



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 05:31 PM UTC

PDB ID : 6ZXJ / pdb_00006zxj
EMDB ID : EMD-11522
Title : Fully-loaded anthrax lethal toxin in its heptameric pre-pore state, in which the third lethal factor is masked out (PA7LF3-masked)
Authors : Quentin, D.; Antoni, C.; Gatsogiannis, C.; Raunser, S.
Deposited on : 2020-07-29
Resolution : 3.50 Å (reported)
Based on initial models : 3HVD, 1J7N

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

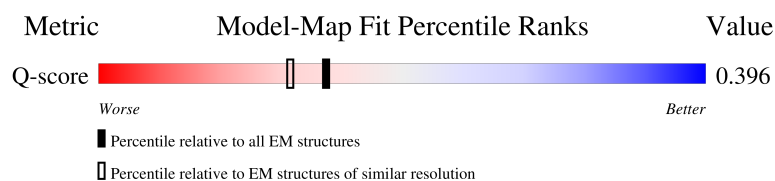
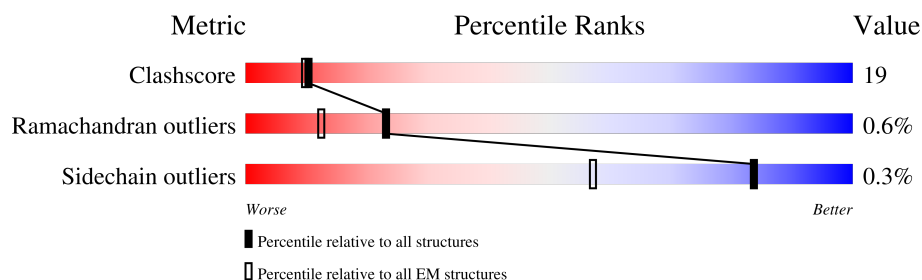
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



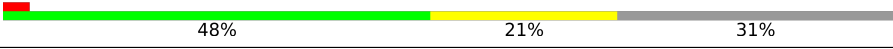
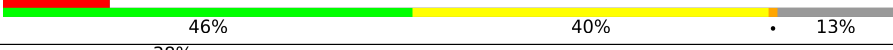
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	759	
1	B	759	
1	C	759	
1	D	759	

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Mol	Chain	Length	Quality of chain
1	E	759	
1	F	759	
1	G	759	
2	H	809	
2	I	809	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 38244 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	527	Total	C	N	O	S	0	0
			3963	2481	690	788	4		
1	B	527	Total	C	N	O	S	0	0
			3966	2482	690	790	4		
1	C	527	Total	C	N	O	S	0	0
			3962	2479	689	790	4		
1	D	527	Total	C	N	O	S	0	0
			3962	2479	689	790	4		
1	E	527	Total	C	N	O	S	0	0
			3966	2482	690	790	4		
1	F	527	Total	C	N	O	S	0	0
			3962	2479	689	790	4		
1	G	527	Total	C	N	O	S	0	0
			3966	2482	690	790	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

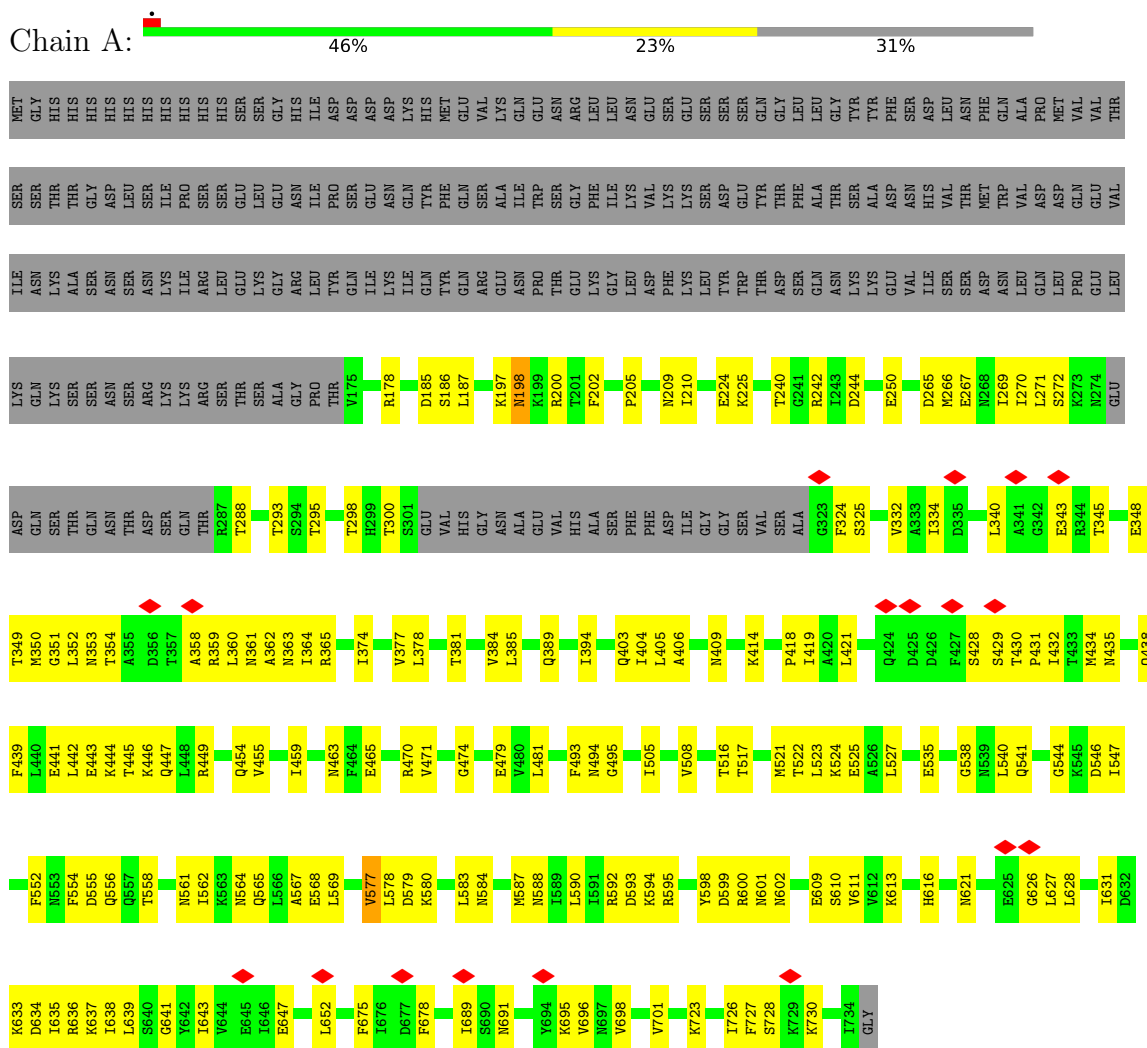
- Molecule 2 is a protein called Lethal factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	700	Total	C	N	O	S	0	0
			5618	3572	943	1097	6		
2	I	710	Total	C	N	O	S	0	0
			4879	3081	865	929	4		

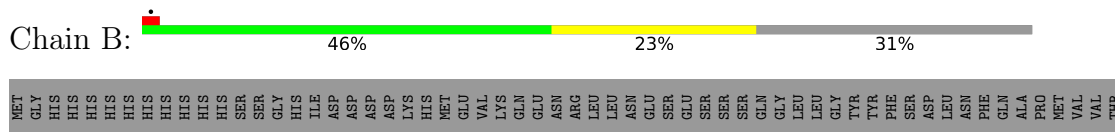
3 Residue-property plots

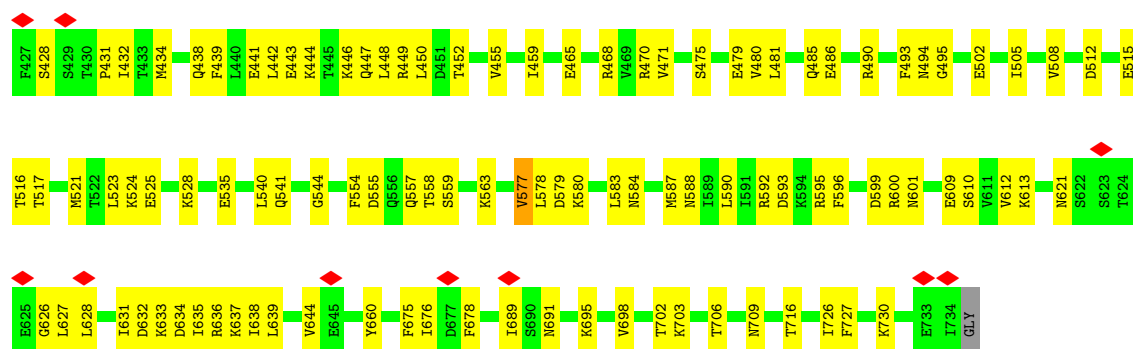
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



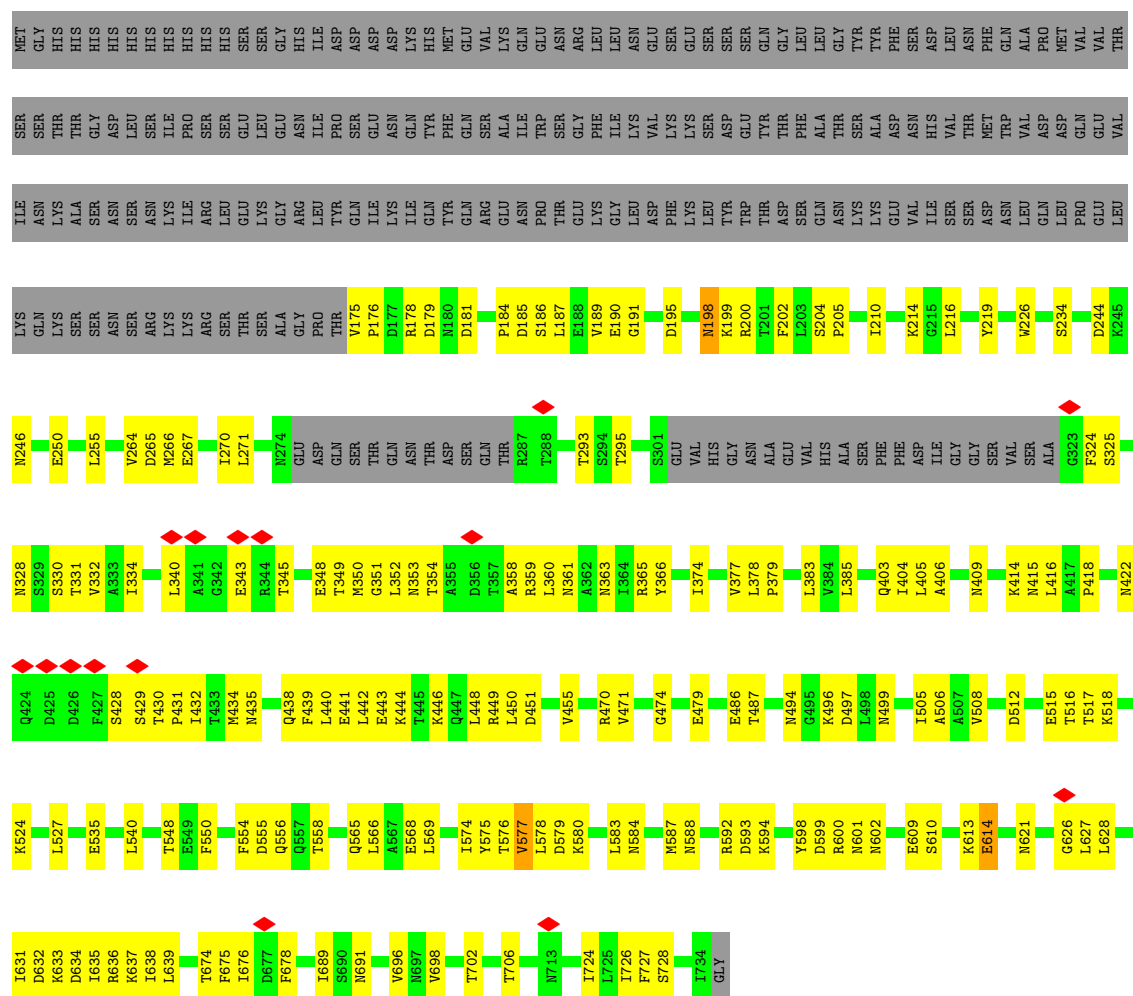
• Molecule 1: Protective antigen





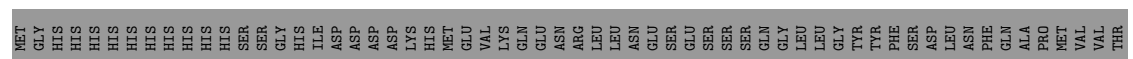
• Molecule 1: Protective antigen

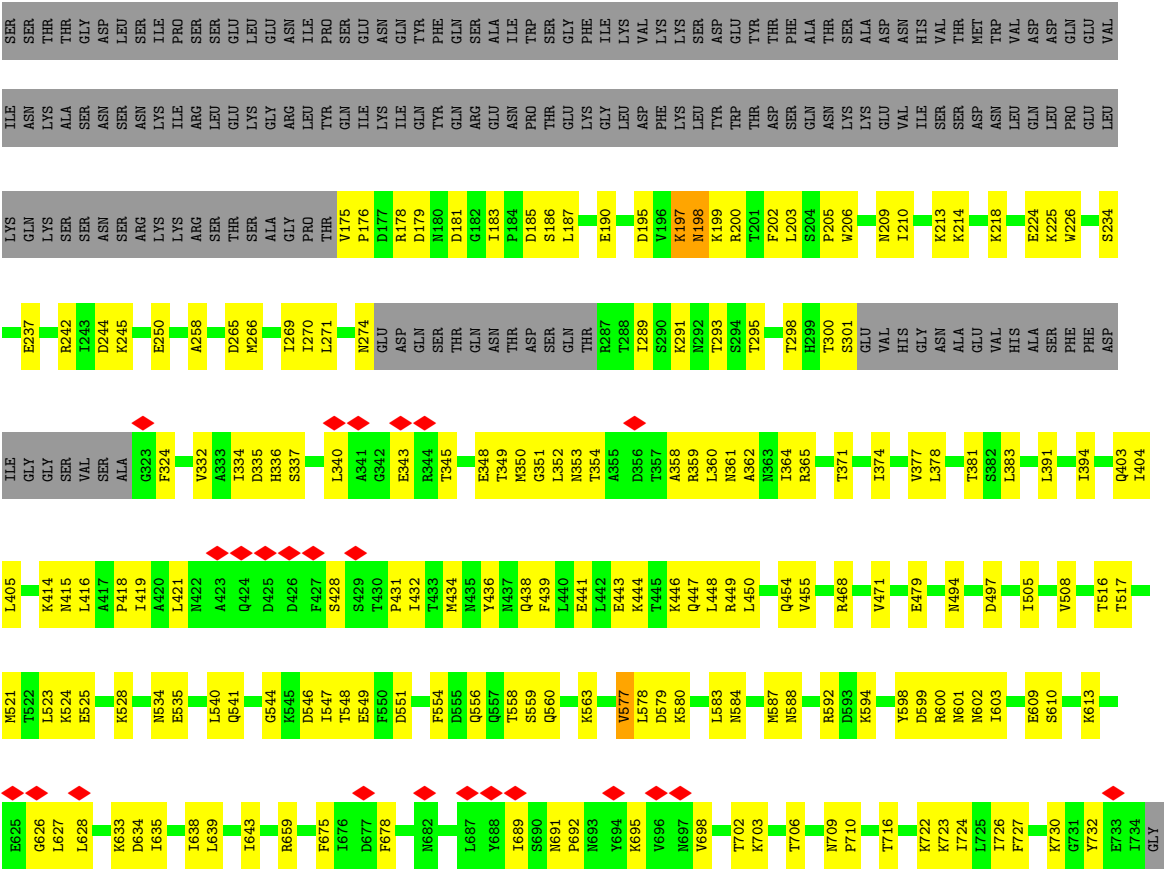
Chain D: 46% 23% 31%



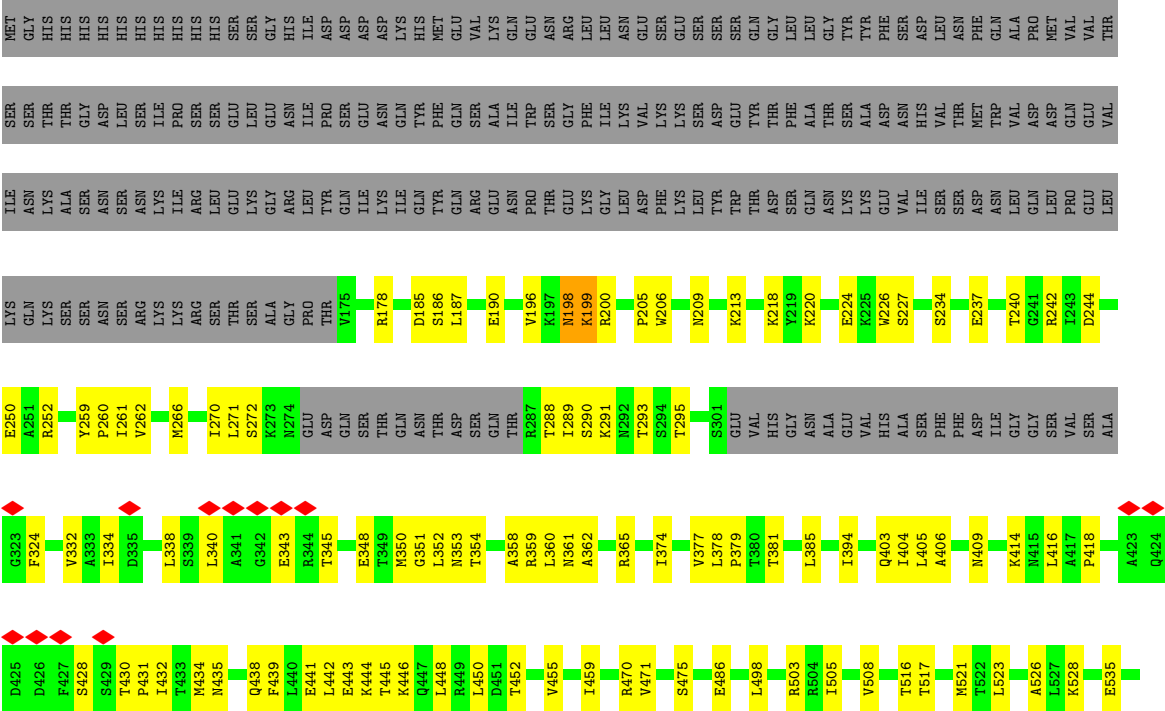
• Molecule 1: Protective antigen

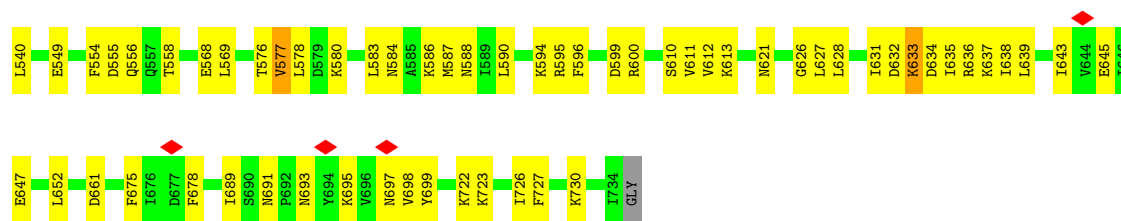
Chain E: 45% 24% 31%



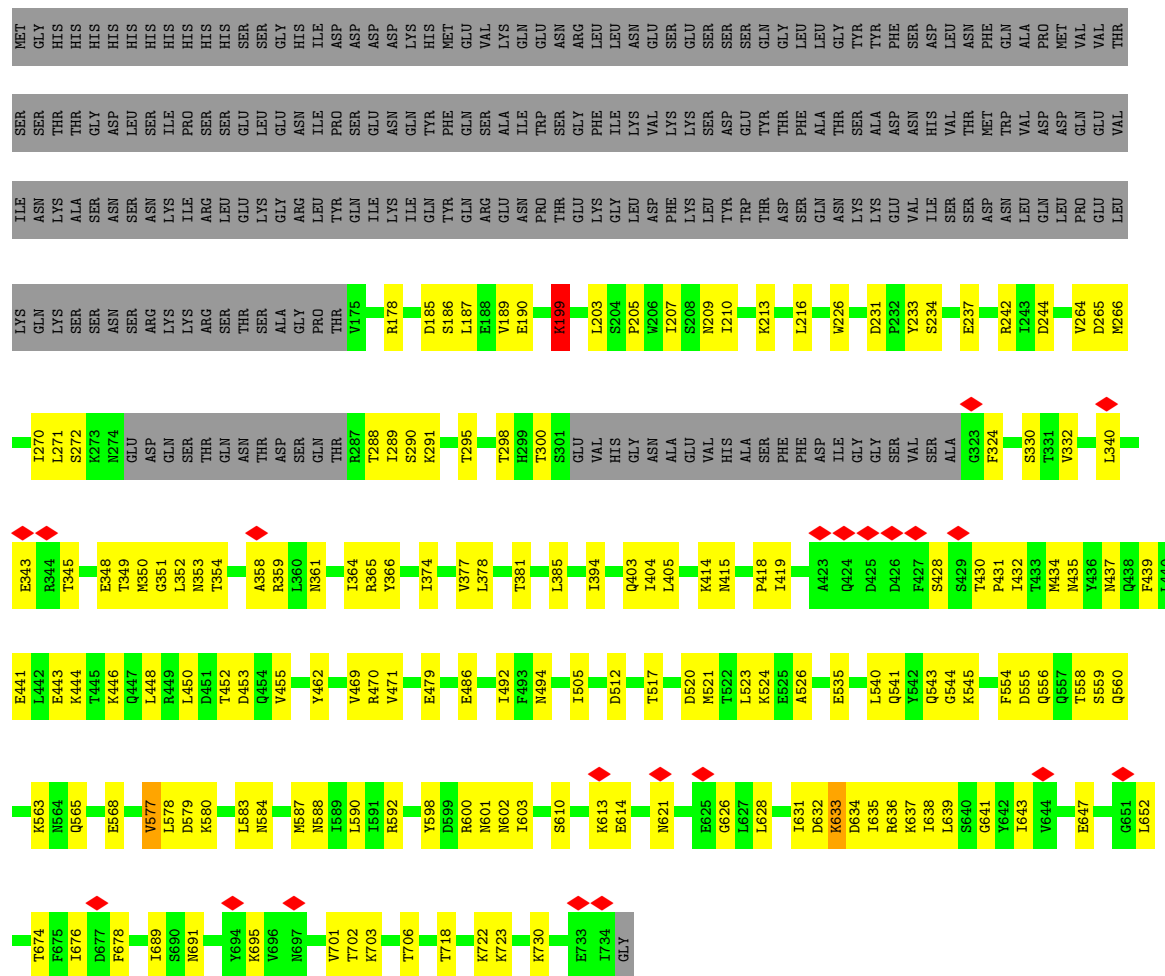


• Molecule 1: Protective antigen

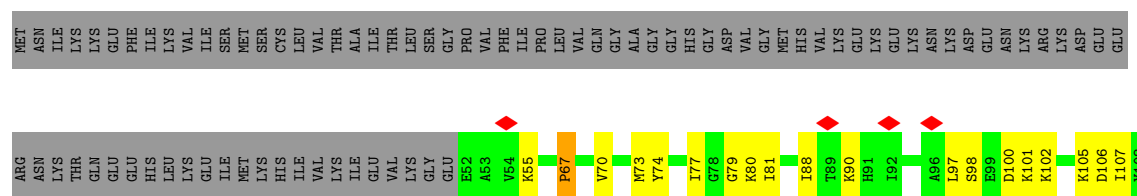




• Molecule 1: Protective antigen



• Molecule 2: Lethal factor



I770	K771	F772	I773	ILE	ASN	SER																																																					
T709	N710	S711	K712	K713	F714	L715	D716	I717	F718	K719	E720	E721	G722	S723	N724	L725	S726	Y727	Y728	G729	N730	T731	N732	E733	A734	E735	F736	F737	A738	E739	A740	F741	R742	L743	M744	H745	S746	T747	D748	H749	A750	E751	R752	L753	K754	V755	Q756	K757	N758	A759	P760	K761	T762	F765	I766	N767	D768	Q769	
E648	I649	Y650	E651	Q652	V653	H654	S655	K656	G657	L658	V659	V660	P661	E662	S663	R664	S665	I666	L667	L668	H669	G670	P671	G674	V675	E676	L677	R678	N679	D680	S681	E682	G683	F684	I685	H686	E687	F688	G689	H690	A691	V692	D693	D694	Y695	A696	G697	N698	L699	L700	D701	K702	N703	Q704	S705	D706	L707	V708	
T584	F585	N586	V587	H588	N589	R590	Y591	A592	I595	V596	E597	S598	A599	I602	L603	M604	N608	N609	I610	Q611	S612	D613	I614	I615	K616	K617	V618	T619	N620	Y621	L622	V623	D624	G625	N626	G627	R628	F629	V630	F631	T632	D633	I634	T635	L636	P637	N638	I639	A640	E641	Q642	Y643	T644	H645	Q646	D647			
T509	Y513	L514	E515	N516	Q517	K518	I525	G526	L527	E528	I529	K530	Q533	I534	K540	E541	Y542	I543	R544	K548	V549	V550	F551	K552	S553	K554	I555	D556	T557	K558	I559	Q560	E561	A562	Q563	L564	N565	I566	N567	Q568	E569	K572	A573	L574	G575	L576	P577	K578	Y579	T580	K581	L582	I583						
LEU	TYR	N433	K434	I435	Y436	L437	Y438	M442	I443	T447	A448	G451	L454	V455	D456	S457	I463	M464	G466	M469	E470	F471	K472	K473	M474	F475	K476	Y477	S478	I479	S480	S481	M482	Y483	M484	I485	V486	D487	I488	A493	L494	R498	L499	K500	M501	R502	L505	D508											
P40	L368	S369	E370	K371	E372	K373	E374	F375	L376	K377	K378	L379	K380	L381	D382	I383	Q384	D387	I388	N389	Q393	G396	G397	LEU	ILE	ASP	S401	P402	I404	M405	L406	D407	V408	R409	K410	Q411	Y412	K413	R414	S414	D415	I416	Q417	M418	I419	D420	A421	L422	L423	H424	Q425	S426	I427	G428	S429	THR			
I307	I308	H309	S310	L311	S312	Q313	E314	E315	K316	E317	L318	L319	K320	R321	I322	Q323	I324	D325	S326	S327	D328	F329	L330	S331	T332	E333	E334	K335	E336	F337	L338	LYS	LYS	LEU	GLN	I343	D344	I345	ARG	ASP	SER	LEU	SER	GLU	GLU	LYS	GLU	LEU	LEU	ASN	ASN	ARG	ILE	GLN	VAL	ASP	SER	SER	ASN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	210000	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	1.927	Depositor
Minimum map value	-1.088	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.032	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	0.70	0/4030	0.72	0/5490
1	B	0.76	0/4033	0.77	1/5494 (0.0%)
1	C	0.73	0/4029	0.74	0/5490
1	D	0.77	0/4029	0.80	3/5490 (0.1%)
1	E	0.69	0/4033	0.75	1/5494 (0.0%)
1	F	0.69	0/4029	0.72	0/5490
1	G	0.72	0/4033	0.78	0/5494
2	H	0.48	0/5719	0.83	1/7729 (0.0%)
2	I	0.46	0/4950	0.75	4/6751 (0.1%)
All	All	0.66	0/38885	0.77	10/52922 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	44	VAL	N-CA-C	8.43	118.78	106.55
1	D	198	ASN	CA-C-N	-7.03	111.60	122.49
1	D	198	ASN	C-N-CA	-7.03	111.60	122.49
1	E	197	LYS	N-CA-C	-6.13	99.24	109.24
2	I	44	VAL	CA-C-N	-5.84	112.82	121.24

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	3963	0	3753	149	0
1	B	3966	0	3755	150	0
1	C	3962	0	3744	149	0
1	D	3962	0	3744	164	0
1	E	3966	0	3755	151	0
1	F	3962	0	3744	128	0
1	G	3966	0	3755	130	0
2	H	5618	0	5483	302	0
2	I	4879	0	4045	138	0
All	All	38244	0	35778	1403	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 19.

The worst 5 of 1403 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:584:ASN:H	1:A:587:MET:HE3	1.15	1.07
1:F:584:ASN:H	1:F:587:MET:HE3	1.22	1.01
2:H:446:LEU:HD11	2:H:590:ARG:HB2	1.43	0.98
1:E:365:ARG:HH12	1:E:414:LYS:HA	1.31	0.96
2:H:563:GLN:HE22	2:H:584:THR:HA	1.33	0.93

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	521/759 (69%)	473 (91%)	45 (9%)	3 (1%)	21	54
1	B	521/759 (69%)	474 (91%)	44 (8%)	3 (1%)	21	54
1	C	521/759 (69%)	473 (91%)	45 (9%)	3 (1%)	21	54
1	D	521/759 (69%)	473 (91%)	45 (9%)	3 (1%)	21	54
1	E	521/759 (69%)	474 (91%)	44 (8%)	3 (1%)	21	54
1	F	521/759 (69%)	472 (91%)	44 (8%)	5 (1%)	12	44
1	G	521/759 (69%)	474 (91%)	43 (8%)	4 (1%)	16	49
2	H	696/809 (86%)	632 (91%)	59 (8%)	5 (1%)	18	51
2	I	700/809 (86%)	648 (93%)	51 (7%)	1 (0%)	48	79
All	All	5043/6931 (73%)	4593 (91%)	420 (8%)	30 (1%)	23	54

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	B	198	ASN
1	C	198	ASN
1	D	198	ASN
1	E	198	ASN

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	413/683 (60%)	413 (100%)	0	100	100
1	B	414/683 (61%)	414 (100%)	0	100	100
1	C	413/683 (60%)	413 (100%)	0	100	100
1	D	413/683 (60%)	413 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	414/683 (61%)	414 (100%)	0	100	100
1	F	413/683 (60%)	412 (100%)	1 (0%)	87	85
1	G	414/683 (61%)	413 (100%)	1 (0%)	87	85
2	H	607/739 (82%)	602 (99%)	5 (1%)	73	77
2	I	373/739 (50%)	370 (99%)	3 (1%)	73	77
All	All	3874/6259 (62%)	3864 (100%)	10 (0%)	84	83

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	40	MET
2	I	118	TYR
2	I	138	VAL
2	H	138	VAL
2	H	254	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	168	GLN
2	H	769	GLN
2	H	228	GLN
2	H	440	ASN
2	I	175	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	517:THR	C	518:LYS	N	1.18
1	B	517:THR	C	518:LYS	N	1.16
1	C	517:THR	C	518:LYS	N	1.15

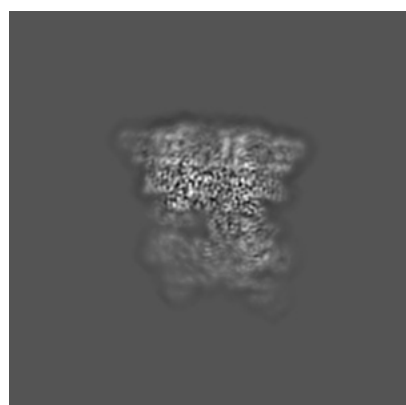
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11522. These allow visual inspection of the internal detail of the map and identification of artifacts.

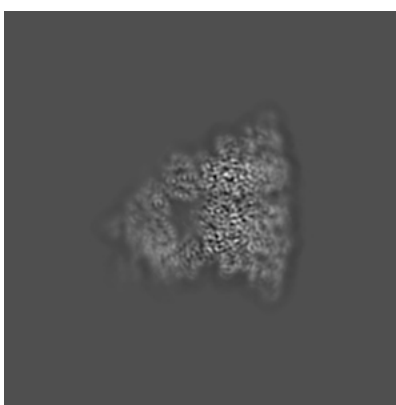
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

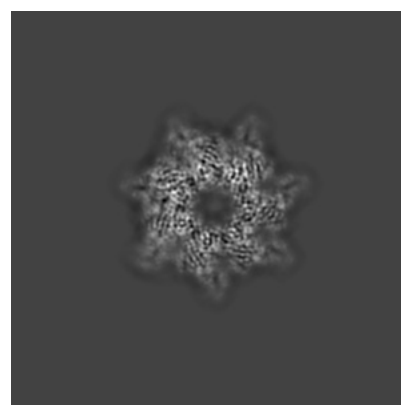
6.1.1 Primary map



X



Y

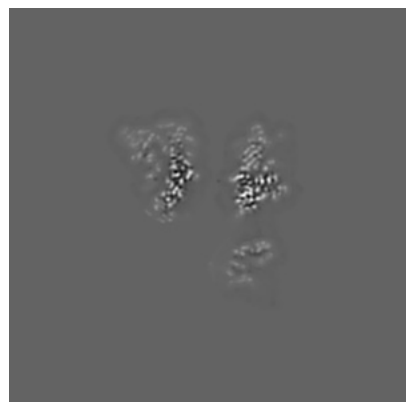


Z

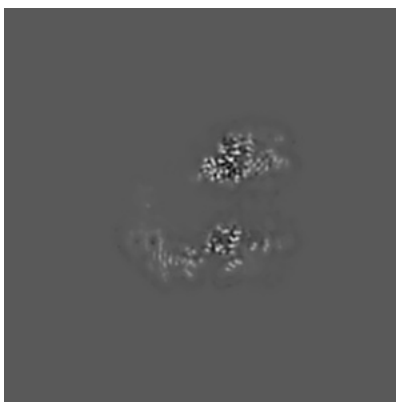
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

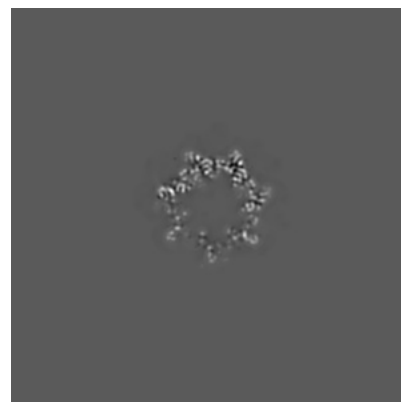
6.2.1 Primary map



X Index: 168



Y Index: 168

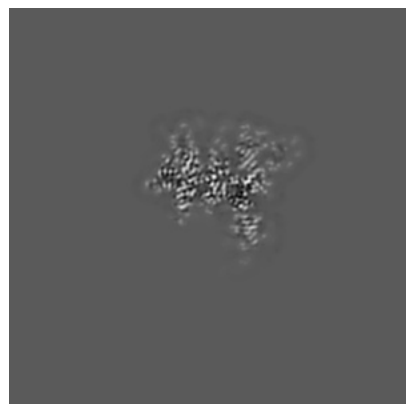


Z Index: 168

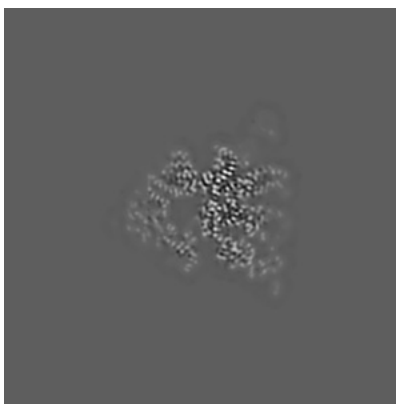
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

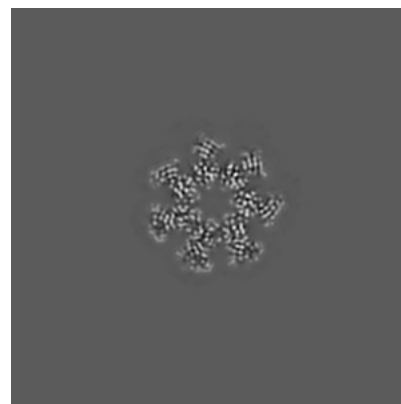
6.3.1 Primary map



X Index: 196



Y Index: 199

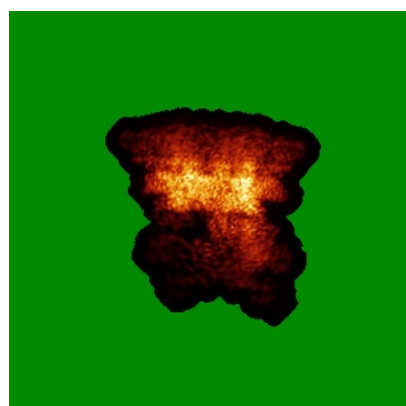


Z Index: 194

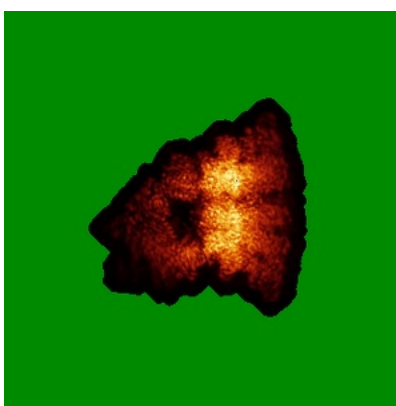
The images above show the largest variance slices of the map in three orthogonal directions.

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

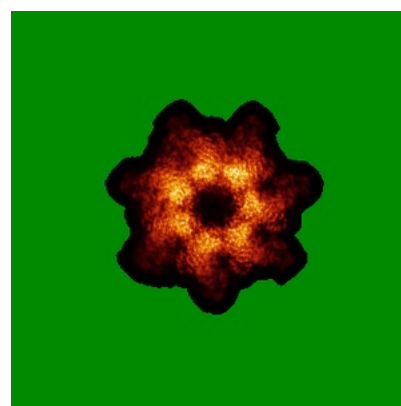
6.4.1 Primary map



X



Y

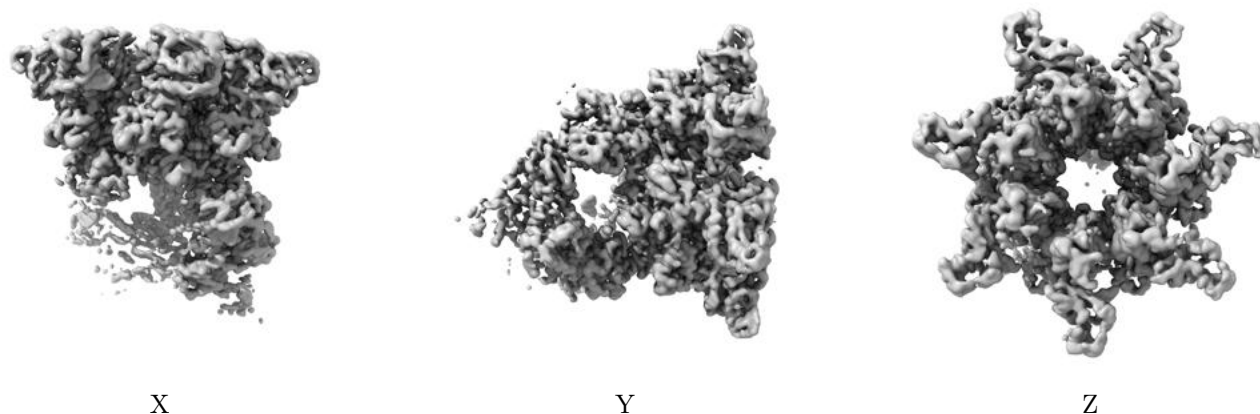


Z

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.

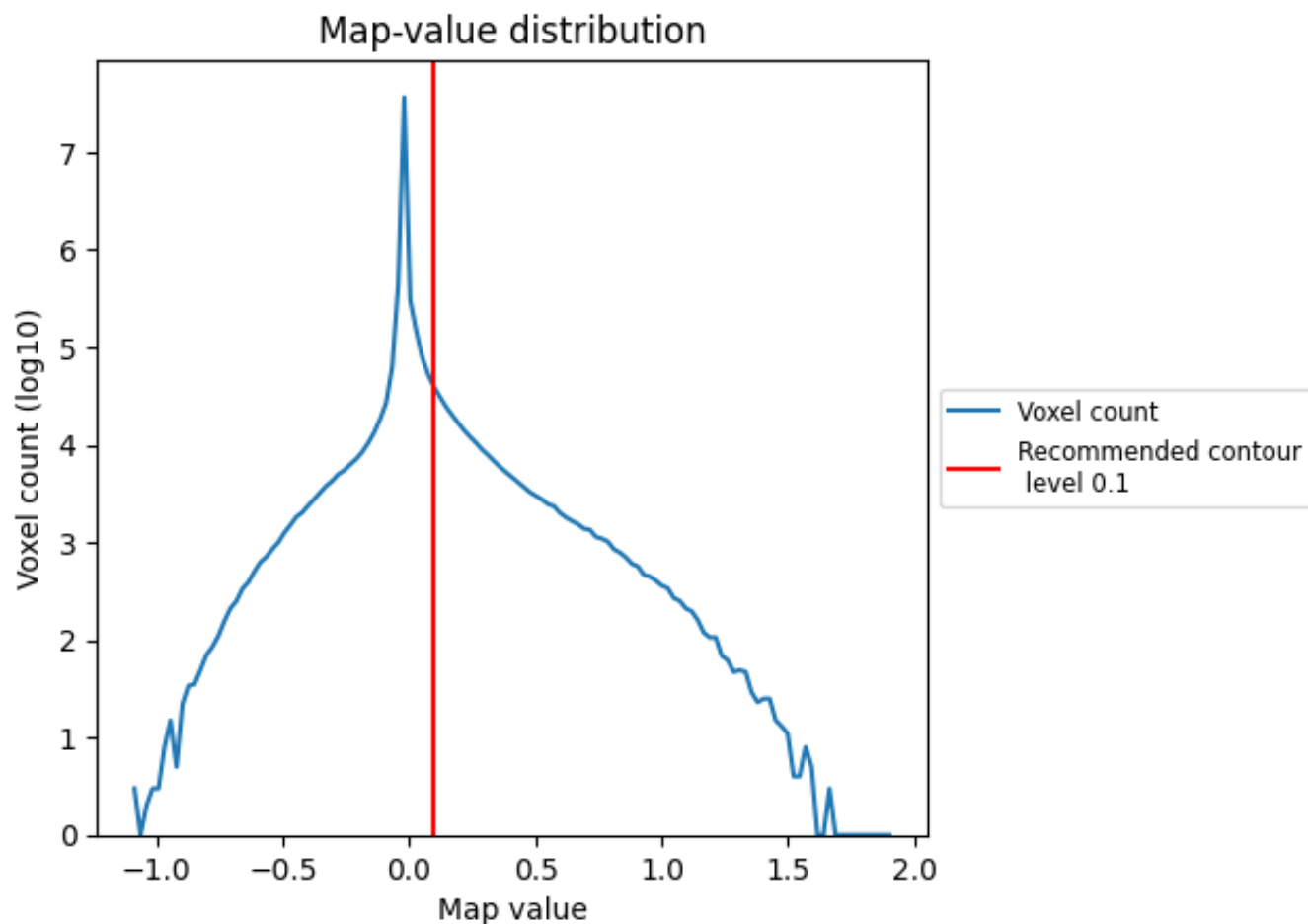
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

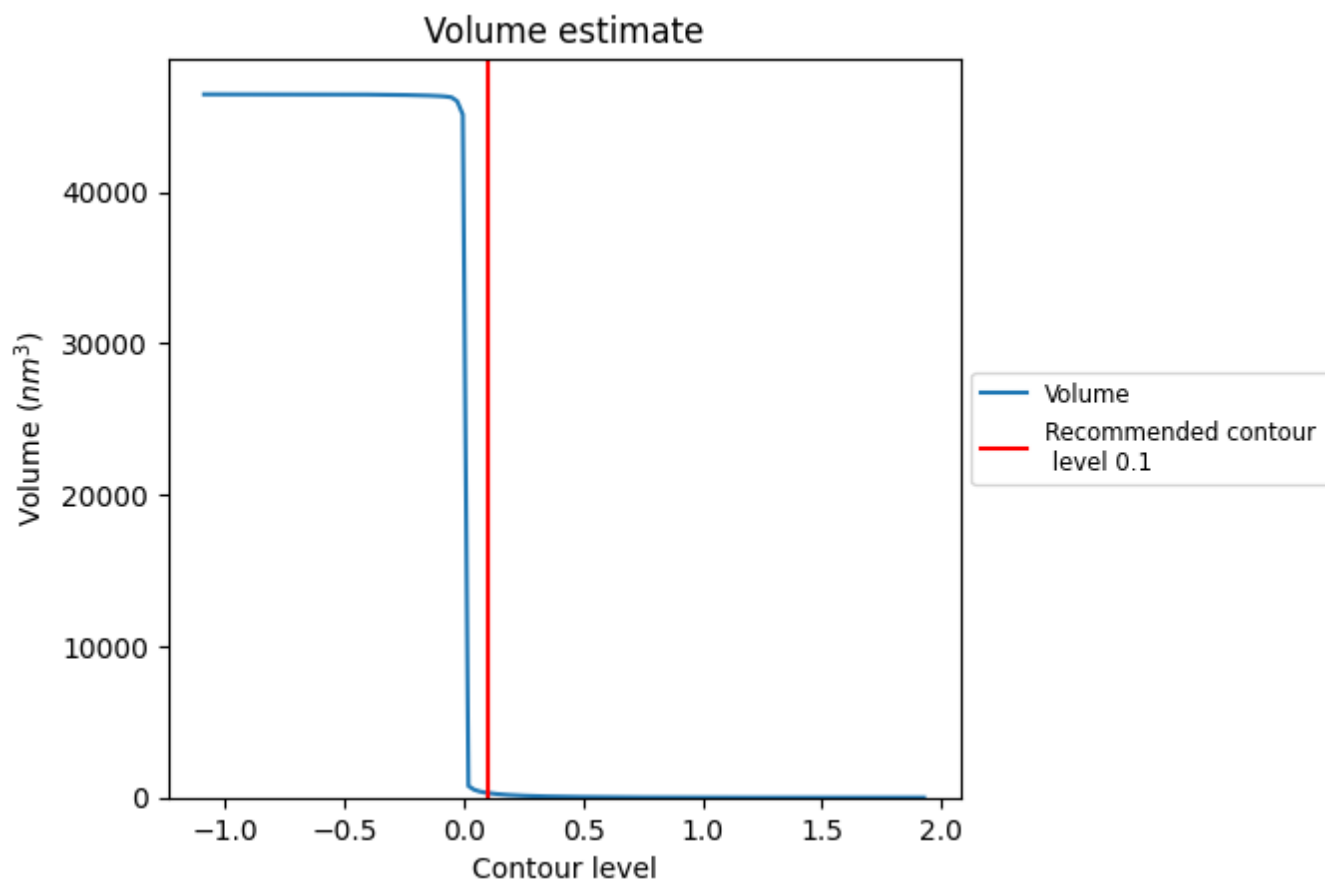
This section contains the results of statistical analysis of the map.

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.

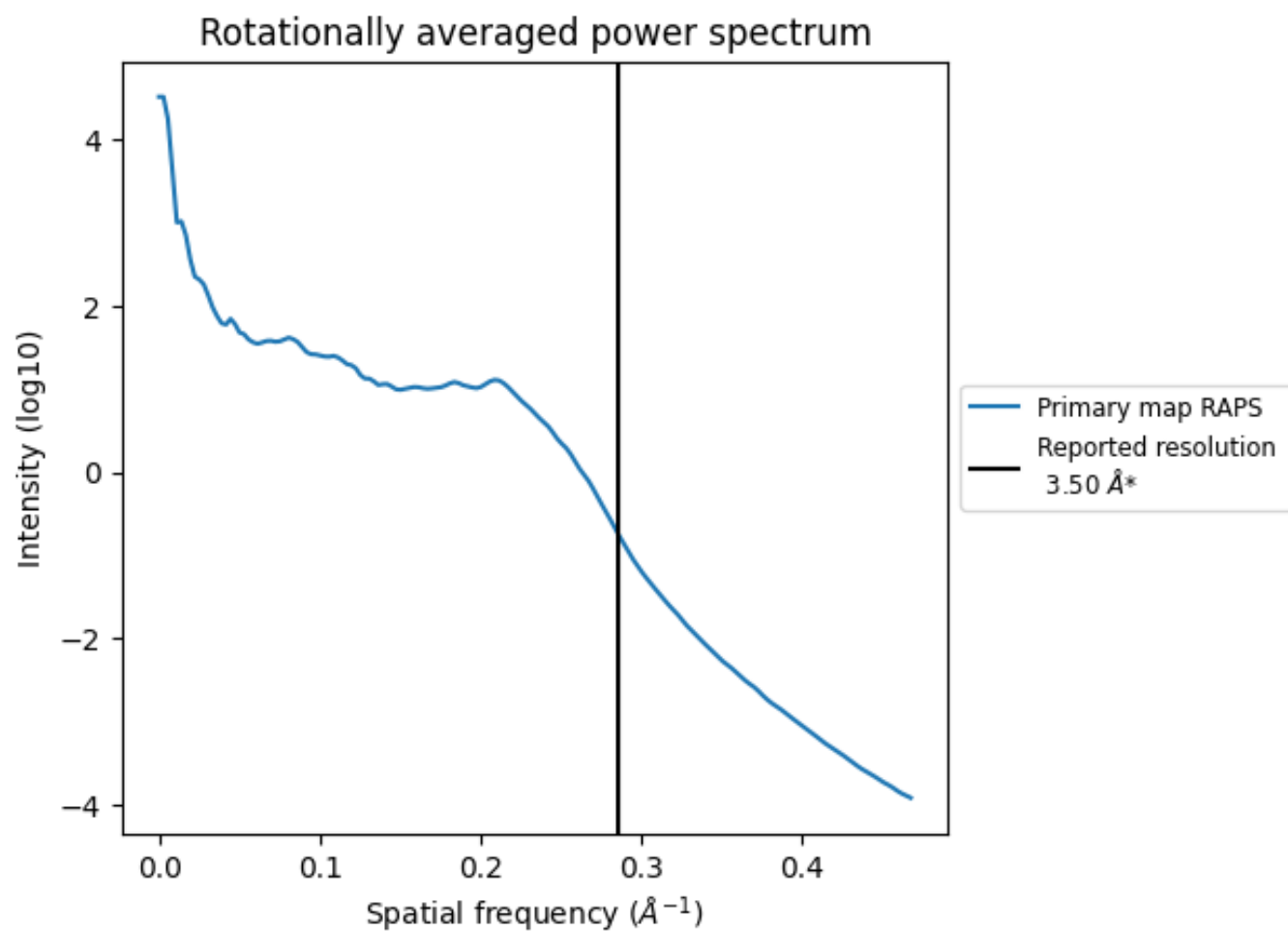
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 305 nm³; this corresponds to an approximate mass of 276 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 0.286 Å⁻¹

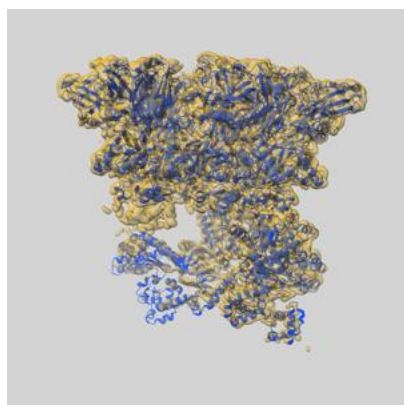
8 Fourier-Shell correlation

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

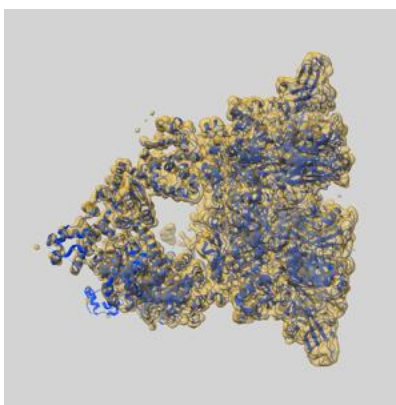
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11522 and PDB model 6ZXJ. Per-residue inclusion information can be found in section [3](#) on page [9](#).

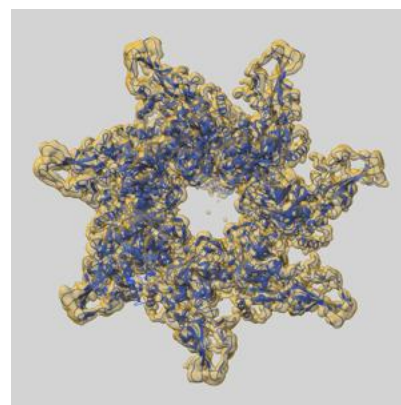
9.1 Map-model overlay [i](#)



X



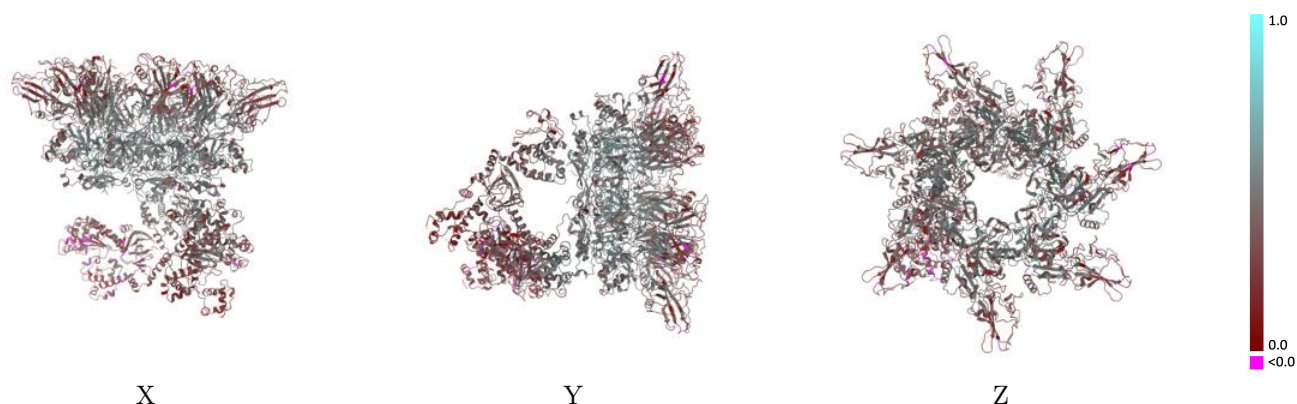
Y



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](#)

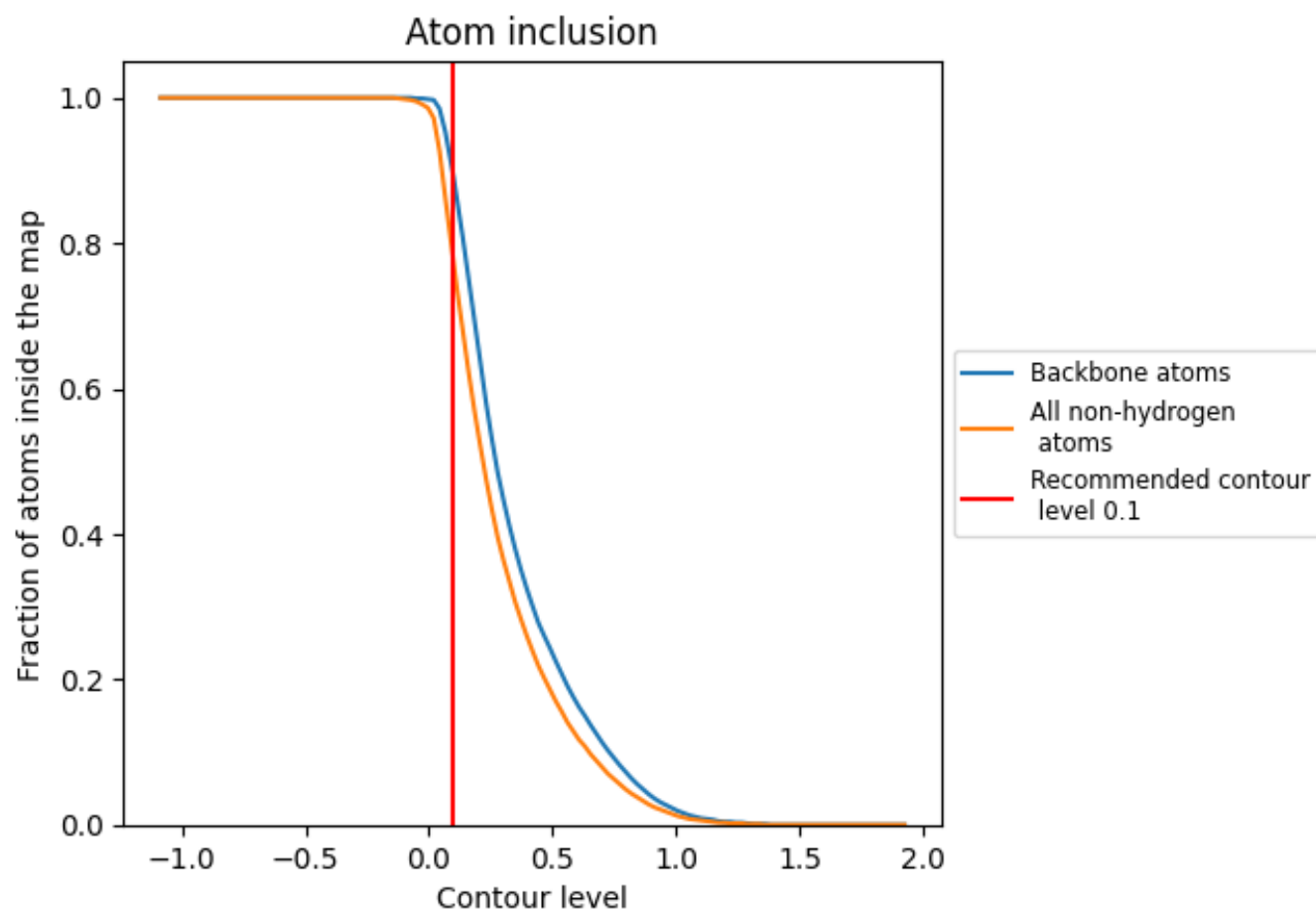


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 77% 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	0.7730	0.3960
A	0.8360	0.4270
B	0.8440	0.4340
C	0.8440	0.4310
D	0.8490	0.4340
E	0.8290	0.4230
F	0.8220	0.4200
G	0.8260	0.4200
H	0.6820	0.3330
I	0.5190	0.2900

1.0

0.0

<0.0