Full wwPDB EM Validation 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 Full wwPDB EM Validation 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:

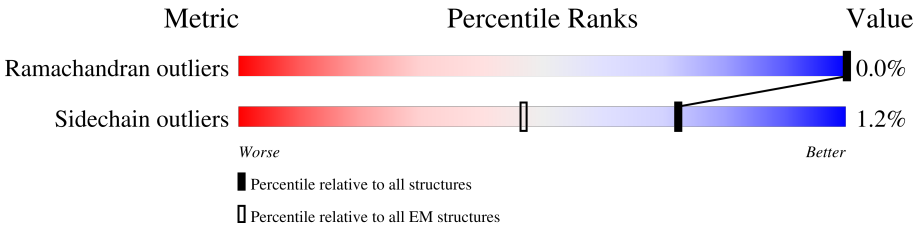
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 <=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	12% 72% · 27%
1	AB	252	10% 72% · 27%
1	AC	252	12% 73% 27%
1	AD	252	12% 73% 27%
1	AE	252	9% 71% · 27%
1	AF	252	11% 72% · 27%
1	AG	252	11% 72% · 27%
1	AH	252	12% 73% 27%
1	AI	252	12% 72% · 27%

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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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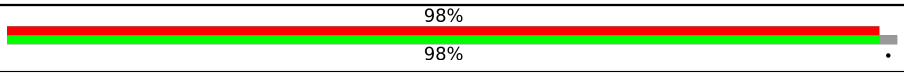
Mol	Chain	Length	Quality of chain
8	BV	80	

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

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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 Protein PrgH.

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

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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 405	C 276	N 61	O 67	S 1	0	0
6	7	84	Total 644	C 436	N 97	O 109	S 2	0	0
6	8	84	Total 644	C 436	N 97	O 109	S 2	0	0
6	9	84	Total 647	C 438	N 97	O 109	S 3	0	0

- Molecule 7 is a protein called Protein PrgJ.

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

- Molecule 8 is a protein called Protein PrgI.

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

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

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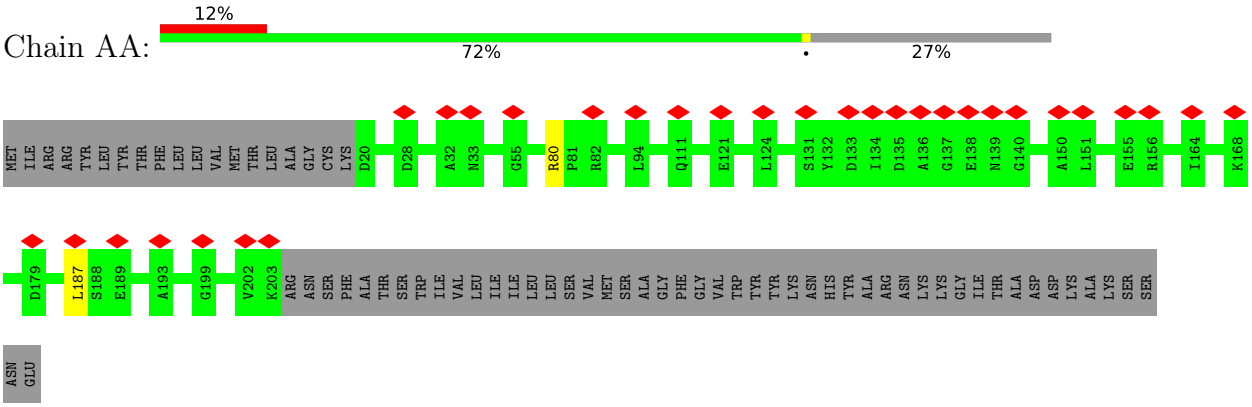
Mol	Chain	Residues	Atoms				AltConf	Trace
8	BR	78	Total	C	N	O	0	0
			612	387	101	124		

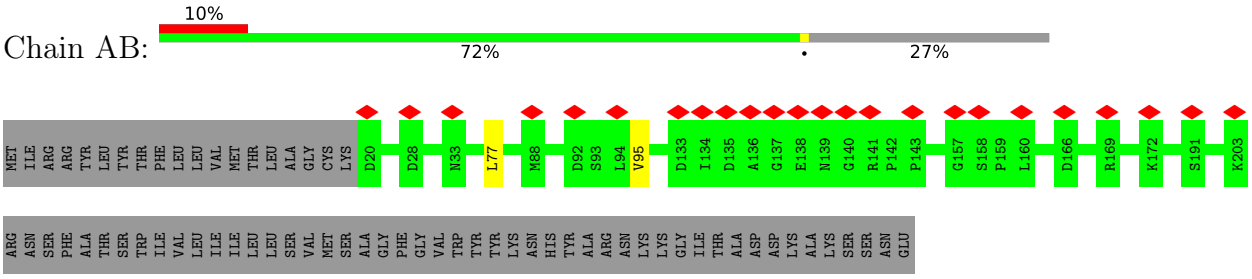
3 Residue-property plots (i)

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.

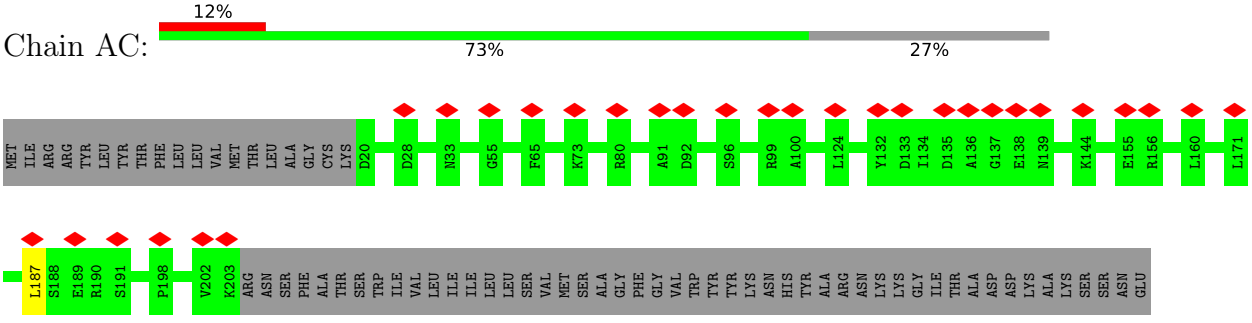
• Molecule 1: Lipoprotein PrgK



• Molecule 1: Lipoprotein PrgK

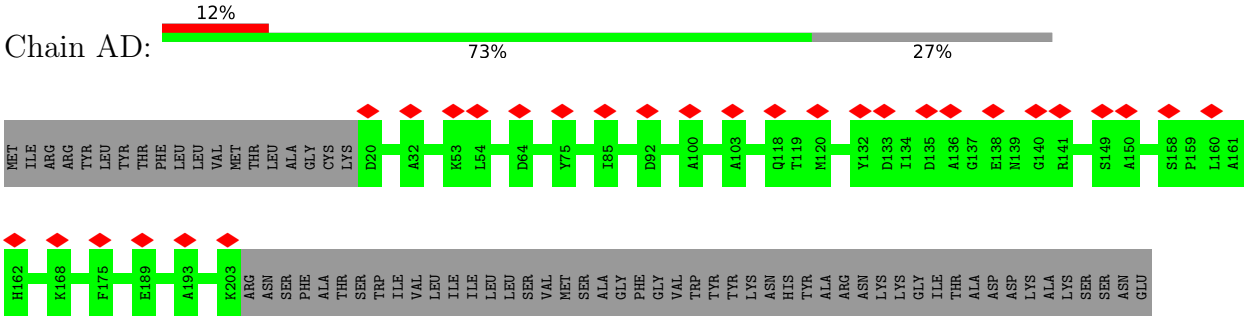


• Molecule 1: Lipoprotein PrgK



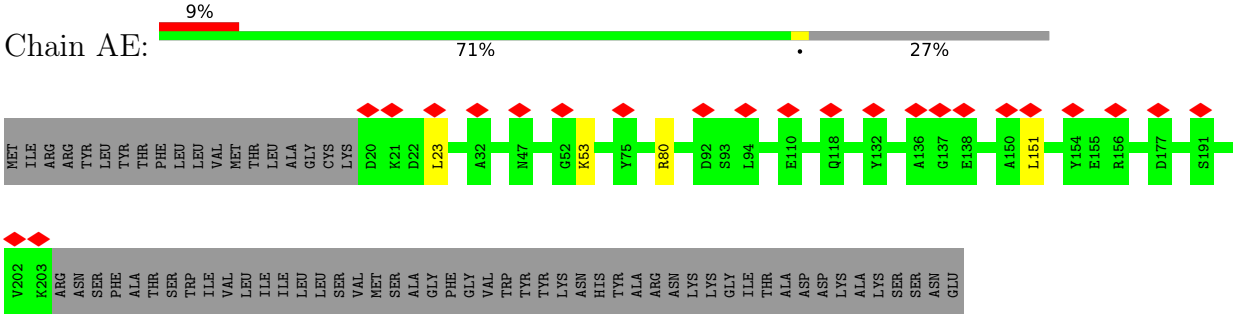
• Molecule 1: Lipoprotein PrgK

Chain AD:



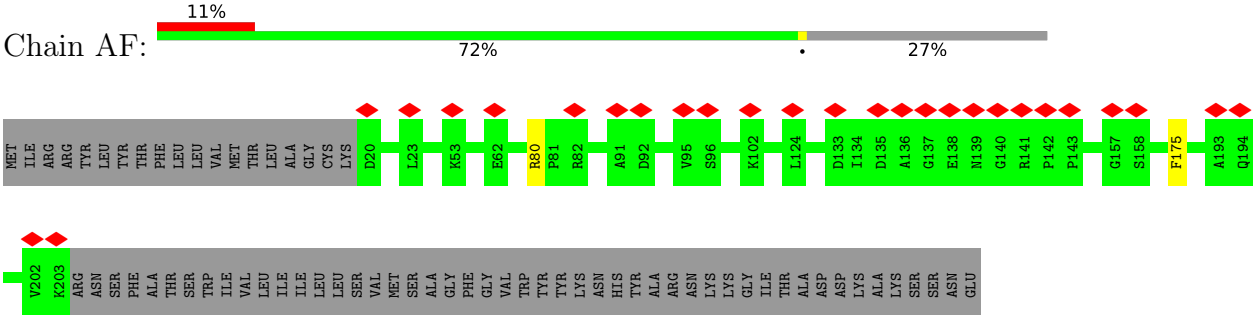
• Molecule 1: Lipoprotein PrgK

Chain AE:



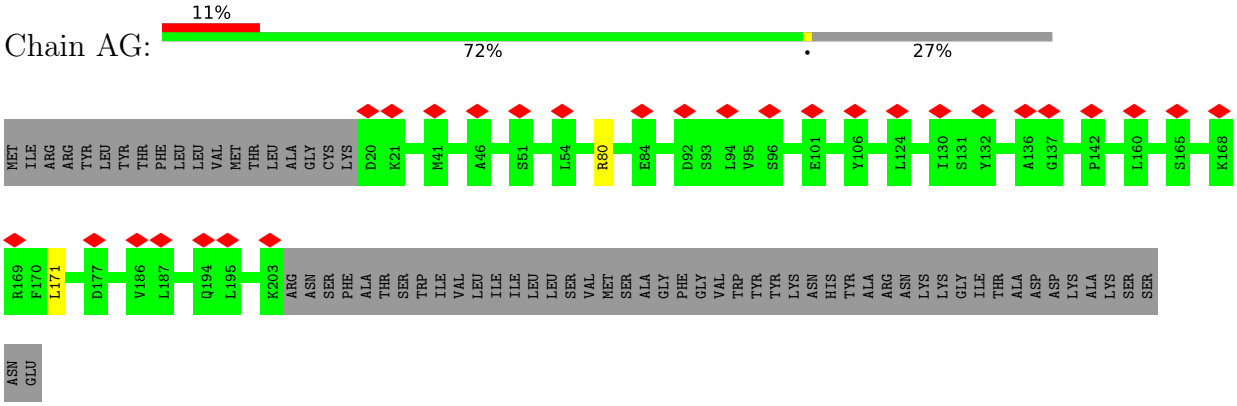
• Molecule 1: Lipoprotein PrgK

Chain AF:



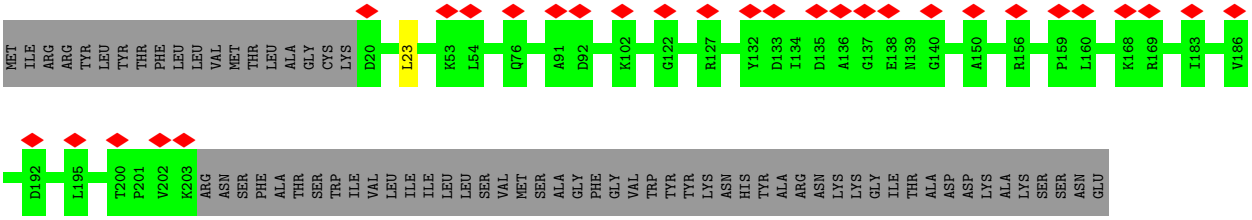
• Molecule 1: Lipoprotein PrgK

Chain AG:



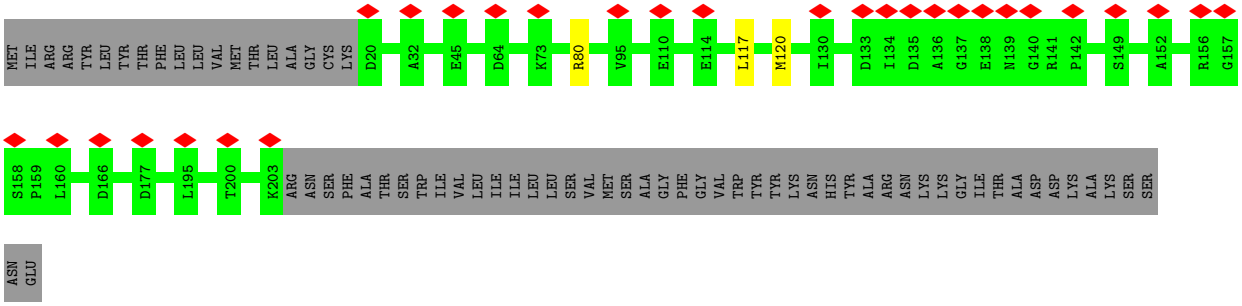
• Molecule 1: Lipoprotein PrgK

Chain AH:



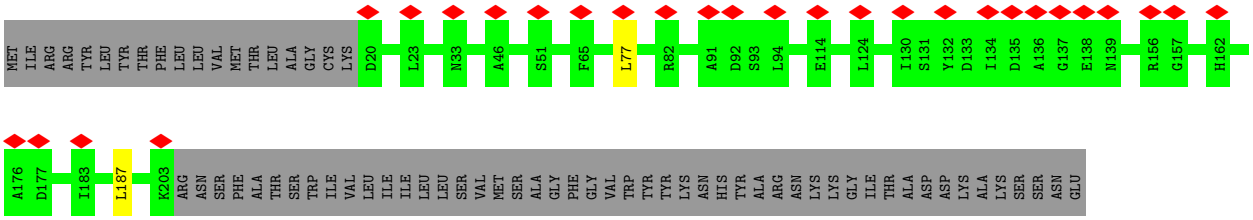
• Molecule 1: Lipoprotein PrgK

Chain AI:



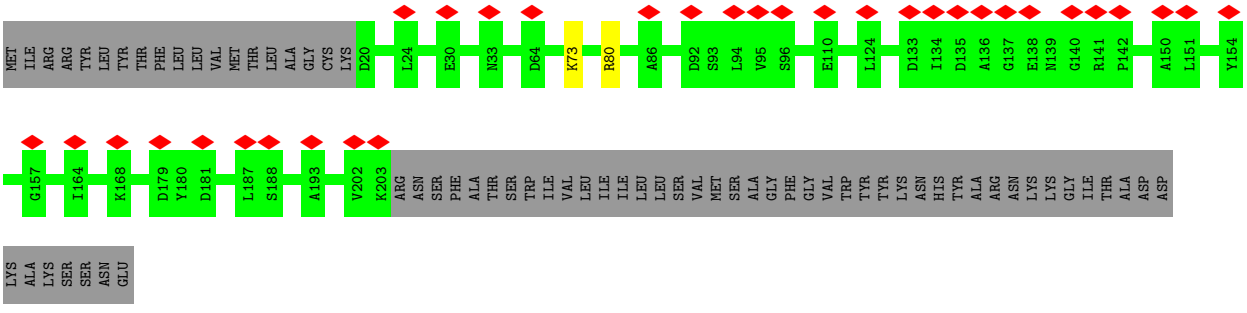
• Molecule 1: Lipoprotein PrgK

Chain AL:



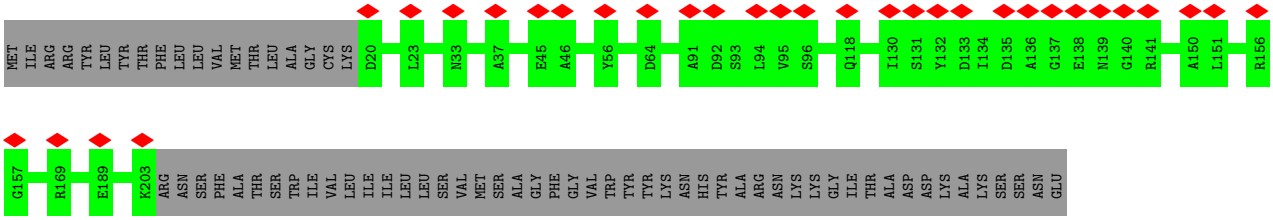
• Molecule 1: Lipoprotein PrgK

Chain o:



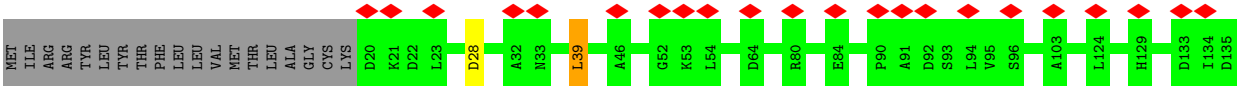
• Molecule 1: Lipoprotein PrgK

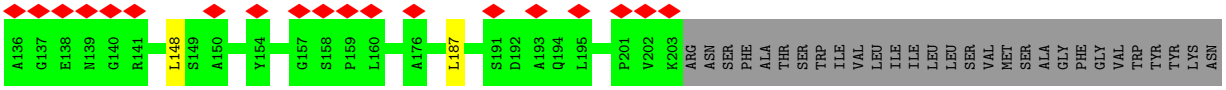
Chain p:



• Molecule 1: Lipoprotein PrgK

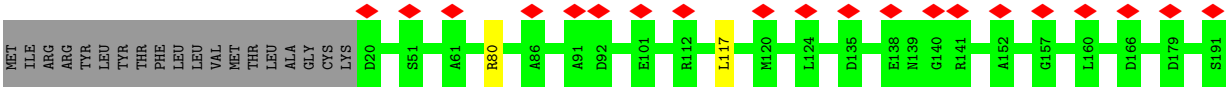
Chain q:

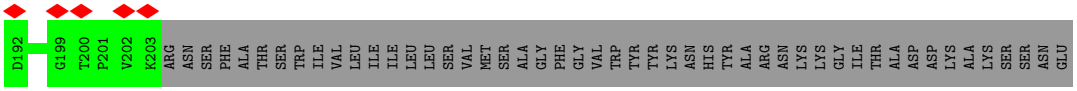




• Molecule 1: Lipoprotein PrgK

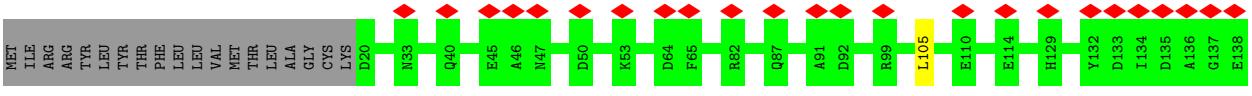
Chain r:

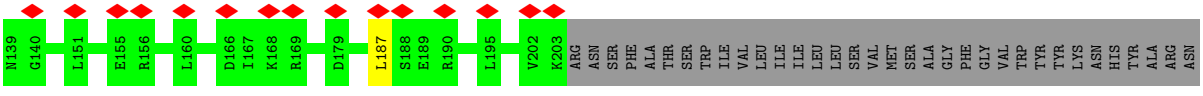


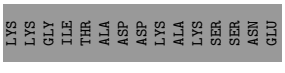


• Molecule 1: Lipoprotein PrgK

Chain s:

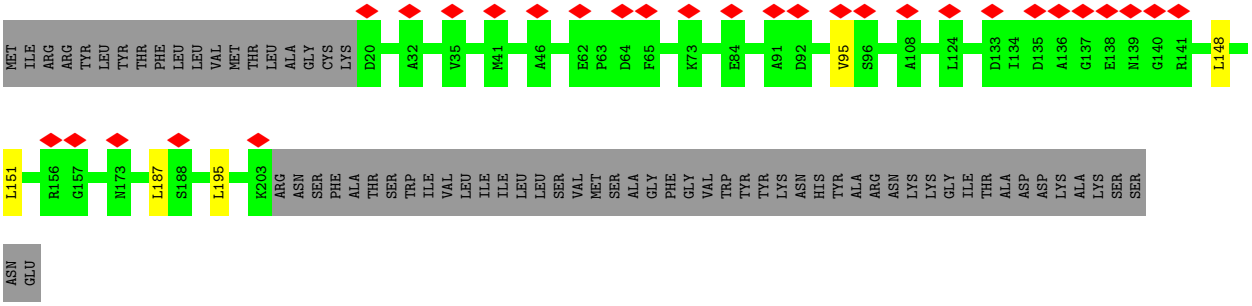






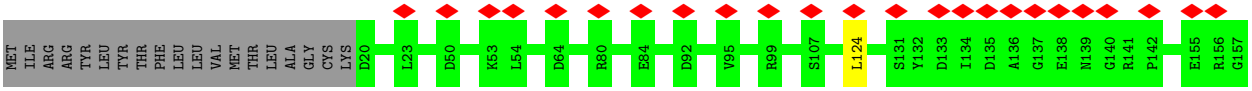
• Molecule 1: Lipoprotein PrgK

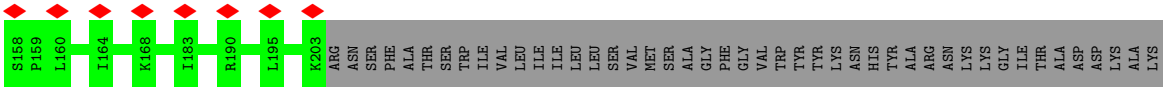
Chain t:



• Molecule 1: Lipoprotein PrgK

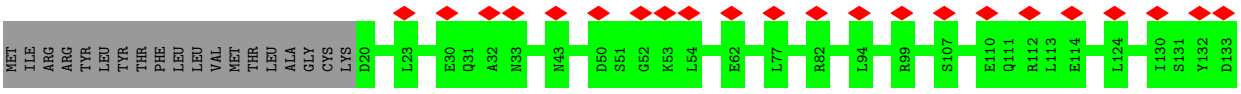
Chain u:

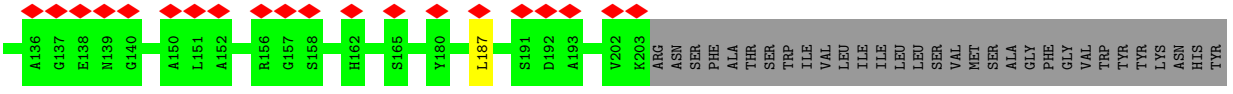




• Molecule 1: Lipoprotein PrgK

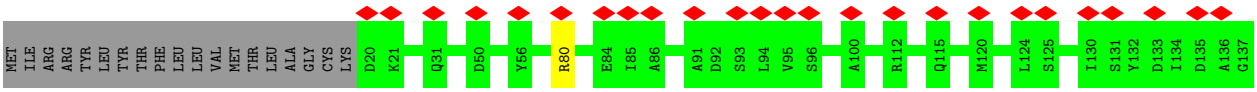
Chain v:

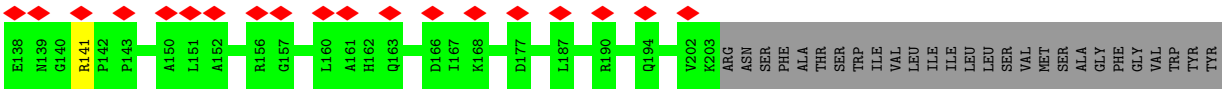


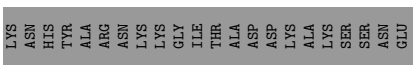


• Molecule 1: Lipoprotein PrgK

Chain w:

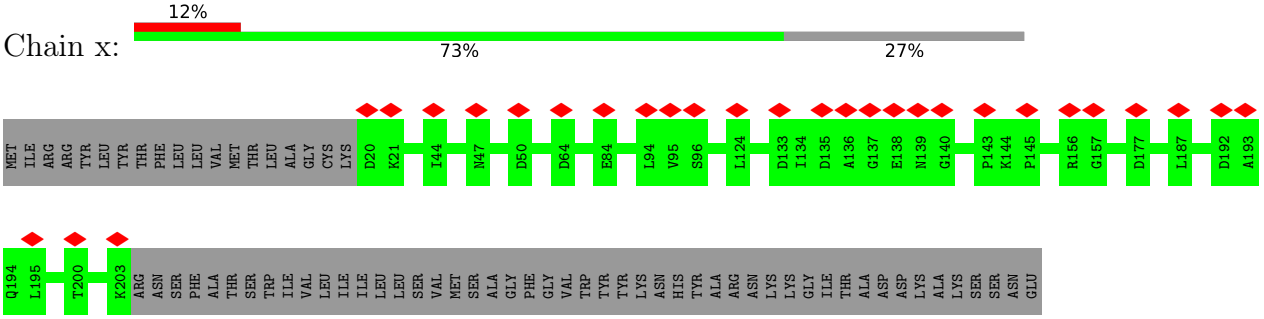






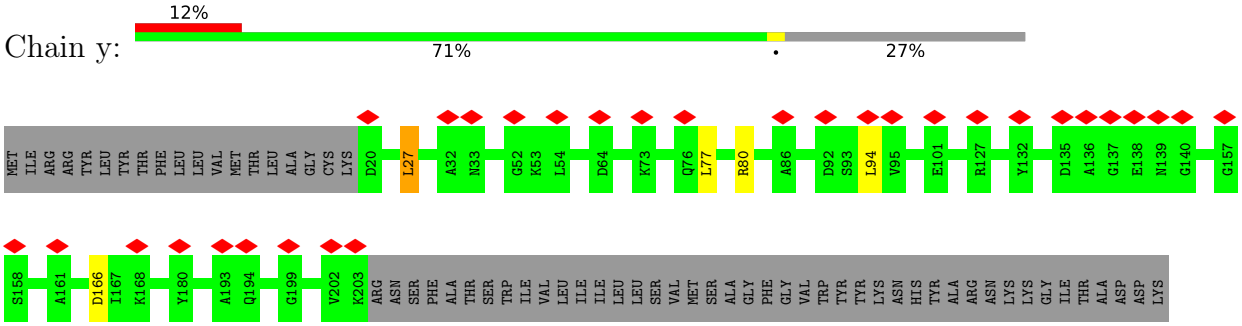
• Molecule 1: Lipoprotein PrgK

Chain x:



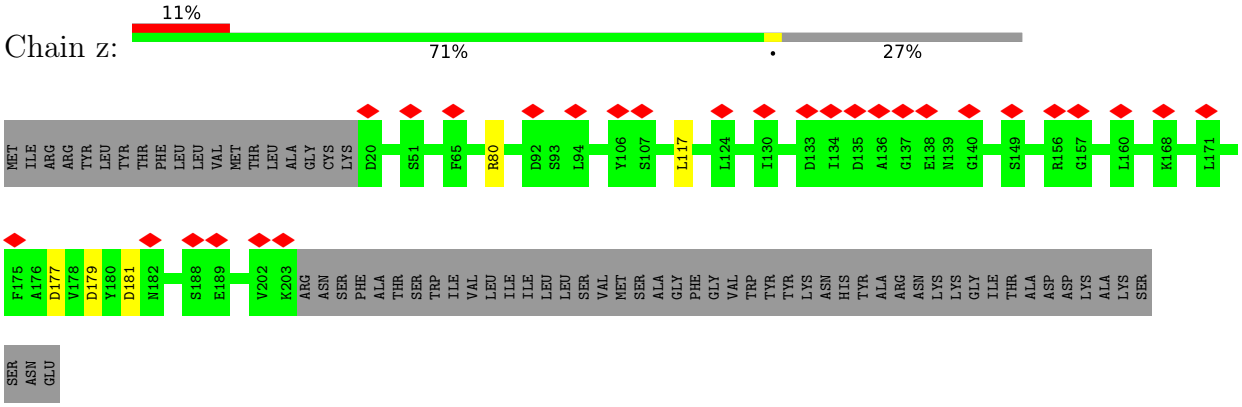
• Molecule 1: Lipoprotein PrgK

Chain y:



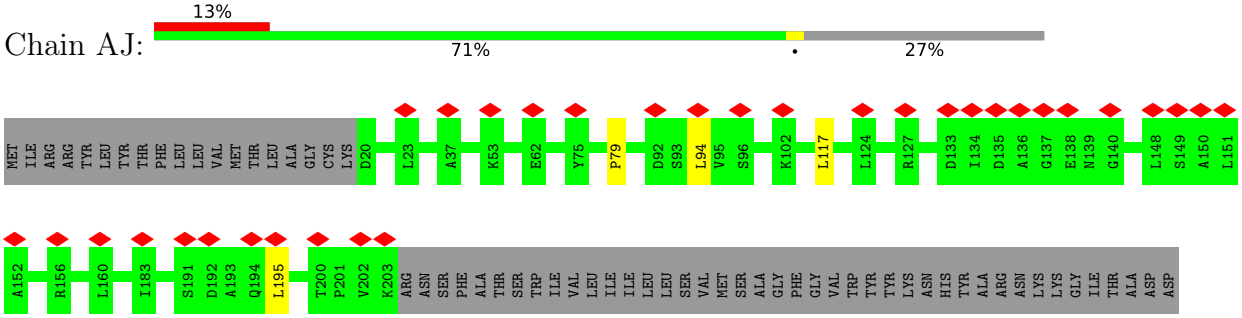
• Molecule 1: Lipoprotein PrgK

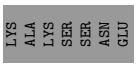
Chain z:



• Molecule 1: Lipoprotein PrgK

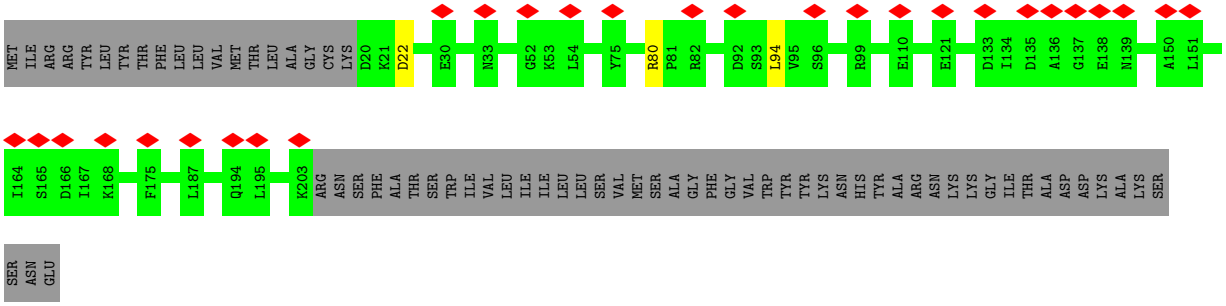
Chain AJ:





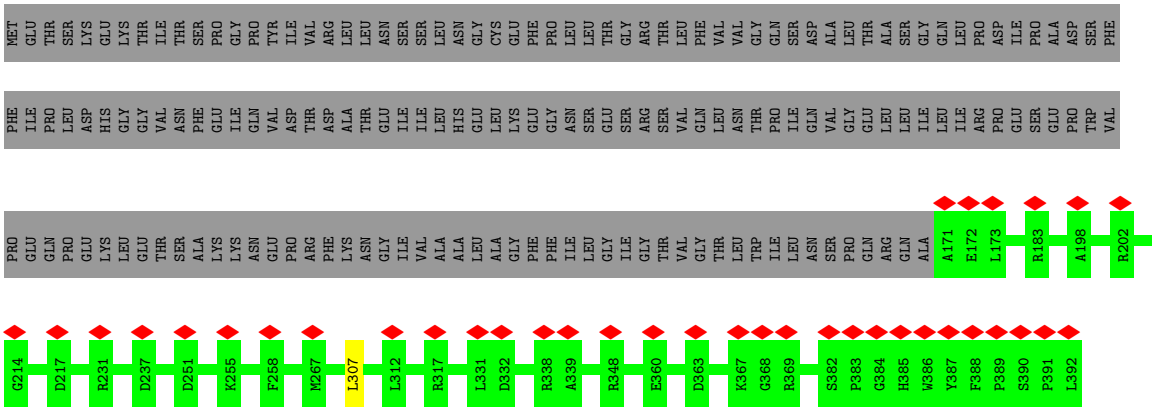
• Molecule 1: Lipoprotein PrgK

Chain AK:



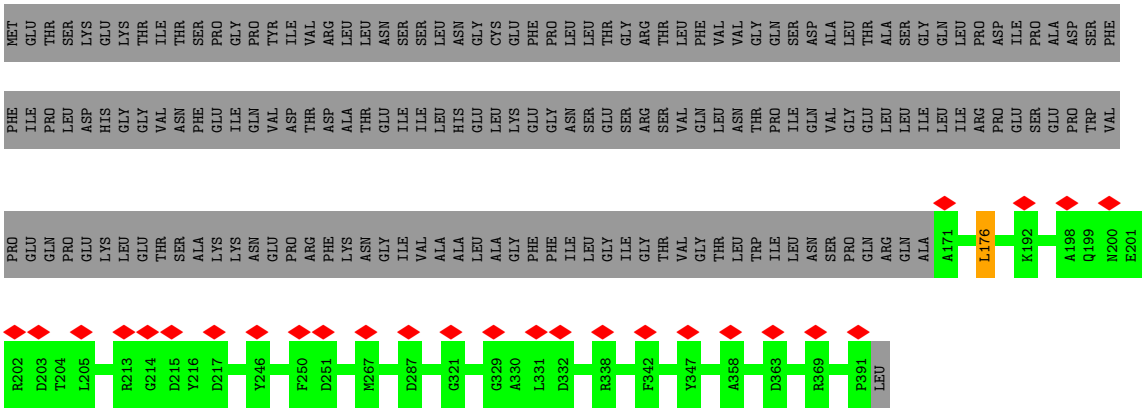
• Molecule 2: Protein PrgH

Chain E:



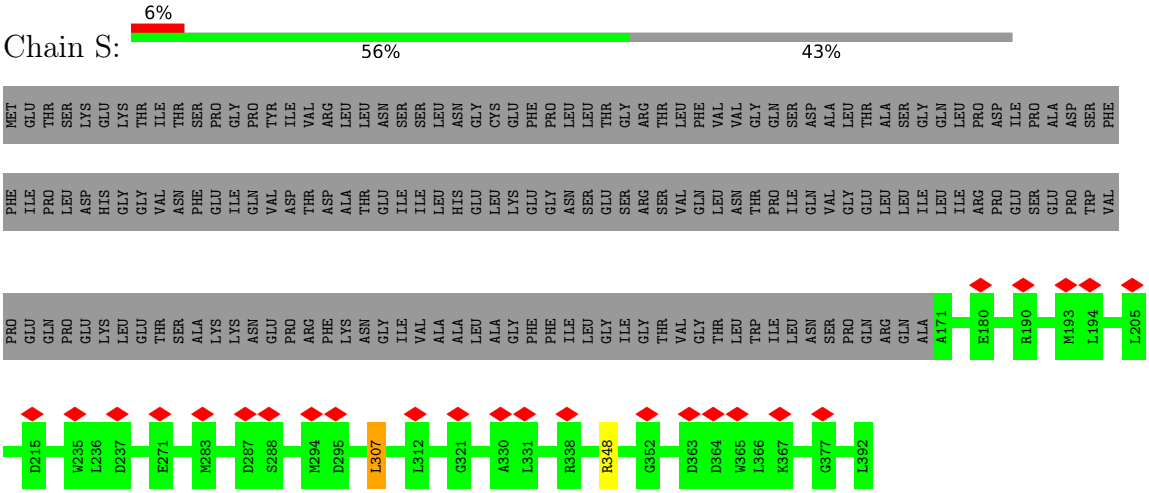
• Molecule 2: Protein PrgH

Chain R:



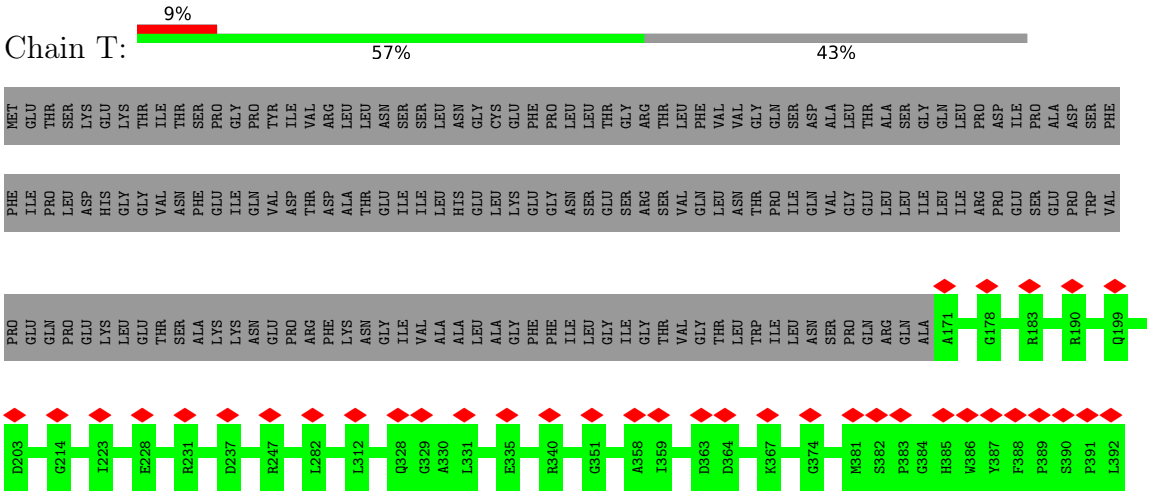
• Molecule 2: Protein PrgH

Chain S:



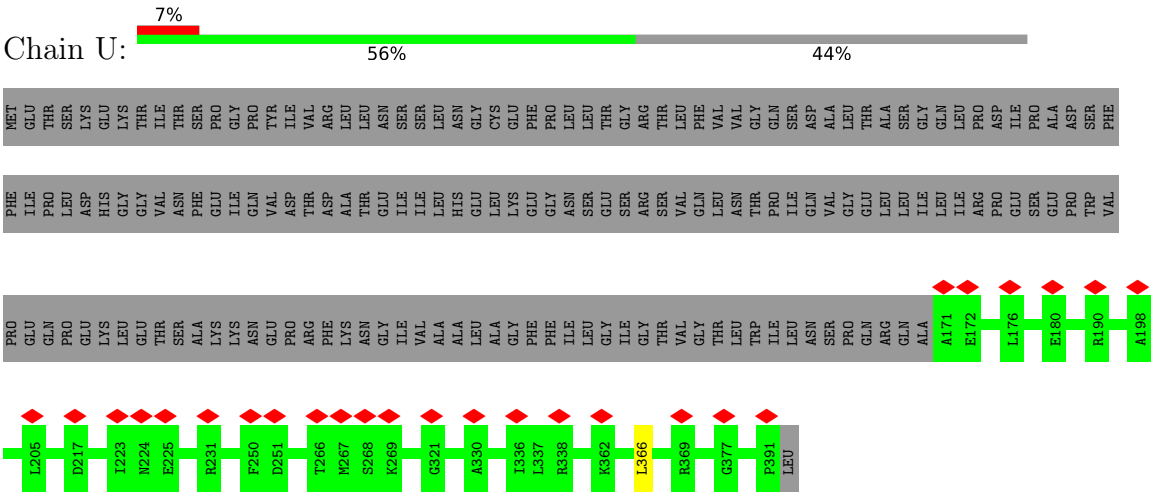
• Molecule 2: Protein PrgH

Chain T:



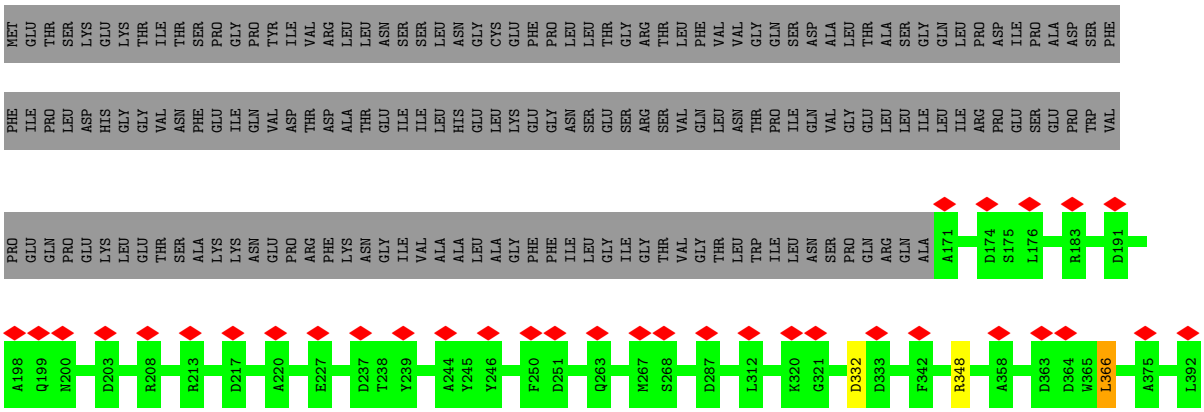
• Molecule 2: Protein PrgH

Chain U:

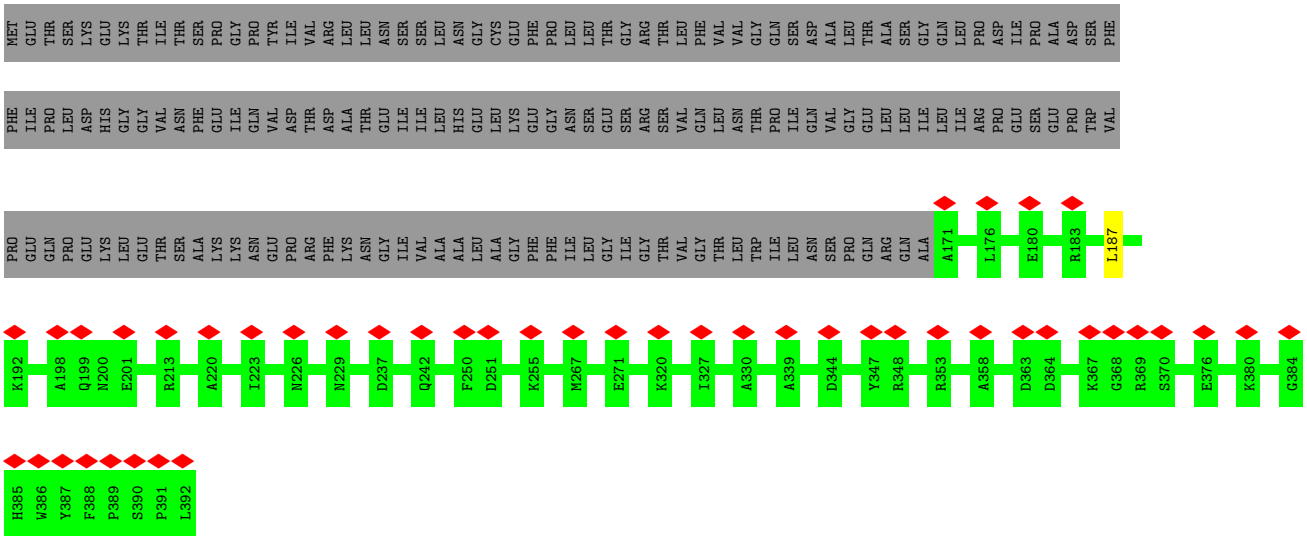


• Molecule 2: Protein PrgH

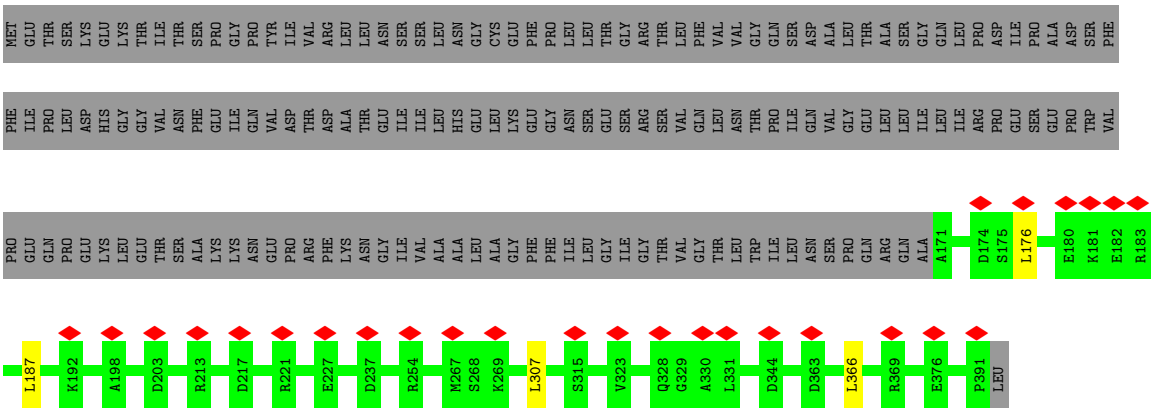
Chain V:



• Molecule 2: Protein PrgH

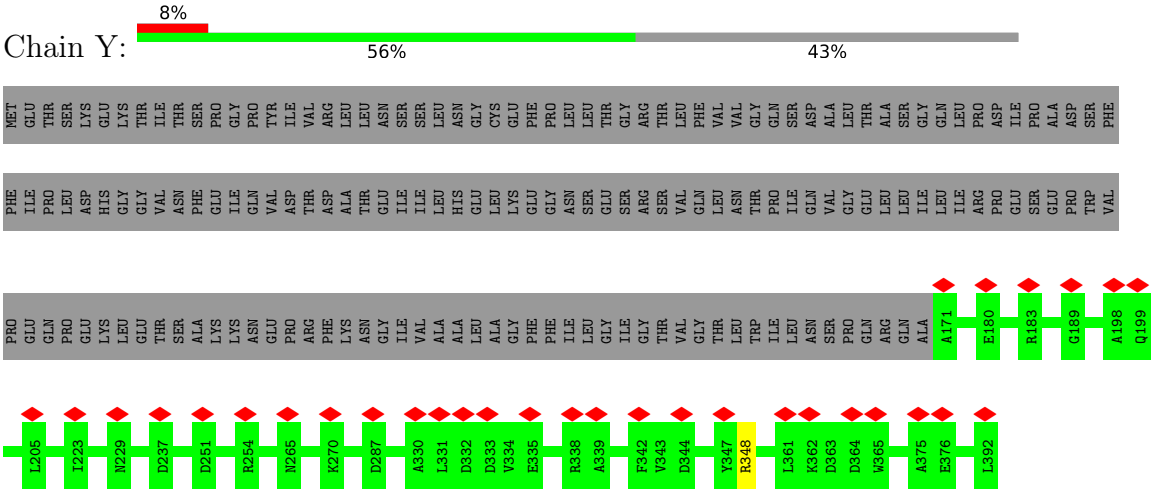


• Molecule 2: Protein PrgH



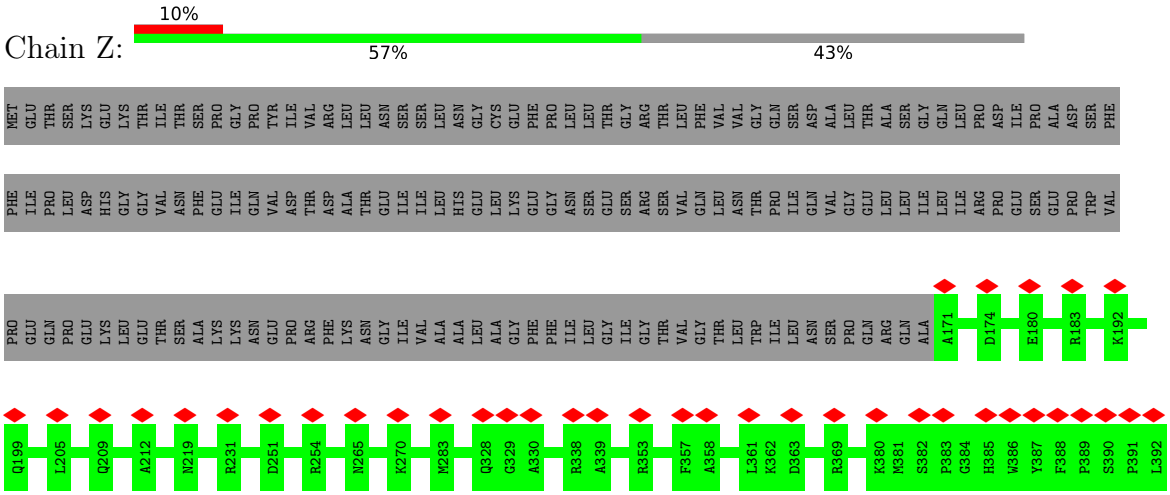
• Molecule 2: Protein PrgH

Chain Y:



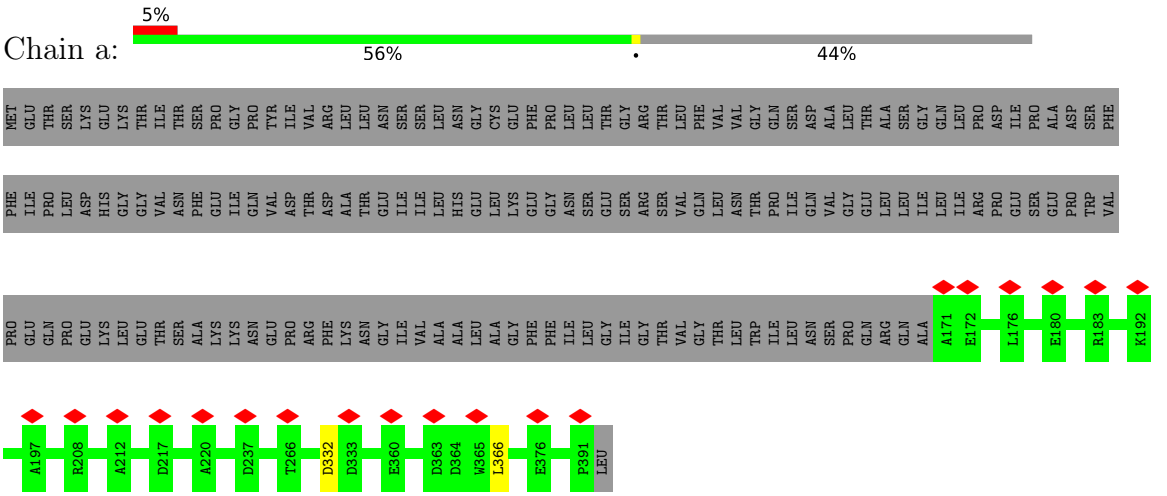
• Molecule 2: Protein PrgH

Chain Z:



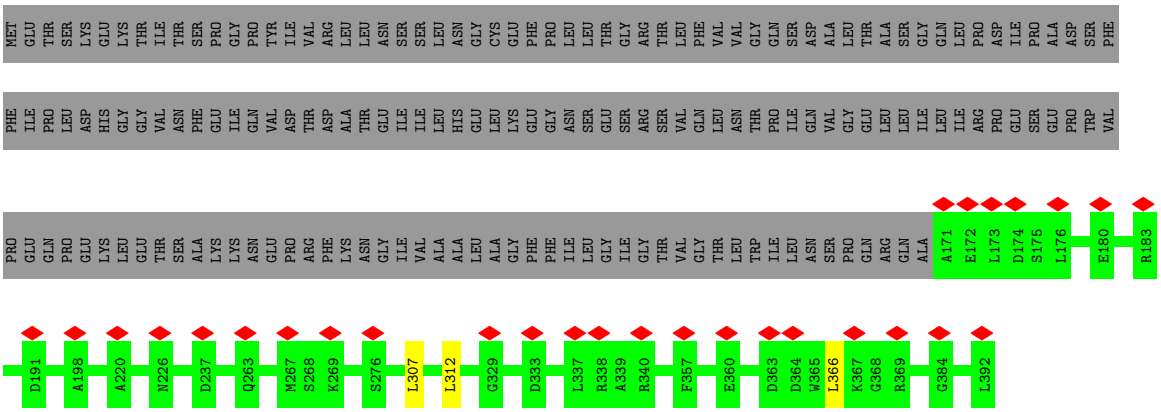
• Molecule 2: Protein PrgH

Chain a:

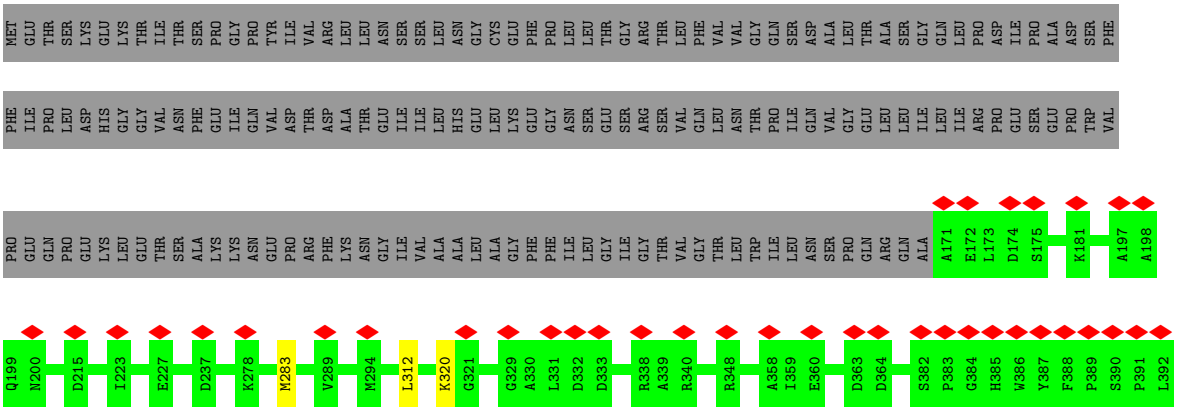


• Molecule 2: Protein PrgH

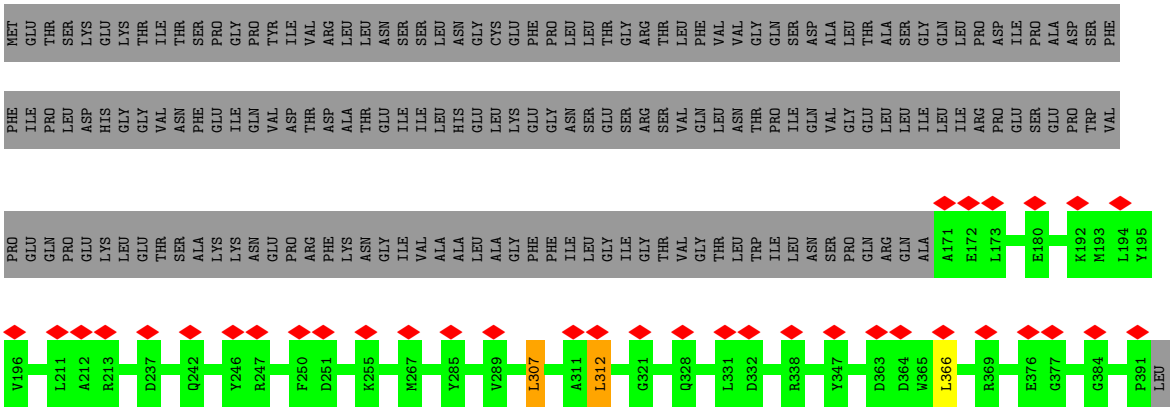
Chain b:



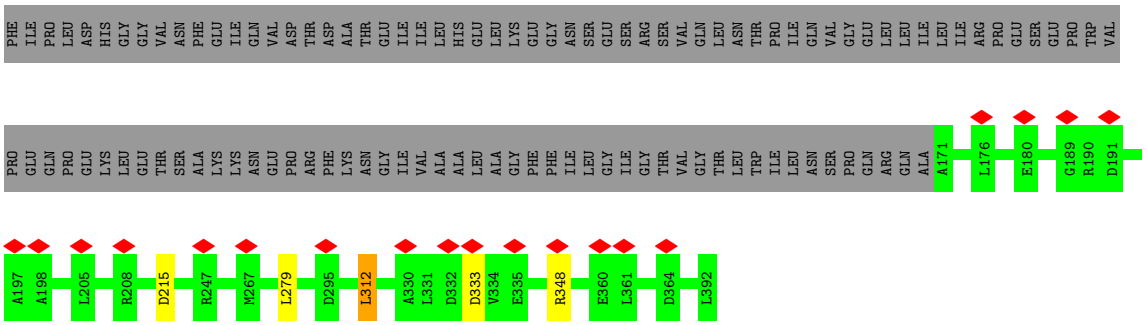
• Molecule 2: Protein PrgH



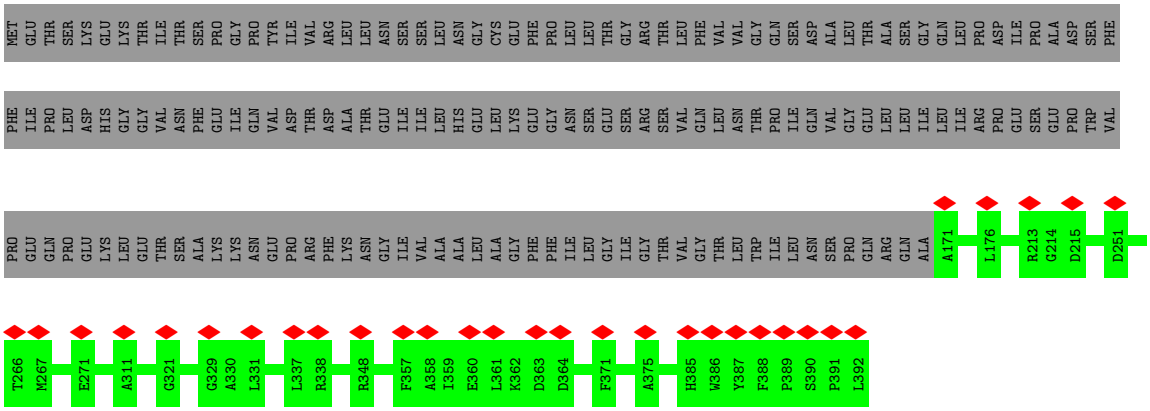
• Molecule 2: Protein PrgH



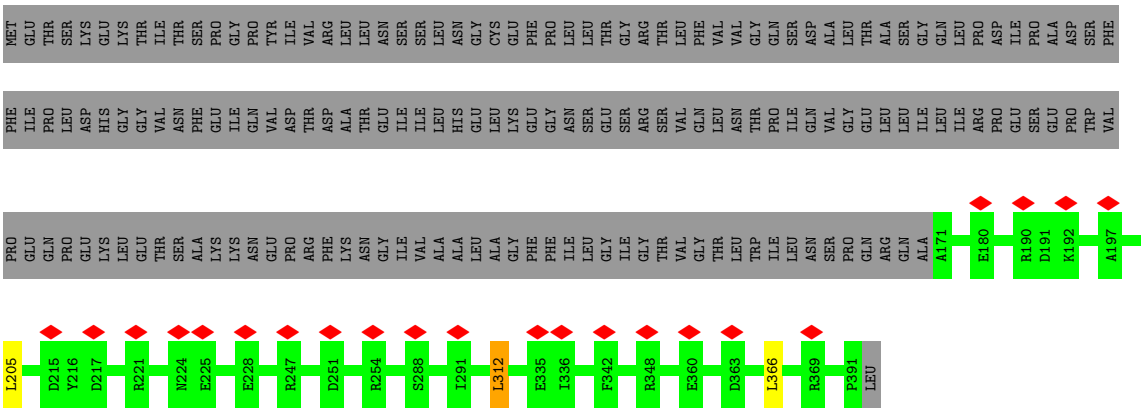
• Molecule 2: Protein PrgH



• Molecule 2: Protein PrgH



• Molecule 2: Protein PrgH



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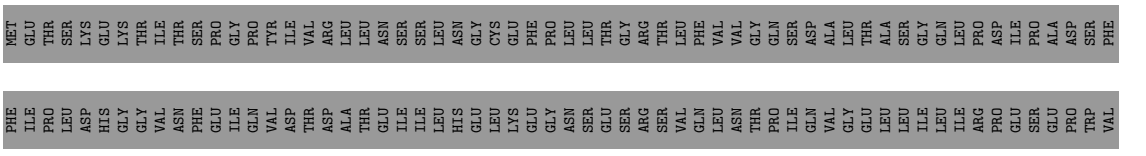
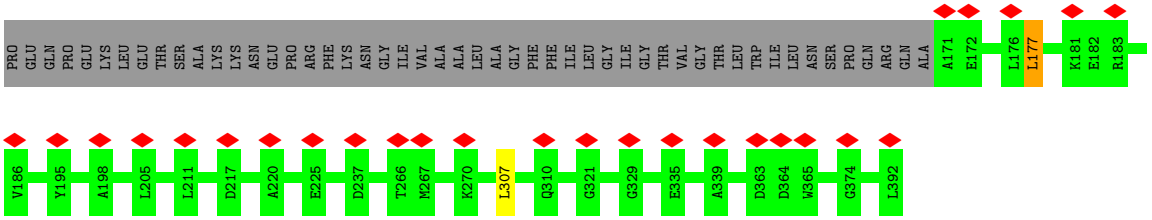
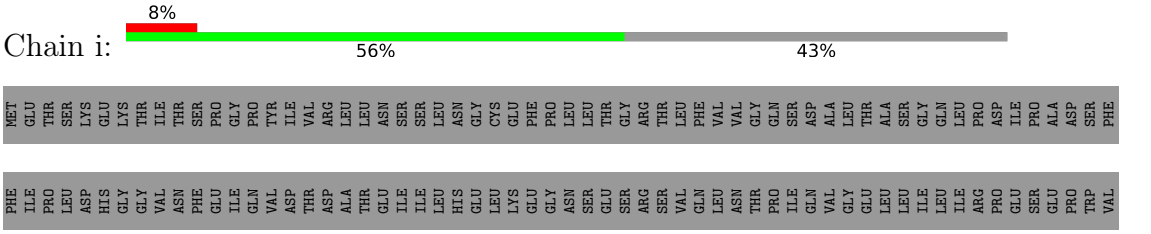
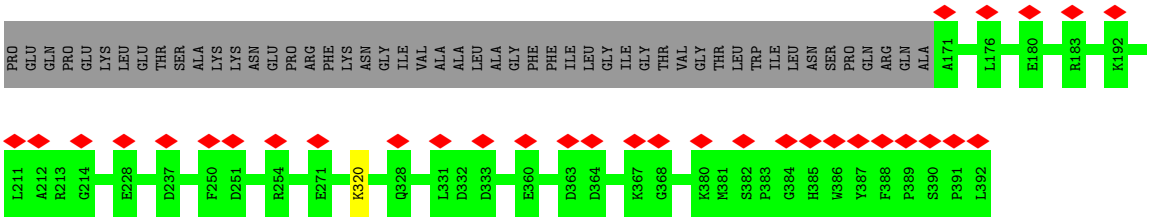


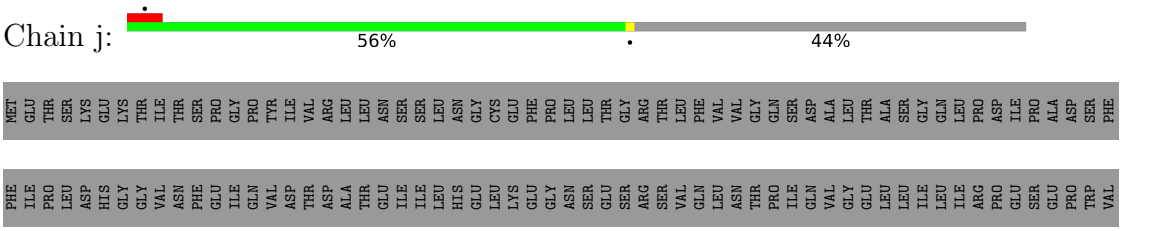


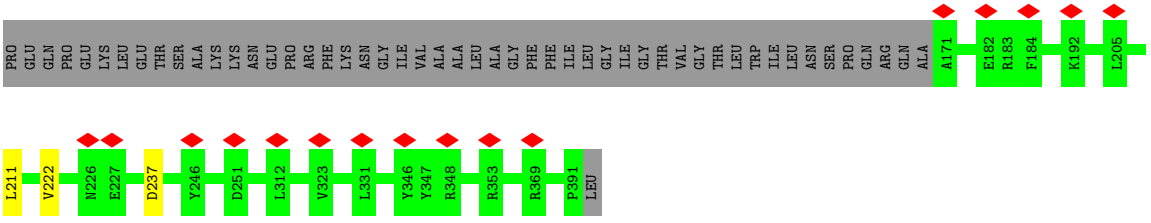
• Molecule 2: Protein PrgH



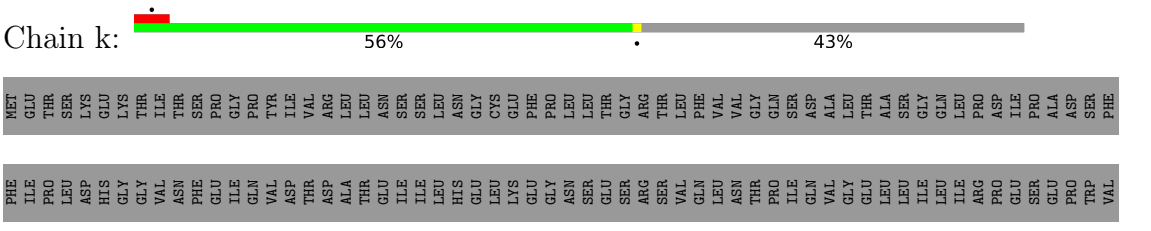


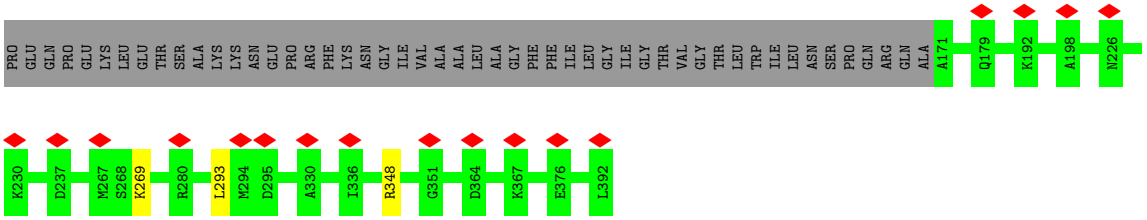
• Molecule 2: Protein PrgH



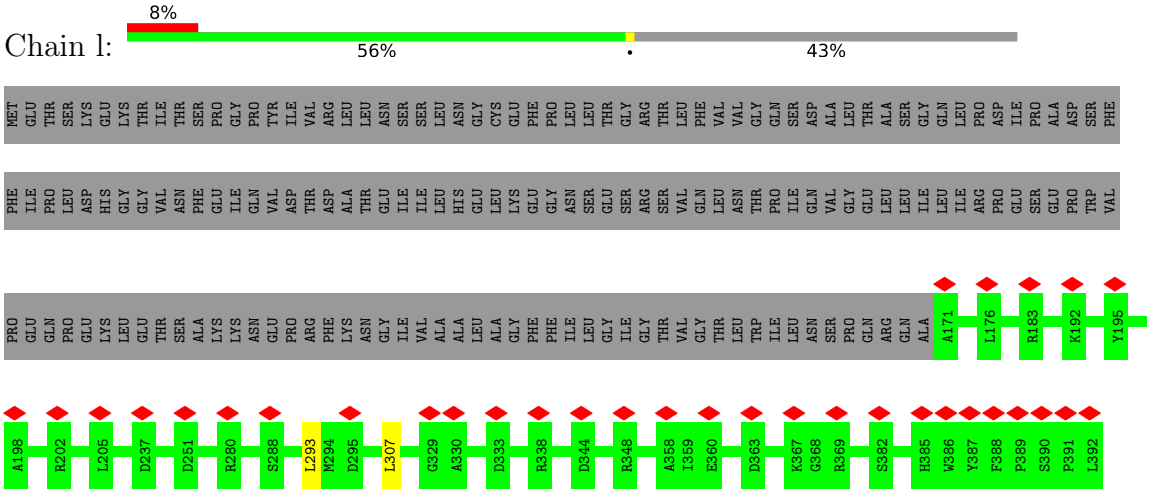


• Molecule 2: Protein PrgH

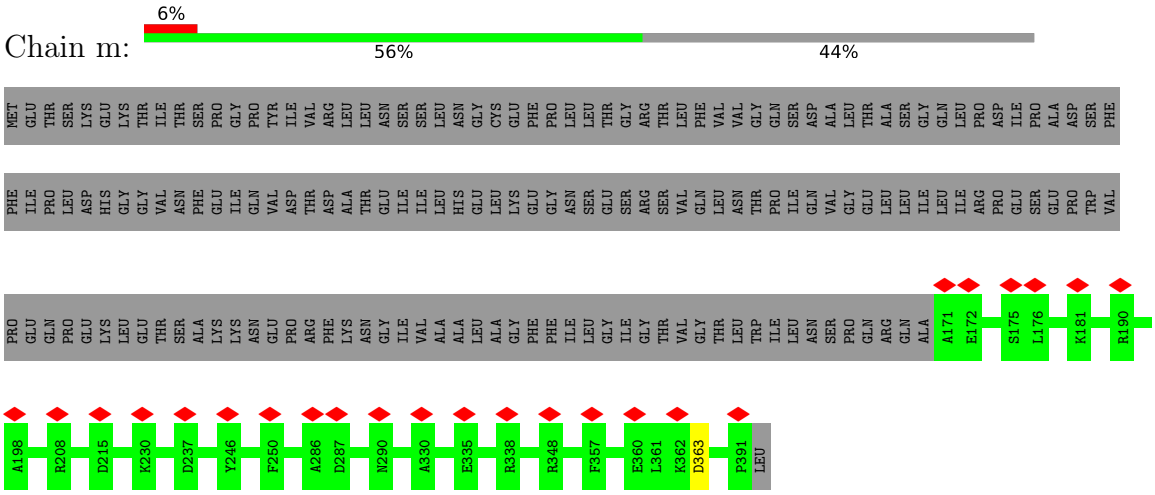




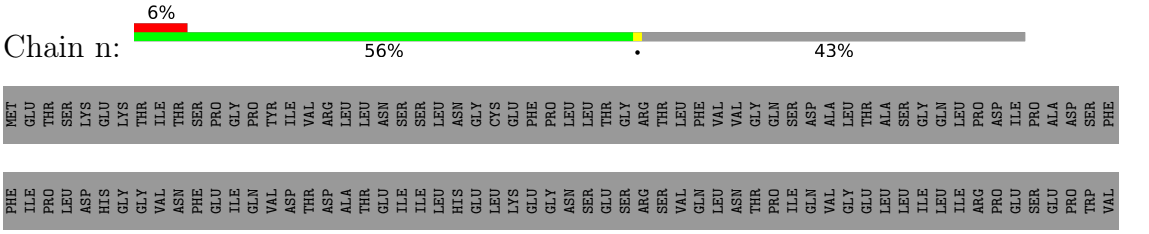
• Molecule 2: Protein PrgH

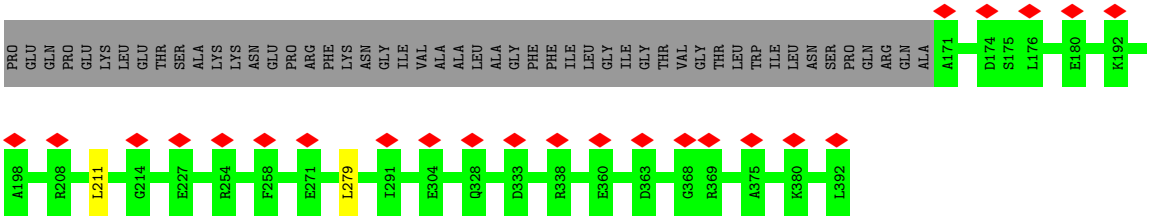


• Molecule 2: Protein PrgH

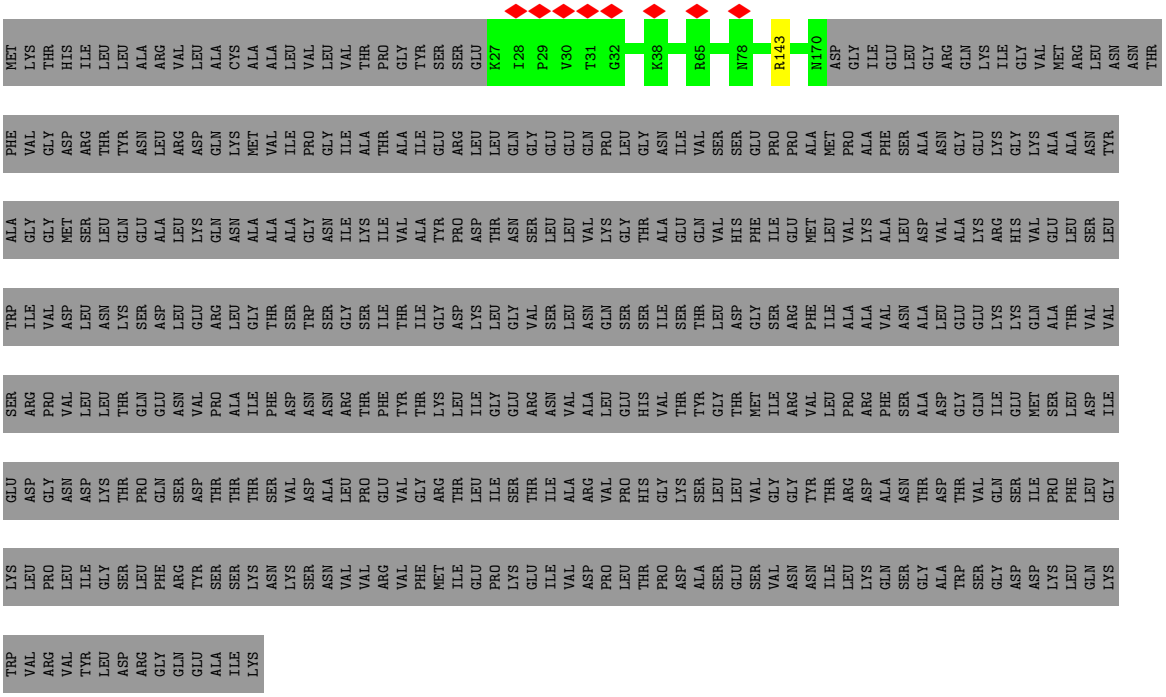


• Molecule 2: Protein PrgH

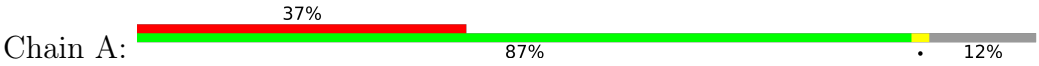


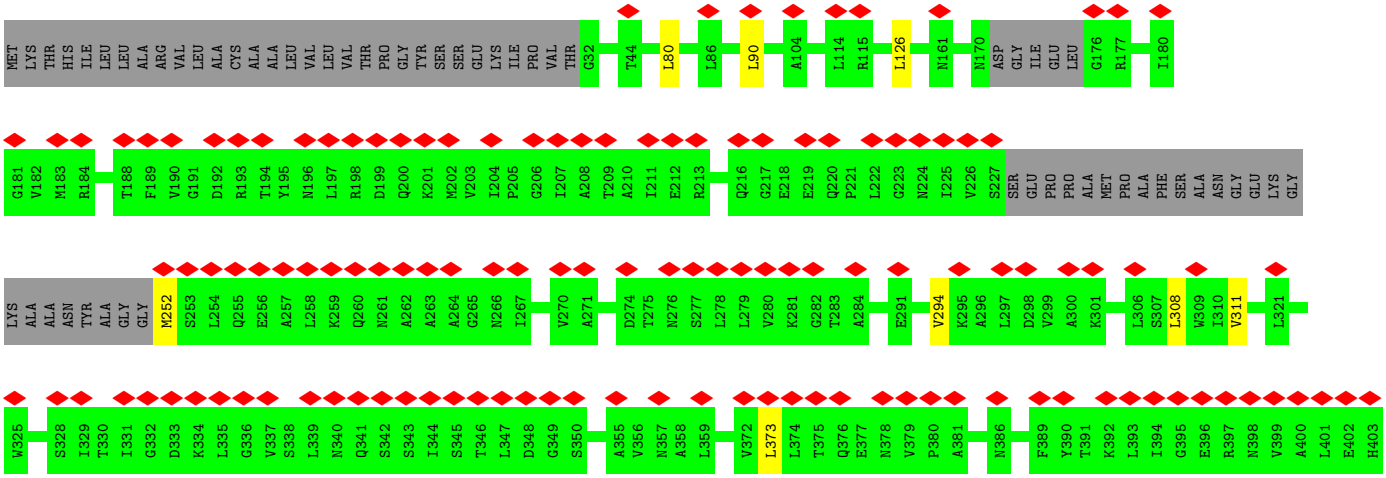


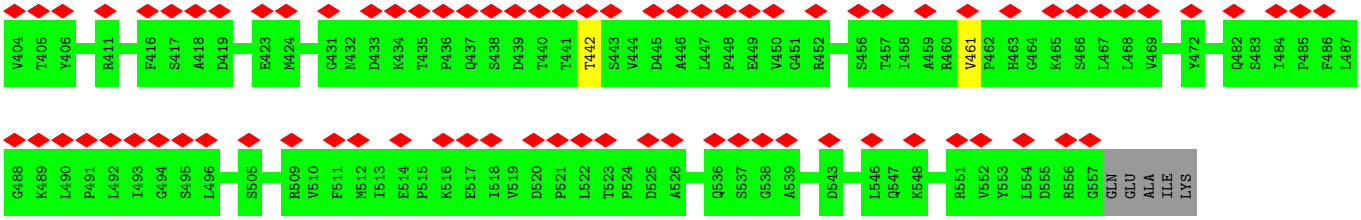
• Molecule 3: Protein InvG



• Molecule 3: Protein InvG

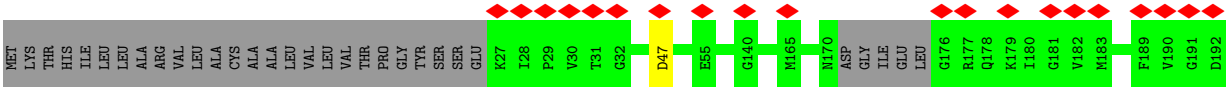






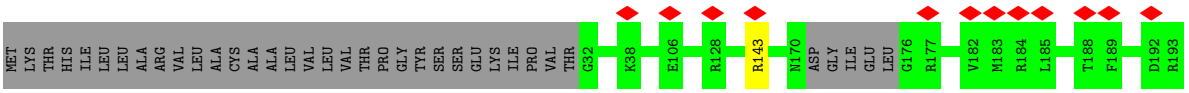
• Molecule 3: Protein InvG

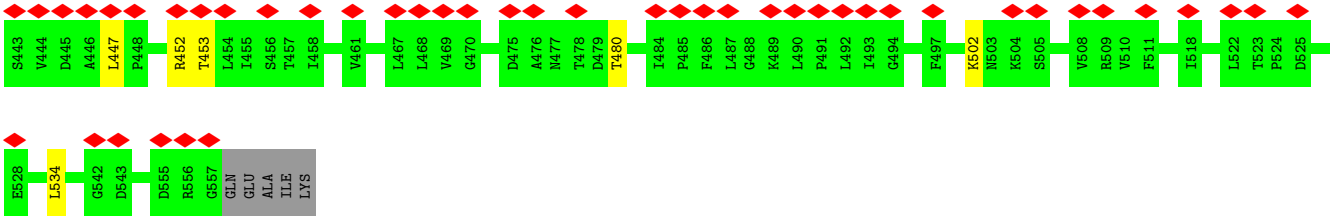
Chain B:



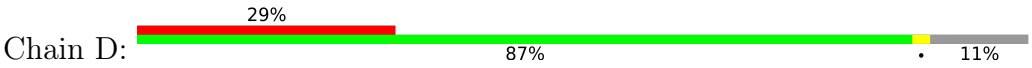
• Molecule 3: Protein InvG

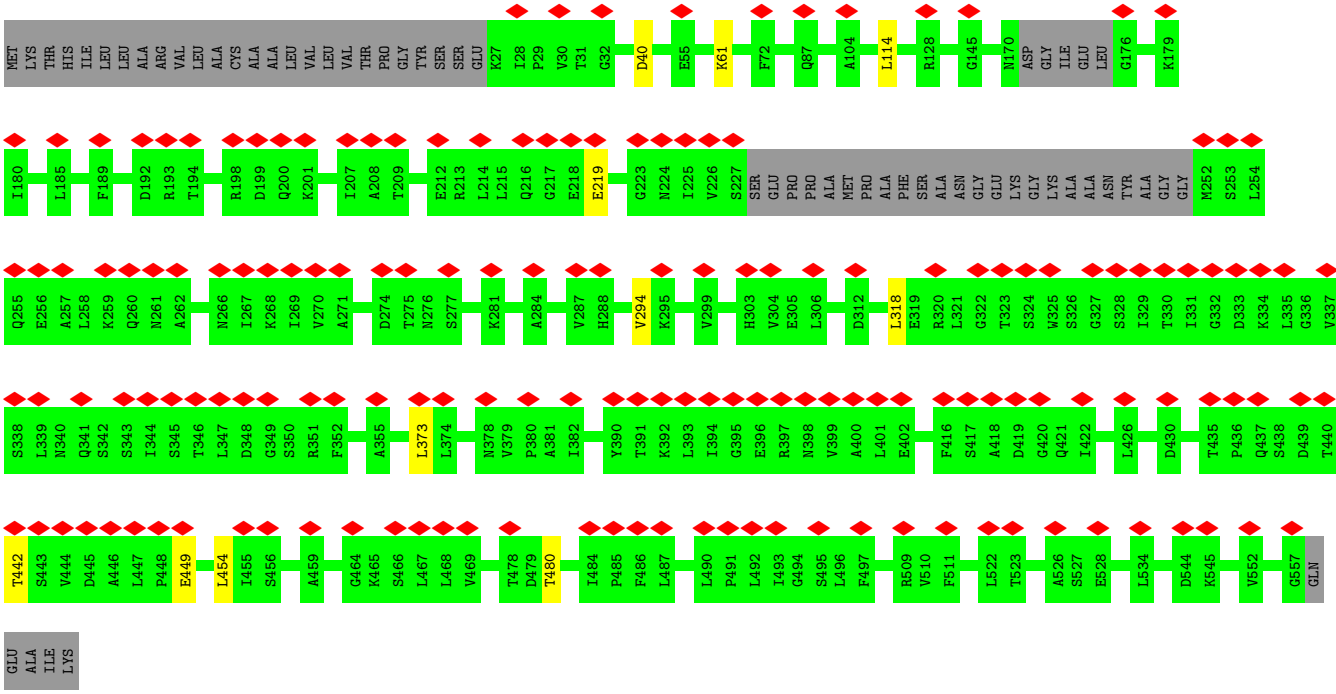
Chain C:



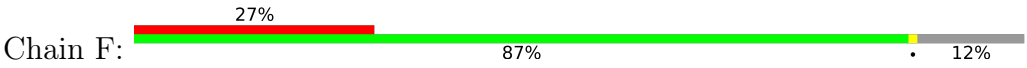


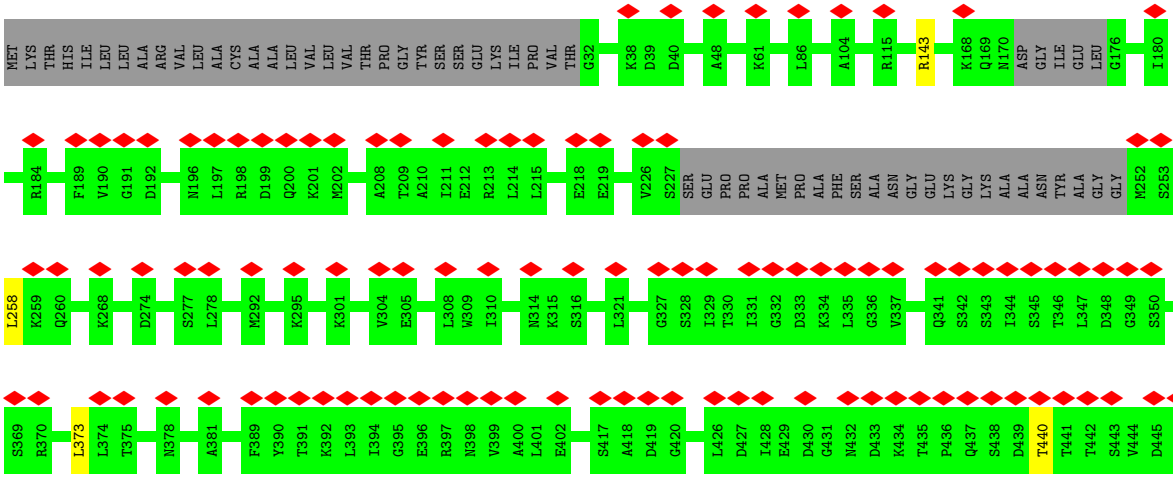
• Molecule 3: Protein InvG

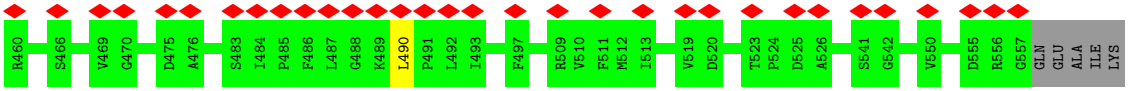




• Molecule 3: Protein InvG

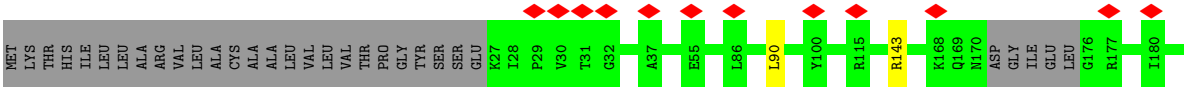


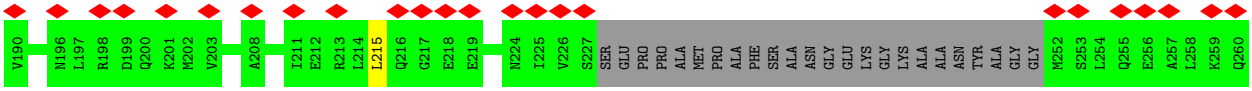


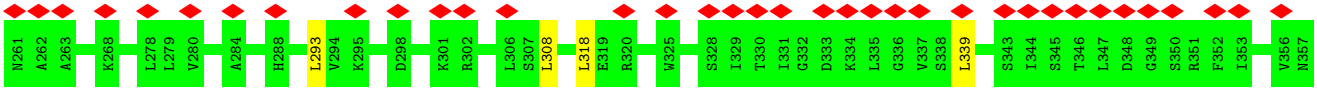


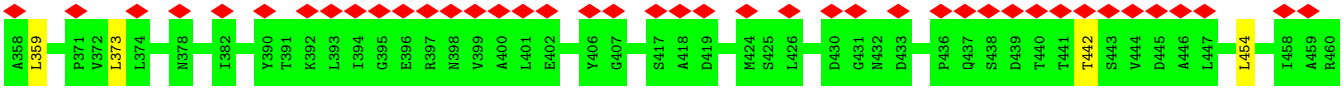
• Molecule 3: Protein InvG

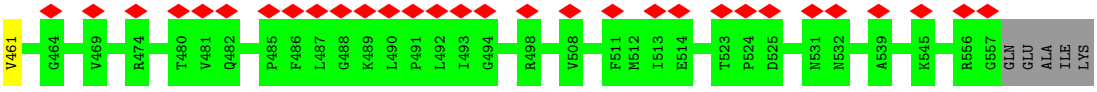
Chain G:





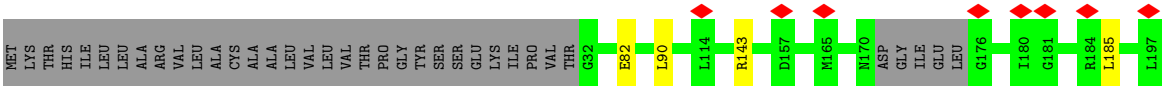


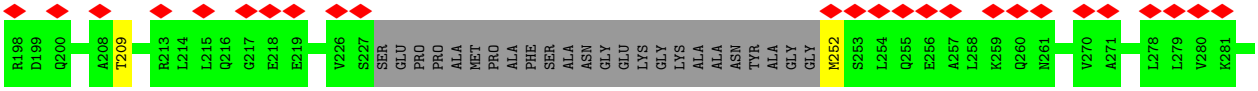


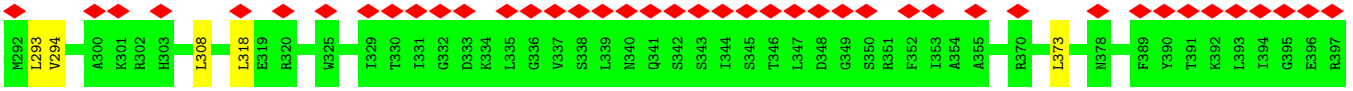


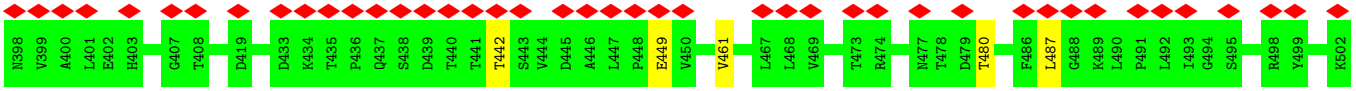
• Molecule 3: Protein InvG

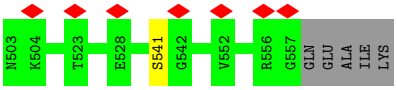
Chain H:





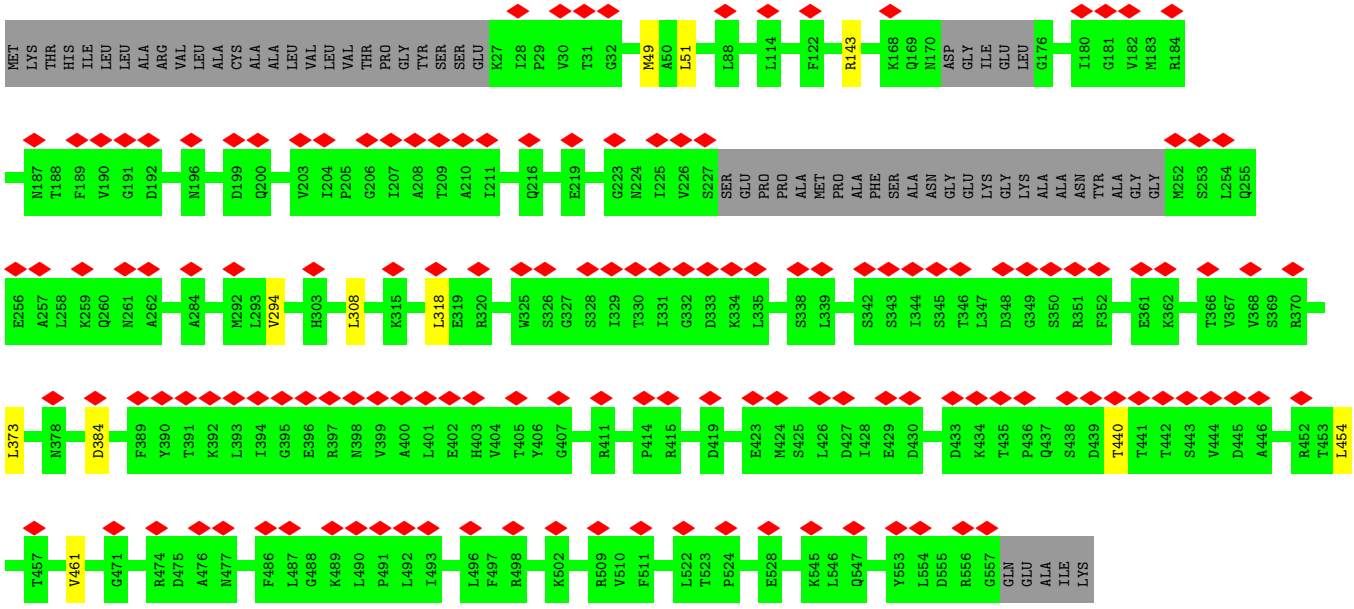






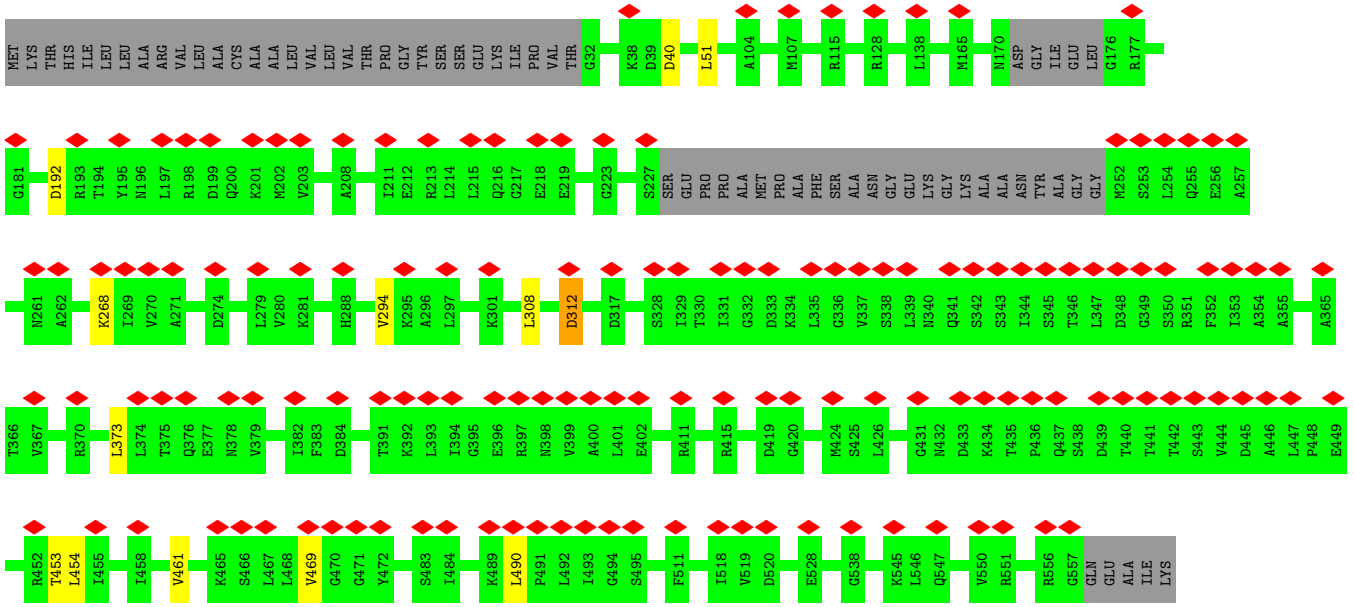
• Molecule 3: Protein InvG

Chain I:



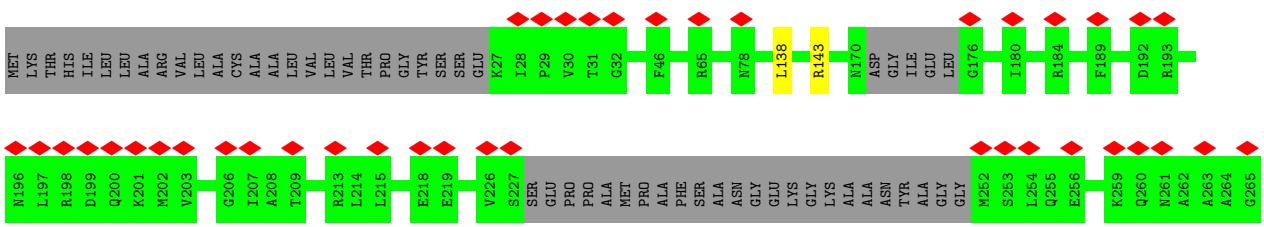
• Molecule 3: Protein InvG

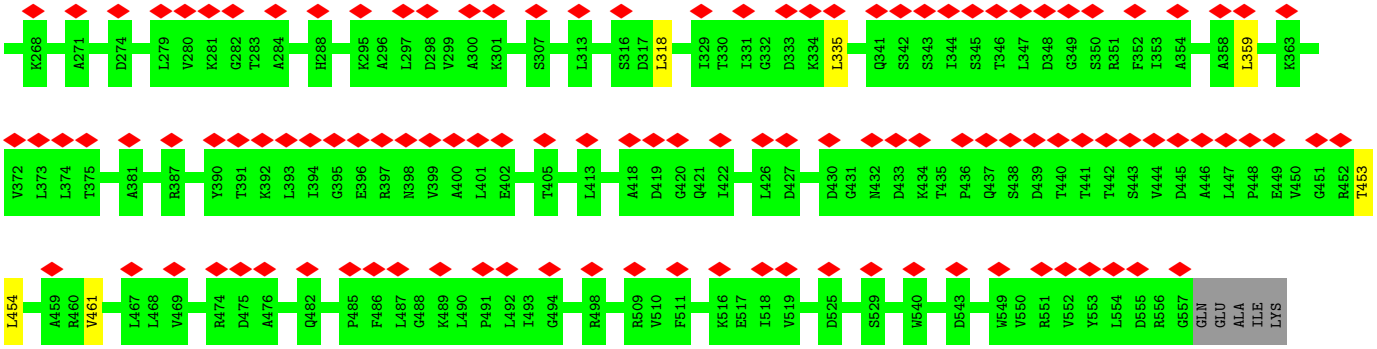
Chain J:



• Molecule 3: Protein InvG

Chain K:





• Molecule 3: Protein InvG

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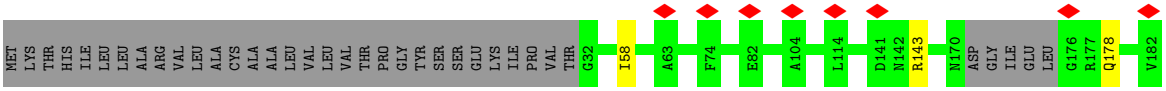
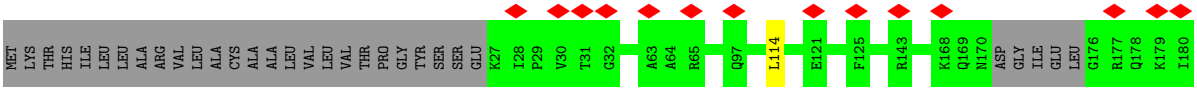
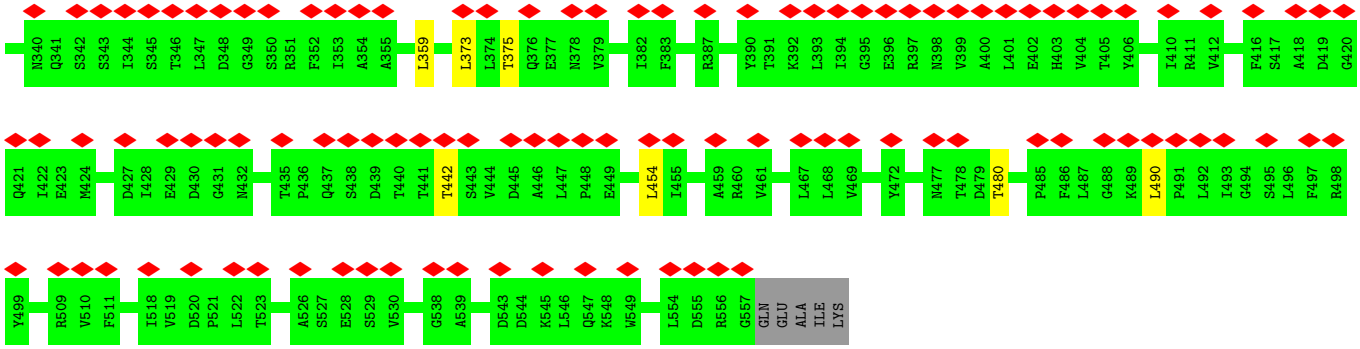


• Molecule 3: Protein InvG

Chain M:





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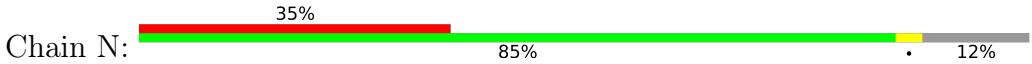
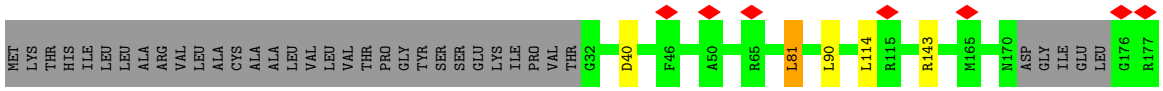
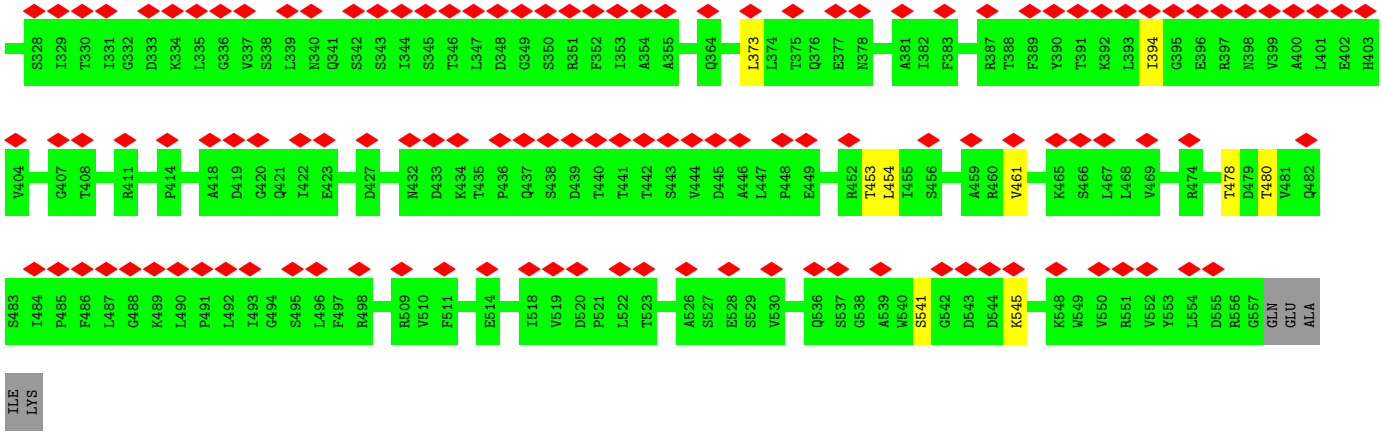
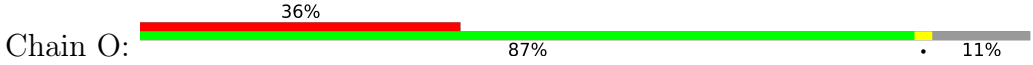
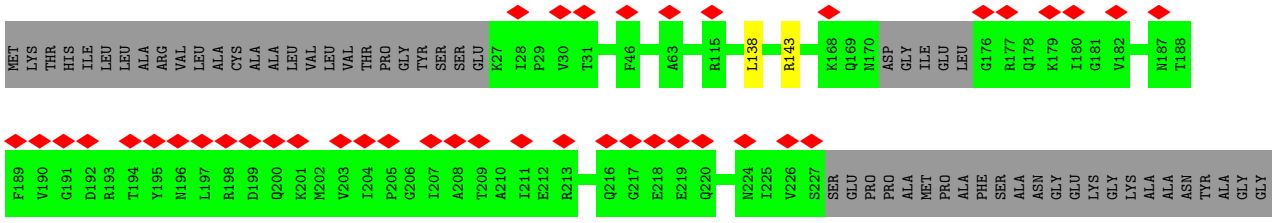


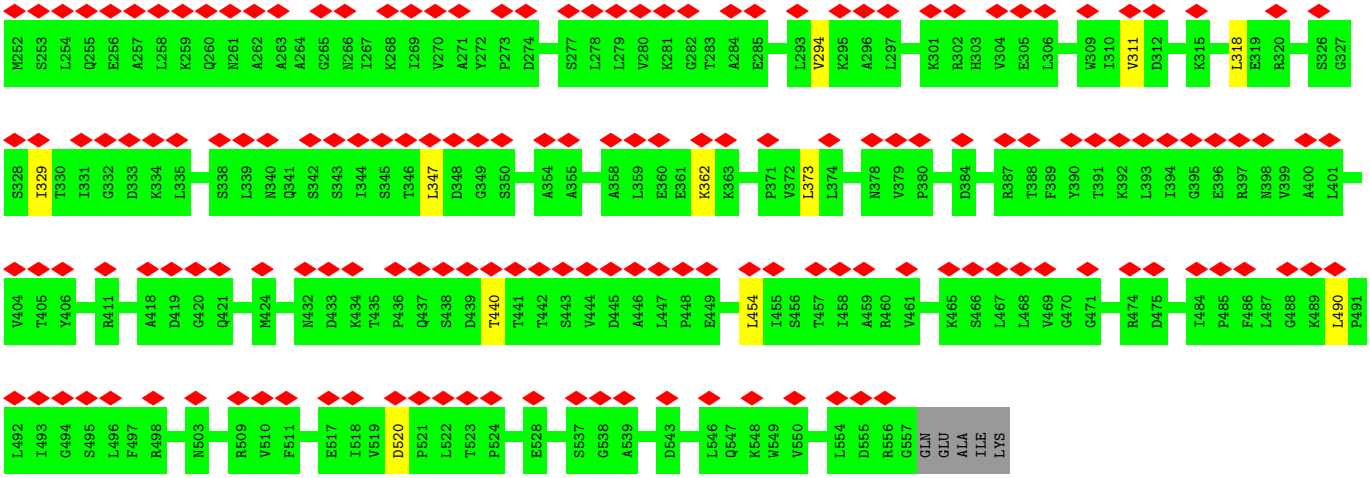




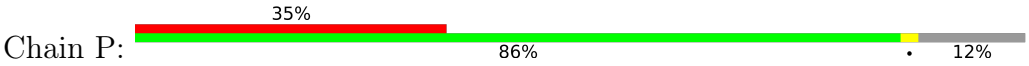
• Molecule 3: Protein InvG

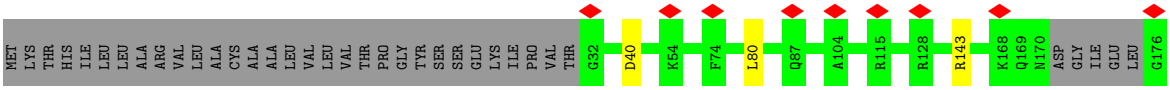




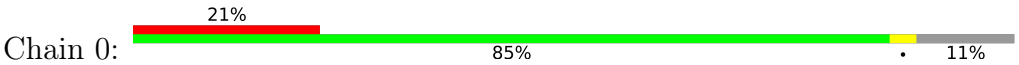


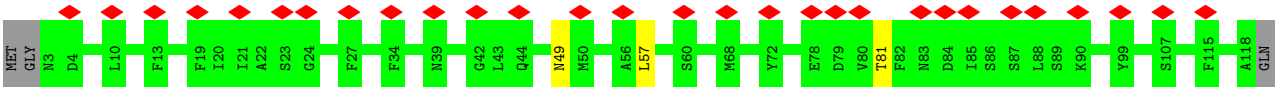
• Molecule 3: Protein InvG

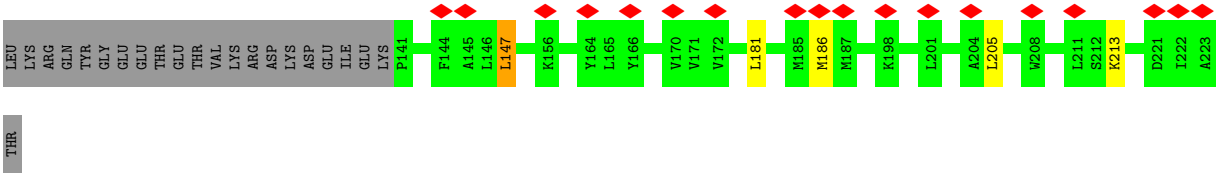




• Molecule 4: Surface presentation of antigens protein SpaP

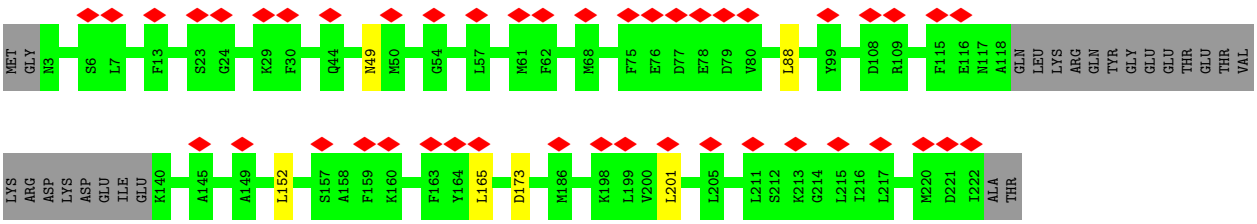






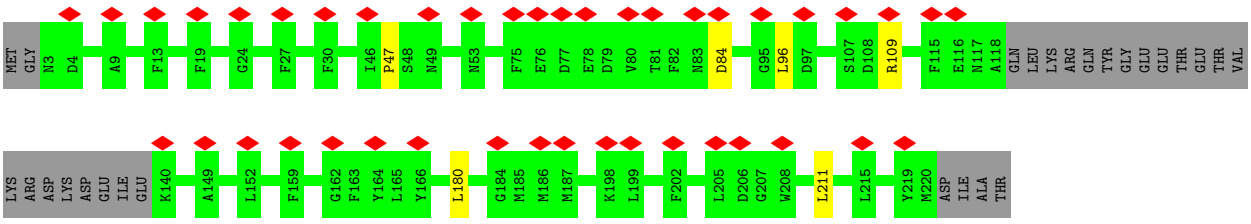
• Molecule 4: Surface presentation of antigens protein SpaP

Chain 1:



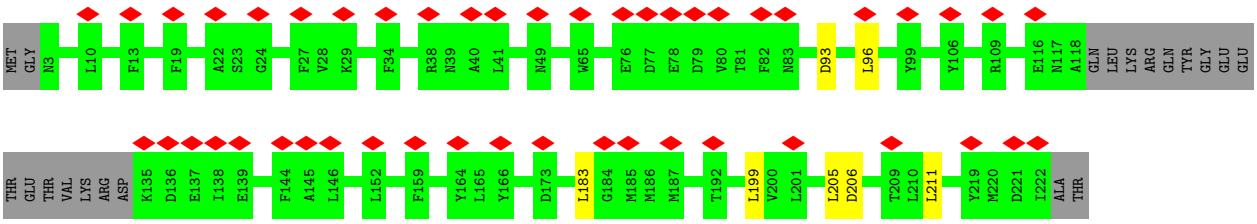
• Molecule 4: Surface presentation of antigens protein SpaP

Chain 2:



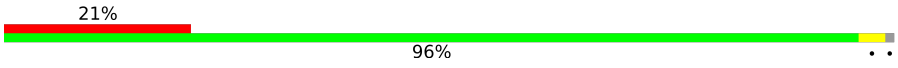
• Molecule 4: Surface presentation of antigens protein SpaP

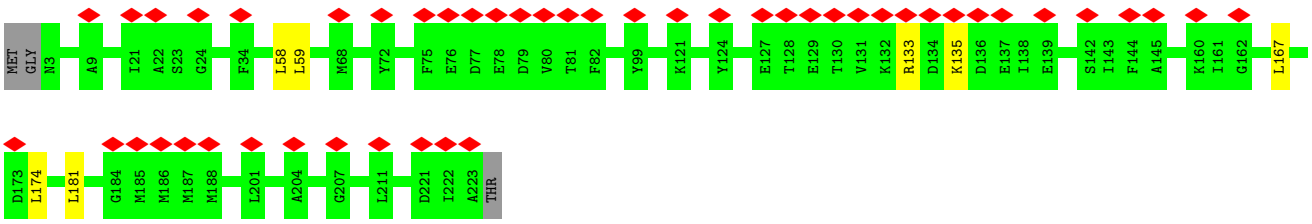
Chain 3:



• Molecule 4: Surface presentation of antigens protein SpaP

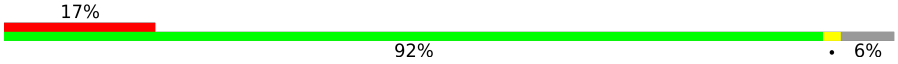
Chain 4:

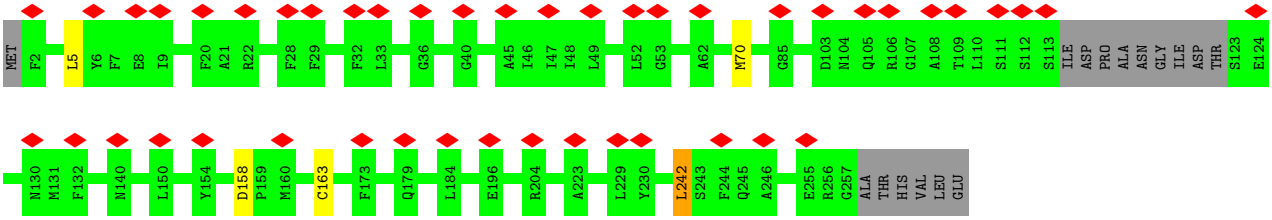




• Molecule 5: Surface presentation of antigens protein SpaR

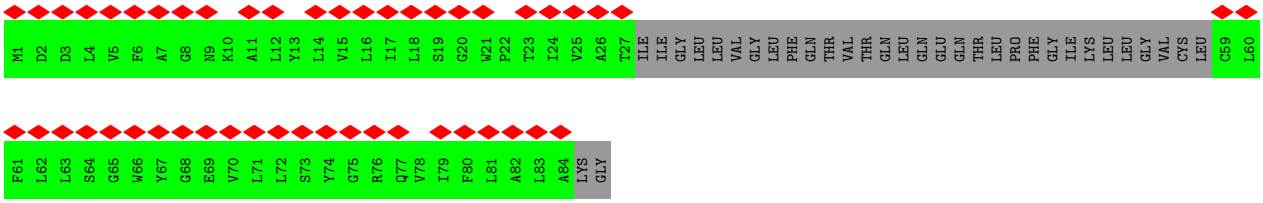
Chain 5:





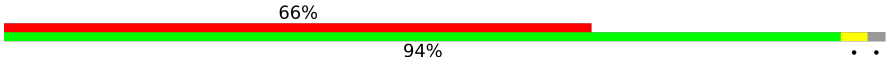
• Molecule 6: Surface presentation of antigens protein SpaQ

Chain 6:



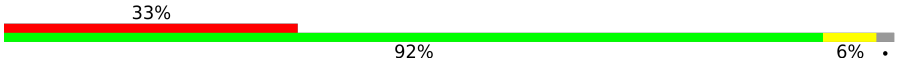
• Molecule 6: Surface presentation of antigens protein SpaQ

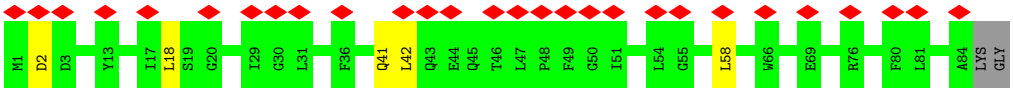
Chain 7:



• Molecule 6: Surface presentation of antigens protein SpaQ

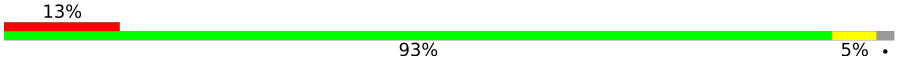
Chain 8:

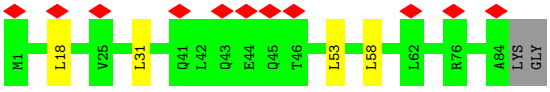




• Molecule 6: Surface presentation of antigens protein SpaQ

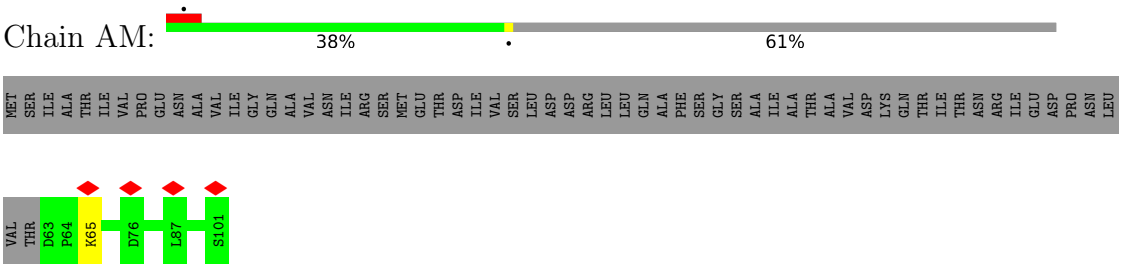
Chain 9:





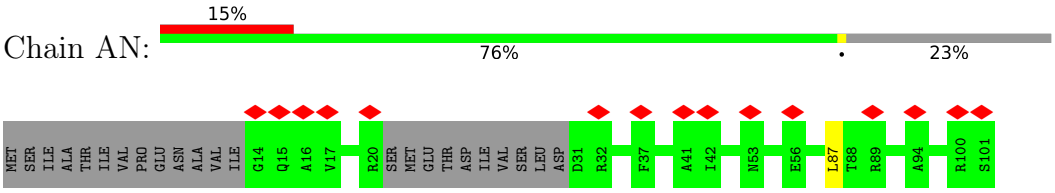
• Molecule 7: Protein PrgJ

Chain AM:



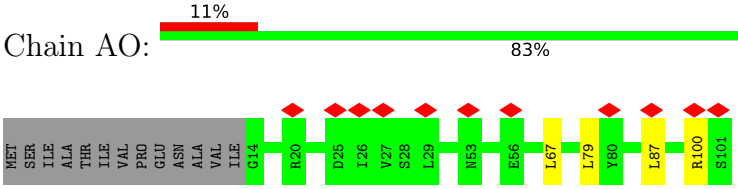
• Molecule 7: Protein PrgJ

Chain AN:



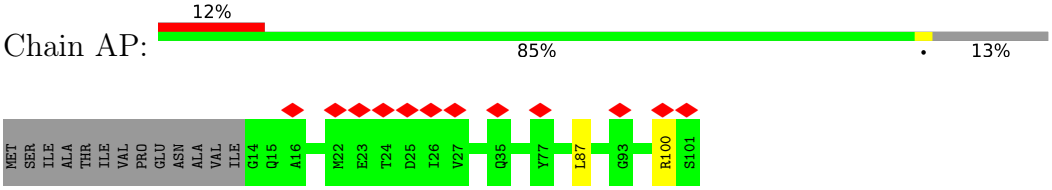
• Molecule 7: Protein PrgJ

Chain AO:



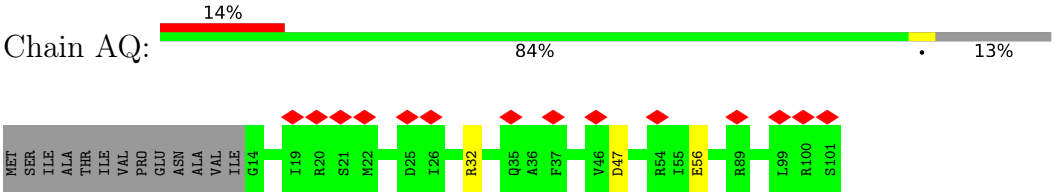
• Molecule 7: Protein PrgJ

Chain AP:



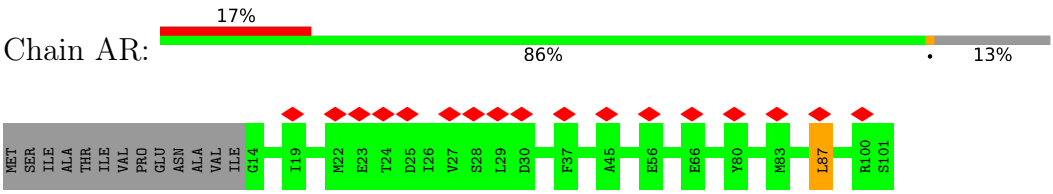
• Molecule 7: Protein PrgJ

Chain AQ:



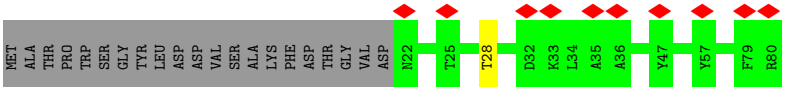
• Molecule 7: Protein PrgJ

Chain AR:

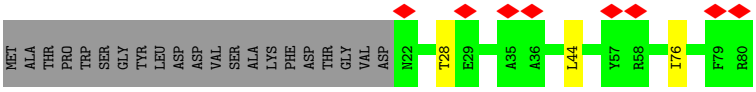


• Molecule 8: Protein PrgI

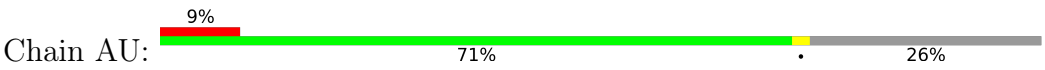
Chain AS:

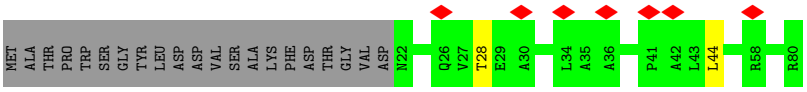


• Molecule 8: Protein PrgI

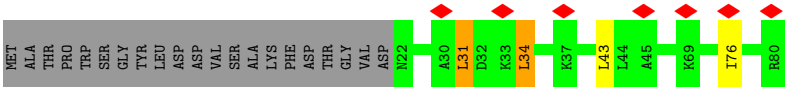


• Molecule 8: Protein PrgI

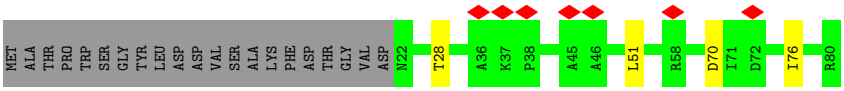




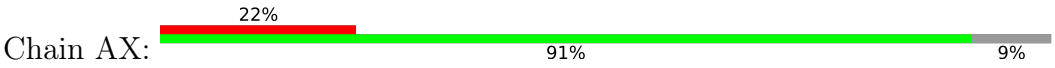
• Molecule 8: Protein PrgI

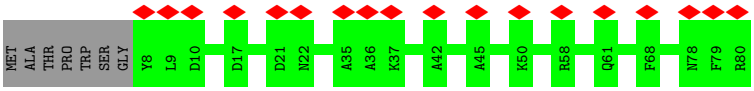


• Molecule 8: Protein PrgI

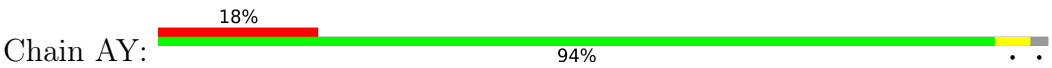


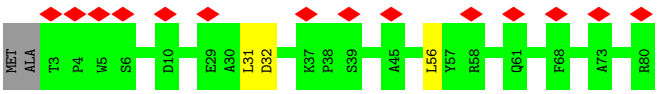
• Molecule 8: Protein PrgI





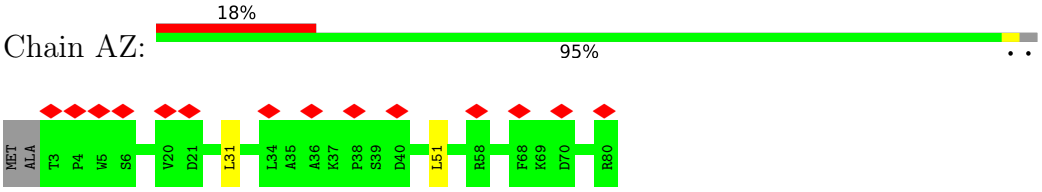
• Molecule 8: Protein PrgI





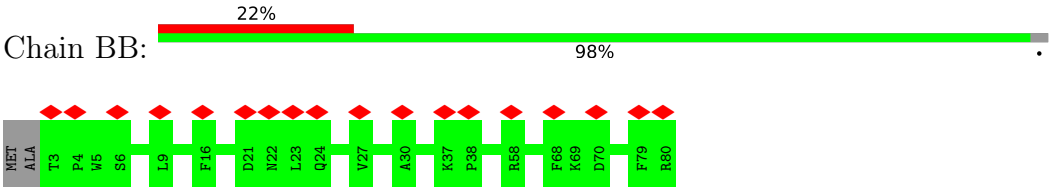
• Molecule 8: Protein PrgI

Chain AZ:



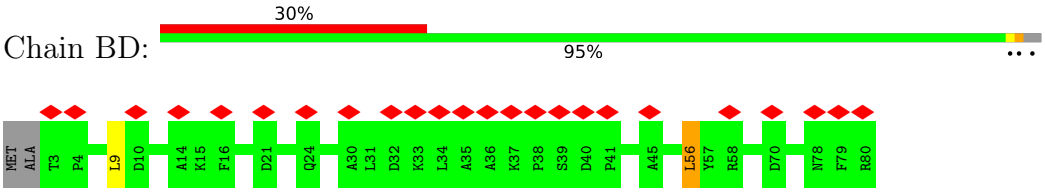
• Molecule 8: Protein PrgI

Chain BB:



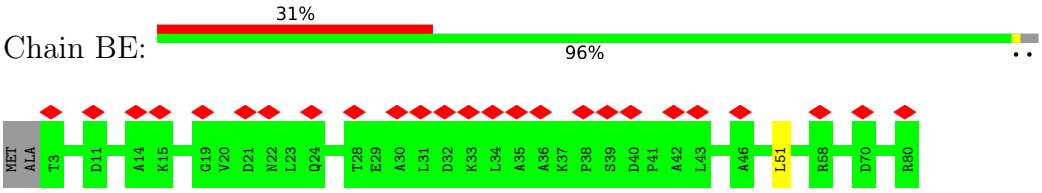
• Molecule 8: Protein PrgI

Chain BD:



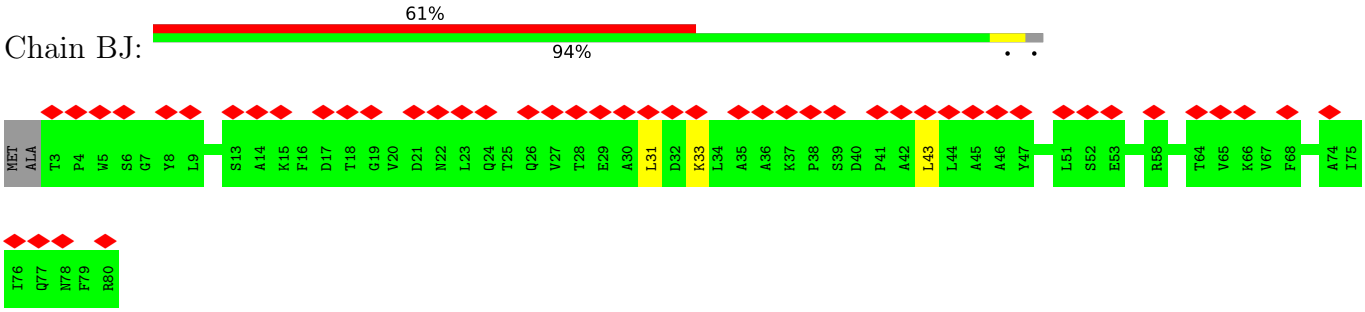
• Molecule 8: Protein PrgI

Chain BE:



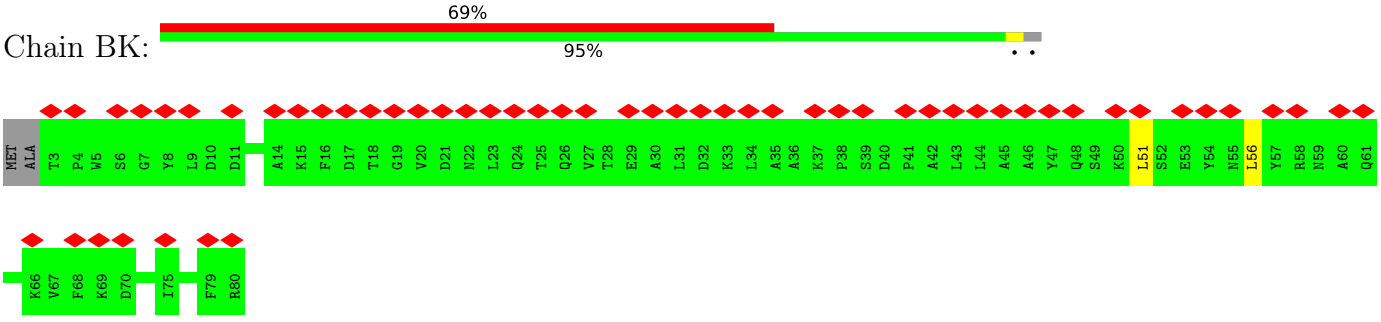
• Molecule 8: Protein PrgI

Chain BJ:



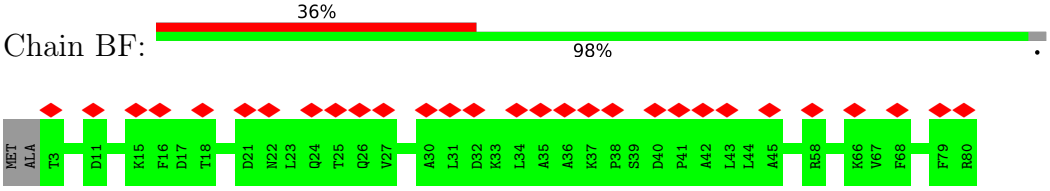
• Molecule 8: Protein PrgI

Chain BK:



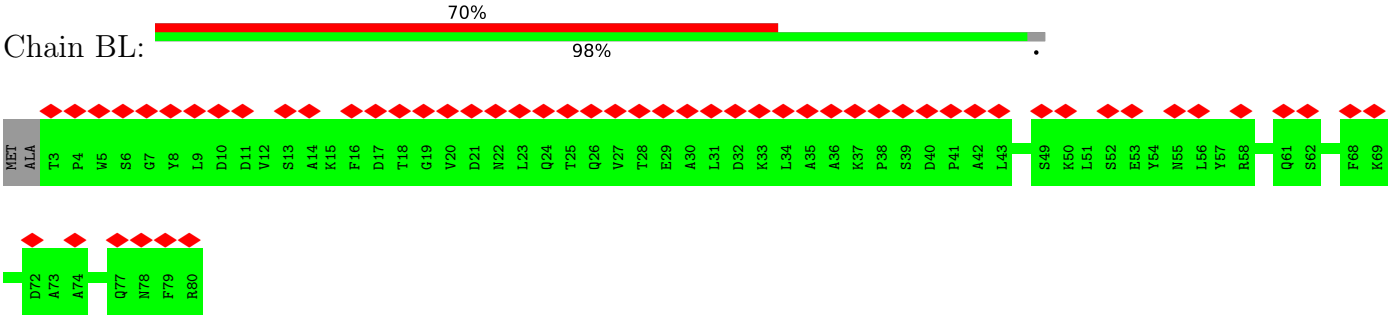
• Molecule 8: Protein PrgI

Chain BF:



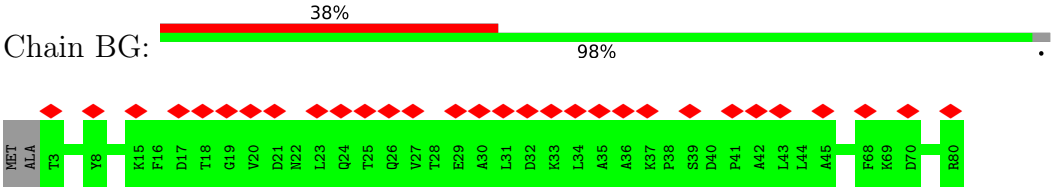
• Molecule 8: Protein PrgI

Chain BL:



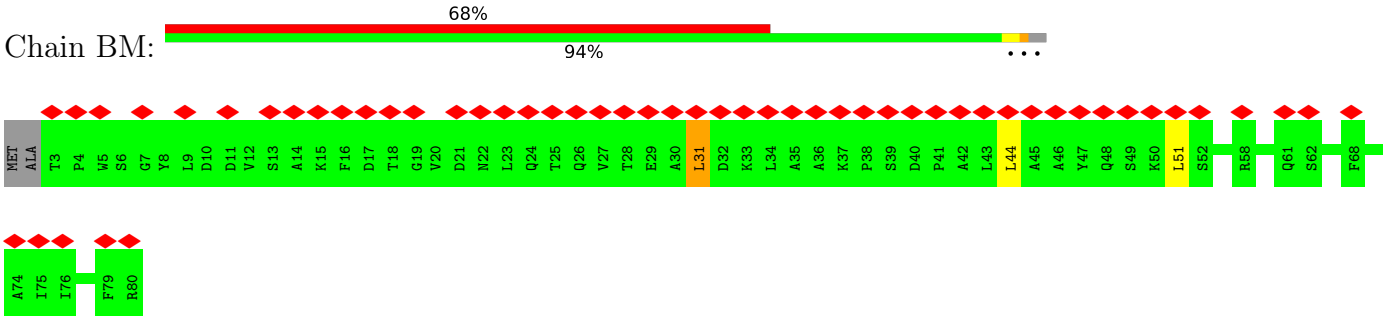
• Molecule 8: Protein PrgI

Chain BG:



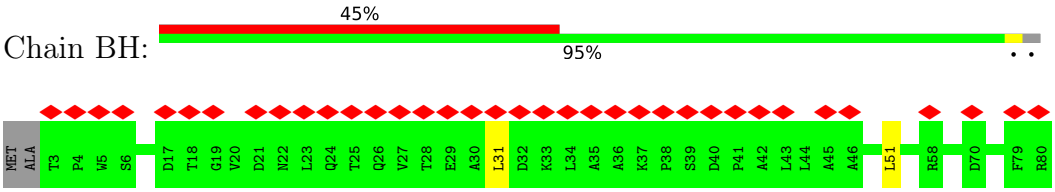
• Molecule 8: Protein PrgI

Chain BM:



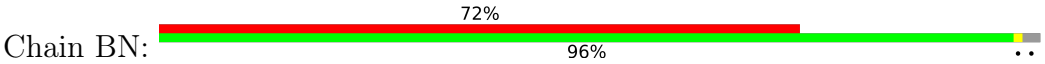
• Molecule 8: Protein PrgI

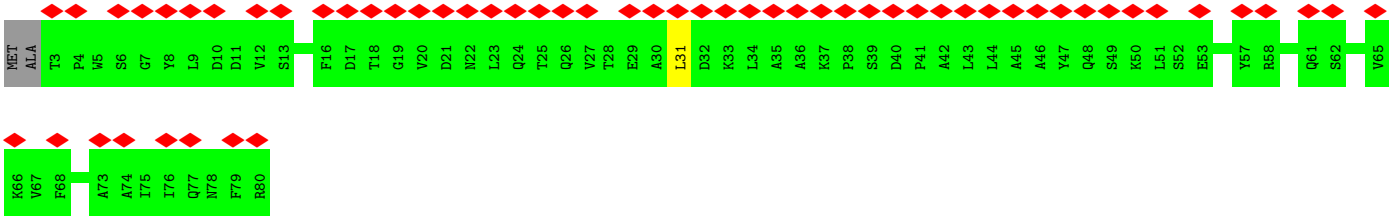
Chain BH:



• Molecule 8: Protein PrgI

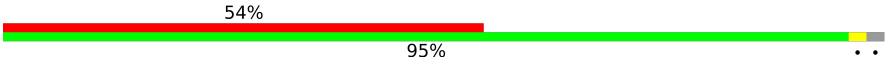
Chain BN:

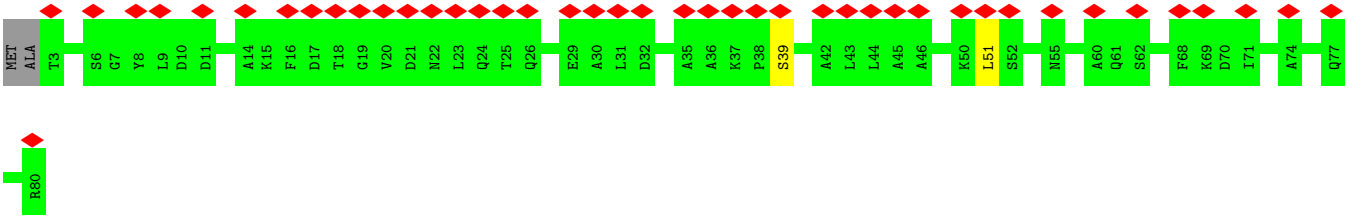




• Molecule 8: Protein PrgI

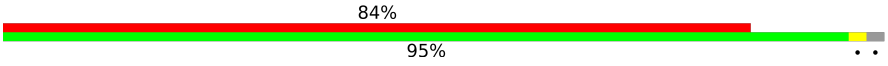
Chain BI:





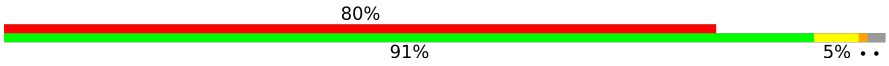
• Molecule 8: Protein PrgI

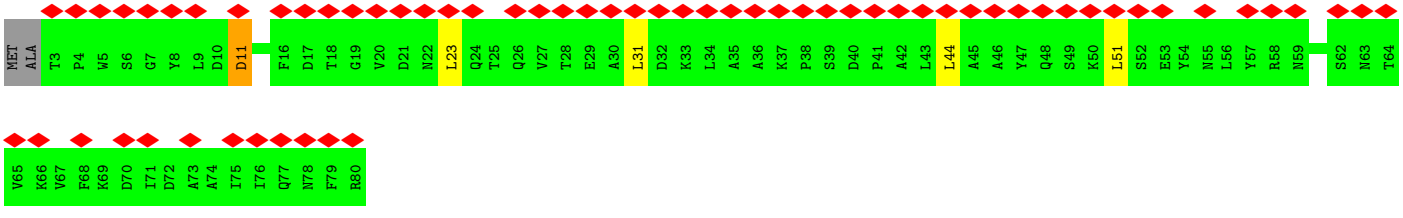
Chain BO:



• Molecule 8: Protein PrgI

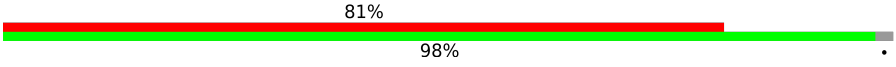
Chain BP:

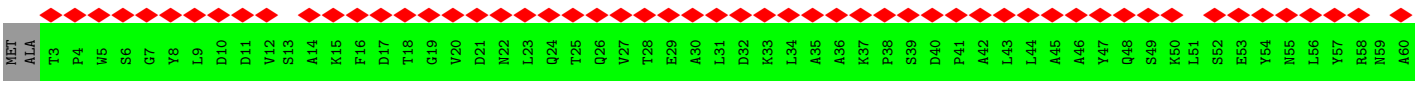


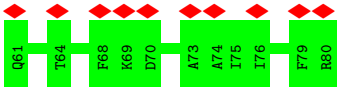


• Molecule 8: Protein PrgI

Chain BQ:

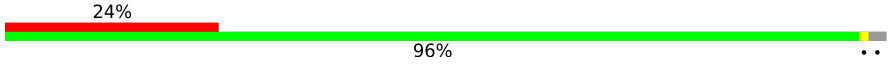


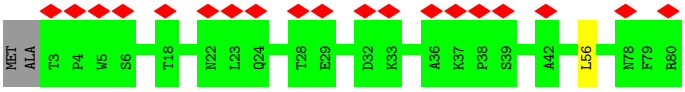




• Molecule 8: Protein PrgI

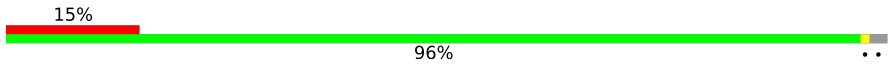
Chain BC:

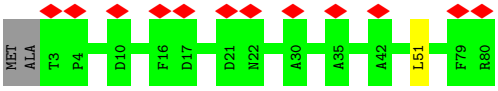




• Molecule 8: Protein PrgI

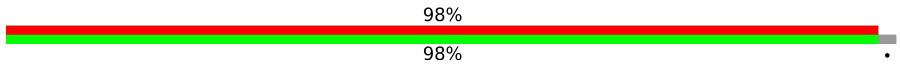
Chain BA:

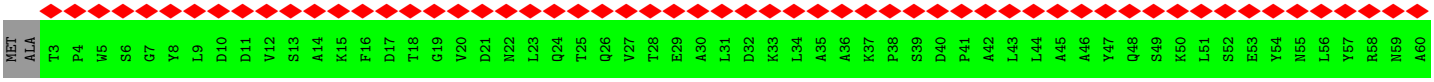


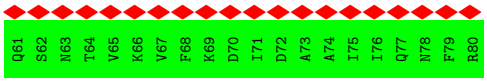


• Molecule 8: Protein PrgI

Chain BV:

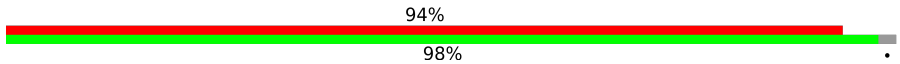


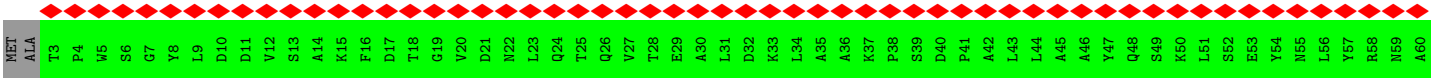


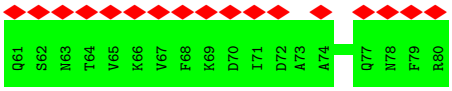


• Molecule 8: Protein PrgI

Chain BU:

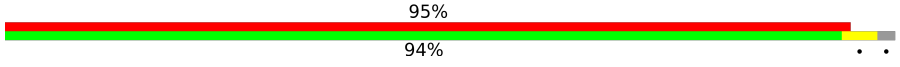


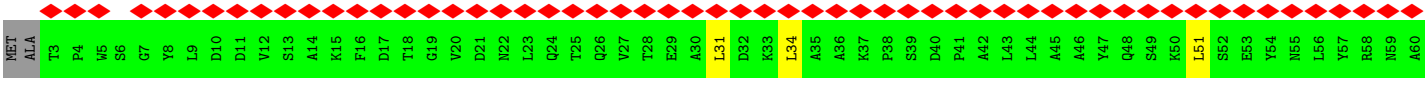


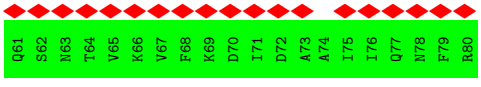


• Molecule 8: Protein PrgI

Chain BT:

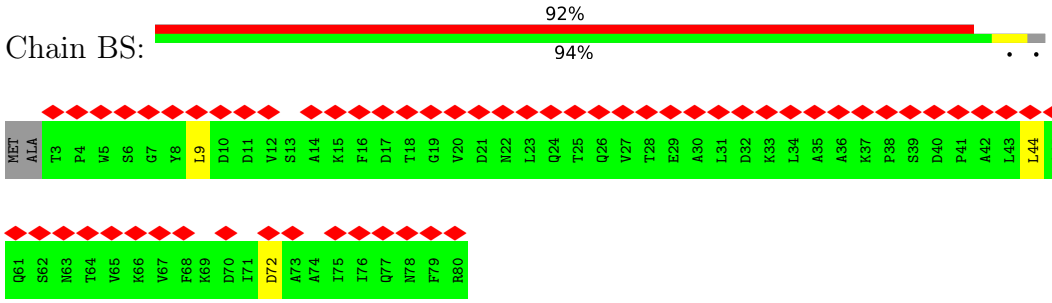






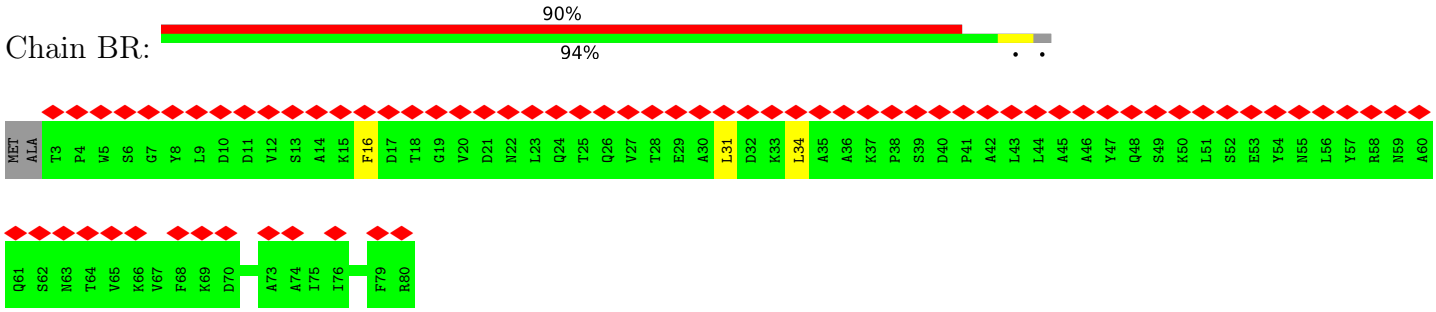
• Molecule 8: Protein PrgI

Chain BS:



• Molecule 8: Protein PrgI

Chain BR:



4 Experimental information (i)

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 ($e^-/Å^2$)	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

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
3	G	339	LEU	CA-CB-CG	8.54	134.93	115.30
8	BO	31	LEU	CA-CB-CG	8.51	134.88	115.30
1	AL	77	LEU	CA-CB-CG	8.48	134.80	115.30
8	BH	31	LEU	CA-CB-CG	8.48	134.80	115.30
3	O	520	ASP	CB-CG-OD1	8.47	125.92	118.30
7	AR	87	LEU	CA-CB-CG	8.40	134.63	115.30
4	3	96	LEU	CA-CB-CG	8.27	134.32	115.30
8	BR	16	PHE	CB-CG-CD2	-8.24	115.03	120.80
8	BP	23	LEU	CA-CB-CG	8.13	134.00	115.30
6	7	58	LEU	CA-CB-CG	7.89	133.45	115.30
8	BT	31	LEU	CA-CB-CG	7.79	133.23	115.30
1	AF	175	PHE	CB-CG-CD1	7.78	126.25	120.80
8	BI	51	LEU	CA-CB-CG	7.72	133.06	115.30
8	BT	51	LEU	CA-CB-CG	7.71	133.03	115.30
3	H	318	LEU	CA-CB-CG	7.66	132.92	115.30
2	n	279	LEU	CA-CB-CG	7.64	132.88	115.30
8	BP	51	LEU	CA-CB-CG	7.63	132.85	115.30
4	3	93	ASP	CB-CG-OD1	7.58	125.12	118.30
8	BR	34	LEU	CA-CB-CG	7.57	132.71	115.30
8	BM	51	LEU	CA-CB-CG	7.54	132.64	115.30
3	M	373	LEU	CA-CB-CG	7.53	132.62	115.30
8	AZ	31	LEU	CA-CB-CG	7.48	132.50	115.30
3	G	293	LEU	CA-CB-CG	7.46	132.46	115.30
8	BP	31	LEU	CA-CB-CG	7.43	132.39	115.30
3	B	47	ASP	CB-CG-OD1	7.40	124.96	118.30
8	BR	31	LEU	CA-CB-CG	7.40	132.32	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	BT	34	LEU	CA-CB-CG	7.38	132.28	115.30
3	O	373	LEU	CA-CB-CG	7.34	132.19	115.30
8	BK	51	LEU	CA-CB-CG	7.34	132.18	115.30
1	t	151	LEU	CA-CB-CG	7.32	132.15	115.30
6	7	62	LEU	CA-CB-CG	7.29	132.06	115.30
4	0	57	LEU	CA-CB-CG	7.28	132.04	115.30
2	j	211	LEU	CA-CB-CG	7.26	132.00	115.30
8	BN	31	LEU	CA-CB-CG	7.26	132.00	115.30
2	S	307	LEU	CA-CB-CG	7.25	131.97	115.30
2	e	312	LEU	CA-CB-CG	7.24	131.96	115.30
3	I	49	MET	CB-CG-SD	7.23	134.08	112.40
1	AI	117	LEU	CA-CB-CG	7.21	131.88	115.30
1	r	117	LEU	CA-CB-CG	7.21	131.87	115.30
8	BO	51	LEU	CA-CB-CG	7.18	131.82	115.30
8	BH	51	LEU	CA-CB-CG	7.17	131.80	115.30
8	BA	51	LEU	CA-CB-CG	7.13	131.70	115.30
8	BE	51	LEU	CA-CB-CG	7.12	131.69	115.30
3	H	308	LEU	CA-CB-CG	7.08	131.59	115.30
3	I	318	LEU	CA-CB-CG	7.08	131.59	115.30
2	d	312	LEU	CA-CB-CG	7.08	131.58	115.30
2	h	177	LEU	CA-CB-CG	7.08	131.57	115.30
8	BR	16	PHE	CB-CG-CD1	7.05	125.74	120.80
3	A	373	LEU	CA-CB-CG	7.05	131.51	115.30
3	N	81	LEU	CA-CB-CG	6.99	131.38	115.30
3	P	454	LEU	CA-CB-CG	6.98	131.36	115.30
8	AZ	51	LEU	CA-CB-CG	6.97	131.33	115.30
8	AY	56	LEU	CA-CB-CG	6.90	131.18	115.30
2	h	307	LEU	CA-CB-CG	6.87	131.09	115.30
3	I	51	LEU	CA-CB-CG	6.86	131.07	115.30
1	s	105	LEU	CA-CB-CG	6.86	131.07	115.30
3	H	373	LEU	CA-CB-CG	6.86	131.07	115.30
2	e	279	LEU	CA-CB-CG	6.85	131.05	115.30
5	5	5	LEU	CA-CB-CG	6.83	131.01	115.30
7	AO	79	LEU	CB-CG-CD1	6.82	122.60	111.00
2	c	283	MET	CA-CB-CG	6.79	124.84	113.30
4	3	183	LEU	CA-CB-CG	6.77	130.87	115.30
2	d	307	LEU	CA-CB-CG	6.71	130.74	115.30
7	AQ	47	ASP	CB-CG-OD2	6.71	124.34	118.30
3	P	373	LEU	CA-CB-CG	6.68	130.68	115.30
3	K	359	LEU	CA-CB-CG	6.67	130.63	115.30
1	z	179	ASP	CB-CG-OD1	6.61	124.25	118.30
1	y	27	LEU	CA-CB-CG	6.61	130.49	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	n	211	LEU	CA-CB-CG	6.59	130.47	115.30
2	V	332	ASP	CB-CG-OD1	6.52	124.17	118.30
2	g	312	LEU	CA-CB-CG	6.47	130.18	115.30
1	u	124	LEU	CA-CB-CG	6.45	130.14	115.30
5	5	158	ASP	CB-CG-OD2	6.42	124.08	118.30
3	I	373	LEU	CA-CB-CG	6.38	129.97	115.30
2	l	307	LEU	CA-CB-CG	6.31	129.81	115.30
3	H	293	LEU	CA-CB-CG	6.30	129.79	115.30
2	X	307	LEU	CA-CB-CG	6.30	129.79	115.30
2	W	187	LEU	CA-CB-CG	6.30	129.78	115.30
4	4	58	LEU	CA-CB-CG	6.30	129.78	115.30
2	l	293	LEU	CA-CB-CG	6.27	129.72	115.30
2	b	307	LEU	CA-CB-CG	6.24	129.66	115.30
8	BJ	31	LEU	CA-CB-CG	6.20	129.57	115.30
4	1	88	LEU	CA-CB-CG	6.20	129.56	115.30
1	AG	171	LEU	CA-CB-CG	6.19	129.54	115.30
2	X	176	LEU	CA-CB-CG	6.16	129.47	115.30
3	O	347	LEU	CA-CB-CG	6.15	129.45	115.30
6	9	53	LEU	CA-CB-CG	6.15	129.45	115.30
3	L	214	LEU	CA-CB-CG	6.12	129.38	115.30
8	AV	31	LEU	CA-CB-CG	6.11	129.36	115.30
5	5	242	LEU	CA-CB-CG	6.10	129.33	115.30
3	N	373	LEU	CA-CB-CG	6.09	129.31	115.30
6	7	42	LEU	CA-CB-CG	6.08	129.29	115.30
6	8	58	LEU	CA-CB-CG	6.08	129.28	115.30
1	z	181	ASP	CB-CG-OD1	6.08	123.77	118.30
3	L	373	LEU	CA-CB-CG	6.07	129.26	115.30
3	A	90	LEU	CA-CB-CG	6.07	129.25	115.30
6	9	31	LEU	CA-CB-CG	6.04	129.18	115.30
4	2	96	LEU	CA-CB-CG	6.02	129.15	115.30
1	y	94	LEU	CA-CB-CG	6.00	129.10	115.30
8	AU	44	LEU	CA-CB-CG	5.99	129.08	115.30
4	1	201	LEU	CA-CB-CG	5.98	129.06	115.30
3	L	214	LEU	CB-CG-CD2	5.96	121.14	111.00
2	V	366	LEU	CA-CB-CG	5.96	129.01	115.30
1	z	117	LEU	CA-CB-CG	5.93	128.94	115.30
2	b	312	LEU	CA-CB-CG	5.92	128.93	115.30
1	AI	120	MET	CA-CB-CG	5.92	123.36	113.30
2	E	307	LEU	CA-CB-CG	5.89	128.84	115.30
2	c	312	LEU	CA-CB-CG	5.87	128.81	115.30
3	M	454	LEU	CA-CB-CG	5.80	128.64	115.30
1	AJ	117	LEU	CA-CB-CG	5.80	128.64	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	k	293	LEU	CA-CB-CG	5.78	128.60	115.30
3	C	534	LEU	CA-CB-CG	5.74	128.50	115.30
3	L	178	GLN	CA-CB-CG	5.72	125.99	113.40
3	P	496	LEU	CA-CB-CG	5.71	128.44	115.30
2	X	187	LEU	CA-CB-CG	5.69	128.40	115.30
1	q	148	LEU	CA-CB-CG	5.68	128.37	115.30
8	BK	56	LEU	CB-CG-CD2	5.66	120.61	111.00
7	AN	87	LEU	CA-CB-CG	5.65	128.30	115.30
1	AJ	195	LEU	CA-CB-CG	5.65	128.29	115.30
4	1	173	ASP	CB-CG-OD2	5.62	123.36	118.30
3	G	90	LEU	CA-CB-CG	5.62	128.22	115.30
6	8	18	LEU	CA-CB-CG	5.60	128.17	115.30
6	8	2	ASP	CB-CG-OD1	5.58	123.32	118.30
3	A	126	LEU	CA-CB-CG	5.57	128.11	115.30
7	AP	87	LEU	CA-CB-CG	5.55	128.07	115.30
4	0	181	LEU	CA-CB-CG	5.52	128.00	115.30
8	AV	43	LEU	CB-CG-CD1	5.48	120.32	111.00
3	J	312	ASP	CB-CG-OD1	5.48	123.24	118.30
8	BP	44	LEU	CA-CB-CG	5.47	127.89	115.30
4	0	147	LEU	CA-CB-CG	5.47	127.88	115.30
1	q	39	LEU	CA-CB-CG	5.45	127.84	115.30
8	BJ	43	LEU	CA-CB-CG	5.45	127.83	115.30
8	BS	44	LEU	CA-CB-CG	5.44	127.81	115.30
4	2	180	LEU	CA-CB-CG	5.43	127.78	115.30
1	y	77	LEU	CA-CB-CG	5.42	127.76	115.30
3	H	90	LEU	CA-CB-CG	5.40	127.71	115.30
8	BD	56	LEU	CA-CB-CG	5.39	127.70	115.30
8	BM	44	LEU	CA-CB-CG	5.38	127.68	115.30
3	J	308	LEU	CA-CB-CG	5.38	127.67	115.30
1	t	195	LEU	CA-CB-CG	5.37	127.65	115.30
3	I	308	LEU	CA-CB-CG	5.37	127.65	115.30
4	4	181	LEU	CA-CB-CG	5.37	127.64	115.30
1	AK	94	LEU	CA-CB-CG	5.36	127.63	115.30
8	BC	56	LEU	CA-CB-CG	5.35	127.61	115.30
3	P	80	LEU	CA-CB-CG	5.35	127.60	115.30
2	R	176	LEU	CB-CG-CD2	5.33	120.07	111.00
8	AY	32	ASP	CB-CG-OD1	5.33	123.09	118.30
3	O	318	LEU	CA-CB-CG	5.32	127.54	115.30
3	C	212	GLU	CA-CB-CG	5.31	125.08	113.40
8	AY	31	LEU	CA-CB-CG	5.30	127.50	115.30
2	g	205	LEU	CB-CG-CD1	5.30	120.01	111.00
3	A	308	LEU	CA-CB-CG	5.30	127.49	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	534	LEU	CA-CB-CG	5.28	127.45	115.30
3	I	454	LEU	CA-CB-CG	5.27	127.42	115.30
7	AO	79	LEU	CB-CG-CD2	-5.26	102.06	111.00
8	BS	9	LEU	CB-CG-CD1	5.25	119.92	111.00
1	t	148	LEU	CA-CB-CG	5.24	127.34	115.30
3	H	487	LEU	CA-CB-CG	5.22	127.30	115.30
3	G	454	LEU	CA-CB-CG	5.20	127.27	115.30
3	N	90	LEU	CA-CB-CG	5.20	127.27	115.30
2	j	237	ASP	CB-CG-OD2	5.20	122.98	118.30
3	I	384	ASP	CB-CG-OD1	5.20	122.97	118.30
4	3	205	LEU	CA-CB-CG	5.19	127.24	115.30
3	K	335	LEU	CA-CB-CG	5.18	127.20	115.30
3	L	258	LEU	CA-CB-CG	5.17	127.20	115.30
3	N	308	LEU	CA-CB-CG	5.17	127.20	115.30
8	BH	51	LEU	CB-CG-CD1	5.17	119.79	111.00
1	y	166	ASP	CB-CG-OD1	5.17	122.95	118.30
8	BP	11	ASP	CB-CG-OD2	5.17	122.95	118.30
3	A	252	MET	CA-CB-CG	5.17	122.08	113.30
4	4	59	LEU	CB-CG-CD2	5.16	119.78	111.00
3	O	454	LEU	CA-CB-CG	5.16	127.17	115.30
3	L	308	LEU	CA-CB-CG	5.12	127.08	115.30
4	4	174	LEU	CB-CG-CD2	5.12	119.70	111.00
4	0	205	LEU	CA-CB-CG	5.10	127.04	115.30
4	3	199	LEU	CA-CB-CG	5.09	127.02	115.30
2	V	366	LEU	CB-CG-CD1	5.08	119.63	111.00
3	B	339	LEU	CA-CB-CG	5.08	126.97	115.30
3	L	318	LEU	CA-CB-CG	5.08	126.97	115.30
8	BS	72	ASP	CB-CG-OD1	5.07	122.86	118.30
3	H	252	MET	CA-CB-CG	5.07	121.91	113.30
4	3	211	LEU	CA-CB-CG	5.06	126.93	115.30
1	AJ	94	LEU	CA-CB-CG	5.05	126.93	115.30
3	G	308	LEU	CA-CB-CG	5.05	126.91	115.30
1	AE	151	LEU	CA-CB-CG	5.02	126.84	115.30
6	9	58	LEU	CA-CB-CG	5.00	126.80	115.30
8	BD	9	LEU	CA-CB-CG	5.00	126.80	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Res	Type
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	80	ARG

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Mol	Chain	Res	Type
1	AA	187	LEU
1	AB	95	VAL
1	AC	187	LEU
1	AE	23	LEU
1	AE	53	LYS
1	AE	80	ARG
1	AF	80	ARG
1	AG	80	ARG
1	AH	23	LEU
1	AI	80	ARG
3	Q	143	ARG
2	R	176	LEU
2	S	307	LEU
2	S	348	ARG
2	U	366	LEU
2	V	348	ARG
2	V	366	LEU
2	X	366	LEU
2	Y	348	ARG
1	AL	187	LEU
2	a	332	ASP
2	a	366	LEU
2	c	320	LYS
2	d	307	LEU
2	d	312	LEU
2	d	366	LEU
2	e	215	ASP
2	e	312	LEU
2	e	333	ASP
2	e	348	ARG
2	g	312	LEU
2	g	366	LEU
2	h	177	LEU
2	i	320	LYS
2	j	222	VAL
2	k	269	LYS
2	k	348	ARG
2	m	363	ASP
1	o	73	LYS
1	o	80	ARG
1	q	28	ASP
1	q	39	LEU

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Mol	Chain	Res	Type
1	q	187	LEU
1	r	80	ARG
1	s	187	LEU
1	t	95	VAL
1	t	187	LEU
1	v	187	LEU
1	w	80	ARG
1	w	141	ARG
1	y	27	LEU
1	y	80	ARG
1	z	80	ARG
1	z	177	ASP
1	AK	22	ASP
1	AK	80	ARG
4	0	81	THR
4	0	147	LEU
4	0	186	MET
4	0	213	LYS
4	1	152	LEU
4	1	165	LEU
4	2	84	ASP
4	2	109	ARG
4	2	211	LEU
4	4	133	ARG
4	4	135	LYS
4	4	167	LEU
5	5	70	MET
5	5	163	CYS
5	5	242	LEU
6	9	18	LEU
7	AM	65	LYS
7	AO	67	LEU
7	AO	87	LEU
7	AO	100	ARG
7	AP	100	ARG
7	AQ	32	ARG
7	AQ	56	GLU
7	AR	87	LEU
8	AS	28	THR
8	AT	28	THR
8	AT	44	LEU
8	AT	76	ILE

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Mol	Chain	Res	Type
8	AU	28	THR
8	AV	31	LEU
8	AV	34	LEU
8	AV	76	ILE
8	AW	28	THR
8	AW	51	LEU
8	AW	70	ASP
8	AW	76	ILE
3	A	80	LEU
3	A	294	VAL
3	A	311	VAL
3	A	442	THR
3	A	461	VAL
3	B	215	LEU
3	B	293	LEU
3	B	373	LEU
3	B	442	THR
3	B	454	LEU
3	B	480	THR
3	B	490	LEU
3	C	143	ARG
3	C	254	LEU
3	C	294	VAL
3	C	318	LEU
3	C	363	LYS
3	C	373	LEU
3	C	447	LEU
3	C	452	ARG
3	C	453	THR
3	C	480	THR
3	C	502	LYS
3	D	40	ASP
3	D	61	LYS
3	D	114	LEU
3	D	219	GLU
3	D	294	VAL
3	D	318	LEU
3	D	373	LEU
3	D	442	THR
3	D	449	GLU
3	D	454	LEU
3	D	480	THR

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Mol	Chain	Res	Type
3	F	143	ARG
3	F	254	LEU
3	F	258	LEU
3	F	359	LEU
3	F	373	LEU
3	F	440	THR
3	F	449	GLU
3	F	490	LEU
3	G	143	ARG
3	G	215	LEU
3	G	318	LEU
3	G	359	LEU
3	G	373	LEU
3	G	442	THR
3	G	461	VAL
3	H	82	GLU
3	H	143	ARG
3	H	185	LEU
3	H	209	THR
3	H	294	VAL
3	H	442	THR
3	H	449	GLU
3	H	461	VAL
3	H	480	THR
3	H	541	SER
3	I	143	ARG
3	I	294	VAL
3	I	440	THR
3	I	461	VAL
3	J	40	ASP
3	J	51	LEU
3	J	192	ASP
3	J	268	LYS
3	J	294	VAL
3	J	312	ASP
3	J	373	LEU
3	J	453	THR
3	J	454	LEU
3	J	461	VAL
3	J	469	VAL
3	J	490	LEU
3	K	138	LEU

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Mol	Chain	Res	Type
3	K	143	ARG
3	K	318	LEU
3	K	453	THR
3	K	454	LEU
3	K	461	VAL
3	L	58	ILE
3	L	143	ARG
3	L	294	VAL
3	L	311	VAL
3	L	318	LEU
3	L	442	THR
3	L	454	LEU
3	L	480	THR
3	L	534	LEU
3	M	114	LEU
3	M	294	VAL
3	M	321	LEU
3	M	359	LEU
3	M	375	THR
3	M	442	THR
3	M	480	THR
3	M	490	LEU
3	N	40	ASP
3	N	81	LEU
3	N	114	LEU
3	N	143	ARG
3	N	254	LEU
3	N	311	VAL
3	N	318	LEU
3	N	394	ILE
3	N	453	THR
3	N	454	LEU
3	N	461	VAL
3	N	478	THR
3	N	480	THR
3	N	541	SER
3	N	545	LYS
3	O	138	LEU
3	O	143	ARG
3	O	294	VAL
3	O	311	VAL
3	O	329	ILE

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Mol	Chain	Res	Type
3	O	362	LYS
3	O	440	THR
3	O	490	LEU
3	P	40	ASP
3	P	143	ARG
3	P	295	LYS
3	P	329	ILE
3	P	440	THR
3	P	454	LEU
3	P	461	VAL
3	P	541	SER
8	BD	56	LEU
8	BJ	33	LYS
8	BM	31	LEU
8	BI	39	SER
8	BP	11	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (232) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	33	ASN
1	AA	162	HIS
1	AB	29	GLN
1	AB	139	ASN
1	AB	162	HIS
1	AC	29	GLN
1	AC	33	ASN
1	AD	29	GLN
1	AE	29	GLN
1	AE	129	HIS
1	AF	33	ASN
1	AF	129	HIS
1	AF	139	ASN
1	AG	40	GLN
1	AI	118	GLN
1	AI	129	HIS
1	AI	162	HIS
2	E	199	GLN
3	Q	97	GLN
3	Q	169	GLN
2	R	229	ASN
2	R	356	GLN

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Mol	Chain	Res	Type
2	S	219	ASN
2	S	318	ASN
2	S	319	HIS
2	T	209	GLN
2	T	229	ASN
2	T	309	GLN
2	V	219	ASN
2	V	229	ASN
2	V	318	ASN
2	V	319	HIS
2	W	318	ASN
2	W	372	GLN
2	X	318	ASN
2	Y	229	ASN
2	Y	318	ASN
2	Z	199	GLN
2	Z	209	GLN
2	Z	265	ASN
1	AL	33	ASN
2	a	318	ASN
2	a	356	GLN
2	b	219	ASN
2	b	310	GLN
2	b	318	ASN
2	b	341	GLN
2	c	219	ASN
2	c	290	ASN
2	c	318	ASN
2	d	242	GLN
2	d	356	GLN
2	e	310	GLN
2	e	318	ASN
2	f	263	GLN
2	g	356	GLN
2	h	224	ASN
2	h	310	GLN
2	h	318	ASN
2	i	219	ASN
2	i	318	ASN
2	i	319	HIS
2	j	318	ASN
2	j	328	GLN

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Mol	Chain	Res	Type
2	k	318	ASN
2	l	229	ASN
2	l	328	GLN
2	l	356	GLN
2	m	209	GLN
2	m	219	ASN
2	m	310	GLN
2	m	318	ASN
2	m	319	HIS
2	n	319	HIS
1	o	29	GLN
1	o	33	ASN
1	p	29	GLN
1	p	33	ASN
1	q	33	ASN
1	r	162	HIS
1	s	29	GLN
1	s	33	ASN
1	s	111	GLN
1	t	29	GLN
1	t	33	ASN
1	t	163	GLN
1	u	29	GLN
1	u	173	ASN
1	v	29	GLN
1	v	33	ASN
1	v	139	ASN
1	v	162	HIS
1	w	129	HIS
1	x	76	GLN
1	x	162	HIS
1	y	162	HIS
1	z	162	HIS
1	AJ	139	ASN
1	AJ	162	HIS
4	2	83	ASN
4	3	69	HIS
4	3	113	GLN
4	3	117	ASN
4	4	44	GLN
5	5	76	GLN
5	5	104	ASN

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Mol	Chain	Res	Type
5	5	105	GLN
5	5	130	ASN
5	5	245	GLN
6	7	37	GLN
6	7	45	GLN
6	8	9	ASN
6	8	37	GLN
6	9	37	GLN
6	9	43	GLN
7	AM	71	GLN
7	AO	53	ASN
7	AP	53	ASN
7	AP	59	ASN
7	AP	71	GLN
7	AQ	71	GLN
7	AR	35	GLN
8	AS	22	ASN
8	AT	48	GLN
8	AT	61	GLN
8	AV	24	GLN
8	AW	24	GLN
8	AX	78	ASN
8	AY	61	GLN
3	A	71	ASN
3	A	87	GLN
3	A	97	GLN
3	A	216	GLN
3	A	220	GLN
3	A	378	ASN
3	A	421	GLN
3	B	87	GLN
3	B	170	ASN
3	B	276	ASN
3	B	286	GLN
3	B	376	GLN
3	B	421	GLN
3	B	547	GLN
3	C	123	ASN
3	C	276	ASN
3	C	421	GLN
3	C	547	GLN
3	D	286	GLN

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Mol	Chain	Res	Type
3	D	421	GLN
3	F	169	GLN
3	F	276	ASN
3	F	286	GLN
3	F	378	ASN
3	G	97	GLN
3	G	120	ASN
3	G	124	ASN
3	G	170	ASN
3	G	220	GLN
3	G	286	GLN
3	G	357	ASN
3	G	421	GLN
3	G	547	GLN
3	H	97	GLN
3	H	178	GLN
3	H	220	GLN
3	H	276	ASN
3	H	286	GLN
3	H	376	GLN
3	H	421	GLN
3	I	169	GLN
3	I	276	ASN
3	I	286	GLN
3	I	421	GLN
3	I	547	GLN
3	J	97	GLN
3	J	276	ASN
3	J	421	GLN
3	J	506	ASN
3	J	536	GLN
3	K	97	GLN
3	K	161	ASN
3	K	169	GLN
3	K	276	ASN
3	K	286	GLN
3	K	421	GLN
3	L	97	GLN
3	L	178	GLN
3	L	196	ASN
3	L	216	GLN
3	L	421	GLN

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Mol	Chain	Res	Type
3	M	97	GLN
3	M	161	ASN
3	M	261	ASN
3	M	276	ASN
3	M	286	GLN
3	M	314	ASN
3	M	421	GLN
3	M	547	GLN
3	N	97	GLN
3	N	170	ASN
3	N	276	ASN
3	N	286	GLN
3	N	421	GLN
3	N	536	GLN
3	O	169	GLN
3	O	200	GLN
3	O	220	GLN
3	O	276	ASN
3	O	286	GLN
3	O	421	GLN
3	P	87	GLN
3	P	196	ASN
3	P	276	ASN
3	P	378	ASN
3	P	421	GLN
3	P	547	GLN
8	BB	78	ASN
8	BD	26	GLN
8	BE	59	ASN
8	BJ	59	ASN
8	BF	61	GLN
8	BL	61	GLN
8	BL	77	GLN
8	BN	26	GLN
8	BN	63	ASN
8	BN	77	GLN
8	BI	26	GLN
8	BP	59	ASN
8	BQ	61	GLN
8	BC	26	GLN
8	BA	26	GLN
8	BT	63	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

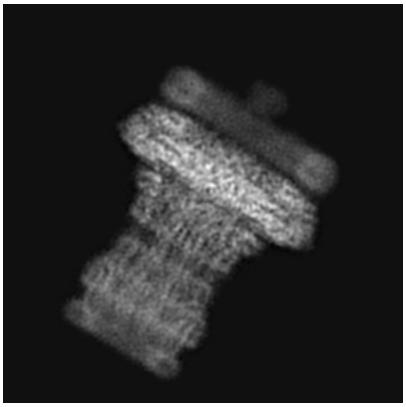
6 Map visualisation

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.

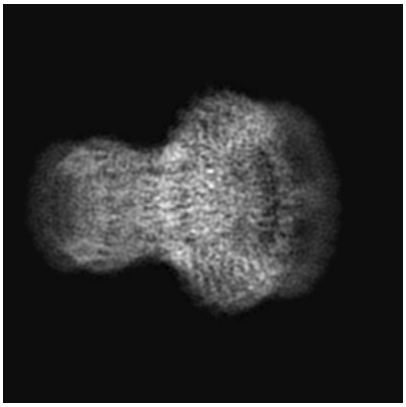
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

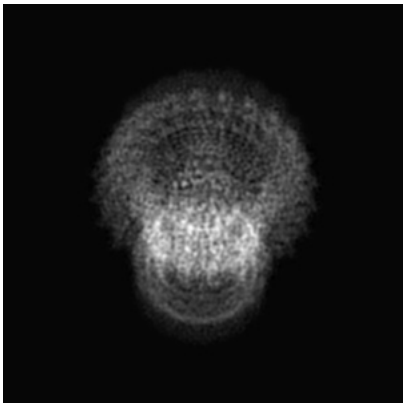
6.1.1 Primary map



X



Y

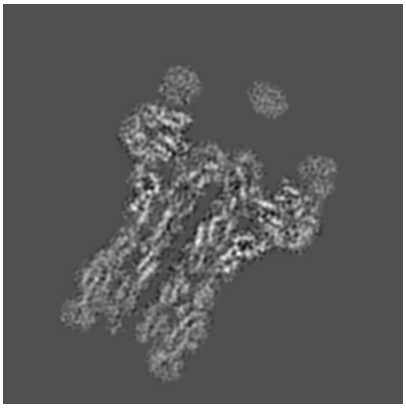


Z

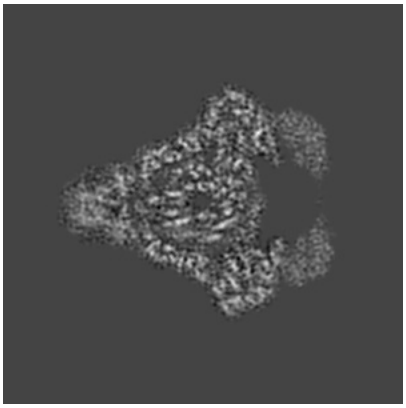
The images above show the map projected in three orthogonal directions.

6.2 Central slices

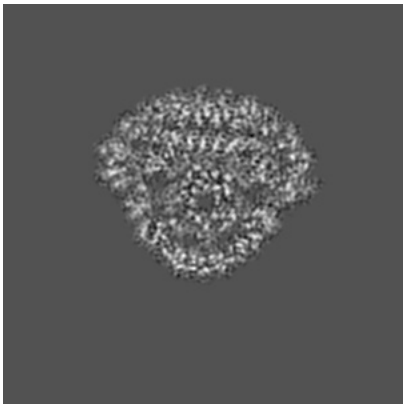
6.2.1 Primary map



X Index: 125



Y Index: 125

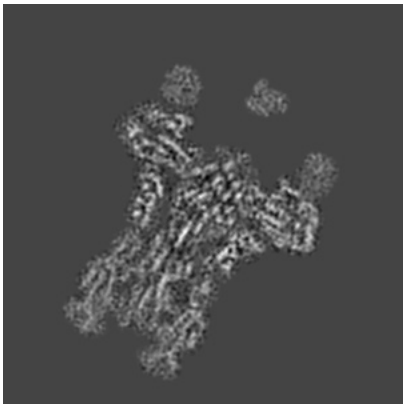


Z Index: 125

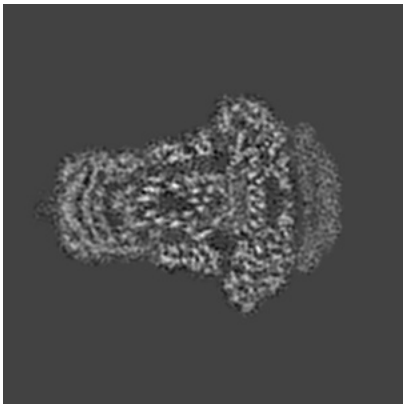
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 136



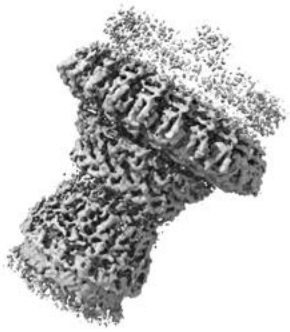
Y Index: 113

Z Index: 123

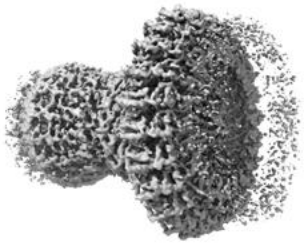
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

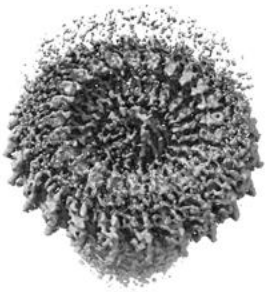
6.4.1 Primary map



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.

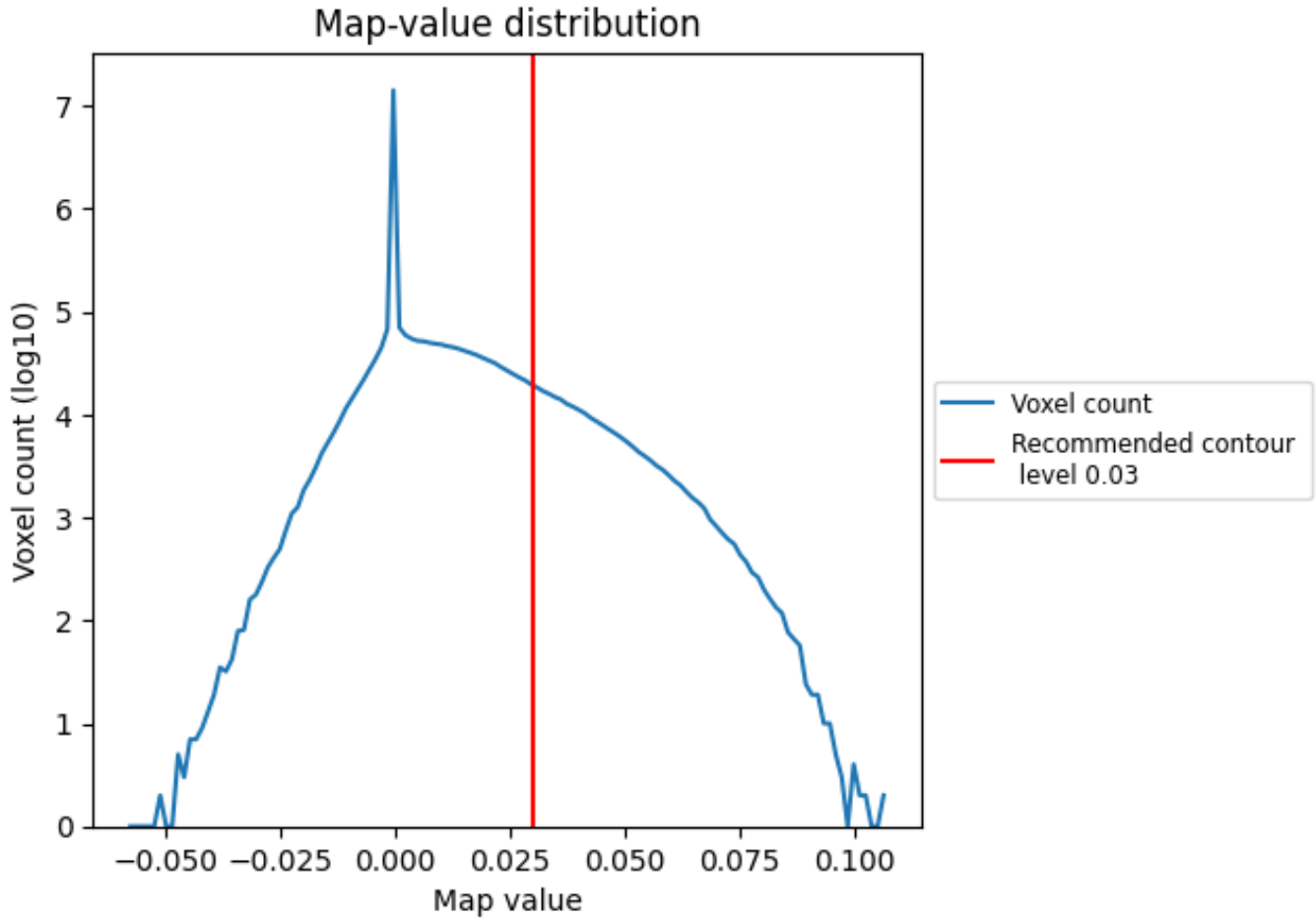
6.5 Mask visualisation (i)

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

7 Map analysis

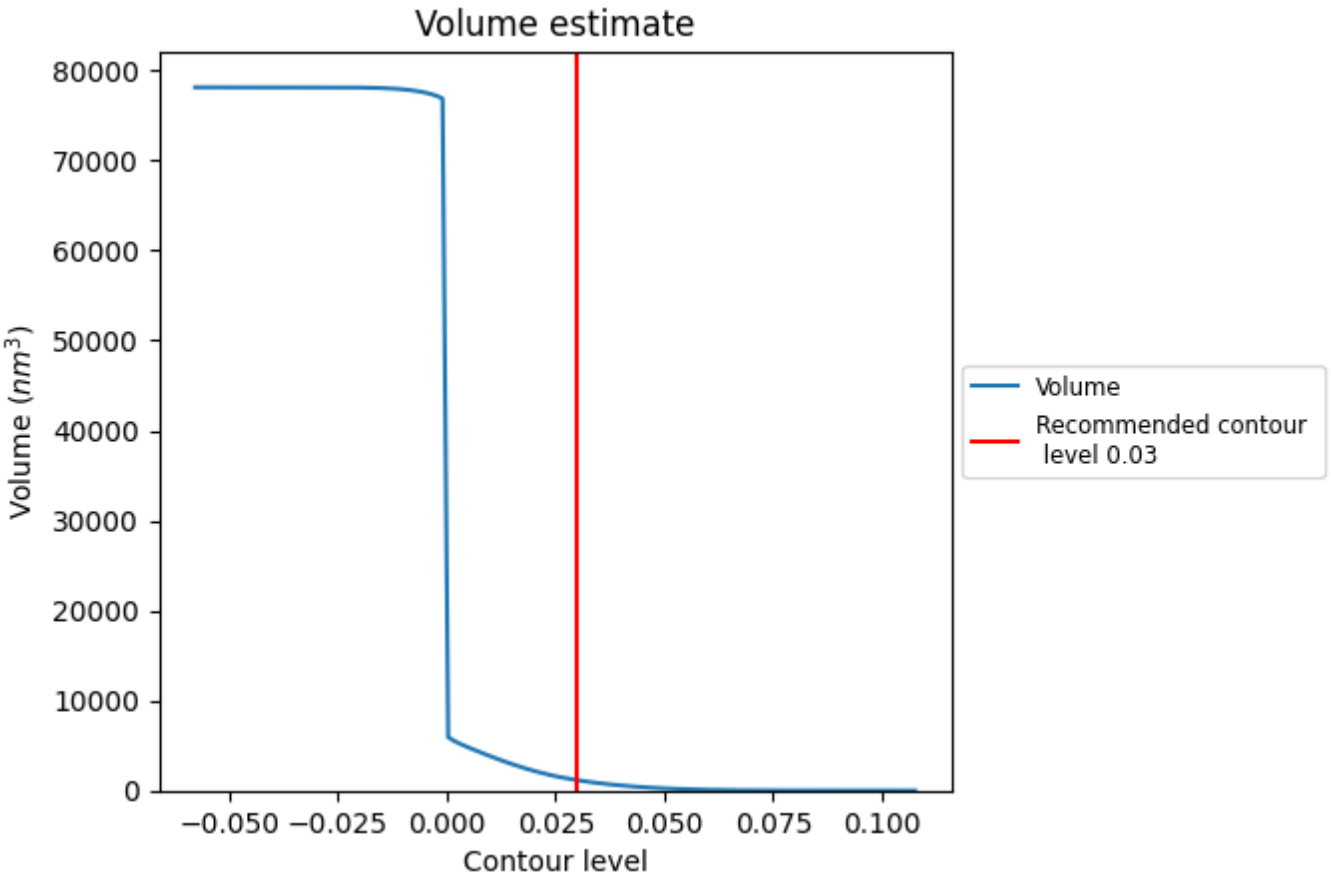
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

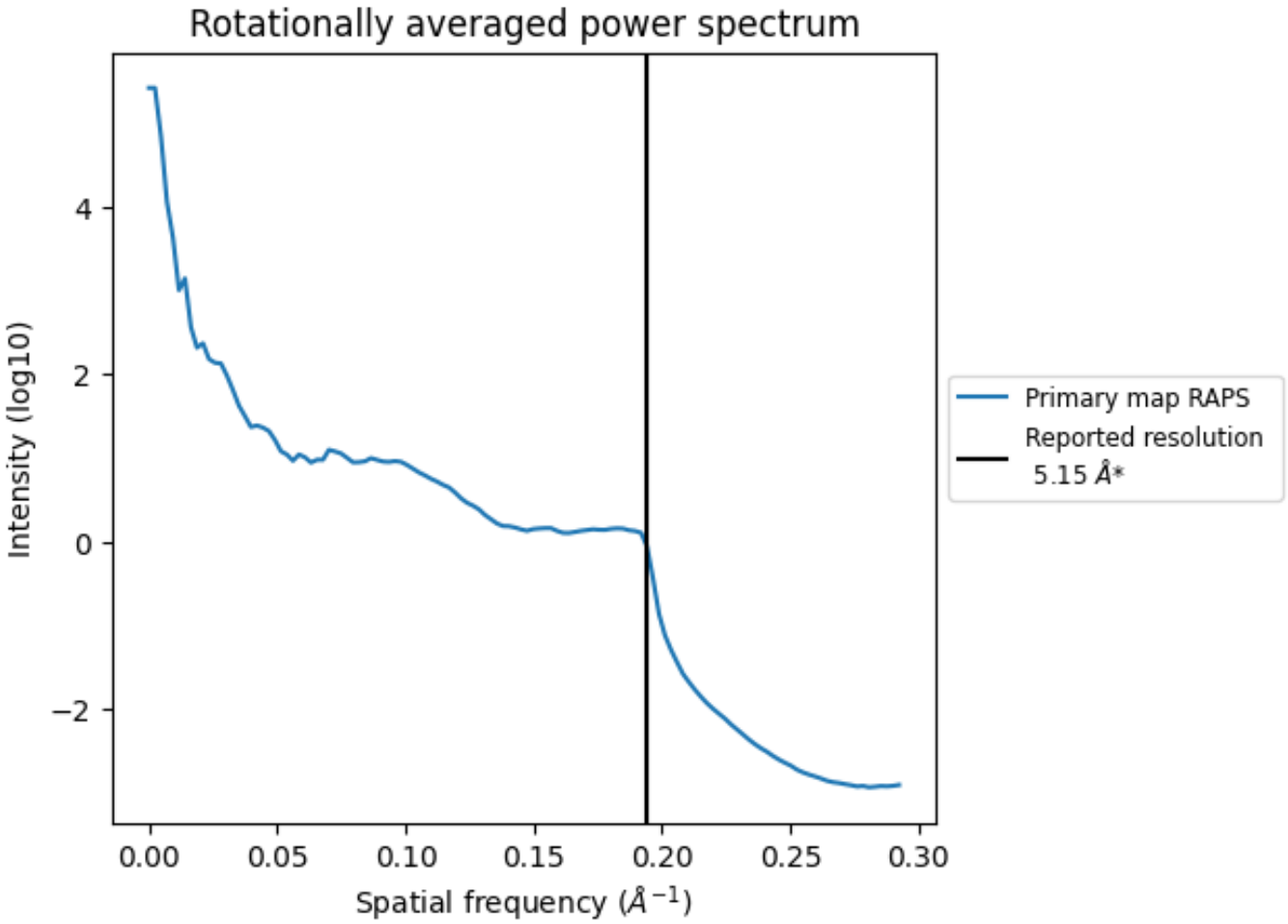
7.2 Volume estimate



The volume at the recommended contour level is 1154 nm^3; 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 Å^{-1}

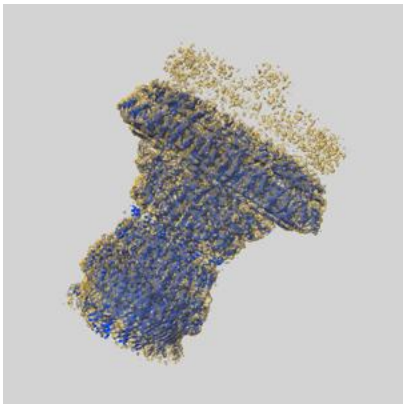
8 Fourier-Shell correlation (i)

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

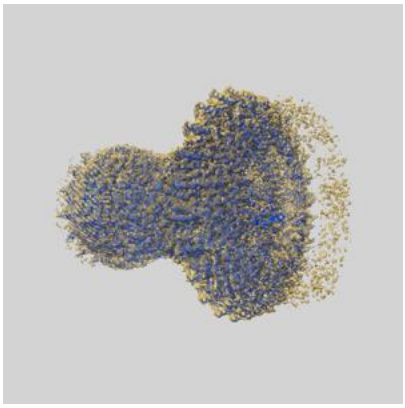
9 Map-model fit

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.

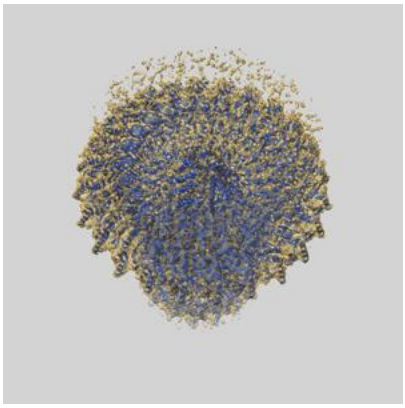
9.1 Map-model overlay



X



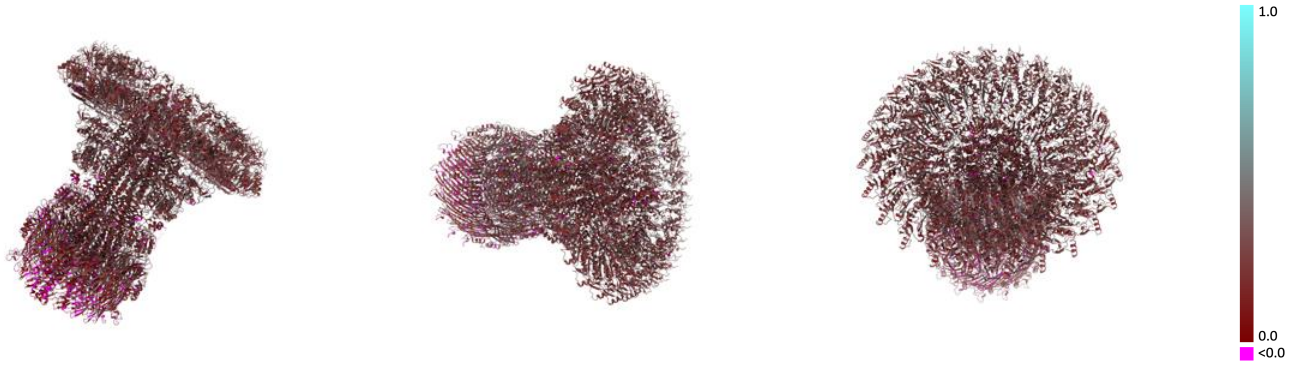
Y



Z

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.

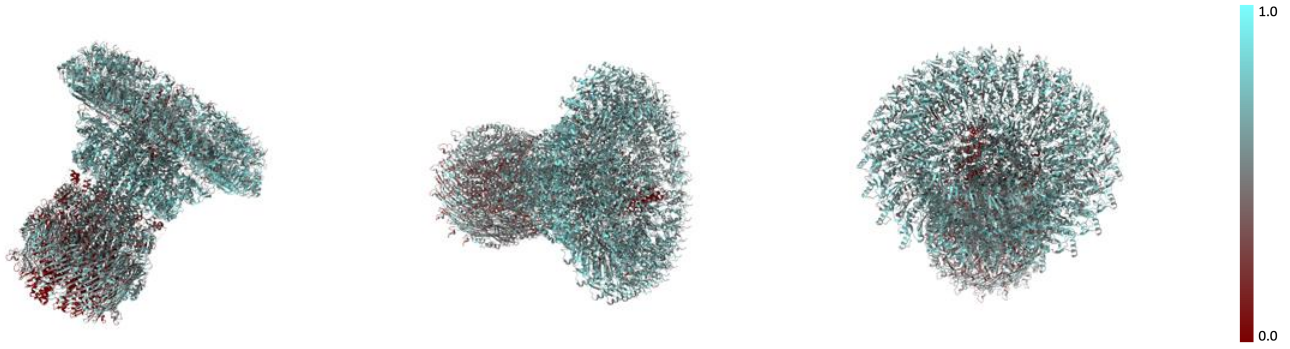
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

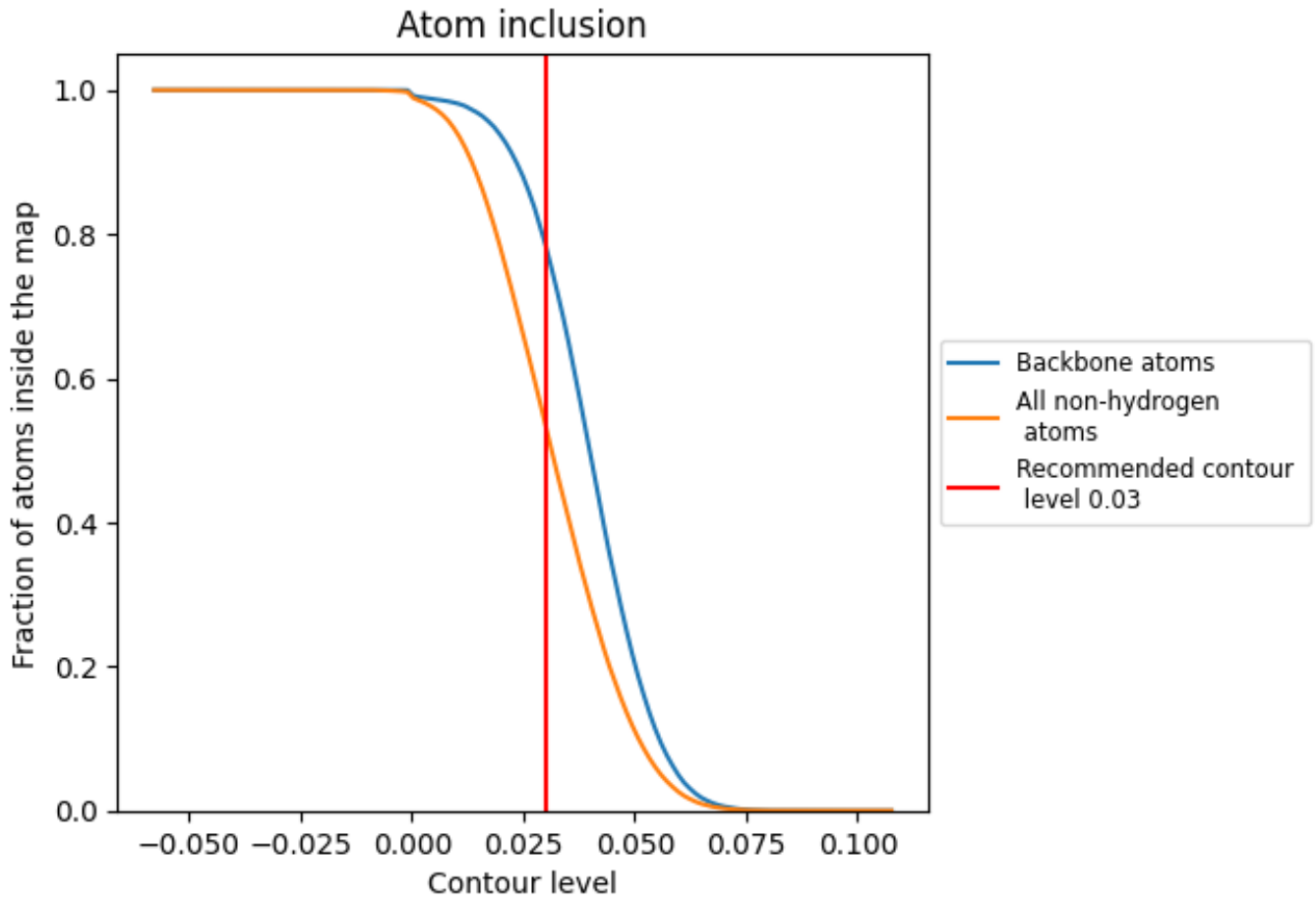
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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