



## Full wwPDB EM Validation Report ⓘ

Oct 26, 2024 – 07:35 PM EDT

PDB ID : 6Q16  
EMDB ID : EMD-20556  
Title : Focussed refinement of InvGN0N1:PrgHK:SpaPQR:PrgIJ from Salmonella SPI-1 injectisome NC-base  
Authors : Hu, J.; Worrall, L.J.; Strynadka, N.C.J.  
Deposited on : 2019-08-02  
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

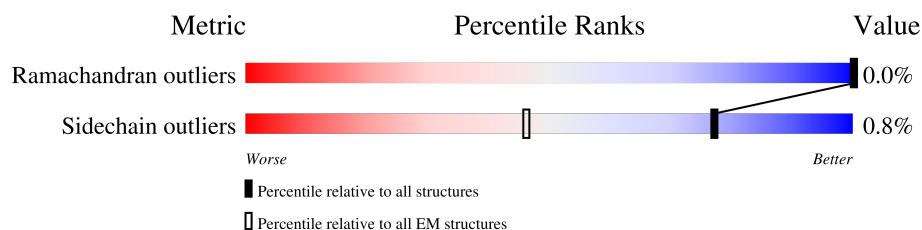
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 4.10 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.






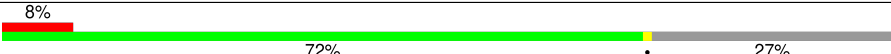
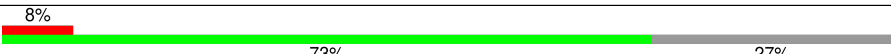
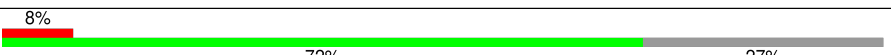
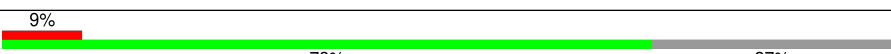
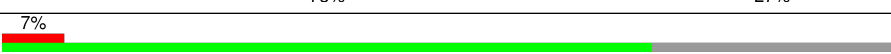

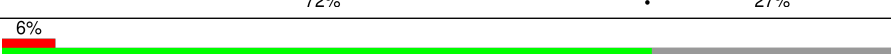
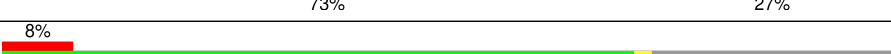
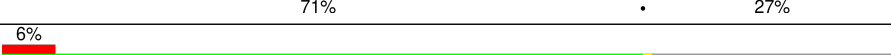
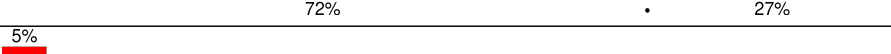
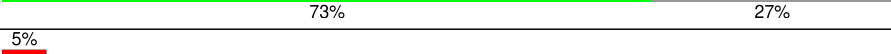











Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	252	
1	AB	252	
1	AC	252	
1	AD	252	
1	AE	252	
1	AF	252	
1	AG	252	
1	AH	252	
1	AI	252	






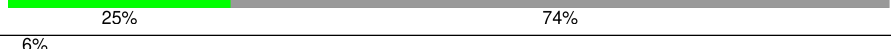
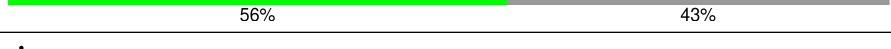
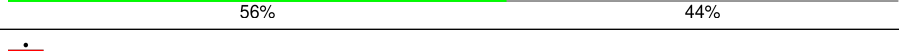
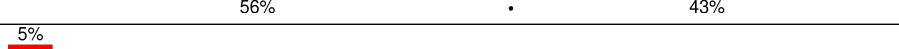
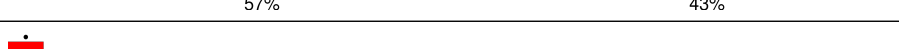
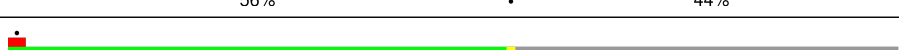

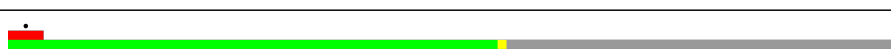

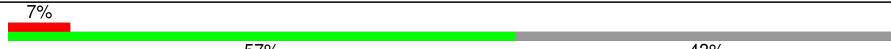





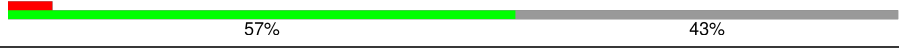
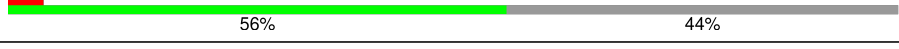



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Mol	Chain	Length	Quality of chain
1	AJ	252	
1	AK	252	
1	AL	252	
1	o	252	
1	p	252	
1	q	252	
1	r	252	
1	s	252	
1	t	252	
1	u	252	
1	v	252	
1	w	252	
1	x	252	
1	y	252	
1	z	252	
2	A	562	
2	B	562	
2	C	562	
2	D	562	
2	F	562	
2	G	562	
2	H	562	
2	I	562	
2	J	562	
2	K	562	

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Mol	Chain	Length	Quality of chain
2	L	562	
2	M	562	
2	N	562	
2	O	562	
2	P	562	
2	Q	562	
3	E	392	
3	R	392	
3	S	392	
3	T	392	
3	U	392	
3	V	392	
3	W	392	
3	X	392	
3	Y	392	
3	Z	392	
3	a	392	
3	b	392	
3	c	392	
3	d	392	
3	e	392	
3	f	392	
3	g	392	
3	h	392	
3	i	392	

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Mol	Chain	Length	Quality of chain
3	j	392	
3	k	392	
3	l	392	
3	m	392	
3	n	392	
4	0	224	
4	1	224	
4	2	224	
4	3	224	
4	4	224	
5	5	263	
6	6	86	
6	7	86	
6	8	86	
6	9	86	
7	AM	101	
7	AN	101	
7	AO	101	
7	AP	101	
7	AQ	101	
7	AR	101	
8	AS	80	
8	AT	80	
8	AU	80	
8	AV	80	

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Mol	Chain	Length	Quality of chain
8	AW	80	
8	AX	80	
8	AY	80	
8	AZ	80	
8	BA	80	
8	BB	80	
8	BC	80	
8	BD	80	
8	BE	80	

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 118198 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 1431	C 901	N 250	O 277	S 3	0	0
1	AB	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AC	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AD	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AE	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AF	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AG	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AH	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AI	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AL	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	o	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	p	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	q	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	r	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	s	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	t	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	u	184	Total 1431	C 901	N 250	O 277	S 3	0	0

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

- Molecule 2 is a protein called Protein InvG.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
2	B	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
2	C	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
2	D	144	Total	C	N	O	S	0	0
			1146	736	195	209	6		
2	F	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
2	G	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
2	H	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
2	I	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
2	J	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
2	K	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
2	L	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
2	M	144	Total	C	N	O	S	0	0
			1146	736	195	209	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
2	O	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
2	P	139	Total	C	N	O	S	0	0
			1108	710	189	203	6		
2	Q	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		

- Molecule 3 is a protein called Protein PrgH.

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

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

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

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

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

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

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

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

- Molecule 7 is a protein called Protein PrgJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AM	39	Total	C	N	O	S	0	0
			298	187	49	60	2		
7	AN	78	Total	C	N	O	S	7	0
			644	396	116	130	2		
7	AO	88	Total	C	N	O	S	0	0
			667	410	114	140	3		
7	AP	89	Total	C	N	O	S	0	0
			675	416	115	141	3		
7	AQ	89	Total	C	N	O	S	0	0
			675	416	115	141	3		
7	AR	88	Total	C	N	O	S	0	0
			667	410	114	140	3		

- Molecule 8 is a protein called Protein PrgI.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AS	59	Total	C	N	O	0	0
			466	294	80	92		
8	AT	59	Total	C	N	O	0	0
			466	294	80	92		
8	AU	59	Total	C	N	O	0	0
			466	294	80	92		
8	AV	59	Total	C	N	O	0	0
			466	294	80	92		
8	AW	59	Total	C	N	O	0	0
			466	294	80	92		
8	AX	73	Total	C	N	O	0	0
			574	362	95	117		
8	AY	78	Total	C	N	O	0	0
			612	387	101	124		
8	AZ	57	Total	C	N	O	0	0
			460	289	76	95		

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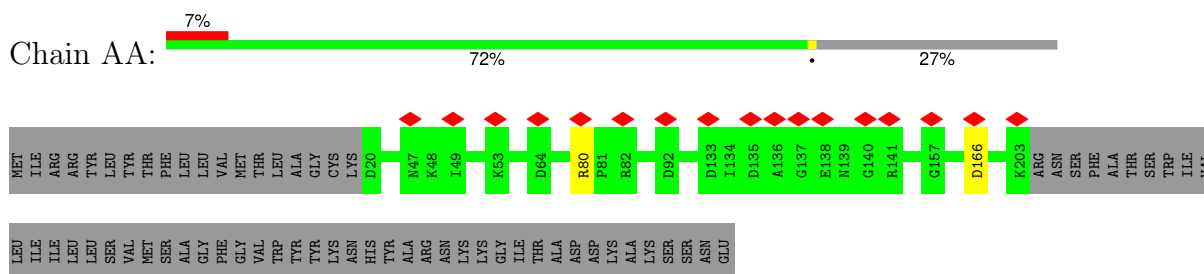
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Mol	Chain	Residues	Atoms				AltConf	Trace
8	BA	54	Total	C	N	O	0	0
			437	275	73	89		
8	BB	48	Total	C	N	O	0	0
			388	247	64	77		
8	BC	48	Total	C	N	O	0	0
			388	247	64	77		
8	BD	48	Total	C	N	O	0	0
			388	247	64	77		
8	BE	43	Total	C	N	O	0	0
			346	219	59	68		

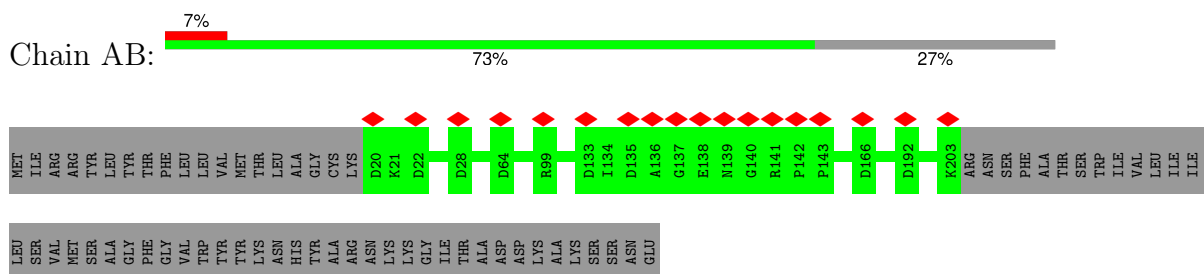
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

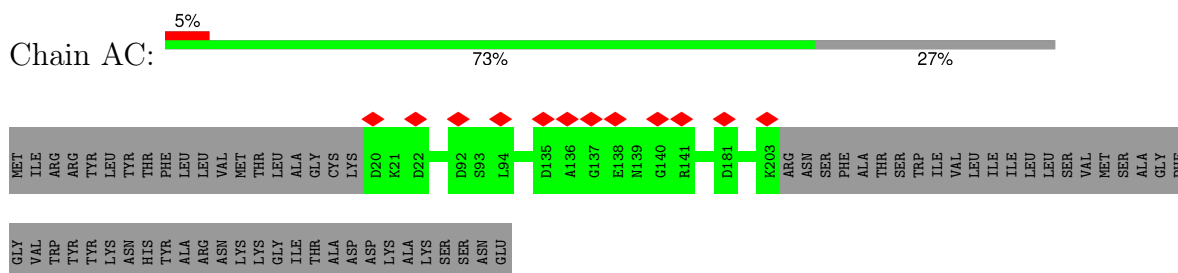
#### • Molecule 1: Lipoprotein PrgK



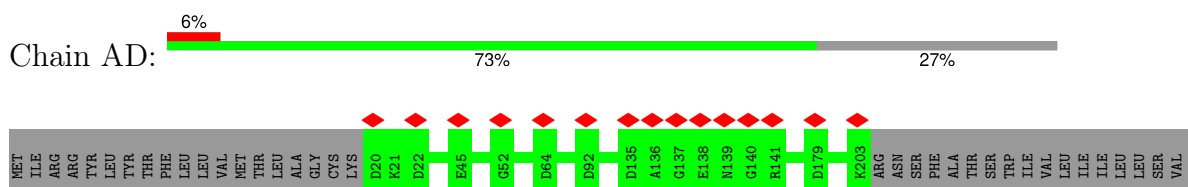
#### • Molecule 1: Lipoprotein PrgK



#### • Molecule 1: Lipoprotein PrgK



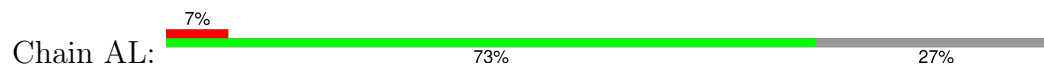
#### • Molecule 1: Lipoprotein PrgK





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

• Molecule 1: Lipoprotein PrgK



MET ILE ARG ARG MET SER LEU TYR TYR PHE GLY PHE GLY VAL TRP TRP TYR TYR MET THR ASN HIS TYR ALA ARG ASN LYS D20 D92 S93 L94 E121 I134 D135 A136 G137 E138 N139 G140 R141 P142 G157 D177 V178 D179 A193 K203 ARG ASN SER PHE ALA THR SER TRP ILE VAL ILE ILE LEU

LEU VAL MET MET SER ARG ALA PHE GLY PHE GLY VAL TRP TRP TYR TYR MET THR LYS ASN HIS TYR ALA ARG ASN LYS D20 D92 S93 L94 E121 I134 D135 A136 G137 E138 N139 G140 R141 P142 G157 D177 V178 D179 A193 K203 ARG ASN SER PHE ALA THR SER TRP ILE VAL ILE ILE LEU

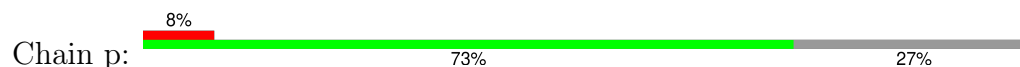
• Molecule 1: Lipoprotein PrgK



MET ILE ARG ARG MET SER LEU TYR TYR PHE GLY PHE GLY VAL TRP TRP TYR TYR MET THR LYS D20 K53 E62 P63 D64 R60 D92 S93 L94 Y95 E121 D133 I134 D135 A136 G137 E138 N139 G140 R141 G157 L160 D179 Y180 D181 K203 ARG ASN SER PHE ALA

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

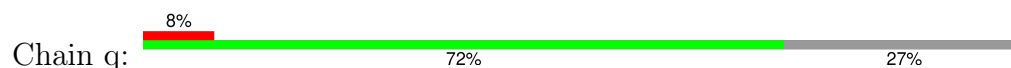
• Molecule 1: Lipoprotein PrgK



MET ILE ARG ARG MET SER LEU TYR TYR PHE GLY PHE GLY VAL TRP TRP TYR TYR MET THR LYS D20 G52 K53 L54 D64 D92 S93 D133 I134 D135 A136 G137 E138 N139 G140 L160 Q163 R190 S191 D192 K203 ARG ASN SER PHE ALA THR SER TRP ILE VAL LEU ILE

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

• Molecule 1: Lipoprotein PrgK



MET ILE ARG ARG MET SER LEU TYR TYR PHE GLY PHE GLY VAL TRP TRP TYR TYR MET THR LYS D20 L24 E30 L54 D64 Q76 R82 D92 S93 L94 D133 I134 D135 A136 G137 E138 N139 G140 R141 G157 K172 D177 G199 V202 K203 ARG ASN SER

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

• Molecule 1: Lipoprotein PrgK



MET ILE ARG ARG MET SER LEU TYR TYR PHE GLY PHE GLY VAL TRP TRP TYR TYR MET THR LYS D20 K21 D22 D23 D50 S51 G52 K53 L54 E62 P63 D64 R80 D92 D135 A136 G137 E138 D166 A176 D177 V178 D179 D192 V202 K203 ARG ASN SER PHE ALA

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

• Molecule 1: Lipoprotein PrgK

Chain s:  7% 73% 27%

MET ILE ARG ARG TYR LEU THR THR PHE LEU VAL MET THR ALA GLY TYR CYS LYS D20 D41 K53 D64 R80 A91 D92 S93 L94 V95 E110 D133 I134 D135 A136 G137 E138 N139 G140 R141 G157 K203 ARG ASN SER PHE ALA THR SER TRP ILE VAL

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


• Molecule 1: Lipoprotein PrgK

Chain t:  8% 72% 27%

MET ILE ARG ARG TYR LEU THR THR PHE LEU VAL MET THR ALA GLY TYR CYS LYS D20 G52 D64 Q76 R98 A91 D92 S93 L94 V95 K102 I134 D135 A136 G137 E138 N139 G140 R141 G157 L195 K203 ARG ASN SER PHE ALA THR SER TRP ILE

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

• Molecule 1: Lipoprotein PrgK

Chain u:  6% 73% 27%

MET ILE ARG ARG TYR LEU THR THR PHE LEU VAL MET THR ALA GLY TYR CYS LYS D20 V95 R99 E121 D133 I134 D135 A136 G137 E138 N139 G140 R141 P142 L171 D192 K203 ARG ASN SER PHE ALA THR SER TRP ILE VAL ILE ILE LEU LEU VAL

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


• Molecule 1: Lipoprotein PrgK

Chain v:  8% 71% 27%

MET ILE ARG ARG TYR LEU THR THR PHE LEU VAL MET THR ALA GLY TYR CYS LYS D20 K53 L54 D64 I72 R80 P81 R82 A91 D92 S93 L94 V95 D133 I134 D135 A136 G137 E138 N139 G140 S158 D179 V202 K203 ARG ASN SER PHE ALA THR SER

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

• Molecule 1: Lipoprotein PrgK


Chain w:  6% 72% 27%

MET ILE ARG ARG TYR LEU THR THR PHE LEU VAL MET THR ALA GLY TYR CYS LYS D20 D28 E62 R80 D92 S93 L94 V95 D133 I134 D135 A136 G137 E138 N139 G140 R141 D177 V178 D179 Y180 D181 K203 ARG ASN SER PHE ALA THR SER TRP ILE VAL LEU



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• Molecule 1: Lipoprotein PrgK

Chain x:  5% 73% 27%

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S93  
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A136  
G137  
E138  
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G140  
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• Molecule 1: Lipoprotein PrgK

Chain y:  5% 72% 27%

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• Molecule 1: Lipoprotein PrgK

Chain z:  6% 72% 27%

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• Molecule 1: Lipoprotein PrgK

Chain AJ:  8% 72% 27%

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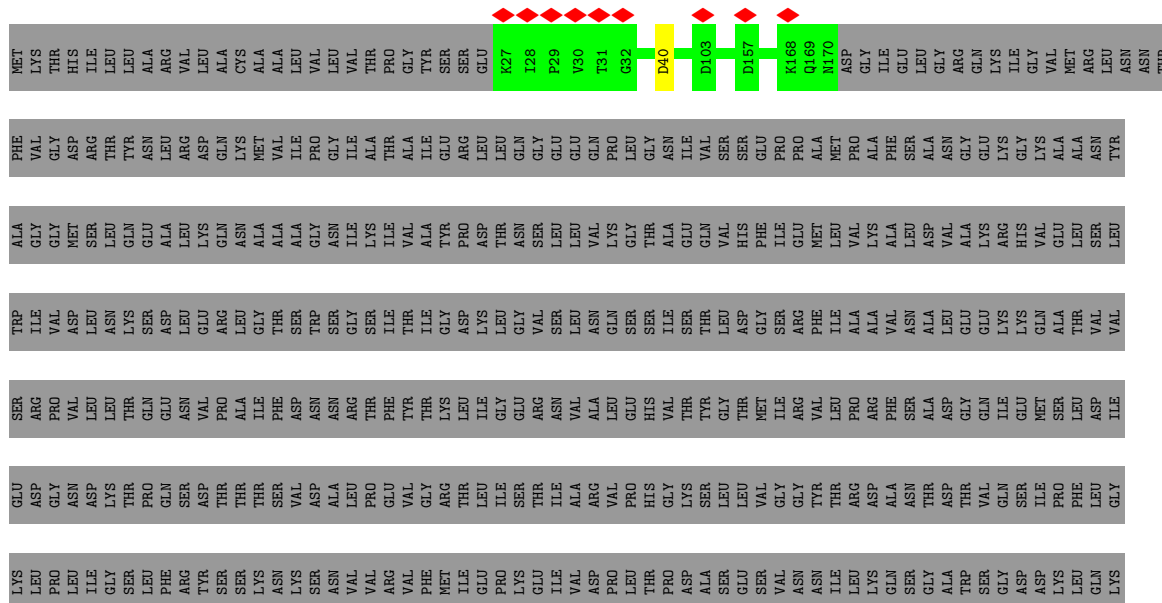
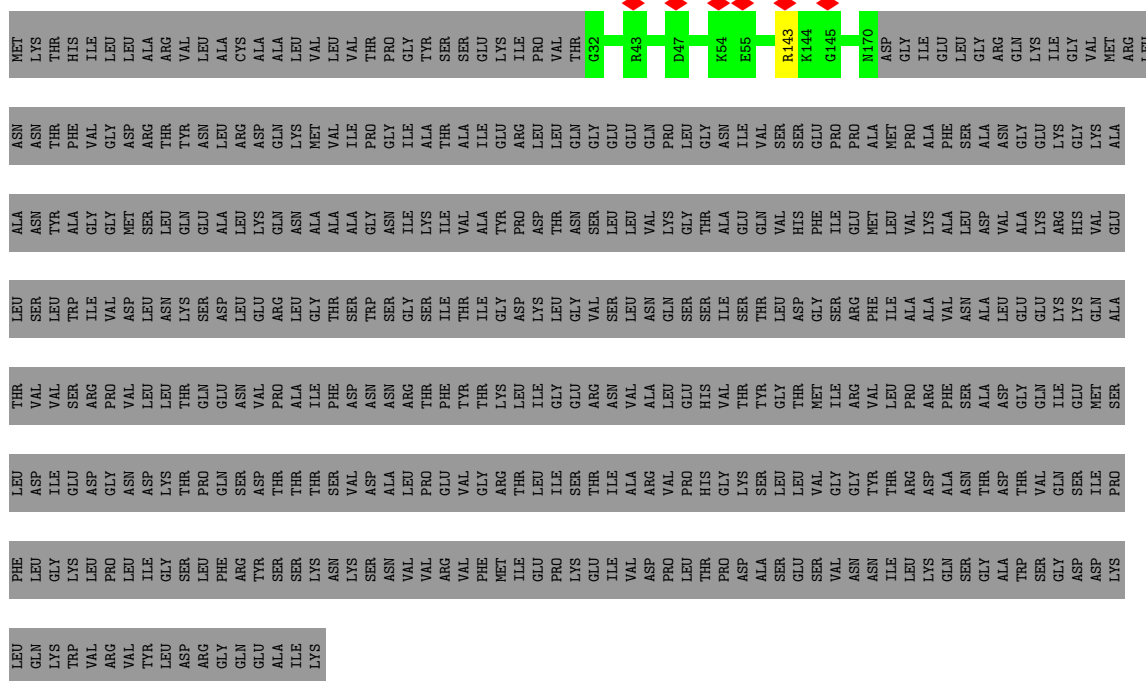
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• Molecule 1: Lipoprotein PrgK

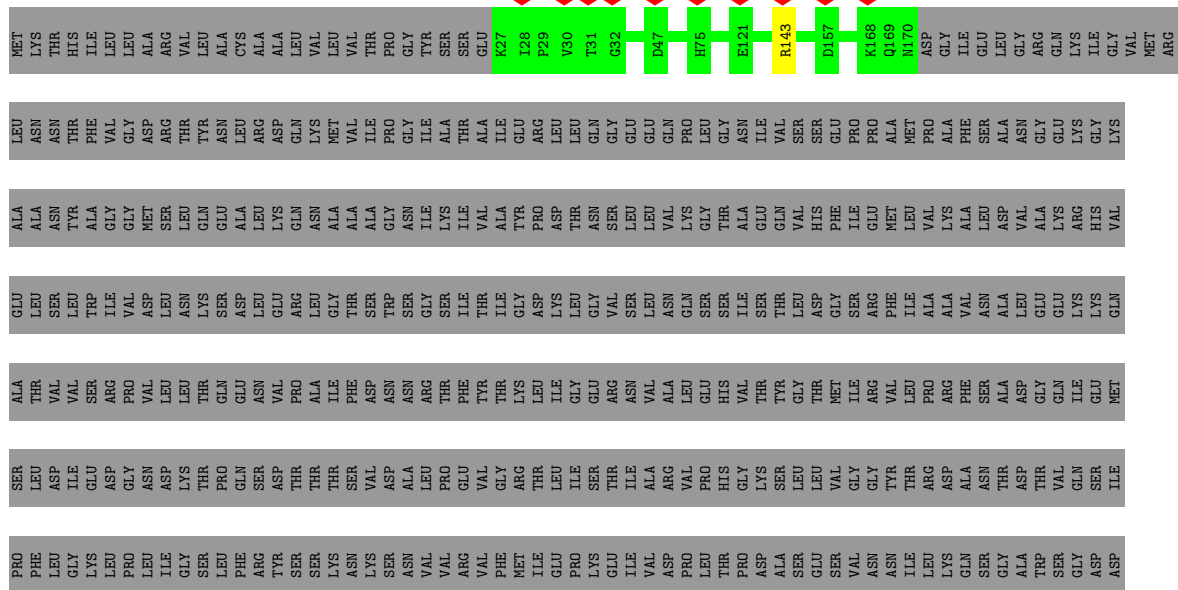
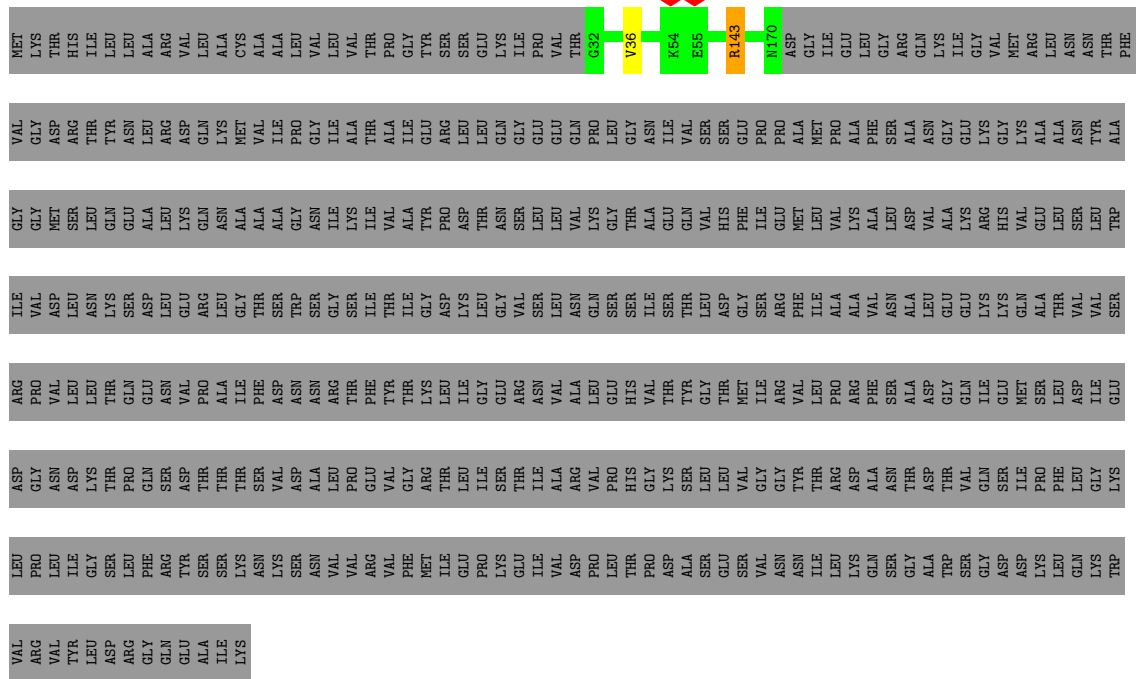
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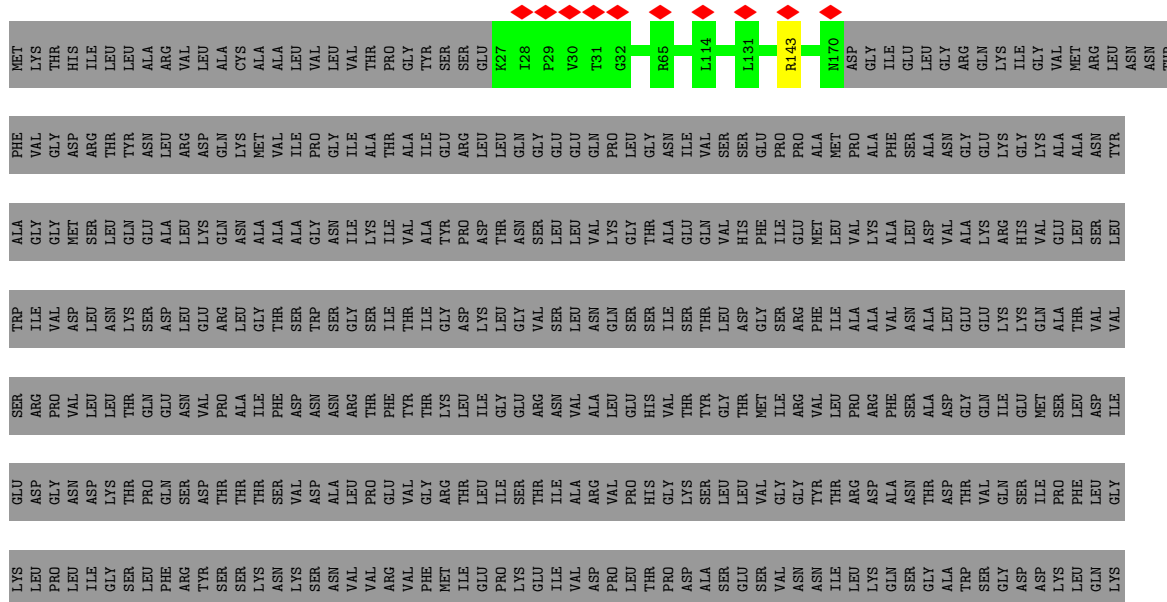
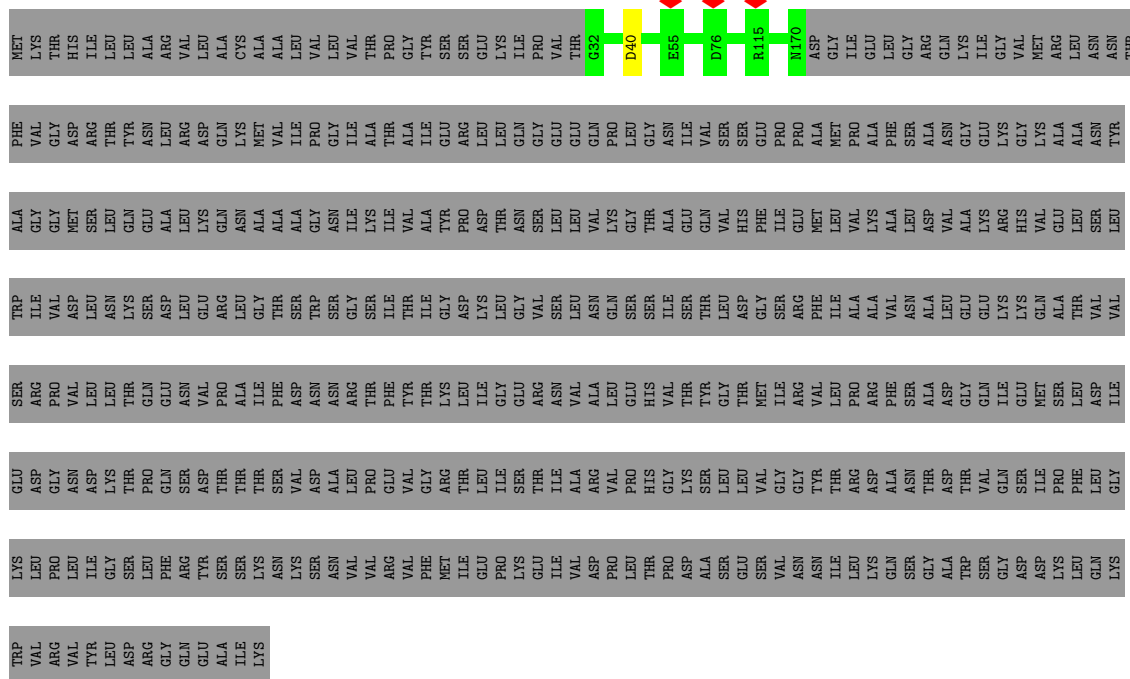
MET  
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CYS  
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D20  
M41  
D64  
R80  
D92  
V95  
D133  
I134  
D135  
A136  
G137  
E138  
N139  
G140  
R141  
G157  
D179  
K203  
ARG  
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ASP  
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GLY  
GLN  
GLU  
ALA  
ILE  
LYS

● Molecule 2: Protein InvG



LYS	GLY	LYS	ILE	SER	VAL	LEU	THR	GLY	ASP	ASN	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY</
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● Molecule 2: Protein InvG



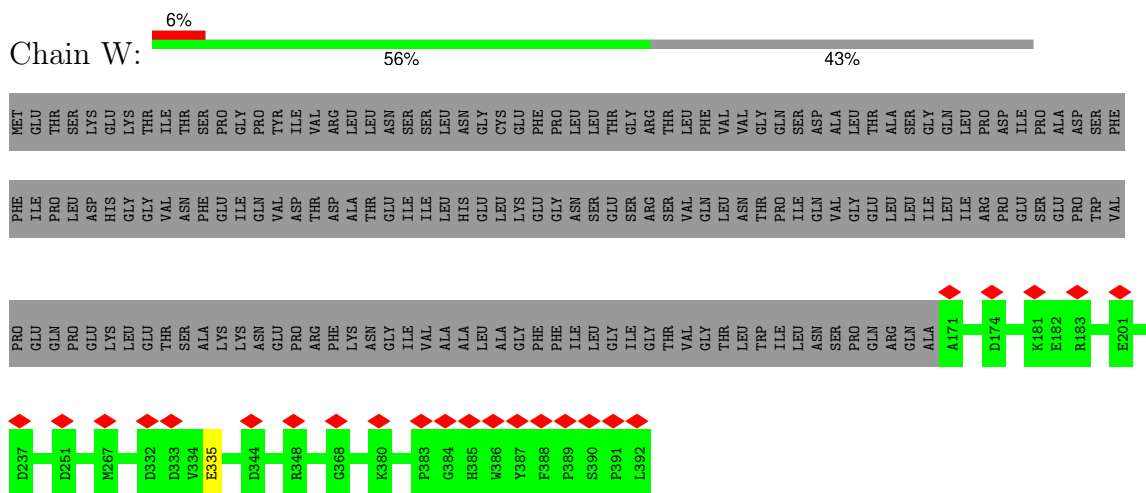
MET	LYS	THR	HIS	VAL	ASP	VAL	LEU	LEU	ALA	VAL	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
TYR	ASN	LEU	ARG	VAL	ASP	GLN	GLY	LYS	MET	VAL	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
GLN	GLU	ALA	LEU	LEU	GLY	GLN	ASN	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY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



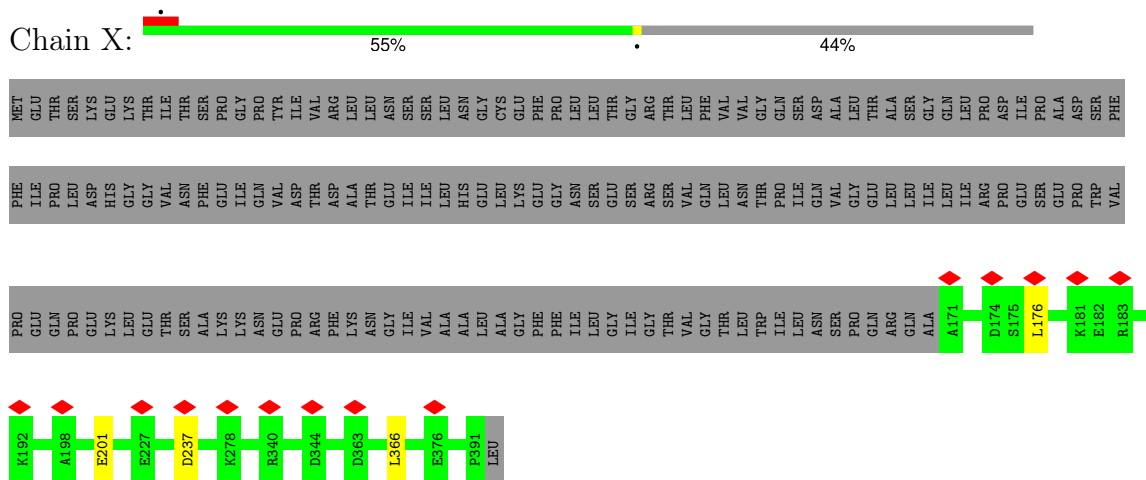




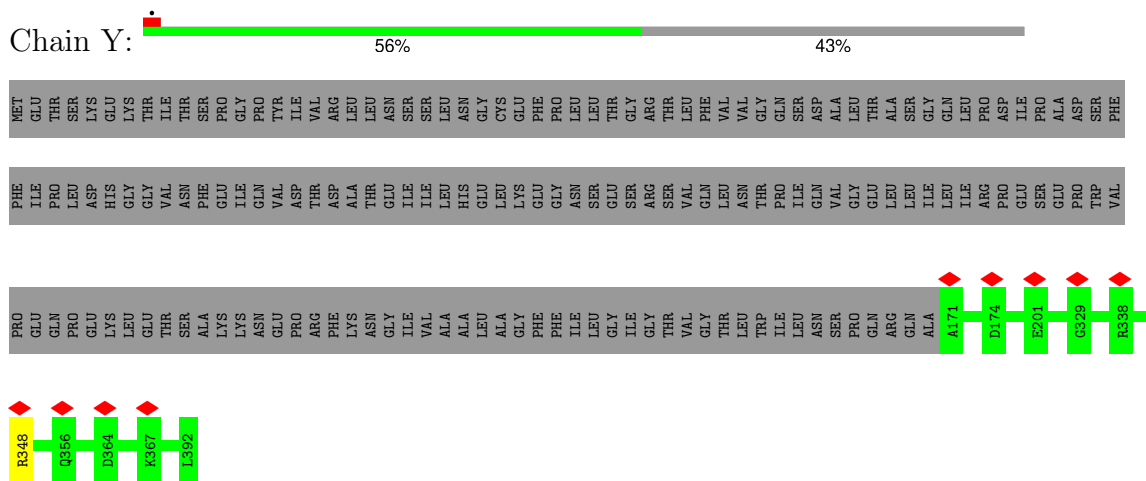




- Molecule 3: Protein PrgH

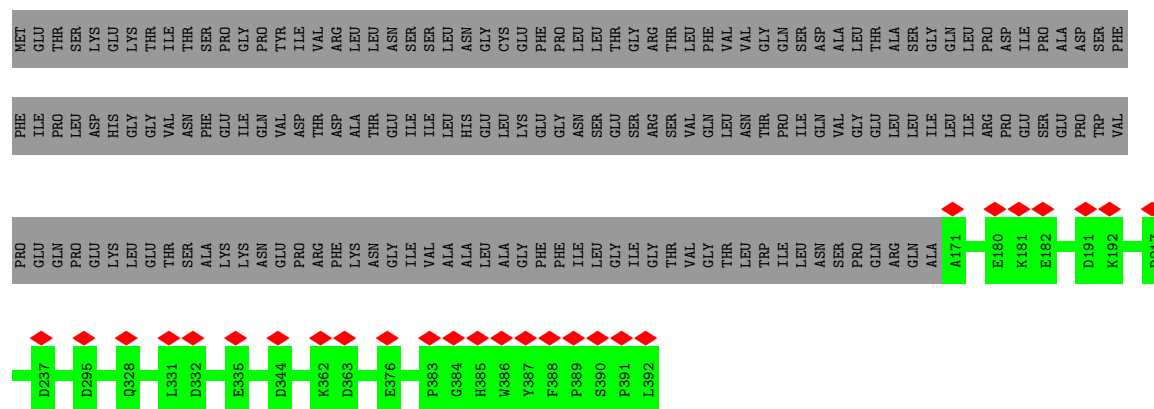


- Molecule 3: Protein PrgH

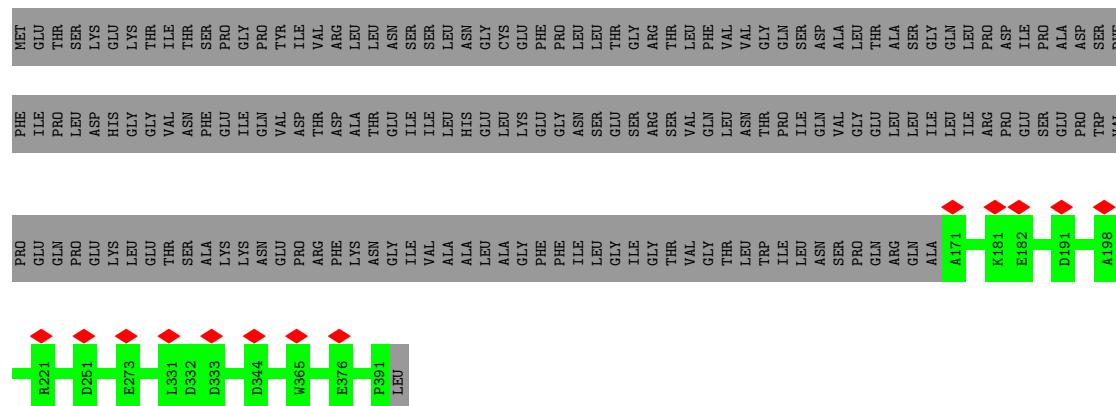


- Molecule 3: Protein PrgH

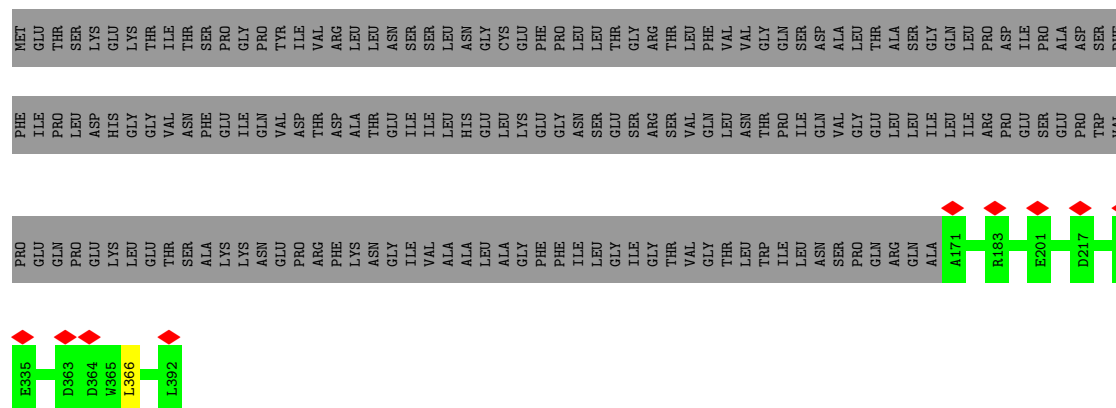




- Molecule 3: Protein PrgH

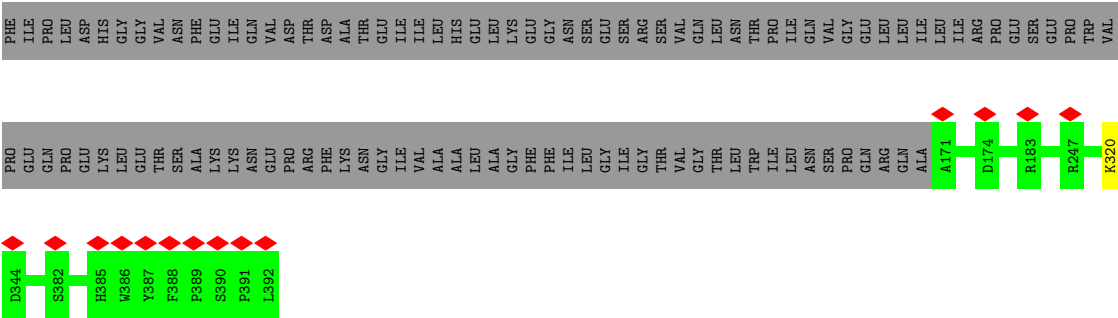


- Molecule 3: Protein PrgH

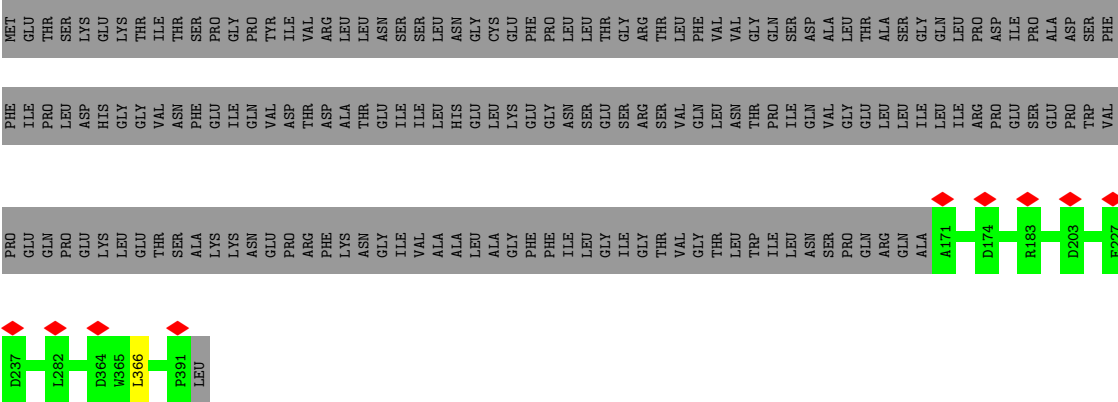


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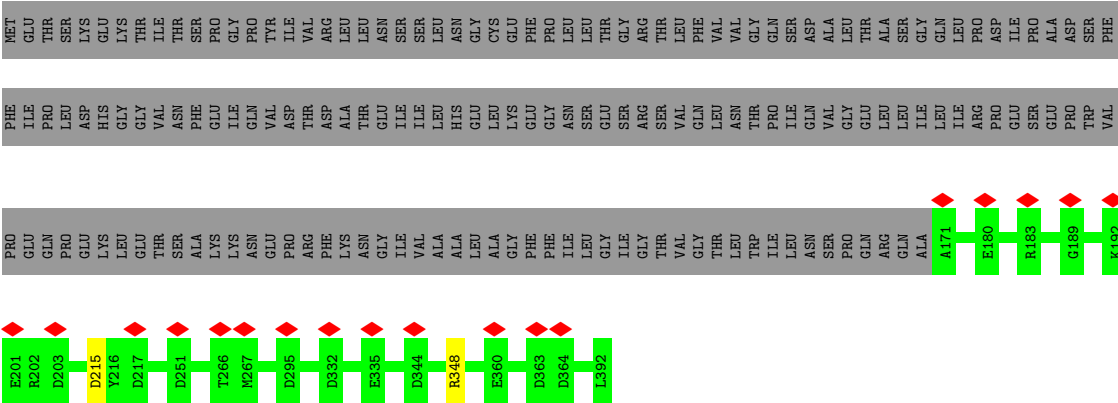




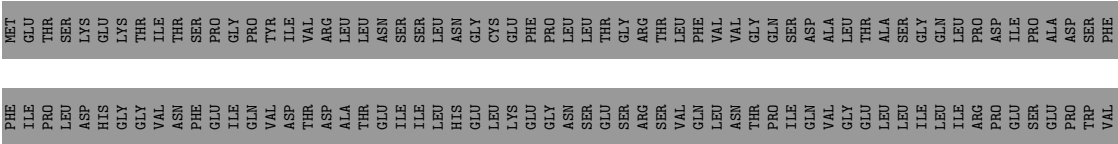
• Molecule 3: Protein PrgH

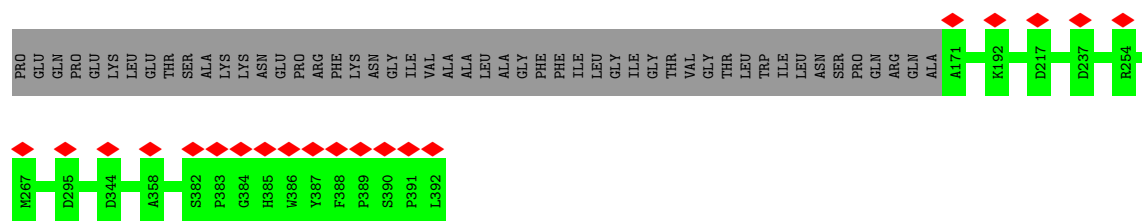


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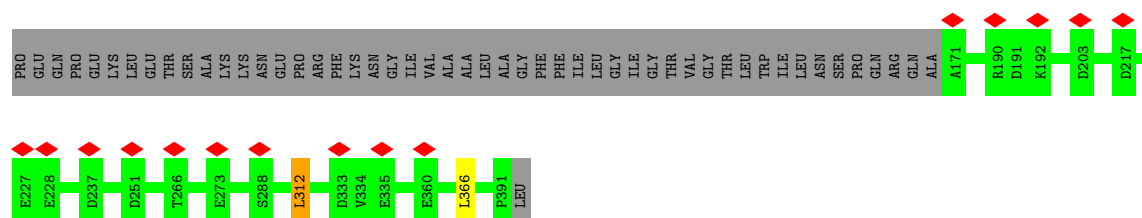


• Molecule 3: Protein PrgH

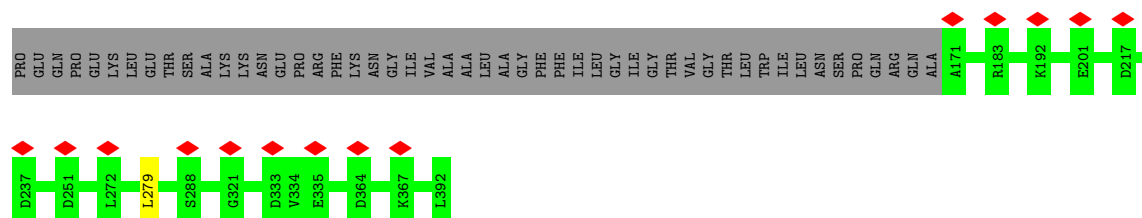
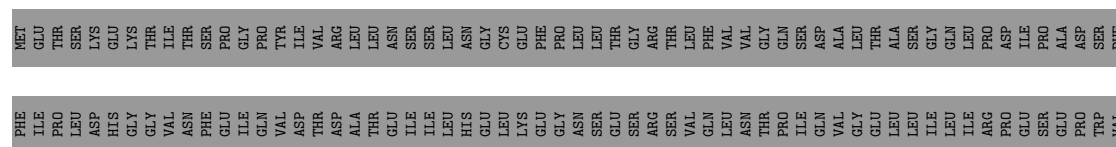




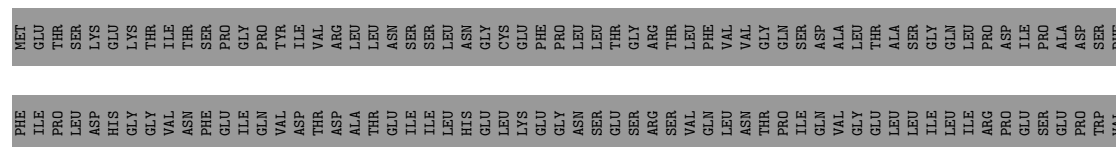
- Molecule 3: Protein PrgH

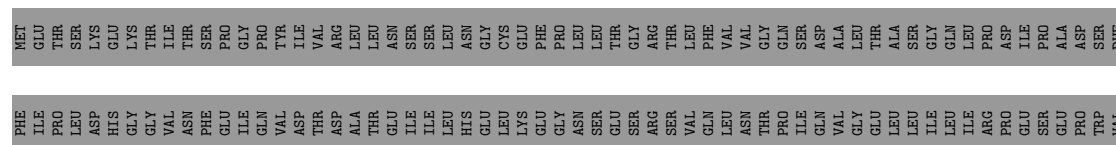


- Molecule 3: Protein PrgH



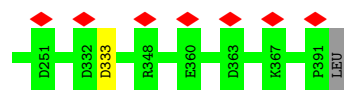
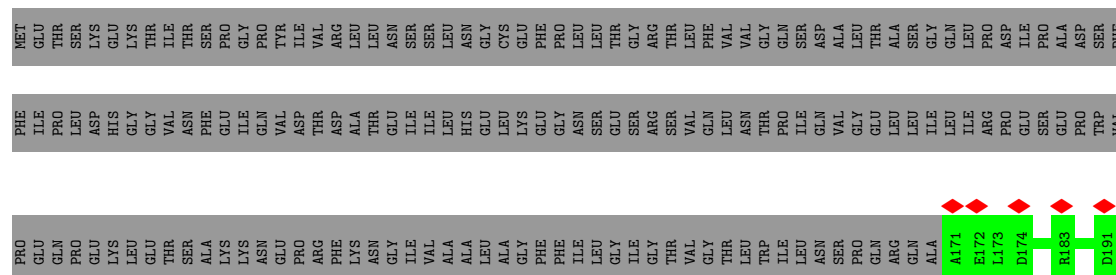
- Molecule 3: Protein PrgH



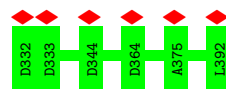
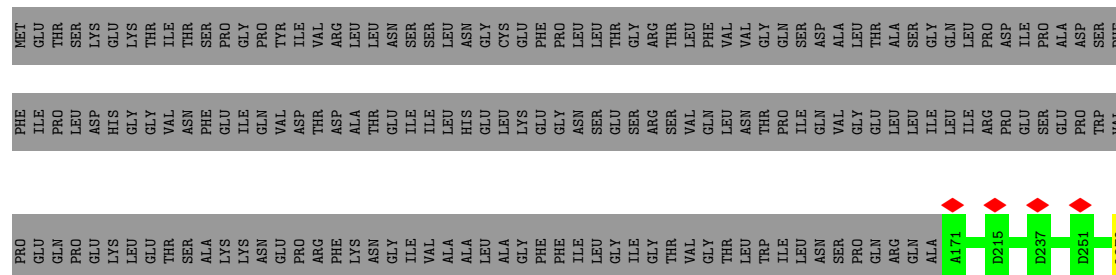




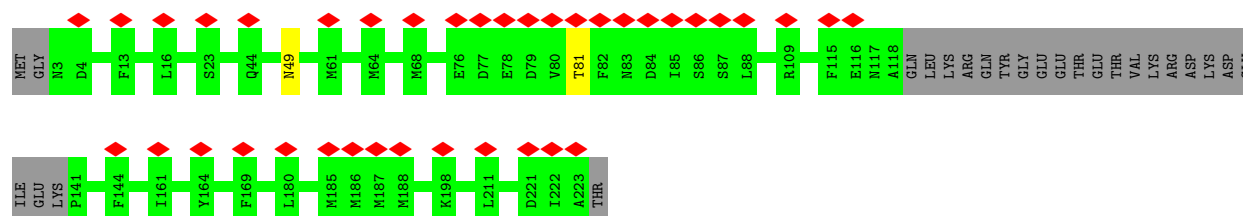
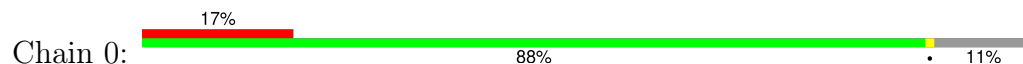
- Molecule 3: Protein PrgH



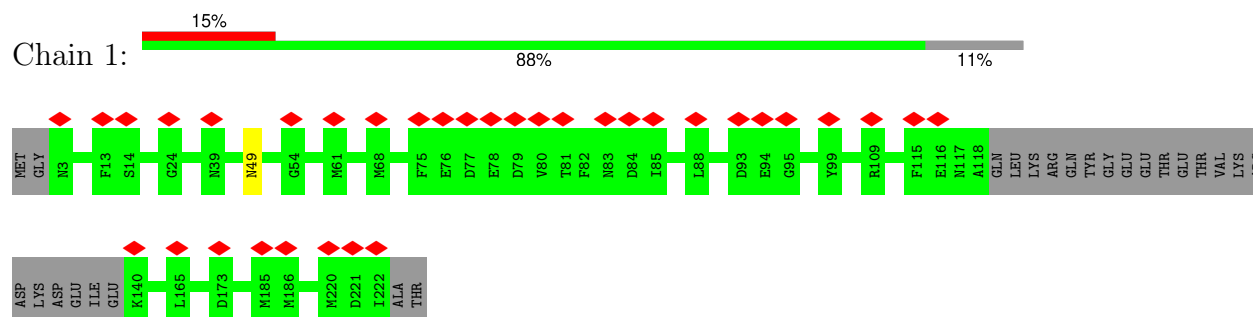
- Molecule 3: Protein PrgH



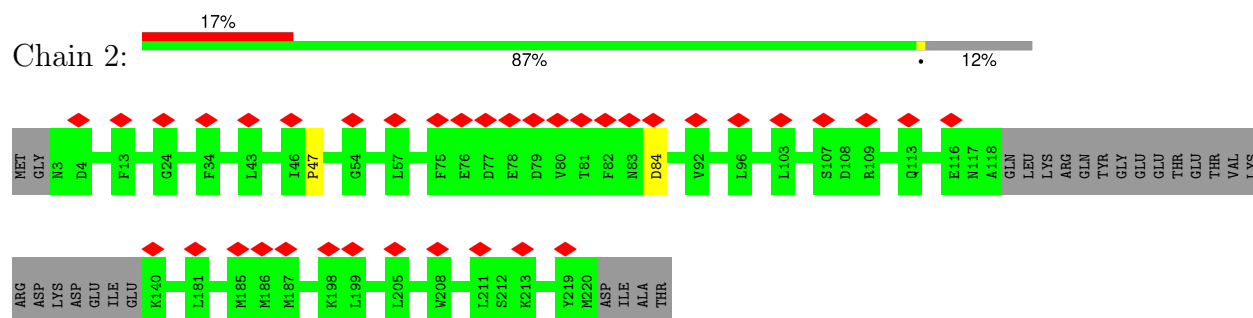
- Molecule 4: Surface presentation of antigens protein SpaP



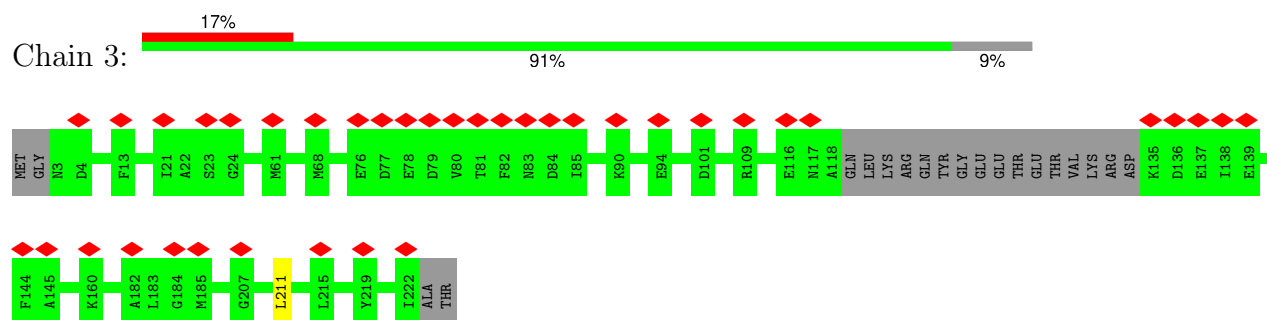
- Molecule 4: Surface presentation of antigens protein SpaP



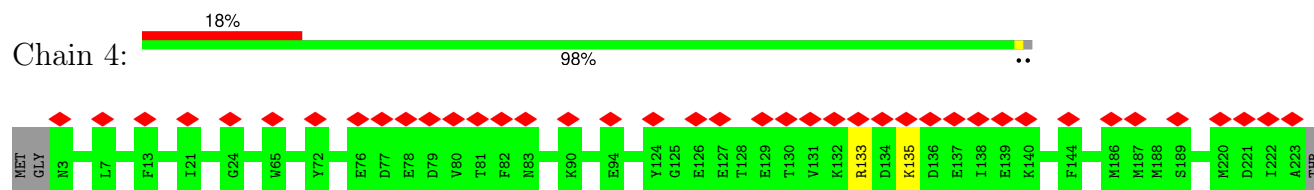
- Molecule 4: Surface presentation of antigens protein SpaP



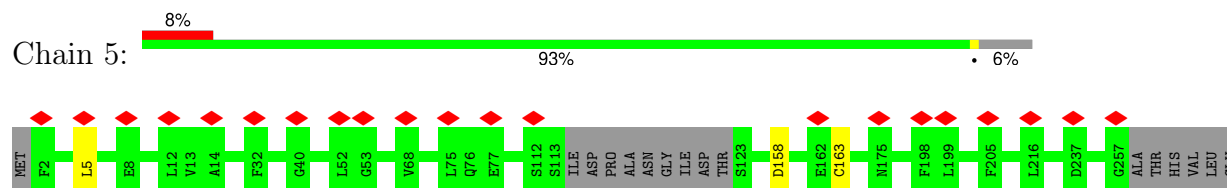
- Molecule 4: Surface presentation of antigens protein SpaP



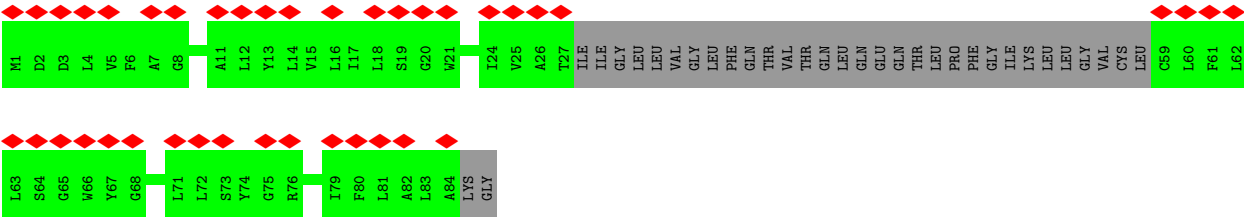
- Molecule 4: Surface presentation of antigens protein SpaP



- Molecule 5: Surface presentation of antigens protein SpaR



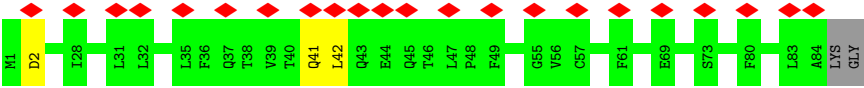
- Molecule 6: Surface presentation of antigens protein SpaQ



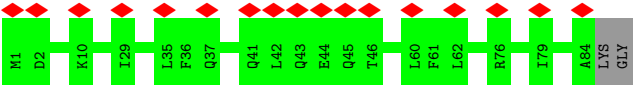
• Molecule 6: Surface presentation of antigens protein SpaQ



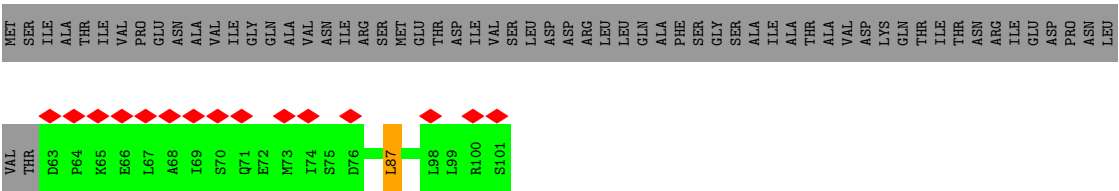
• Molecule 6: Surface presentation of antigens protein SpaQ



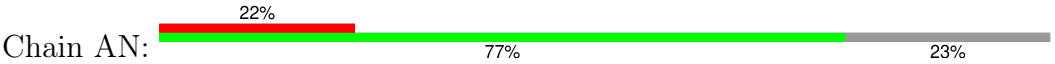
• Molecule 6: Surface presentation of antigens protein SpaQ

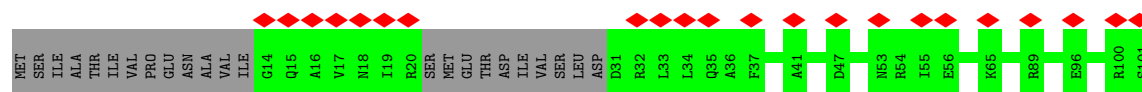


• Molecule 7: Protein PrgJ

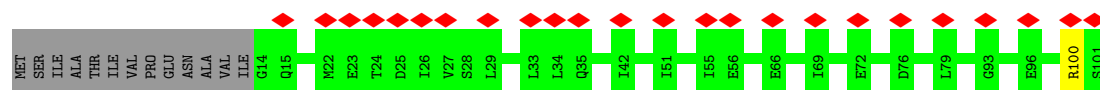
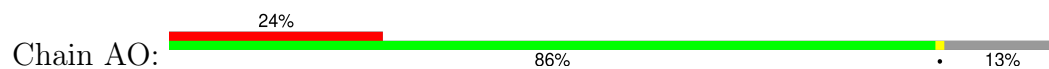


• Molecule 7: Protein PrgJ

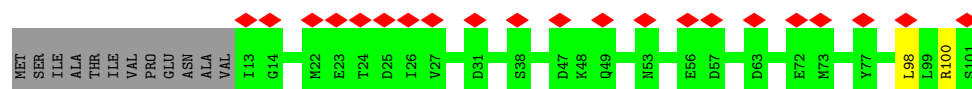
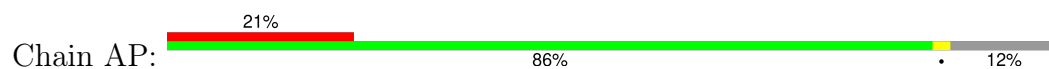




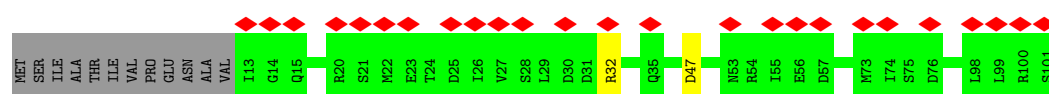
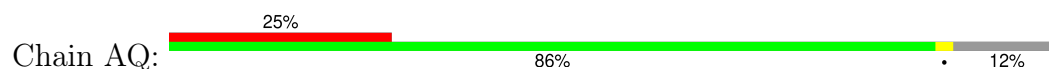
• Molecule 7: Protein PrgJ



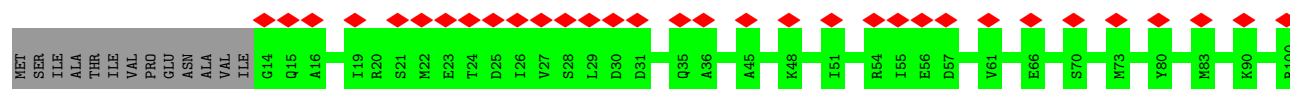
• Molecule 7: Protein PrgJ



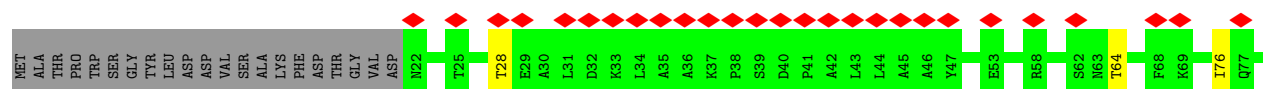
• Molecule 7: Protein PrgJ



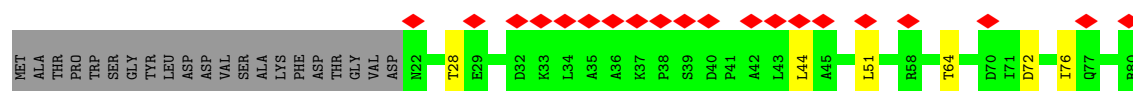
• Molecule 7: Protein PrgJ



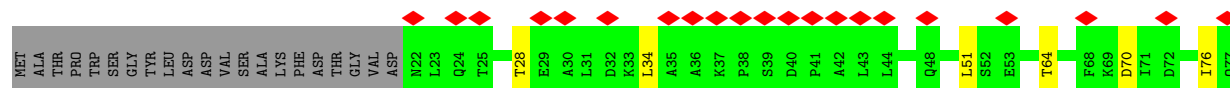
• Molecule 8: Protein PrgI



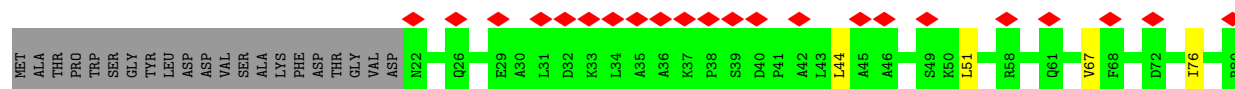
• Molecule 8: Protein PrgI



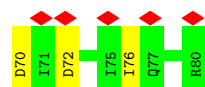
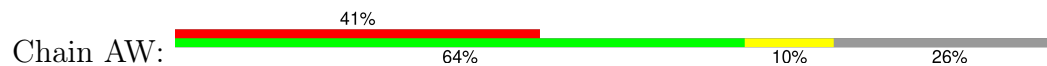
- Molecule 8: Protein PrgI



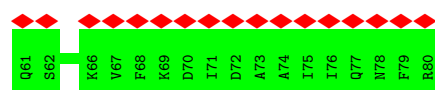
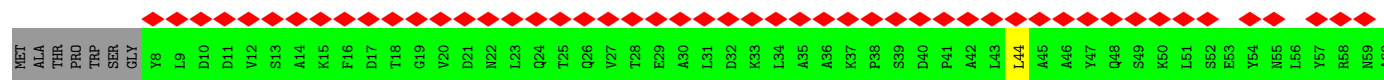
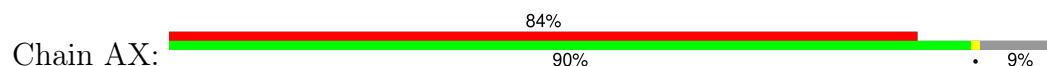
- Molecule 8: Protein PrgI



- Molecule 8: Protein PrgI

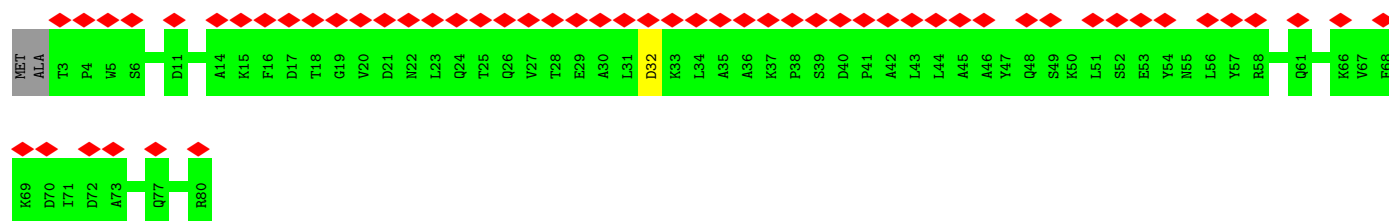


- Molecule 8: Protein PrgI

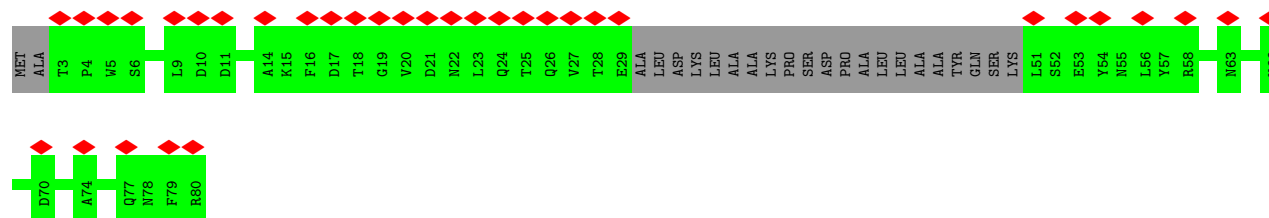
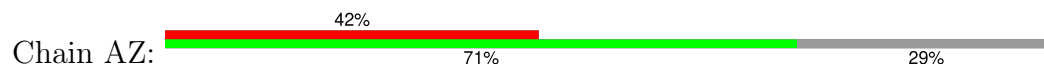


- Molecule 8: Protein PrgI

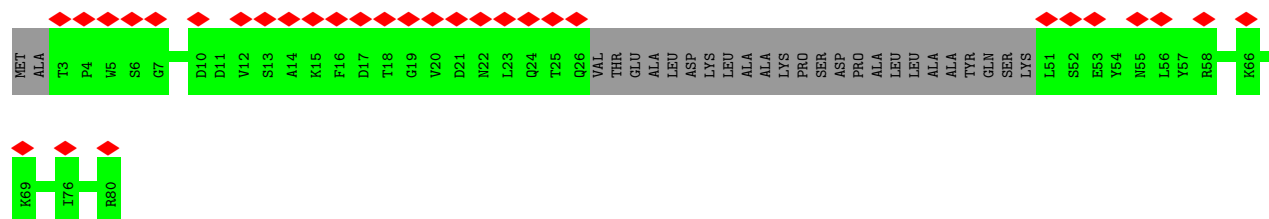
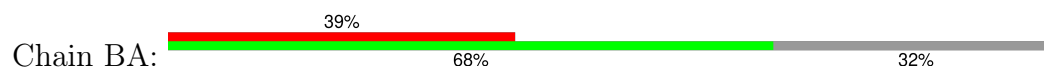




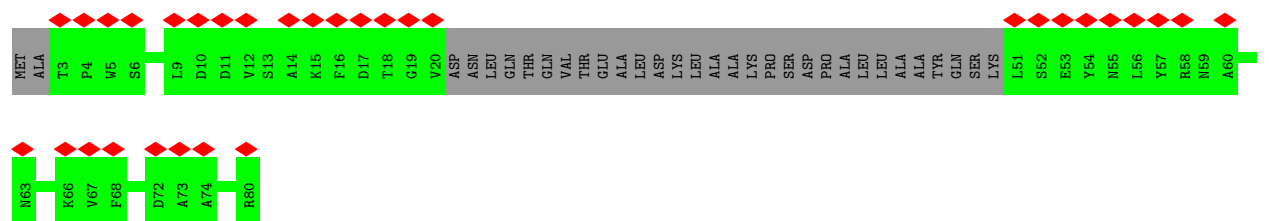
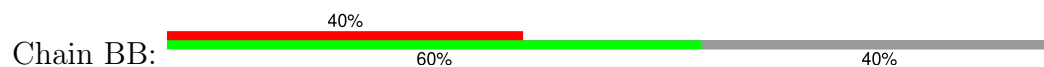
• Molecule 8: Protein PrgI



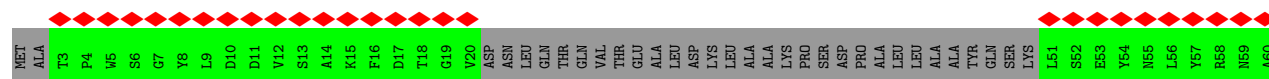
• Molecule 8: Protein PrgI

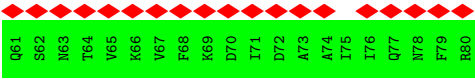


• Molecule 8: Protein PrgI

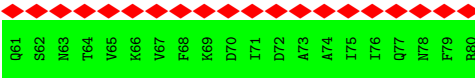
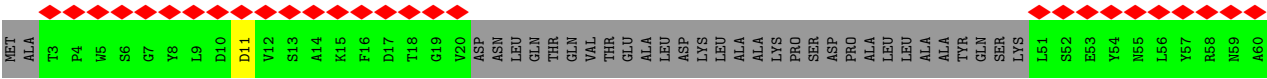


• Molecule 8: Protein PrgI

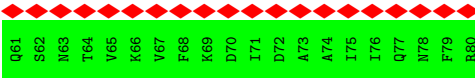
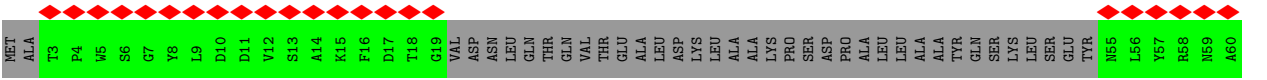




● Molecule 8: Protein PrgI



● Molecule 8: Protein PrgI



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19141	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	51.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.147	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.035	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	0.43	0/1458	0.61	0/1979
1	AB	0.40	0/1458	0.59	0/1979
1	AC	0.43	0/1458	0.60	0/1979
1	AD	0.40	0/1458	0.61	0/1979
1	AE	0.42	0/1458	0.60	0/1979
1	AF	0.42	0/1458	0.59	0/1979
1	AG	0.42	0/1458	0.59	0/1979
1	AH	0.41	0/1458	0.58	0/1979
1	AI	0.41	0/1458	0.61	0/1979
1	AJ	0.41	0/1458	0.64	2/1979 (0.1%)
1	AK	0.40	0/1458	0.59	0/1979
1	AL	0.41	0/1458	0.60	0/1979
1	o	0.41	0/1458	0.59	1/1979 (0.1%)
1	p	0.40	0/1458	0.57	0/1979
1	q	0.42	1/1458 (0.1%)	0.58	1/1979 (0.1%)
1	r	0.39	0/1458	0.60	0/1979
1	s	0.40	0/1458	0.59	0/1979
1	t	0.42	1/1458 (0.1%)	0.63	1/1979 (0.1%)
1	u	0.40	0/1458	0.62	1/1979 (0.1%)
1	v	0.42	0/1458	0.60	1/1979 (0.1%)
1	w	0.40	0/1458	0.61	1/1979 (0.1%)
1	x	0.41	0/1458	0.61	0/1979
1	y	0.42	0/1458	0.62	1/1979 (0.1%)
1	z	0.41	0/1458	0.63	1/1979 (0.1%)
2	A	0.39	0/1131	0.65	3/1525 (0.2%)
2	B	0.41	0/1181	0.65	1/1593 (0.1%)
2	C	0.40	0/1131	0.60	0/1525
2	D	0.41	0/1170	0.59	0/1579
2	F	0.41	0/1131	0.59	0/1525
2	G	0.40	0/1181	0.60	0/1593
2	H	0.45	0/1131	0.63	1/1525 (0.1%)
2	I	0.39	0/1181	0.59	0/1593
2	J	0.42	0/1131	0.58	0/1525
2	K	0.41	0/1181	0.61	0/1593

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	L	0.41	0/1131	0.59	0/1525
2	M	0.39	0/1170	0.61	1/1579 (0.1%)
2	N	0.42	0/1131	0.59	0/1525
2	O	0.40	0/1181	0.63	0/1593
2	P	0.41	0/1131	0.58	0/1525
2	Q	0.41	0/1181	0.62	0/1593
3	E	0.39	0/1881	0.58	0/2541
3	R	0.39	0/1872	0.62	2/2530 (0.1%)
3	S	0.40	0/1876	0.58	1/2536 (0.0%)
3	T	0.38	0/1881	0.56	0/2541
3	U	0.38	0/1872	0.60	1/2530 (0.0%)
3	V	0.38	0/1876	0.63	2/2536 (0.1%)
3	W	0.38	0/1881	0.58	0/2541
3	X	0.38	0/1872	0.63	2/2530 (0.1%)
3	Y	0.40	0/1876	0.59	0/2536
3	Z	0.39	0/1881	0.57	0/2541
3	a	0.40	0/1872	0.58	0/2530
3	b	0.39	0/1876	0.57	0/2536
3	c	0.40	0/1881	0.58	0/2541
3	d	0.39	0/1872	0.56	0/2530
3	e	0.39	0/1876	0.59	0/2536
3	f	0.39	0/1881	0.58	0/2541
3	g	0.37	0/1872	0.59	1/2530 (0.0%)
3	h	0.41	0/1876	0.62	1/2536 (0.0%)
3	i	0.38	0/1881	0.56	0/2541
3	j	0.39	0/1872	0.59	0/2530
3	k	0.41	0/1876	0.59	0/2536
3	l	0.41	0/1881	0.60	0/2541
3	m	0.40	0/1872	0.62	0/2530
3	n	0.38	0/1876	0.59	1/2536 (0.0%)
4	0	0.40	0/1598	0.64	0/2172
4	1	0.37	0/1605	0.64	0/2181
4	2	0.36	0/1589	0.63	0/2159
4	3	0.38	0/1642	0.60	0/2230
4	4	0.39	0/1799	0.63	0/2441
5	5	0.39	0/1935	0.68	2/2647 (0.1%)
6	6	0.32	0/414	0.72	0/565
6	7	0.35	0/657	0.69	0/897
6	8	0.37	0/657	0.69	1/897 (0.1%)
6	9	0.38	0/660	0.64	0/900
7	AM	0.40	0/300	0.78	1/403 (0.2%)
7	AN	0.35	0/646	0.59	0/870
7	AO	0.33	0/671	0.59	0/908

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
7	AP	0.36	0/679	0.64	0/919
7	AQ	0.32	0/679	0.63	1/919 (0.1%)
7	AR	0.33	0/671	0.62	0/908
8	AS	0.35	0/472	0.65	0/638
8	AT	0.35	0/472	0.59	0/638
8	AU	0.37	0/472	0.62	0/638
8	AV	0.39	0/472	0.70	1/638 (0.2%)
8	AW	0.35	0/472	0.56	0/638
8	AX	0.33	0/582	0.56	1/788 (0.1%)
8	AY	0.39	0/623	0.62	1/846 (0.1%)
8	AZ	0.31	0/467	0.50	0/632
8	BA	0.31	0/444	0.49	0/600
8	BB	0.33	0/395	0.66	0/533
8	BC	0.30	0/395	0.54	0/533
8	BD	0.32	0/395	0.61	1/533 (0.2%)
8	BE	0.32	0/352	0.59	0/474
All	All	0.40	2/120713 (0.0%)	0.60	36/163413 (0.0%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	q	76	GLN	C-N	-5.89	1.20	1.34
1	t	76	GLN	C-N	-5.27	1.22	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	90	LEU	CA-CB-CG	8.54	134.93	115.30
2	B	47	ASP	CB-CG-OD1	8.49	125.94	118.30
7	AQ	47	ASP	CB-CG-OD2	7.27	124.84	118.30
5	5	158	ASP	CB-CG-OD2	7.17	124.75	118.30
3	h	279	LEU	CA-CB-CG	7.15	131.74	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	n	279	LEU	CA-CB-CG	7.12	131.67	115.30
8	AV	51	LEU	CA-CB-CG	6.98	131.35	115.30
5	5	5	LEU	CA-CB-CG	6.78	130.89	115.30
3	g	312	LEU	CA-CB-CG	6.62	130.53	115.30
3	V	366	LEU	CA-CB-CG	6.38	129.97	115.30
3	X	176	LEU	CA-CB-CG	6.27	129.73	115.30
3	U	287	ASP	CB-CG-OD1	6.26	123.94	118.30
3	V	332	ASP	CB-CG-OD1	6.25	123.93	118.30
1	z	181	ASP	CB-CG-OD1	6.03	123.72	118.30
1	q	24	LEU	CA-CB-CG	5.99	129.06	115.30
3	R	366	LEU	CB-CG-CD2	5.93	121.07	111.00
7	AM	87	LEU	CA-CB-CG	5.82	128.69	115.30
1	v	94	LEU	CA-CB-CG	5.81	128.66	115.30
1	t	195	LEU	CA-CB-CG	5.80	128.65	115.30
3	R	366	LEU	CA-CB-CG	5.66	128.31	115.30
1	y	94	LEU	CA-CB-CG	5.63	128.26	115.30
6	8	2	ASP	CB-CG-OD1	5.41	123.17	118.30
1	AJ	195	LEU	CA-CB-CG	5.37	127.65	115.30
1	o	160	LEU	CA-CB-CG	5.36	127.63	115.30
8	AY	32	ASP	CB-CG-OD1	5.36	123.12	118.30
8	AX	44	LEU	CA-CB-CG	5.29	127.46	115.30
3	X	237	ASP	CB-CG-OD2	5.26	123.03	118.30
1	u	171	LEU	CA-CB-CG	5.23	127.32	115.30
2	M	126	LEU	CA-CB-CG	5.17	127.20	115.30
1	w	179	ASP	CB-CG-OD2	5.17	122.95	118.30
8	BD	11	ASP	CB-CG-OD2	5.10	122.89	118.30
1	AJ	94	LEU	CA-CB-CG	5.08	126.99	115.30
2	A	126	LEU	CB-CG-CD1	5.04	119.58	111.00
2	H	143	ARG	CA-CB-CG	5.03	124.47	113.40
2	A	126	LEU	CA-CB-CG	5.01	126.83	115.30
3	S	331	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

## 5.2 Too-close contacts

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	182/252 (72%)	173 (95%)	9 (5%)	0	100	100
1	AB	182/252 (72%)	178 (98%)	4 (2%)	0	100	100
1	AC	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	AD	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
1	AE	182/252 (72%)	177 (97%)	5 (3%)	0	100	100
1	AF	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	AG	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	AH	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	AI	182/252 (72%)	177 (97%)	5 (3%)	0	100	100
1	AJ	182/252 (72%)	177 (97%)	5 (3%)	0	100	100
1	AK	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	AL	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	o	182/252 (72%)	177 (97%)	5 (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%)	176 (97%)	6 (3%)	0	100	100
1	t	182/252 (72%)	179 (98%)	3 (2%)	0	100	100
1	u	182/252 (72%)	177 (97%)	5 (3%)	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%)	175 (96%)	7 (4%)	0	100	100
2	A	137/562 (24%)	136 (99%)	1 (1%)	0	100	100
2	B	143/562 (25%)	139 (97%)	4 (3%)	0	100	100
2	C	137/562 (24%)	134 (98%)	3 (2%)	0	100	100
2	D	142/562 (25%)	138 (97%)	4 (3%)	0	100	100
2	F	137/562 (24%)	135 (98%)	2 (2%)	0	100	100
2	G	143/562 (25%)	137 (96%)	6 (4%)	0	100	100
2	H	137/562 (24%)	134 (98%)	3 (2%)	0	100	100
2	I	143/562 (25%)	141 (99%)	2 (1%)	0	100	100
2	J	137/562 (24%)	134 (98%)	3 (2%)	0	100	100
2	K	143/562 (25%)	139 (97%)	4 (3%)	0	100	100
2	L	137/562 (24%)	135 (98%)	2 (2%)	0	100	100
2	M	142/562 (25%)	137 (96%)	5 (4%)	0	100	100
2	N	137/562 (24%)	134 (98%)	3 (2%)	0	100	100
2	O	143/562 (25%)	140 (98%)	3 (2%)	0	100	100
2	P	137/562 (24%)	136 (99%)	1 (1%)	0	100	100
2	Q	143/562 (25%)	139 (97%)	4 (3%)	0	100	100
3	E	220/392 (56%)	212 (96%)	8 (4%)	0	100	100
3	R	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
3	S	220/392 (56%)	209 (95%)	11 (5%)	0	100	100
3	T	220/392 (56%)	210 (96%)	10 (4%)	0	100	100
3	U	219/392 (56%)	213 (97%)	6 (3%)	0	100	100
3	V	220/392 (56%)	207 (94%)	13 (6%)	0	100	100
3	W	220/392 (56%)	211 (96%)	9 (4%)	0	100	100
3	X	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
3	Y	220/392 (56%)	204 (93%)	16 (7%)	0	100	100
3	Z	220/392 (56%)	210 (96%)	10 (4%)	0	100	100
3	a	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
3	b	220/392 (56%)	207 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	220/392 (56%)	210 (96%)	10 (4%)	0	100	100
3	d	219/392 (56%)	213 (97%)	6 (3%)	0	100	100
3	e	220/392 (56%)	208 (94%)	12 (6%)	0	100	100
3	f	220/392 (56%)	209 (95%)	11 (5%)	0	100	100
3	g	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
3	h	220/392 (56%)	207 (94%)	13 (6%)	0	100	100
3	i	220/392 (56%)	211 (96%)	9 (4%)	0	100	100
3	j	219/392 (56%)	213 (97%)	6 (3%)	0	100	100
3	k	220/392 (56%)	206 (94%)	14 (6%)	0	100	100
3	l	220/392 (56%)	210 (96%)	10 (4%)	0	100	100
3	m	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
3	n	220/392 (56%)	207 (94%)	13 (6%)	0	100	100
4	0	195/224 (87%)	189 (97%)	5 (3%)	1 (0%)	25	62
4	1	195/224 (87%)	186 (95%)	8 (4%)	1 (0%)	25	62
4	2	193/224 (86%)	187 (97%)	5 (3%)	1 (0%)	25	62
4	3	200/224 (89%)	195 (98%)	5 (2%)	0	100	100
4	4	220/224 (98%)	209 (95%)	11 (5%)	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%)	11	44
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	87/101 (86%)	87 (100%)	0	0	100	100
7	AQ	87/101 (86%)	87 (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	53/80 (66%)	52 (98%)	1 (2%)	0	100	100
8	BA	50/80 (62%)	47 (94%)	3 (6%)	0	100	100
8	BB	44/80 (55%)	43 (98%)	1 (2%)	0	100	100
8	BC	44/80 (55%)	44 (100%)	0	0	100	100
8	BD	44/80 (55%)	43 (98%)	1 (2%)	0	100	100
8	BE	39/80 (49%)	37 (95%)	2 (5%)	0	100	100
All	All	14587/27821 (52%)	14062 (96%)	521 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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%)	65	77
1	AB	155/215 (72%)	155 (100%)	0	100	100
1	AC	155/215 (72%)	155 (100%)	0	100	100
1	AD	155/215 (72%)	155 (100%)	0	100	100
1	AE	155/215 (72%)	152 (98%)	3 (2%)	52	69
1	AF	155/215 (72%)	154 (99%)	1 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AG	155/215 (72%)	154 (99%)	1 (1%)	84	88
1	AH	155/215 (72%)	155 (100%)	0	100	100
1	AI	155/215 (72%)	153 (99%)	2 (1%)	65	77
1	AJ	155/215 (72%)	154 (99%)	1 (1%)	84	88
1	AK	155/215 (72%)	154 (99%)	1 (1%)	84	88
1	AL	155/215 (72%)	155 (100%)	0	100	100
1	o	155/215 (72%)	153 (99%)	2 (1%)	65	77
1	p	155/215 (72%)	155 (100%)	0	100	100
1	q	155/215 (72%)	154 (99%)	1 (1%)	84	88
1	r	155/215 (72%)	154 (99%)	1 (1%)	84	88
1	s	155/215 (72%)	155 (100%)	0	100	100
1	t	155/215 (72%)	155 (100%)	0	100	100
1	u	155/215 (72%)	155 (100%)	0	100	100
1	v	155/215 (72%)	152 (98%)	3 (2%)	52	69
1	w	155/215 (72%)	153 (99%)	2 (1%)	65	77
1	x	155/215 (72%)	155 (100%)	0	100	100
1	y	155/215 (72%)	154 (99%)	1 (1%)	84	88
1	z	155/215 (72%)	154 (99%)	1 (1%)	84	88
2	A	119/477 (25%)	119 (100%)	0	100	100
2	B	125/477 (26%)	125 (100%)	0	100	100
2	C	119/477 (25%)	118 (99%)	1 (1%)	79	84
2	D	124/477 (26%)	123 (99%)	1 (1%)	79	84
2	F	119/477 (25%)	118 (99%)	1 (1%)	79	84
2	G	125/477 (26%)	124 (99%)	1 (1%)	79	84
2	H	119/477 (25%)	117 (98%)	2 (2%)	56	72
2	I	125/477 (26%)	124 (99%)	1 (1%)	79	84
2	J	119/477 (25%)	118 (99%)	1 (1%)	79	84
2	K	125/477 (26%)	124 (99%)	1 (1%)	79	84
2	L	119/477 (25%)	118 (99%)	1 (1%)	79	84
2	M	124/477 (26%)	123 (99%)	1 (1%)	79	84
2	N	119/477 (25%)	118 (99%)	1 (1%)	79	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	125/477 (26%)	124 (99%)	1 (1%)	79	84
2	P	119/477 (25%)	118 (99%)	1 (1%)	79	84
2	Q	125/477 (26%)	123 (98%)	2 (2%)	58	74
3	E	190/337 (56%)	189 (100%)	1 (0%)	86	90
3	R	189/337 (56%)	187 (99%)	2 (1%)	70	80
3	S	188/337 (56%)	187 (100%)	1 (0%)	86	90
3	T	190/337 (56%)	190 (100%)	0	100	100
3	U	189/337 (56%)	188 (100%)	1 (0%)	86	90
3	V	188/337 (56%)	186 (99%)	2 (1%)	70	80
3	W	190/337 (56%)	189 (100%)	1 (0%)	86	90
3	X	189/337 (56%)	187 (99%)	2 (1%)	70	80
3	Y	188/337 (56%)	187 (100%)	1 (0%)	86	90
3	Z	190/337 (56%)	190 (100%)	0	100	100
3	a	189/337 (56%)	189 (100%)	0	100	100
3	b	188/337 (56%)	188 (100%)	0	100	100
3	c	190/337 (56%)	189 (100%)	1 (0%)	86	90
3	d	189/337 (56%)	188 (100%)	1 (0%)	86	90
3	e	188/337 (56%)	186 (99%)	2 (1%)	70	80
3	f	190/337 (56%)	190 (100%)	0	100	100
3	g	189/337 (56%)	187 (99%)	2 (1%)	70	80
3	h	188/337 (56%)	188 (100%)	0	100	100
3	i	190/337 (56%)	189 (100%)	1 (0%)	86	90
3	j	189/337 (56%)	189 (100%)	0	100	100
3	k	188/337 (56%)	187 (100%)	1 (0%)	86	90
3	l	190/337 (56%)	189 (100%)	1 (0%)	86	90
3	m	189/337 (56%)	188 (100%)	1 (0%)	86	90
3	n	188/337 (56%)	188 (100%)	0	100	100
4	0	175/199 (88%)	174 (99%)	1 (1%)	84	88
4	1	177/199 (89%)	177 (100%)	0	100	100
4	2	175/199 (88%)	174 (99%)	1 (1%)	84	88
4	3	180/199 (90%)	179 (99%)	1 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	4	197/199 (99%)	195 (99%)	2 (1%)	73	81
5	5	205/219 (94%)	204 (100%)	1 (0%)	86	90
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%)	70 (100%)	0	100	100
7	AM	34/88 (39%)	33 (97%)	1 (3%)	37	58
7	AN	71/88 (81%)	71 (100%)	0	100	100
7	AO	76/88 (86%)	75 (99%)	1 (1%)	65	77
7	AP	77/88 (88%)	75 (97%)	2 (3%)	41	61
7	AQ	77/88 (88%)	76 (99%)	1 (1%)	65	77
7	AR	76/88 (86%)	76 (100%)	0	100	100
8	AS	50/67 (75%)	47 (94%)	3 (6%)	16	39
8	AT	50/67 (75%)	44 (88%)	6 (12%)	4	18
8	AU	50/67 (75%)	44 (88%)	6 (12%)	4	18
8	AV	50/67 (75%)	47 (94%)	3 (6%)	16	39
8	AW	50/67 (75%)	42 (84%)	8 (16%)	2	13
8	AX	62/67 (92%)	62 (100%)	0	100	100
8	AY	66/67 (98%)	66 (100%)	0	100	100
8	AZ	51/67 (76%)	51 (100%)	0	100	100
8	BA	48/67 (72%)	48 (100%)	0	100	100
8	BB	42/67 (63%)	42 (100%)	0	100	100
8	BC	42/67 (63%)	42 (100%)	0	100	100
8	BD	42/67 (63%)	42 (100%)	0	100	100
8	BE	37/67 (55%)	37 (100%)	0	100	100
All	All	12615/23777 (53%)	12519 (99%)	96 (1%)	77	84

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	80	ARG
1	AA	166	ASP
1	AE	34	GLU

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Mol	Chain	Res	Type
1	AE	53	LYS
1	AE	80	ARG
1	AF	80	ARG
1	AG	80	ARG
1	AI	60	VAL
1	AI	80	ARG
2	C	143	ARG
2	D	40	ASP
3	E	340	ARG
2	F	143	ARG
2	G	143	ARG
2	H	36	VAL
2	H	143	ARG
2	I	143	ARG
2	J	40	ASP
2	K	143	ARG
2	L	143	ARG
2	M	126	LEU
2	N	143	ARG
2	O	143	ARG
2	P	143	ARG
2	Q	40	ASP
2	Q	143	ARG
3	R	192	LYS
3	R	366	LEU
3	S	348	ARG
3	U	366	LEU
3	V	348	ARG
3	V	366	LEU
3	W	335	GLU
3	X	201	GLU
3	X	366	LEU
3	Y	348	ARG
3	c	320	LYS
3	d	366	LEU
3	e	215	ASP
3	e	348	ARG
3	g	312	LEU
3	g	366	LEU
3	i	320	LYS
3	k	348	ARG
3	l	196	VAL

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Mol	Chain	Res	Type
3	m	333	ASP
1	o	53	LYS
1	o	80	ARG
1	q	24	LEU
1	r	80	ARG
1	v	72	ILE
1	v	80	ARG
1	v	82	ARG
1	w	80	ARG
1	w	141	ARG
1	y	80	ARG
1	z	80	ARG
1	AJ	77	LEU
1	AK	80	ARG
4	0	81	THR
4	2	84	ASP
4	3	211	LEU
4	4	133	ARG
4	4	135	LYS
5	5	163	CYS
7	AM	87	LEU
7	AO	100	ARG
7	AP	98	LEU
7	AP	100	ARG
7	AQ	32	ARG
8	AS	28	THR
8	AS	64	THR
8	AS	76	ILE
8	AT	28	THR
8	AT	44	LEU
8	AT	51	LEU
8	AT	64	THR
8	AT	72	ASP
8	AT	76	ILE
8	AU	28	THR
8	AU	34	LEU
8	AU	51	LEU
8	AU	64	THR
8	AU	70	ASP
8	AU	76	ILE
8	AV	44	LEU
8	AV	67	VAL

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Mol	Chain	Res	Type
8	AV	76	ILE
8	AW	28	THR
8	AW	34	LEU
8	AW	44	LEU
8	AW	51	LEU
8	AW	64	THR
8	AW	70	ASP
8	AW	72	ASP
8	AW	76	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	29	GLN
1	AB	139	ASN
1	AC	29	GLN
1	AD	29	GLN
1	AE	29	GLN
1	AE	162	HIS
1	AF	162	HIS
1	AI	162	HIS
2	A	71	ASN
2	A	87	GLN
2	B	87	GLN
2	B	170	ASN
2	C	123	ASN
2	C	161	ASN
2	D	87	GLN
3	E	199	GLN
3	E	341	GLN
2	F	71	ASN
2	G	97	GLN
2	G	124	ASN
2	G	170	ASN
2	H	97	GLN
2	I	169	GLN
2	J	87	GLN
2	J	97	GLN
2	L	87	GLN
2	L	97	GLN
2	L	169	GLN
2	M	161	ASN

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Mol	Chain	Res	Type
2	M	169	GLN
2	N	97	GLN
2	N	170	ASN
2	P	87	GLN
2	P	169	GLN
2	Q	87	GLN
2	Q	97	GLN
2	Q	169	GLN
3	R	219	ASN
3	R	229	ASN
3	R	265	ASN
3	R	318	ASN
3	S	219	ASN
3	S	318	ASN
3	T	309	GLN
3	U	318	ASN
3	V	219	ASN
3	V	229	ASN
3	V	318	ASN
3	W	318	ASN
3	X	229	ASN
3	X	318	ASN
3	Y	318	ASN
3	Z	199	GLN
3	Z	209	GLN
3	Z	265	ASN
3	Z	309	GLN
3	Z	356	GLN
1	AL	111	GLN
1	AL	162	HIS
3	a	229	ASN
3	a	310	GLN
3	a	318	ASN
3	b	219	ASN
3	b	318	ASN
3	c	219	ASN
3	c	318	ASN
3	d	356	GLN
3	e	219	ASN
3	e	310	GLN
3	e	318	ASN
3	f	356	GLN

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Mol	Chain	Res	Type
3	g	229	ASN
3	g	309	GLN
3	g	310	GLN
3	g	356	GLN
3	h	224	ASN
3	h	310	GLN
3	h	318	ASN
3	i	318	ASN
3	j	328	GLN
3	k	310	GLN
3	k	356	GLN
3	l	209	GLN
3	l	310	GLN
3	m	219	ASN
3	m	318	ASN
1	o	47	ASN
1	o	115	GLN
1	o	162	HIS
1	p	163	GLN
1	r	163	GLN
1	s	139	ASN
1	s	163	GLN
1	t	173	ASN
1	u	29	GLN
1	u	139	ASN
1	u	173	ASN
1	v	29	GLN
1	v	139	ASN
1	v	162	HIS
1	x	111	GLN
1	x	162	HIS
1	x	163	GLN
1	AJ	162	HIS
1	AK	29	GLN
4	3	117	ASN
4	4	44	GLN
5	5	104	ASN
5	5	130	ASN
5	5	245	GLN
6	7	37	GLN
6	8	9	ASN
6	8	37	GLN

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Mol	Chain	Res	Type
6	9	37	GLN
7	AN	78	ASN
7	AO	53	ASN
7	AP	59	ASN
7	AQ	71	GLN
8	AS	26	GLN
8	AS	48	GLN
8	AT	26	GLN
8	AT	48	GLN
8	AU	55	ASN
8	AU	78	ASN
8	AV	22	ASN
8	AW	22	ASN
8	AW	63	ASN
8	AX	59	ASN
8	AX	78	ASN
8	AZ	26	GLN
8	AZ	78	ASN
8	BA	24	GLN
8	BA	26	GLN
8	BD	59	ASN
8	BD	61	GLN
8	BD	78	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

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.

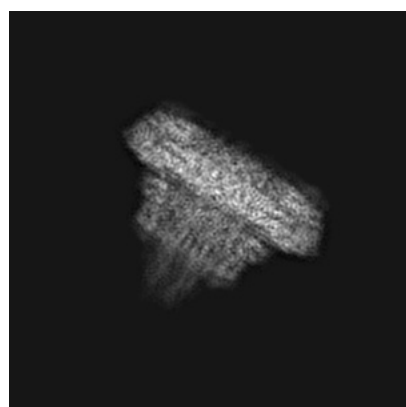
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20556. These allow visual inspection of the internal detail of the map and identification of artifacts.

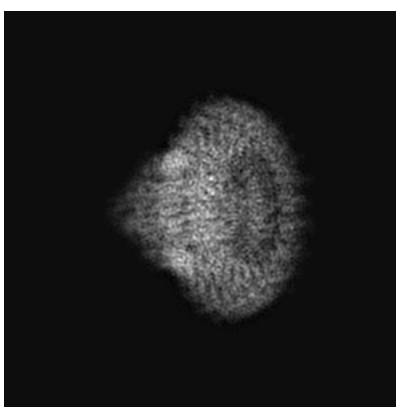
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

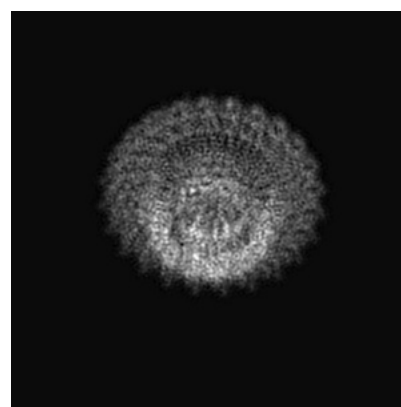
#### 6.1.1 Primary map



X



Y

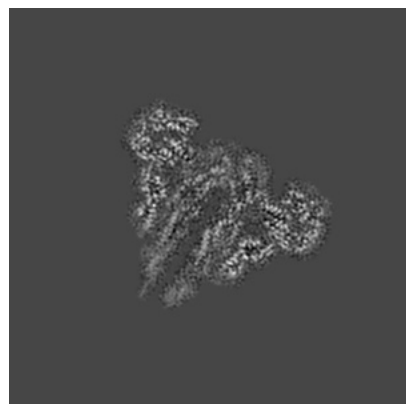


Z

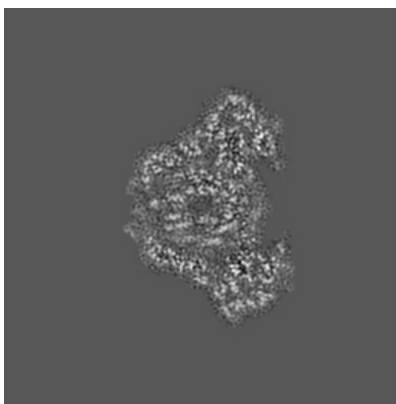
The images above show the map projected in three orthogonal directions.

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

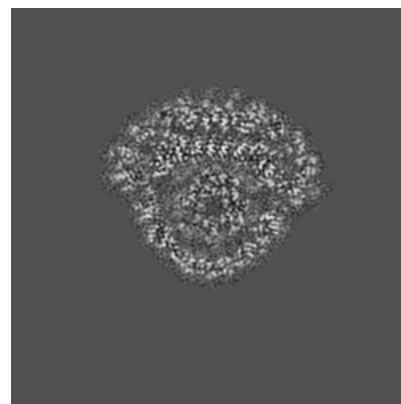
#### 6.2.1 Primary map



X Index: 125



Y Index: 125



Z Index: 125

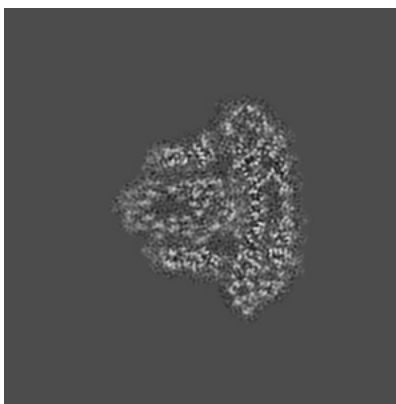
The images above show central slices of the map in three orthogonal directions.

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

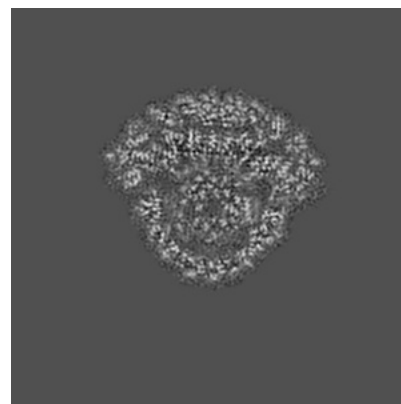
### 6.3.1 Primary map



X Index: 114



Y Index: 112

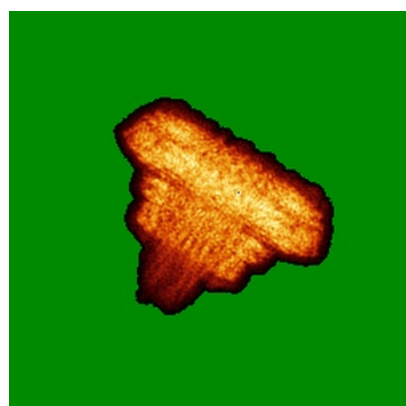


Z Index: 123

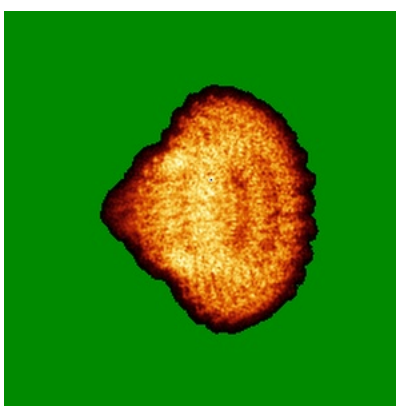
The images above show the largest variance slices of the map in three orthogonal directions.

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

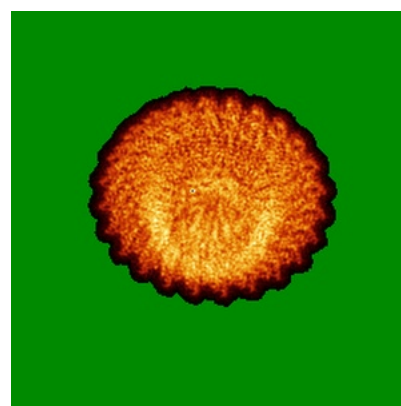
### 6.4.1 Primary map



X



Y

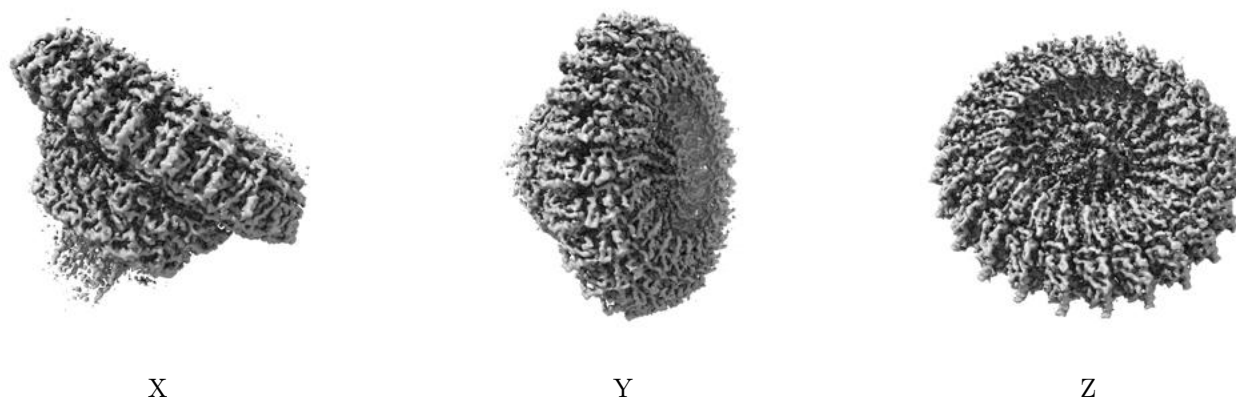


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

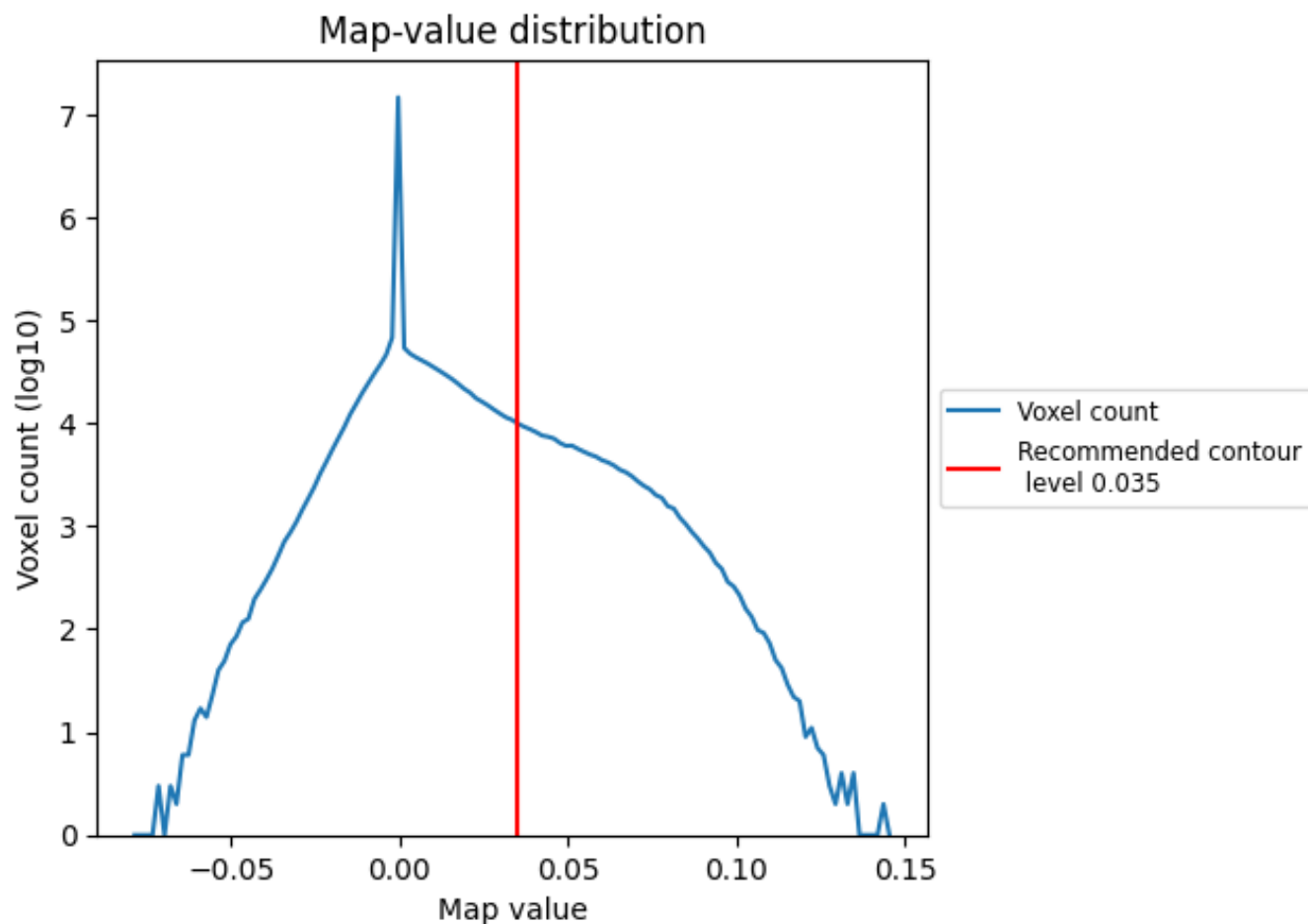
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

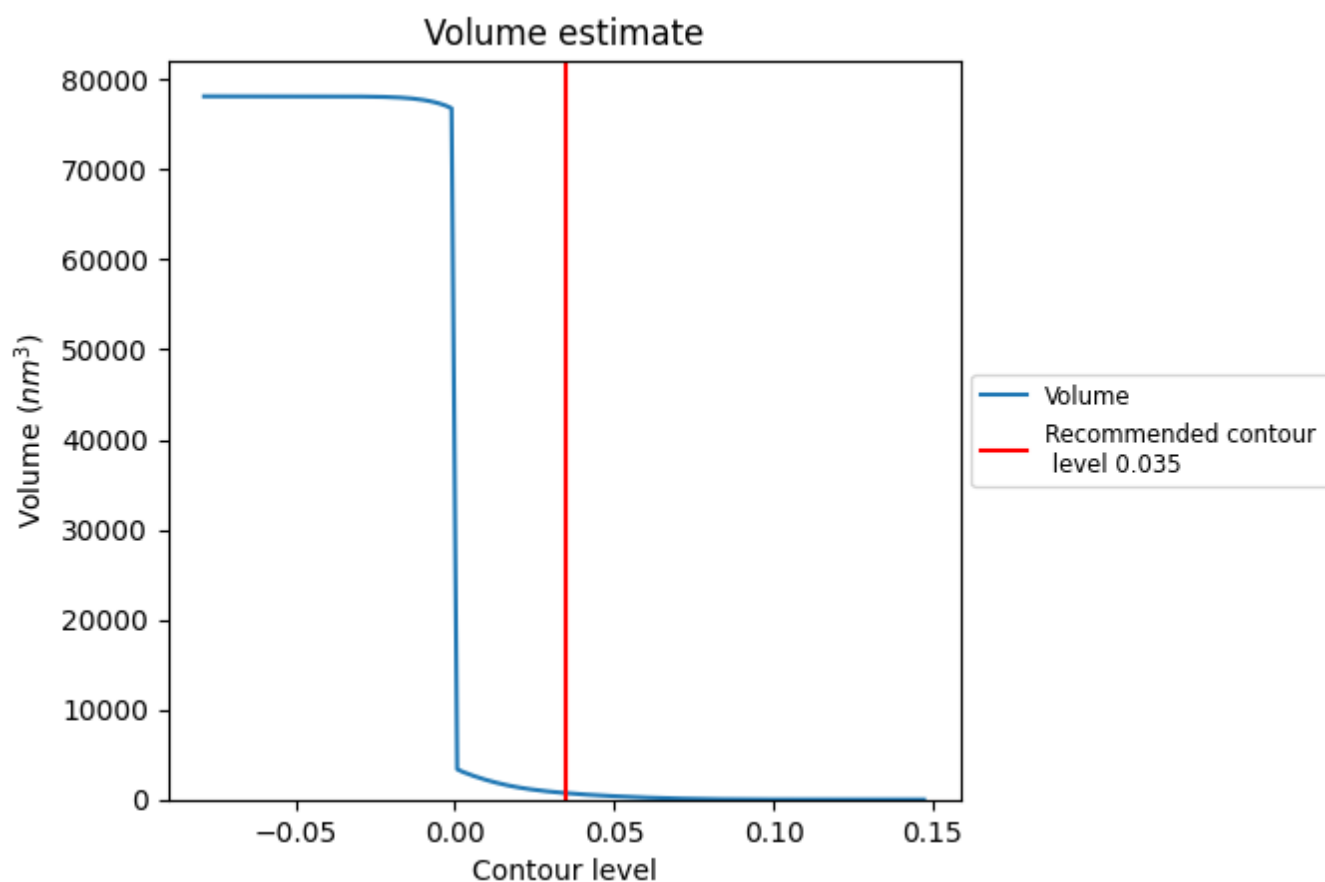
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

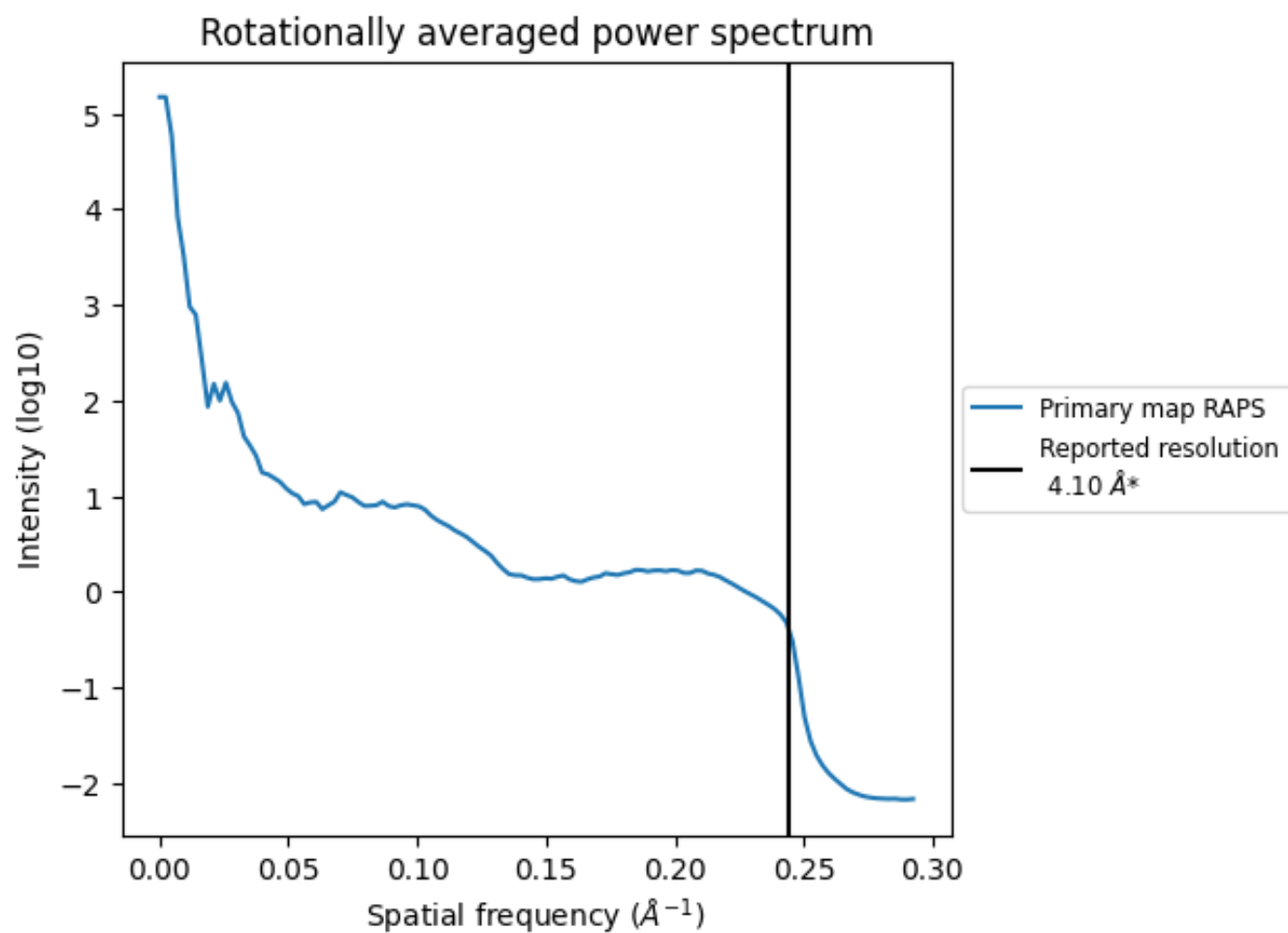
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 715 nm<sup>3</sup>; this corresponds to an approximate mass of 646 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>



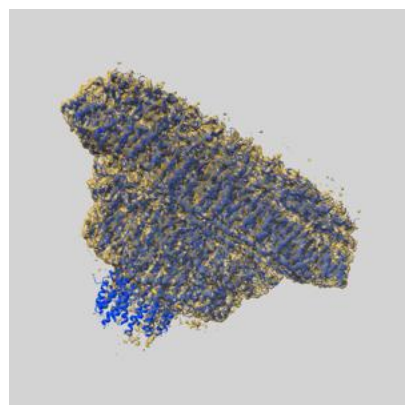
## 8 Fourier-Shell correlation ⓘ

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

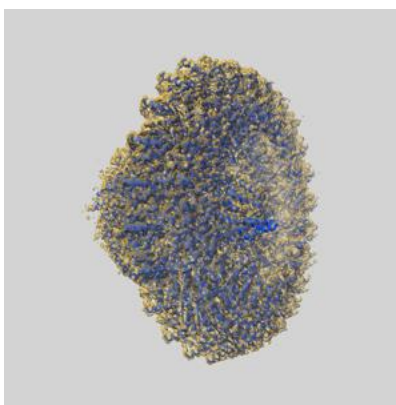
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20556 and PDB model 6Q16. Per-residue inclusion information can be found in section 3 on page 13.

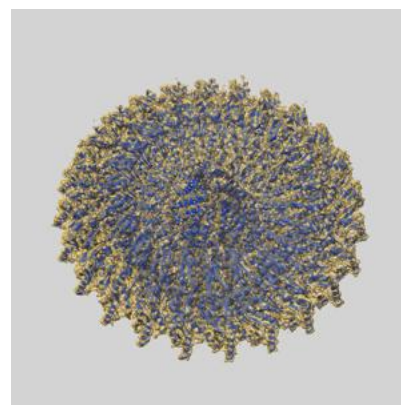
### 9.1 Map-model overlay [i](#)



X



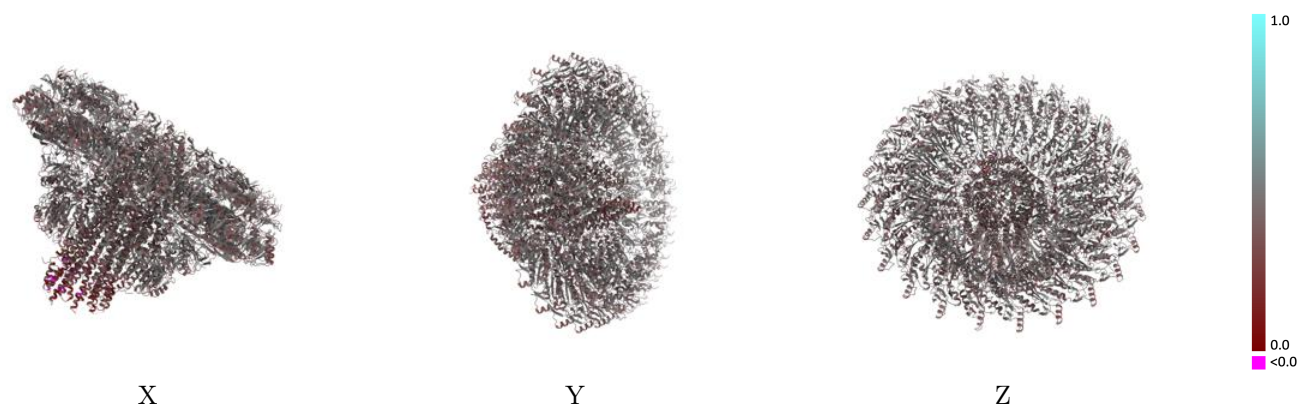
Y



Z

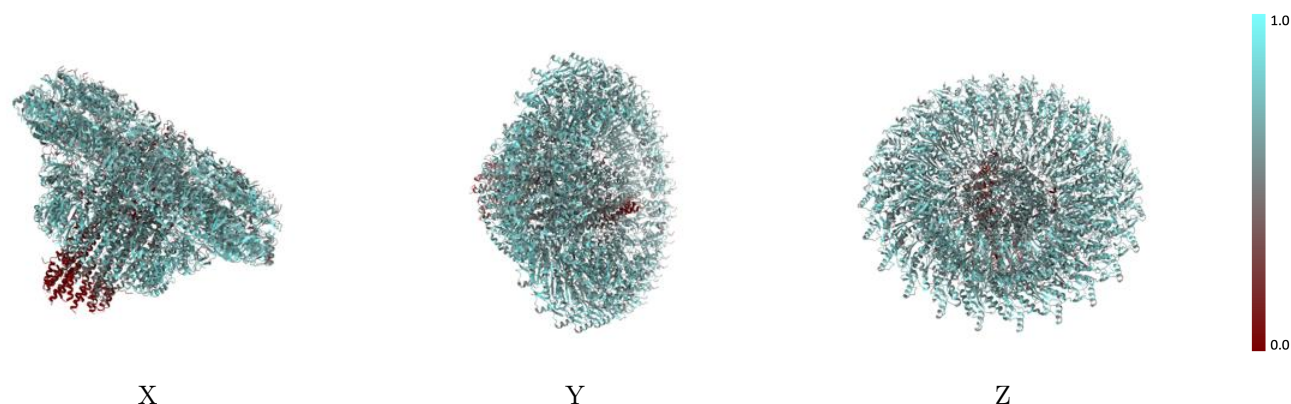
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



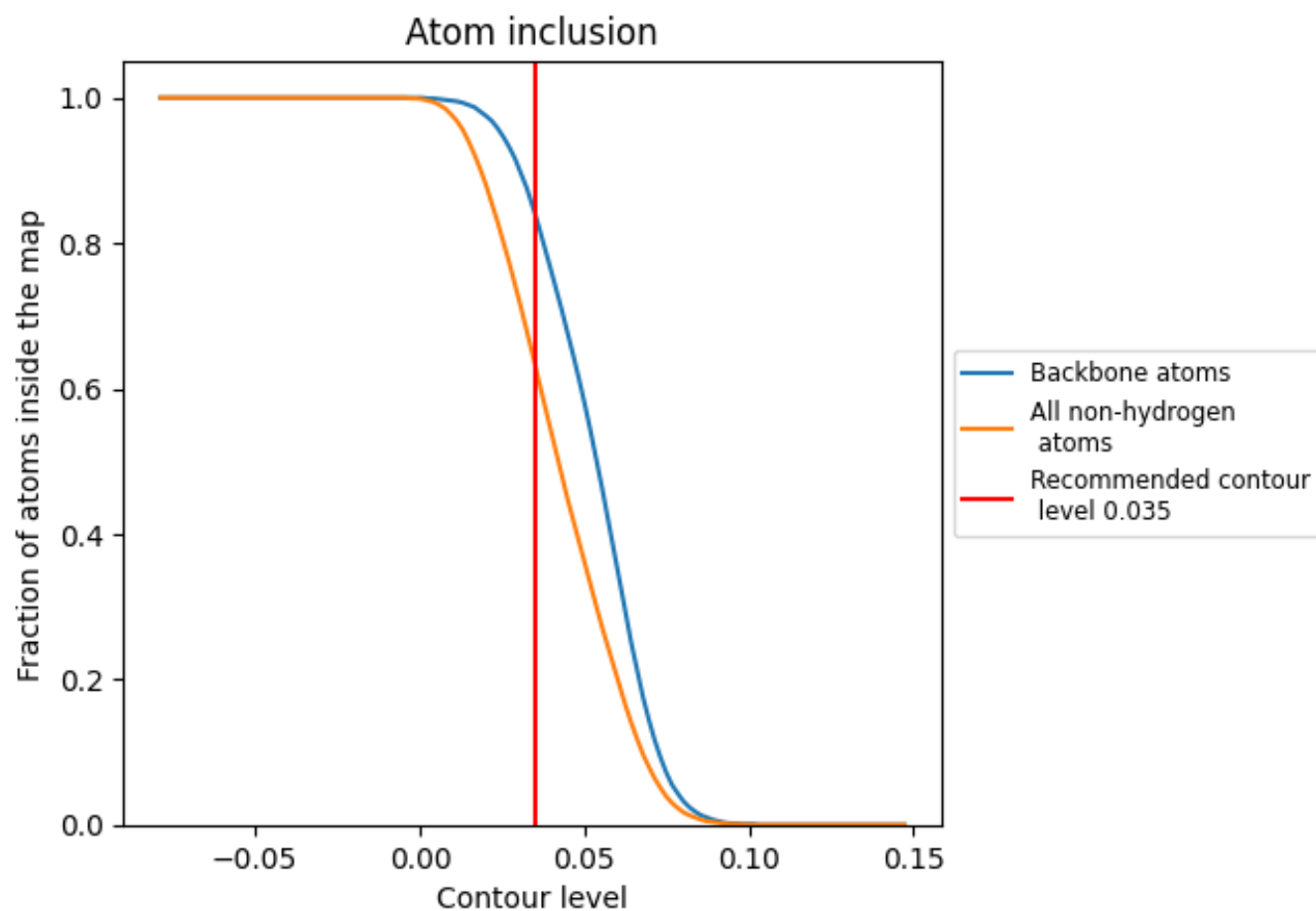
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 63% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6340	 0.4040
0	 0.5530	 0.3700
1	 0.5440	 0.3610
2	 0.5420	 0.3690
3	 0.5660	 0.3750
4	 0.5500	 0.3790
5	 0.6250	 0.4070
6	 0.2590	 0.3530
7	 0.3120	 0.3520
8	 0.4930	 0.3670
9	 0.5500	 0.3760
A	 0.7020	 0.4050
AA	 0.6490	 0.4220
AB	 0.6600	 0.4270
AC	 0.6740	 0.4340
AD	 0.6530	 0.4250
AE	 0.6660	 0.4250
AF	 0.6490	 0.4340
AG	 0.6650	 0.4230
AH	 0.6550	 0.4280
AI	 0.6610	 0.4230
AJ	 0.6460	 0.4260
AK	 0.6520	 0.4200
AL	 0.6710	 0.4290
AM	 0.5000	 0.3590
AN	 0.4840	 0.3490
AO	 0.4990	 0.3630
AP	 0.5130	 0.3510
AQ	 0.5020	 0.3480
AR	 0.4460	 0.3380
AS	 0.4200	 0.3130
AT	 0.4790	 0.2900
AU	 0.4640	 0.3050
AV	 0.4490	 0.2850
AW	 0.3640	 0.2910





































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Chain	Atom inclusion	Q-score
AX	 0.0990	 0.2850
AY	 0.2520	 0.2530
AZ	 0.3190	 0.2720
B	 0.6950	 0.4010
BA	 0.3150	 0.2660
BB	 0.2760	 0.2440
BC	 0.0660	 0.2520
BD	 0.0260	 0.2330
BE	 0.0500	 0.1660
C	 0.7160	 0.4140
D	 0.6910	 0.4050
E	 0.6390	 0.3980
F	 0.7000	 0.4120
G	 0.6950	 0.4180
H	 0.7220	 0.4150
I	 0.6920	 0.4060
J	 0.7120	 0.4160
K	 0.6890	 0.4050
L	 0.7250	 0.4150
M	 0.6940	 0.4100
N	 0.7120	 0.4160
O	 0.6950	 0.4080
P	 0.7000	 0.4010
Q	 0.6930	 0.4000
R	 0.6950	 0.4100
S	 0.6930	 0.4120
T	 0.6500	 0.4110
U	 0.6840	 0.4200
V	 0.6810	 0.4160
W	 0.6290	 0.4120
X	 0.6900	 0.4150
Y	 0.6880	 0.4200
Z	 0.6350	 0.4150
a	 0.6790	 0.4200
b	 0.6940	 0.4240
c	 0.6660	 0.4180
d	 0.7110	 0.4240
e	 0.6930	 0.4110
f	 0.6700	 0.4150
g	 0.6890	 0.4160
h	 0.6940	 0.4150
i	 0.6620	 0.4160

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Chain	Atom inclusion	Q-score
j	 0.6930	 0.4180
k	 0.6980	 0.4150
l	 0.6540	 0.4130
m	 0.6910	 0.4140
n	 0.7010	 0.4220
o	 0.6520	 0.4300
p	 0.6420	 0.4230
q	 0.6450	 0.4220
r	 0.6410	 0.4270
s	 0.6340	 0.4220
t	 0.6320	 0.4230
u	 0.6380	 0.4220
v	 0.6290	 0.4140
w	 0.6410	 0.4230
x	 0.6620	 0.4300
y	 0.6620	 0.4170
z	 0.6540	 0.4280