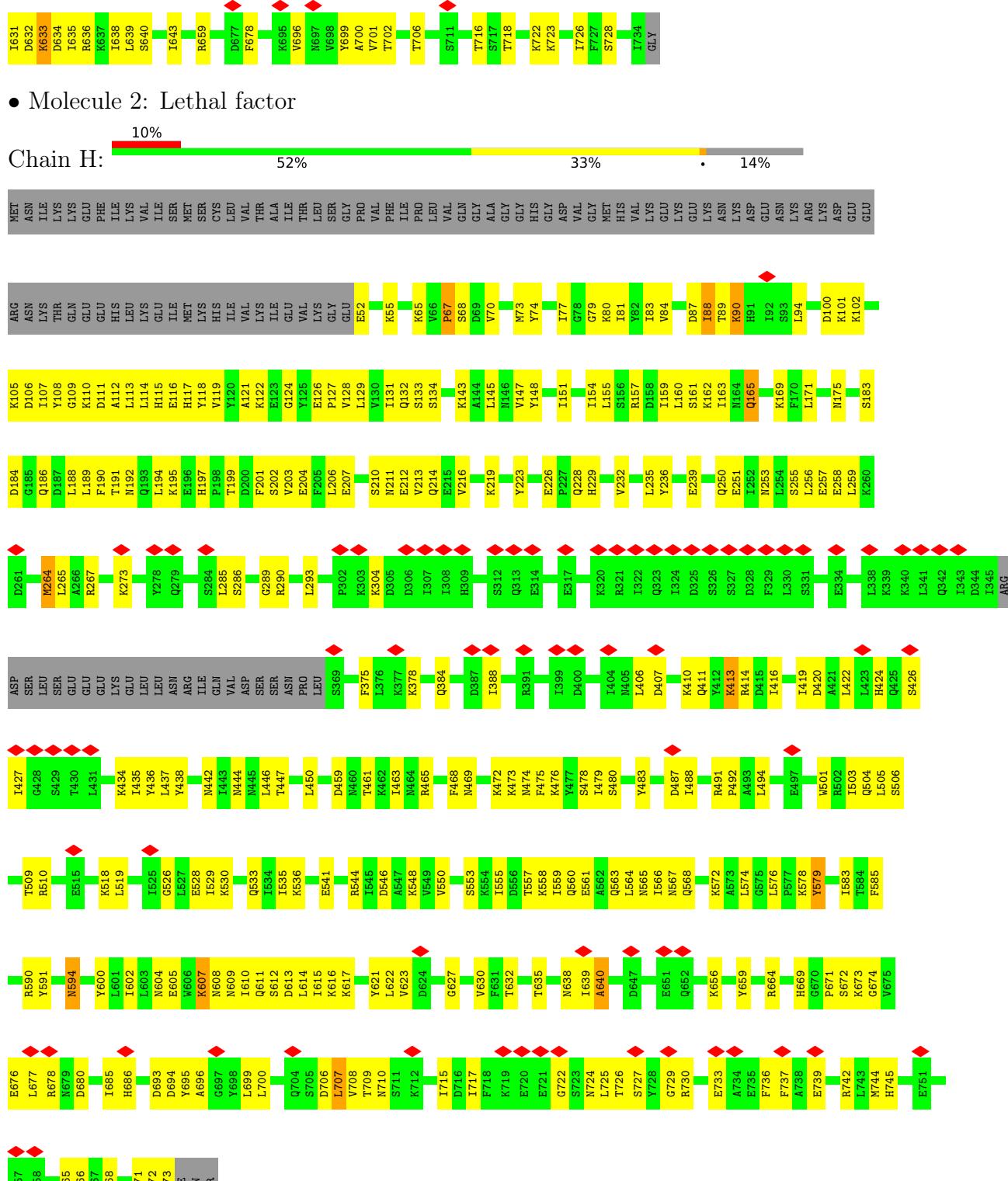
P5.33	N5.34	E5.35	L5.40	Y5.41	T5.42	Q5.43	G5.44	K5.45	D5.46	M5.47	T5.48	F5.49	F5.50	D5.51	N5.52	N5.53	F5.54	T5.58	S5.59	Q5.60	N5.61	T5.62	R5.63	L5.69	Y5.75	T5.76	V5.77	L5.78	D5.79	K5.80	L5.83	N5.84	M5.87	N5.88	R5.92	D5.93	R5.94	R5.95	F5.96	D5.99	H6.02	I6.03	A6.04	S6.09	E6.10	V6.11	V6.12
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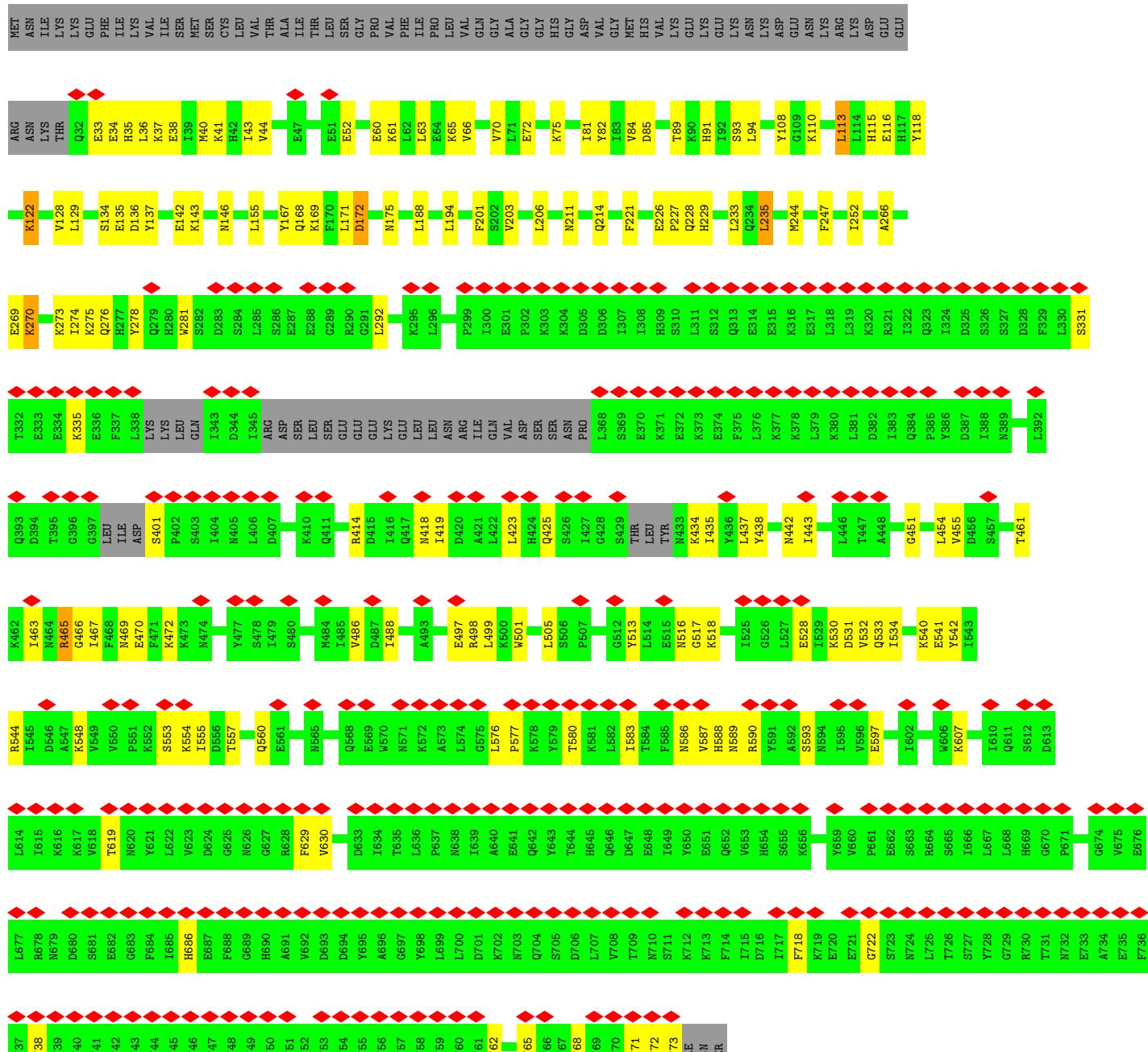
- Molecule 1: Protective antigen





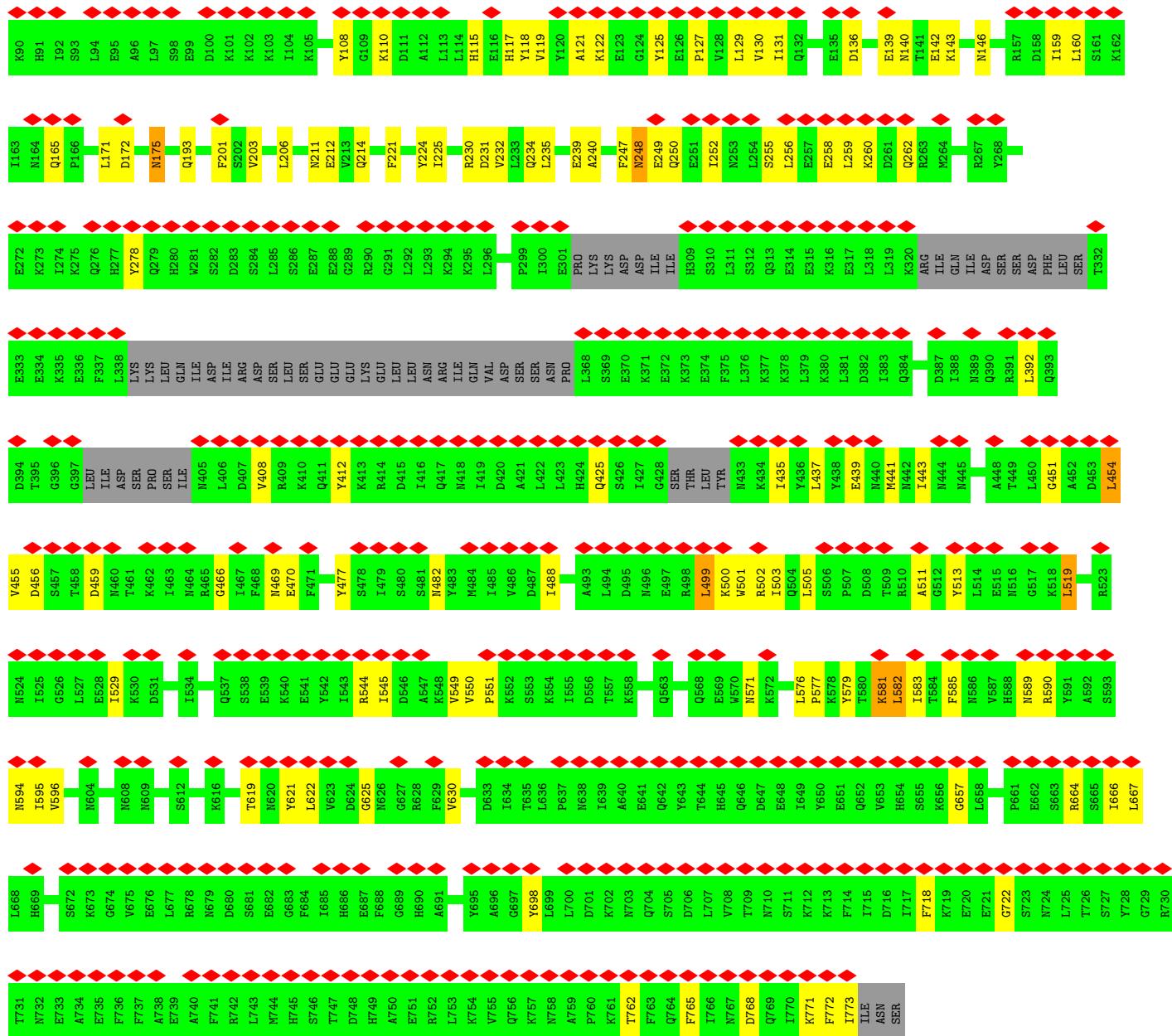




- Molecule 2: Lethal factor

Chain J: 50% Red, 65% Green, 16% Yellow, 18% Grey





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	99000	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 ($e^-/\text{\AA}^2$)	74.4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.696	Depositor
Minimum map value	-1.033	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	359.52002, 359.52002, 359.52002	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	0.62	1/4054 (0.0%)	0.68	3/5524 (0.1%)
1	B	0.65	1/4045 (0.0%)	0.70	5/5511 (0.1%)
1	C	0.63	0/4045	0.68	2/5511 (0.0%)
1	D	0.64	0/4037	0.72	4/5500 (0.1%)
1	E	0.60	0/4045	0.69	2/5511 (0.0%)
1	F	0.60	0/4045	0.68	3/5511 (0.1%)
1	G	0.61	0/4045	0.66	1/5511 (0.0%)
2	H	0.44	0/5499	0.67	3/7464 (0.0%)
2	I	0.40	0/4799	0.57	2/6559 (0.0%)
2	J	0.36	0/4380	0.59	7/6015 (0.1%)
All	All	0.56	2/42994 (0.0%)	0.66	32/58617 (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
2	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	517	THR	C-N	-5.67	1.21	1.34
1	B	517	THR	C-N	-5.23	1.22	1.34

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	88	ILE	C-N-CA	14.34	157.54	121.70
2	J	499	LEU	CB-CG-CD2	-8.26	96.96	111.00
1	A	434	MET	CA-CB-CG	6.90	125.04	113.30
1	D	517	THR	C-N-CA	-6.83	104.64	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	628	LEU	CA-CB-CG	6.58	130.45	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	165	GLN	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3984	0	3762	164	0
1	B	3977	0	3761	147	0
1	C	3977	0	3761	173	0
1	D	3970	0	3753	172	0
1	E	3977	0	3761	165	0
1	F	3977	0	3761	171	0
1	G	3977	0	3761	153	0
2	H	5401	0	5036	270	0
2	I	4734	0	3781	134	0
2	J	4318	0	3304	117	0
All	All	42292	0	38441	1610	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 20.

The worst 5 of 1610 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (\AA)	Clash overlap (\AA)
2:I:89:THR:CG2	2:I:115:HIS:HA	1.42	1.48
1:F:643:ILE:CD1	1:F:723:LYS:HD3	1.56	1.33
2:J:89:THR:CG2	2:J:115:HIS:HA	1.59	1.32
1:D:176:PRO:HG2	1:D:185:ASP:OD2	1.25	1.25
2:I:89:THR:HG21	2:I:115:HIS:CB	1.74	1.17

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	523/759 (69%)	479 (92%)	40 (8%)	4 (1%)	19 57
1	B	523/759 (69%)	477 (91%)	44 (8%)	2 (0%)	34 70
1	C	523/759 (69%)	477 (91%)	44 (8%)	2 (0%)	34 70
1	D	522/759 (69%)	474 (91%)	46 (9%)	2 (0%)	34 70
1	E	523/759 (69%)	477 (91%)	45 (9%)	1 (0%)	47 79
1	F	523/759 (69%)	474 (91%)	47 (9%)	2 (0%)	34 70
1	G	523/759 (69%)	478 (91%)	42 (8%)	3 (1%)	25 62
2	H	695/809 (86%)	638 (92%)	53 (8%)	4 (1%)	25 62
2	I	700/809 (86%)	648 (93%)	51 (7%)	1 (0%)	51 83
2	J	649/809 (80%)	606 (93%)	41 (6%)	2 (0%)	41 74
All	All	5704/7740 (74%)	5228 (92%)	453 (8%)	23 (0%)	38 70

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	A	663	LEU
1	B	198	ASN
1	C	198	ASN
1	D	198	ASN

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	414/683 (61%)	410 (99%)	4 (1%)	76	86
1	B	415/683 (61%)	414 (100%)	1 (0%)	93	97
1	C	415/683 (61%)	414 (100%)	1 (0%)	93	97
1	D	414/683 (61%)	413 (100%)	1 (0%)	93	97
1	E	415/683 (61%)	409 (99%)	6 (1%)	67	81
1	F	415/683 (61%)	412 (99%)	3 (1%)	84	91
1	G	415/683 (61%)	415 (100%)	0	100	100
2	H	551/739 (75%)	542 (98%)	9 (2%)	62	79
2	I	338/739 (46%)	333 (98%)	5 (2%)	65	81
2	J	292/739 (40%)	285 (98%)	7 (2%)	49	71
All	All	4084/6998 (58%)	4047 (99%)	37 (1%)	79	88

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	465	ARG
2	J	581	LYS
2	I	607	LYS
2	J	175	ASN
1	E	636	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	186	GLN
2	H	563	GLN
2	J	690	HIS
2	I	228	GLN
2	H	417	GLN

5.3.3 RNA

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.

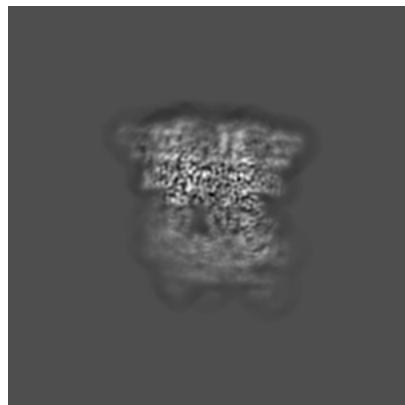
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11523. These allow visual inspection of the internal detail of the map and identification of artifacts.

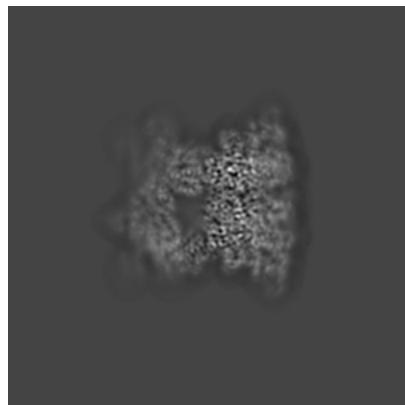
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

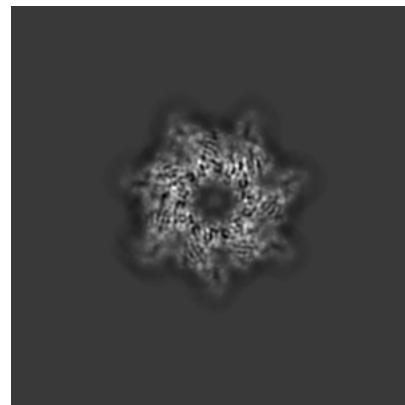
6.1.1 Primary map



X



Y

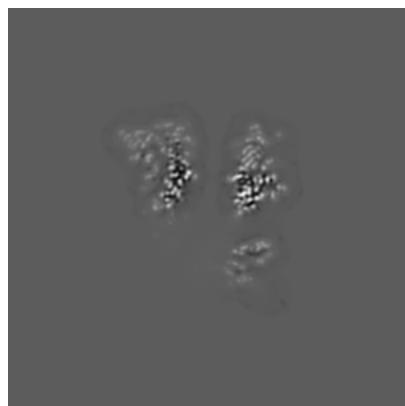


Z

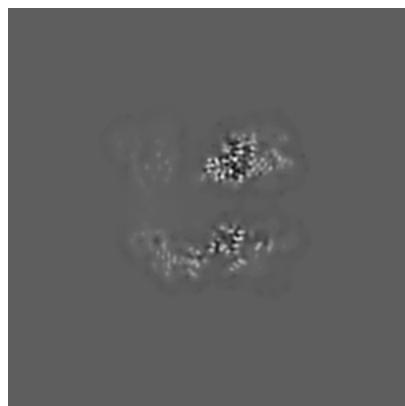
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

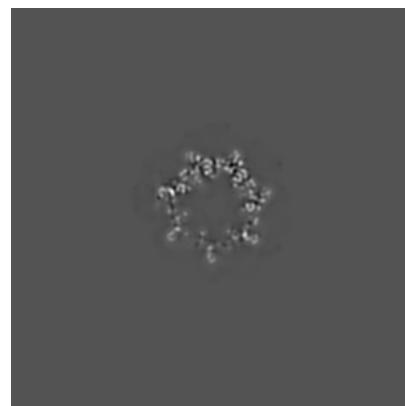
6.2.1 Primary map



X Index: 168



Y Index: 168

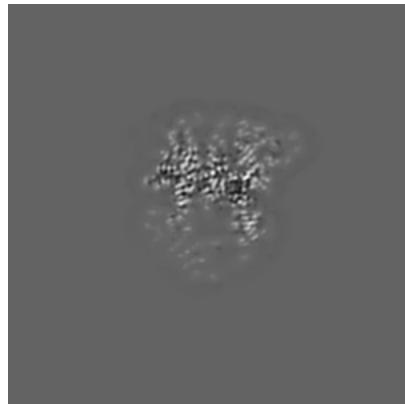


Z Index: 168

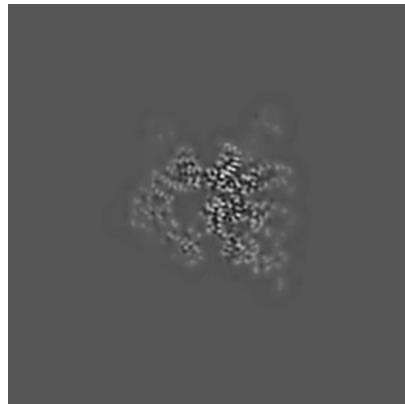
The images above show central slices of the map in three orthogonal directions.

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

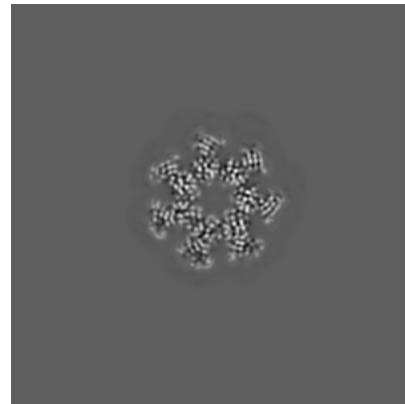
6.3.1 Primary map



X Index: 196



Y Index: 198

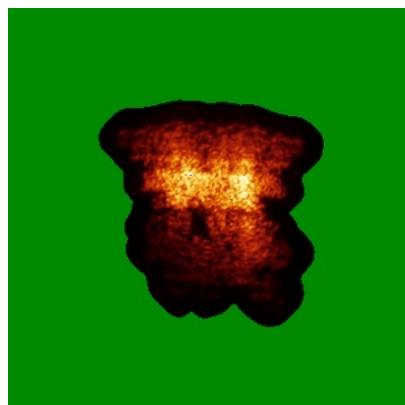


Z Index: 194

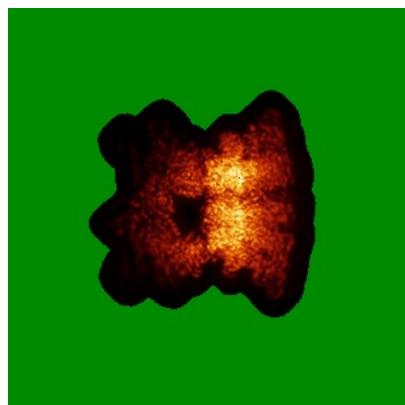
The images above show the largest variance slices of the map in three orthogonal directions.

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

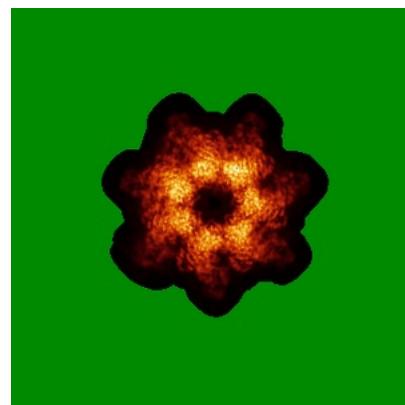
6.4.1 Primary map



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

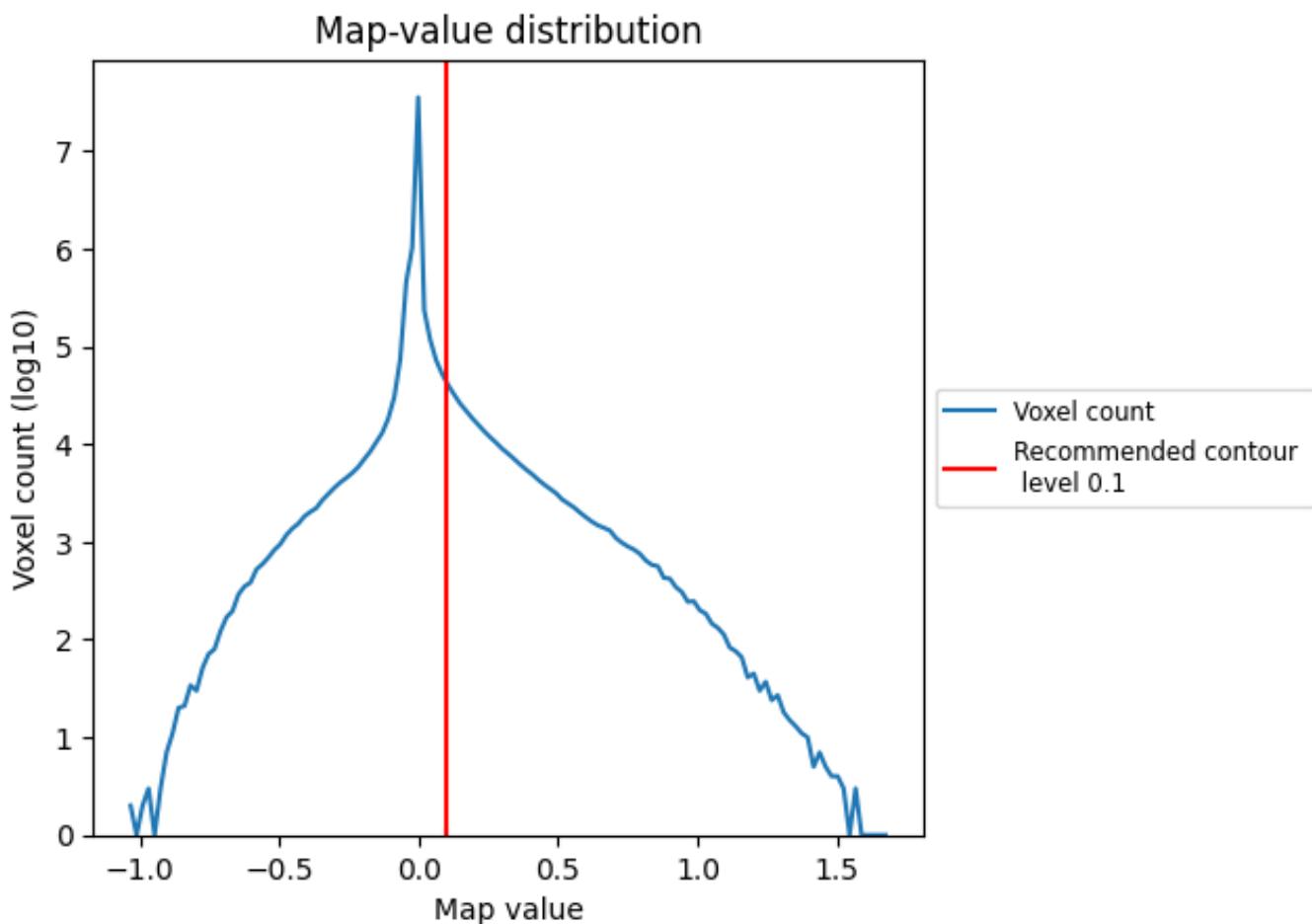
6.6 Mask visualisation [\(i\)](#)

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

7 Map analysis (i)

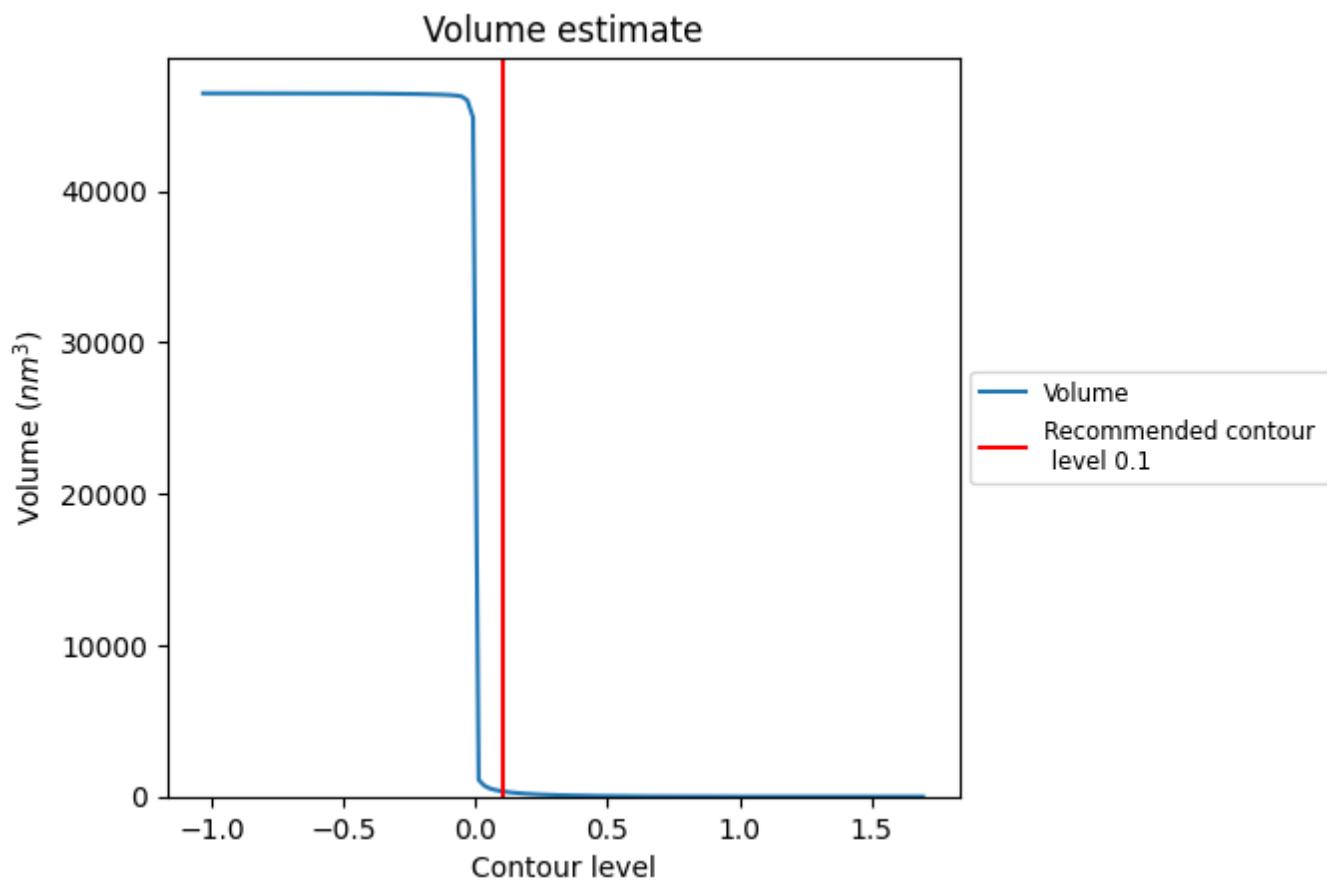
This section contains the results of statistical analysis of the map.

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.

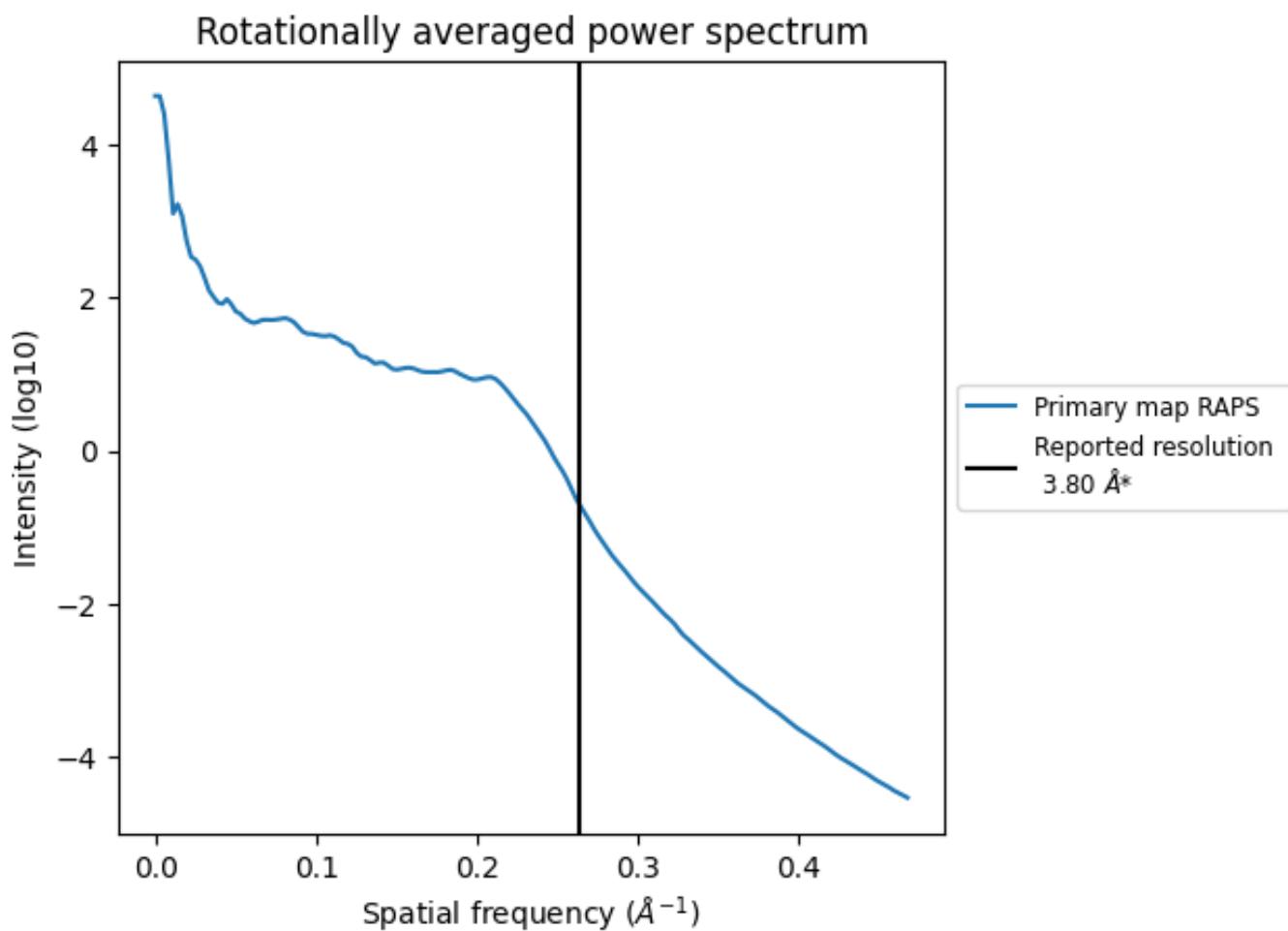
7.2 Volume estimate (i)



The volume at the recommended contour level is 351 nm^3 ; this corresponds to an approximate mass of 317 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 0.263 \AA^{-1}

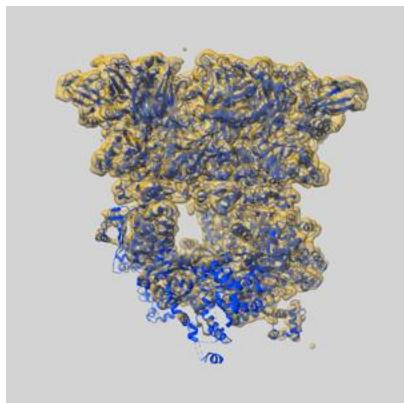
8 Fourier-Shell correlation

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

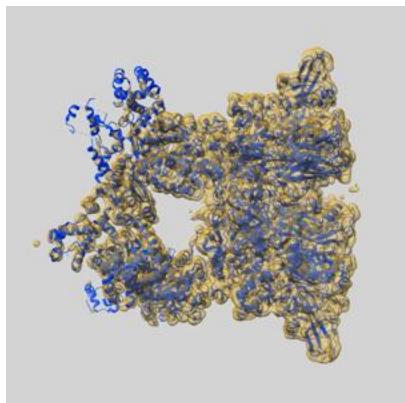
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11523 and PDB model 6ZXK. Per-residue inclusion information can be found in section 3 on page 9.

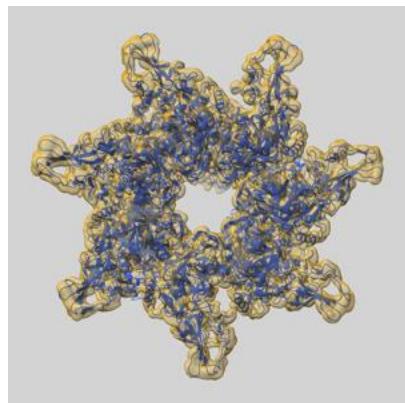
9.1 Map-model overlay (i)



X



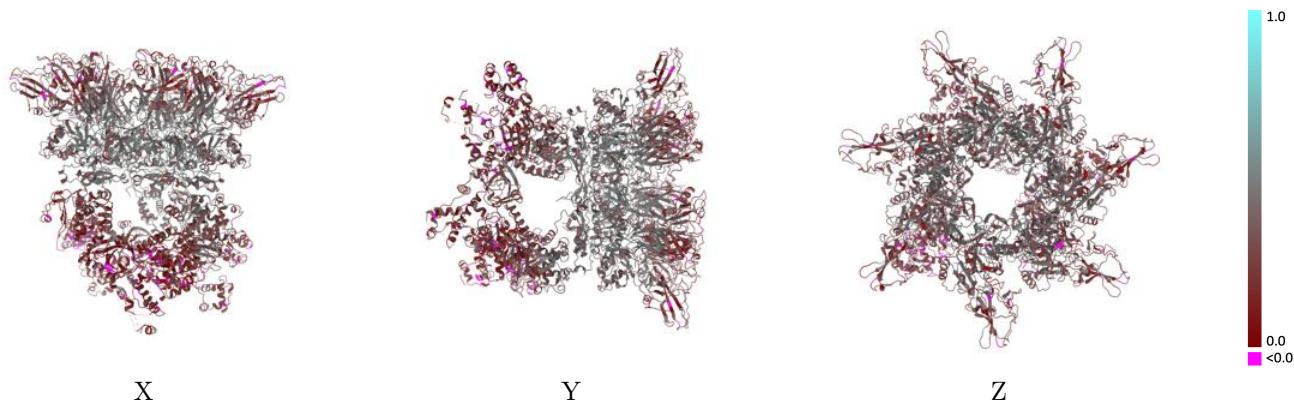
Y



Z

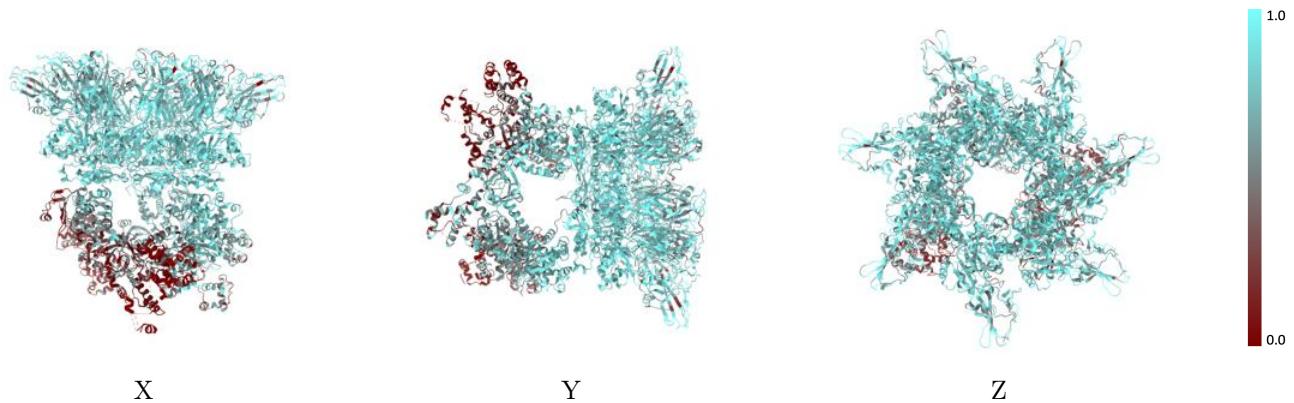
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



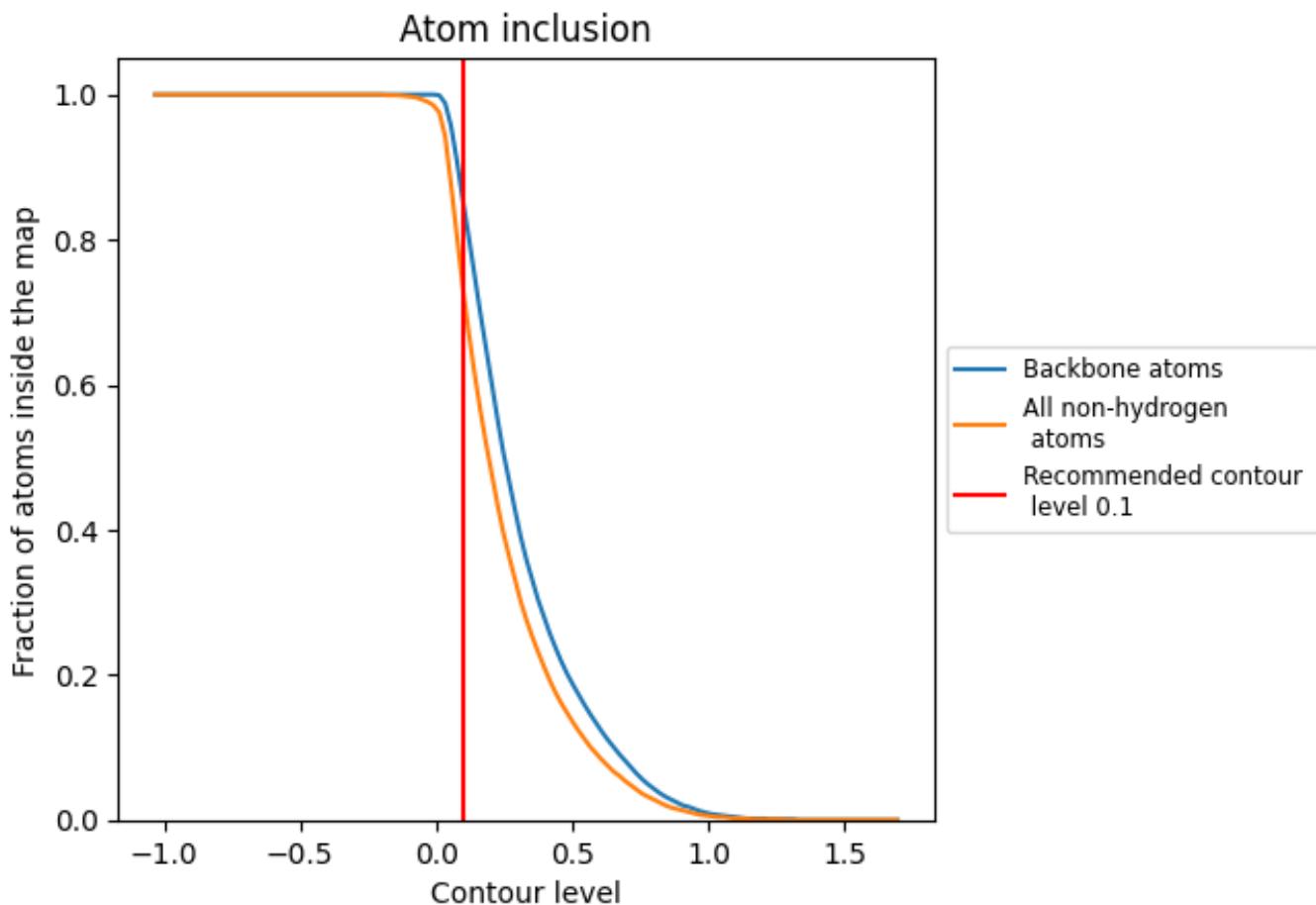
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

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



At the recommended contour level, 85% of all backbone atoms, 73% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7280	0.3400
A	0.8240	0.3850
B	0.8310	0.3890
C	0.8350	0.3890
D	0.8380	0.3880
E	0.8180	0.3790
F	0.8170	0.3750
G	0.8280	0.3840
H	0.6900	0.2920
I	0.5280	0.2510
J	0.3570	0.2100

