



wwPDB EM Validation Summary Report ⓘ

Nov 27, 2022 – 12:11 PM EST

PDB ID : 6Q14
EMDB ID : EMD-20310
Title : Structure of the Salmonella SPI-1 injectisome NC-base
Authors : Hu, J.; Worrall, L.J.; Strynadka, N.C.J.
Deposited on : 2019-08-02
Resolution : 3.80 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:

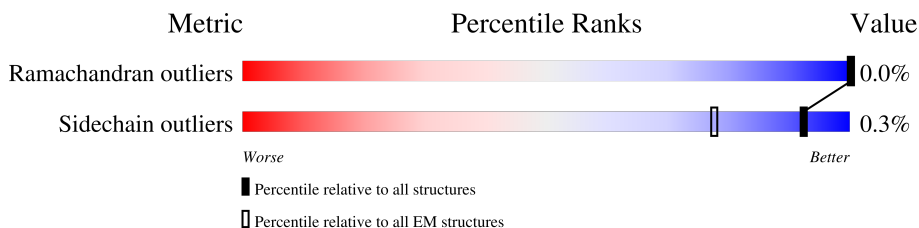
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.80 Å.

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















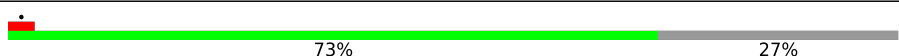
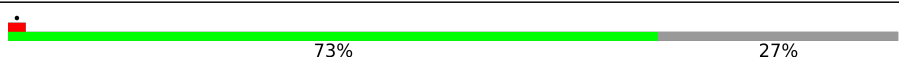
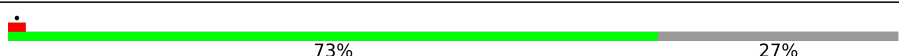

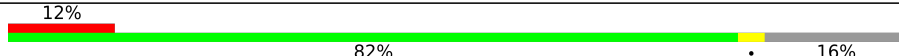
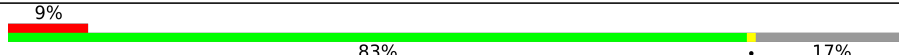
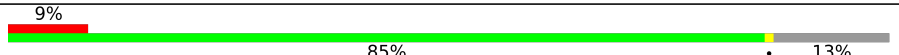
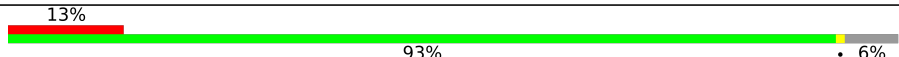
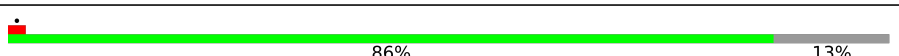

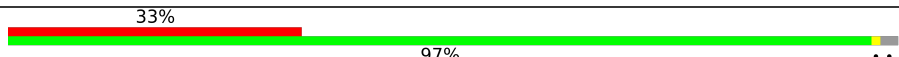
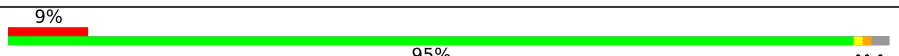
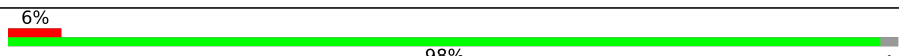
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	 72% 27%
1	AB	252	 73% 27%
1	AC	252	 73% 27%
1	AD	252	 72% 27%
1	AE	252	 72% 27%
1	AF	252	 73% 27%
1	AG	252	 73% 27%
1	AH	252	 73% 27%
1	AI	252	 72% 27%

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Mol	Chain	Length	Quality of chain
1	AJ	252	 73% 27%
1	AK	252	 73% 27%
1	AL	252	 73% 27%
1	o	252	 73% 27%
1	p	252	 73% 27%
1	q	252	 73% 27%
1	r	252	 73% 27%
1	s	252	 73% 27%
1	t	252	 73% 27%
1	u	252	 72% 27%
1	v	252	 73% 27%
1	w	252	 73% 27%
1	x	252	 73% 27%
1	y	252	 73% 27%
1	z	252	 73% 27%
2	0	224	 83% 16% 9%
2	1	224	 82% 16% 12%
2	2	224	 83% 17% 9%
2	3	224	 85% 13% 9%
2	4	224	 93% 6% 13%
3	5	263	 86% 13%
4	6	86	 62% 38% 35%
4	7	86	 97% 33%
4	8	86	 95% 9%
4	9	86	 98% 6%

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Mol	Chain	Length	Quality of chain	
5	E	392	56%	43%
5	R	392	56%	44%
5	S	392	56%	43%
5	T	392	57%	43%
5	U	392	56%	44%
5	V	392	56%	43%
5	W	392	57%	43%
5	X	392	56%	44%
5	Y	392	56%	43%
5	Z	392	56%	43%
5	a	392	56%	44%
5	b	392	56%	43%
5	c	392	57%	43%
5	d	392	56%	44%
5	e	392	56%	43%
5	f	392	56%	43%
5	g	392	56%	44%
5	h	392	57%	43%
5	i	392	56%	43%
5	j	392	56%	44%
5	k	392	56%	43%
5	l	392	57%	43%
5	m	392	56%	44%
5	n	392	57%	43%
6	A	562	20% 86%	14%

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Mol	Chain	Length	Quality of chain
6	B	562	 21% 86% 13%
6	C	562	 19% 86% 14%
6	D	562	 18% 87% 13%
6	F	562	 17% 86% 14%
6	G	562	 17% 86% 13%
6	H	562	 16% 86% 14%
6	I	562	 16% 87% 13%
6	J	562	 16% 86% 14%
6	K	562	 18% 86% 13%
6	L	562	 16% 86% 14%
6	M	562	 20% 87% 13%
6	N	562	 19% 86% 14%
6	O	562	 20% 86% 13%
6	P	562	 19% 86% 14%
6	Q	562	 25% 74%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 147873 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	C	N	O	S	0	0
			1431	901	250	277	3		
1	w	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	x	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	y	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	z	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AJ	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AK	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		

- Molecule 2 is a protein called Surface presentation of antigens protein SpaP.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	189	Total	C	N	O	S	0	0
			1468	982	219	256	11		
2	1	189	Total	C	N	O	S	0	0
			1475	988	220	256	11		
2	2	187	Total	C	N	O	S	0	0
			1464	981	219	253	11		
2	3	194	Total	C	N	O	S	0	0
			1520	1016	227	266	11		
2	4	211	Total	C	N	O	S	1	0
			1672	1108	255	298	11		

- Molecule 3 is a protein called Surface presentation of antigens protein SpaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	228	Total	C	N	O	S	0	0
			1718	1136	276	293	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	53	Total	C	N	O	S	0	0
			405	276	61	67	1		
4	7	84	Total	C	N	O	S	0	0
			644	436	97	109	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	84	Total	C	N	O	S	0	0
			644	436	97	109	2		
4	9	84	Total	C	N	O	S	0	0
			647	438	97	109	3		

- Molecule 5 is a protein called Protein PrgH.

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

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

- Molecule 6 is a protein called Protein InvG.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
6	A	484	Total	C	N	O	S	0	0
			3764	2384	656	712	12		
6	B	489	Total	C	N	O	S	1	0
			3810	2415	665	718	12		
6	C	484	Total	C	N	O	S	0	0
			3764	2384	656	712	12		
6	D	489	Total	C	N	O	S	0	0
			3802	2410	662	718	12		
6	F	484	Total	C	N	O	S	0	0
			3764	2384	656	712	12		
6	G	489	Total	C	N	O	S	1	0
			3810	2415	665	718	12		
6	H	484	Total	C	N	O	S	0	0
			3764	2384	656	712	12		
6	I	489	Total	C	N	O	S	1	0
			3810	2415	665	718	12		
6	J	484	Total	C	N	O	S	0	0
			3764	2384	656	712	12		
6	K	489	Total	C	N	O	S	1	0
			3810	2415	665	718	12		
6	L	484	Total	C	N	O	S	0	0
			3764	2384	656	712	12		

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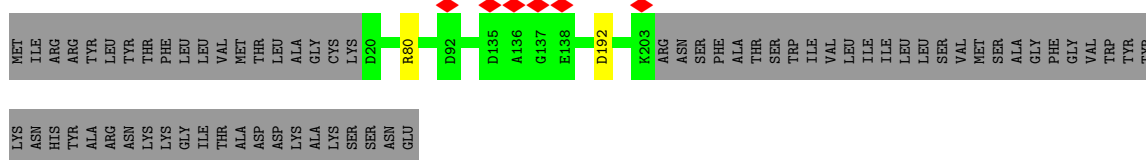
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	M	489	Total 3802	C 2410	N 662	O 718	S 12	0	0
6	N	484	Total 3764	C 2384	N 656	O 712	S 12	0	0
6	O	489	Total 3810	C 2415	N 665	O 718	S 12	1	0
6	P	484	Total 3764	C 2384	N 656	O 712	S 12	0	0

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.

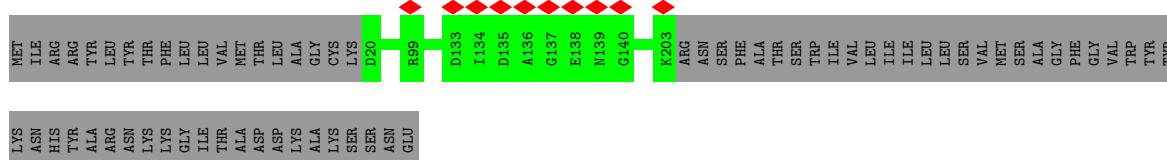
- Molecule 1: Lipoprotein PrgK

Chain AA:  72% 27%




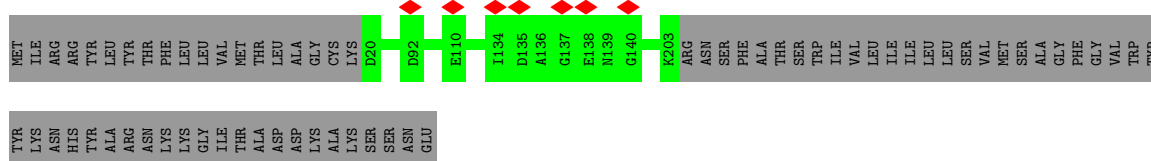
- Molecule 1: Lipoprotein PrgK

Chain AB:  73% 27%



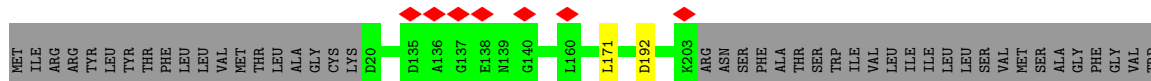
- Molecule 1: Lipoprotein PrgK

Chain AC:  73% 27%



- Molecule 1: Lipoprotein PrgK

Chain AD:  72% 27%



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• Molecule 1: Lipoprotein PrgK



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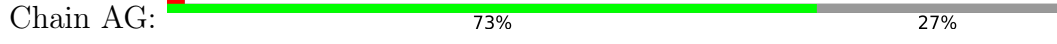
• Molecule 1: Lipoprotein PrgK



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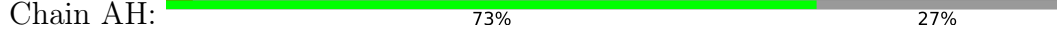
• Molecule 1: Lipoprotein PrgK



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• Molecule 1: Lipoprotein PrgK



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• Molecule 1: Lipoprotein PrgK



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• Molecule 1: Lipoprotein PrgK



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• Molecule 1: Lipoprotein PrgK



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• Molecule 1: Lipoprotein PrgK



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• Molecule 1: Lipoprotein PrgK



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• Molecule 1: Lipoprotein PrgK



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• Molecule 1: Lipoprotein PrgK



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GLY VAL TRP TYR LYS ASN HIS TYR ARG ASN LYS LYS THR LEU LEU VAL MET THR LEU LEU ALA LYS LYS ASP ASP LYS LYS LYS SER SER ASN GLU

• Molecule 1: Lipoprotein PrgK



MET ILE ARG TYR LEU TYR THR PHE LEU LEU VAL MET THR LEU LEU ALA LYS LYS CYS LYS D20 D92 S93 L94 D135 A136 G137 E138 K203 ARG ASN SER PHE ALA THR SER TRP ILE VAL LEU ILE LEU LEU LEU VAL MET MET SER VAL MET MET SER ALA GLY PHE VAL TRP TYR TYR LYS ASN

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• Molecule 1: Lipoprotein PrgK



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• Molecule 1: Lipoprotein PrgK



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• Molecule 1: Lipoprotein PrgK



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• Molecule 1: Lipoprotein PrgK



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• Molecule 1: Lipoprotein PrgK



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• Molecule 1: Lipoprotein PrgK



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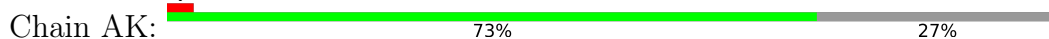
• Molecule 1: Lipoprotein PrgK



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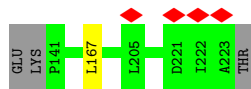
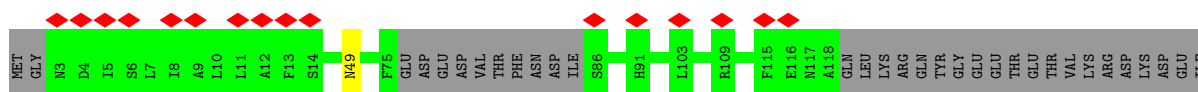
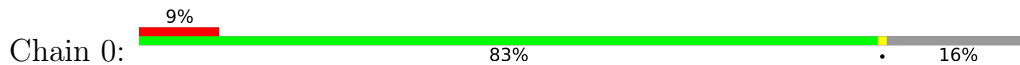
• Molecule 1: Lipoprotein PrgK



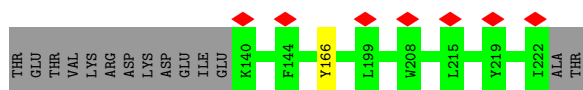
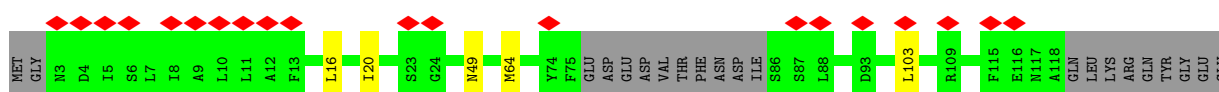
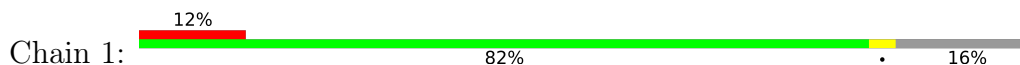
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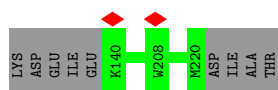
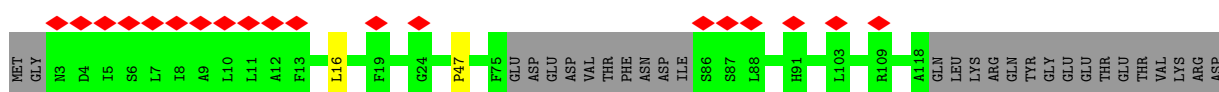
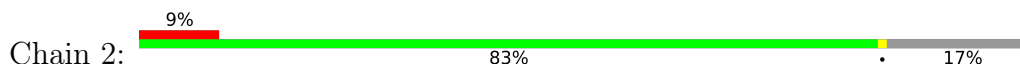
• Molecule 2: Surface presentation of antigens protein SpaP



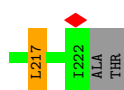
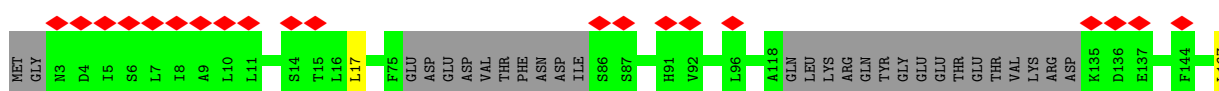
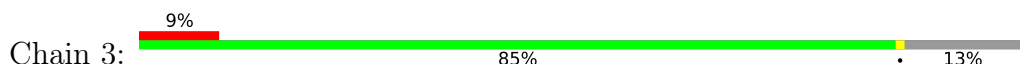
• Molecule 2: Surface presentation of antigens protein SpaP



• Molecule 2: Surface presentation of antigens protein SpaP

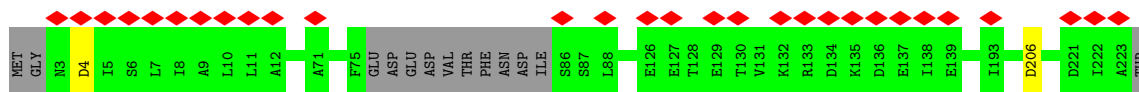


• Molecule 2: Surface presentation of antigens protein SpaP

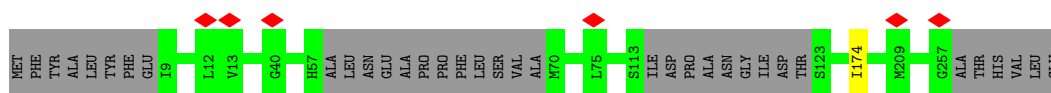
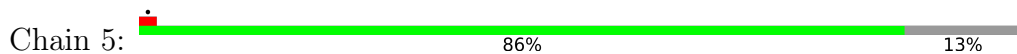


• Molecule 2: Surface presentation of antigens protein SpaP

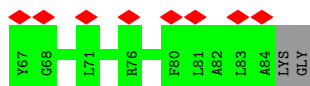
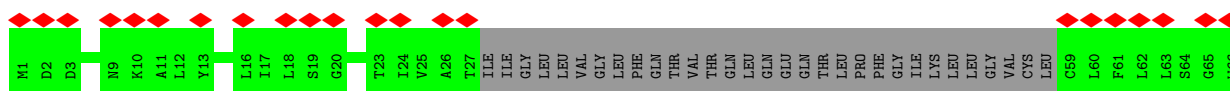




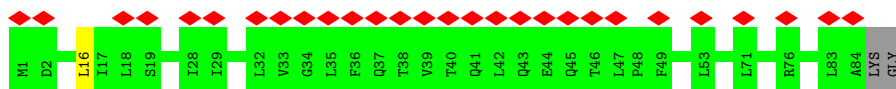
• Molecule 3: Surface presentation of antigens protein SpaR



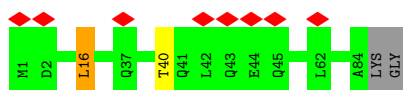
• Molecule 4: Surface presentation of antigens protein SpaQ



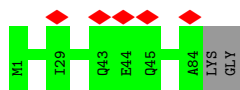
• Molecule 4: Surface presentation of antigens protein SpaQ



• Molecule 4: Surface presentation of antigens protein SpaQ

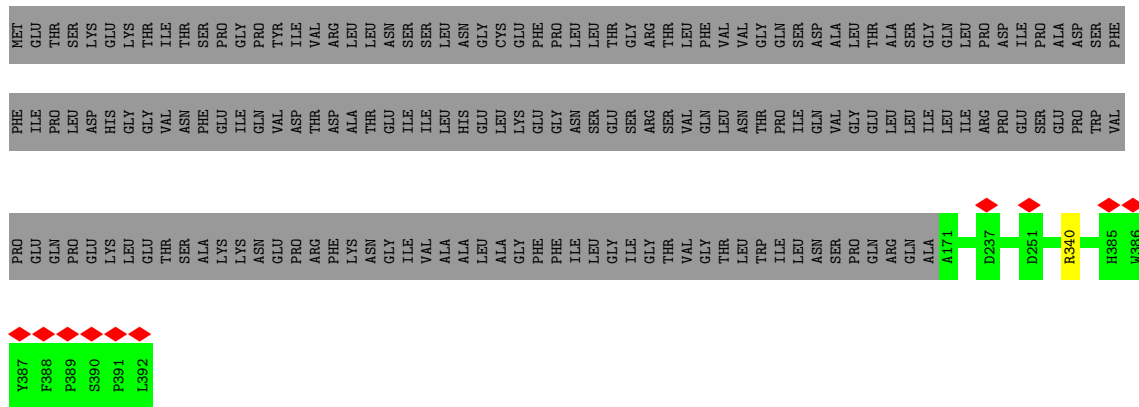


• Molecule 4: Surface presentation of antigens protein SpaQ

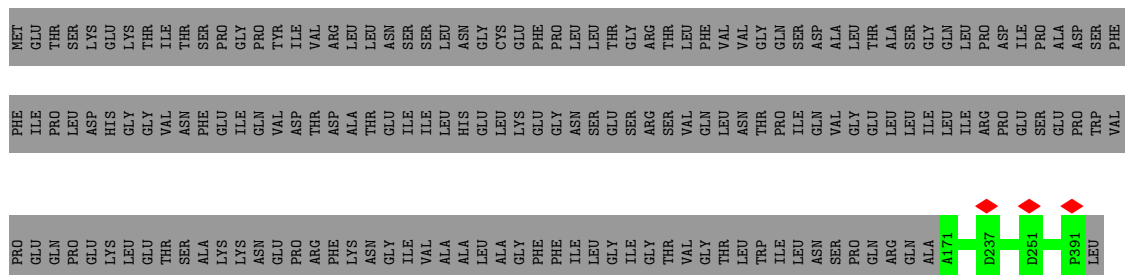


• Molecule 5: Protein PrgH

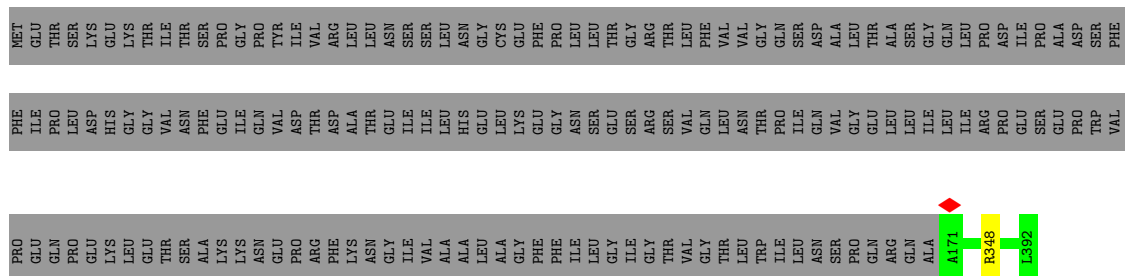




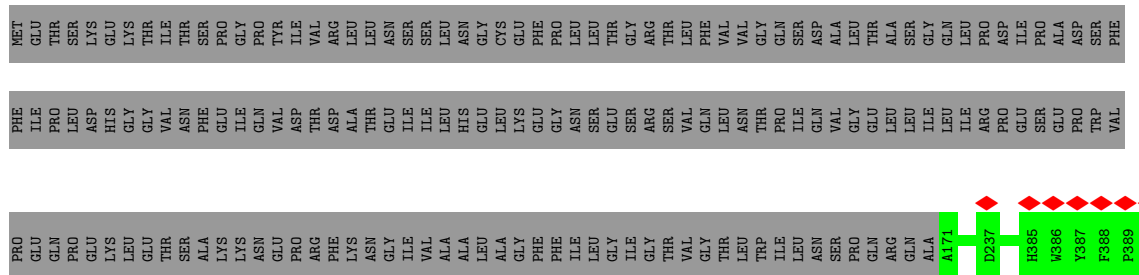
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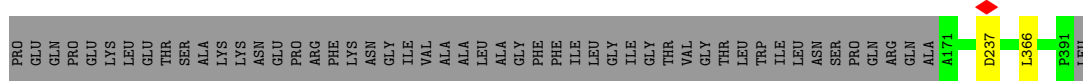


• Molecule 5: Protein PrgH



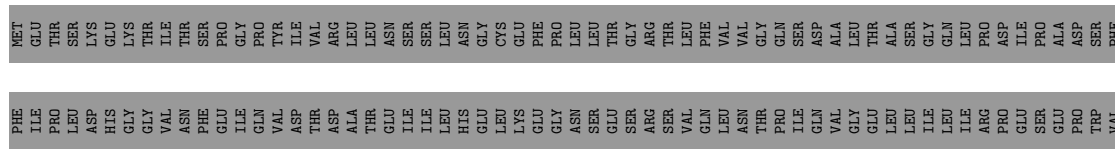
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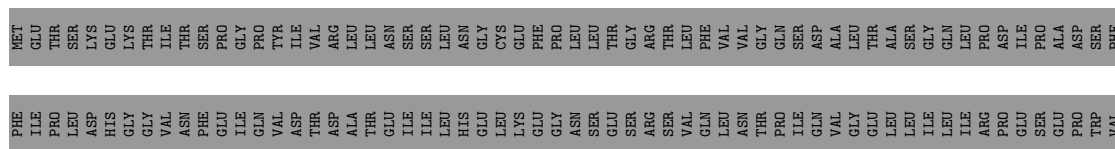
• Molecule 5: Protein PrgH

Chain Y: 56% 43%



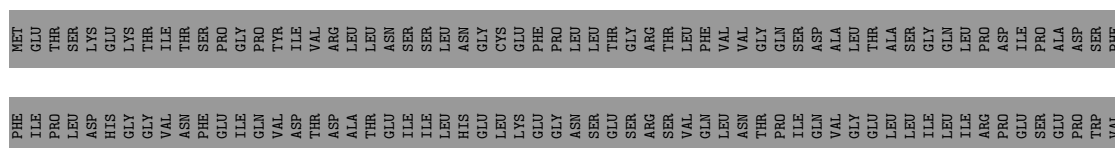
• Molecule 5: Protein PrgH

Chain Z: 56% 43%



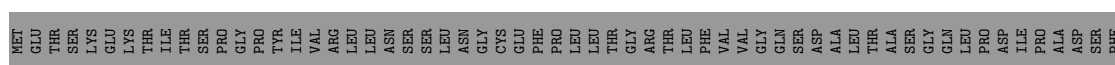
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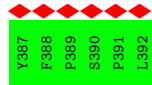
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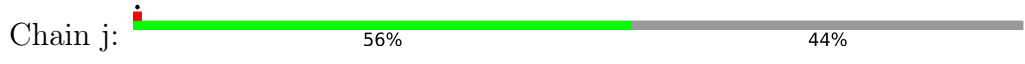
• Molecule 5: Protein PrgH

Chain b: 56% 43%





• Molecule 5: Protein PrgH



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• Molecule 5: Protein PrgH



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• Molecule 5: Protein PrgH



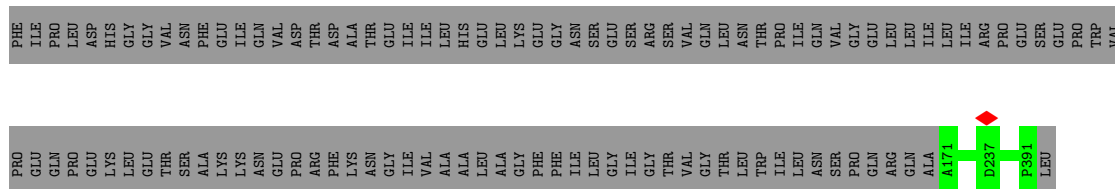
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PHE	ILE	PRO	LEU	ASP	HIS	GLY	THR	VAL	ASN	PHE	GLY	GLN	VAL	TYR	ASP	THR	VAL	ARG	PHE	ALA	THR	LEU	ASN	GLY	LEU	ALA	GLY	PHE	GLY	ASN	SER	GLY	THR	THR	THR	VAL	GLN	LEU	ASN	VAL	THR	TRP	TRP	ILE	GLY	VAL	GLY	LEU	LEU	GLY	ARG	PRO	PRO	ASP	GLY	THR	GLY	LEU	LEU	GLY	ASP	PRO	ALA	ASP	TRP	TRP	VAL	
PRO	GLU	GLN	PRO	GLU	ASP	LYS	LEU	GLY	THR	ILE	THR	ASN	ALA	PRO	ASP	THR	VAL	ARG	PHE	ALA	THR	LEU	ASN	GLY	LEU	ALA	GLY	PHE	GLY	ASN	SER	GLY	THR	THR	THR	VAL	GLN	LEU	ASN	VAL	THR	TRP	TRP	ILE	GLY	VAL	GLY	LEU	LEU	GLY	ARG	PRO	PRO	ASP	GLY	THR	GLY	LEU	LEU	GLY	ASP	PRO	ALA	ASP	TRP	TRP	VAL	



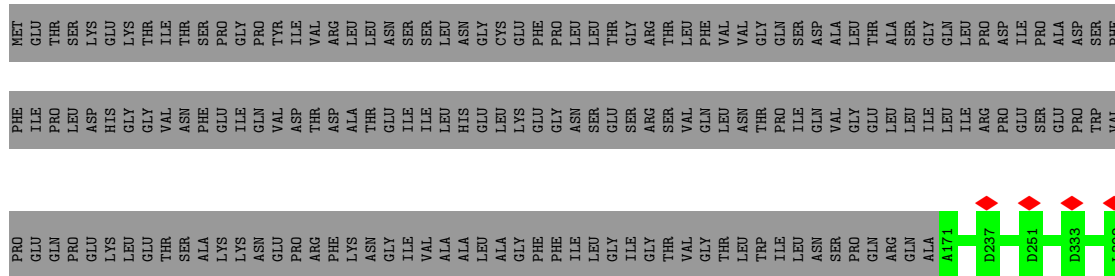
• Molecule 5: Protein PrgH



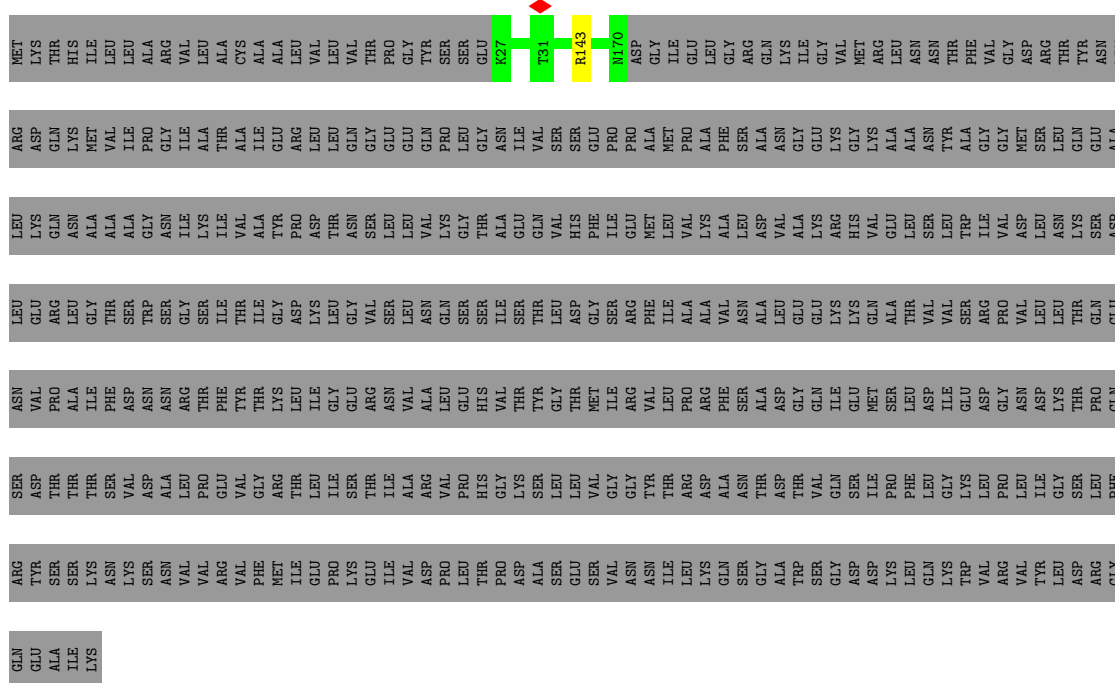
MET	GLU	THR	THR	LEU	SER	LYS	GLU	LYS	THR	ILE	THR	ASN	SER	PRO	GLY	PRO	TYR	VAL	ARG	THR	LEU	ASN	GLY	CYS	GLY	PHE	GLU	PHE	GLY	LEU	LEU	GLY	THR	THR	THR	THR	PHE	VAL	VAL	VAL	VAL	GLN	PRO	GLY	ASP	ASP	ALA	LEU	THR	GLN	GLY	ILE	LEU	LEU	PRO	ASP	PRO	ILE	PRO	ALA	ASP	TRP	TRP	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



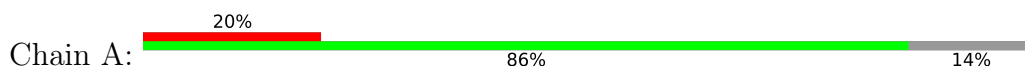
● Molecule 5: Protein PrgH

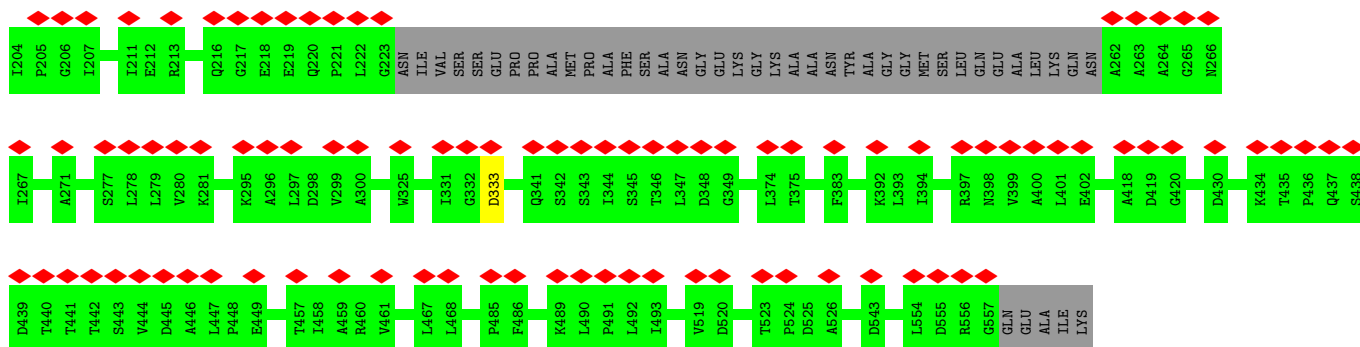


● Molecule 6: Protein InvG

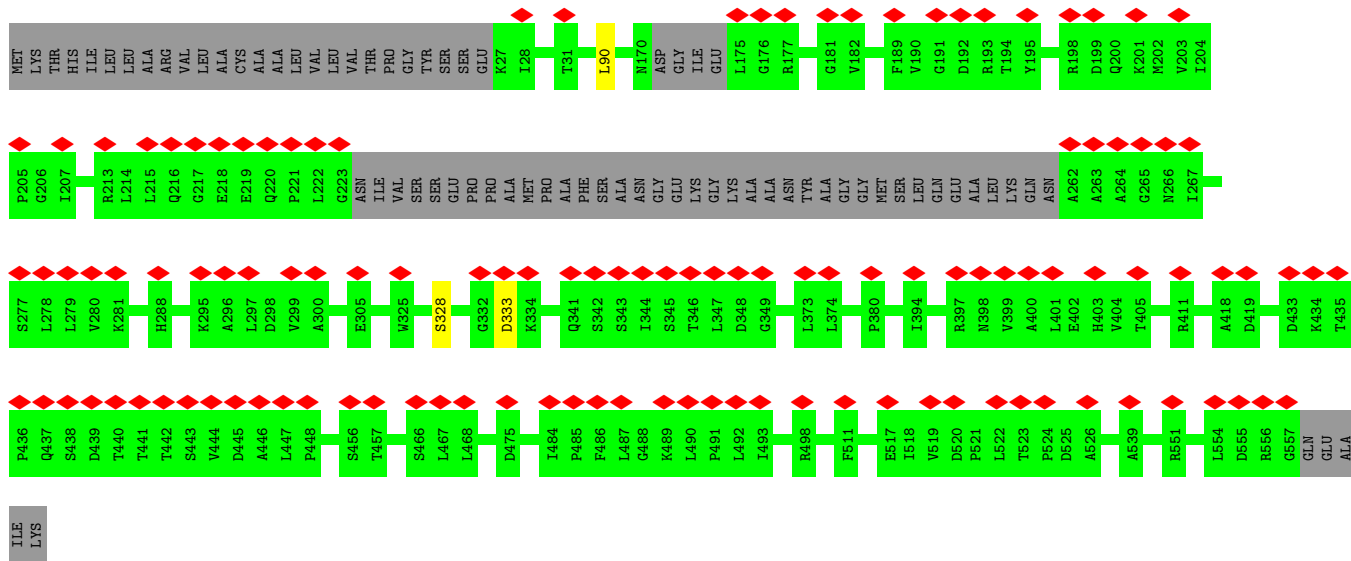
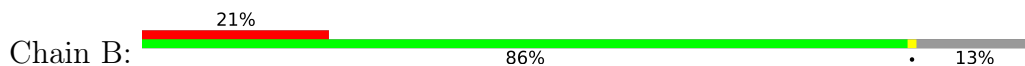


● Molecule 6: Protein InvG

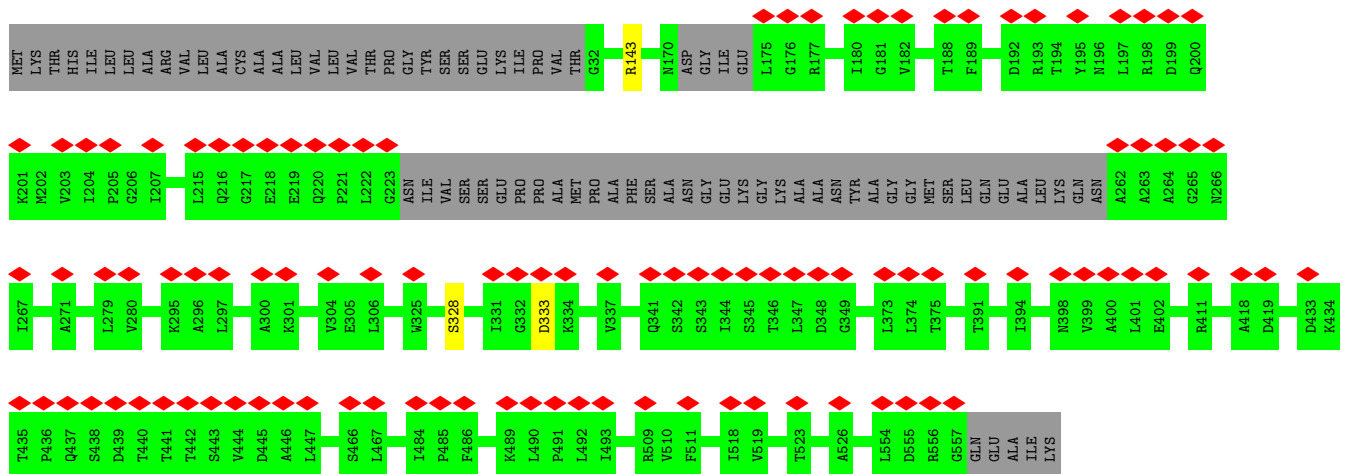
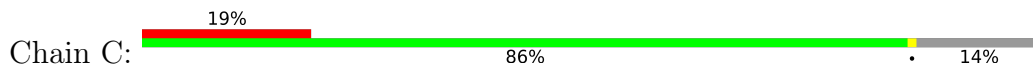




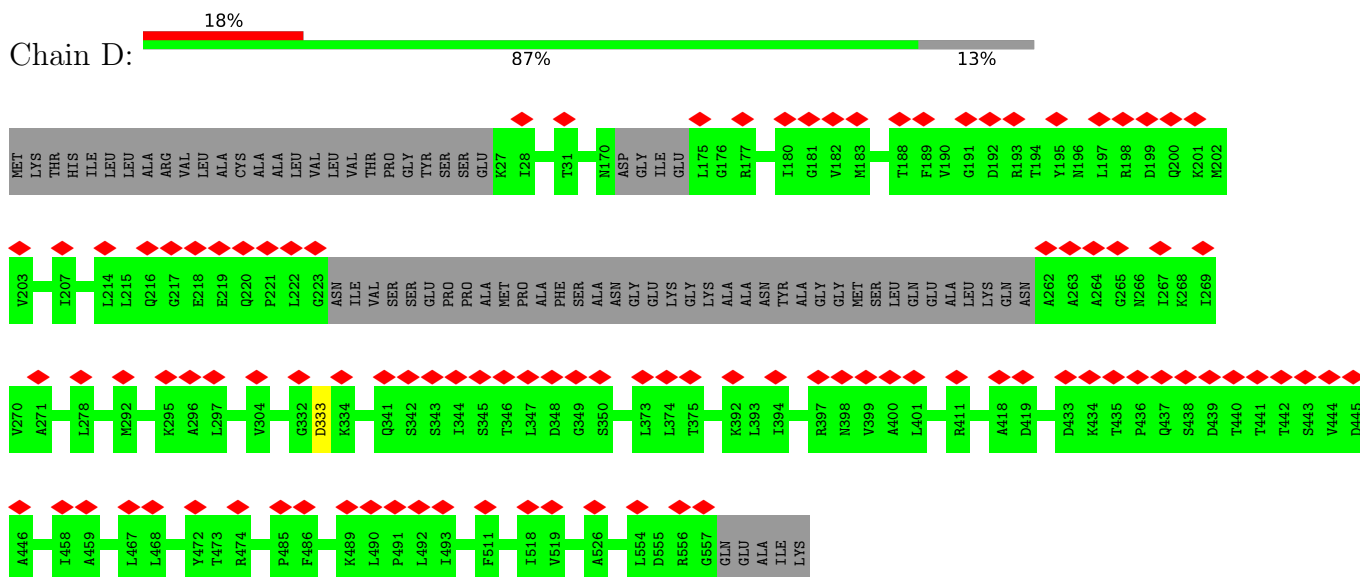
• Molecule 6: Protein InvG



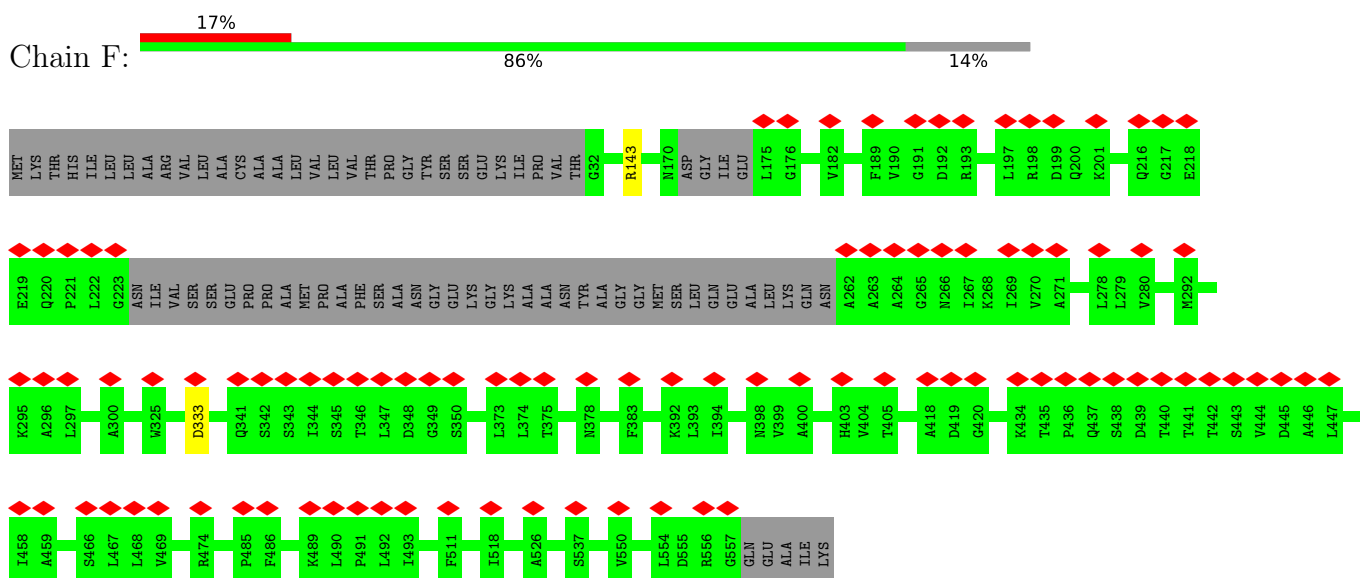
• Molecule 6: Protein InvG



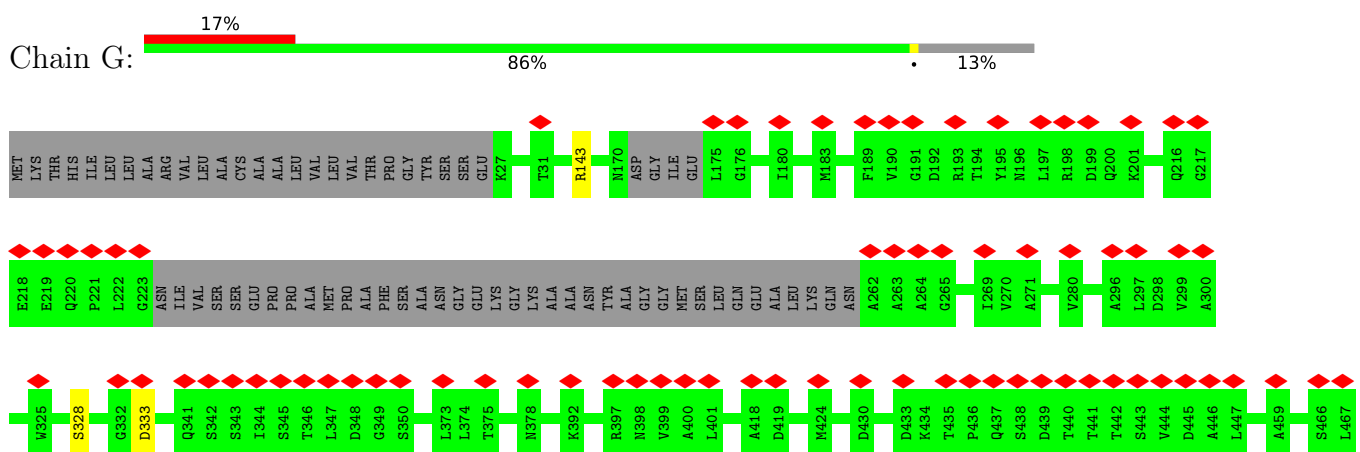
• Molecule 6: Protein InvG

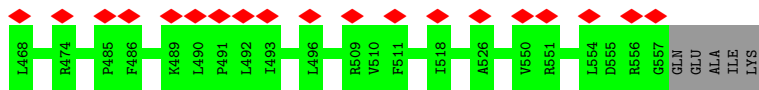


• Molecule 6: Protein InvG

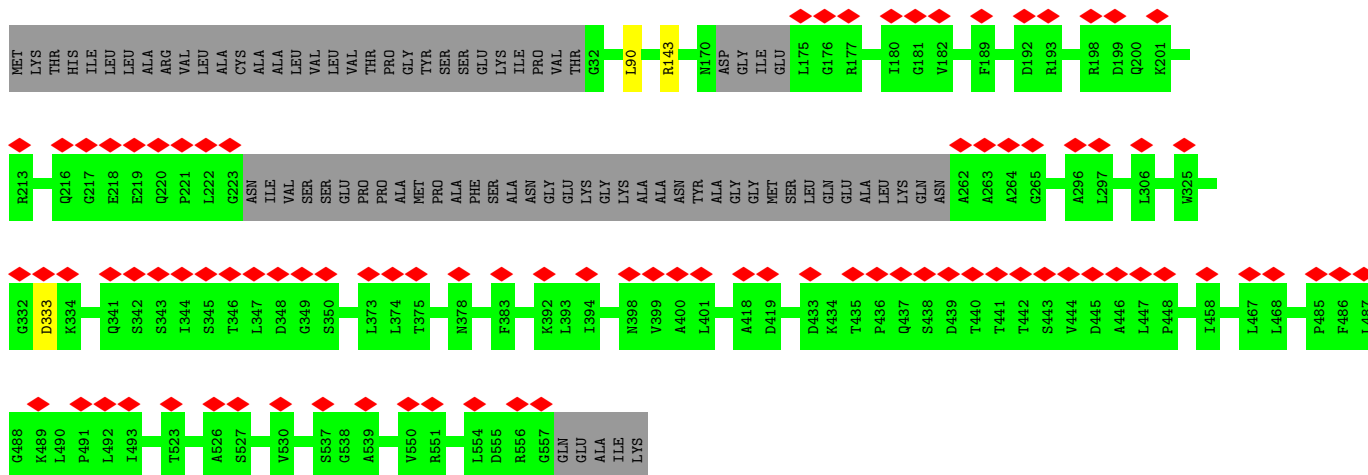
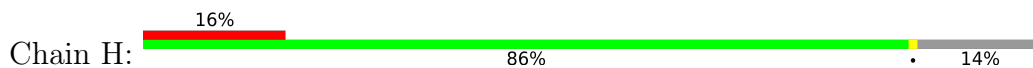


• Molecule 6: Protein InvG

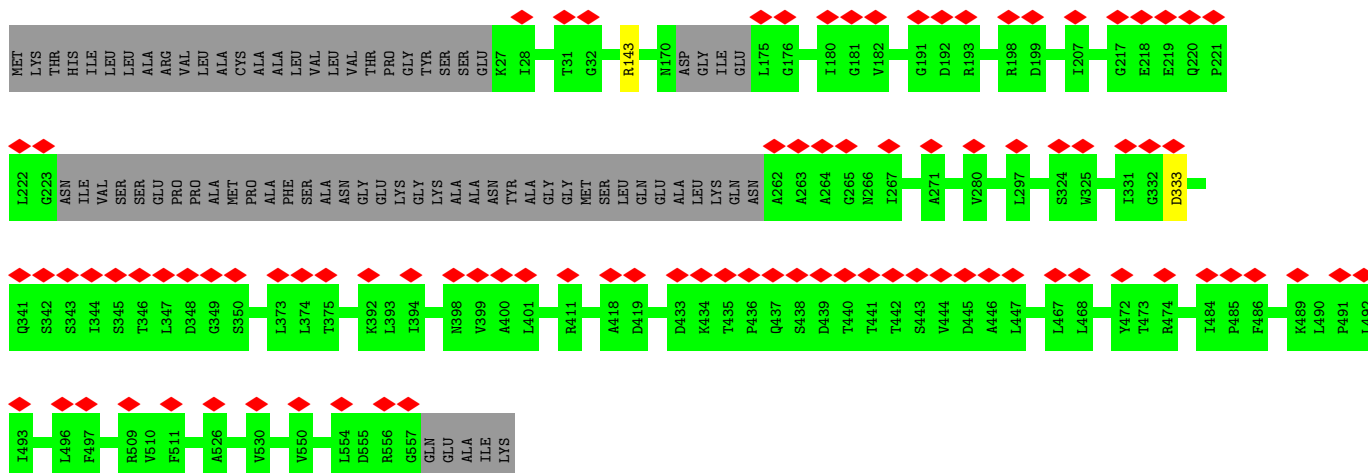
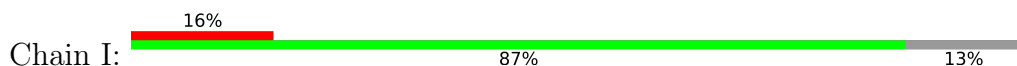




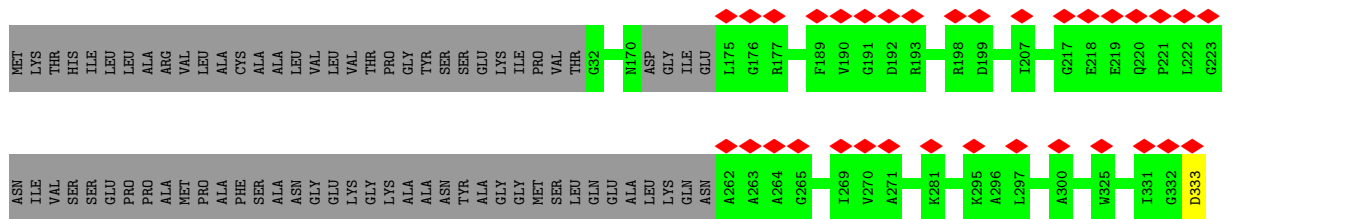
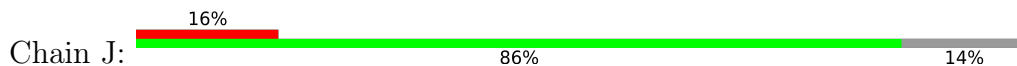
• Molecule 6: Protein InvG

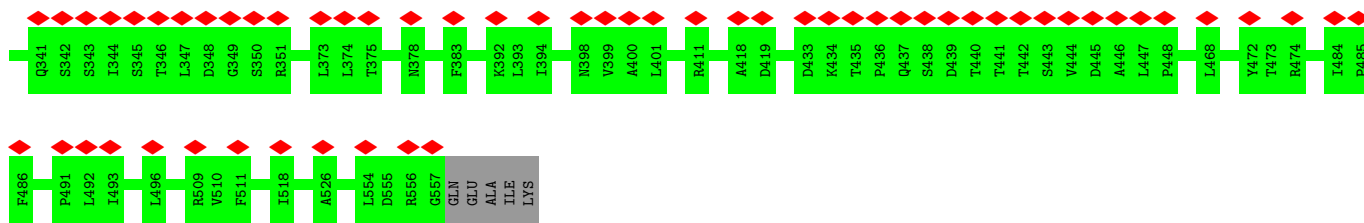


• Molecule 6: Protein InvG

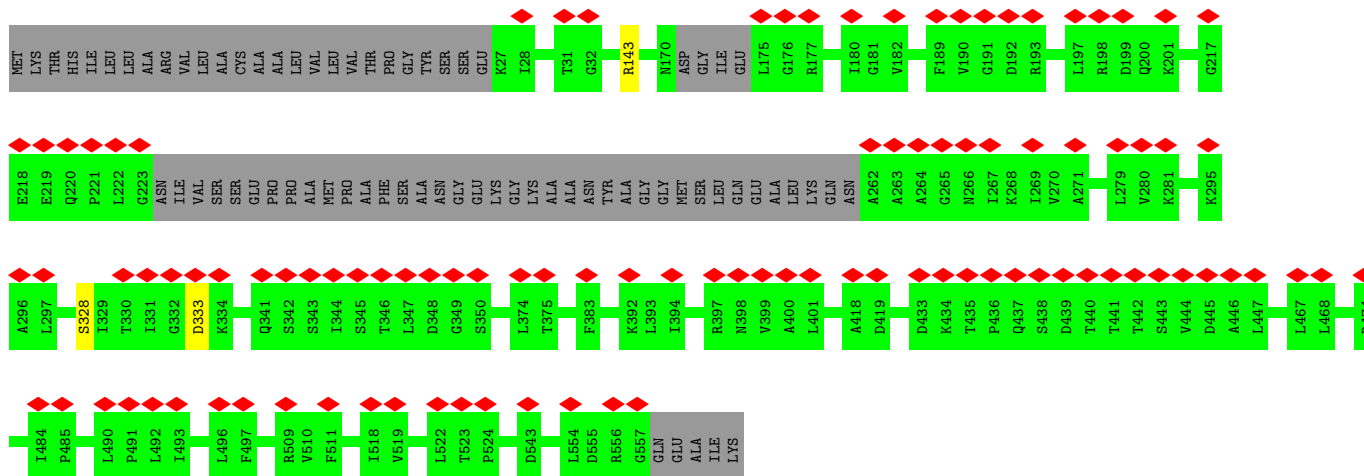
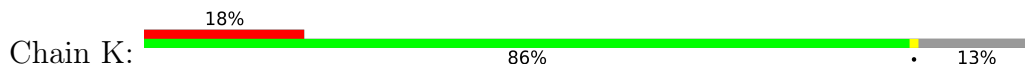


• Molecule 6: Protein InvG

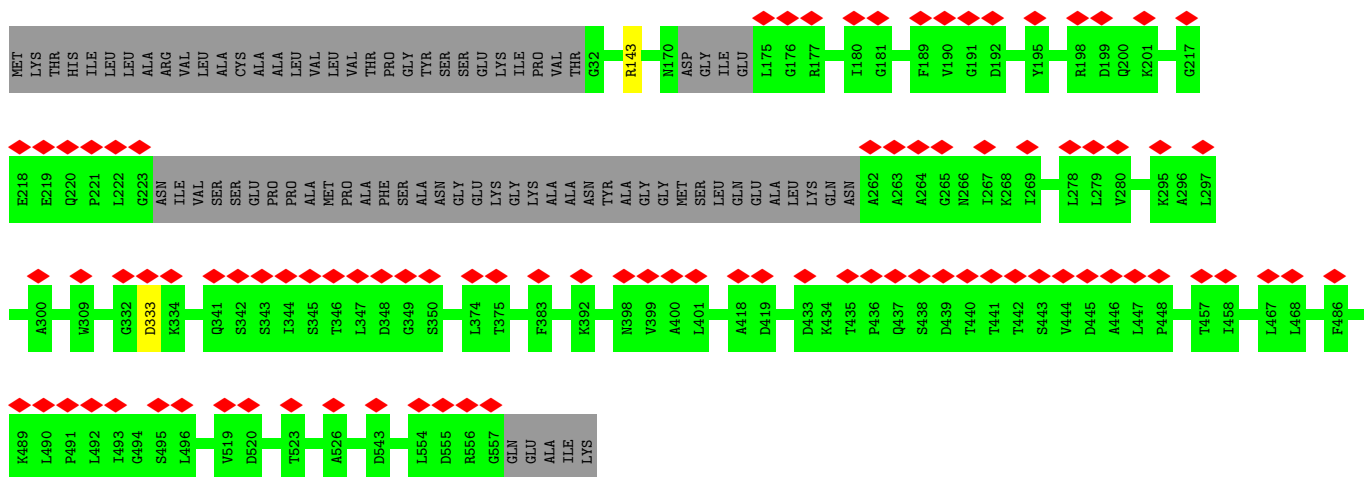
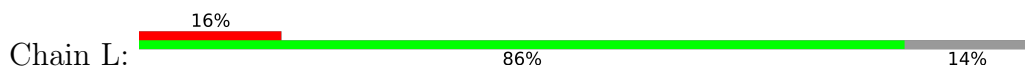




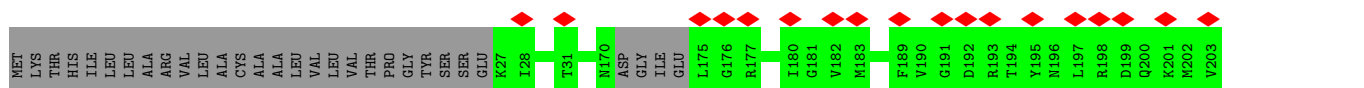
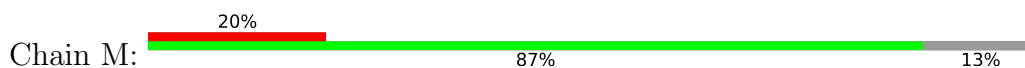
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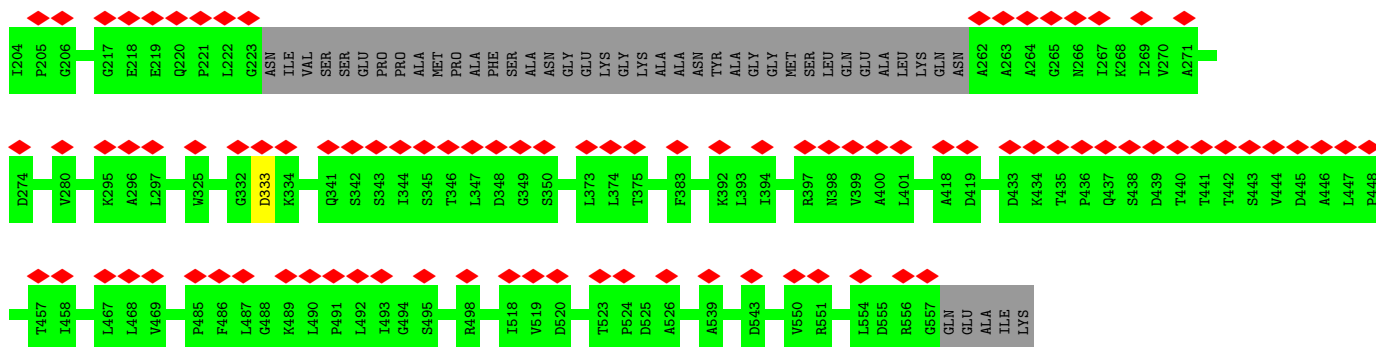


• Molecule 6: Protein InvG

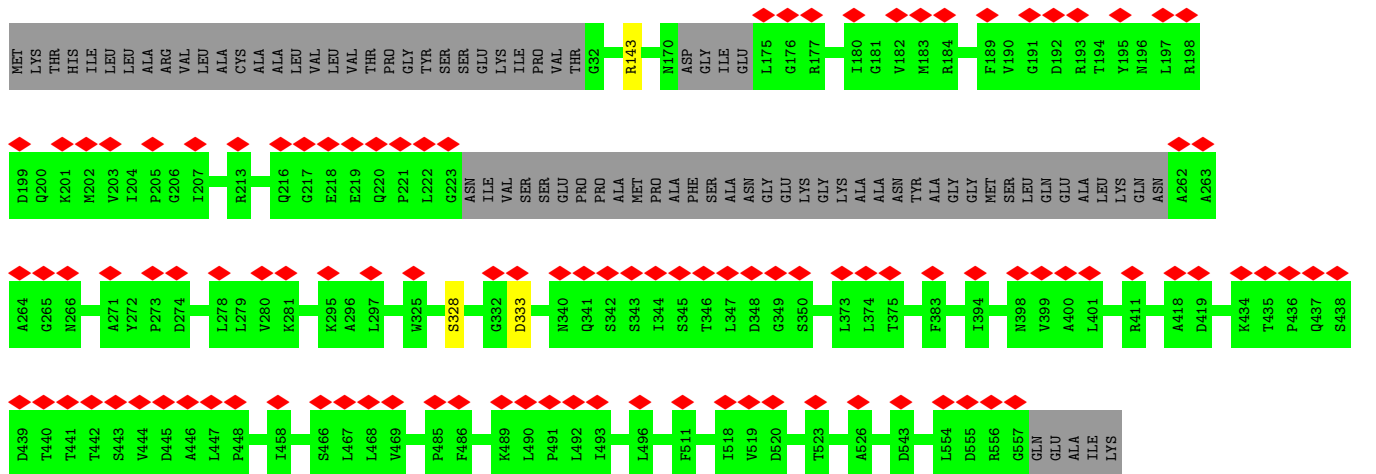
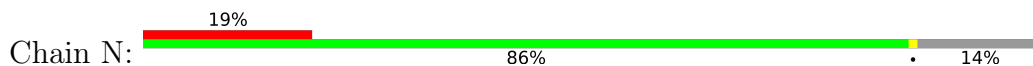


• Molecule 6: Protein InvG

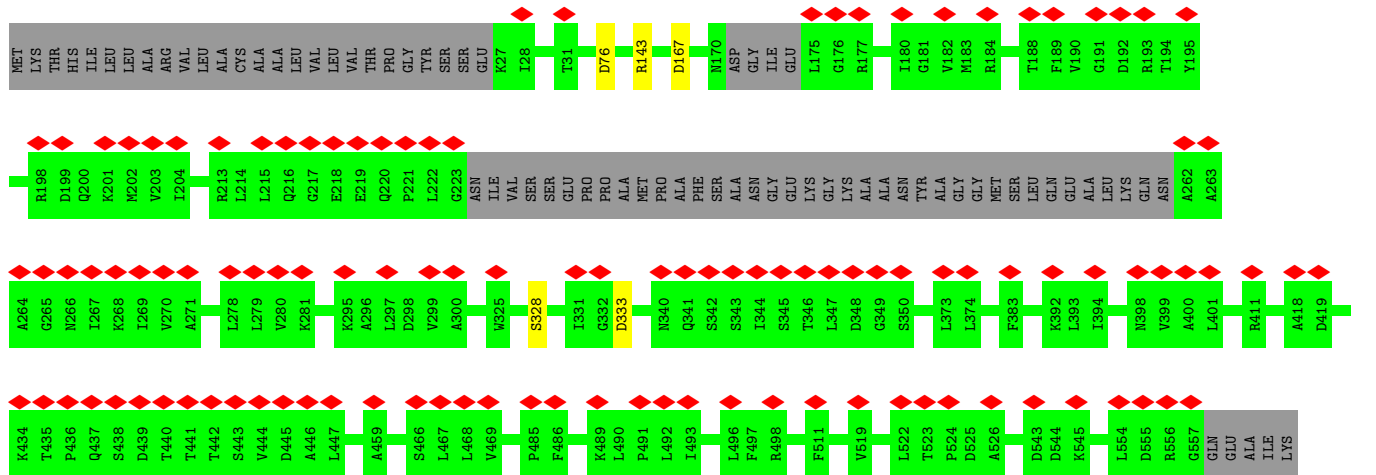
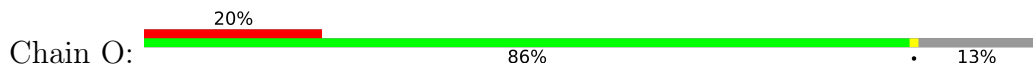




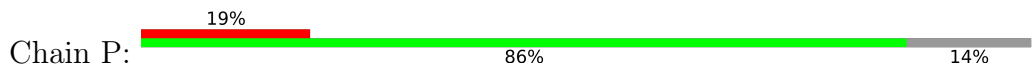
• Molecule 6: Protein InvG

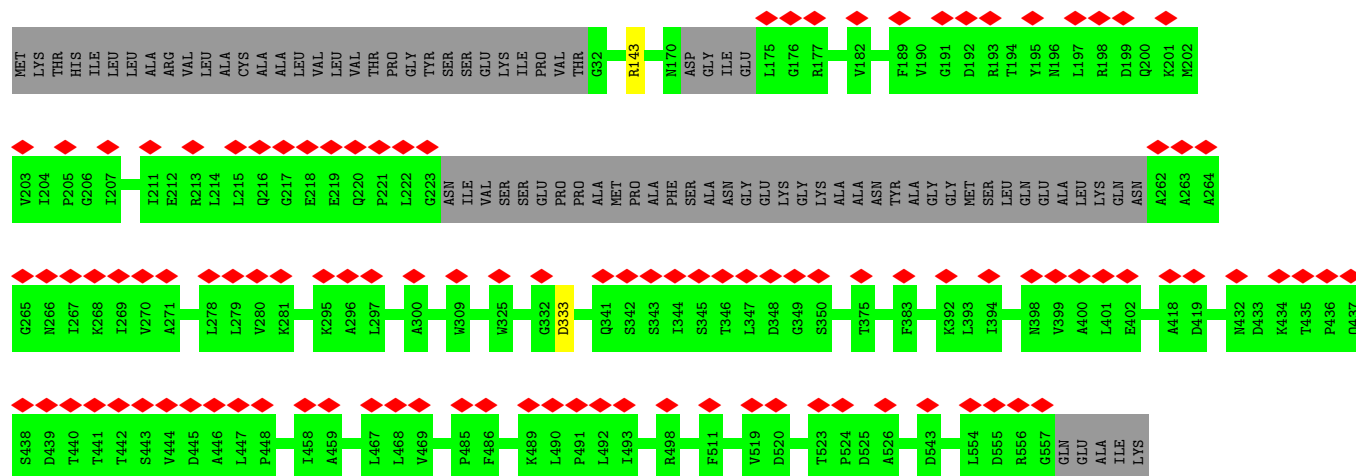


• Molecule 6: Protein InvG



• Molecule 6: Protein InvG





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51816	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	0.087	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	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 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	AA	0.41	0/1458	0.58	1/1979 (0.1%)
1	AB	0.40	0/1458	0.57	0/1979
1	AC	0.39	0/1458	0.55	0/1979
1	AD	0.39	0/1458	0.60	2/1979 (0.1%)
1	AE	0.40	0/1458	0.58	1/1979 (0.1%)
1	AF	0.42	0/1458	0.55	0/1979
1	AG	0.39	0/1458	0.54	0/1979
1	AH	0.39	0/1458	0.54	0/1979
1	AI	0.40	0/1458	0.58	0/1979
1	AJ	0.41	0/1458	0.59	0/1979
1	AK	0.40	0/1458	0.56	0/1979
1	AL	0.40	0/1458	0.57	1/1979 (0.1%)
1	o	0.38	0/1458	0.57	0/1979
1	p	0.38	0/1458	0.53	0/1979
1	q	0.39	0/1458	0.54	0/1979
1	r	0.39	0/1458	0.57	0/1979
1	s	0.40	0/1458	0.55	0/1979
1	t	0.40	0/1458	0.59	0/1979
1	u	0.38	0/1458	0.58	1/1979 (0.1%)
1	v	0.42	1/1458 (0.1%)	0.57	0/1979
1	w	0.39	0/1458	0.56	0/1979
1	x	0.40	0/1458	0.55	0/1979
1	y	0.39	0/1458	0.54	0/1979
1	z	0.41	0/1458	0.58	0/1979
2	0	0.34	0/1501	0.65	0/2040
2	1	0.38	0/1508	0.72	2/2049 (0.1%)
2	2	0.37	0/1497	0.68	1/2032 (0.0%)
2	3	0.34	0/1553	0.64	2/2107 (0.1%)
2	4	0.37	0/1710	0.62	1/2318 (0.0%)
3	5	0.35	0/1758	0.62	0/2402
4	6	0.30	0/414	0.60	0/565
4	7	0.33	0/657	0.77	1/897 (0.1%)
4	8	0.33	0/657	0.72	1/897 (0.1%)
4	9	0.35	0/660	0.61	0/900

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	E	0.38	0/1881	0.54	0/2541
5	R	0.39	0/1872	0.55	0/2530
5	S	0.38	0/1876	0.55	0/2536
5	T	0.39	0/1881	0.53	0/2541
5	U	0.37	0/1872	0.56	0/2530
5	V	0.38	0/1876	0.53	0/2536
5	W	0.38	0/1881	0.52	0/2541
5	X	0.37	0/1872	0.55	1/2530 (0.0%)
5	Y	0.40	0/1876	0.54	0/2536
5	Z	0.38	0/1881	0.53	0/2541
5	a	0.38	0/1872	0.55	0/2530
5	b	0.40	0/1876	0.55	0/2536
5	c	0.39	0/1881	0.53	0/2541
5	d	0.38	0/1872	0.53	0/2530
5	e	0.39	0/1876	0.53	0/2536
5	f	0.39	0/1881	0.53	0/2541
5	g	0.39	0/1872	0.55	0/2530
5	h	0.39	0/1876	0.54	0/2536
5	i	0.38	0/1881	0.55	1/2541 (0.0%)
5	j	0.39	0/1872	0.55	0/2530
5	k	0.38	0/1876	0.53	0/2536
5	l	0.38	0/1881	0.52	0/2541
5	m	0.38	0/1872	0.54	0/2530
5	n	0.39	0/1876	0.55	0/2536
6	A	0.32	0/3827	0.55	1/5180 (0.0%)
6	B	0.32	0/3877	0.55	2/5248 (0.0%)
6	C	0.33	0/3827	0.55	1/5180 (0.0%)
6	D	0.32	0/3866	0.55	1/5234 (0.0%)
6	F	0.33	0/3827	0.54	1/5180 (0.0%)
6	G	0.33	0/3877	0.56	1/5248 (0.0%)
6	H	0.32	0/3827	0.55	2/5180 (0.0%)
6	I	0.32	0/3877	0.55	1/5248 (0.0%)
6	J	0.32	0/3827	0.55	1/5180 (0.0%)
6	K	0.33	0/3877	0.56	1/5248 (0.0%)
6	L	0.33	0/3827	0.55	1/5180 (0.0%)
6	M	0.32	0/3866	0.55	1/5234 (0.0%)
6	N	0.33	0/3827	0.55	1/5180 (0.0%)
6	O	0.33	0/3877	0.57	3/5248 (0.1%)
6	P	0.33	0/3827	0.55	1/5180 (0.0%)
6	Q	0.37	0/1181	0.57	0/1593
All	All	0.36	1/150853 (0.0%)	0.56	35/204300 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	8	0	2
5	b	0	1
5	k	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	v	76	GLN	C-N	-5.20	1.22	1.34

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	333	ASP	CB-CG-OD2	7.26	124.83	118.30
6	F	333	ASP	CB-CG-OD2	7.20	124.78	118.30
6	K	333	ASP	CB-CG-OD2	7.19	124.77	118.30
6	M	333	ASP	CB-CG-OD2	7.19	124.77	118.30
6	J	333	ASP	CB-CG-OD2	7.17	124.75	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	8	16	LEU	Mainchain
4	8	40	THR	Peptide
5	b	366	LEU	Peptide
5	k	366	LEU	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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%)	178 (98%)	4 (2%)	0	100	100
1	AC	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	AD	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	AE	182/252 (72%)	177 (97%)	5 (3%)	0	100	100
1	AF	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	AG	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	AH	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	AI	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	AJ	182/252 (72%)	178 (98%)	4 (2%)	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%)	172 (94%)	10 (6%)	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%)	175 (96%)	7 (4%)	0	100	100
1	t	182/252 (72%)	179 (98%)	3 (2%)	0	100	100
1	u	182/252 (72%)	178 (98%)	4 (2%)	0	100	100
1	v	182/252 (72%)	175 (96%)	7 (4%)	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	0	183/224 (82%)	178 (97%)	4 (2%)	1 (0%)	29	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	183/224 (82%)	176 (96%)	6 (3%)	1 (0%)	29	66
2	2	181/224 (81%)	174 (96%)	6 (3%)	1 (1%)	25	62
2	3	188/224 (84%)	185 (98%)	3 (2%)	0	100	100
2	4	208/224 (93%)	199 (96%)	9 (4%)	0	100	100
3	5	222/263 (84%)	216 (97%)	6 (3%)	0	100	100
4	6	49/86 (57%)	48 (98%)	1 (2%)	0	100	100
4	7	82/86 (95%)	80 (98%)	2 (2%)	0	100	100
4	8	82/86 (95%)	79 (96%)	3 (4%)	0	100	100
4	9	82/86 (95%)	81 (99%)	1 (1%)	0	100	100
5	E	220/392 (56%)	213 (97%)	7 (3%)	0	100	100
5	R	219/392 (56%)	213 (97%)	6 (3%)	0	100	100
5	S	220/392 (56%)	208 (94%)	12 (6%)	0	100	100
5	T	220/392 (56%)	210 (96%)	10 (4%)	0	100	100
5	U	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
5	V	220/392 (56%)	207 (94%)	13 (6%)	0	100	100
5	W	220/392 (56%)	212 (96%)	8 (4%)	0	100	100
5	X	219/392 (56%)	213 (97%)	6 (3%)	0	100	100
5	Y	220/392 (56%)	205 (93%)	15 (7%)	0	100	100
5	Z	220/392 (56%)	210 (96%)	10 (4%)	0	100	100
5	a	219/392 (56%)	213 (97%)	6 (3%)	0	100	100
5	b	220/392 (56%)	206 (94%)	14 (6%)	0	100	100
5	c	220/392 (56%)	211 (96%)	9 (4%)	0	100	100
5	d	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
5	e	220/392 (56%)	208 (94%)	12 (6%)	0	100	100
5	f	220/392 (56%)	209 (95%)	11 (5%)	0	100	100
5	g	219/392 (56%)	210 (96%)	9 (4%)	0	100	100
5	h	220/392 (56%)	207 (94%)	13 (6%)	0	100	100
5	i	220/392 (56%)	212 (96%)	8 (4%)	0	100	100
5	j	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
5	k	220/392 (56%)	205 (93%)	15 (7%)	0	100	100
5	l	220/392 (56%)	210 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	m	219/392 (56%)	214 (98%)	5 (2%)	0	100	100
5	n	220/392 (56%)	207 (94%)	13 (6%)	0	100	100
6	A	478/562 (85%)	458 (96%)	20 (4%)	0	100	100
6	B	484/562 (86%)	461 (95%)	23 (5%)	0	100	100
6	C	478/562 (85%)	455 (95%)	23 (5%)	0	100	100
6	D	483/562 (86%)	459 (95%)	24 (5%)	0	100	100
6	F	478/562 (85%)	457 (96%)	21 (4%)	0	100	100
6	G	484/562 (86%)	458 (95%)	26 (5%)	0	100	100
6	H	478/562 (85%)	456 (95%)	22 (5%)	0	100	100
6	I	484/562 (86%)	462 (96%)	22 (4%)	0	100	100
6	J	478/562 (85%)	456 (95%)	22 (5%)	0	100	100
6	K	484/562 (86%)	460 (95%)	24 (5%)	0	100	100
6	L	478/562 (85%)	456 (95%)	22 (5%)	0	100	100
6	M	483/562 (86%)	458 (95%)	25 (5%)	0	100	100
6	N	478/562 (85%)	455 (95%)	23 (5%)	0	100	100
6	O	484/562 (86%)	461 (95%)	23 (5%)	0	100	100
6	P	478/562 (85%)	457 (96%)	21 (4%)	0	100	100
6	Q	143/562 (25%)	139 (97%)	4 (3%)	0	100	100
All	All	18453/26175 (70%)	17682 (96%)	768 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	0	49	ASN
2	2	47	PRO
2	1	49	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	155/215 (72%)	154 (99%)	1 (1%)	86	92
1	AB	155/215 (72%)	155 (100%)	0	100	100
1	AC	155/215 (72%)	155 (100%)	0	100	100
1	AD	155/215 (72%)	155 (100%)	0	100	100
1	AE	155/215 (72%)	154 (99%)	1 (1%)	86	92
1	AF	155/215 (72%)	154 (99%)	1 (1%)	86	92
1	AG	155/215 (72%)	154 (99%)	1 (1%)	86	92
1	AH	155/215 (72%)	155 (100%)	0	100	100
1	AI	155/215 (72%)	153 (99%)	2 (1%)	69	82
1	AJ	155/215 (72%)	155 (100%)	0	100	100
1	AK	155/215 (72%)	154 (99%)	1 (1%)	86	92
1	AL	155/215 (72%)	155 (100%)	0	100	100
1	o	155/215 (72%)	154 (99%)	1 (1%)	86	92
1	p	155/215 (72%)	155 (100%)	0	100	100
1	q	155/215 (72%)	155 (100%)	0	100	100
1	r	155/215 (72%)	154 (99%)	1 (1%)	86	92
1	s	155/215 (72%)	155 (100%)	0	100	100
1	t	155/215 (72%)	155 (100%)	0	100	100
1	u	155/215 (72%)	154 (99%)	1 (1%)	86	92
1	v	155/215 (72%)	155 (100%)	0	100	100
1	w	155/215 (72%)	154 (99%)	1 (1%)	86	92
1	x	155/215 (72%)	155 (100%)	0	100	100
1	y	155/215 (72%)	154 (99%)	1 (1%)	86	92
1	z	155/215 (72%)	154 (99%)	1 (1%)	86	92
2	0	162/199 (81%)	161 (99%)	1 (1%)	86	92
2	1	164/199 (82%)	161 (98%)	3 (2%)	59	77
2	2	164/199 (82%)	164 (100%)	0	100	100
2	3	170/199 (85%)	168 (99%)	2 (1%)	71	84
2	4	187/199 (94%)	186 (100%)	1 (0%)	88	94
3	5	187/219 (85%)	186 (100%)	1 (0%)	88	94
4	6	41/71 (58%)	41 (100%)	0	100	100
4	7	69/71 (97%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	8	69/71 (97%)	69 (100%)	0	100	100
4	9	70/71 (99%)	70 (100%)	0	100	100
5	E	190/337 (56%)	189 (100%)	1 (0%)	88	94
5	R	189/337 (56%)	189 (100%)	0	100	100
5	S	188/337 (56%)	187 (100%)	1 (0%)	88	94
5	T	190/337 (56%)	190 (100%)	0	100	100
5	U	189/337 (56%)	188 (100%)	1 (0%)	88	94
5	V	188/337 (56%)	186 (99%)	2 (1%)	73	85
5	W	190/337 (56%)	190 (100%)	0	100	100
5	X	189/337 (56%)	188 (100%)	1 (0%)	88	94
5	Y	188/337 (56%)	187 (100%)	1 (0%)	88	94
5	Z	190/337 (56%)	189 (100%)	1 (0%)	88	94
5	a	189/337 (56%)	189 (100%)	0	100	100
5	b	188/337 (56%)	188 (100%)	0	100	100
5	c	190/337 (56%)	190 (100%)	0	100	100
5	d	189/337 (56%)	188 (100%)	1 (0%)	88	94
5	e	188/337 (56%)	187 (100%)	1 (0%)	88	94
5	f	190/337 (56%)	189 (100%)	1 (0%)	88	94
5	g	189/337 (56%)	187 (99%)	2 (1%)	73	85
5	h	188/337 (56%)	188 (100%)	0	100	100
5	i	190/337 (56%)	189 (100%)	1 (0%)	88	94
5	j	189/337 (56%)	189 (100%)	0	100	100
5	k	188/337 (56%)	187 (100%)	1 (0%)	88	94
5	l	190/337 (56%)	190 (100%)	0	100	100
5	m	189/337 (56%)	189 (100%)	0	100	100
5	n	188/337 (56%)	188 (100%)	0	100	100
6	A	414/477 (87%)	414 (100%)	0	100	100
6	B	420/477 (88%)	419 (100%)	1 (0%)	93	97
6	C	414/477 (87%)	412 (100%)	2 (0%)	88	94
6	D	419/477 (88%)	419 (100%)	0	100	100
6	F	414/477 (87%)	413 (100%)	1 (0%)	93	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	420/477 (88%)	418 (100%)	2 (0%)	88	94
6	H	414/477 (87%)	413 (100%)	1 (0%)	93	97
6	I	420/477 (88%)	419 (100%)	1 (0%)	93	97
6	J	414/477 (87%)	414 (100%)	0	100	100
6	K	420/477 (88%)	418 (100%)	2 (0%)	88	94
6	L	414/477 (87%)	413 (100%)	1 (0%)	93	97
6	M	419/477 (88%)	419 (100%)	0	100	100
6	N	414/477 (87%)	412 (100%)	2 (0%)	88	94
6	O	420/477 (88%)	418 (100%)	2 (0%)	88	94
6	P	414/477 (87%)	413 (100%)	1 (0%)	93	97
6	Q	125/477 (26%)	124 (99%)	1 (1%)	81	89
All	All	15914/22378 (71%)	15861 (100%)	53 (0%)	92	96

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	i	176	LEU
1	z	80	ARG
6	N	328	SER
5	k	348	ARG
1	u	177	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
5	k	318	ASN
6	P	169	GLN
1	AJ	162	HIS
6	P	87	GLN
6	L	169	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 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.

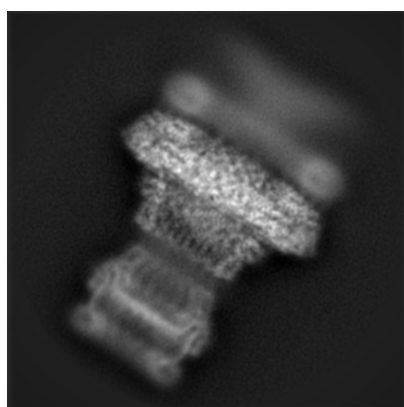
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20310. These allow visual inspection of the internal detail of the map and identification of artifacts.

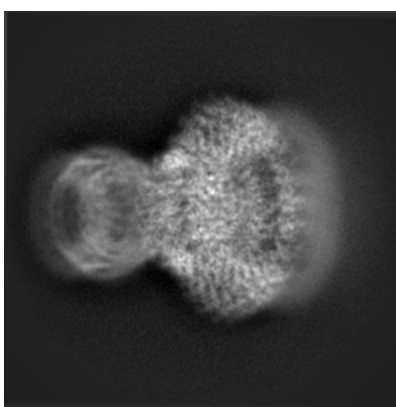
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

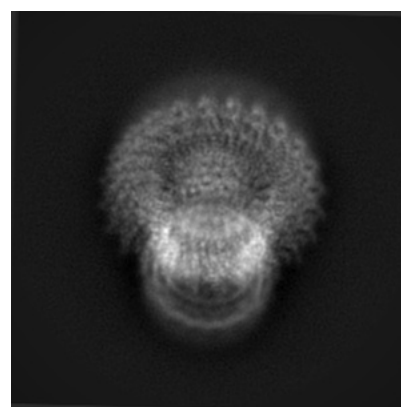
6.1.1 Primary map



X



Y

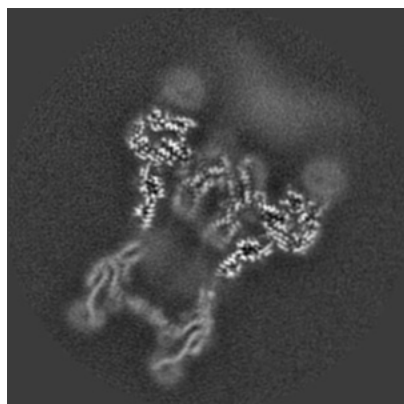


Z

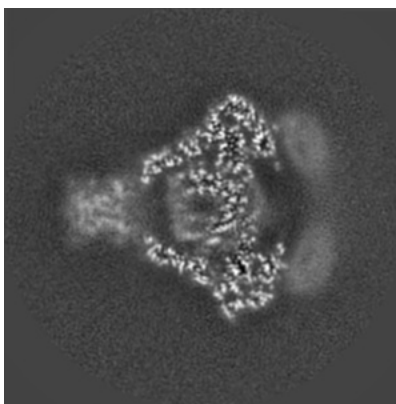
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

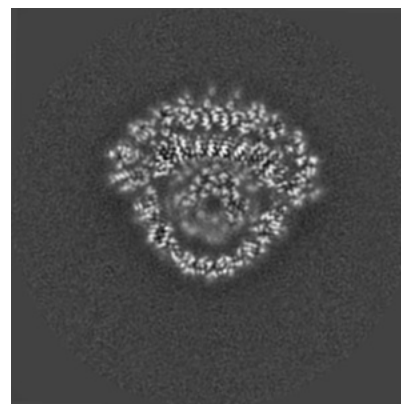
6.2.1 Primary map



X Index: 125



Y Index: 125

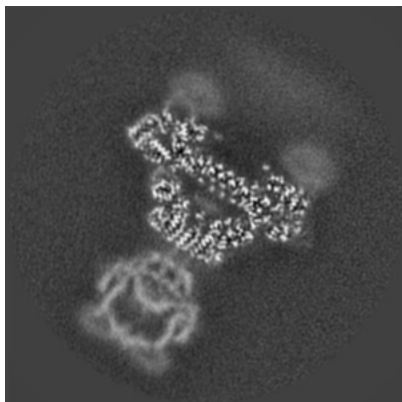


Z Index: 125

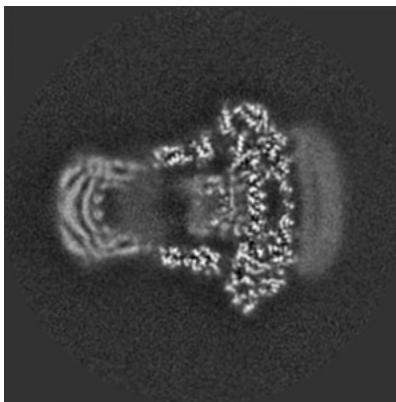
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

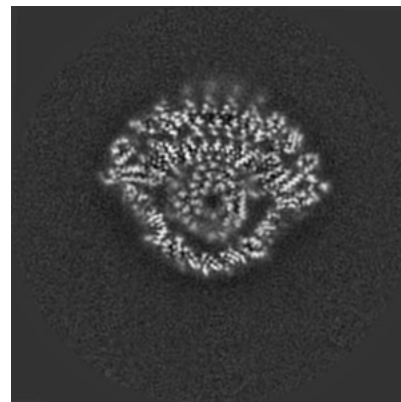
6.3.1 Primary map



X Index: 97



Y Index: 113



Z Index: 129

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

6.4 Orthogonal surface views [i](#)

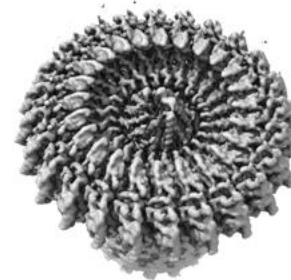
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

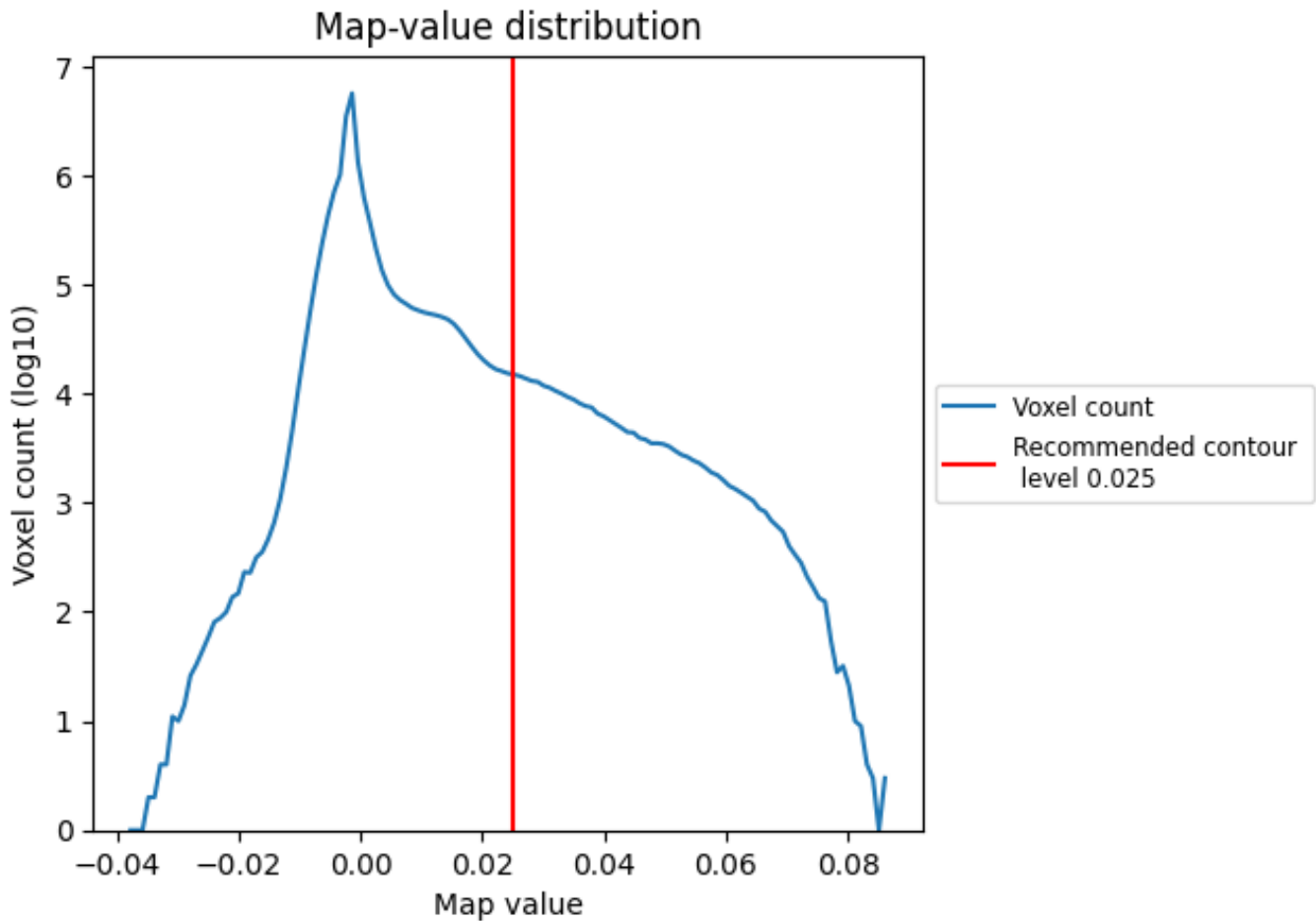
6.5 Mask visualisation

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

7 Map analysis [i](#)

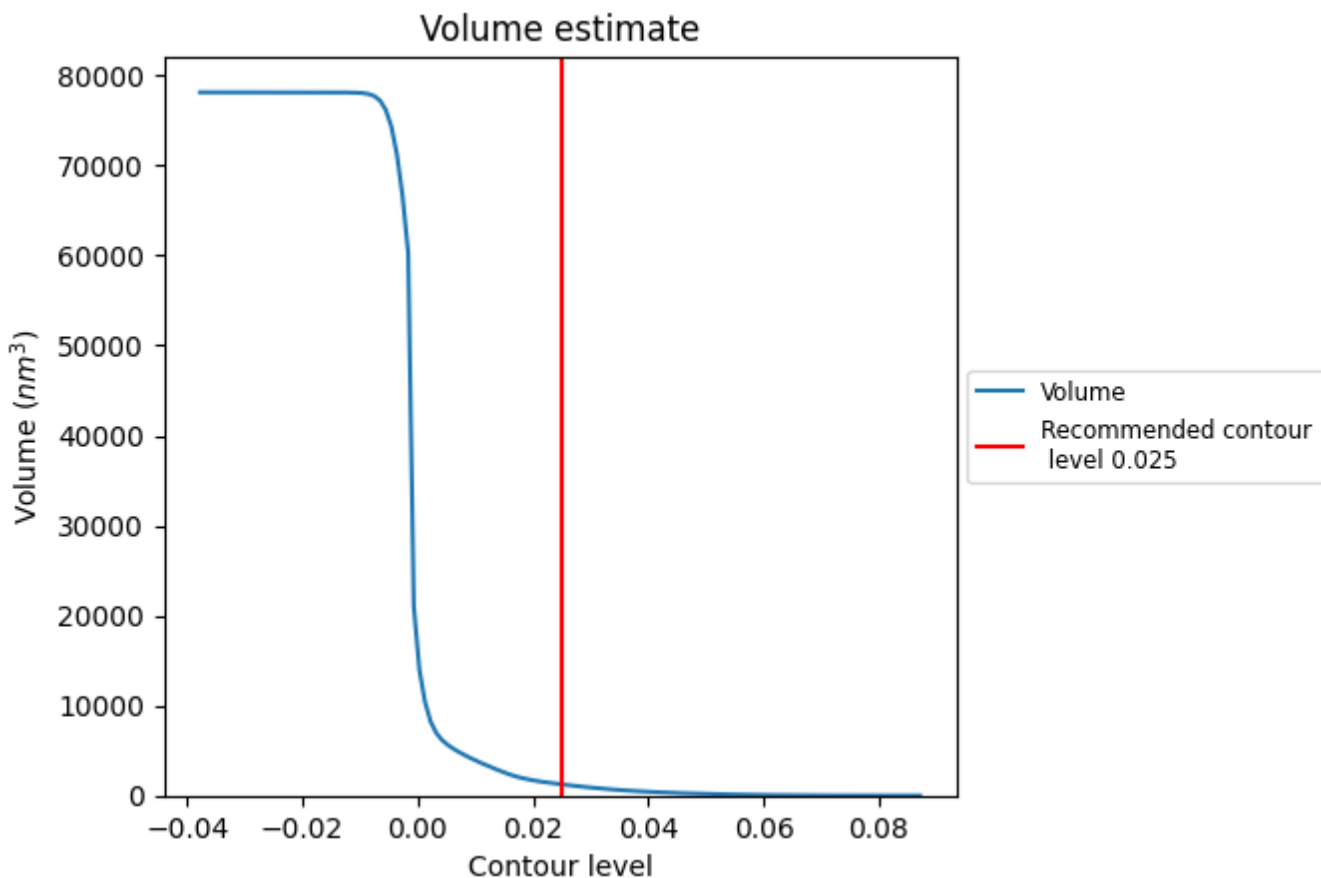
This section contains the results of statistical analysis of the map.

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.

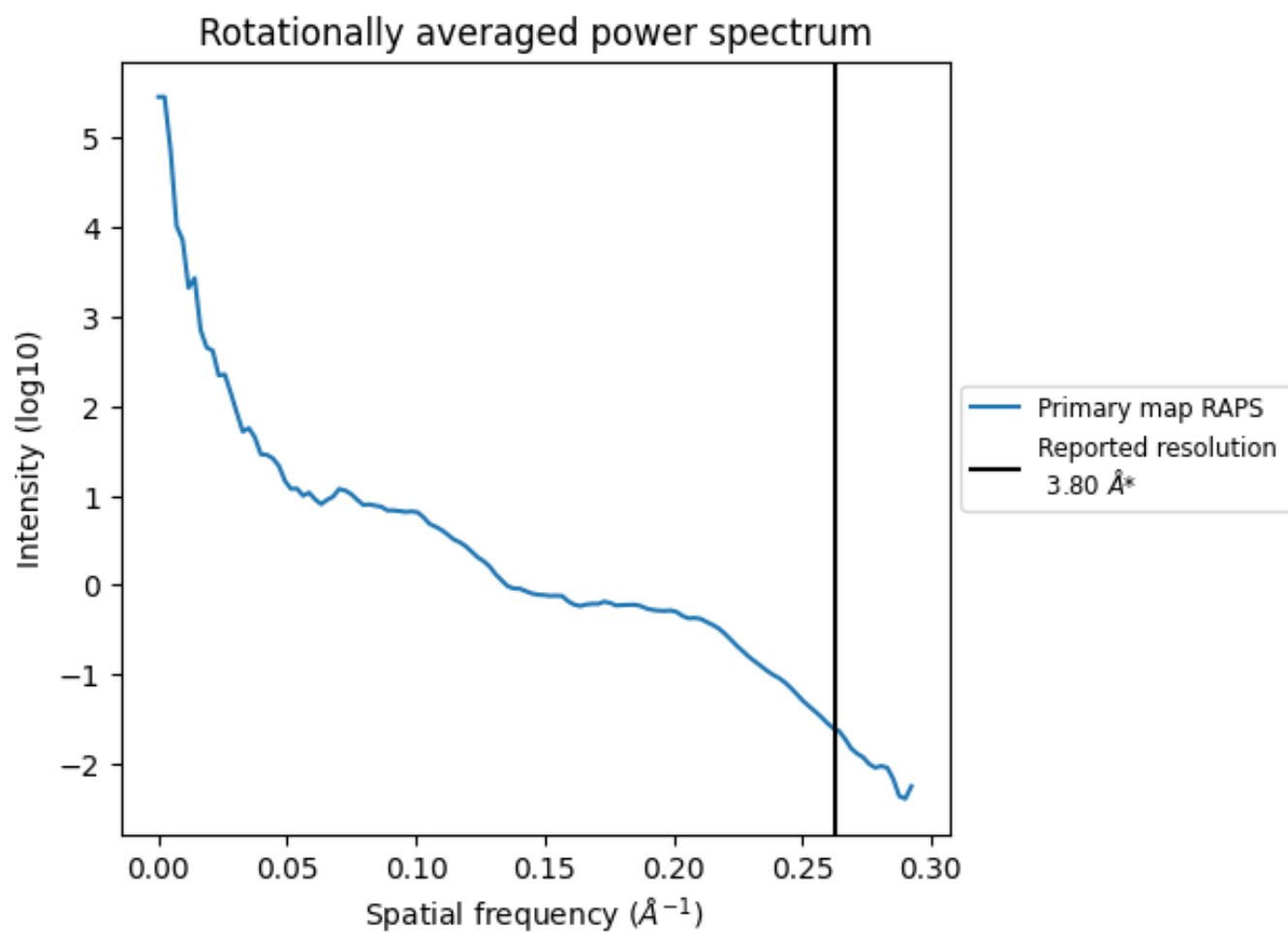
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1245 nm³; this corresponds to an approximate mass of 1124 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

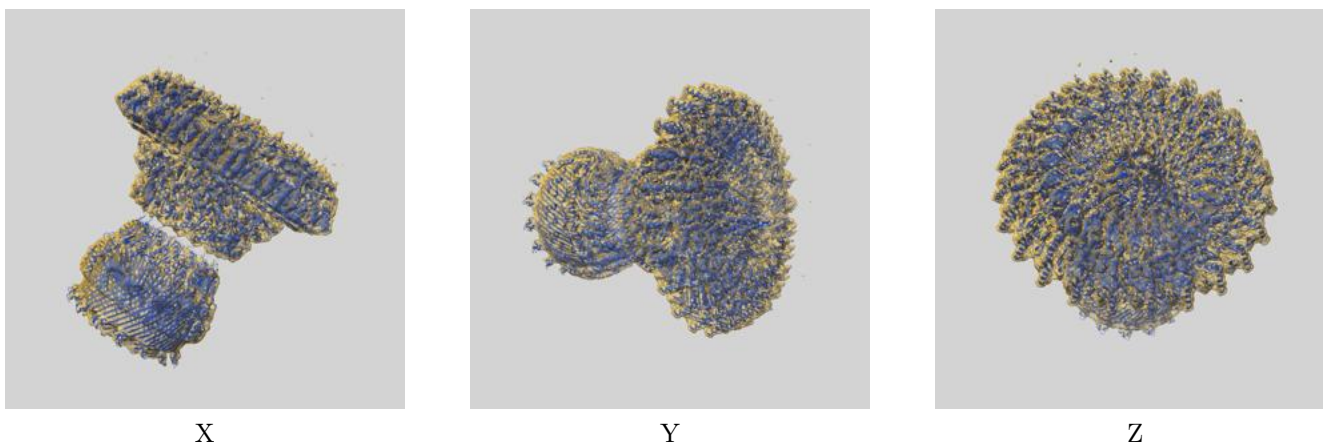
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

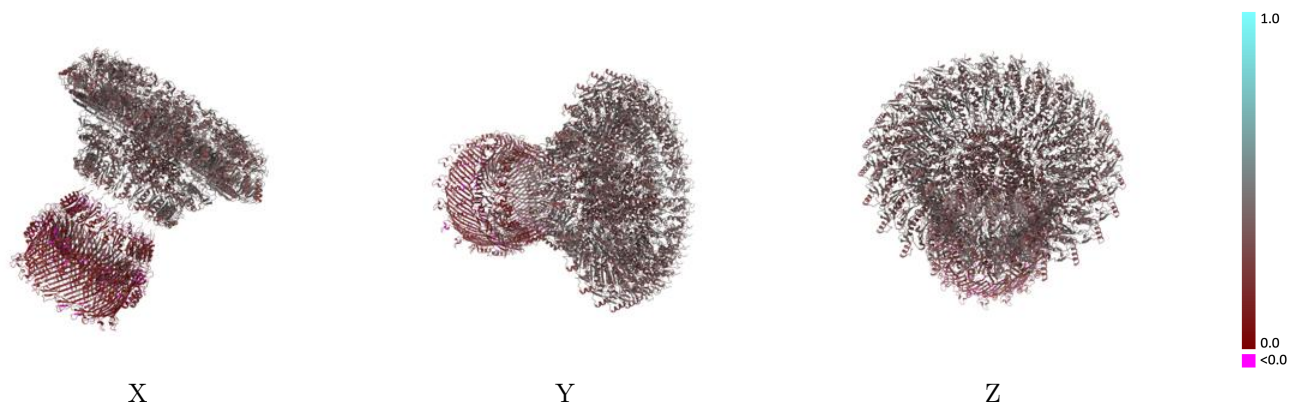
This section contains information regarding the fit between EMDB map EMD-20310 and PDB model 6Q14. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



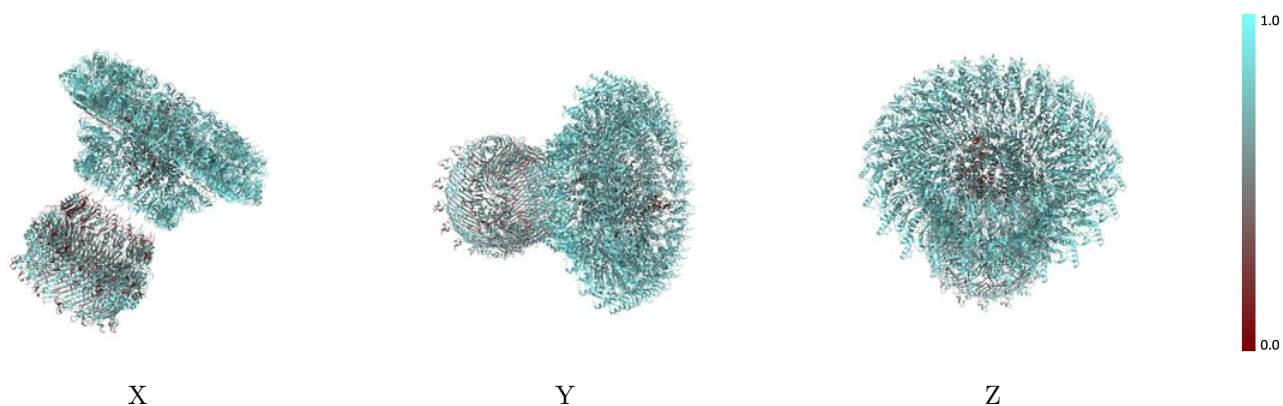
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



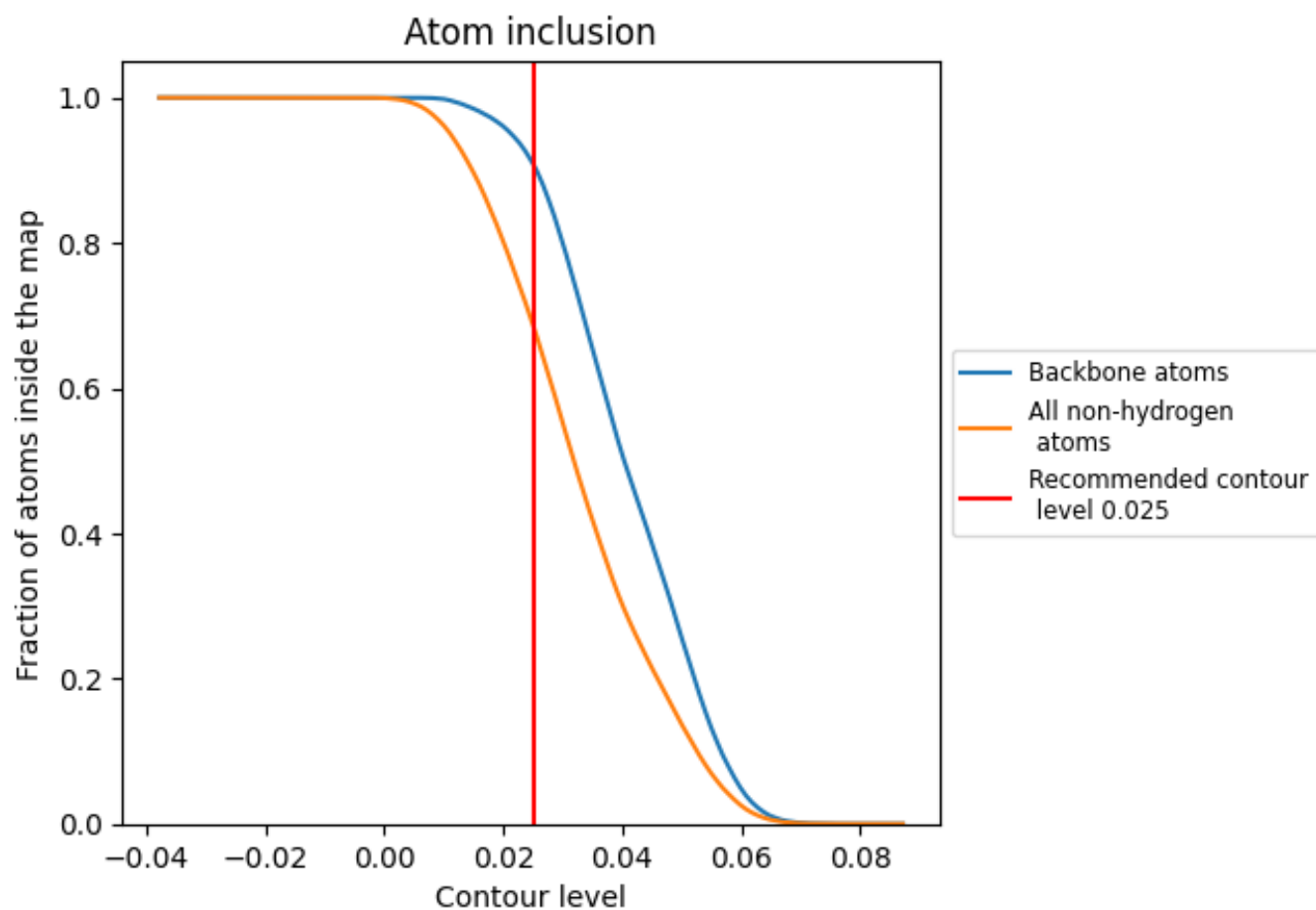
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 69% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6875	 0.3220
0	 0.6196	 0.3330
1	 0.5837	 0.3070
2	 0.5888	 0.3140
3	 0.5975	 0.3190
4	 0.5876	 0.3200
5	 0.6908	 0.3510
6	 0.3693	 0.3360
7	 0.4286	 0.3130
8	 0.5871	 0.3110
9	 0.6406	 0.3330
A	 0.5898	 0.2300
AA	 0.7413	 0.3980
AB	 0.7227	 0.3880
AC	 0.7384	 0.3910
AD	 0.7334	 0.3860
AE	 0.7270	 0.3780
AF	 0.7356	 0.3910
AG	 0.7491	 0.3920
AH	 0.7406	 0.3950
AI	 0.7470	 0.3990
AJ	 0.7441	 0.3960
AK	 0.7541	 0.3980
AL	 0.7327	 0.3870
B	 0.5894	 0.2220
C	 0.5917	 0.2230
D	 0.6053	 0.2310
E	 0.7475	 0.3760
F	 0.6058	 0.2290
G	 0.6101	 0.2370
H	 0.6180	 0.2470
I	 0.6230	 0.2440
J	 0.6177	 0.2370
K	 0.6104	 0.2370
L	 0.6080	 0.2380



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Chain	Atom inclusion	Q-score
M	0.5991	0.2300
N	0.5917	0.2320
O	0.5902	0.2320
P	0.5923	0.2290
Q	0.8078	0.3950
R	0.7824	0.3740
S	0.7823	0.3700
T	0.7565	0.3730
U	0.7863	0.3760
V	0.7840	0.3770
W	0.7778	0.3920
X	0.7863	0.3790
Y	0.7902	0.3730
Z	0.7655	0.3820
a	0.7886	0.3790
b	0.8082	0.3910
c	0.7818	0.3920
d	0.7976	0.3900
e	0.7947	0.3910
f	0.7677	0.3820
g	0.7858	0.3730
h	0.7896	0.3870
i	0.7615	0.3850
j	0.7993	0.3940
k	0.7970	0.3890
l	0.7582	0.3770
m	0.7891	0.3840
n	0.7772	0.3660
o	0.7434	0.3990
p	0.7249	0.3840
q	0.7220	0.3790
r	0.7320	0.3840
s	0.7277	0.3830
t	0.7384	0.3980
u	0.7491	0.3980
v	0.7313	0.3880
w	0.7249	0.3800
x	0.7242	0.3770
y	0.7413	0.3880
z	0.7505	0.4020