



wwPDB EM Validation Summary Report ⓘ

Nov 27, 2022 – 12:31 PM EST

PDB ID : 6Q15
EMDB ID : EMD-20312
Title : Structure of the Salmonella SPI-1 injectisome needle complex
Authors : Hu, J.; Worrall, L.J.; Strynadka, N.C.J.
Deposited on : 2019-08-02
Resolution : 5.15 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

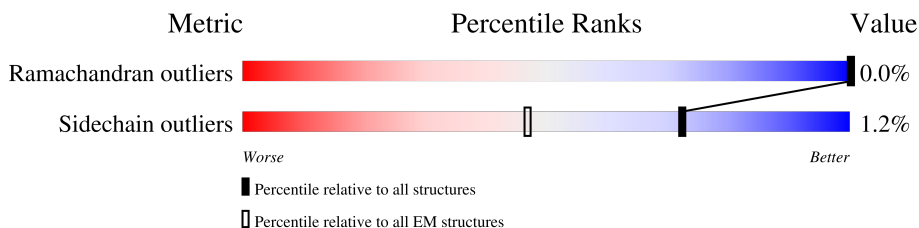
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 5.15 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)
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 $\leq 5\%$. 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	AA	252	
1	AB	252	
1	AC	252	
1	AD	252	
1	AE	252	
1	AF	252	
1	AG	252	
1	AH	252	
1	AI	252	

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Mol	Chain	Length	Quality of chain	
1	AJ	252	13%	71% 27%
1	AK	252	11%	72% 27%
1	AL	252	11%	72% 27%
1	o	252	13%	72% 27%
1	p	252	13%	73% 27%
1	q	252	16%	71% 27%
1	r	252	10%	72% 27%
1	s	252	15%	72% 27%
1	t	252	12%	71% 27%
1	u	252	13%	73% 27%
1	v	252	17%	73% 27%
1	w	252	17%	72% 27%
1	x	252	12%	73% 27%
1	y	252	12%	71% 27%
1	z	252	11%	71% 27%
2	E	392	9%	56% 43%
2	R	392	7%	56% 44%
2	S	392	6%	56% 43%
2	T	392	9%	57% 43%
2	U	392	7%	56% 44%
2	V	392	9%	56% 43%
2	W	392	12%	56% 43%
2	X	392	7%	55% 44%
2	Y	392	8%	56% 43%
2	Z	392	10%	57% 43%

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Mol	Chain	Length	Quality of chain	
2	a	392	5%	56% 44%
2	b	392	7%	56% 43%
2	c	392	10%	56% 43%
2	d	392	9%	56% 44%
2	e	392	5%	55% 43%
2	f	392	8%	57% 43%
2	g	392	6%	56% 44%
2	h	392	7%	56% 43%
2	i	392	8%	56% 43%
2	j	392	•	56% 44%
2	k	392	•	56% 43%
2	l	392	8%	56% 43%
2	m	392	6%	56% 44%
2	n	392	6%	56% 43%
3	A	562	37%	87% 12%
3	B	562	34%	88% 11%
3	C	562	30%	86% 12%
3	D	562	29%	87% 11%
3	F	562	27%	87% 12%
3	G	562	25%	87% 11%
3	H	562	22%	85% 12%
3	I	562	26%	87% 11%
3	J	562	26%	86% 12%
3	K	562	28%	88% 11%
3	L	562	28%	86% 12%

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Mol	Chain	Length	Quality of chain
3	M	562	34% 88% 11%
3	N	562	35% 85% 12%
3	O	562	36% 87% 11%
3	P	562	35% 86% 12%
3	Q	562	25% 74%
4	0	224	21% 85% 11%
4	1	224	20% 86% 11%
4	2	224	19% 85% 12%
4	3	224	21% 88% 9%
4	4	224	21% 96%
5	5	263	17% 92% 6%
6	6	86	57% 62% 38%
6	7	86	66% 94% ..
6	8	86	33% 92% 6% .
6	9	86	13% 93% 5% .
7	AM	101	38% 61%
7	AN	101	15% 76% 23%
7	AO	101	11% 83% 13%
7	AP	101	12% 85% 13%
7	AQ	101	14% 84% 13%
7	AR	101	17% 86% 13%
8	AS	80	12% 72% 26%
8	AT	80	10% 70% 26%
8	AU	80	9% 71% 26%
8	AV	80	9% 69% 26%

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Mol	Chain	Length	Quality of chain
8	AW	80	9% 69% 5% 26%
8	AX	80	22% 91% 9%
8	AY	80	18% 94% ..
8	AZ	80	18% 95% ..
8	BA	80	15% 96% ..
8	BB	80	22% 98% .
8	BC	80	24% 96% ..
8	BD	80	30% 95% ...
8	BE	80	31% 96% ..
8	BF	80	36% 98% .
8	BG	80	38% 98% .
8	BH	80	45% 95% ..
8	BI	80	54% 95% ..
8	BJ	80	61% 94% ..
8	BK	80	69% 95% ..
8	BL	80	70% 98% .
8	BM	80	68% 94% ...
8	BN	80	72% 96% ..
8	BO	80	84% 95% ..
8	BP	80	80% 91% 5% ..
8	BQ	80	81% 98% .
8	BR	80	90% 94% ..
8	BS	80	92% 94% ..
8	BT	80	95% 94% ..
8	BU	80	94% 98% .

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Mol	Chain	Length	Quality of chain
8	BV	80	 <p>98% 98%</p>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 170801 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 Lipoprotein PrgK.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	184	1431	901	250	277	3	0	0
1	AB	184	1431	901	250	277	3	0	0
1	AC	184	1431	901	250	277	3	0	0
1	AD	184	1431	901	250	277	3	0	0
1	AE	184	1431	901	250	277	3	0	0
1	AF	184	1431	901	250	277	3	0	0
1	AG	184	1431	901	250	277	3	0	0
1	AH	184	1431	901	250	277	3	0	0
1	AI	184	1431	901	250	277	3	0	0
1	AL	184	1431	901	250	277	3	0	0
1	o	184	1431	901	250	277	3	0	0
1	p	184	1431	901	250	277	3	0	0
1	q	184	1431	901	250	277	3	0	0
1	r	184	1431	901	250	277	3	0	0
1	s	184	1431	901	250	277	3	0	0
1	t	184	1431	901	250	277	3	0	0
1	u	184	1431	901	250	277	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	v	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	w	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	x	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	y	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	z	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AJ	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AK	184	Total 1431	C 901	N 250	O 277	S 3	0	0

- Molecule 2 is a protein called Protein PrgH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	222	Total 1836	C 1170	N 326	O 335	S 5	0	0
2	R	221	Total 1827	C 1164	N 325	O 333	S 5	0	0
2	S	222	Total 1831	C 1167	N 326	O 333	S 5	0	0
2	T	222	Total 1836	C 1170	N 326	O 335	S 5	0	0
2	U	221	Total 1827	C 1164	N 325	O 333	S 5	0	0
2	V	222	Total 1831	C 1167	N 326	O 333	S 5	0	0
2	W	222	Total 1836	C 1170	N 326	O 335	S 5	0	0
2	X	221	Total 1827	C 1164	N 325	O 333	S 5	0	0
2	Y	222	Total 1831	C 1167	N 326	O 333	S 5	0	0
2	Z	222	Total 1836	C 1170	N 326	O 335	S 5	0	0
2	a	221	Total 1827	C 1164	N 325	O 333	S 5	0	0
2	b	222	Total 1831	C 1167	N 326	O 333	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
2	d	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
2	e	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
2	f	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
2	g	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
2	h	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
2	i	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
2	j	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
2	k	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
2	l	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
2	m	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
2	n	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		

- Molecule 3 is a protein called Protein InvG.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
3	A	497	Total	C	N	O	S	0	0
			3838	2428	664	733	13		
3	B	502	Total	C	N	O	S	1	0
			3884	2459	673	739	13		
3	C	497	Total	C	N	O	S	0	0
			3838	2428	664	733	13		
3	D	502	Total	C	N	O	S	0	0
			3876	2454	670	739	13		
3	F	497	Total	C	N	O	S	0	0
			3838	2428	664	733	13		
3	G	502	Total	C	N	O	S	1	0
			3884	2459	673	739	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	497	Total	C	N	O	S	0	0
			3838	2428	664	733	13		
3	I	502	Total	C	N	O	S	1	0
			3884	2459	673	739	13		
3	J	497	Total	C	N	O	S	0	0
			3838	2428	664	733	13		
3	K	502	Total	C	N	O	S	1	0
			3884	2459	673	739	13		
3	L	497	Total	C	N	O	S	0	0
			3838	2428	664	733	13		
3	M	502	Total	C	N	O	S	0	0
			3876	2454	670	739	13		
3	N	497	Total	C	N	O	S	0	0
			3838	2428	664	733	13		
3	O	502	Total	C	N	O	S	1	0
			3884	2459	673	739	13		
3	P	497	Total	C	N	O	S	0	0
			3838	2428	664	733	13		

- Molecule 4 is a protein called Surface presentation of antigens protein SpaP.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	0	199	Total	C	N	O	S	0	0
			1562	1041	231	279	11		
4	1	199	Total	C	N	O	S	0	0
			1569	1047	232	279	11		
4	2	197	Total	C	N	O	S	0	0
			1553	1037	230	275	11		
4	3	204	Total	C	N	O	S	0	0
			1606	1071	238	286	11		
4	4	221	Total	C	N	O	S	1	0
			1758	1163	266	318	11		

- Molecule 5 is a protein called Surface presentation of antigens protein SpaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	247	Total	C	N	O	S	0	0
			1885	1252	300	320	13		

- Molecule 6 is a protein called Surface presentation of antigens protein SpaQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	53	Total	C	N	O	S	0	0
			405	276	61	67	1		
6	7	84	Total	C	N	O	S	0	0
			644	436	97	109	2		
6	8	84	Total	C	N	O	S	0	0
			644	436	97	109	2		
6	9	84	Total	C	N	O	S	0	0
			647	438	97	109	3		

- Molecule 7 is a protein called Protein PrgJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AM	39	Total	C	N	O	S	0	0
			298	187	49	60	2		
7	AN	78	Total	C	N	O	S	7	0
			644	396	116	130	2		
7	AO	88	Total	C	N	O	S	0	0
			667	410	114	140	3		
7	AP	88	Total	C	N	O	S	0	0
			667	410	114	140	3		
7	AQ	88	Total	C	N	O	S	0	0
			667	410	114	140	3		
7	AR	88	Total	C	N	O	S	0	0
			667	410	114	140	3		

- Molecule 8 is a protein called Protein PrgI.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AS	59	Total	C	N	O	0	0
			466	294	80	92		
8	AT	59	Total	C	N	O	0	0
			466	294	80	92		
8	AU	59	Total	C	N	O	0	0
			466	294	80	92		
8	AV	59	Total	C	N	O	0	0
			466	294	80	92		
8	AW	59	Total	C	N	O	0	0
			466	294	80	92		
8	AX	73	Total	C	N	O	0	0
			574	362	95	117		
8	AY	78	Total	C	N	O	0	0
			612	387	101	124		
8	AZ	78	Total	C	N	O	0	0
			612	387	101	124		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	BB	78	Total 612	C 387	N 101	O 124	0	0
8	BD	78	Total 612	C 387	N 101	O 124	0	0
8	BE	78	Total 612	C 387	N 101	O 124	0	0
8	BJ	78	Total 612	C 387	N 101	O 124	0	0
8	BK	78	Total 612	C 387	N 101	O 124	0	0
8	BF	78	Total 612	C 387	N 101	O 124	0	0
8	BL	78	Total 612	C 387	N 101	O 124	0	0
8	BG	78	Total 612	C 387	N 101	O 124	0	0
8	BM	78	Total 612	C 387	N 101	O 124	0	0
8	BH	78	Total 612	C 387	N 101	O 124	0	0
8	BN	78	Total 612	C 387	N 101	O 124	0	0
8	BI	78	Total 612	C 387	N 101	O 124	0	0
8	BO	78	Total 612	C 387	N 101	O 124	0	0
8	BP	78	Total 612	C 387	N 101	O 124	0	0
8	BQ	78	Total 612	C 387	N 101	O 124	0	0
8	BC	78	Total 612	C 387	N 101	O 124	0	0
8	BA	78	Total 612	C 387	N 101	O 124	0	0
8	BV	78	Total 612	C 387	N 101	O 124	0	0
8	BU	78	Total 612	C 387	N 101	O 124	0	0
8	BT	78	Total 612	C 387	N 101	O 124	0	0
8	BS	78	Total 612	C 387	N 101	O 124	0	0

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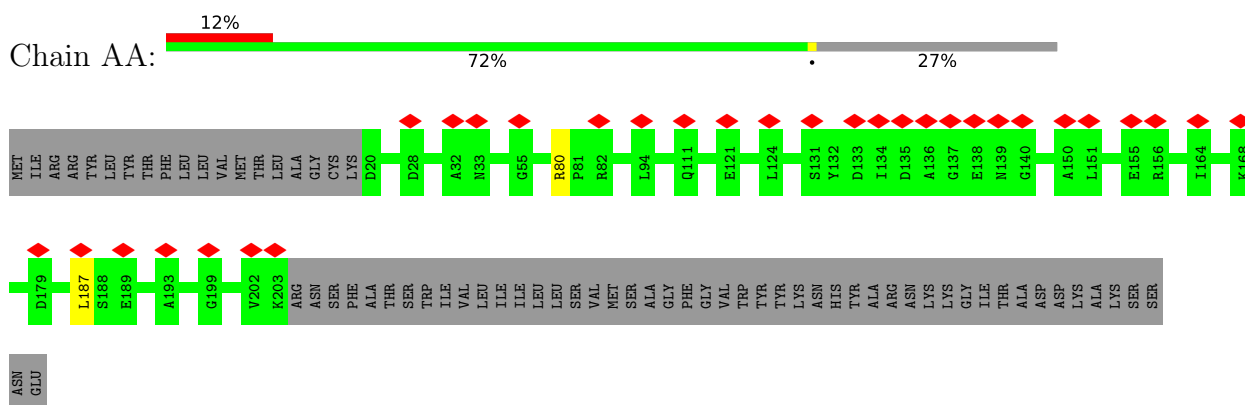
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Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
8	BR	78	612	387	101	124	0	0

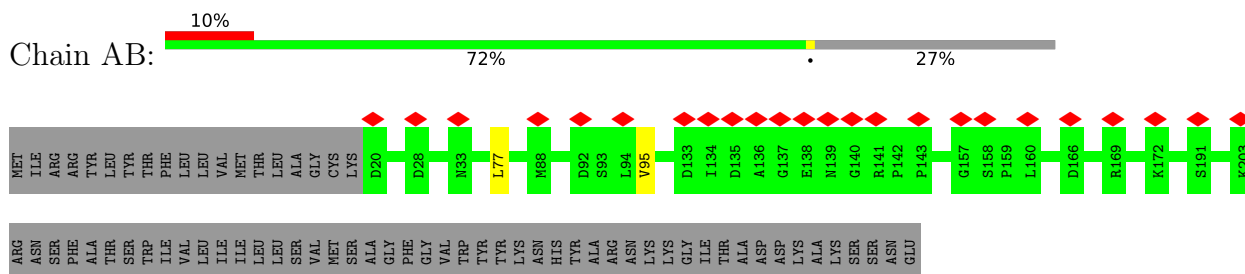
3 Residue-property plots [i](#)

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.

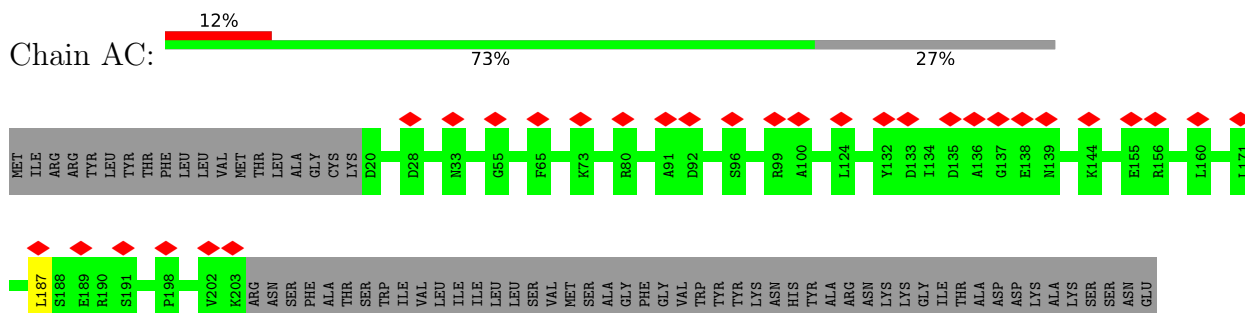
- Molecule 1: Lipoprotein PrgK



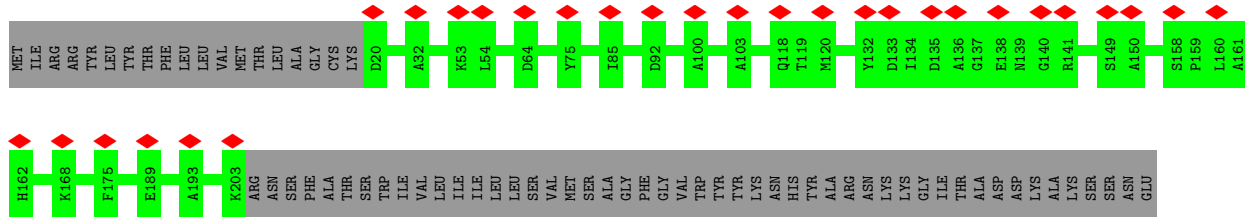
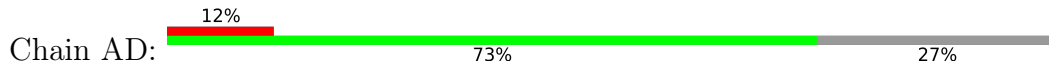
- Molecule 1: Lipoprotein PrgK



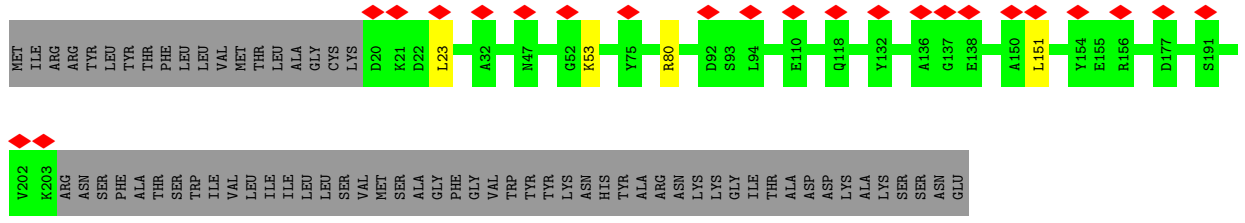
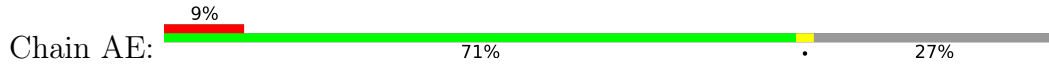
- Molecule 1: Lipoprotein PrgK



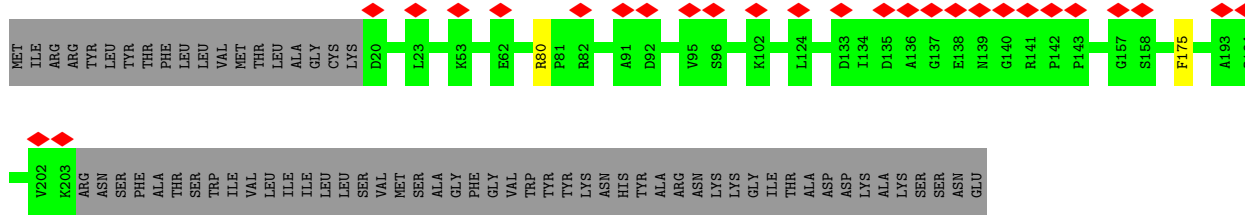
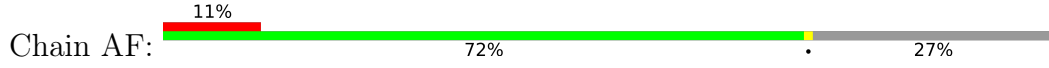
- Molecule 1: Lipoprotein PrgK



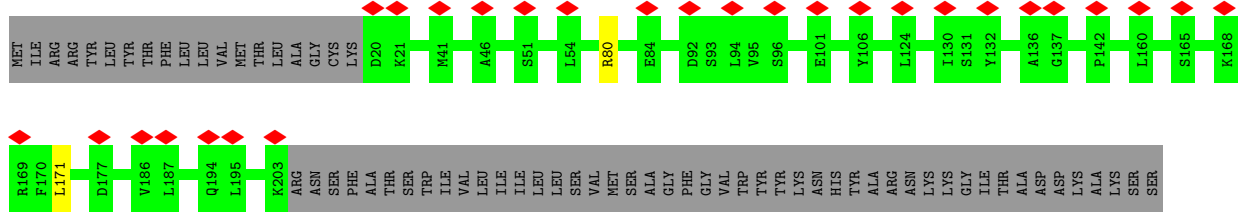
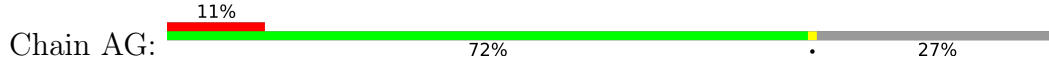
• Molecule 1: Lipoprotein PrgK



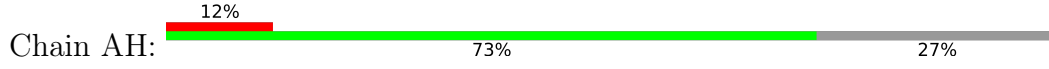
• Molecule 1: Lipoprotein PrgK

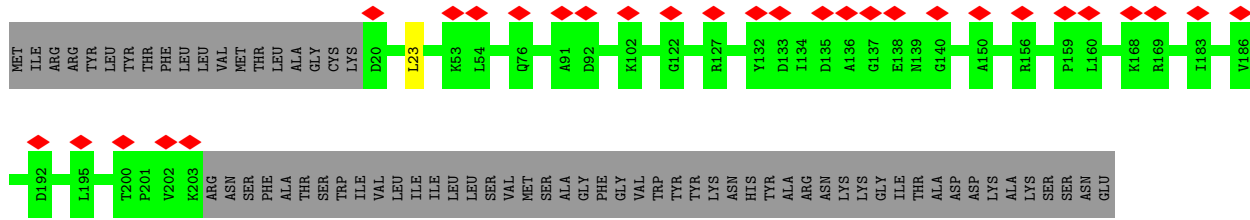


• Molecule 1: Lipoprotein PrgK

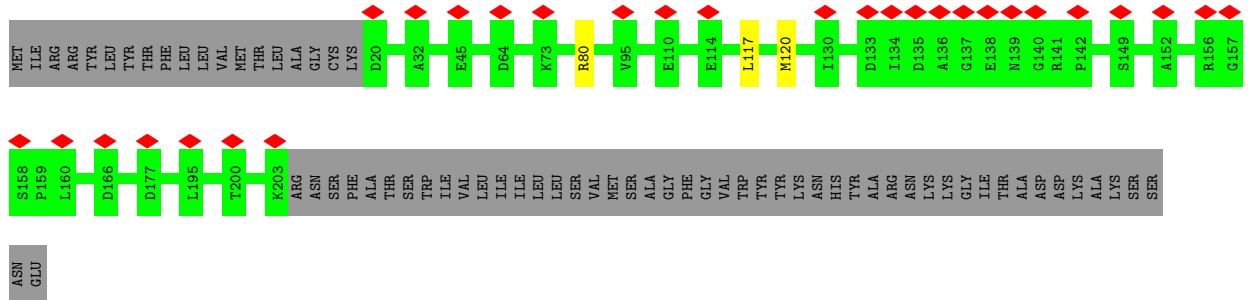
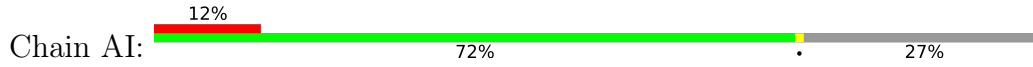


• Molecule 1: Lipoprotein PrgK

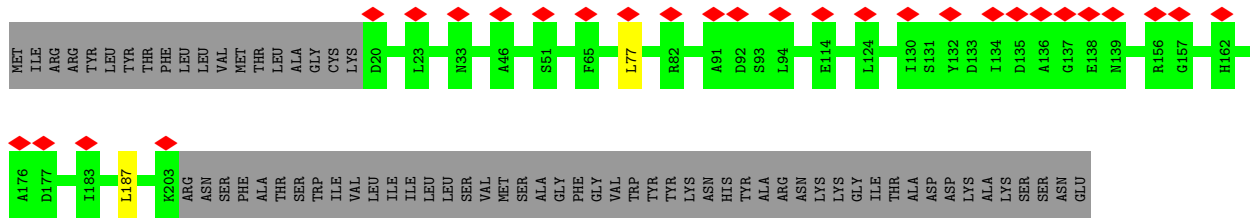
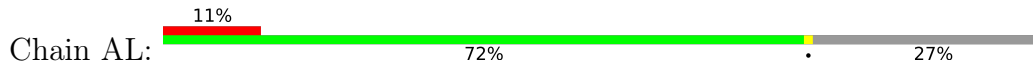




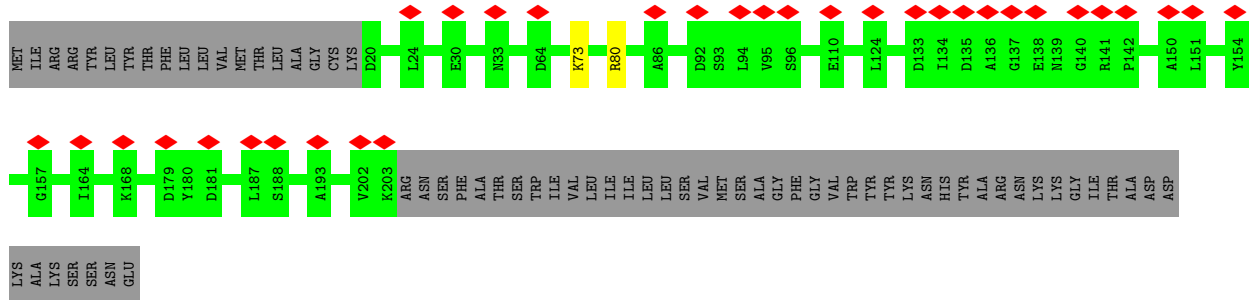
• Molecule 1: Lipoprotein PrgK



• Molecule 1: Lipoprotein PrgK

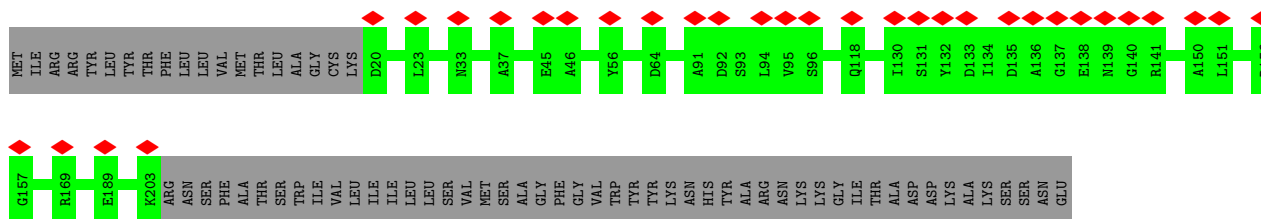


• Molecule 1: Lipoprotein PrgK

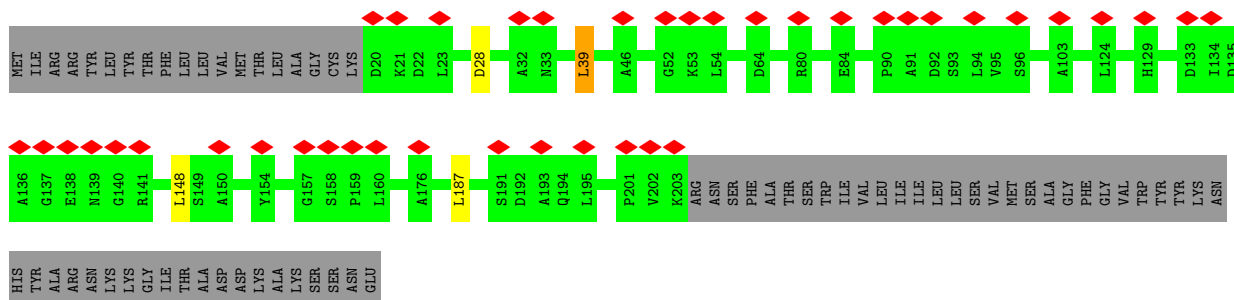


• Molecule 1: Lipoprotein PrgK

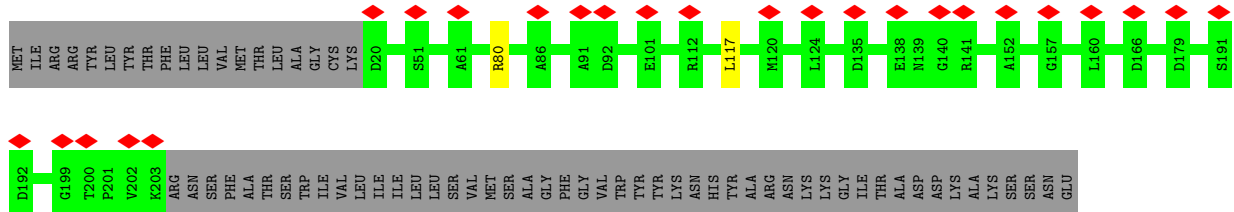




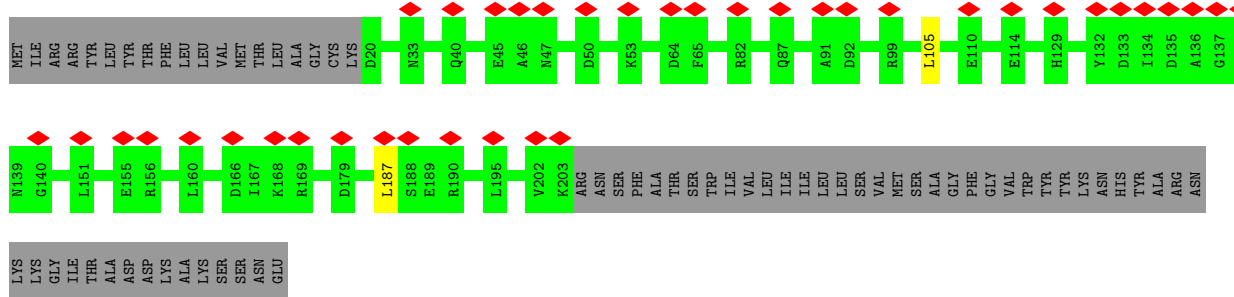
• Molecule 1: Lipoprotein PrgK



• Molecule 1: Lipoprotein PrgK



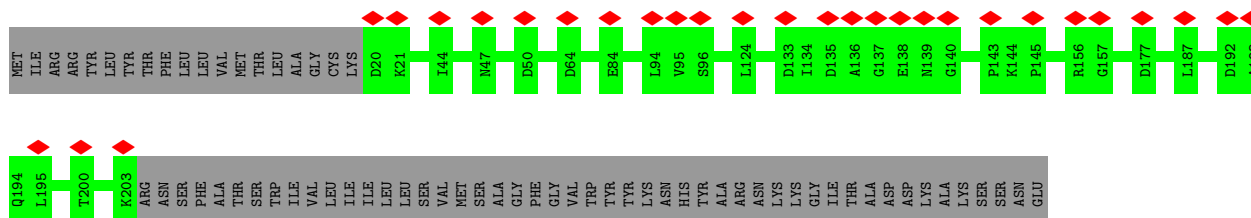
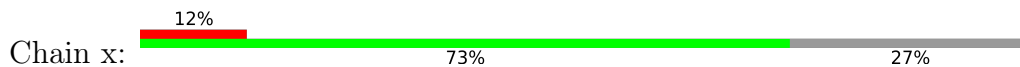
• Molecule 1: Lipoprotein PrgK



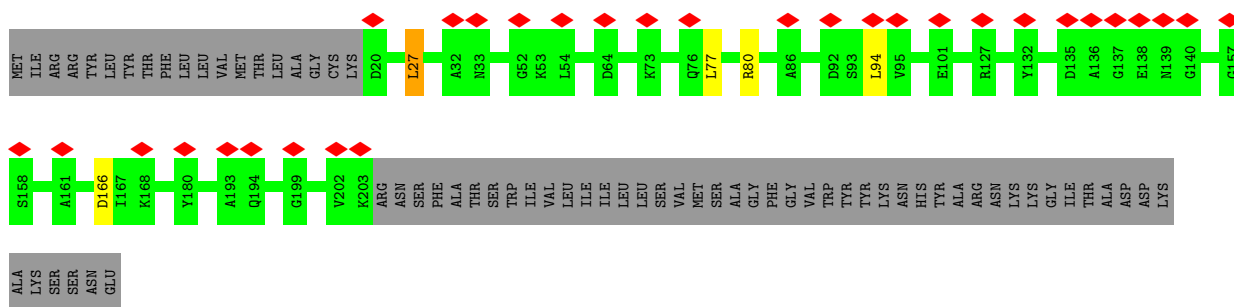
• Molecule 1: Lipoprotein PrgK



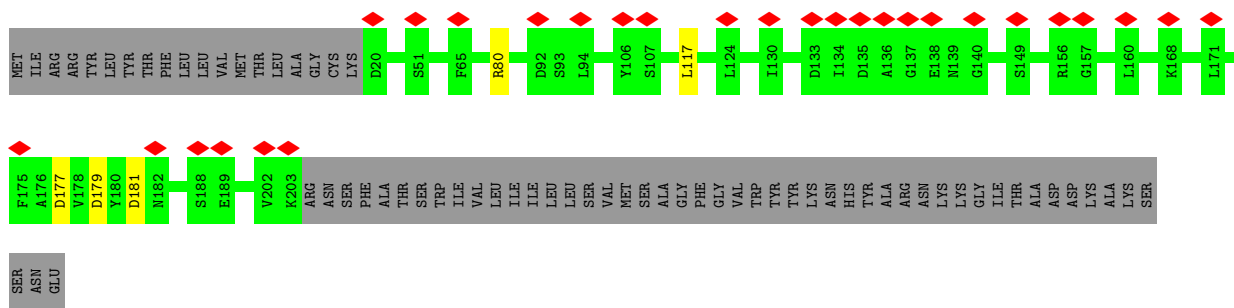
• Molecule 1: Lipoprotein PrgK



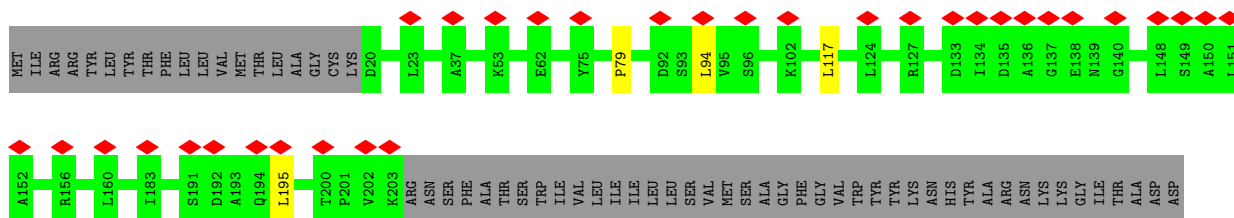
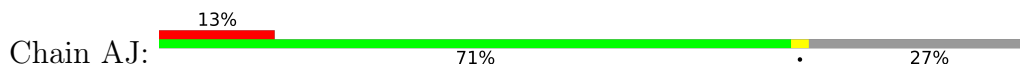
• Molecule 1: Lipoprotein PrgK

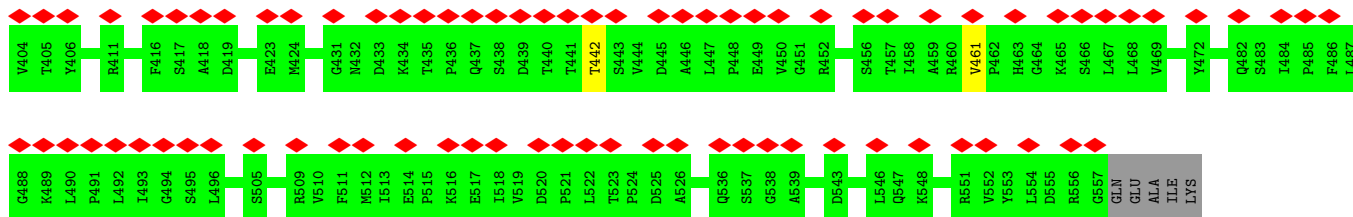


• Molecule 1: Lipoprotein PrgK



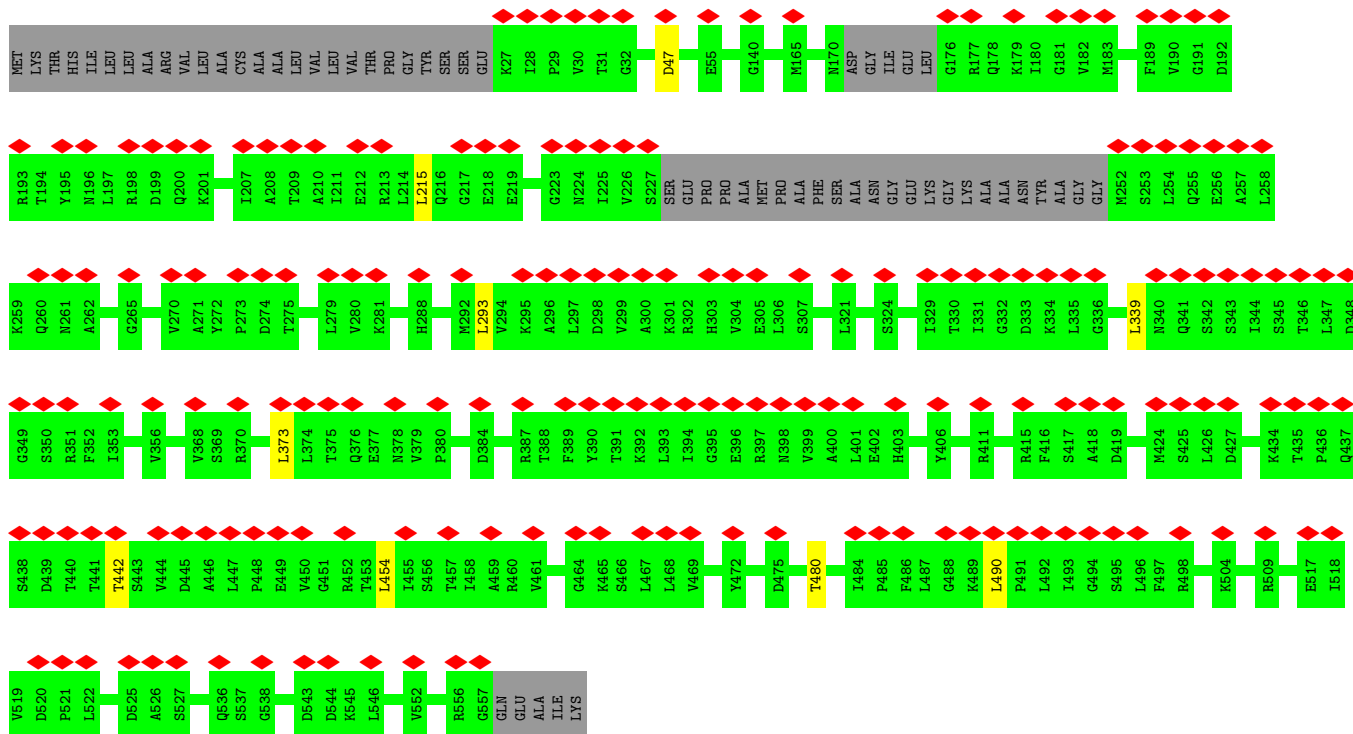
• Molecule 1: Lipoprotein PrgK





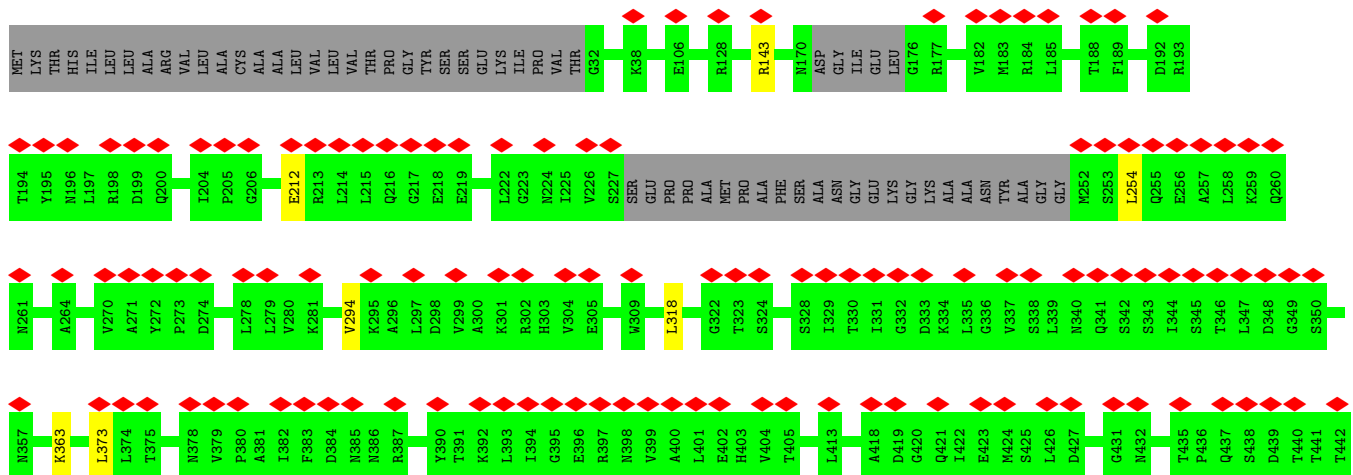
• Molecule 3: Protein InvG

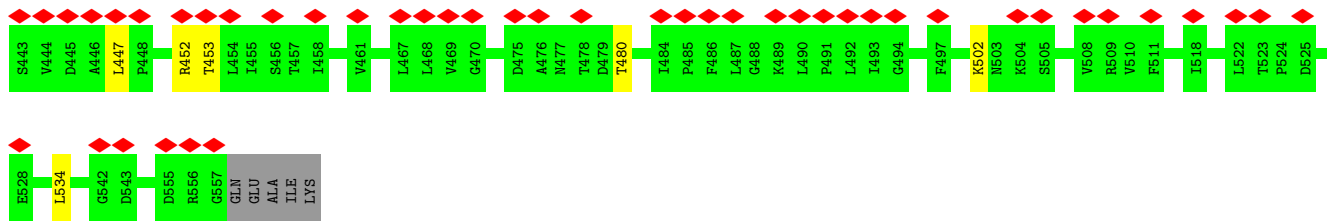
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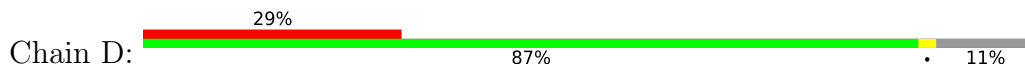
• Molecule 3: Protein InvG

Chain C:

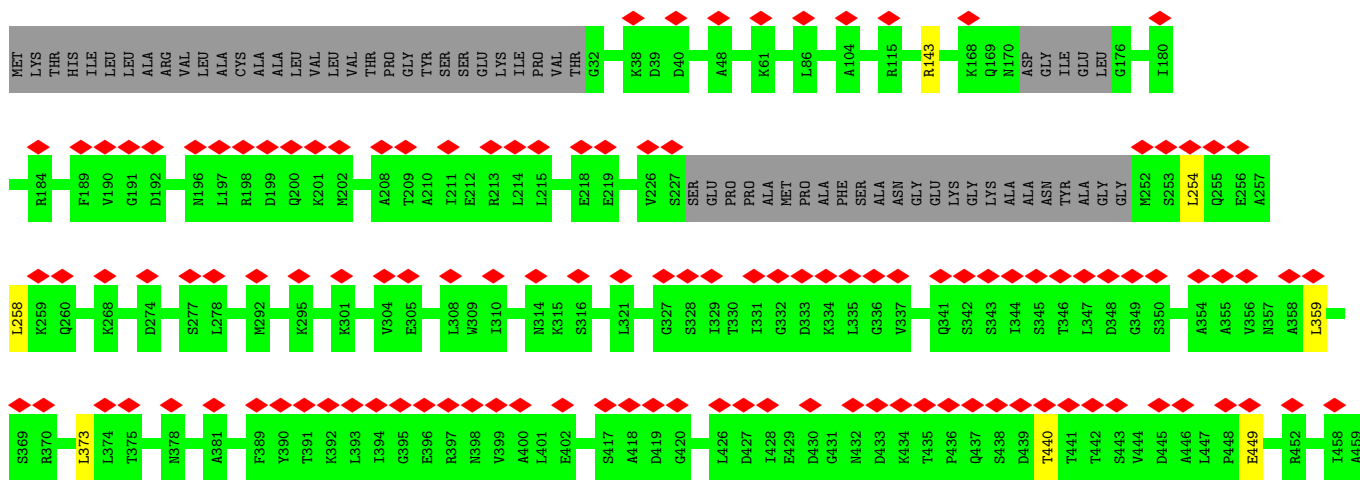
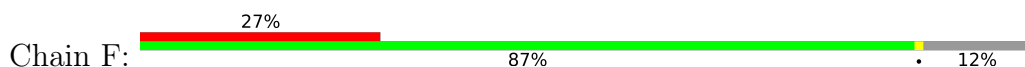


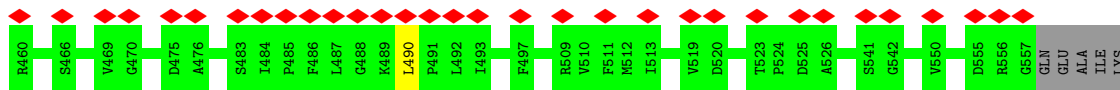


• Molecule 3: Protein InvG

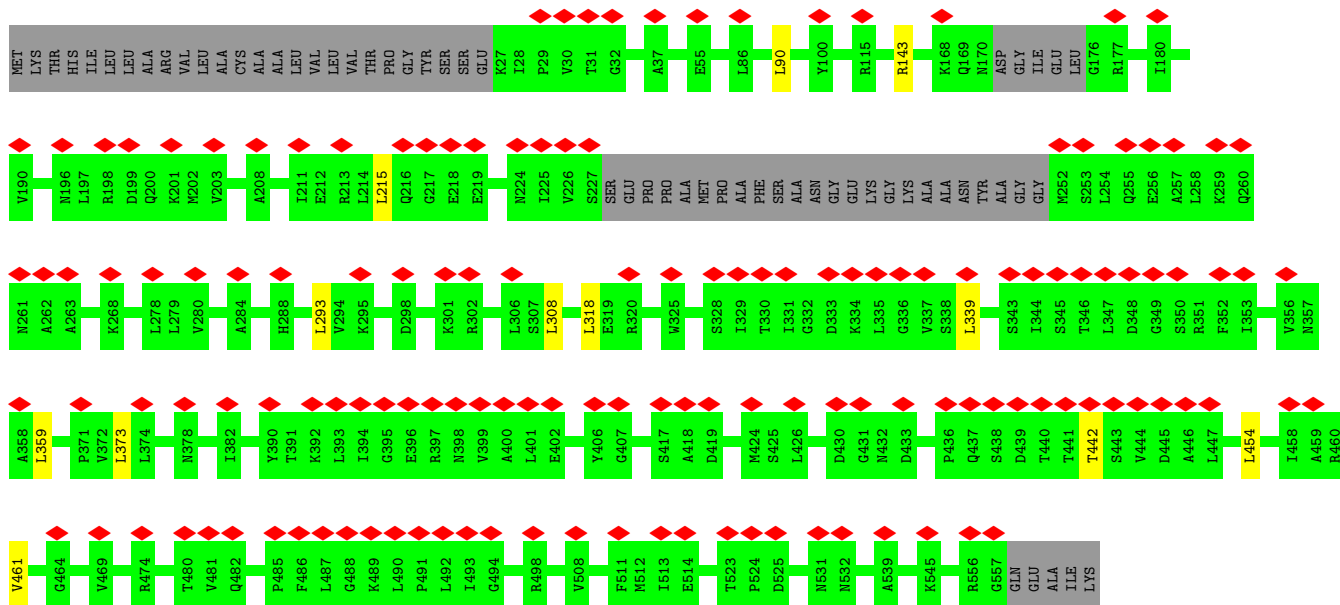
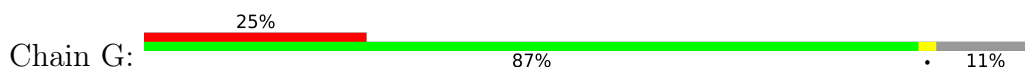


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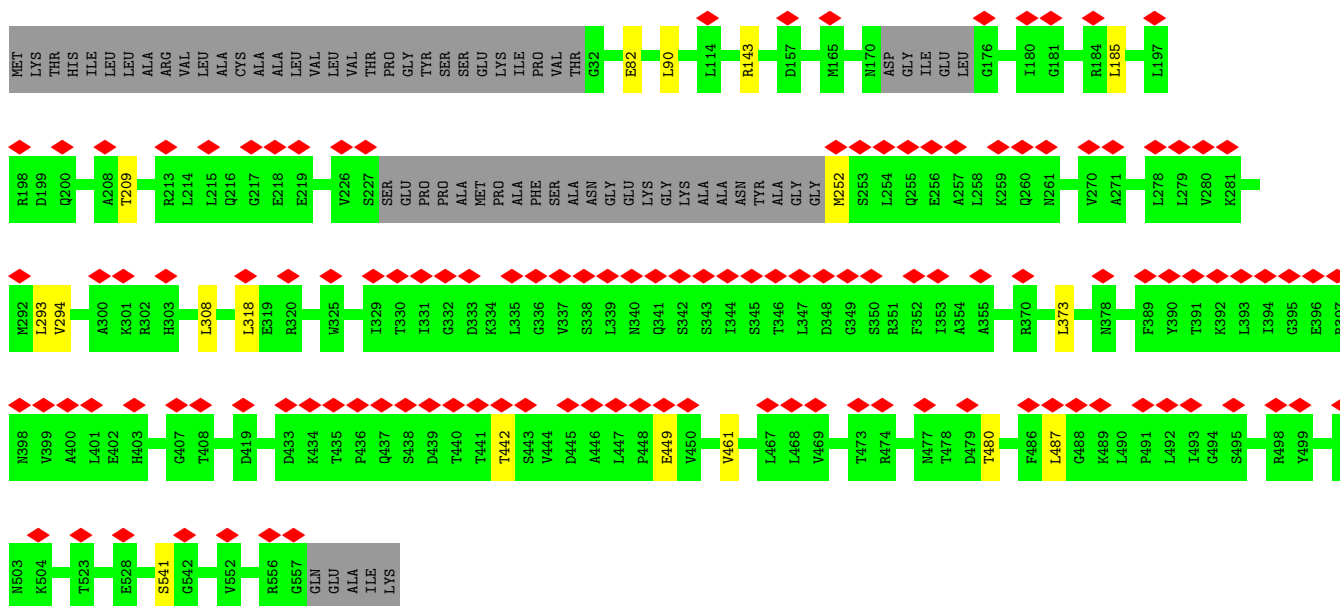
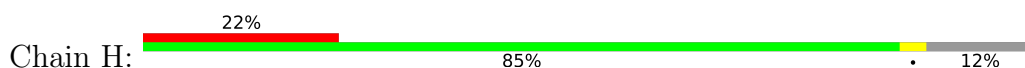




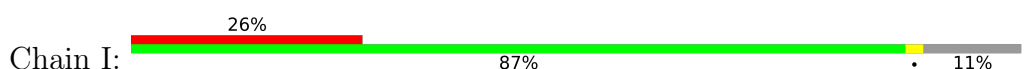
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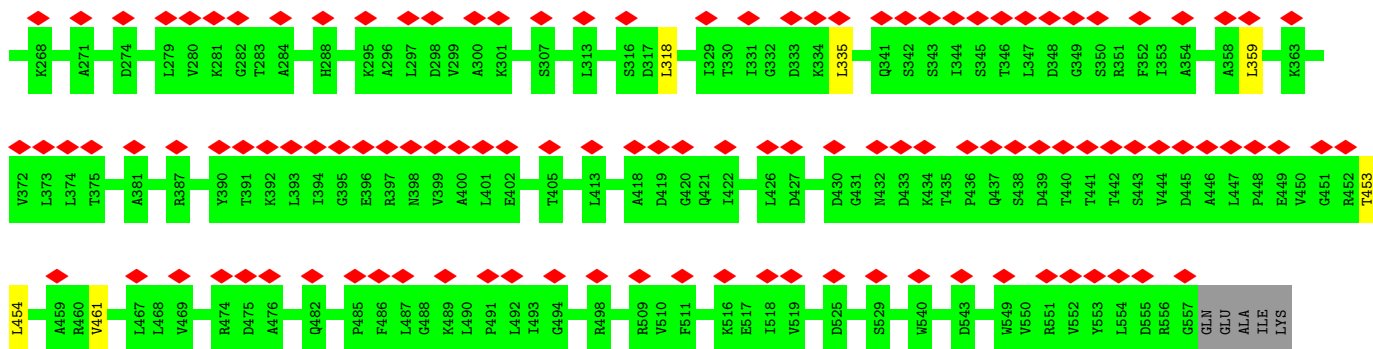


• Molecule 3: Protein InvG



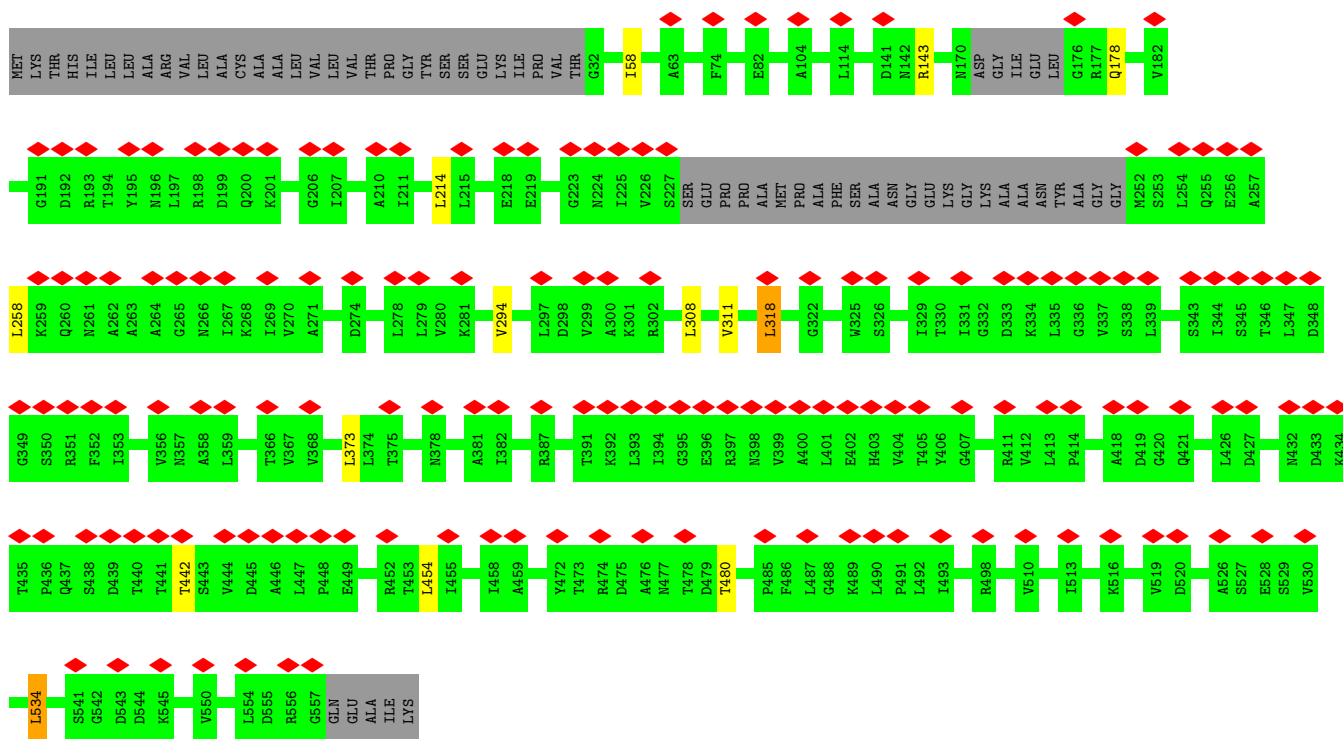
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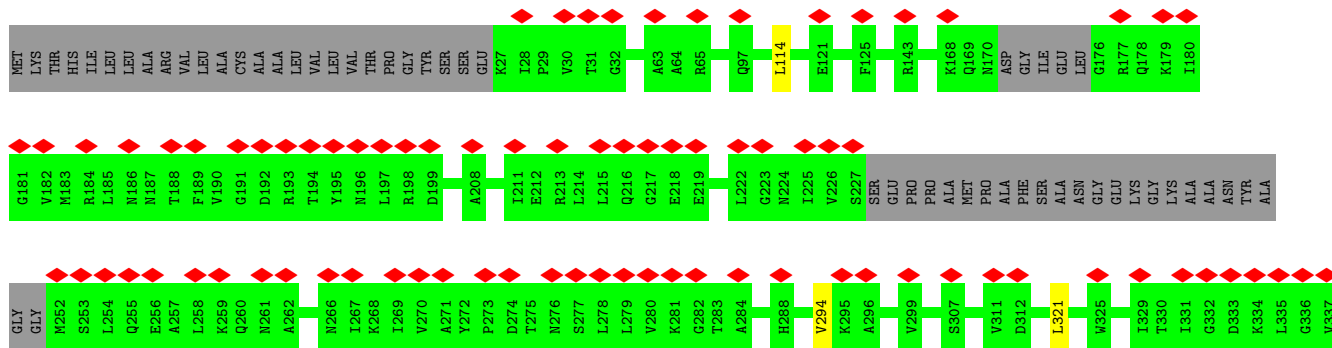
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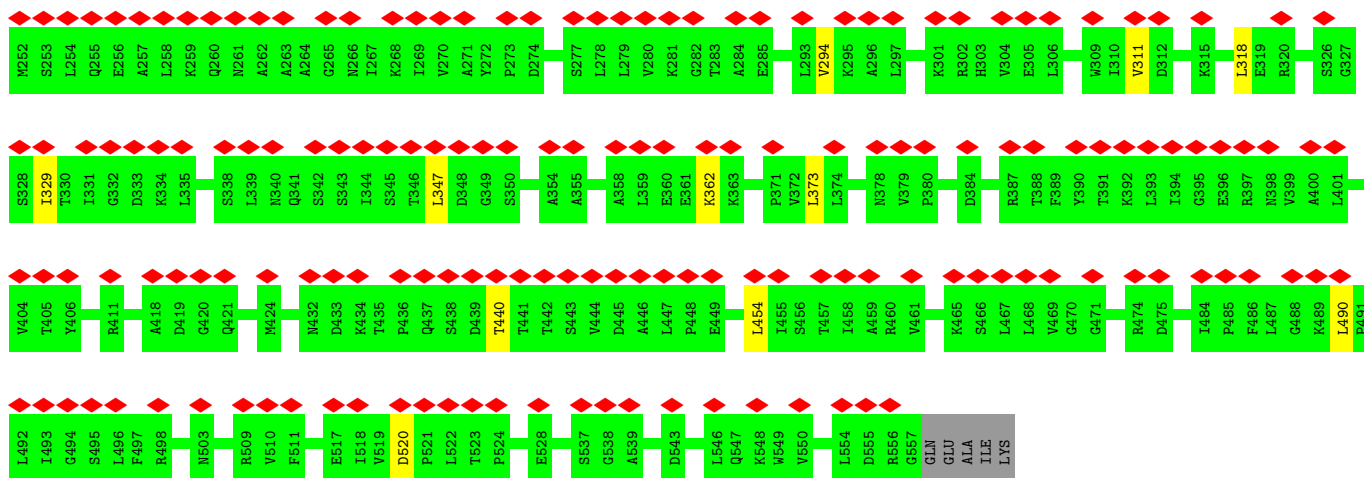
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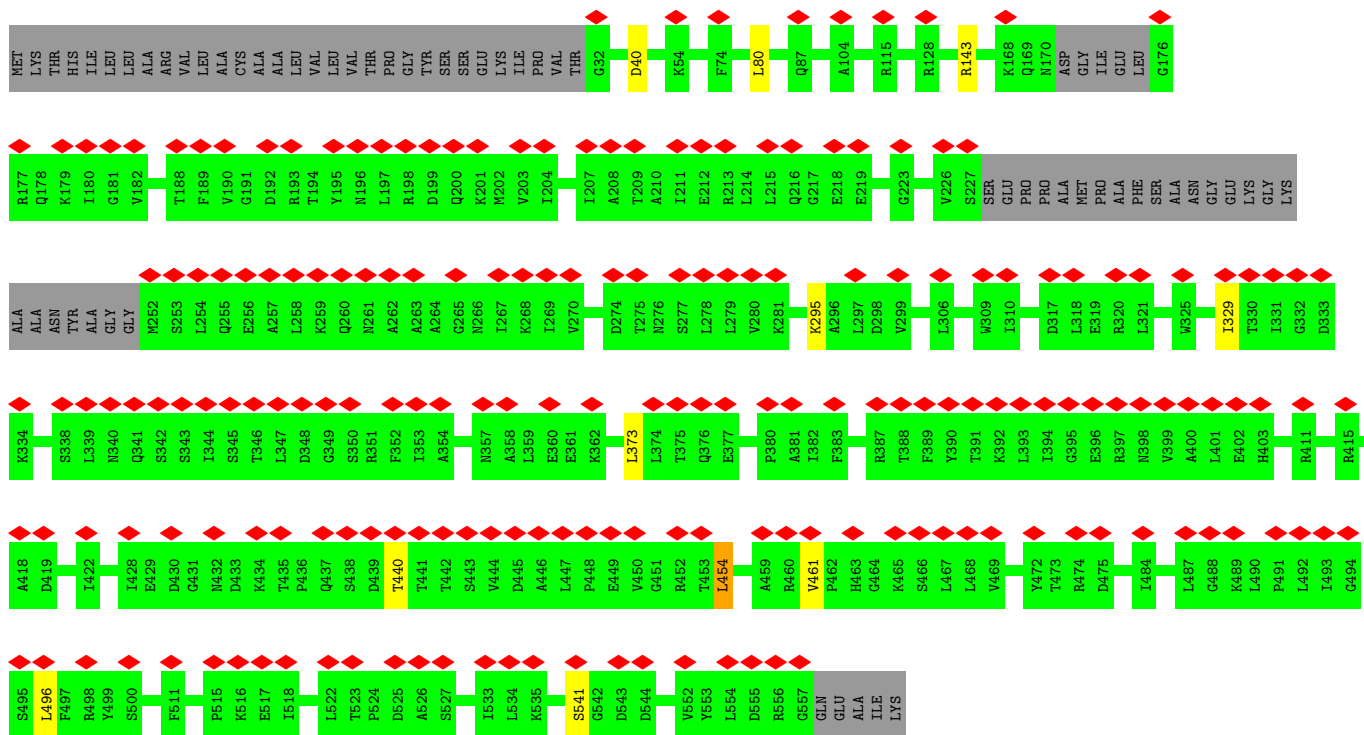
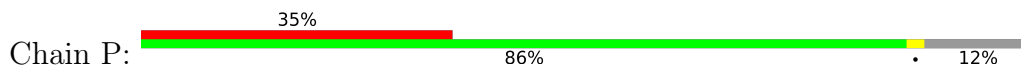
• Molecule 3: Protein InvG

Chain M:

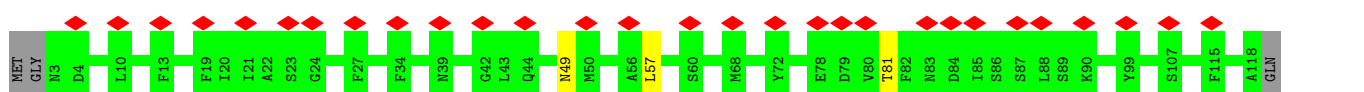
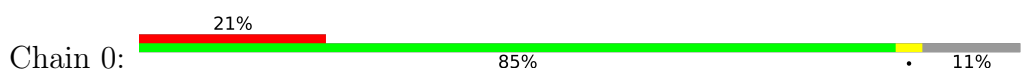




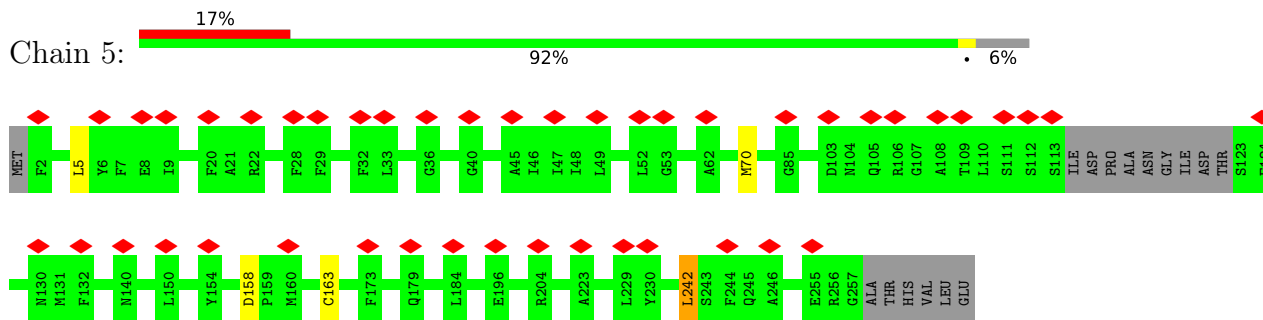
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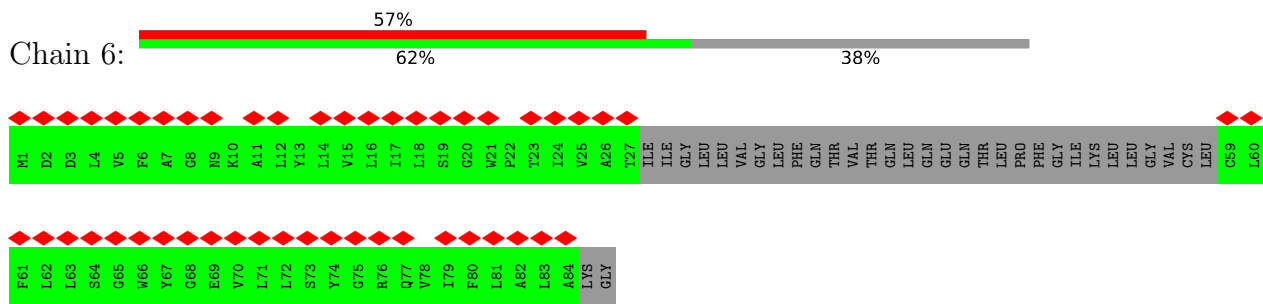
• Molecule 4: Surface presentation of antigens protein SpaP



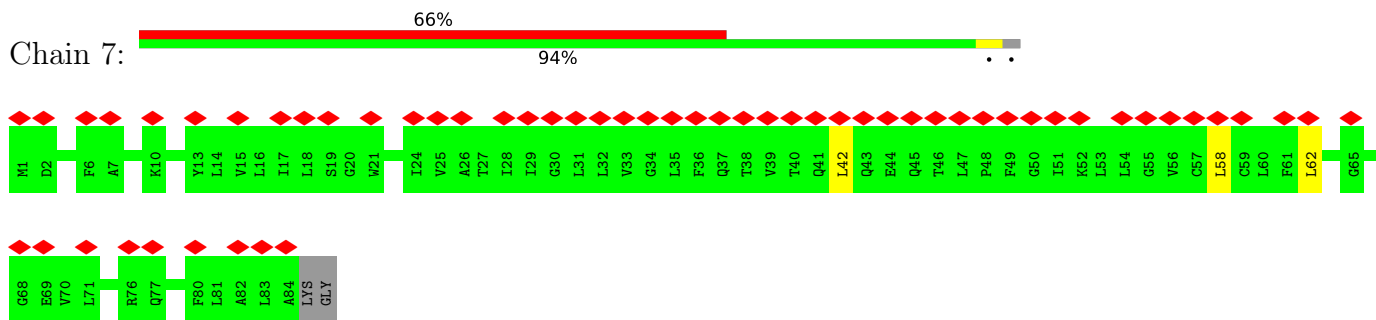
• Molecule 5: Surface presentation of antigens protein SpaR



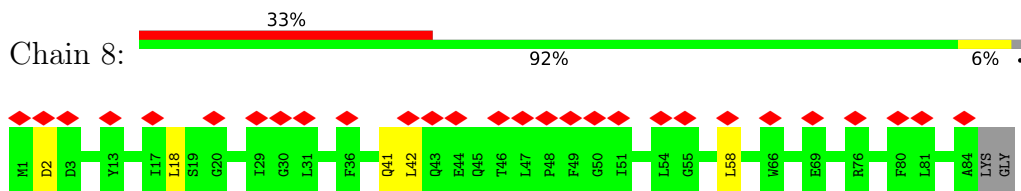
• Molecule 6: Surface presentation of antigens protein SpaQ



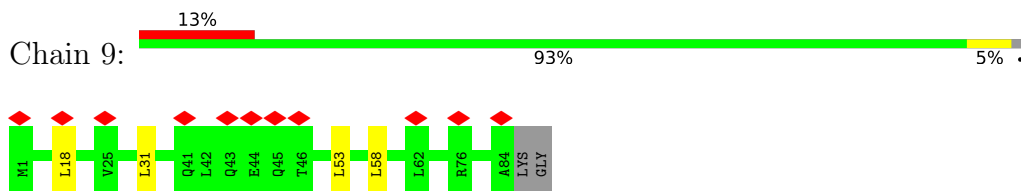
• Molecule 6: Surface presentation of antigens protein SpaQ



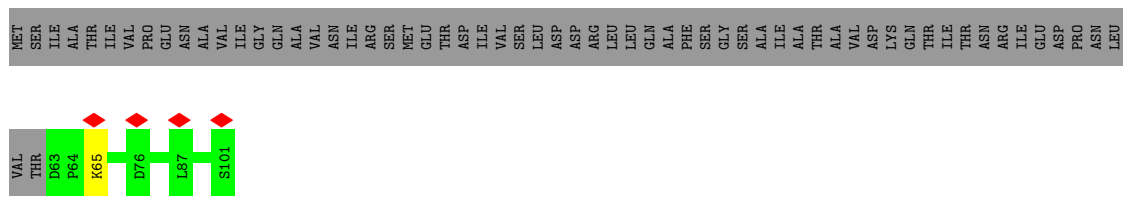
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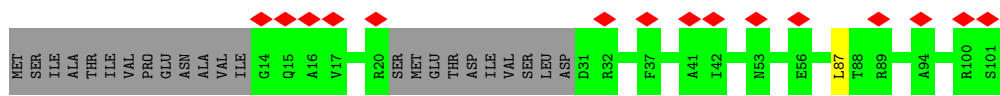
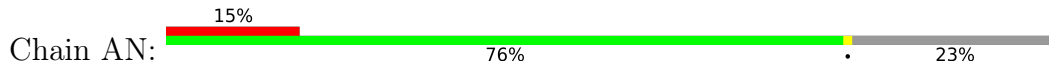
• Molecule 6: Surface presentation of antigens protein SpaQ



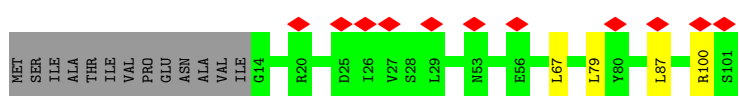
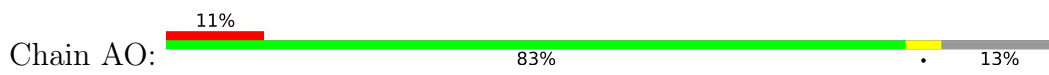
• Molecule 7: Protein PrgJ



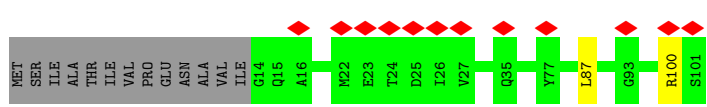
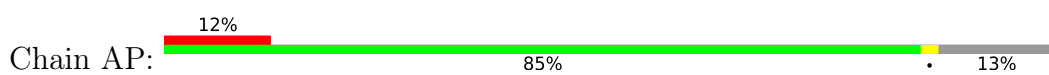
• Molecule 7: Protein PrgJ



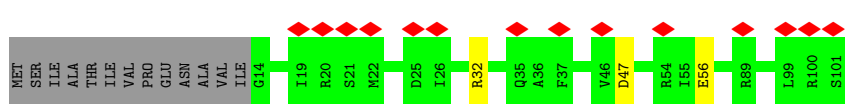
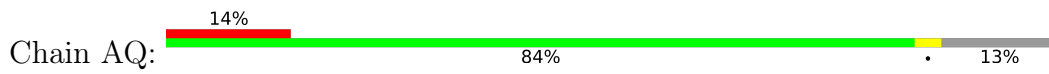
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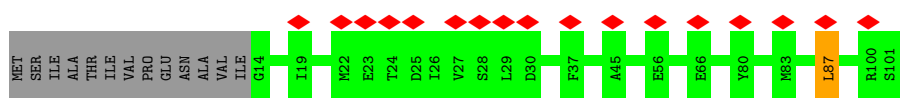
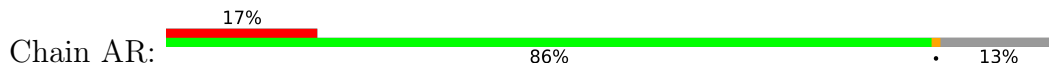
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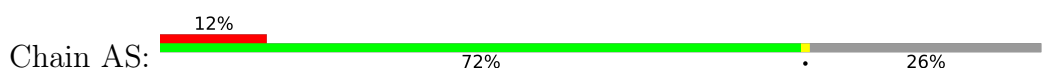
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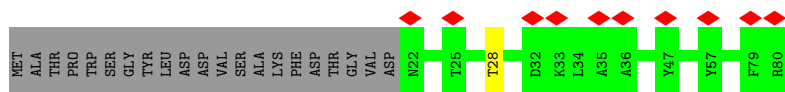


• Molecule 7: Protein PrgJ

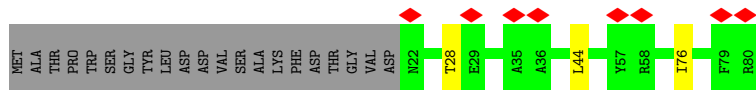
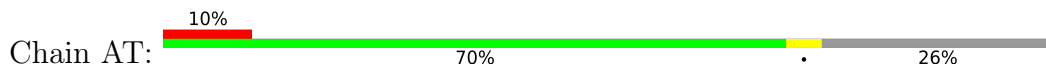


• Molecule 8: Protein PrgI

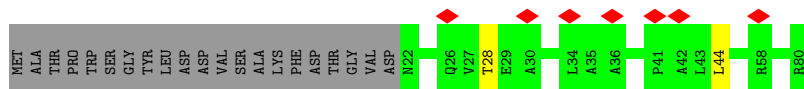
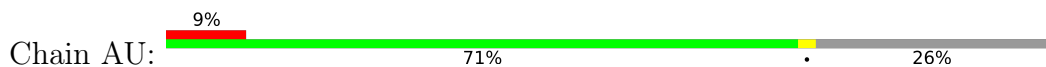




• Molecule 8: Protein PrgI



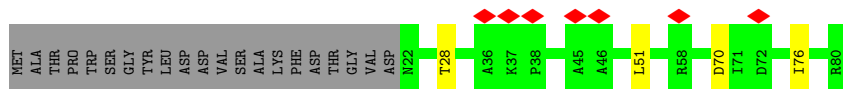
• Molecule 8: Protein PrgI



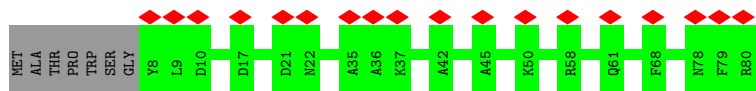
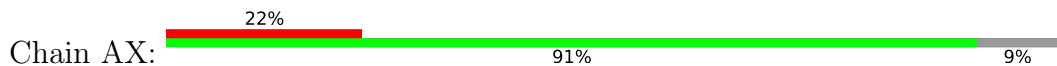
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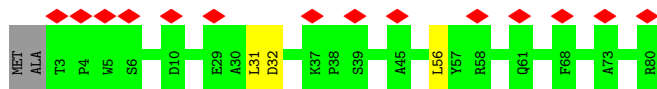
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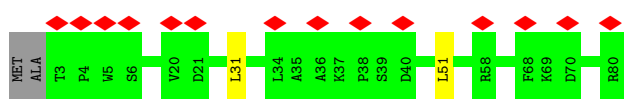
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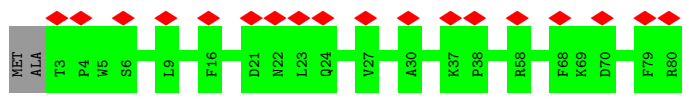
• Molecule 8: Protein PrgI



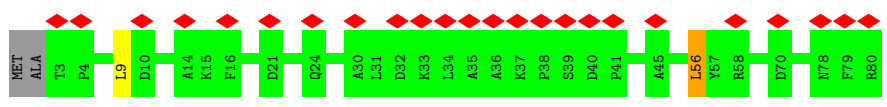
• Molecule 8: Protein PrgI



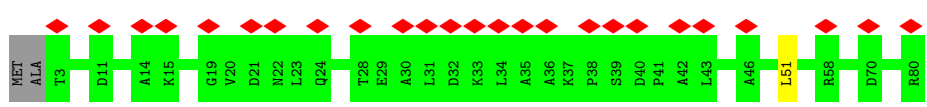
● Molecule 8: Protein PrgI



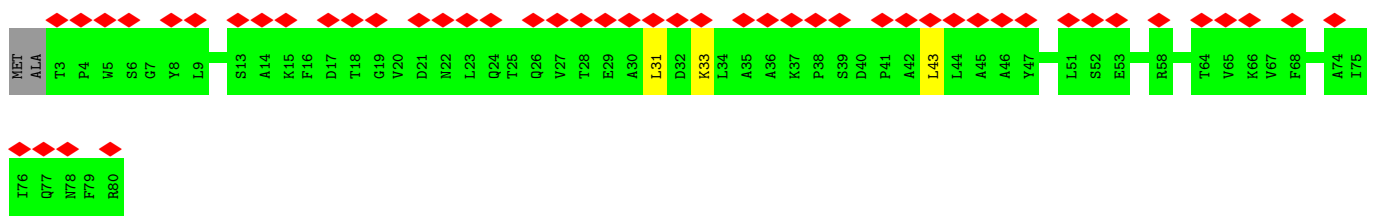
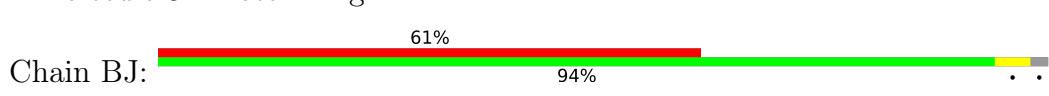
● Molecule 8: Protein PrgI



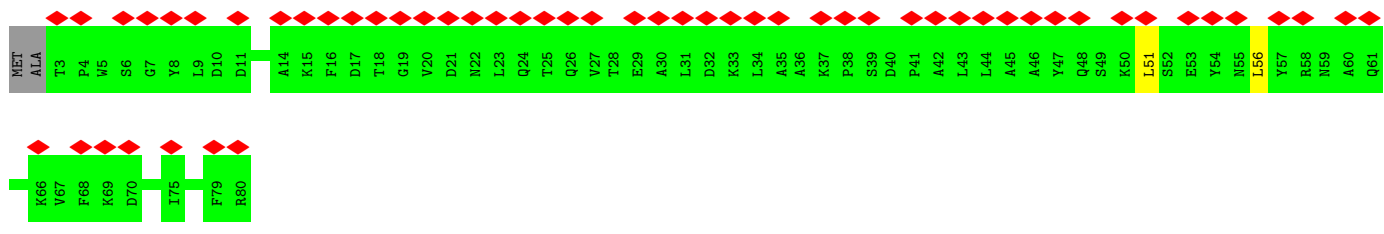
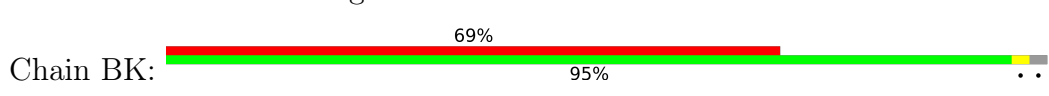
● Molecule 8: Protein PrgI



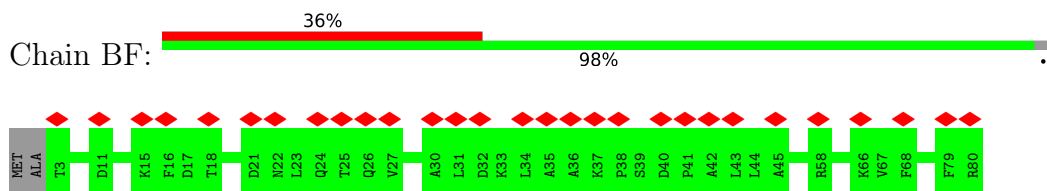
● Molecule 8: Protein PrgI



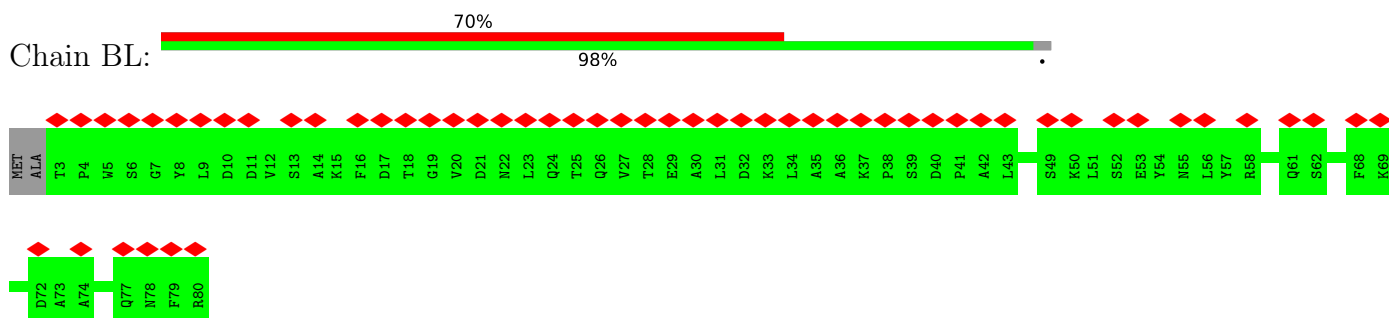
● Molecule 8: Protein PrgI



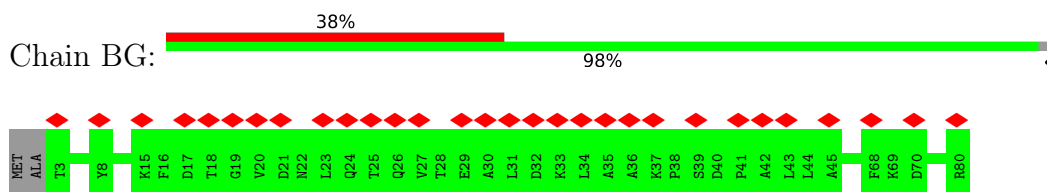
• Molecule 8: Protein PrgI



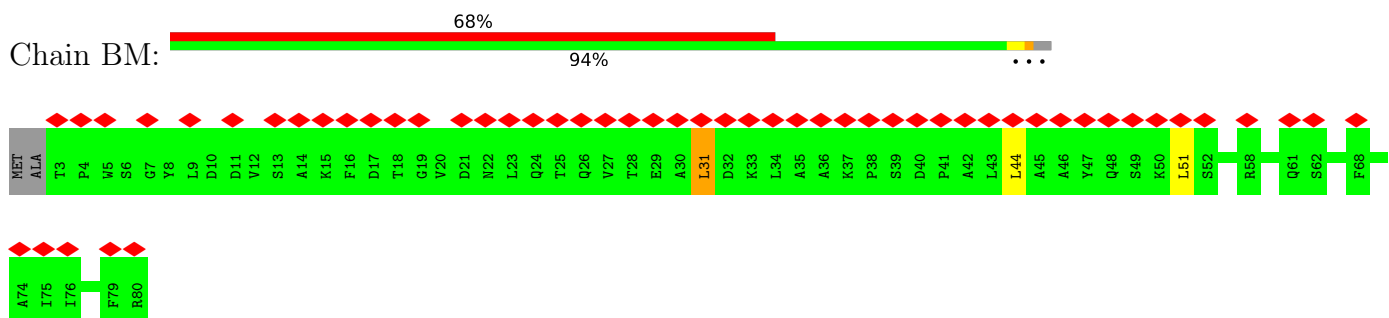
• Molecule 8: Protein PrgI



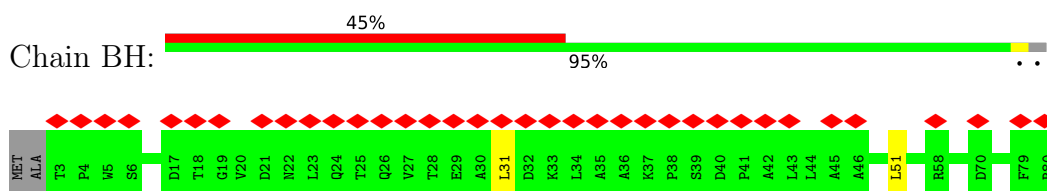
• Molecule 8: Protein PrgI



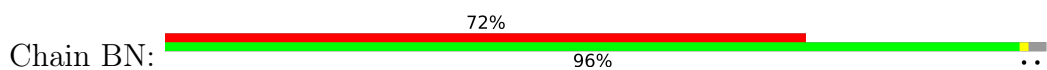
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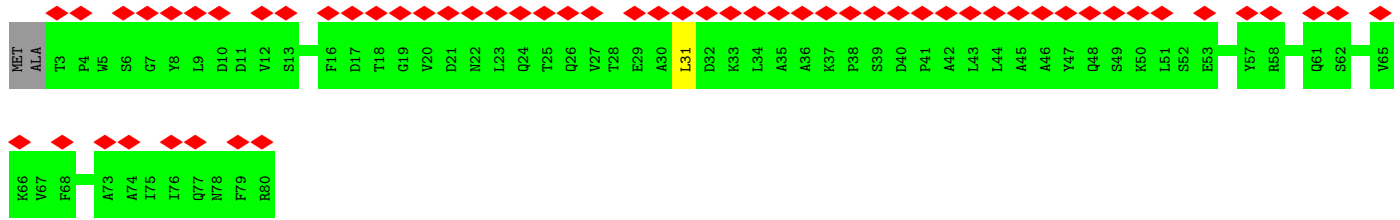


• Molecule 8: Protein PrgI

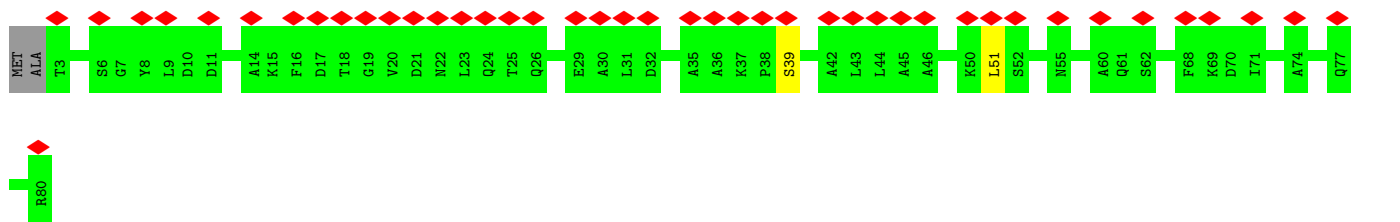


• Molecule 8: Protein PrgI

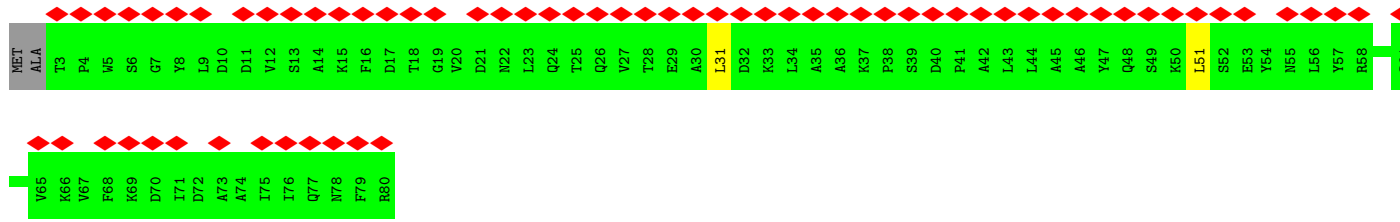
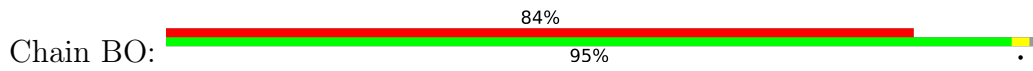




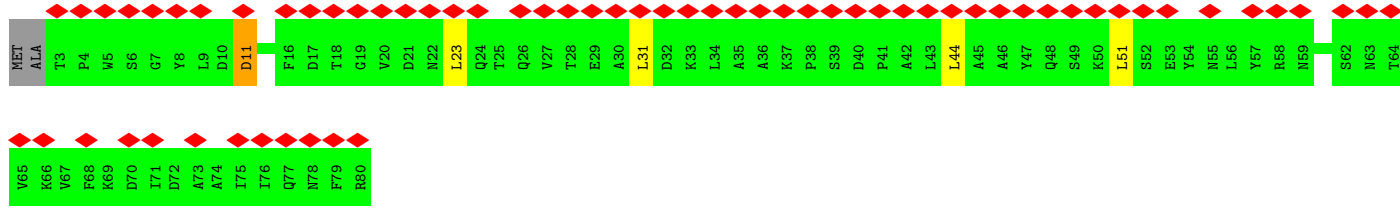
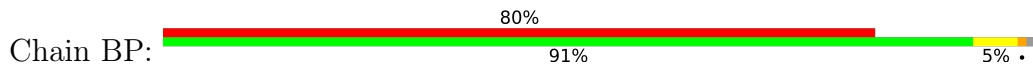
• Molecule 8: Protein PrgI



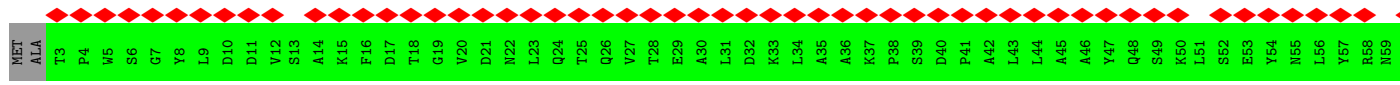
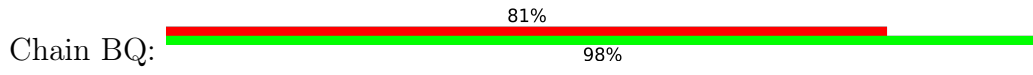
• Molecule 8: Protein PrgI

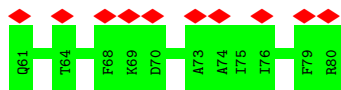


• Molecule 8: Protein PrgI

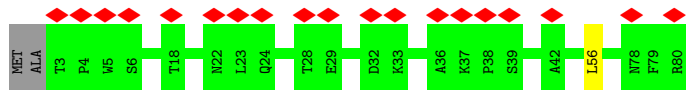


• Molecule 8: Protein PrgI





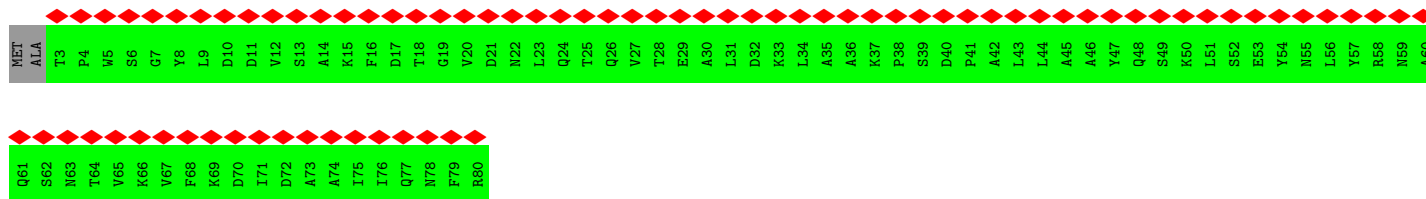
• Molecule 8: Protein PrgI



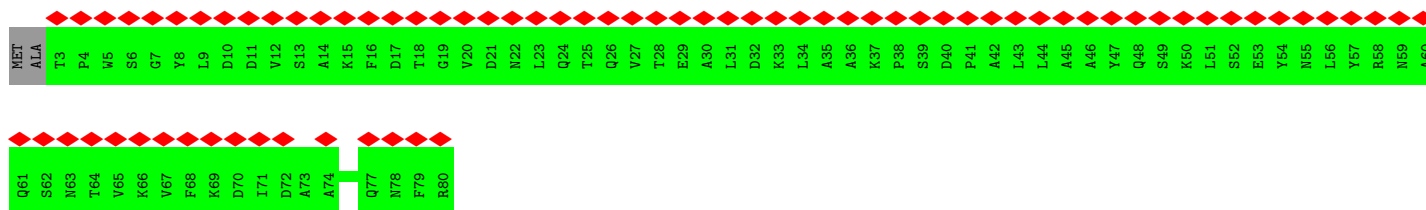
• Molecule 8: Protein PrgI



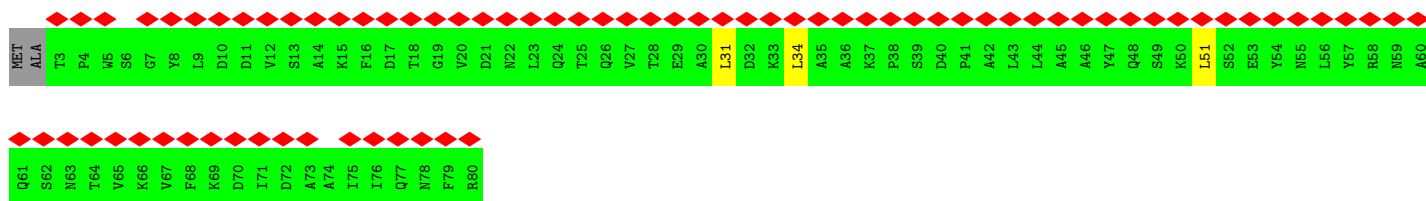
• Molecule 8: Protein PrgI



• Molecule 8: Protein PrgI



• Molecule 8: Protein PrgI



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5018	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 ($e^-/\text{\AA}^2$)	51.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.108	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	427.5, 427.5, 427.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.71, 1.71, 1.71	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.35	0/1458	0.63	0/1979
1	AB	0.34	0/1458	0.61	1/1979 (0.1%)
1	AC	0.35	0/1458	0.64	0/1979
1	AD	0.35	0/1458	0.64	0/1979
1	AE	0.36	0/1458	0.65	1/1979 (0.1%)
1	AF	0.37	0/1458	0.70	2/1979 (0.1%)
1	AG	0.37	0/1458	0.61	1/1979 (0.1%)
1	AH	0.34	0/1458	0.59	0/1979
1	AI	0.35	0/1458	0.67	2/1979 (0.1%)
1	AJ	0.38	1/1458 (0.1%)	0.65	3/1979 (0.2%)
1	AK	0.35	0/1458	0.63	1/1979 (0.1%)
1	AL	0.37	0/1458	0.67	1/1979 (0.1%)
1	o	0.35	0/1458	0.63	0/1979
1	p	0.37	0/1458	0.65	0/1979
1	q	0.36	0/1458	0.65	2/1979 (0.1%)
1	r	0.34	0/1458	0.63	1/1979 (0.1%)
1	s	0.34	0/1458	0.62	1/1979 (0.1%)
1	t	0.36	0/1458	0.65	3/1979 (0.2%)
1	u	0.36	0/1458	0.67	1/1979 (0.1%)
1	v	0.35	0/1458	0.61	0/1979
1	w	0.34	0/1458	0.64	0/1979
1	x	0.34	0/1458	0.65	0/1979
1	y	0.38	0/1458	0.69	4/1979 (0.2%)
1	z	0.35	0/1458	0.69	3/1979 (0.2%)
2	E	0.34	0/1881	0.59	1/2541 (0.0%)
2	R	0.34	0/1872	0.64	1/2530 (0.0%)
2	S	0.35	0/1876	0.63	1/2536 (0.0%)
2	T	0.34	0/1881	0.59	0/2541
2	U	0.35	0/1872	0.61	0/2530
2	V	0.34	0/1876	0.62	3/2536 (0.1%)
2	W	0.35	0/1881	0.62	1/2541 (0.0%)
2	X	0.35	0/1872	0.67	3/2530 (0.1%)
2	Y	0.35	0/1876	0.60	0/2536
2	Z	0.33	0/1881	0.57	0/2541

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	a	0.34	0/1872	0.61	0/2530
2	b	0.35	0/1876	0.64	2/2536 (0.1%)
2	c	0.36	0/1881	0.63	2/2541 (0.1%)
2	d	0.35	0/1872	0.63	2/2530 (0.1%)
2	e	0.35	0/1876	0.63	2/2536 (0.1%)
2	f	0.34	0/1881	0.62	0/2541
2	g	0.36	0/1872	0.64	2/2530 (0.1%)
2	h	0.35	0/1876	0.65	2/2536 (0.1%)
2	i	0.35	0/1881	0.58	0/2541
2	j	0.36	0/1872	0.65	2/2530 (0.1%)
2	k	0.35	0/1876	0.60	1/2536 (0.0%)
2	l	0.35	0/1881	0.59	2/2541 (0.1%)
2	m	0.35	0/1872	0.61	0/2530
2	n	0.35	0/1876	0.64	2/2536 (0.1%)
3	A	0.33	0/3901	0.69	5/5284 (0.1%)
3	B	0.34	0/3951	0.70	2/5352 (0.0%)
3	C	0.34	0/3901	0.67	2/5284 (0.0%)
3	D	0.33	0/3940	0.69	0/5338
3	F	0.34	0/3901	0.66	0/5284
3	G	0.34	0/3951	0.74	5/5352 (0.1%)
3	H	0.35	0/3901	0.71	7/5284 (0.1%)
3	I	0.34	0/3951	0.71	7/5352 (0.1%)
3	J	0.34	0/3901	0.66	2/5284 (0.0%)
3	K	0.33	0/3951	0.69	2/5352 (0.0%)
3	L	0.34	0/3901	0.70	8/5284 (0.2%)
3	M	0.34	0/3940	0.69	2/5338 (0.0%)
3	N	0.34	0/3901	0.70	4/5284 (0.1%)
3	O	0.34	0/3951	0.74	5/5352 (0.1%)
3	P	0.33	0/3901	0.68	4/5284 (0.1%)
3	Q	0.38	0/1181	0.66	0/1593
4	0	0.35	0/1598	0.70	4/2172 (0.2%)
4	1	0.36	0/1605	0.72	3/2181 (0.1%)
4	2	0.35	0/1589	0.69	2/2159 (0.1%)
4	3	0.35	0/1642	0.77	7/2230 (0.3%)
4	4	0.37	0/1799	0.79	4/2441 (0.2%)
5	5	0.35	0/1935	0.74	3/2647 (0.1%)
6	6	0.29	0/414	0.65	0/565
6	7	0.36	0/657	0.86	3/897 (0.3%)
6	8	0.33	0/657	0.76	3/897 (0.3%)
6	9	0.36	0/660	0.76	3/900 (0.3%)
7	AM	0.36	0/300	0.66	0/403
7	AN	0.33	0/646	0.70	1/870 (0.1%)
7	AO	0.31	0/671	0.67	2/908 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	AP	0.32	0/671	0.60	1/908 (0.1%)
7	AQ	0.31	0/671	0.66	1/908 (0.1%)
7	AR	0.33	0/671	0.70	1/908 (0.1%)
8	AS	0.33	0/472	0.63	0/638
8	AT	0.34	0/472	0.56	0/638
8	AU	0.34	0/472	0.65	1/638 (0.2%)
8	AV	0.34	0/472	0.83	3/638 (0.5%)
8	AW	0.34	0/472	0.57	0/638
8	AX	0.38	0/582	0.67	0/788
8	AY	0.37	0/623	0.77	3/846 (0.4%)
8	AZ	0.35	0/623	0.68	2/846 (0.2%)
8	BA	0.33	0/623	0.66	1/846 (0.1%)
8	BB	0.35	0/623	0.57	0/846
8	BC	0.34	0/623	0.56	1/846 (0.1%)
8	BD	0.34	0/623	0.60	2/846 (0.2%)
8	BE	0.35	0/623	0.67	1/846 (0.1%)
8	BF	0.32	0/623	0.57	0/846
8	BG	0.35	0/623	0.52	0/846
8	BH	0.34	0/623	0.73	3/846 (0.4%)
8	BI	0.35	0/623	0.63	1/846 (0.1%)
8	BJ	0.34	0/623	0.65	2/846 (0.2%)
8	BK	0.31	0/623	0.70	2/846 (0.2%)
8	BL	0.31	0/623	0.50	0/846
8	BM	0.32	0/623	0.73	3/846 (0.4%)
8	BN	0.32	0/623	0.70	1/846 (0.1%)
8	BO	0.35	0/623	0.70	2/846 (0.2%)
8	BP	0.32	0/623	0.81	5/846 (0.6%)
8	BQ	0.32	0/623	0.62	0/846
8	BR	0.33	0/623	0.80	4/846 (0.5%)
8	BS	0.34	0/623	0.71	3/846 (0.4%)
8	BT	0.33	0/623	0.79	3/846 (0.4%)
8	BU	0.32	0/623	0.68	0/846
8	BV	0.30	0/623	0.55	0/846
All	All	0.35	1/174128 (0.0%)	0.67	192/235929 (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	b	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	8	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AJ	79	PRO	C-N	-5.20	1.22	1.34

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AV	34	LEU	CA-CB-CG	9.89	138.05	115.30
4	3	206	ASP	CB-CG-OD1	9.84	127.16	118.30
1	AF	175	PHE	CB-CG-CD2	-9.13	114.41	120.80
8	BM	31	LEU	CA-CB-CG	8.73	135.38	115.30
1	AB	77	LEU	CA-CB-CG	8.58	135.04	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	8	41	GLN	Peptide
2	b	366	LEU	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	AA	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
1	AB	182/252 (72%)	177 (97%)	5 (3%)	0	100	100
1	AC	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
1	AD	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	AE	182/252 (72%)	178 (98%)	4 (2%)	0	100	100
1	AF	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	AG	182/252 (72%)	173 (95%)	9 (5%)	0	100	100
1	AH	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	AI	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
1	AJ	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	AK	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	AL	182/252 (72%)	177 (97%)	5 (3%)	0	100	100
1	o	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	p	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	q	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	r	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
1	s	182/252 (72%)	177 (97%)	5 (3%)	0	100	100
1	t	182/252 (72%)	178 (98%)	4 (2%)	0	100	100
1	u	182/252 (72%)	178 (98%)	4 (2%)	0	100	100
1	v	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	w	182/252 (72%)	177 (97%)	5 (3%)	0	100	100
1	x	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	y	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	z	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
2	E	220/392 (56%)	212 (96%)	8 (4%)	0	100	100
2	R	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
2	S	220/392 (56%)	208 (94%)	12 (6%)	0	100	100
2	T	220/392 (56%)	209 (95%)	11 (5%)	0	100	100
2	U	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
2	V	220/392 (56%)	206 (94%)	14 (6%)	0	100	100
2	W	220/392 (56%)	212 (96%)	8 (4%)	0	100	100
2	X	219/392 (56%)	211 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Y	220/392 (56%)	206 (94%)	14 (6%)	0	100	100
2	Z	220/392 (56%)	210 (96%)	10 (4%)	0	100	100
2	a	219/392 (56%)	214 (98%)	5 (2%)	0	100	100
2	b	220/392 (56%)	209 (95%)	11 (5%)	0	100	100
2	c	220/392 (56%)	210 (96%)	10 (4%)	0	100	100
2	d	219/392 (56%)	213 (97%)	6 (3%)	0	100	100
2	e	220/392 (56%)	207 (94%)	13 (6%)	0	100	100
2	f	220/392 (56%)	209 (95%)	11 (5%)	0	100	100
2	g	219/392 (56%)	213 (97%)	6 (3%)	0	100	100
2	h	220/392 (56%)	207 (94%)	13 (6%)	0	100	100
2	i	220/392 (56%)	212 (96%)	8 (4%)	0	100	100
2	j	219/392 (56%)	213 (97%)	6 (3%)	0	100	100
2	k	220/392 (56%)	206 (94%)	14 (6%)	0	100	100
2	l	220/392 (56%)	209 (95%)	11 (5%)	0	100	100
2	m	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
2	n	220/392 (56%)	209 (95%)	11 (5%)	0	100	100
3	A	491/562 (87%)	471 (96%)	20 (4%)	0	100	100
3	B	497/562 (88%)	474 (95%)	23 (5%)	0	100	100
3	C	491/562 (87%)	471 (96%)	20 (4%)	0	100	100
3	D	496/562 (88%)	473 (95%)	23 (5%)	0	100	100
3	F	491/562 (87%)	471 (96%)	20 (4%)	0	100	100
3	G	497/562 (88%)	472 (95%)	25 (5%)	0	100	100
3	H	491/562 (87%)	471 (96%)	20 (4%)	0	100	100
3	I	497/562 (88%)	477 (96%)	20 (4%)	0	100	100
3	J	491/562 (87%)	468 (95%)	23 (5%)	0	100	100
3	K	497/562 (88%)	473 (95%)	24 (5%)	0	100	100
3	L	491/562 (87%)	469 (96%)	22 (4%)	0	100	100
3	M	496/562 (88%)	472 (95%)	24 (5%)	0	100	100
3	N	491/562 (87%)	469 (96%)	22 (4%)	0	100	100
3	O	497/562 (88%)	474 (95%)	23 (5%)	0	100	100
3	P	491/562 (87%)	469 (96%)	22 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	143/562 (25%)	139 (97%)	4 (3%)	0	100	100
4	0	195/224 (87%)	189 (97%)	5 (3%)	1 (0%)	29	68
4	1	195/224 (87%)	188 (96%)	6 (3%)	1 (0%)	29	68
4	2	193/224 (86%)	186 (96%)	6 (3%)	1 (0%)	29	68
4	3	200/224 (89%)	195 (98%)	5 (2%)	0	100	100
4	4	220/224 (98%)	207 (94%)	13 (6%)	0	100	100
5	5	243/263 (92%)	224 (92%)	19 (8%)	0	100	100
6	6	49/86 (57%)	46 (94%)	3 (6%)	0	100	100
6	7	82/86 (95%)	80 (98%)	2 (2%)	0	100	100
6	8	82/86 (95%)	80 (98%)	1 (1%)	1 (1%)	13	50
6	9	82/86 (95%)	81 (99%)	1 (1%)	0	100	100
7	AM	37/101 (37%)	37 (100%)	0	0	100	100
7	AN	79/101 (78%)	79 (100%)	0	0	100	100
7	AO	86/101 (85%)	84 (98%)	2 (2%)	0	100	100
7	AP	86/101 (85%)	86 (100%)	0	0	100	100
7	AQ	86/101 (85%)	86 (100%)	0	0	100	100
7	AR	86/101 (85%)	83 (96%)	3 (4%)	0	100	100
8	AS	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
8	AT	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
8	AU	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
8	AV	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
8	AW	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
8	AX	71/80 (89%)	68 (96%)	3 (4%)	0	100	100
8	AY	76/80 (95%)	73 (96%)	3 (4%)	0	100	100
8	AZ	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BA	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BB	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BC	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
8	BD	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
8	BE	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BF	76/80 (95%)	74 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	BG	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
8	BH	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
8	BI	76/80 (95%)	73 (96%)	3 (4%)	0	100	100
8	BJ	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
8	BK	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
8	BL	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BM	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BN	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BO	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BP	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BQ	76/80 (95%)	73 (96%)	3 (4%)	0	100	100
8	BR	76/80 (95%)	73 (96%)	3 (4%)	0	100	100
8	BS	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BT	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
8	BU	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
8	BV	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
All	All	21369/29181 (73%)	20501 (96%)	864 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	8	42	LEU
4	0	49	ASN
4	1	49	ASN
4	2	47	PRO

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	AA	155/215 (72%)	153 (99%)	2 (1%)	69	82
1	AB	155/215 (72%)	154 (99%)	1 (1%)	86	91
1	AC	155/215 (72%)	154 (99%)	1 (1%)	86	91
1	AD	155/215 (72%)	155 (100%)	0	100	100
1	AE	155/215 (72%)	152 (98%)	3 (2%)	57	75
1	AF	155/215 (72%)	154 (99%)	1 (1%)	86	91
1	AG	155/215 (72%)	154 (99%)	1 (1%)	86	91
1	AH	155/215 (72%)	154 (99%)	1 (1%)	86	91
1	AI	155/215 (72%)	154 (99%)	1 (1%)	86	91
1	AJ	155/215 (72%)	155 (100%)	0	100	100
1	AK	155/215 (72%)	153 (99%)	2 (1%)	69	82
1	AL	155/215 (72%)	154 (99%)	1 (1%)	86	91
1	o	155/215 (72%)	153 (99%)	2 (1%)	69	82
1	p	155/215 (72%)	155 (100%)	0	100	100
1	q	155/215 (72%)	152 (98%)	3 (2%)	57	75
1	r	155/215 (72%)	154 (99%)	1 (1%)	86	91
1	s	155/215 (72%)	154 (99%)	1 (1%)	86	91
1	t	155/215 (72%)	153 (99%)	2 (1%)	69	82
1	u	155/215 (72%)	155 (100%)	0	100	100
1	v	155/215 (72%)	154 (99%)	1 (1%)	86	91
1	w	155/215 (72%)	153 (99%)	2 (1%)	69	82
1	x	155/215 (72%)	155 (100%)	0	100	100
1	y	155/215 (72%)	153 (99%)	2 (1%)	69	82
1	z	155/215 (72%)	153 (99%)	2 (1%)	69	82
2	E	190/337 (56%)	190 (100%)	0	100	100
2	R	189/337 (56%)	188 (100%)	1 (0%)	88	93
2	S	188/337 (56%)	186 (99%)	2 (1%)	73	84
2	T	190/337 (56%)	190 (100%)	0	100	100
2	U	189/337 (56%)	188 (100%)	1 (0%)	88	93
2	V	188/337 (56%)	186 (99%)	2 (1%)	73	84
2	W	190/337 (56%)	190 (100%)	0	100	100
2	X	189/337 (56%)	188 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Y	188/337 (56%)	187 (100%)	1 (0%)	88	93
2	Z	190/337 (56%)	190 (100%)	0	100	100
2	a	189/337 (56%)	187 (99%)	2 (1%)	73	84
2	b	188/337 (56%)	188 (100%)	0	100	100
2	c	190/337 (56%)	189 (100%)	1 (0%)	88	93
2	d	189/337 (56%)	186 (98%)	3 (2%)	62	79
2	e	188/337 (56%)	184 (98%)	4 (2%)	53	72
2	f	190/337 (56%)	190 (100%)	0	100	100
2	g	189/337 (56%)	187 (99%)	2 (1%)	73	84
2	h	188/337 (56%)	187 (100%)	1 (0%)	88	93
2	i	190/337 (56%)	189 (100%)	1 (0%)	88	93
2	j	189/337 (56%)	188 (100%)	1 (0%)	88	93
2	k	188/337 (56%)	186 (99%)	2 (1%)	73	84
2	l	190/337 (56%)	190 (100%)	0	100	100
2	m	189/337 (56%)	188 (100%)	1 (0%)	88	93
2	n	188/337 (56%)	188 (100%)	0	100	100
3	A	420/477 (88%)	415 (99%)	5 (1%)	71	84
3	B	426/477 (89%)	419 (98%)	7 (2%)	62	79
3	C	420/477 (88%)	409 (97%)	11 (3%)	46	66
3	D	425/477 (89%)	414 (97%)	11 (3%)	46	66
3	F	420/477 (88%)	412 (98%)	8 (2%)	57	75
3	G	426/477 (89%)	419 (98%)	7 (2%)	62	79
3	H	420/477 (88%)	410 (98%)	10 (2%)	49	69
3	I	426/477 (89%)	422 (99%)	4 (1%)	78	87
3	J	420/477 (88%)	408 (97%)	12 (3%)	42	64
3	K	426/477 (89%)	420 (99%)	6 (1%)	67	80
3	L	420/477 (88%)	411 (98%)	9 (2%)	53	72
3	M	425/477 (89%)	417 (98%)	8 (2%)	57	75
3	N	420/477 (88%)	405 (96%)	15 (4%)	35	59
3	O	426/477 (89%)	418 (98%)	8 (2%)	57	75
3	P	420/477 (88%)	412 (98%)	8 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	125/477 (26%)	124 (99%)	1 (1%)	81	89
4	0	175/199 (88%)	171 (98%)	4 (2%)	50	70
4	1	177/199 (89%)	175 (99%)	2 (1%)	73	84
4	2	175/199 (88%)	172 (98%)	3 (2%)	60	78
4	3	180/199 (90%)	180 (100%)	0	100	100
4	4	197/199 (99%)	194 (98%)	3 (2%)	65	80
5	5	205/219 (94%)	202 (98%)	3 (2%)	65	80
6	6	41/71 (58%)	41 (100%)	0	100	100
6	7	69/71 (97%)	69 (100%)	0	100	100
6	8	69/71 (97%)	69 (100%)	0	100	100
6	9	70/71 (99%)	69 (99%)	1 (1%)	67	80
7	AM	34/88 (39%)	33 (97%)	1 (3%)	42	64
7	AN	71/88 (81%)	71 (100%)	0	100	100
7	AO	76/88 (86%)	73 (96%)	3 (4%)	32	56
7	AP	76/88 (86%)	75 (99%)	1 (1%)	69	82
7	AQ	76/88 (86%)	74 (97%)	2 (3%)	46	66
7	AR	76/88 (86%)	75 (99%)	1 (1%)	69	82
8	AS	50/67 (75%)	49 (98%)	1 (2%)	55	73
8	AT	50/67 (75%)	47 (94%)	3 (6%)	19	46
8	AU	50/67 (75%)	49 (98%)	1 (2%)	55	73
8	AV	50/67 (75%)	47 (94%)	3 (6%)	19	46
8	AW	50/67 (75%)	46 (92%)	4 (8%)	12	37
8	AX	62/67 (92%)	62 (100%)	0	100	100
8	AY	66/67 (98%)	66 (100%)	0	100	100
8	AZ	66/67 (98%)	66 (100%)	0	100	100
8	BA	66/67 (98%)	66 (100%)	0	100	100
8	BB	66/67 (98%)	66 (100%)	0	100	100
8	BC	66/67 (98%)	66 (100%)	0	100	100
8	BD	66/67 (98%)	65 (98%)	1 (2%)	65	80
8	BE	66/67 (98%)	66 (100%)	0	100	100
8	BF	66/67 (98%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	BG	66/67 (98%)	66 (100%)	0	100	100
8	BH	66/67 (98%)	66 (100%)	0	100	100
8	BI	66/67 (98%)	65 (98%)	1 (2%)	65	80
8	BJ	66/67 (98%)	65 (98%)	1 (2%)	65	80
8	BK	66/67 (98%)	66 (100%)	0	100	100
8	BL	66/67 (98%)	66 (100%)	0	100	100
8	BM	66/67 (98%)	65 (98%)	1 (2%)	65	80
8	BN	66/67 (98%)	66 (100%)	0	100	100
8	BO	66/67 (98%)	66 (100%)	0	100	100
8	BP	66/67 (98%)	65 (98%)	1 (2%)	65	80
8	BQ	66/67 (98%)	66 (100%)	0	100	100
8	BR	66/67 (98%)	66 (100%)	0	100	100
8	BS	66/67 (98%)	66 (100%)	0	100	100
8	BT	66/67 (98%)	66 (100%)	0	100	100
8	BU	66/67 (98%)	66 (100%)	0	100	100
8	BV	66/67 (98%)	66 (100%)	0	100	100
All	All	18384/24916 (74%)	18157 (99%)	227 (1%)	72	84

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	502	LYS
3	P	541	SER
3	H	143	ARG
3	P	454	LEU
3	N	453	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 232 such sidechains are listed below:

Mol	Chain	Res	Type
7	AM	71	GLN
8	BL	61	GLN
3	C	123	ASN
8	BJ	59	ASN
3	N	170	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

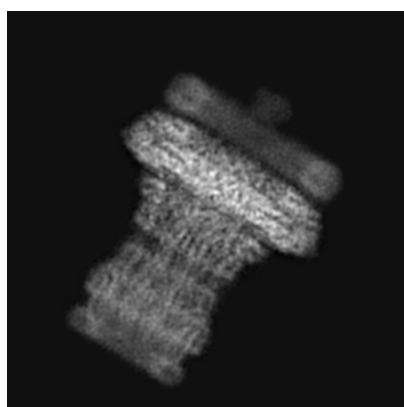
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20312. These allow visual inspection of the internal detail of the map and identification of artifacts.

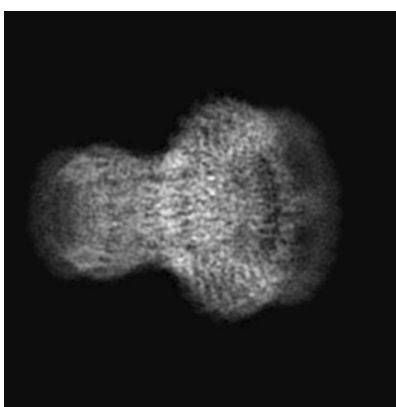
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

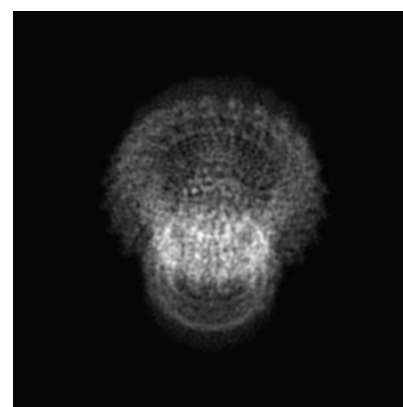
6.1.1 Primary map



X



Y

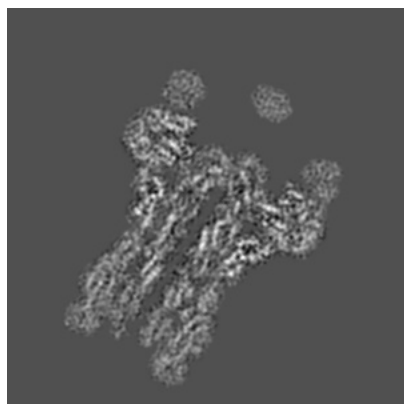


Z

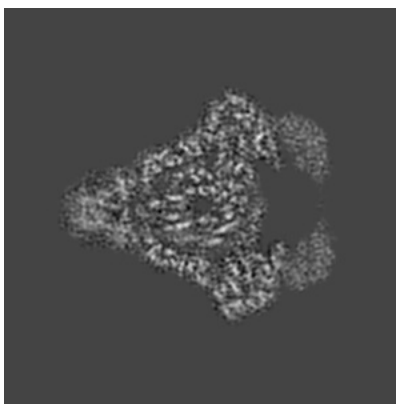
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

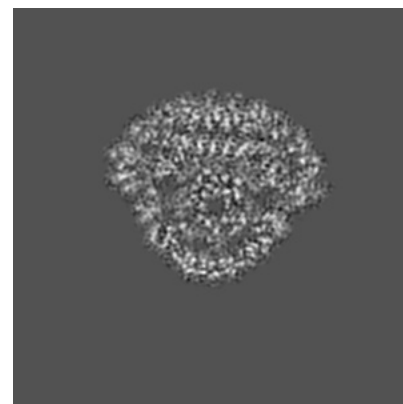
6.2.1 Primary map



X Index: 125



Y Index: 125

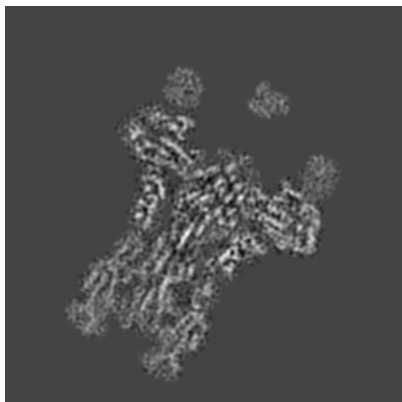


Z Index: 125

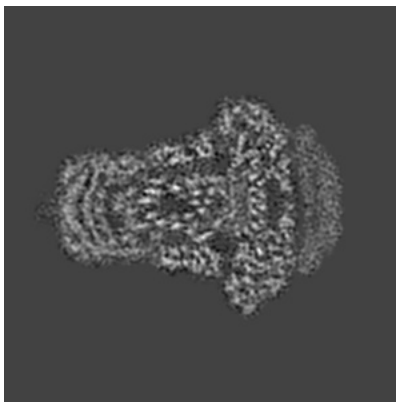
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

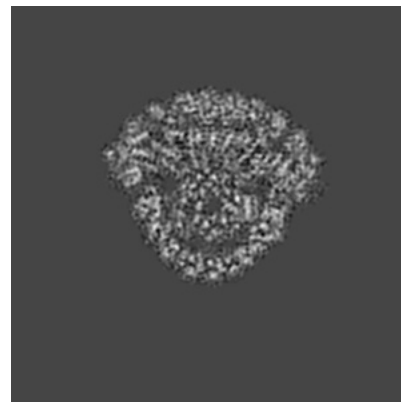
6.3.1 Primary map



X Index: 136



Y Index: 113

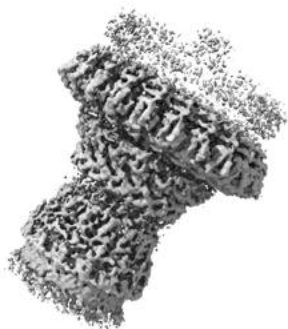


Z Index: 123

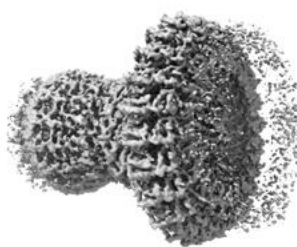
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

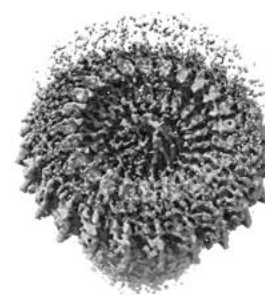
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

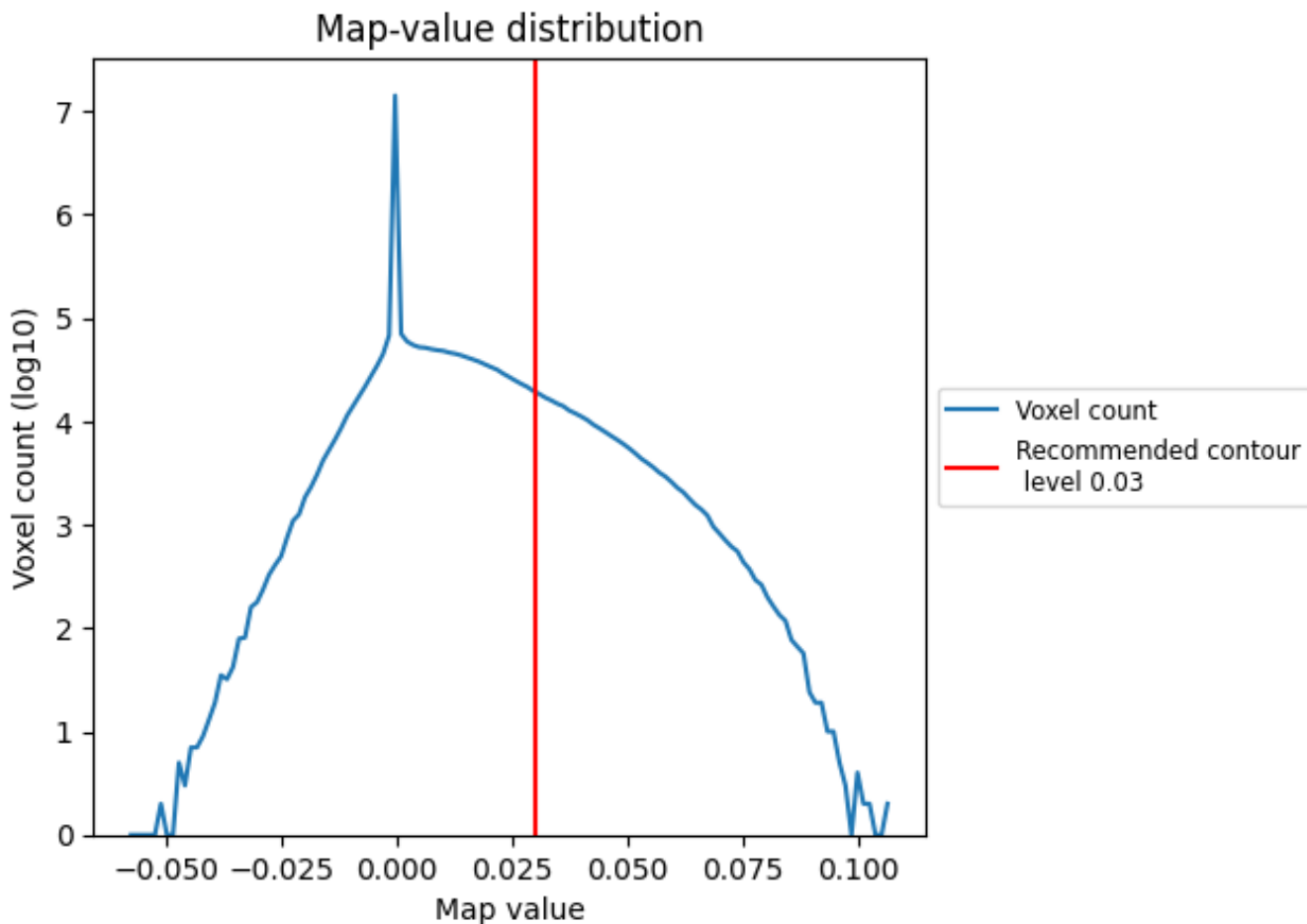
6.5 Mask visualisation

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

7 Map analysis [i](#)

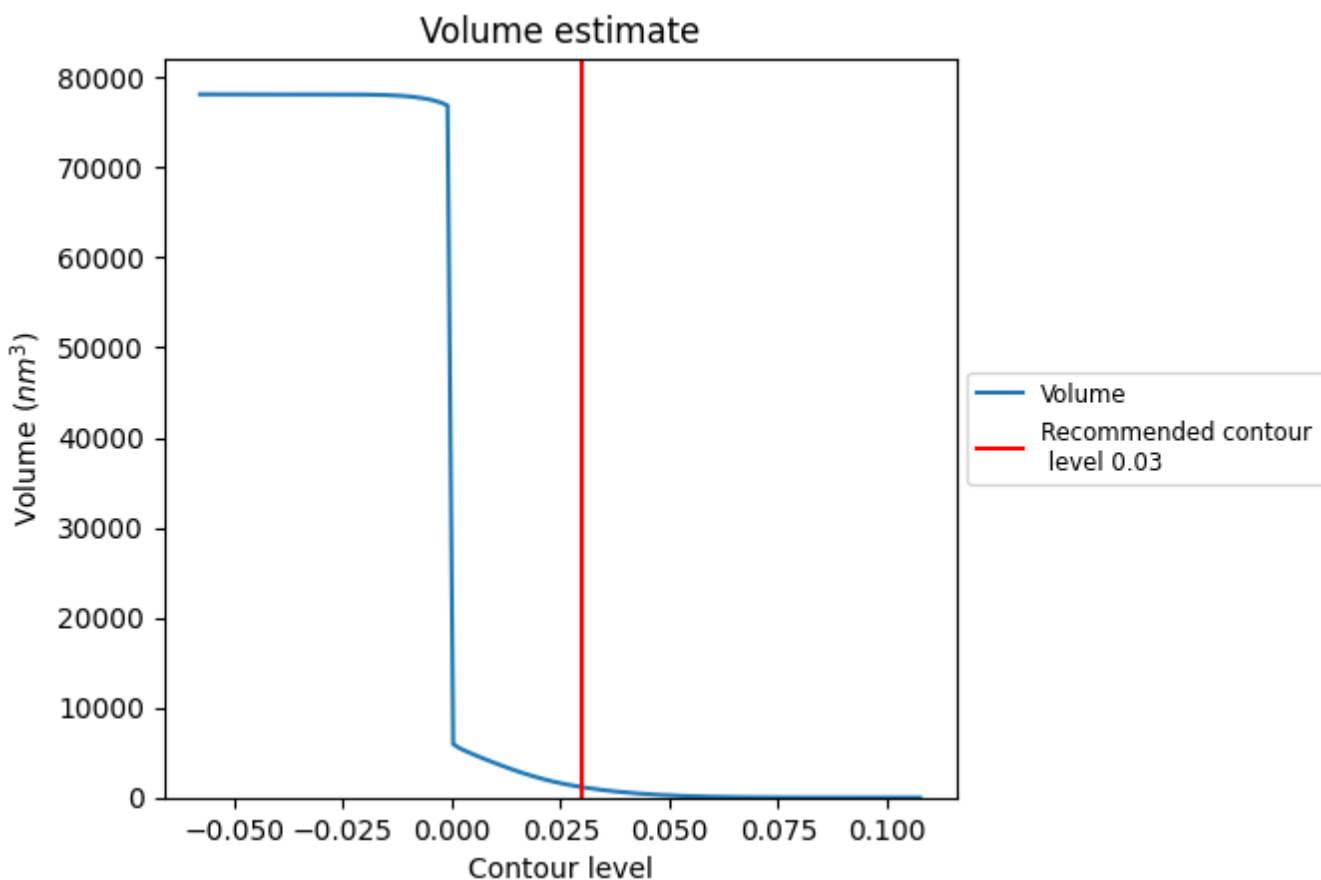
This section contains the results of statistical analysis of the map.

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.

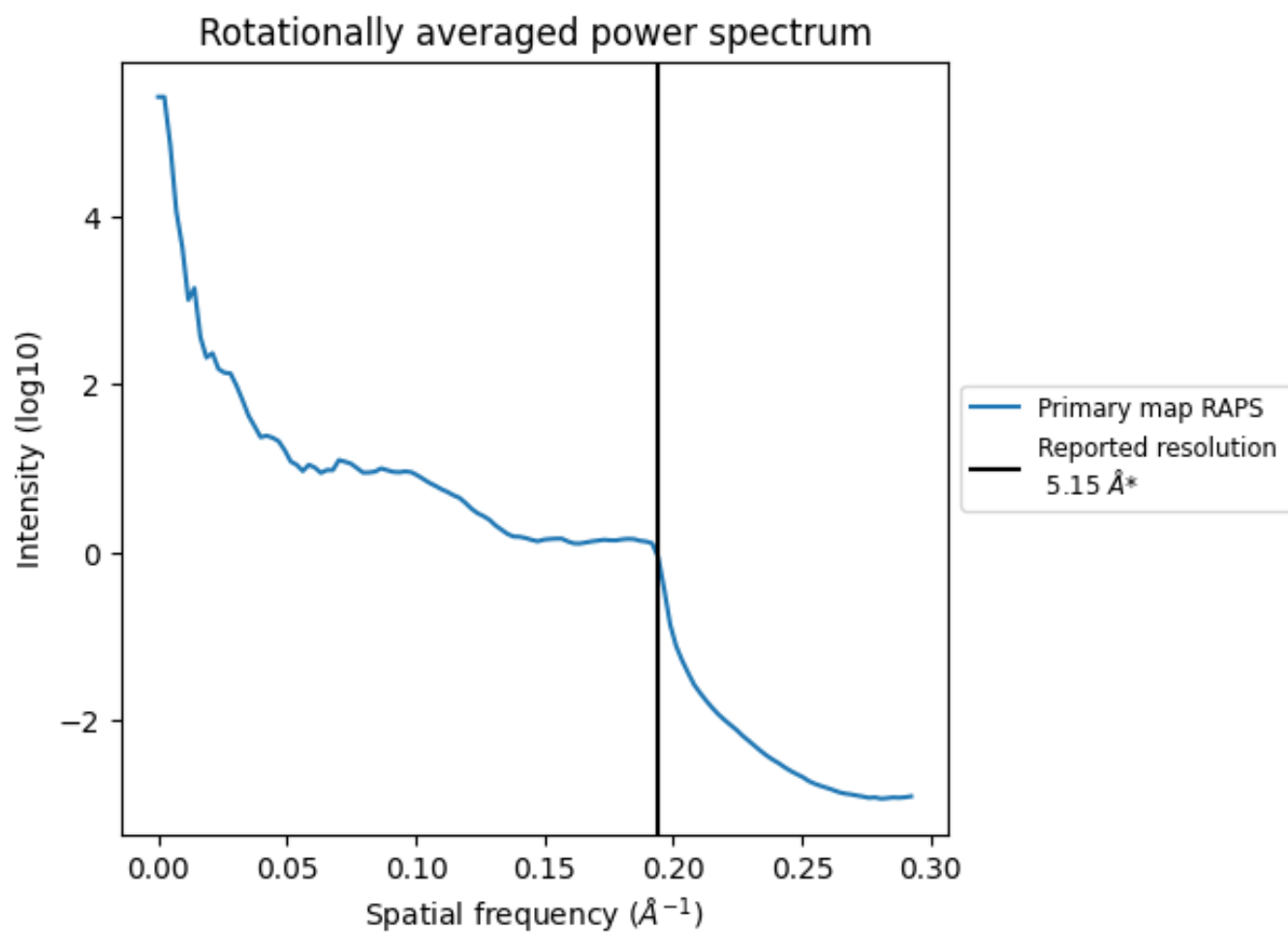
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1154 nm³; this corresponds to an approximate mass of 1042 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 0.194\AA^{-1}

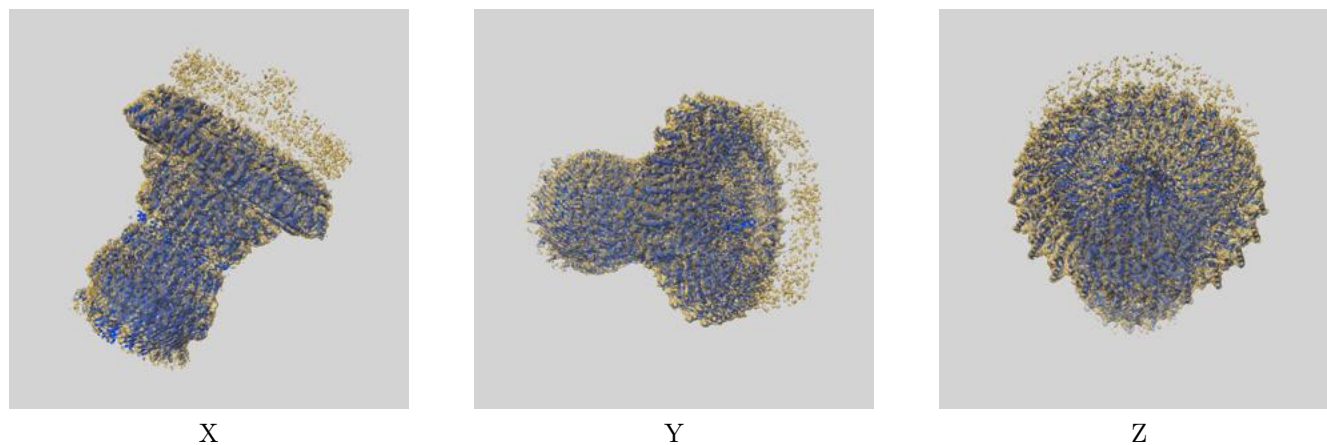
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

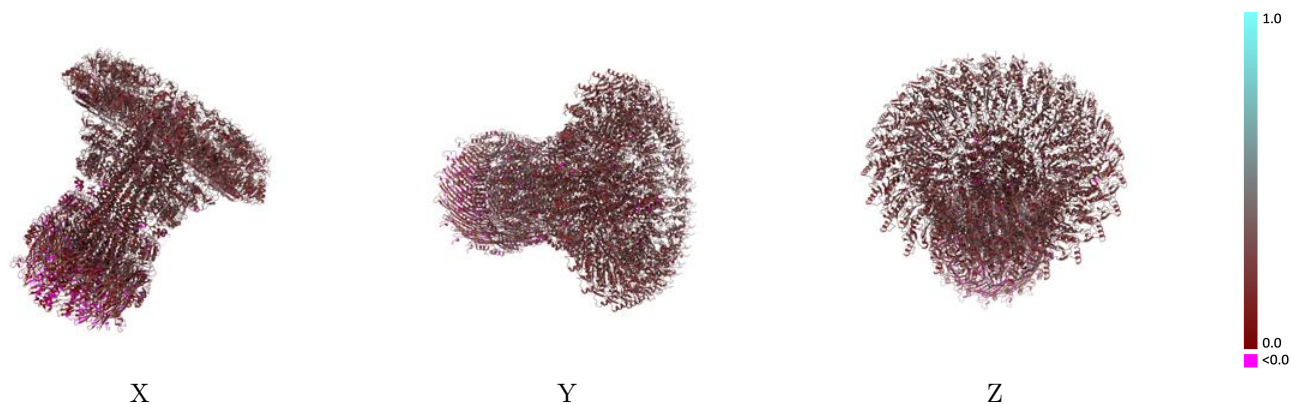
This section contains information regarding the fit between EMDB map EMD-20312 and PDB model 6Q15. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



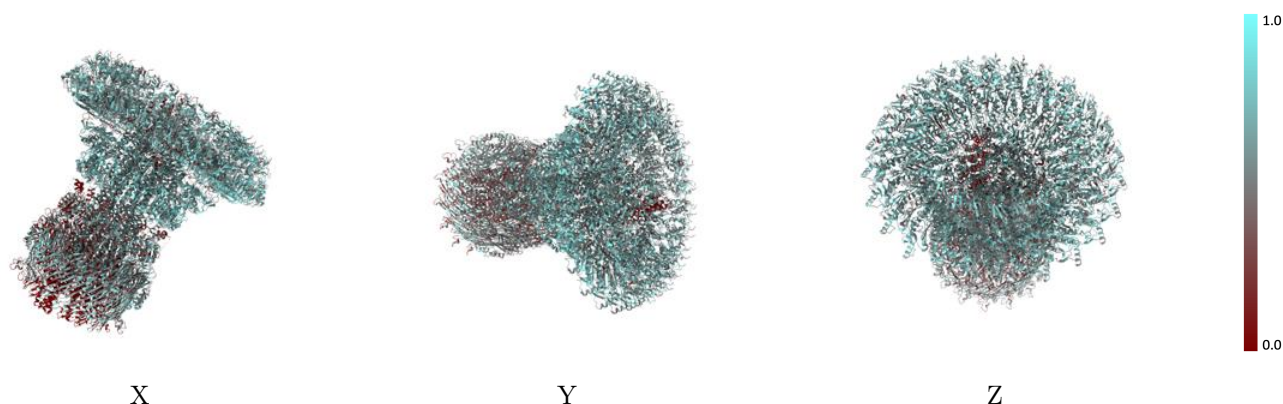
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



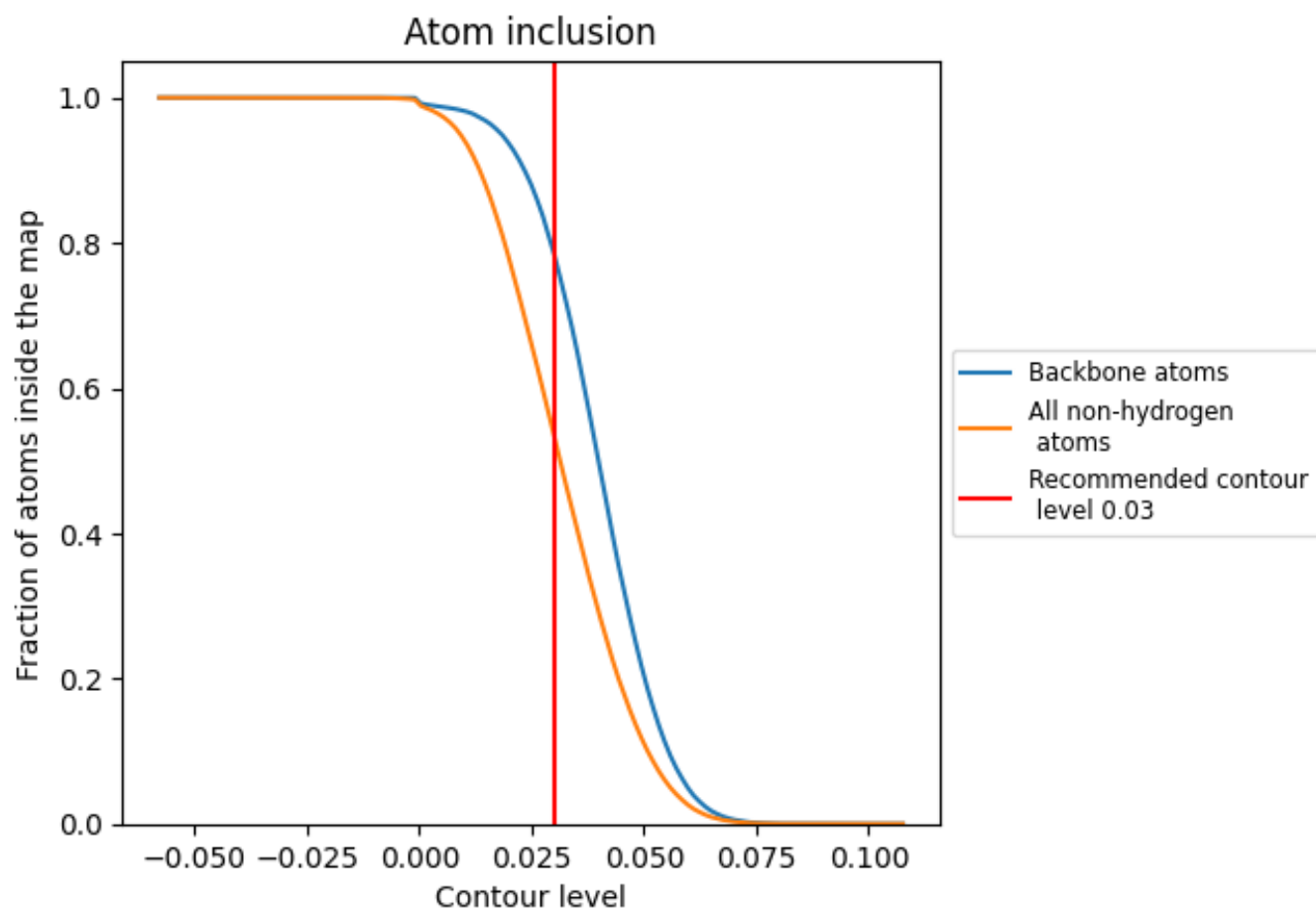
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 53% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5346	 0.2430
0	 0.5191	 0.2350
1	 0.5258	 0.2250
2	 0.5280	 0.2250
3	 0.5387	 0.2310
4	 0.5179	 0.2320
5	 0.5743	 0.2550
6	 0.1407	 0.2290
7	 0.2732	 0.2060
8	 0.4772	 0.2210
9	 0.5563	 0.2320
A	 0.4540	 0.2070
AA	 0.5916	 0.2810
AB	 0.5873	 0.2980
AC	 0.6037	 0.2980
AD	 0.5980	 0.2920
AE	 0.6108	 0.2980
AF	 0.6016	 0.3000
AG	 0.6080	 0.2910
AH	 0.5973	 0.2860
AI	 0.6137	 0.2870
AJ	 0.5873	 0.3010
AK	 0.5987	 0.2890
AL	 0.5973	 0.3010
AM	 0.5548	 0.2100
AN	 0.5638	 0.2250
AO	 0.5557	 0.2230
AP	 0.5695	 0.2400
AQ	 0.5557	 0.2440
AR	 0.5359	 0.2320
AS	 0.5686	 0.2260
AT	 0.5577	 0.2000
AU	 0.5403	 0.2020
AV	 0.5512	 0.2130
AW	 0.5991	 0.2350







































































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Chain	Atom inclusion	Q-score
AX	0.5035	0.2080
AY	0.5257	0.2020
AZ	0.5406	0.2230
B	0.4623	0.1990
BA	0.5224	0.2010
BB	0.5224	0.2090
BC	0.4959	0.2100
BD	0.4610	0.1980
BE	0.4726	0.2220
BF	0.4511	0.2120
BG	0.4362	0.2090
BH	0.4196	0.1870
BI	0.3715	0.1950
BJ	0.3333	0.1930
BK	0.2869	0.1790
BL	0.2720	0.1920
BM	0.2653	0.1780
BN	0.2255	0.1630
BO	0.1758	0.1350
BP	0.1758	0.1330
BQ	0.1443	0.1270
BR	0.0945	0.0810
BS	0.0630	0.0660
BT	0.0531	0.0810
BU	0.0415	0.0480
BV	0.0199	0.0380
C	0.4940	0.2160
D	0.5075	0.2250
E	0.5956	0.2700
F	0.5129	0.2290
G	0.5248	0.2240
H	0.5471	0.2390
I	0.5327	0.2290
J	0.5261	0.2330
K	0.5204	0.2280
L	0.5015	0.2170
M	0.4836	0.2130
N	0.4633	0.1990
O	0.4605	0.1970
P	0.4548	0.1950
Q	0.6726	0.2720
R	0.6230	0.2710

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Chain	Atom inclusion	Q-score
S	 0.6159	 0.2680
T	 0.5951	 0.2680
U	 0.6343	 0.2710
V	 0.6136	 0.2710
W	 0.5664	 0.2610
X	 0.6354	 0.2800
Y	 0.6153	 0.2690
Z	 0.5911	 0.2690
a	 0.6444	 0.2790
b	 0.6317	 0.2680
c	 0.5967	 0.2610
d	 0.6280	 0.2750
e	 0.6582	 0.2730
f	 0.6080	 0.2750
g	 0.6433	 0.2740
h	 0.6492	 0.2720
i	 0.6091	 0.2750
j	 0.6682	 0.2830
k	 0.6458	 0.2780
l	 0.5917	 0.2770
m	 0.6456	 0.2740
n	 0.6362	 0.2790
o	 0.5745	 0.2860
p	 0.5852	 0.2840
q	 0.5567	 0.2880
r	 0.5845	 0.2900
s	 0.5595	 0.2860
t	 0.5773	 0.2900
u	 0.5709	 0.2830
v	 0.5652	 0.2860
w	 0.5617	 0.2800
x	 0.5823	 0.2880
y	 0.5930	 0.2970
z	 0.5937	 0.2920