



## Full wwPDB EM Validation Report ⓘ

May 31, 2025 – 02:15 PM EDT

PDB ID : 9D94 / pdb\_00009d94  
EMDB ID : EMD-46669  
Title : Mycobacteriophage Bxb1 portal and connector assembly - Composite map and model  
Authors : Freeman, K.G.  
Deposited on : 2024-08-20  
Resolution : 3.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

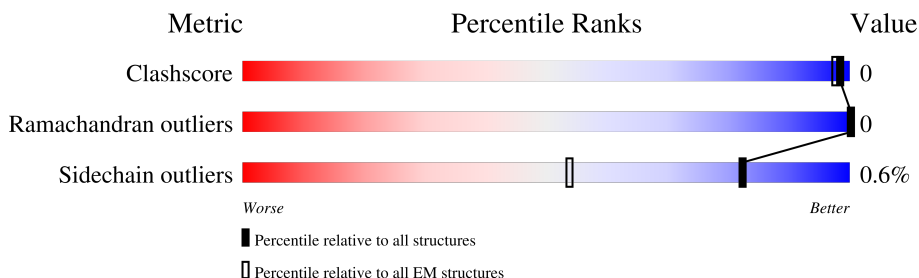
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	Fa	488	<div> <div>21%</div> <div>89%</div> <div>8%</div> </div>
1	Fb	488	<div> <div>19%</div> <div>89%</div> <div>8%</div> </div>
1	Fc	488	<div> <div>22%</div> <div>90%</div> <div>8%</div> </div>
1	Fd	488	<div> <div>20%</div> <div>91%</div> <div>8%</div> </div>
1	Fe	488	<div> <div>22%</div> <div>90%</div> <div>8%</div> </div>
1	Ff	488	<div> <div>19%</div> <div>89%</div> <div>8%</div> </div>
1	Fg	488	<div> <div>20%</div> <div>90%</div> <div>8%</div> </div>
1	Fh	488	<div> <div>21%</div> <div>89%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	Fi	488	
1	Fj	488	
1	Fk	488	
1	Fl	488	
2	Ga	125	
2	Gb	125	
2	Gc	125	
2	Gd	125	
2	Ge	125	
2	Gf	125	
2	Gg	125	
2	Gh	125	
2	Gi	125	
2	Gj	125	
2	Gk	125	
2	Gl	125	
3	Ha	126	
3	Hb	126	
3	Hc	126	
3	Hd	126	
3	He	126	
3	Hf	126	
4	Ia	148	
4	Ib	148	
4	Ic	148	

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Mol	Chain	Length	Quality of chain
4	Id	148	
4	Ie	148	
4	If	148	
5	Ja	283	
5	Jb	283	
5	Jc	283	
5	Jd	283	
5	Je	283	
5	Jf	283	
5	Jg	283	
5	Jh	283	
5	Ji	283	
5	Jj	283	
5	Jk	283	
5	Jl	283	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 181089 atoms, of which 89475 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 Portal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	Fa	450	Total 6952	C 2219	H 3426	N 603	O 690	S 14	0	0
1	Fb	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
1	Fc	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
1	Fd	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
1	Fe	450	Total 6952	C 2219	H 3426	N 603	O 690	S 14	0	0
1	Ff	450	Total 6952	C 2219	H 3426	N 603	O 690	S 14	0	0
1	Fg	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
1	Fh	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
1	Fi	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
1	Fj	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
1	Fk	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
1	Fl	450	Total 6952	C 2219	H 3426	N 603	O 690	S 14	0	0

- Molecule 2 is a protein called Head-to-tail adaptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Ga	124	Total 1981	C 624	H 1000	N 169	O 186	S 2	0	0
2	Gb	124	Total 1981	C 624	H 1000	N 169	O 186	S 2	0	0
2	Gc	124	Total 1981	C 624	H 1000	N 169	O 186	S 2	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	Gd	124	Total 1981	C 624	H 1000	N 169	O 186	S 2	0	0
2	Ge	124	Total 1981	C 624	H 1000	N 169	O 186	S 2	0	0
2	Gf	124	Total 1981	C 624	H 1000	N 169	O 186	S 2	0	0
2	Gg	124	Total 1981	C 624	H 1000	N 169	O 186	S 2	0	0
2	Gh	124	Total 1981	C 624	H 1000	N 169	O 186	S 2	0	0
2	Gi	124	Total 1981	C 624	H 1000	N 169	O 186	S 2	0	0
2	Gj	124	Total 1981	C 624	H 1000	N 169	O 186	S 2	0	0
2	Gk	124	Total 1981	C 624	H 1000	N 169	O 186	S 2	0	0
2	Gl	124	Total 1981	C 624	H 1000	N 169	O 186	S 2	0	0

- Molecule 3 is a protein called Head-to-tail stopper.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	Ha	125	Total 1970	C 617	H 973	N 185	O 192	S 3	0	0
3	Hb	125	Total 1970	C 617	H 973	N 185	O 192	S 3	0	0
3	Hc	125	Total 1971	C 617	H 974	N 185	O 192	S 3	0	0
3	Hd	125	Total 1971	C 617	H 974	N 185	O 192	S 3	0	0
3	He	125	Total 1970	C 617	H 973	N 185	O 192	S 3	0	0
3	Hf	125	Total 1971	C 617	H 974	N 185	O 192	S 3	0	0

- Molecule 4 is a protein called Tail terminator.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	Ia	147	Total	C	H	N	O	S	0	0
			2279	723	1143	200	211	2		
4	Ib	147	Total	C	H	N	O	S	0	0
			2279	723	1143	200	211	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ic	147	Total	C	H	N	O	S	
			2279	723	1143	200	211	2	0
4	Id	147	Total	C	H	N	O	S	
			2279	723	1143	200	211	2	0
4	Ie	147	Total	C	H	N	O	S	
			2279	723	1143	200	211	2	0
4	If	147	Total	C	H	N	O	S	
			2280	723	1144	200	211	2	0

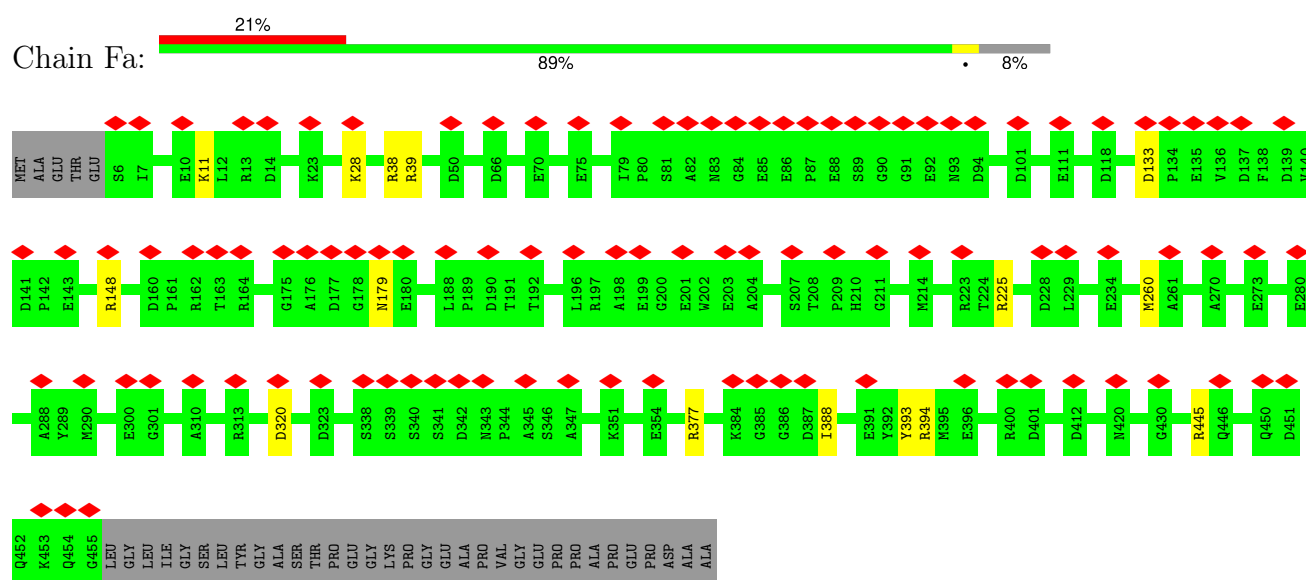
- Molecule 5 is a protein called Major tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ja	282	Total	C	H	N	O		
			4163	1345	2039	344	435	0	0
5	Jb	267	Total	C	H	N	O		
			3895	1264	1900	318	413	0	0
5	Jc	282	Total	C	H	N	O		
			4163	1345	2039	344	435	0	0
5	Jd	270	Total	C	H	N	O		
			3949	1279	1929	324	417	0	0
5	Je	282	Total	C	H	N	O		
			4163	1345	2039	344	435	0	0
5	Jf	282	Total	C	H	N	O		
			4163	1345	2039	344	435	0	0
5	Jg	282	Total	C	H	N	O		
			4163	1345	2039	344	435	0	0
5	Jh	267	Total	C	H	N	O		
			3894	1263	1901	318	412	0	0
5	Ji	265	Total	C	H	N	O		
			3869	1256	1889	316	408	0	0
5	Jj	282	Total	C	H	N	O		
			4163	1345	2039	344	435	0	0
5	Jk	265	Total	C	H	N	O		
			3869	1256	1889	316	408	0	0
5	Jl	270	Total	C	H	N	O		
			3949	1279	1929	324	417	0	0

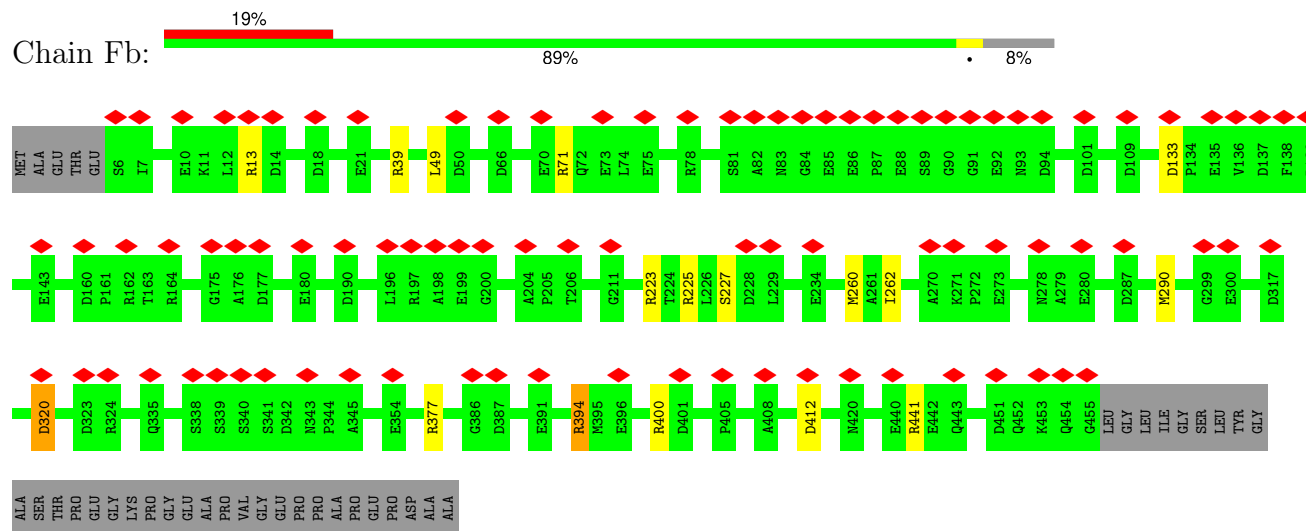
### 3 Residue-property plots

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: Portal protein

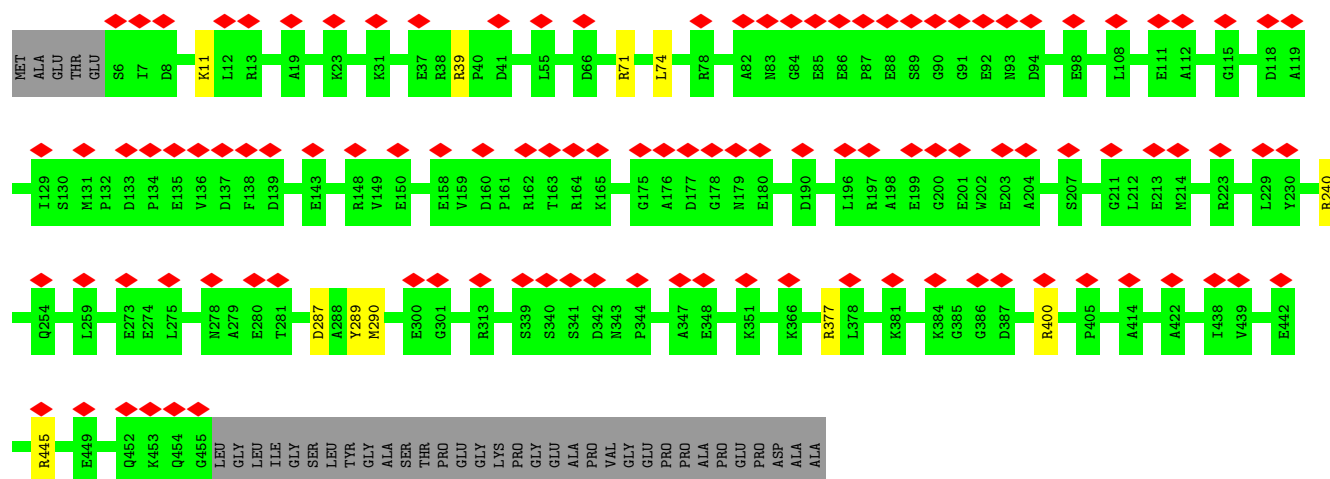
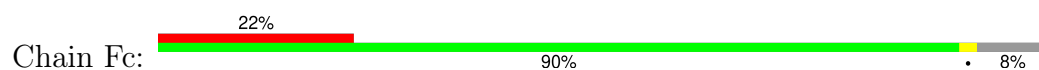


- Molecule 1: Portal protein

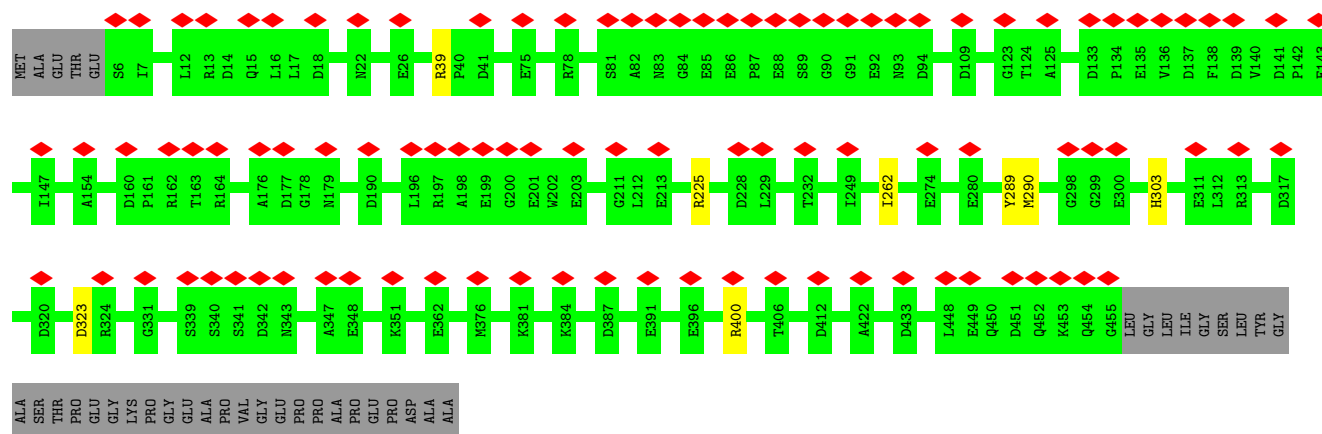
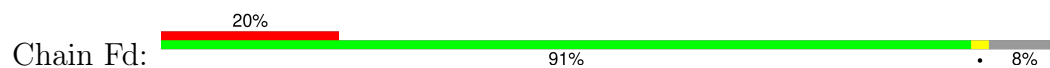


- Molecule 1: Portal protein

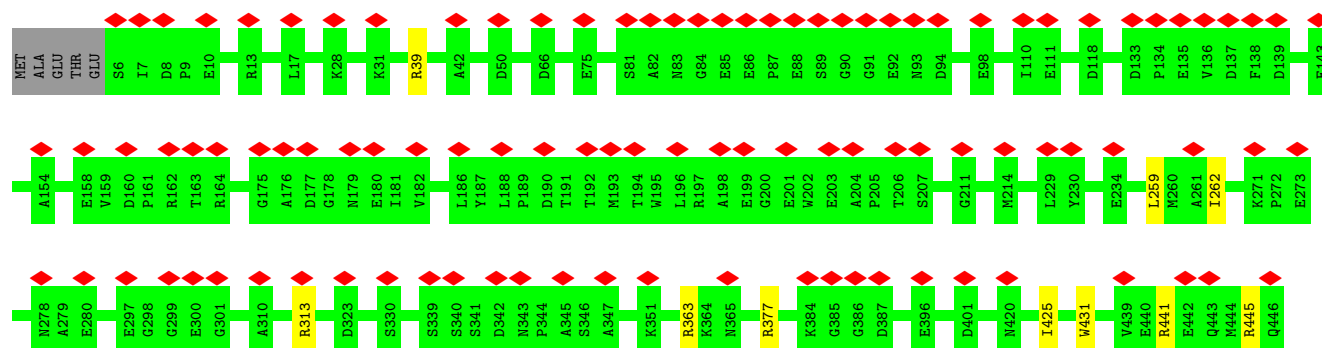
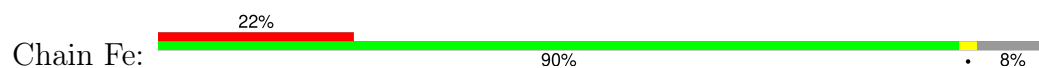


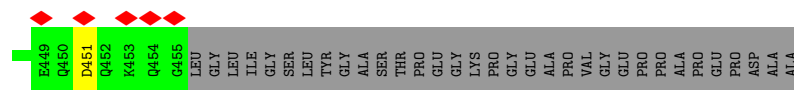


• Molecule 1: Portal protein

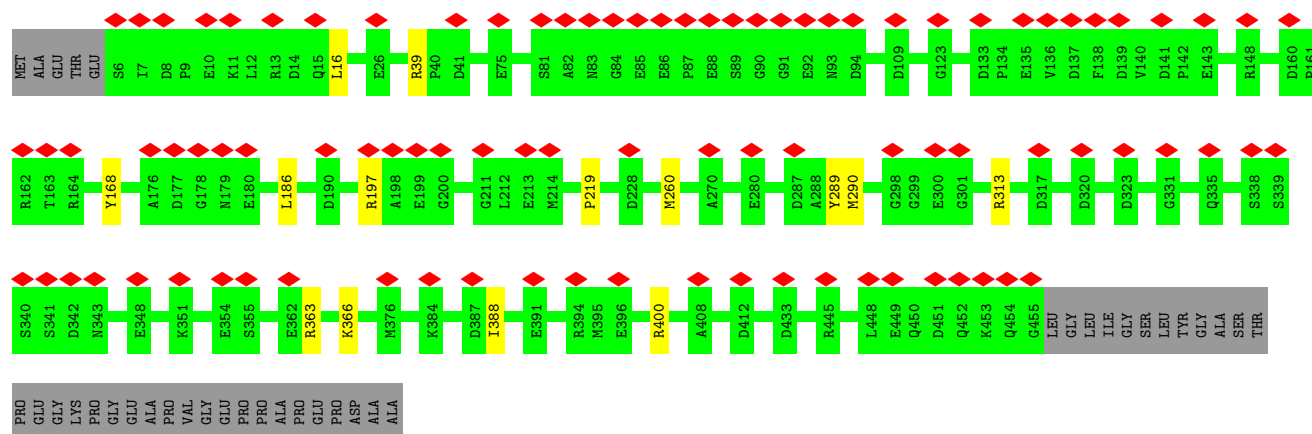
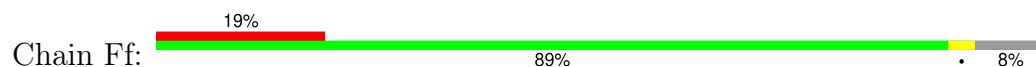


• Molecule 1: Portal protein

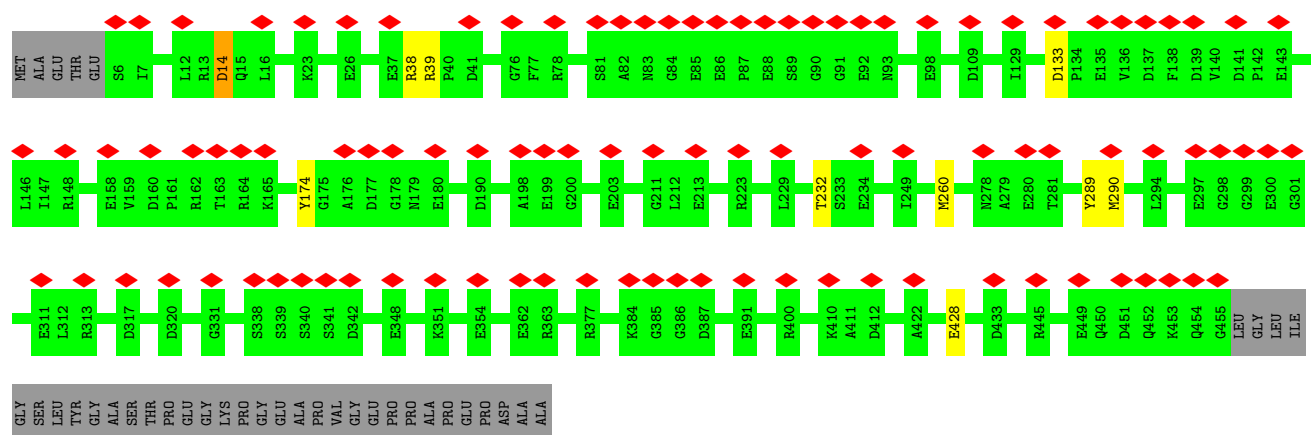
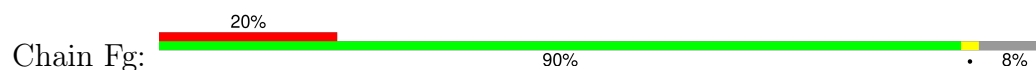




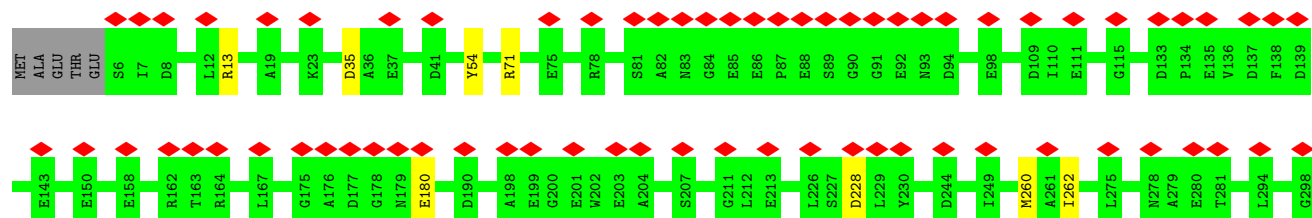
- Molecule 1: Portal protein

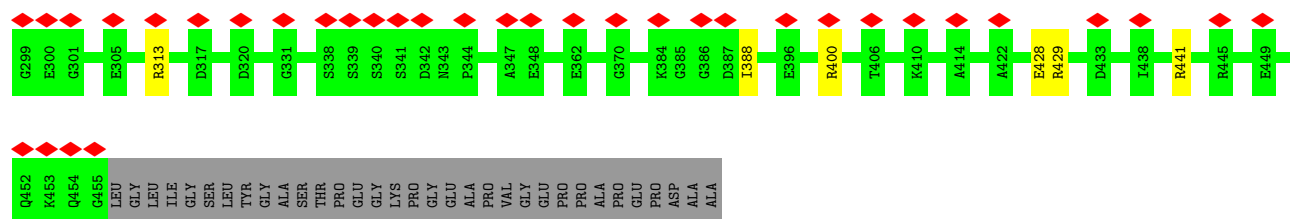


- Molecule 1: Portal protein

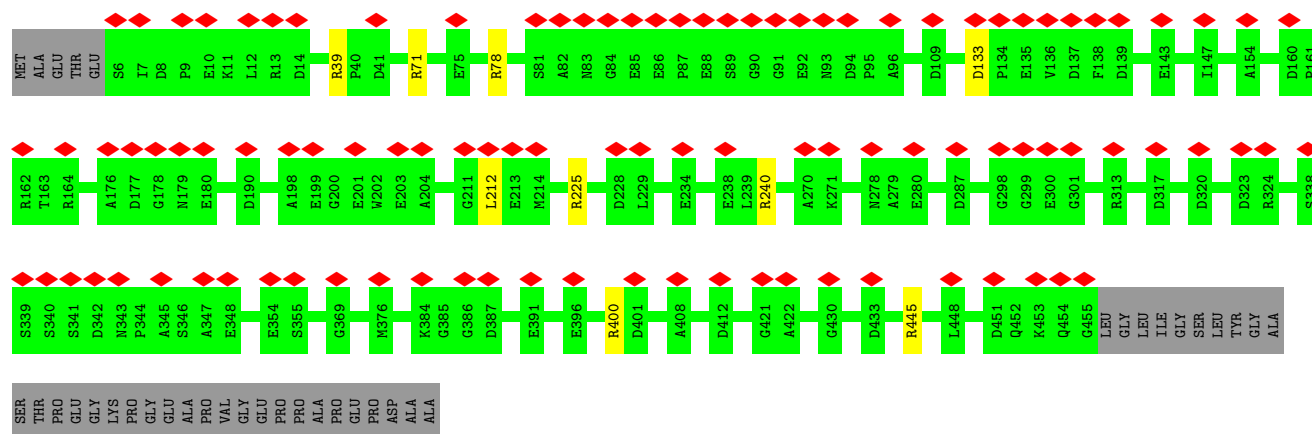
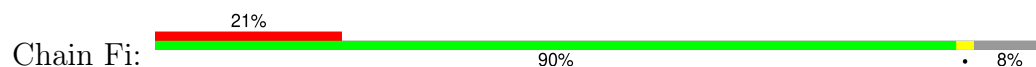


- Molecule 1: Portal protein

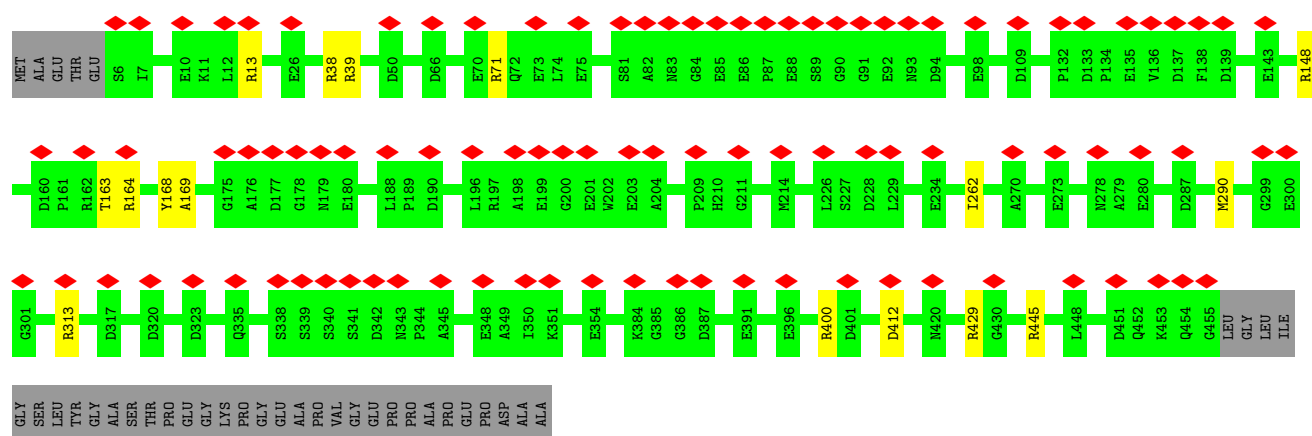
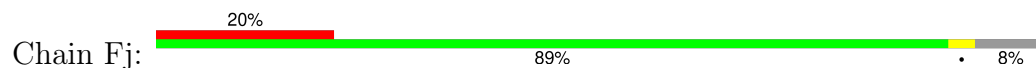




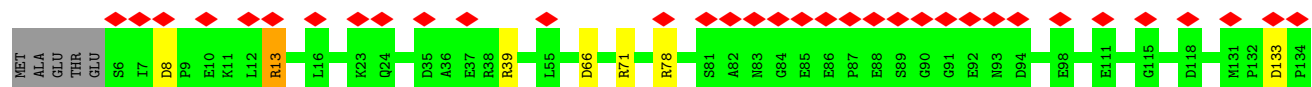
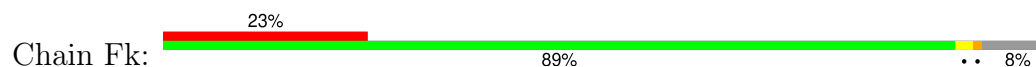
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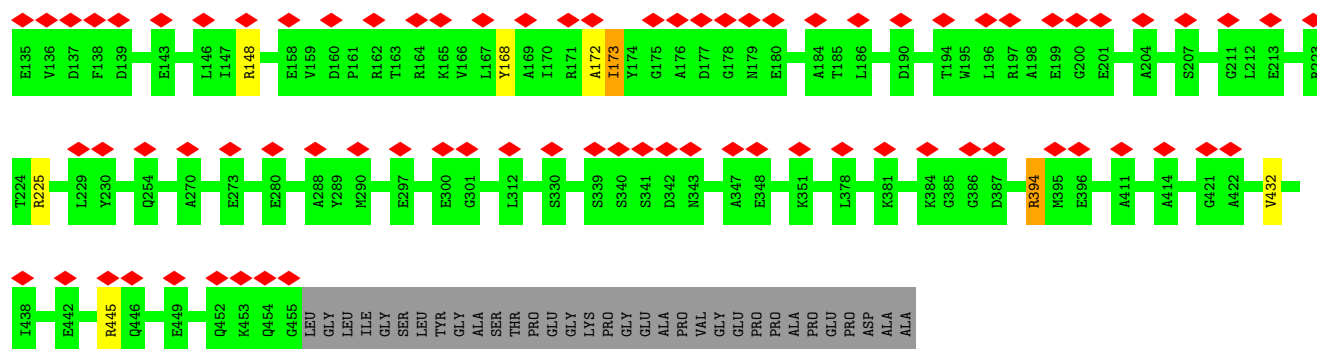


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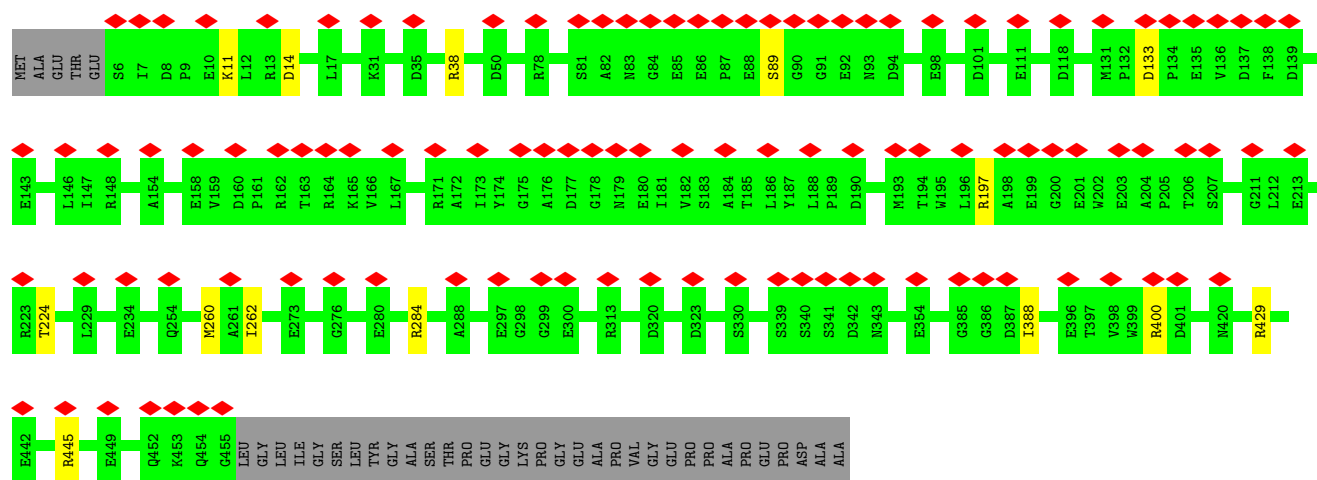
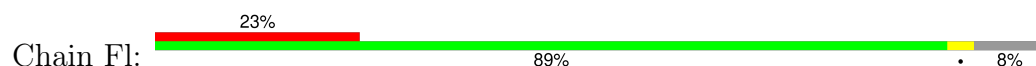


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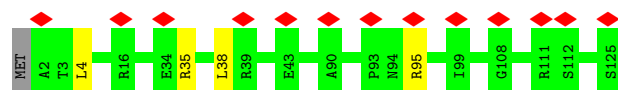




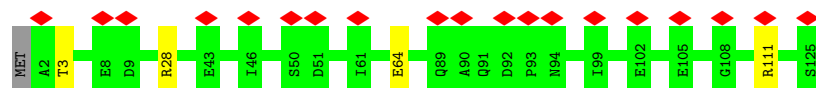
- Molecule 1: Portal protein



- Molecule 2: Head-to-tail adaptor

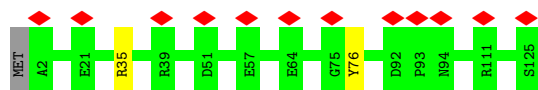


- Molecule 2: Head-to-tail adaptor

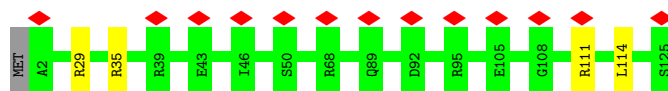


- Molecule 2: Head-to-tail adaptor

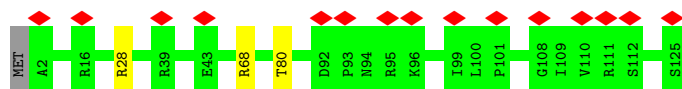




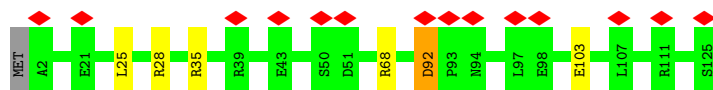
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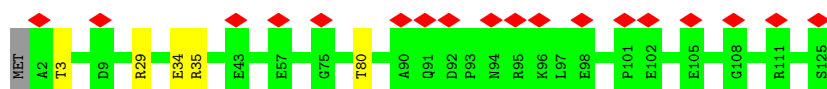
- Molecule 2: Head-to-tail adaptor



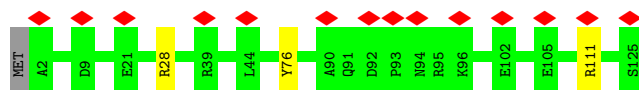
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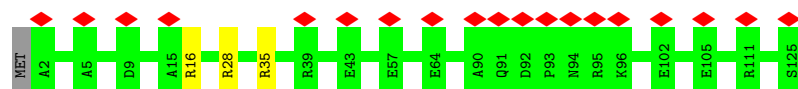
- Molecule 2: Head-to-tail adaptor



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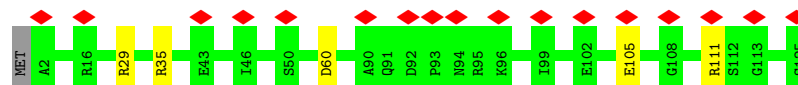
- Molecule 2: Head-to-tail adaptor



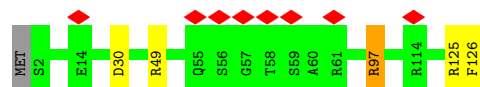
- Molecule 2: Head-to-tail adaptor



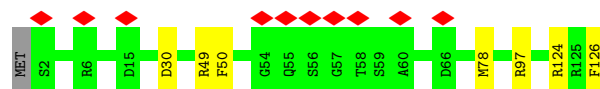
- Molecule 2: Head-to-tail adaptor



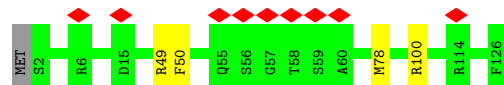
- Molecule 3: Head-to-tail stopper



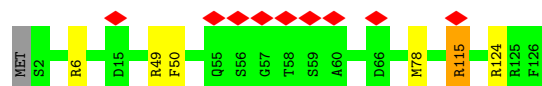
- Molecule 3: Head-to-tail stopper



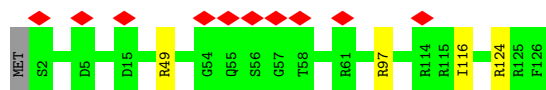
- Molecule 3: Head-to-tail stopper



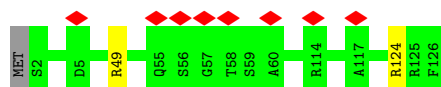
- Molecule 3: Head-to-tail stopper



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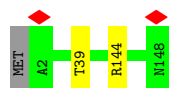
- Molecule 4: Tail terminator



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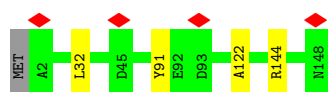


- Molecule 4: Tail terminator

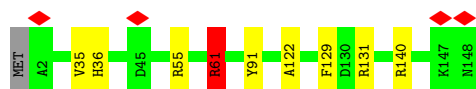


- Molecule 4: Tail terminator

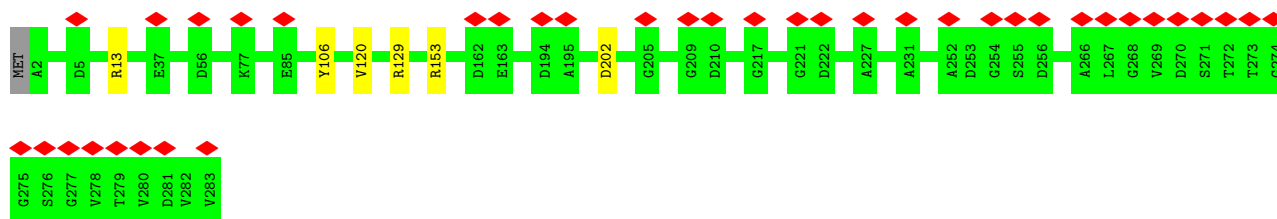




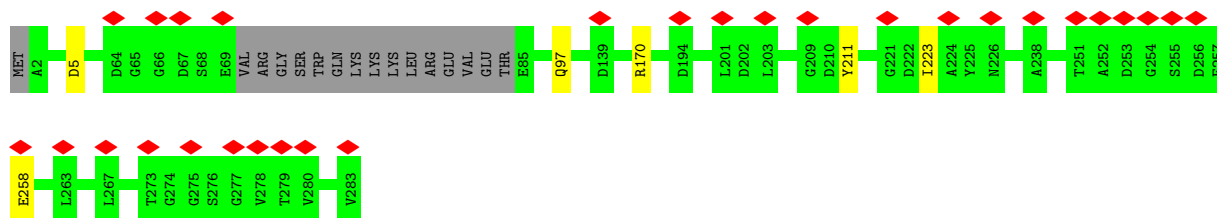
- Molecule 4: Tail terminator



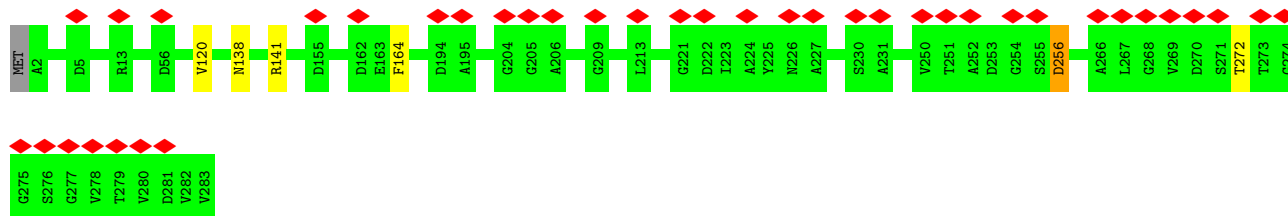
- Molecule 5: Major tail protein



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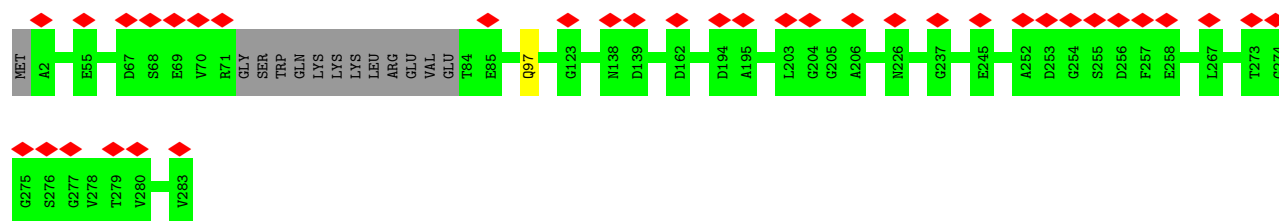
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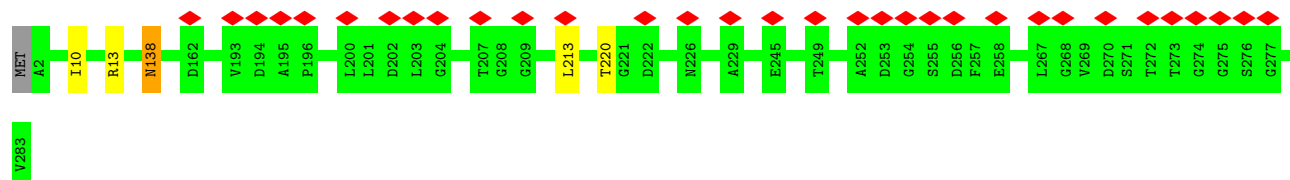






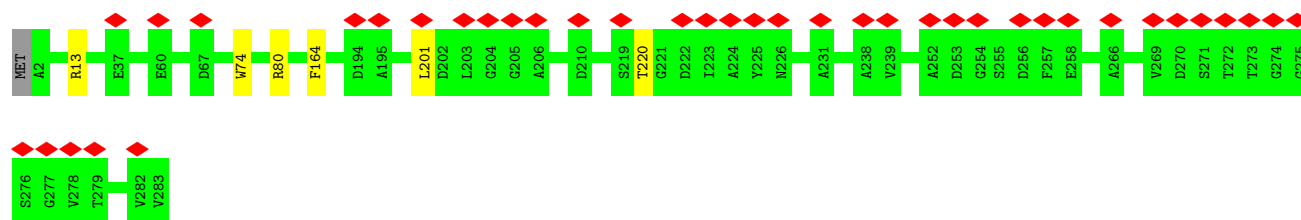
- Molecule 5: Major tail protein

Chain Je: 11% 98%



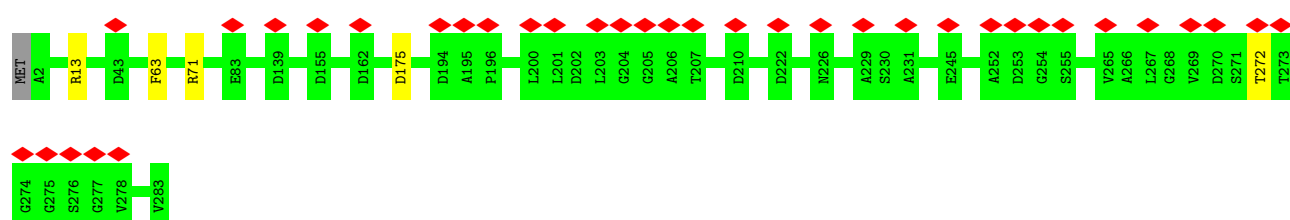
- Molecule 5: Major tail protein

Chain Jf: 14% 98%



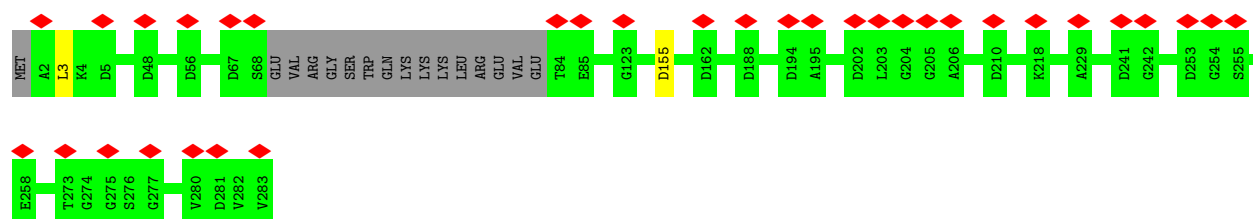
- Molecule 5: Major tail protein

Chain Jg: 13% 98%

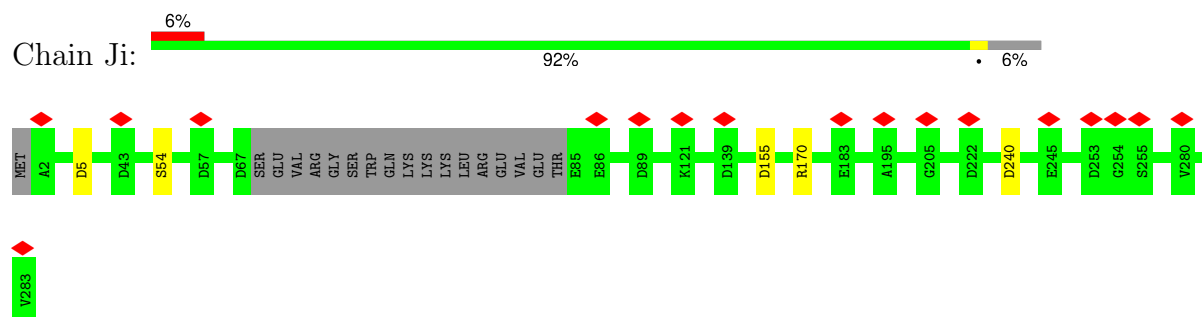


- Molecule 5: Major tail protein

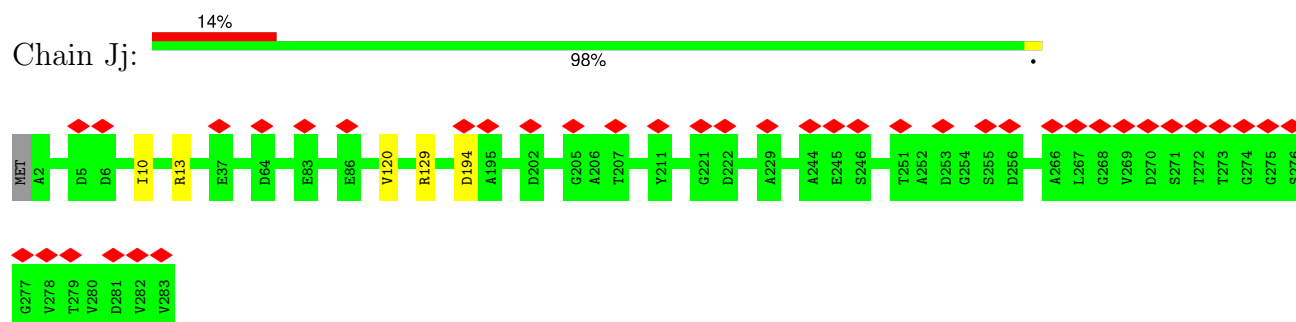
Chain Jh: 12% 94% 6%



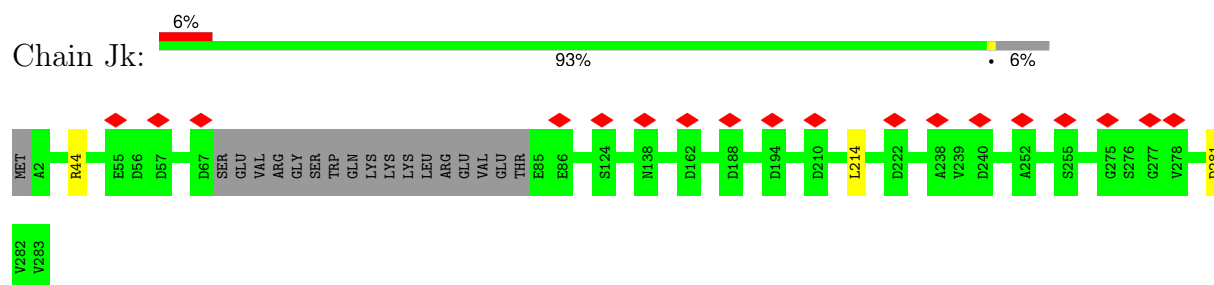
## • Molecule 5: Major tail protein



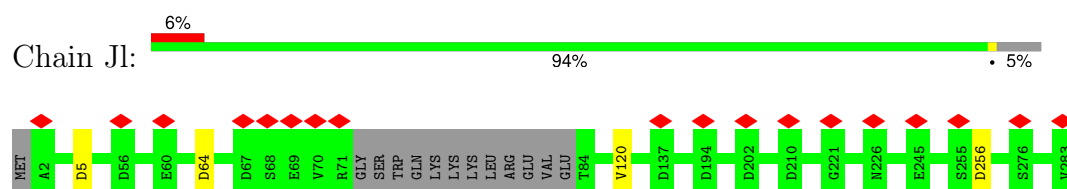
## • Molecule 5: Major tail protein



## • Molecule 5: Major tail protein



## • Molecule 5: Major tail protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	22590	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	50.461	Depositor
Minimum map value	-20.836	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.996	Depositor
Recommended contour level	6	Depositor
Map size (Å)	539.84, 539.84, 539.84	wwPDB
Map dimensions	482, 482, 482	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	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	Fa	0.73	0/3606	1.26	9/4901 (0.2%)
1	Fb	0.73	0/3606	1.25	10/4901 (0.2%)
1	Fc	0.73	0/3606	1.25	6/4901 (0.1%)
1	Fd	0.73	0/3606	1.25	5/4901 (0.1%)
1	Fe	0.72	0/3606	1.24	7/4901 (0.1%)
1	Ff	0.73	0/3606	1.24	6/4901 (0.1%)
1	Fg	0.72	0/3606	1.25	5/4901 (0.1%)
1	Fh	0.73	0/3606	1.24	6/4901 (0.1%)
1	Fi	0.73	0/3606	1.26	6/4901 (0.1%)
1	Fj	0.73	0/3606	1.26	11/4901 (0.2%)
1	Fk	0.72	0/3606	1.26	11/4901 (0.2%)
1	Fl	0.73	0/3606	1.26	9/4901 (0.2%)
2	Ga	0.73	0/998	1.29	2/1360 (0.1%)
2	Gb	0.71	0/998	1.25	2/1360 (0.1%)
2	Gc	0.71	0/998	1.23	1/1360 (0.1%)
2	Gd	0.72	0/998	1.28	4/1360 (0.3%)
2	Ge	0.71	0/998	1.24	2/1360 (0.1%)
2	Gf	0.72	0/998	1.56	7/1360 (0.5%)
2	Gg	0.72	0/998	1.31	2/1360 (0.1%)
2	Gh	0.70	0/998	1.25	2/1360 (0.1%)
2	Gi	0.71	0/998	1.26	3/1360 (0.2%)
2	Gj	0.72	0/998	1.26	2/1360 (0.1%)
2	Gk	0.72	0/998	1.27	3/1360 (0.2%)
2	Gl	0.72	0/998	1.26	3/1360 (0.2%)
3	Ha	0.80	0/1017	1.36	4/1371 (0.3%)
3	Hb	0.80	0/1017	1.32	3/1371 (0.2%)
3	Hc	0.80	0/1017	1.30	2/1371 (0.1%)
3	Hd	0.79	0/1017	1.34	2/1371 (0.1%)
3	He	0.81	0/1017	1.33	2/1371 (0.1%)
3	Hf	0.80	0/1017	1.31	1/1371 (0.1%)
4	Ia	0.78	0/1166	1.28	2/1595 (0.1%)
4	Ib	0.78	0/1166	1.29	4/1595 (0.3%)
4	Ic	0.77	0/1166	1.27	2/1595 (0.1%)
4	Id	0.78	0/1166	1.27	4/1595 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	Ie	0.77	0/1166	1.26	1/1595 (0.1%)
4	If	0.78	0/1166	1.33	5/1595 (0.3%)
5	Ja	0.70	0/2167	1.24	3/2958 (0.1%)
5	Jb	0.70	0/2035	1.21	1/2781 (0.0%)
5	Jc	0.70	0/2167	1.23	2/2958 (0.1%)
5	Jd	0.70	0/2060	1.25	1/2815 (0.0%)
5	Je	0.71	0/2167	1.24	1/2958 (0.0%)
5	Jf	0.69	0/2167	1.24	4/2958 (0.1%)
5	Jg	0.70	0/2167	1.24	2/2958 (0.1%)
5	Jh	0.69	0/2033	1.21	2/2779 (0.1%)
5	Ji	0.70	0/2020	1.24	4/2761 (0.1%)
5	Jj	0.68	0/2167	1.22	3/2958 (0.1%)
5	Jk	0.69	0/2020	1.22	2/2761 (0.1%)
5	Jl	0.68	0/2060	1.22	3/2815 (0.1%)
All	All	0.73	0/93576	1.26	184/127388 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Fb	0	2
1	Fc	0	2
1	Fd	0	1
1	Fe	0	1
1	Ff	0	3
1	Fg	0	1
1	Fh	0	2
1	Fi	0	2
1	Fj	0	2
1	Fk	0	4
1	Fl	0	1
2	Gc	0	1
2	Gh	0	1
2	Gj	0	1
3	Ha	0	2
3	Hb	0	2
3	Hd	0	3
3	He	0	1
3	Hf	0	1
4	Ia	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	Id	0	1
4	If	0	1
5	Ja	0	2
5	Jb	0	1
5	Jc	0	1
5	Je	0	1
5	Jg	0	1
All	All	0	42

There are no bond length outliers.

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Gf	103	GLU	CG-CD-OE1	19.33	162.86	118.40
2	Gf	103	GLU	OE1-CD-OE2	-18.49	78.52	122.90
2	Gf	103	GLU	CG-CD-OE2	-14.78	84.41	118.40
4	If	61	ARG	NE-CZ-NH2	8.24	126.62	119.20
1	Fj	71	ARG	NE-CZ-NH2	7.75	126.17	119.20
1	Fk	445	ARG	NE-CZ-NH2	7.31	125.78	119.20
3	Hc	49	ARG	NE-CZ-NH2	7.30	125.77	119.20
1	Fb	400	ARG	NE-CZ-NH2	7.09	125.58	119.20
5	Ja	106	TYR	CA-C-N	6.95	131.03	119.35
5	Ja	106	TYR	C-N-CA	6.95	131.03	119.35
1	Fg	133	ASP	CA-CB-CG	6.90	119.50	112.60
1	Fd	400	ARG	NE-CZ-NH2	6.84	125.36	119.20
1	Fh	400	ARG	NE-CZ-NH2	6.84	125.36	119.20
1	Fi	400	ARG	NE-CZ-NH2	6.81	125.33	119.20
1	Fe	451	ASP	CA-CB-CG	6.71	119.31	112.60
2	Gf	68	ARG	NE-CZ-NH2	6.69	125.22	119.20
4	Ic	144	ARG	NE-CZ-NH2	6.66	125.19	119.20
2	Gk	35	ARG	NE-CZ-NH2	6.60	125.14	119.20
1	Fd	290	MET	N-CA-C	6.58	118.11	111.07
1	Fb	394	ARG	NE-CZ-NH2	6.57	125.11	119.20
2	Ga	35	ARG	NE-CZ-NH2	6.54	125.08	119.20
1	Fa	133	ASP	CA-CB-CG	6.31	118.91	112.60
1	Fk	394	ARG	NE-CZ-NH2	6.28	124.85	119.20
1	Fg	14	ASP	CA-CB-CG	6.27	118.87	112.60
1	Ff	363	ARG	NE-CZ-NH2	6.26	124.84	119.20
1	Fl	445	ARG	NE-CZ-NH2	6.25	124.82	119.20
2	Gj	28	ARG	NE-CZ-NH2	6.22	124.80	119.20
2	Gf	92	ASP	CA-CB-CG	6.21	118.81	112.60
1	Fi	445	ARG	NE-CZ-NH2	6.13	124.72	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Fh	228	ASP	CA-CB-CG	6.10	118.70	112.60
1	Ff	290	MET	N-CA-C	6.09	118.45	111.02
5	Ji	170	ARG	NE-CZ-NH2	6.09	124.68	119.20
5	Ji	240	ASP	CA-CB-CG	6.08	118.68	112.60
1	Fk	133	ASP	CA-CB-CG	6.04	118.64	112.60
1	Fd	39	ARG	NE-CZ-NH2	6.02	124.61	119.20
1	Ff	39	ARG	NE-CZ-NH2	6.01	124.61	119.20
2	Gi	29	ARG	NE-CZ-NH2	5.99	124.59	119.20
4	Ia	55	ARG	NE-CZ-NH2	5.97	124.57	119.20
4	Id	55	ARG	NE-CZ-NH2	5.96	124.56	119.20
3	Hb	126	PHE	CA-CB-CG	5.95	119.75	113.80
1	Fk	66	ASP	CA-CB-CG	5.91	118.50	112.60
1	Fe	363	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	Fb	320	ASP	CA-CB-CG	5.88	118.48	112.60
1	Fl	133	ASP	CA-CB-CG	5.84	118.44	112.60
4	Id	140	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	Fi	133	ASP	CA-CB-CG	5.82	118.42	112.60
4	If	131	ARG	NE-CZ-NH2	5.81	124.43	119.20
2	Gd	35	ARG	NE-CZ-NH2	5.80	124.42	119.20
2	Gg	35	ARG	NE-CZ-NH2	5.80	124.42	119.20
2	Gb	111	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	Fj	412	ASP	CA-CB-CG	5.78	118.38	112.60
1	Fc	287	ASP	CA-CB-CG	5.78	118.38	112.60
2	Gk	28	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	Fe	313	ARG	NE-CZ-NH2	5.77	124.39	119.20
5	Jg	175	ASP	CA-CB-CG	5.76	118.36	112.60
1	Fj	445	ARG	NE-CZ-NH2	5.75	124.38	119.20
1	Fg	290	MET	N-CA-C	5.73	118.01	111.02
5	Jj	13	ARG	NE-CZ-NH2	5.73	124.35	119.20
4	Ie	144	ARG	NE-CZ-NH2	5.72	124.35	119.20
2	Gf	28	ARG	NE-CZ-NH2	5.72	124.35	119.20
4	Ib	19	HIS	CB-CG-CD2	-5.70	123.80	131.20
1	Fl	197	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	Ff	313	ARG	NE-CZ-NH2	5.69	124.32	119.20
5	Jj	194	ASP	CA-CB-CG	5.68	118.28	112.60
5	Jl	64	ASP	CA-CB-CG	5.68	118.28	112.60
1	Fj	39	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	Ff	400	ARG	NE-CZ-NH2	5.67	124.30	119.20
2	Ge	28	ARG	NE-CZ-NH2	5.65	124.29	119.20
1	Fa	39	ARG	NE-CZ-NH2	5.64	124.28	119.20
2	Gk	60	ASP	CA-CB-CG	5.63	118.23	112.60
4	Ib	131	ARG	NE-CZ-NH2	5.63	124.27	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	If	140	ARG	NE-CZ-NH2	5.63	124.26	119.20
5	Jl	5	ASP	CA-CB-CG	5.62	118.22	112.60
2	Gf	35	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	Fk	13	ARG	NE-CZ-NH2	5.60	124.24	119.20
5	Jf	80	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	Fb	39	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	Fb	13	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	Fl	400	ARG	NE-CZ-NH2	5.54	124.19	119.20
3	Ha	97	ARG	NE-CZ-NH2	5.54	124.18	119.20
1	Fc	400	ARG	NE-CZ-NH2	5.53	124.18	119.20
3	Hd	124	ARG	NE-CZ-NH2	5.53	124.17	119.20
1	Fb	71	ARG	NE-CZ-NH2	5.52	124.17	119.20
2	Gl	35	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	Fj	13	ARG	NE-CZ-NH2	5.51	124.16	119.20
5	Jf	74	TRP	CA-C-N	5.50	128.11	120.63
5	Jf	74	TRP	C-N-CA	5.50	128.11	120.63
1	Fa	320	ASP	CA-CB-CG	5.49	118.09	112.60
3	Ha	30	ASP	CA-CB-CG	5.48	118.08	112.60
2	Gj	35	ARG	NE-CZ-NH2	5.47	124.13	119.20
1	Fj	164	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	Fj	400	ARG	NE-CZ-NH2	5.47	124.12	119.20
4	Id	148	ASN	CA-CB-CG	5.45	118.05	112.60
1	Fa	394	ARG	NE-CZ-NH2	5.43	124.09	119.20
4	Ic	144	ARG	CD-NE-CZ	5.43	132.01	124.40
1	Fj	148	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	Fk	173	ILE	N-CA-C	5.43	117.91	108.95
1	Fl	14	ASP	CA-CB-CG	5.43	118.03	112.60
1	Fg	38	ARG	NE-CZ-NH2	5.42	124.08	119.20
4	If	36	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	Fl	89	SER	CA-C-N	5.41	126.33	120.44
1	Fl	89	SER	C-N-CA	5.41	126.33	120.44
2	Gb	28	ARG	NE-CZ-NH2	5.38	124.05	119.20
5	Jc	256	ASP	CA-CB-CG	5.38	117.98	112.60
1	Fi	71	ARG	NE-CZ-NH2	5.38	124.04	119.20
3	He	97	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	Fc	71	ARG	NE-CZ-NH2	5.36	124.03	119.20
5	Jh	3	LEU	N-CA-C	5.36	117.12	111.28
1	Fa	445	ARG	NE-CZ-NH2	5.35	124.02	119.20
2	Ge	68	ARG	NE-CZ-NH2	5.35	124.02	119.20
5	Jl	256	ASP	CA-CB-CG	5.34	117.94	112.60
3	Ha	126	PHE	CA-CB-CG	5.34	119.14	113.80
1	Ff	197	ARG	NE-CZ-NH2	5.33	124.00	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Fb	133	ASP	CA-CB-CG	5.33	117.93	112.60
1	Fi	78	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	Gc	35	ARG	NE-CZ-NH2	5.29	123.96	119.20
2	Gd	114	LEU	CA-C-N	5.28	126.26	121.82
2	Gd	114	LEU	C-N-CA	5.28	126.26	121.82
1	Fa	377	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	Fk	225	ARG	NE-CZ-NH2	5.28	123.95	119.20
2	Gh	111	ARG	NE-CZ-NH2	5.27	123.94	119.20
4	Ib	19	HIS	CA-CB-CG	5.27	119.07	113.80
1	Fe	377	ARG	NE-CZ-NH2	5.25	123.92	119.20
5	Jg	63	PHE	CA-CB-CG	5.24	119.04	113.80
1	Fc	445	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	Fi	39	ARG	NE-CZ-NH2	5.23	123.91	119.20
5	Je	138	ASN	OD1-CG-ND2	-5.22	117.38	122.60
2	Gd	111	ARG	NE-CZ-NH2	5.22	123.90	119.20
3	Hf	124	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	Fa	225	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	Fa	148	ARG	NE-CZ-NH2	5.21	123.89	119.20
5	Jj	129	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	Fa	38	ARG	NE-CZ-NH2	5.20	123.88	119.20
2	Gl	111	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	Fe	445	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	Fb	441	ARG	NE-CZ-NH2	5.20	123.88	119.20
2	Ga	95	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	Fl	284	ARG	NE-CZ-NH2	5.19	123.87	119.20
2	Gh	28	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	Fk	71	ARG	NE-CZ-NH2	5.18	123.86	119.20
5	Jk	281	ASP	CA-CB-CG	5.18	117.78	112.60
1	Fk	78	ARG	NE-CZ-NH2	5.17	123.86	119.20
3	Ha	125	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	Fb	223	ARG	NE-CZ-NH2	5.17	123.85	119.20
3	Hb	30	ASP	CA-CB-CG	5.17	117.77	112.60
1	Fl	38	ARG	NE-CZ-NH2	5.16	123.84	119.20
3	Hb	124	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	Fe	431	TRP	CA-CB-CG	5.14	123.37	113.60
1	Fe	39	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	Fh	441	ARG	NE-CZ-NH2	5.14	123.83	119.20
4	Id	131	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	Fc	377	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	Fh	71	ARG	NE-CZ-NH2	5.13	123.82	119.20
4	Ia	131	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	Fb	377	ARG	NE-CZ-NH2	5.13	123.81	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Fc	39	ARG	NE-CZ-NH2	5.13	123.81	119.20
5	Ja	13	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	Fg	39	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	Fj	313	ARG	NE-CZ-NH2	5.12	123.81	119.20
5	Jk	44	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	Fh	313	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	Fk	39	ARG	NE-CZ-NH2	5.10	123.79	119.20
4	Ib	36	HIS	CB-CG-CD2	-5.10	124.58	131.20
1	Fh	429	ARG	NE-CZ-NH2	5.08	123.77	119.20
3	He	124	ARG	NE-CZ-NH2	5.08	123.77	119.20
2	Gg	29	ARG	NE-CZ-NH2	5.07	123.76	119.20
2	Gl	29	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	Fd	225	ARG	N-CA-CB	-5.06	103.20	111.24
3	Hc	100	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	Fd	303	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	Fj	38	ARG	NE-CZ-NH2	5.04	123.73	119.20
5	Jc	138	ASN	CA-CB-CG	5.03	117.63	112.60
5	Ji	155	ASP	CA-CB-CG	5.02	117.62	112.60
5	Ji	5	ASP	CA-CB-CG	5.02	117.62	112.60
1	Fk	8	ASP	CA-CB-CG	5.02	117.62	112.60
5	Jf	13	ARG	NE-CZ-NH2	5.02	123.72	119.20
2	Gi	95	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	Fj	169	ALA	N-CA-C	5.01	117.00	109.23
5	Jh	155	ASP	CA-CB-CG	5.01	117.61	112.60
2	Gi	92	ASP	CA-CB-CG	5.00	117.60	112.60
5	Jd	97	GLN	OE1-CD-NE2	-5.00	117.60	122.60
3	Hd	115	ARG	NE-CZ-NH2	5.00	123.70	119.20
4	If	129	PHE	N-CA-C	5.00	117.54	108.69
5	Jb	5	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Fb	225	ARG	Peptide
1	Fb	394	ARG	Sidechain
1	Fc	240	ARG	Sidechain
1	Fc	289	TYR	Sidechain
1	Fd	289	TYR	Sidechain
1	Fe	441	ARG	Sidechain
1	Ff	16	LEU	Peptide
1	Ff	219	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	Ff	289	TYR	Sidechain
1	Fg	289	TYR	Sidechain
1	Fh	13	ARG	Sidechain
1	Fh	54	TYR	Sidechain
1	Fi	225	ARG	Sidechain
1	Fi	240	ARG	Sidechain
1	Fj	168	TYR	Sidechain
1	Fj	429	ARG	Sidechain
1	Fk	13	ARG	Sidechain
1	Fk	148	ARG	Sidechain
1	Fk	172	ALA	Peptide
1	Fk	394	ARG	Sidechain
1	Fl	429	ARG	Sidechain
2	Gc	76	TYR	Sidechain
2	Gh	76	TYR	Sidechain
2	Gj	16	ARG	Sidechain
3	Ha	49	ARG	Sidechain
3	Ha	97	ARG	Sidechain
3	Hb	49	ARG	Sidechain
3	Hb	97	ARG	Sidechain
3	Hd	115	ARG	Sidechain
3	Hd	49	ARG	Sidechain
3	Hd	6	ARG	Peptide
3	He	49	ARG	Sidechain
3	Hf	49	ARG	Sidechain
4	Ia	47	ARG	Sidechain
4	Id	47	ARG	Sidechain
4	If	55	ARG	Sidechain
5	Ja	129	ARG	Sidechain
5	Ja	153	ARG	Sidechain
5	Jb	170	ARG	Sidechain
5	Jc	141	ARG	Sidechain
5	Je	13	ARG	Sidechain
5	Jg	71	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Fa	3526	3426	3424	3	0
1	Fb	3526	3425	3424	4	0
1	Fc	3526	3425	3424	1	0
1	Fd	3526	3425	3424	1	0
1	Fe	3526	3426	3424	2	0
1	Ff	3526	3426	3424	2	0
1	Fg	3526	3425	3424	2	0
1	Fh	3526	3425	3424	2	0
1	Fi	3526	3425	3424	1	0
1	Fj	3526	3425	3424	2	0
1	Fk	3526	3425	3424	0	0
1	Fl	3526	3426	3424	1	0
2	Ga	981	1000	999	0	0
2	Gb	981	1000	999	1	0
2	Gc	981	1000	999	0	0
2	Gd	981	1000	999	1	0
2	Ge	981	1000	999	0	0
2	Gf	981	1000	999	1	0
2	Gg	981	1000	999	1	0
2	Gh	981	1000	999	0	0
2	Gi	981	1000	999	1	0
2	Gj	981	1000	999	0	0
2	Gk	981	1000	999	0	0
2	Gl	981	1000	999	0	0
3	Ha	997	973	972	0	0
3	Hb	997	973	972	1	0
3	Hc	997	974	972	1	0
3	Hd	997	974	972	1	0
3	He	997	973	972	0	0
3	Hf	997	974	972	0	0
4	Ia	1136	1143	1142	1	0
4	Ib	1136	1143	1142	0	0
4	Ic	1136	1143	1142	0	0
4	Id	1136	1143	1142	0	0
4	Ie	1136	1143	1142	1	0
4	If	1136	1144	1142	2	0
5	Ja	2124	2039	2038	0	0
5	Jb	1995	1900	1898	0	0
5	Jc	2124	2039	2038	1	0
5	Jd	2020	1929	1927	0	0
5	Je	2124	2039	2038	2	0
5	Jf	2124	2039	2038	1	0
5	Jg	2124	2039	2038	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Jh	1993	1901	1899	0	0
5	Ji	1980	1889	1887	0	0
5	Jj	2124	2039	2038	1	0
5	Jk	1980	1889	1887	0	0
5	Jl	2020	1929	1927	0	0
All	All	91614	89475	89413	27	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 0.

All (27) 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)
5:Je:213:LEU:H	5:Je:220:THR:HG22	1.69	0.57
1:Fd:262:ILE:HD12	1:Ff:260:MET:HE3	1.90	0.53
1:Fg:260:MET:HE1	1:Fh:262:ILE:HG23	1.92	0.52
1:Fb:290:MET:HE3	1:Fe:259:LEU:HD12	1.92	0.52
1:Fa:388:ILE:HD11	1:Fa:393:TYR:CZ	2.47	0.49
2:Gg:3:THR:HA	2:Gg:34:GLU:HG3	1.96	0.48
1:Fe:262:ILE:HD12	1:Fl:260:MET:HE3	1.96	0.48
3:Hd:50:PHE:CE2	3:Hd:78:MET:HG3	2.51	0.46
4:If:61:ARG:HH21	4:If:61:ARG:HG2	1.80	0.46
1:Fi:212:LEU:H	1:Fi:212:LEU:HD23	1.80	0.46
4:Ia:91:TYR:CE1	4:Ia:122:ALA:HB2	2.52	0.45
2:Gf:25:LEU:HD23	2:Gf:25:LEU:C	2.42	0.44
3:Hb:50:PHE:CE2	3:Hb:78:MET:HG3	2.53	0.44
4:Ie:91:TYR:CE1	4:Ie:122:ALA:HB2	2.53	0.44
1:Fb:260:MET:HE3	1:Fj:262:ILE:HD12	1.99	0.43
5:Jf:164:PHE:CZ	5:Jj:10:ILE:HD11	2.53	0.43
4:If:91:TYR:CE1	4:If:122:ALA:HB2	2.55	0.42
5:Jc:164:PHE:CE2	5:Je:10:ILE:HD11	2.55	0.42
1:Fa:260:MET:HE2	1:Fj:290:MET:HG3	2.02	0.41
3:Hc:50:PHE:CE2	3:Hc:78:MET:HG3	2.56	0.41
1:Fb:49:LEU:HD22	1:Fb:49:LEU:H	1.85	0.41
2:Gb:64:GLU:CD	2:Gd:29:ARG:HH22	2.29	0.41
1:Fa:260:MET:HE1	1:Fb:262:ILE:HB	2.03	0.41
1:Fh:260:MET:C	1:Fh:262:ILE:H	2.29	0.41
1:Ff:168:TYR:CE2	1:Ff:186:LEU:HD22	2.56	0.41
1:Fc:290:MET:HG3	1:Fg:260:MET:HE2	2.03	0.40
2:Gi:77:LEU:C	2:Gi:77:LEU:HD13	2.46	0.40

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	Fa	448/488 (92%)	438 (98%)	10 (2%)	0	100	100
1	Fb	448/488 (92%)	432 (96%)	16 (4%)	0	100	100
1	Fc	448/488 (92%)	434 (97%)	14 (3%)	0	100	100
1	Fd	448/488 (92%)	430 (96%)	18 (4%)	0	100	100
1	Fe	448/488 (92%)	437 (98%)	11 (2%)	0	100	100
1	Ff	448/488 (92%)	434 (97%)	14 (3%)	0	100	100
1	Fg	448/488 (92%)	433 (97%)	15 (3%)	0	100	100
1	Fh	448/488 (92%)	433 (97%)	15 (3%)	0	100	100
1	Fi	448/488 (92%)	436 (97%)	12 (3%)	0	100	100
1	Fj	448/488 (92%)	433 (97%)	15 (3%)	0	100	100
1	Fk	448/488 (92%)	433 (97%)	15 (3%)	0	100	100
1	Fl	448/488 (92%)	431 (96%)	17 (4%)	0	100	100
2	Ga	122/125 (98%)	119 (98%)	3 (2%)	0	100	100
2	Gb	122/125 (98%)	120 (98%)	2 (2%)	0	100	100
2	Gc	122/125 (98%)	120 (98%)	2 (2%)	0	100	100
2	Gd	122/125 (98%)	119 (98%)	3 (2%)	0	100	100
2	Ge	122/125 (98%)	121 (99%)	1 (1%)	0	100	100
2	Gf	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
2	Gg	122/125 (98%)	116 (95%)	6 (5%)	0	100	100
2	Gh	122/125 (98%)	121 (99%)	1 (1%)	0	100	100
2	Gi	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
2	Gj	122/125 (98%)	118 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Gk	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
2	Gl	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
3	Ha	123/126 (98%)	118 (96%)	5 (4%)	0	100	100
3	Hb	123/126 (98%)	116 (94%)	7 (6%)	0	100	100
3	Hc	123/126 (98%)	113 (92%)	10 (8%)	0	100	100
3	Hd	123/126 (98%)	119 (97%)	4 (3%)	0	100	100
3	He	123/126 (98%)	119 (97%)	4 (3%)	0	100	100
3	Hf	123/126 (98%)	116 (94%)	7 (6%)	0	100	100
4	Ia	145/148 (98%)	142 (98%)	3 (2%)	0	100	100
4	Ib	145/148 (98%)	143 (99%)	2 (1%)	0	100	100
4	Ic	145/148 (98%)	141 (97%)	4 (3%)	0	100	100
4	Id	145/148 (98%)	143 (99%)	2 (1%)	0	100	100
4	Ie	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
4	If	145/148 (98%)	141 (97%)	4 (3%)	0	100	100
5	Ja	280/283 (99%)	265 (95%)	15 (5%)	0	100	100
5	Jb	263/283 (93%)	249 (95%)	14 (5%)	0	100	100
5	Jc	280/283 (99%)	262 (94%)	18 (6%)	0	100	100
5	Jd	266/283 (94%)	255 (96%)	11 (4%)	0	100	100
5	Je	280/283 (99%)	258 (92%)	22 (8%)	0	100	100
5	Jf	280/283 (99%)	264 (94%)	16 (6%)	0	100	100
5	Jg	280/283 (99%)	268 (96%)	12 (4%)	0	100	100
5	Jh	263/283 (93%)	254 (97%)	9 (3%)	0	100	100
5	Ji	261/283 (92%)	241 (92%)	20 (8%)	0	100	100
5	Jj	280/283 (99%)	262 (94%)	18 (6%)	0	100	100
5	Jk	261/283 (92%)	250 (96%)	11 (4%)	0	100	100
5	Jl	266/283 (94%)	253 (95%)	13 (5%)	0	100	100
All	All	11708/12396 (94%)	11261 (96%)	447 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	Fa	364/390 (93%)	361 (99%)	3 (1%)	79	90
1	Fb	364/390 (93%)	361 (99%)	3 (1%)	79	90
1	Fc	364/390 (93%)	362 (100%)	2 (0%)	86	94
1	Fd	364/390 (93%)	363 (100%)	1 (0%)	91	96
1	Fe	364/390 (93%)	363 (100%)	1 (0%)	91	96
1	Ff	364/390 (93%)	362 (100%)	2 (0%)	86	94
1	Fg	364/390 (93%)	360 (99%)	4 (1%)	70	87
1	Fh	364/390 (93%)	360 (99%)	4 (1%)	70	87
1	Fi	364/390 (93%)	364 (100%)	0	100	100
1	Fj	364/390 (93%)	363 (100%)	1 (0%)	91	96
1	Fk	364/390 (93%)	361 (99%)	3 (1%)	79	90
1	Fl	364/390 (93%)	360 (99%)	4 (1%)	70	87
2	Ga	106/107 (99%)	104 (98%)	2 (2%)	52	79
2	Gb	106/107 (99%)	105 (99%)	1 (1%)	75	89
2	Gc	106/107 (99%)	106 (100%)	0	100	100
2	Gd	106/107 (99%)	106 (100%)	0	100	100
2	Ge	106/107 (99%)	105 (99%)	1 (1%)	75	89
2	Gf	106/107 (99%)	105 (99%)	1 (1%)	75	89
2	Gg	106/107 (99%)	105 (99%)	1 (1%)	75	89
2	Gh	106/107 (99%)	106 (100%)	0	100	100
2	Gi	106/107 (99%)	105 (99%)	1 (1%)	75	89
2	Gj	106/107 (99%)	106 (100%)	0	100	100
2	Gk	106/107 (99%)	106 (100%)	0	100	100
2	Gl	106/107 (99%)	104 (98%)	2 (2%)	52	79
3	Ha	106/107 (99%)	106 (100%)	0	100	100
3	Hb	106/107 (99%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Hc	106/107 (99%)	106 (100%)	0	100	100
3	Hd	106/107 (99%)	106 (100%)	0	100	100
3	He	106/107 (99%)	105 (99%)	1 (1%)	75	89
3	Hf	106/107 (99%)	106 (100%)	0	100	100
4	Ia	125/126 (99%)	125 (100%)	0	100	100
4	Ib	125/126 (99%)	125 (100%)	0	100	100
4	Ic	125/126 (99%)	124 (99%)	1 (1%)	79	90
4	Id	125/126 (99%)	124 (99%)	1 (1%)	79	90
4	Ie	125/126 (99%)	124 (99%)	1 (1%)	79	90
4	If	125/126 (99%)	123 (98%)	2 (2%)	58	82
5	Ja	220/221 (100%)	218 (99%)	2 (1%)	75	89
5	Jb	206/221 (93%)	202 (98%)	4 (2%)	52	79
5	Jc	220/221 (100%)	217 (99%)	3 (1%)	62	83
5	Jd	209/221 (95%)	209 (100%)	0	100	100
5	Je	220/221 (100%)	219 (100%)	1 (0%)	86	94
5	Jf	220/221 (100%)	218 (99%)	2 (1%)	75	89
5	Jg	220/221 (100%)	218 (99%)	2 (1%)	75	89
5	Jh	206/221 (93%)	206 (100%)	0	100	100
5	Ji	204/221 (92%)	203 (100%)	1 (0%)	86	94
5	Jj	220/221 (100%)	219 (100%)	1 (0%)	86	94
5	Jk	204/221 (92%)	203 (100%)	1 (0%)	86	94
5	Jl	209/221 (95%)	208 (100%)	1 (0%)	86	94
All	All	9584/10014 (96%)	9523 (99%)	61 (1%)	82	93

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Fa	11	LYS
1	Fa	28	LYS
1	Fa	179	ASN
1	Fb	227	SER
1	Fb	320	ASP
1	Fb	412	ASP
1	Fc	11	LYS

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Mol	Chain	Res	Type
1	Fc	74	LEU
1	Fd	323	ASP
1	Fe	425	ILE
1	Ff	366	LYS
1	Ff	388	ILE
1	Fg	14	ASP
1	Fg	174	TYR
1	Fg	232	THR
1	Fg	428	GLU
1	Fh	35	ASP
1	Fh	180	GLU
1	Fh	388	ILE
1	Fh	428	GLU
1	Fj	163	THR
1	Fk	168	TYR
1	Fk	173	ILE
1	Fk	432	VAL
1	Fl	11	LYS
1	Fl	224	THR
1	Fl	262	ILE
1	Fl	388	ILE
2	Ga	4	LEU
2	Ga	38	LEU
2	Gb	3	THR
2	Ge	80	THR
2	Gf	92	ASP
2	Gg	80	THR
2	Gi	97	LEU
2	Gl	60	ASP
2	Gl	105	GLU
3	He	116	ILE
4	Ic	39	THR
4	Id	39	THR
4	Ie	32	LEU
4	If	35	VAL
4	If	61	ARG
5	Ja	120	VAL
5	Ja	202	ASP
5	Jb	97	GLN
5	Jb	211	TYR
5	Jb	223	ILE
5	Jb	258	GLU

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Mol	Chain	Res	Type
5	Jc	120	VAL
5	Jc	256	ASP
5	Jc	272	THR
5	Je	138	ASN
5	Jf	201	LEU
5	Jf	220	THR
5	Jg	13	ARG
5	Jg	272	THR
5	Ji	54	SER
5	Jj	120	VAL
5	Jk	214	LEU
5	Jl	120	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	Fa	72	GLN
1	Fa	258	ASN
1	Fb	72	GLN
1	Fb	252	ASN
1	Fb	283	GLN
1	Fc	72	GLN
1	Fc	93	ASN
1	Fc	179	ASN
1	Fc	254	GLN
1	Fc	258	ASN
1	Fc	278	ASN
1	Fc	374	GLN
1	Fc	443	GLN
1	Fc	446	GLN
1	Fc	454	GLN
1	Fd	15	GLN
1	Fd	72	GLN
1	Fd	278	ASN
1	Fd	335	GLN
1	Fe	252	ASN
1	Fe	335	GLN
1	Fe	343	ASN
1	Fe	374	GLN
1	Fe	420	ASN
1	Fe	450	GLN
1	Ff	254	GLN

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Mol	Chain	Res	Type
1	Ff	258	ASN
1	Ff	343	ASN
1	Ff	443	GLN
1	Ff	454	GLN
1	Fh	72	GLN
1	Fh	83	ASN
1	Fh	248	GLN
1	Fh	252	ASN
1	Fh	452	GLN
1	Fi	72	GLN
1	Fi	179	ASN
1	Fi	252	ASN
1	Fi	258	ASN
1	Fi	365	ASN
1	Fi	374	GLN
1	Fi	446	GLN
1	Fj	72	GLN
1	Fj	252	ASN
1	Fj	258	ASN
1	Fj	283	GLN
1	Fk	252	ASN
1	Fk	446	GLN
1	Fl	258	ASN
1	Fl	278	ASN
1	Fl	420	ASN
2	Gb	7	HIS
2	Gb	27	ASN
2	Gc	27	ASN
2	Gg	32	GLN
2	Gh	91	GLN
2	Gi	7	HIS
2	Gi	27	ASN
2	Gi	94	ASN
2	Gk	27	ASN
2	Gk	94	ASN
3	Hc	55	GLN
3	Hd	53	GLN
3	He	53	GLN
4	Ib	148	ASN
4	Ic	89	GLN
4	Ic	105	GLN
4	Ie	36	HIS

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Mol	Chain	Res	Type
5	Jb	38	HIS
5	Jb	180	ASN
5	Jd	52	HIS
5	Jd	111	GLN
5	Jd	177	GLN
5	Jg	138	ASN
5	Jh	180	ASN
5	Ji	177	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

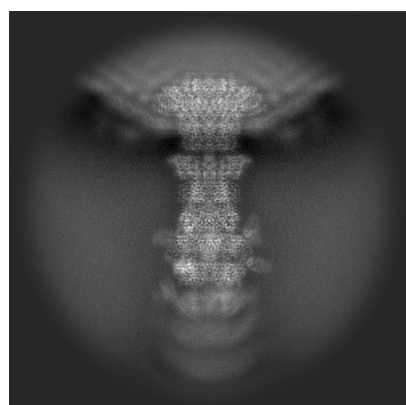
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46669. These allow visual inspection of the internal detail of the map and identification of artifacts.

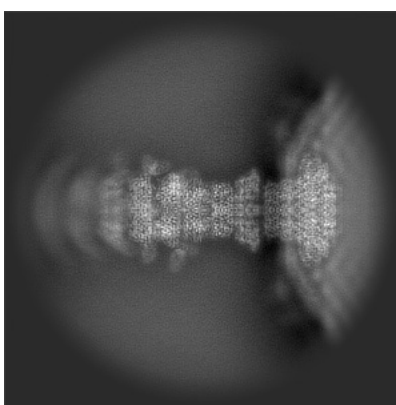
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

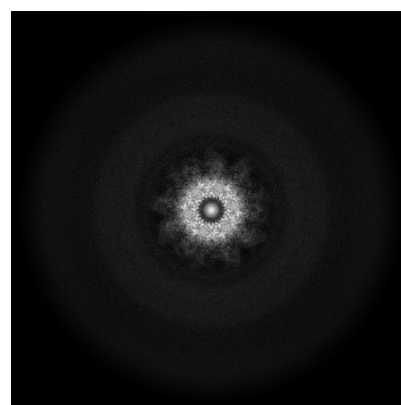
#### 6.1.1 Primary map



X



Y

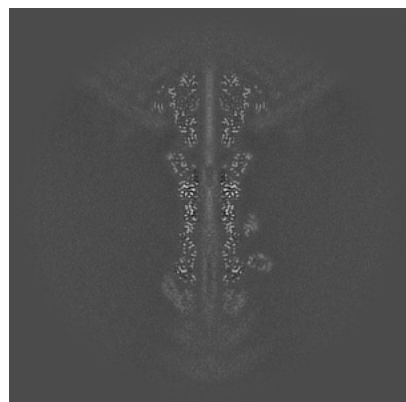


Z

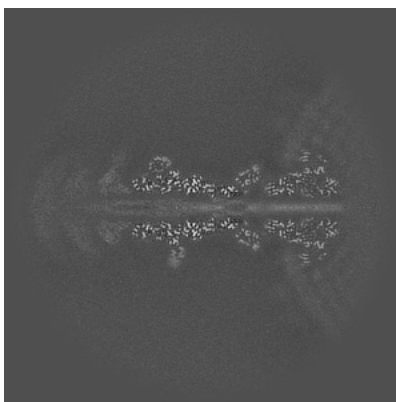
The images above show the map projected in three orthogonal directions.

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

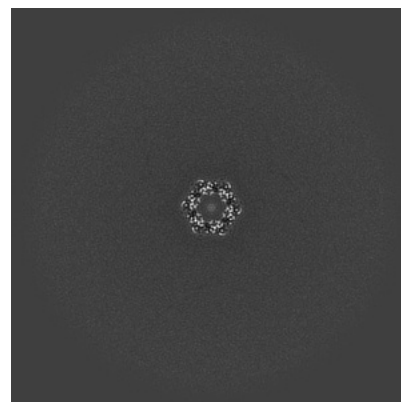
#### 6.2.1 Primary map



X Index: 241



Y Index: 241

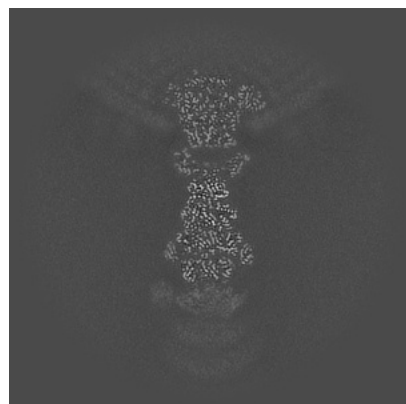


Z Index: 241

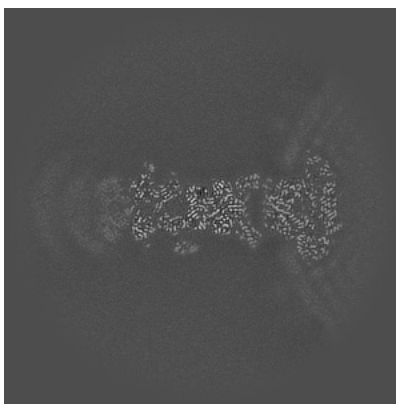
The images above show central slices of the map in three orthogonal directions.

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

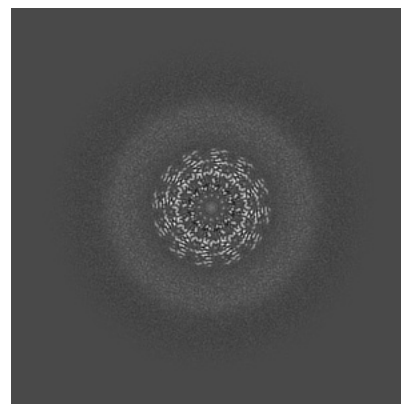
### 6.3.1 Primary map



X Index: 220



Y Index: 224



Z Index: 366

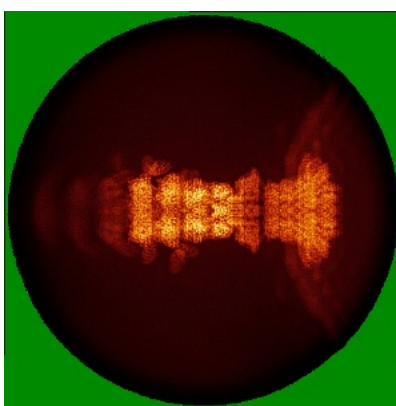
The images above show the largest variance slices of the map in three orthogonal directions.

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

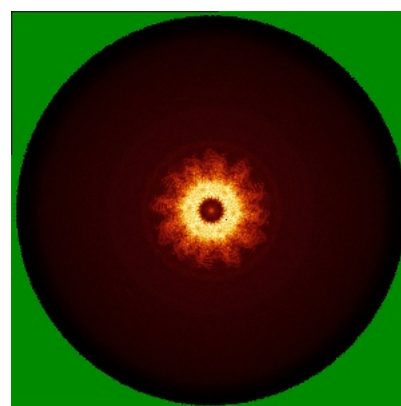
### 6.4.1 Primary map



X



Y

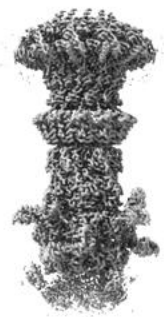


Z

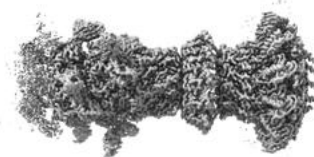
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

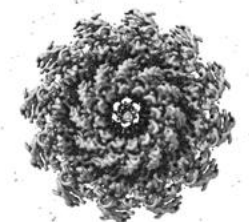
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. 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](#)

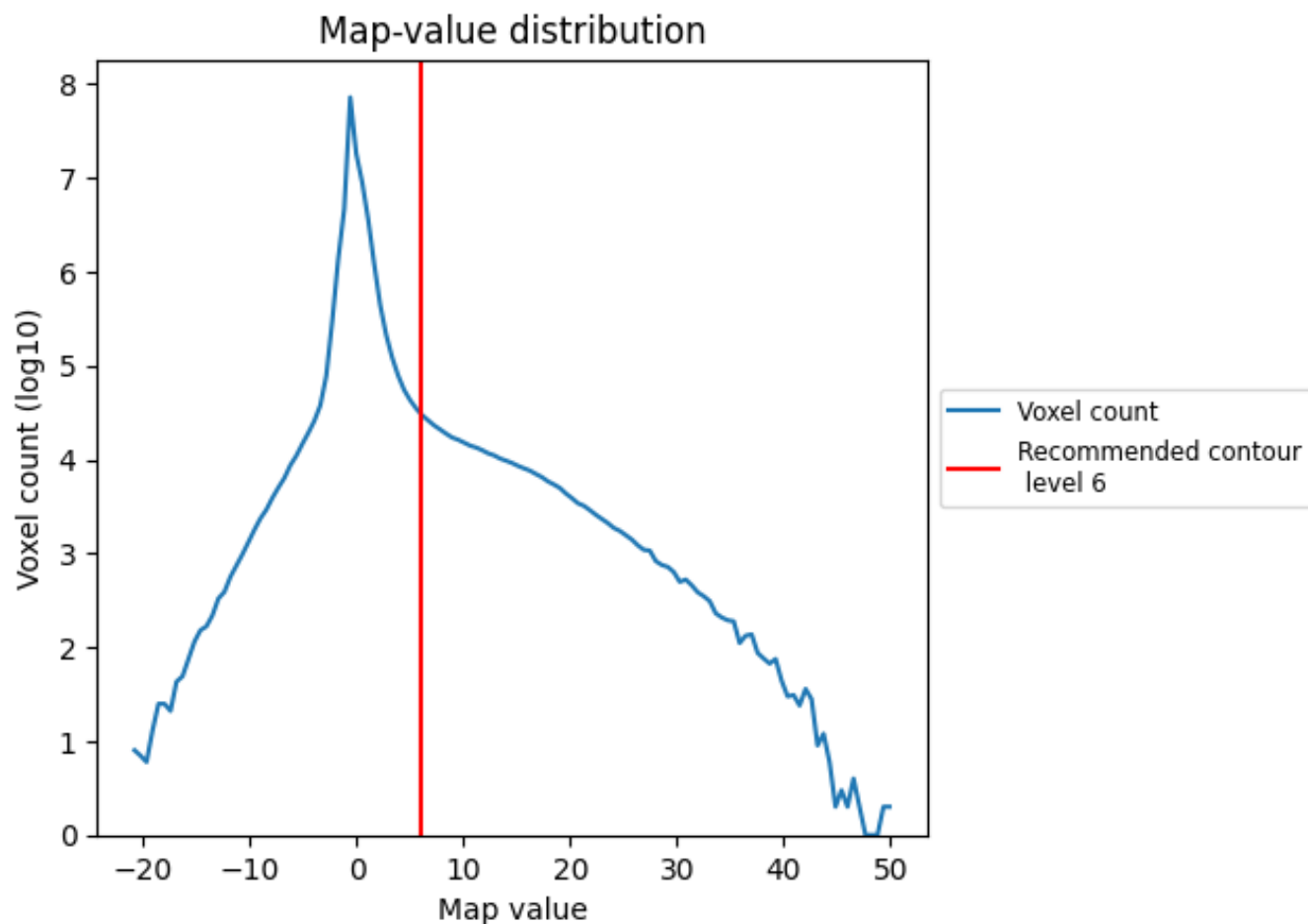
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

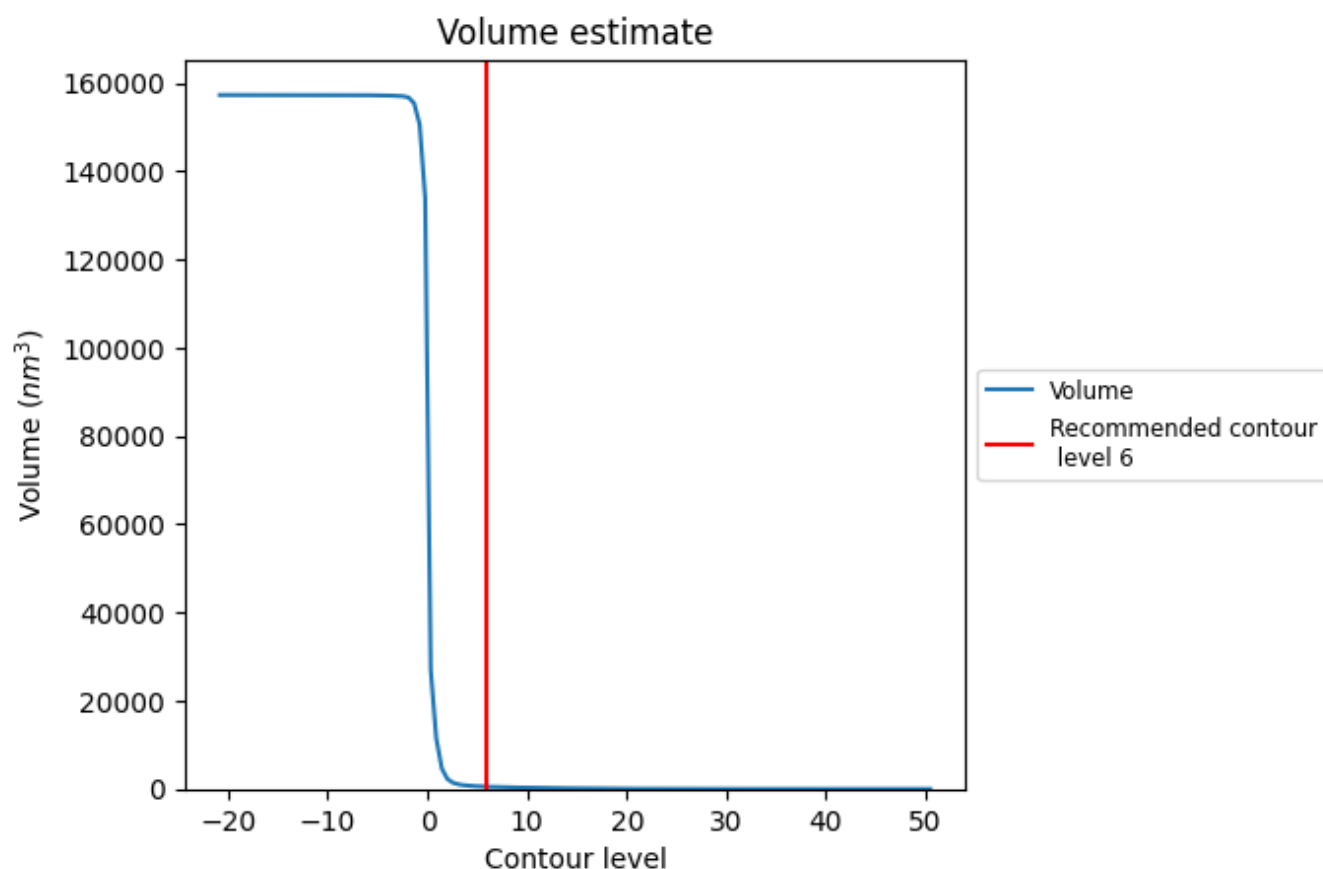
This section contains the results of statistical analysis of the map.

### 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.

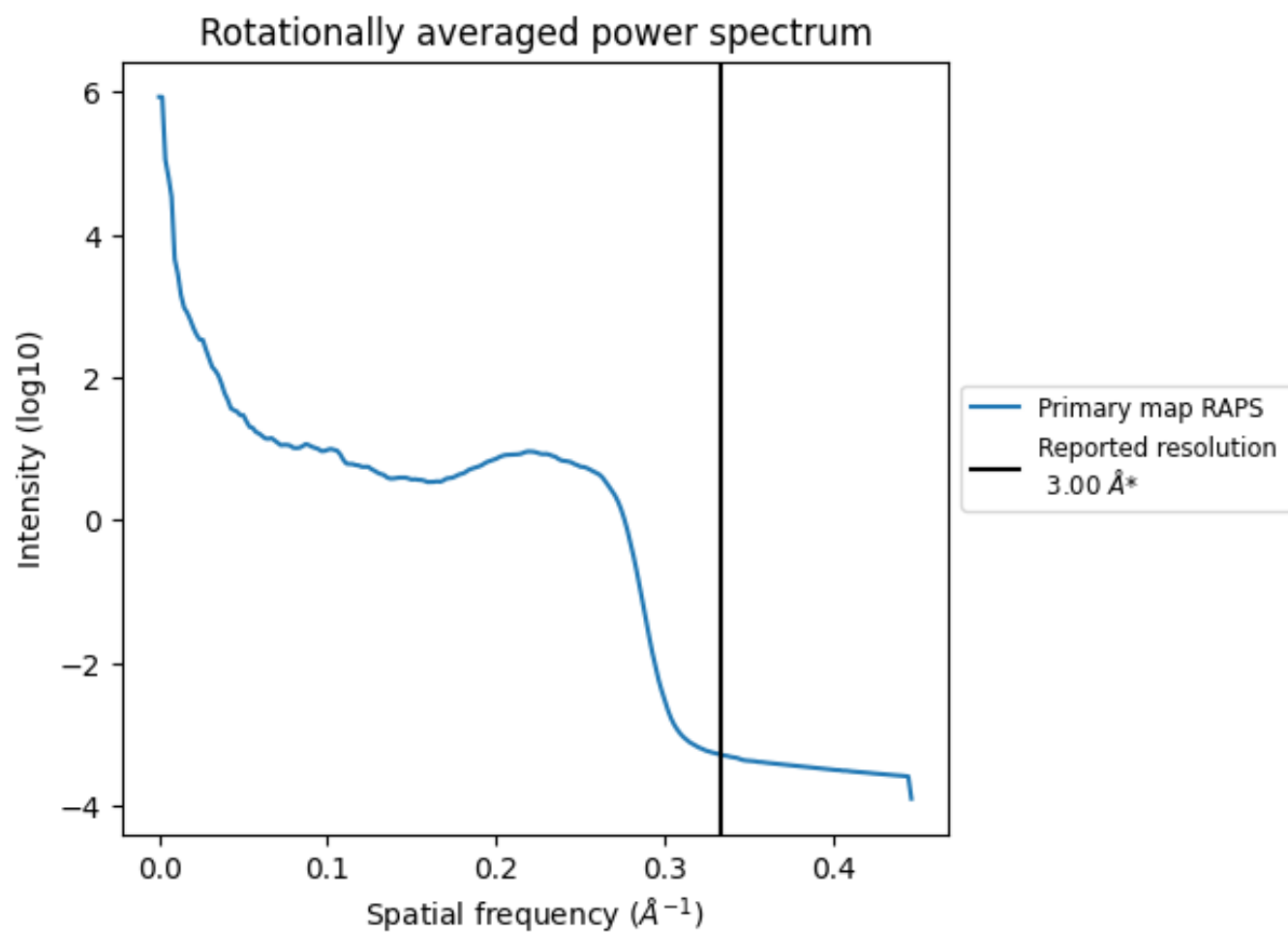
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 508  $\text{nm}^3$ ; this corresponds to an approximate mass of 459 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 0.333 Å<sup>-1</sup>

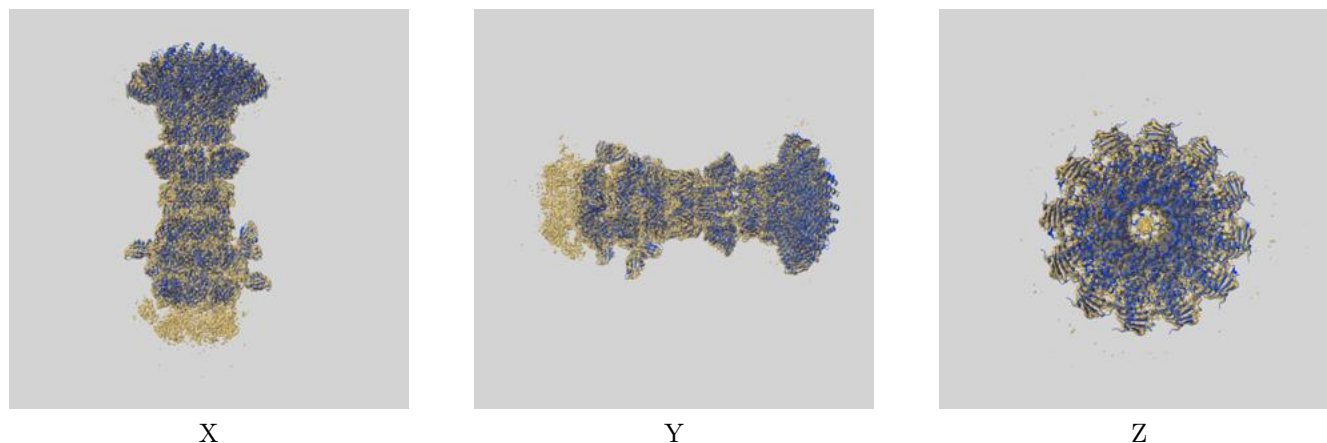
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

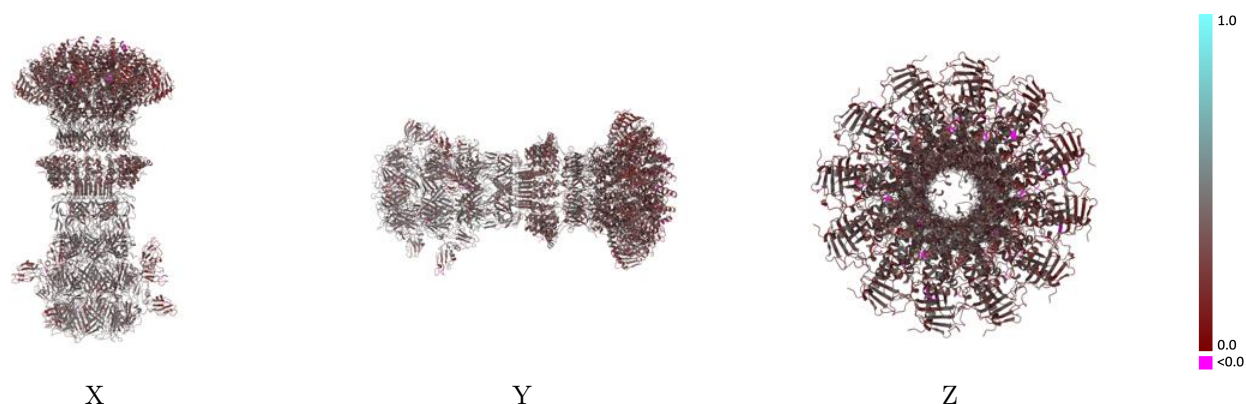
This section contains information regarding the fit between EMDB map EMD-46669 and PDB model 9D94. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

### 9.1 Map-model overlay [i](#)



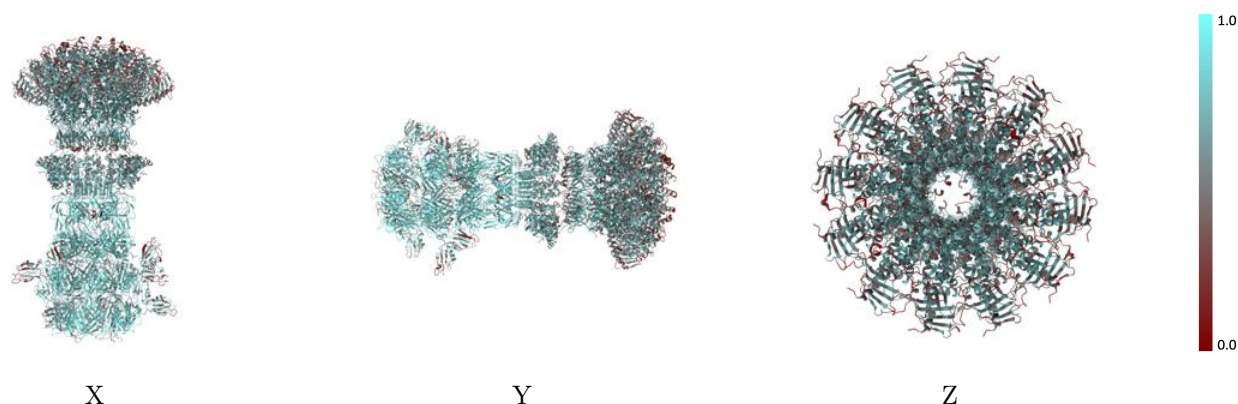
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



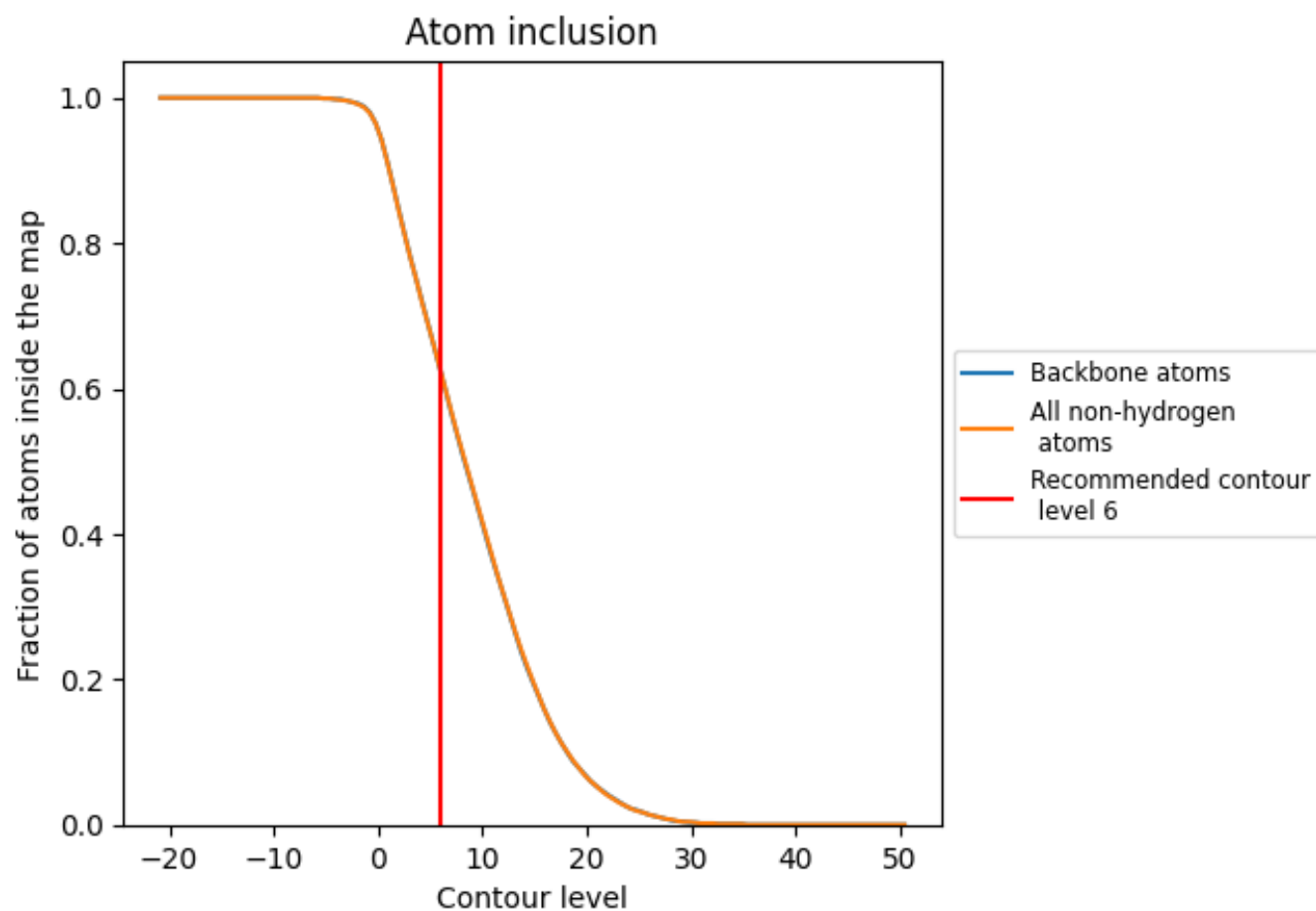
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 62% 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 (6) and Q-score for the entire model and for each chain.





























Chain	Atom inclusion	Q-score
All	 0.6240	 0.3580
Fa	 0.5670	 0.3320
Fb	 0.5810	 0.3380
Fc	 0.5480	 0.3040
Fd	 0.5740	 0.3280
Fe	 0.5630	 0.3130
Ff	 0.5780	 0.3380
Fg	 0.5600	 0.3260
Fh	 0.5600	 0.3250
Fi	 0.5710	 0.3370
Fj	 0.5700	 0.3410
Fk	 0.5470	 0.3010
Fl	 0.5550	 0.3070
Ga	 0.6450	 0.3520
Gb	 0.6130	 0.3500
Gc	 0.6450	 0.3630
Gd	 0.6090	 0.3390
Ge	 0.6180	 0.3450
Gf	 0.6290	 0.3530
Gg	 0.6290	 0.3530
Gh	 0.6370	 0.3730
Gi	 0.6330	 0.3540
Gj	 0.6290	 0.3640
Gk	 0.6230	 0.3530
Gl	 0.6280	 0.3590
Ha	 0.7530	 0.4070
Hb	 0.7580	 0.3980
Hc	 0.7440	 0.3940
Hd	 0.7560	 0.3950
He	 0.7580	 0.4000
Hf	 0.7550	 0.4010
Ia	 0.7890	 0.4210
Ib	 0.8000	 0.4260
Ic	 0.8000	 0.4210
Id	 0.7930	 0.4040



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Chain	Atom inclusion	Q-score
Ie	 0.7710	 0.4080
If	 0.7760	 0.4180
Ja	 0.6790	 0.4020
Jb	 0.6740	 0.3840
Jc	 0.6650	 0.3720
Jd	 0.6650	 0.3740
Je	 0.6760	 0.3940
Jf	 0.6580	 0.3770
Jg	 0.6610	 0.3720
Jh	 0.6930	 0.4100
Ji	 0.7100	 0.4010
Jj	 0.6680	 0.3780
Jk	 0.7230	 0.4140
Jl	 0.7160	 0.4080