Full wwPDB EM Validation Report (i)

Nov 27, 2022 – 10:28 AM EST

PDB ID	:	6PEP
EMDB ID	:	EMD-20317
Title	:	Focussed refinement of InvGN0N1:SpaPQR:PrgIJ from the Salmonella SPI-1 injectisome needle complex
Authors	:	Hu, J.; Worrall, L.J.; Strynadka, N.C.J.
Deposited on	:	2019-06-20
Resolution	:	3.80 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 (i) 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 (i)) were used in the production of this report:

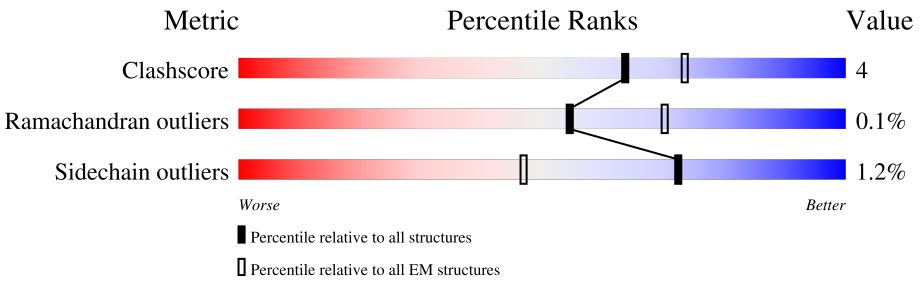
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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	0	224	7% 80% 8% 11%
1	1	224	6% 82% 7% 11%
1	2	224	5% 75% 13% 12%
1	3	224	• 74% 17% 9%
1	4	224	7% 88% 11% •
2	5	263	• 78% 16% 6%
3	6	86	43% 58% • 38%
3	7	86	33% 84% 14% •

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Mol	Chain	Length	Quality of chain
3	8	86	12% 76% 22%
3	9	86	78% 20%
4	A	562	22% 75%
4	B	562	23% 74%
4	C	562	22% 75%
4	D	562	24% 74%
4	F	562	22% 75%
4	G	562	23% 74%
4	H	562	22% 75%
4	I	562	24% 74%
4	J	562	22% 75%
4	K	562	24% 74%
4	L	562	21% 75%
4	M	562	23% 74%
4	N	562	22% 75%
4	O	562	24% 74%
4	P	562	21% 75%
4	Q	562	23% 74%
5	AM	101	7% 37% 61%
5	AN	101	14% 62% 15% 23%
5	AO	101	9% 77% 10% 13%
5	AP	101	15% 77% 11% 12%
5	AQ	101	16% 74% 14% 12%
5	AR	101	22% 76% 11% 13%
6	AS	80	26% 54% 18% 26%

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Mol	Chain	Length	Quality of chain
6	AT	80	20% 59% 15% 26%
6	AU	80	26% 55% 15% • 26%
6	AV	80	34% 58% 16% 26%
6	AW	80	45% 54% 18% • 26%
6	AX	80	88% 75% 16% 9%
6	AY	80	59% 74% 24% •
6	AZ	80	35% 58% 14% 29%
6	BA	80	35% 56% 11% 32%
6	BB	80	35% 54% 6% 40%
6	BC	80	59% 50% 10% 40%
6	BD	80	60% 40% 20% 40%
6	BE	80	45% 42% 11% 46%
7	E	392	• 6% • 93%
7	R	392	• 6% 93%
7	S	392	• 7% 93%
7	T	392	• 7% 93%
7	U	392	• 5% • 93%
7	V	392	• 7% 93%
7	W	392	• 6% • 93%
7	X	392	• 6% • 93%
7	Y	392	• 7% 93%
7	Z	392	• 7% 93%
7	a	392	• 7% 93%
7	b	392	• 7% 93%
7	c	392	• 7% 93%

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Mol	Chain	Length	Quality of chain
7	d	392	7% 93%
7	e	392	7% 93%
7	f	392	7% 93%
7	g	392	7% 93%
7	h	392	7% 93%
7	i	392	7% 93%
7	j	392	7% 93%
7	k	392	7% 93%
7	l	392	7% 93%
7	m	392	7% 93%
7	n	392	7% 93%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 45454 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 Surface presentation of antigens protein SpaP.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	5	247	1885	1252	300	320	13	0	0

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

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

- Molecule 4 is a protein called Protein InvG.

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

- Molecule 5 is a protein called Protein PrgJ.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AQ	89	675	416	115	141	3	0	0
5	AR	88	667	410	114	140	3	0	0

- Molecule 6 is a protein called Protein PrgI.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	AS	59	466	294	80	92	0	0
6	AT	59	466	294	80	92	0	0
6	AU	59	466	294	80	92	0	0
6	AV	59	466	294	80	92	0	0
6	AW	59	466	294	80	92	0	0
6	AX	73	574	362	95	117	0	0
6	AY	78	612	387	101	124	0	0
6	AZ	57	460	289	76	95	0	0
6	BA	54	437	275	73	89	0	0
6	BB	48	388	247	64	77	0	0
6	BC	48	388	247	64	77	0	0
6	BD	48	388	247	64	77	0	0
6	BE	43	346	219	59	68	0	0

- Molecule 7 is a protein called Protein PrgH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	E	28	236	159	38	38	1	0	0
7	R	27	227	153	37	36	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	S	28	231	156	38	36	1	0	0
			Total	C	N	O	S		
7	T	28	236	159	38	38	1	0	0
			Total	C	N	O	S		
7	U	27	227	153	37	36	1	0	0
			Total	C	N	O	S		
7	V	28	231	156	38	36	1	0	0
			Total	C	N	O	S		
7	W	28	236	159	38	38	1	0	0
			Total	C	N	O	S		
7	X	27	227	153	37	36	1	0	0
			Total	C	N	O	S		
7	Y	28	231	156	38	36	1	0	0
			Total	C	N	O	S		
7	Z	28	236	159	38	38	1	0	0
			Total	C	N	O	S		
7	a	27	227	153	37	36	1	0	0
			Total	C	N	O	S		
7	b	28	231	156	38	36	1	0	0
			Total	C	N	O	S		
7	c	28	236	159	38	38	1	0	0
			Total	C	N	O	S		
7	d	27	227	153	37	36	1	0	0
			Total	C	N	O	S		
7	e	28	231	156	38	36	1	0	0
			Total	C	N	O	S		
7	f	28	236	159	38	38	1	0	0
			Total	C	N	O	S		
7	g	27	227	153	37	36	1	0	0
			Total	C	N	O	S		
7	h	28	231	156	38	36	1	0	0
			Total	C	N	O	S		
7	i	28	236	159	38	38	1	0	0
			Total	C	N	O	S		
7	j	27	227	153	37	36	1	0	0
			Total	C	N	O	S		
7	k	28	231	156	38	36	1	0	0
			Total	C	N	O	S		
7	l	28	236	159	38	38	1	0	0
			Total	C	N	O	S		
7	m	27	227	153	37	36	1	0	0

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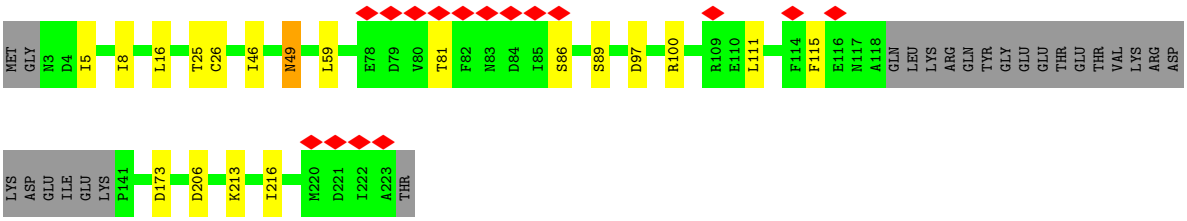
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	n	28	231	156	38	36	1	0	0

3 Residue-property plots (i)

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

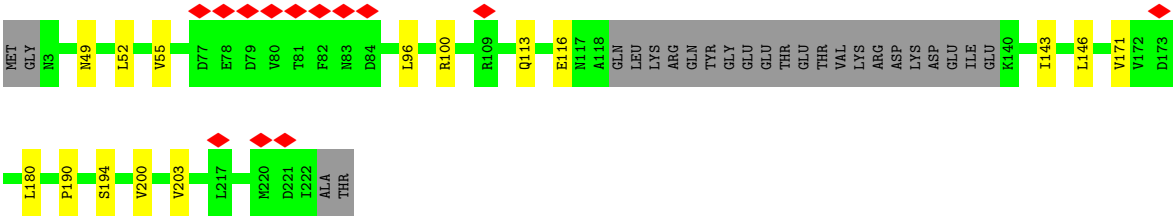
• Molecule 1: Surface presentation of antigens protein SpaP

Chain 0:



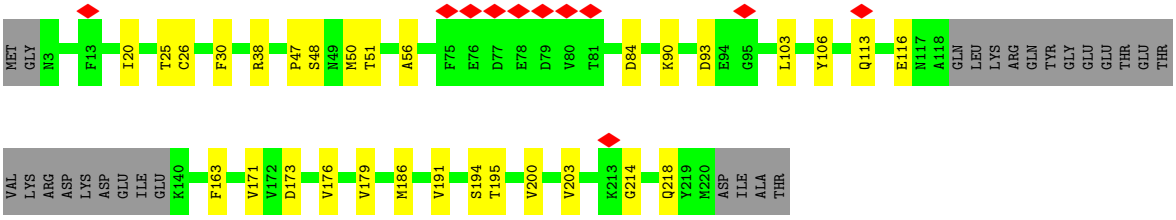
• Molecule 1: Surface presentation of antigens protein SpaP

Chain 1:



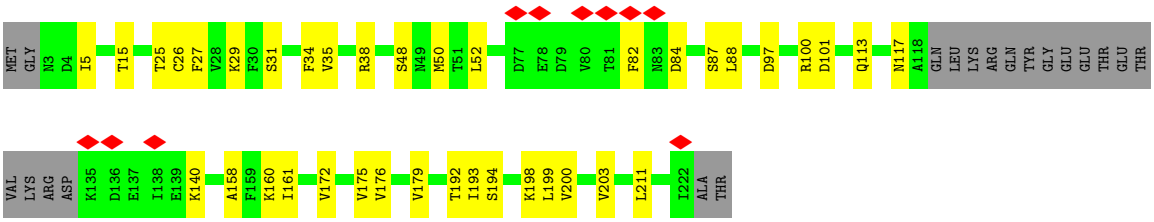
• Molecule 1: Surface presentation of antigens protein SpaP

Chain 2:



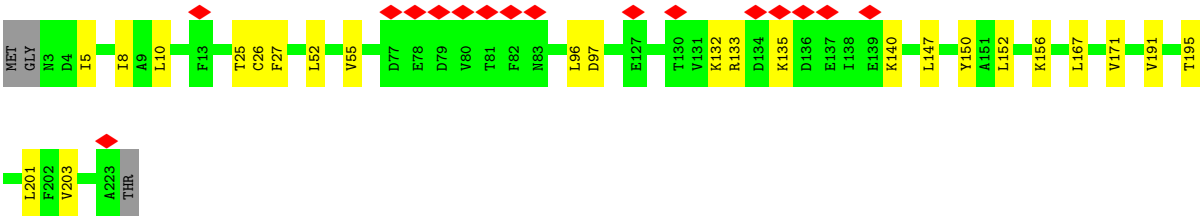
• Molecule 1: Surface presentation of antigens protein SpaP

Chain 3:



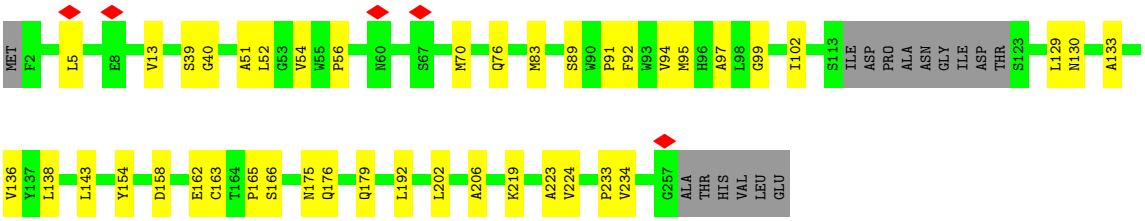
• Molecule 1: Surface presentation of antigens protein SpaP

Chain 4:



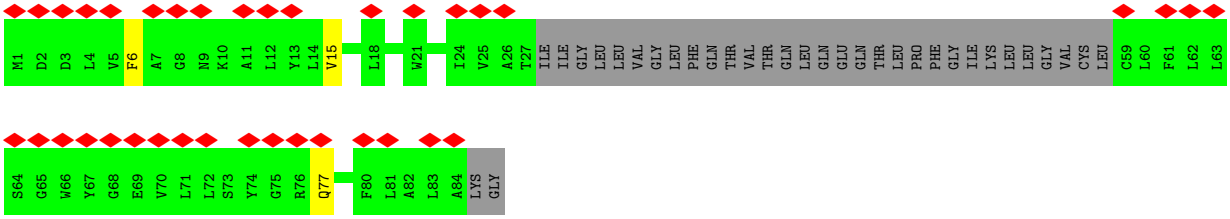
• Molecule 2: Surface presentation of antigens protein SpaR

Chain 5:



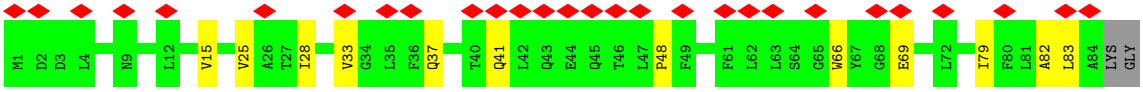
• Molecule 3: Surface presentation of antigens protein SpaQ

Chain 6:



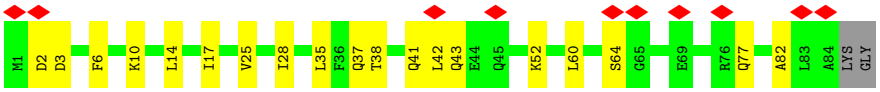
• Molecule 3: Surface presentation of antigens protein SpaQ

Chain 7:



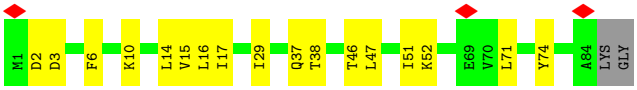
• Molecule 3: Surface presentation of antigens protein SpaQ

Chain 8:



• Molecule 3: Surface presentation of antigens protein SpaQ

Chain 9:

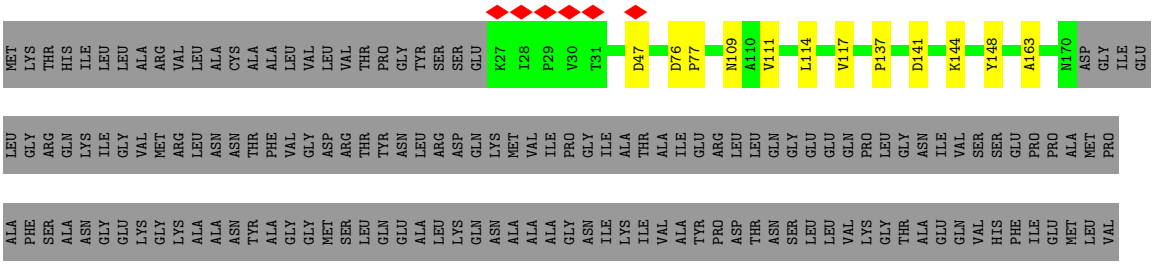


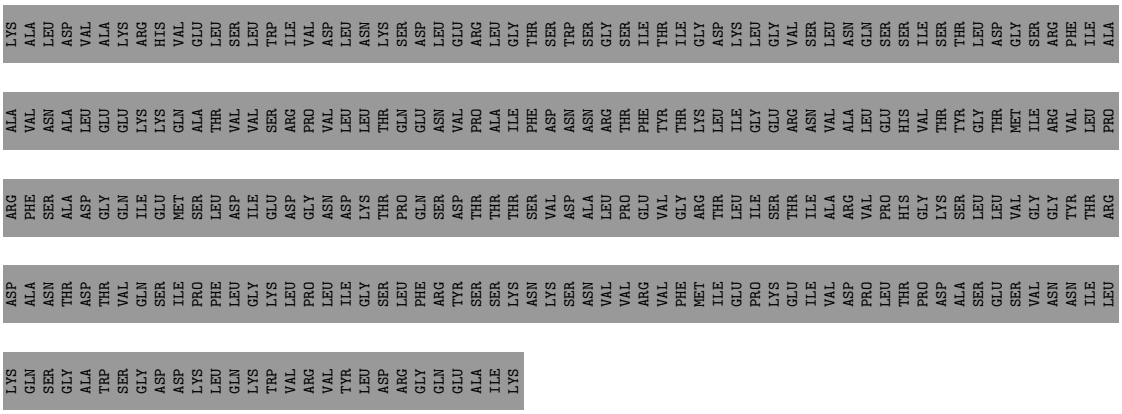
• Molecule 4: Protein InvG

Chain A:

• Molecule 4: Protein InvG

Chain B:



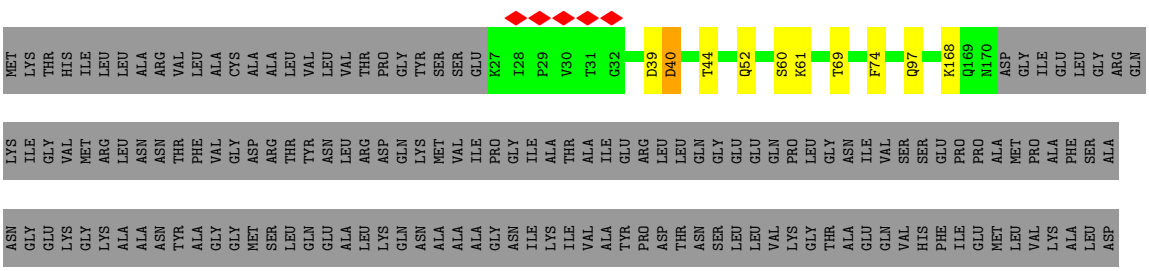


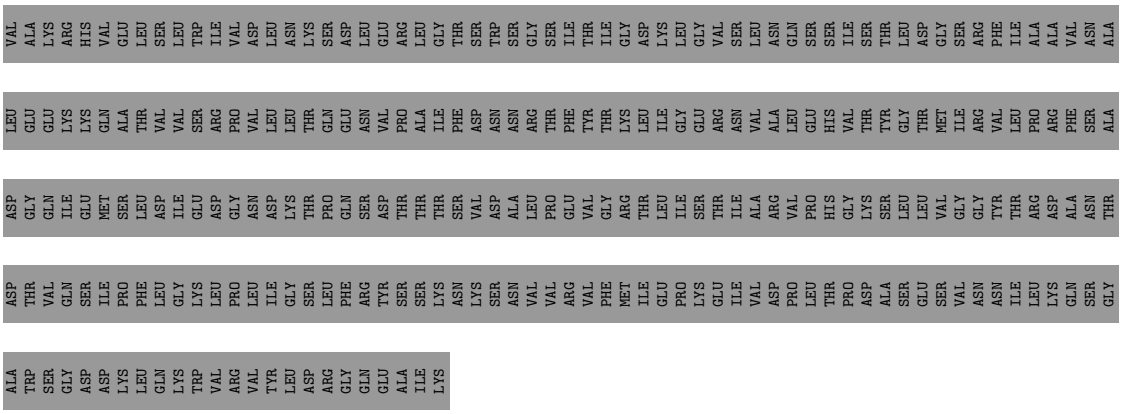
- Molecule 4: Protein InvG

Chain C:

- Molecule 4: Protein InvG

Chain D:



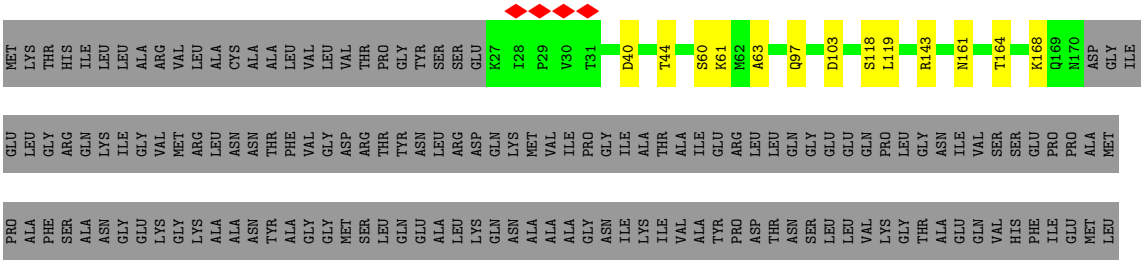


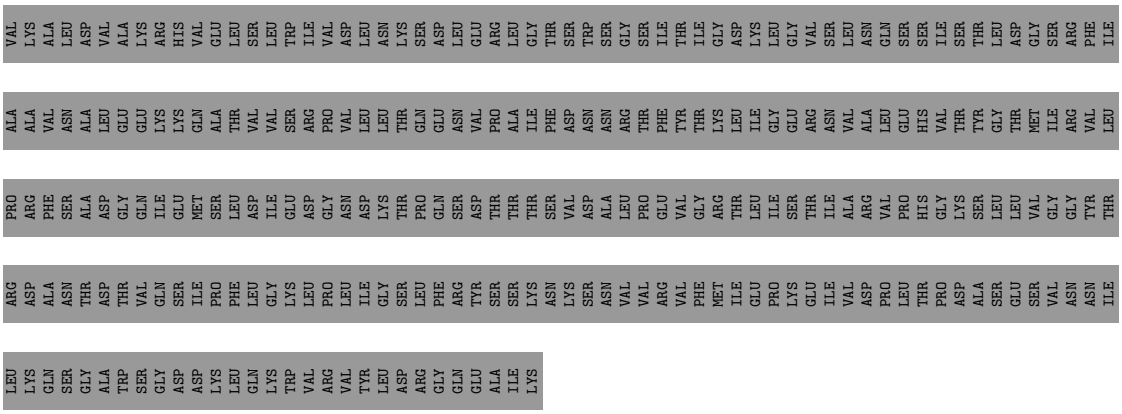
• Molecule 4: Protein InvG

Chain F: 22% 75%

• Molecule 4: Protein InvG

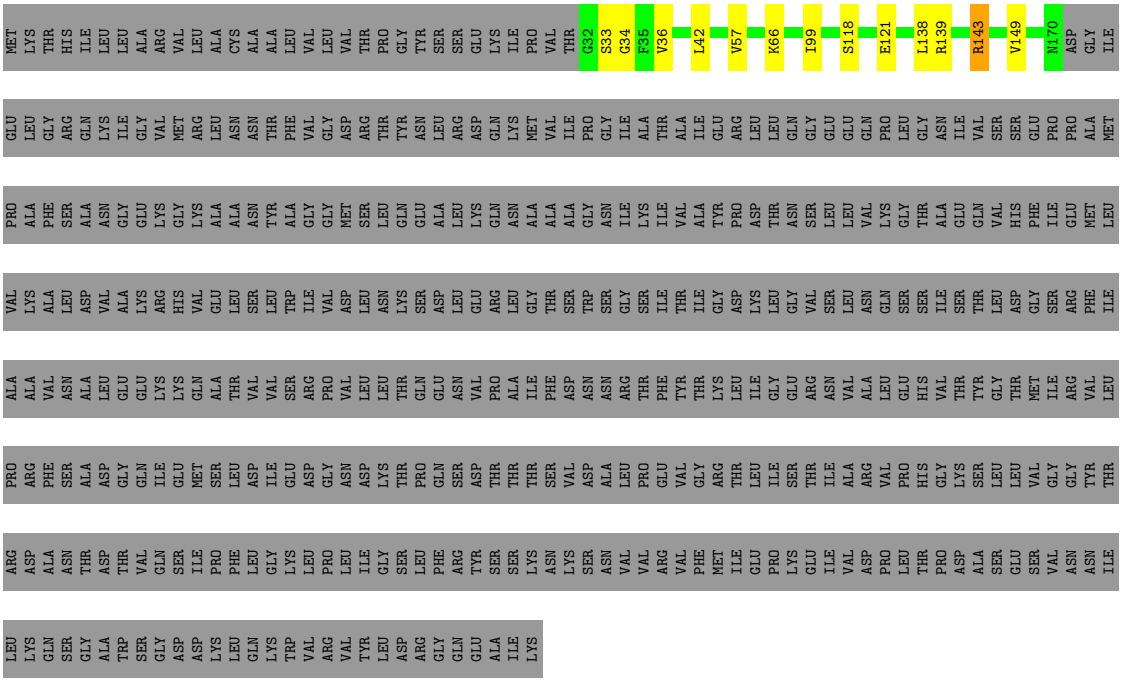
Chain G: 23% 74%





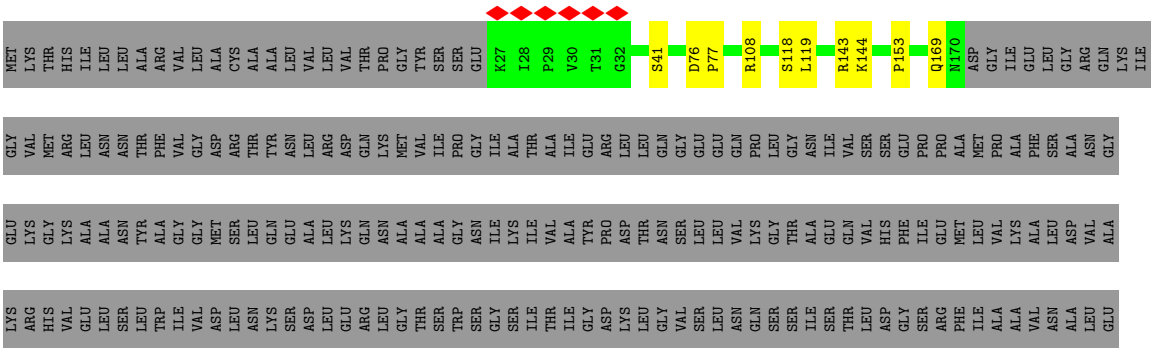
- Molecule 4: Protein InvG

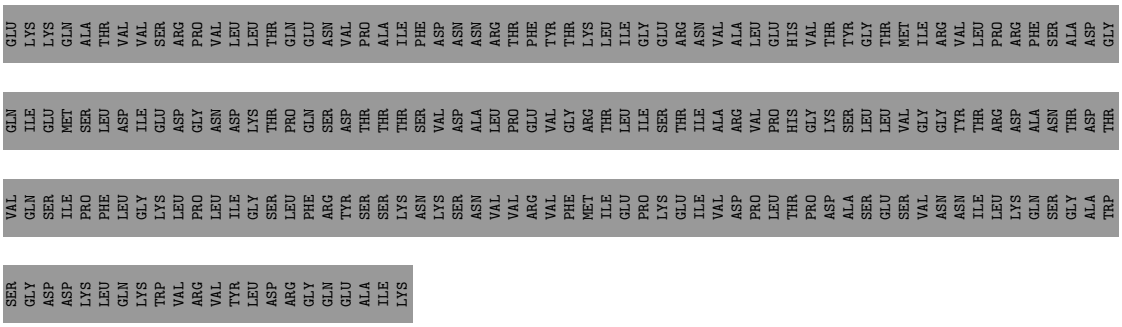
Chain H:



- Molecule 4: Protein InvG

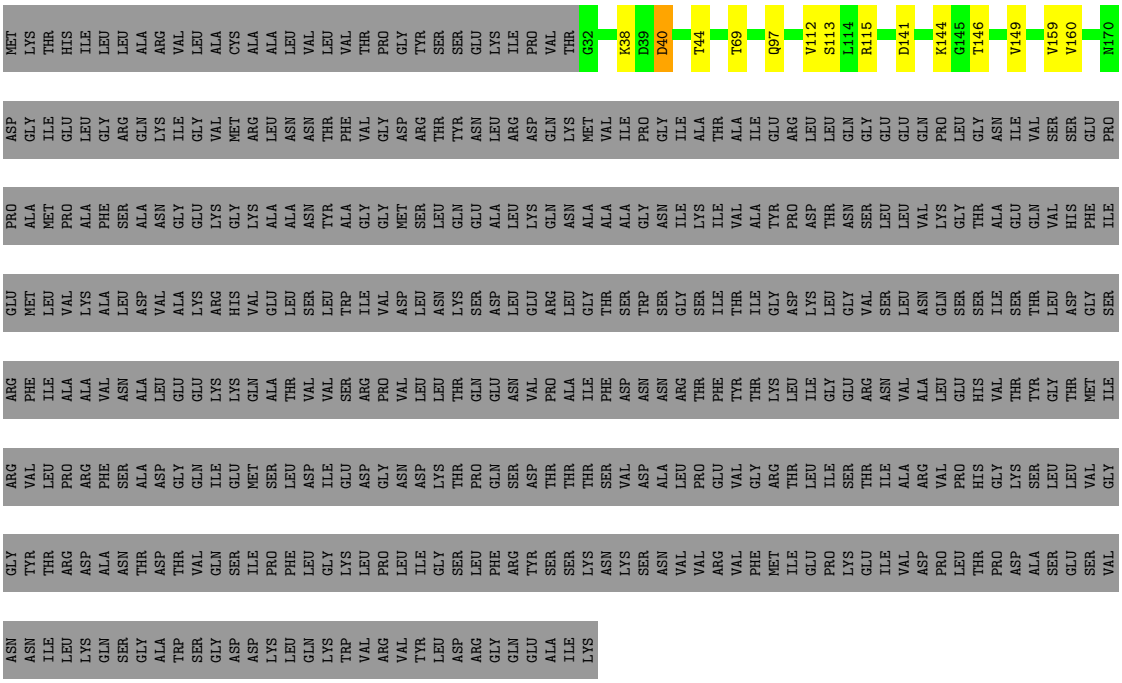
Chain I:





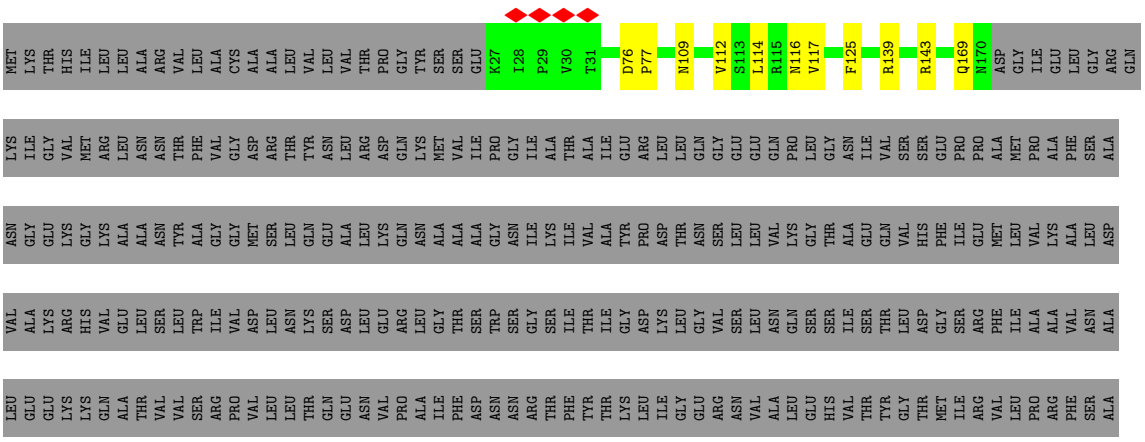
- Molecule 4: Protein InvG

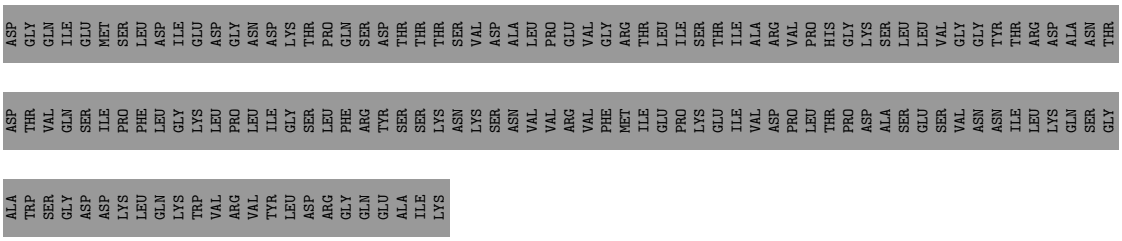
Chain J: 22% 75%



- Molecule 4: Protein InvG

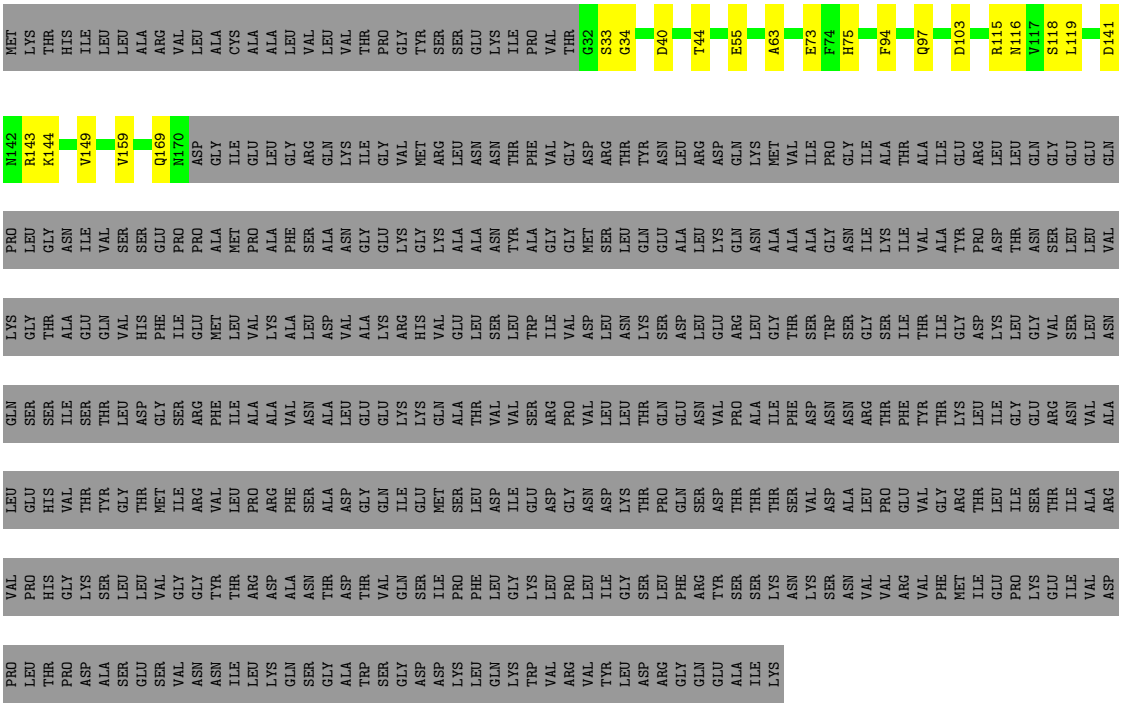
Chain K: 24% 74%





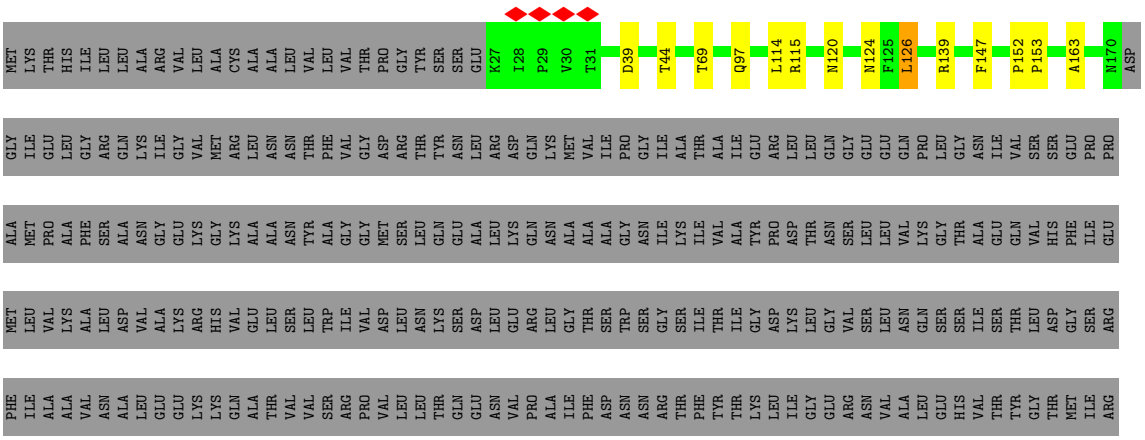
• Molecule 4: Protein InvG

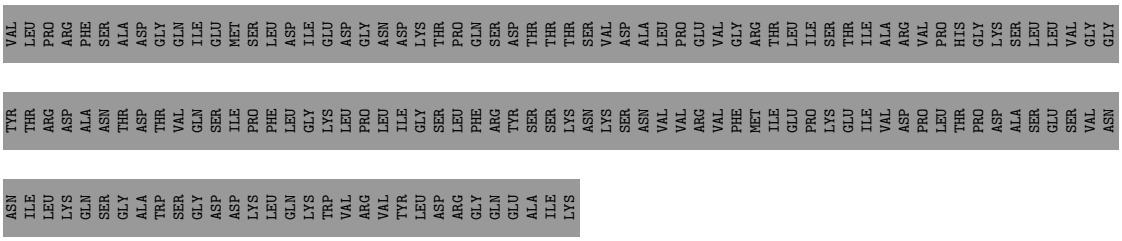
Chain L:



• Molecule 4: Protein InvG

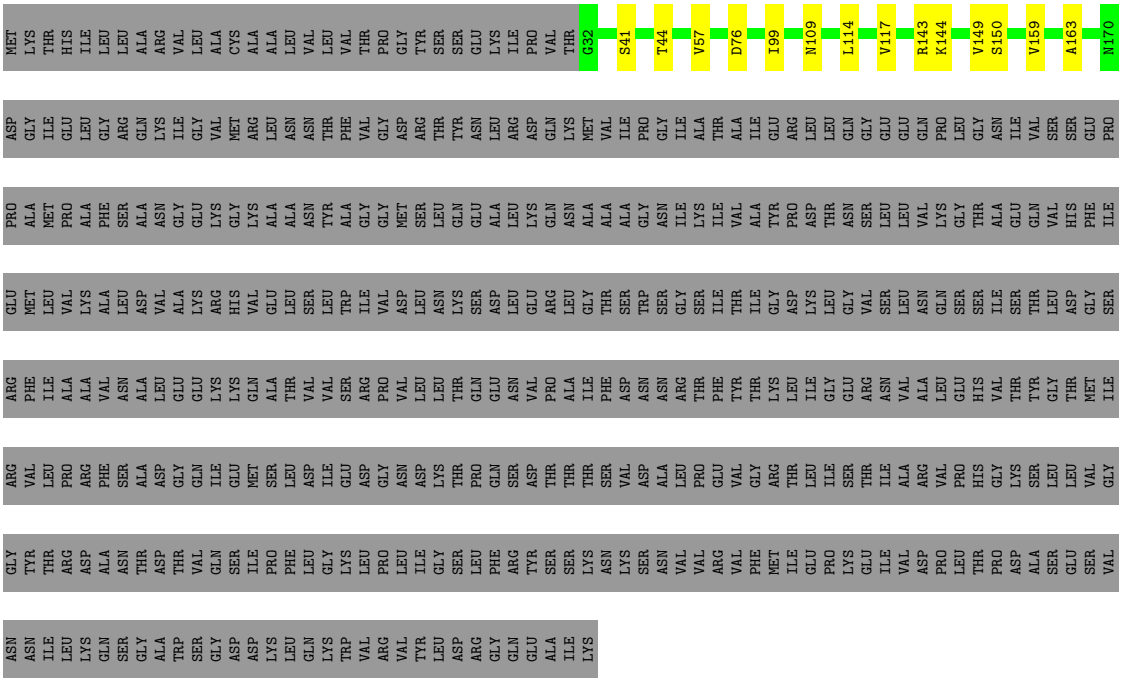
Chain M:





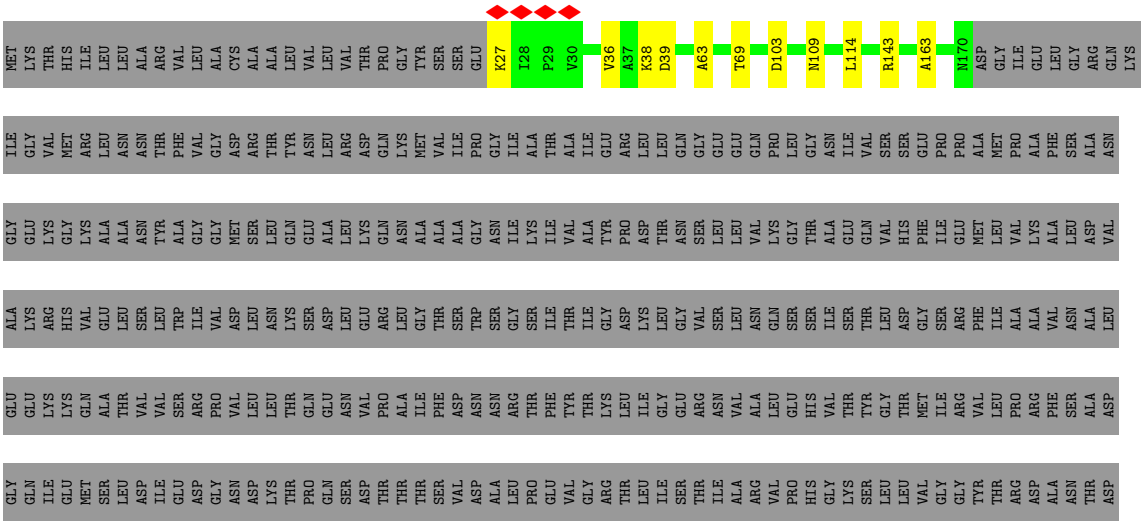
• Molecule 4: Protein InvG

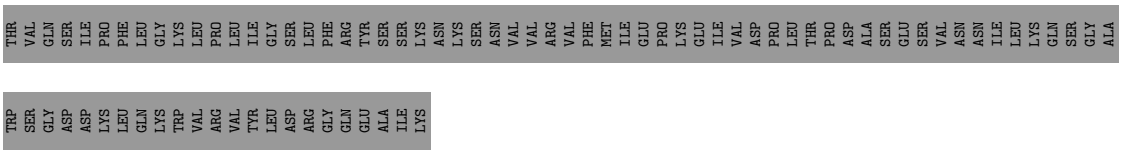
Chain N:



• Molecule 4: Protein InvG

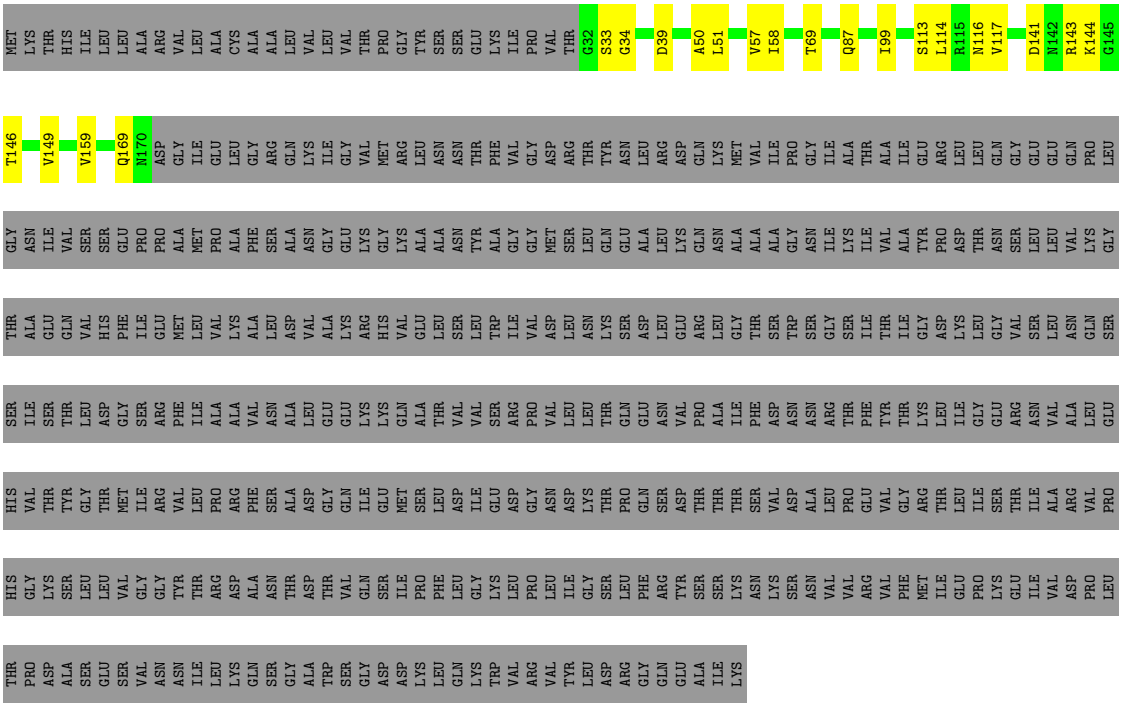
Chain O:





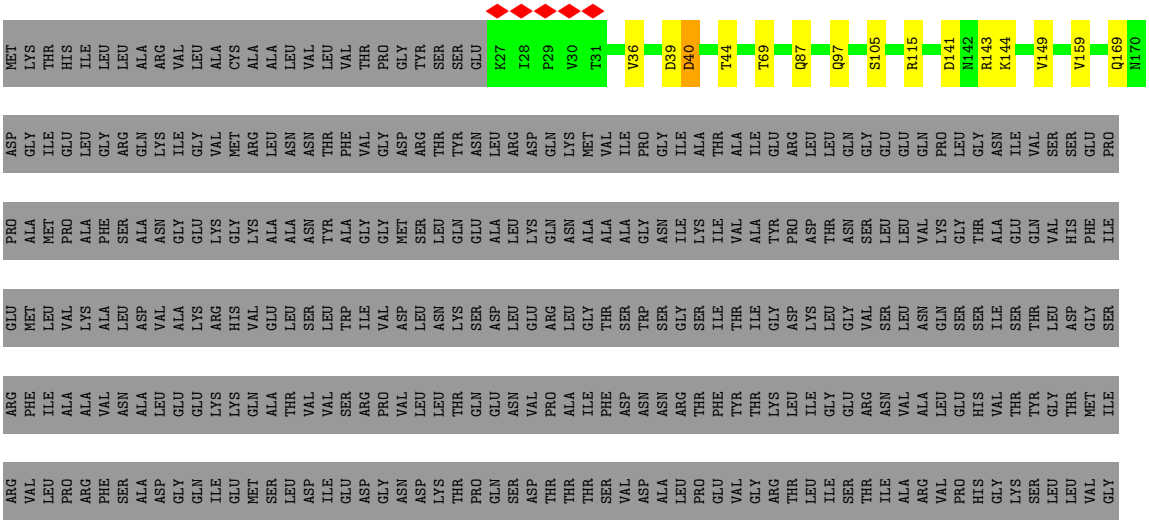
• Molecule 4: Protein InvG

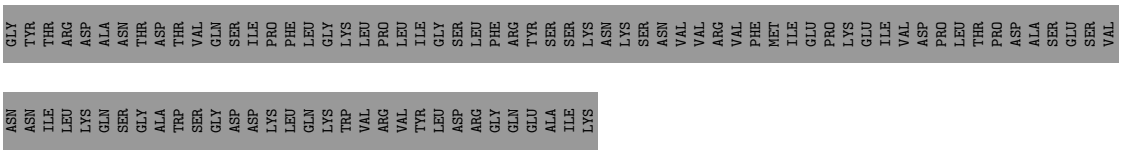
Chain P:



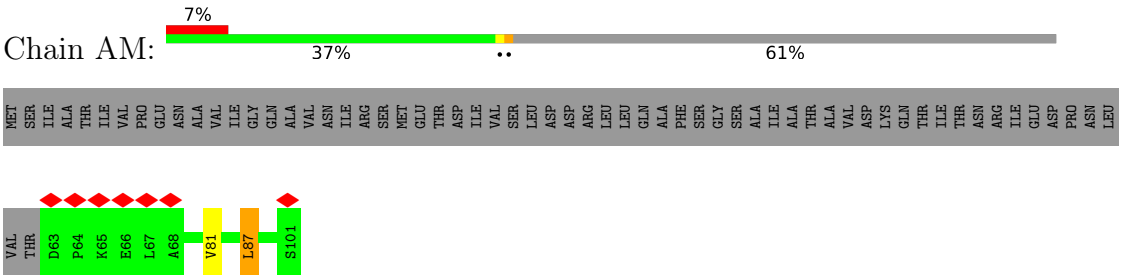
• Molecule 4: Protein InvG

Chain Q:

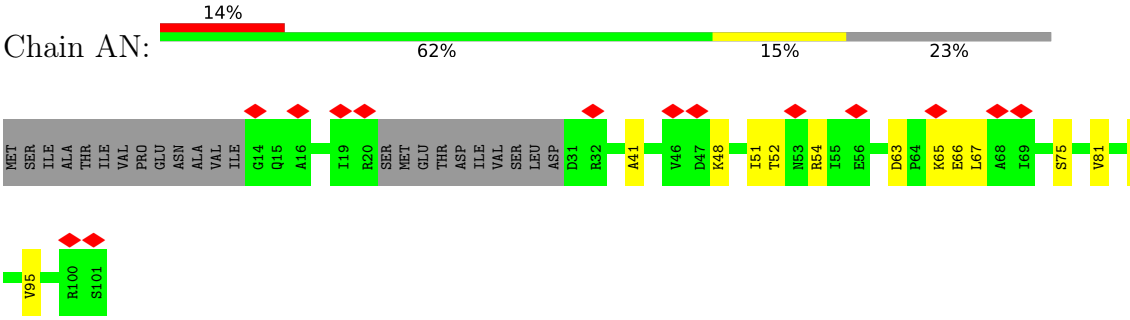




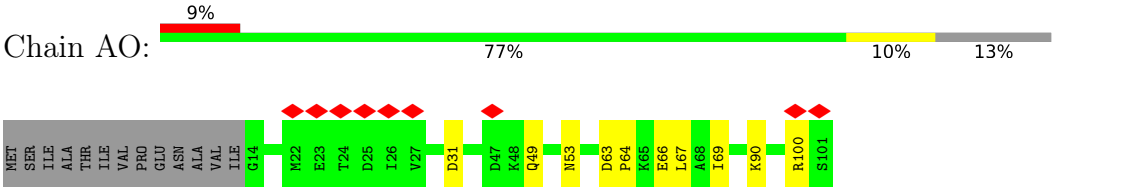
- Molecule 5: Protein PrgJ



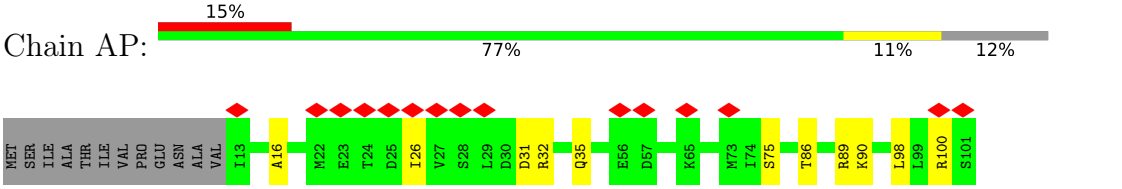
- Molecule 5: Protein PrgJ



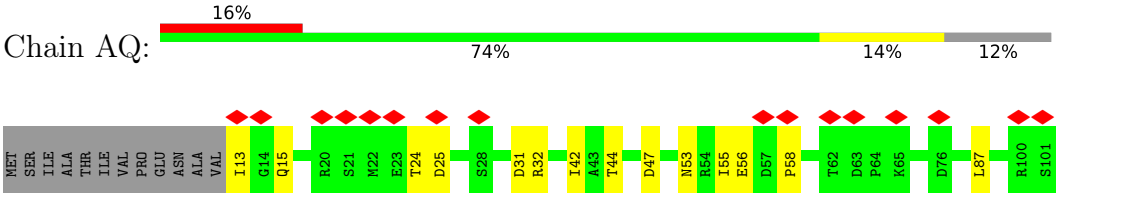
- Molecule 5: Protein PrgJ



- Molecule 5: Protein PrgJ

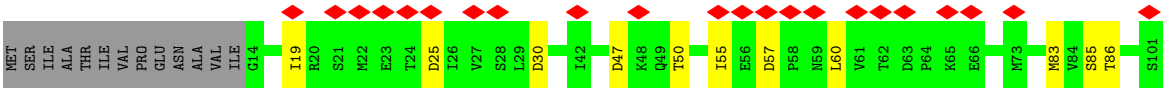


- Molecule 5: Protein PrgJ



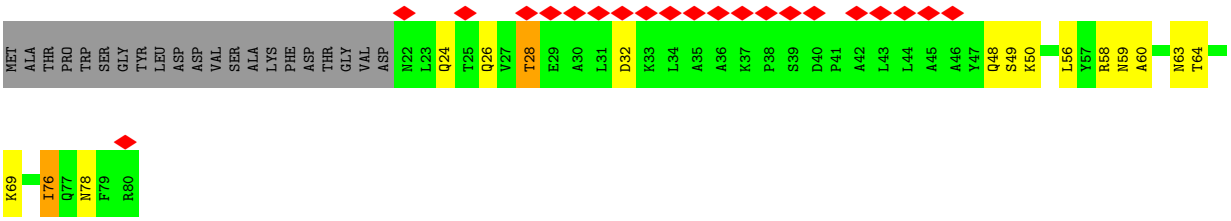
- Molecule 5: Protein PrgJ

Chain AR:



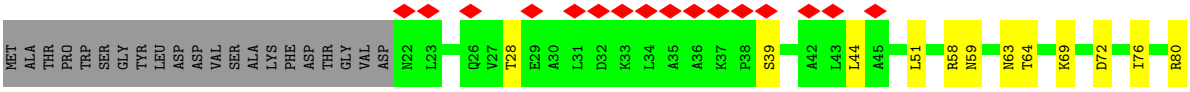
• Molecule 6: Protein PrgI

Chain AS:



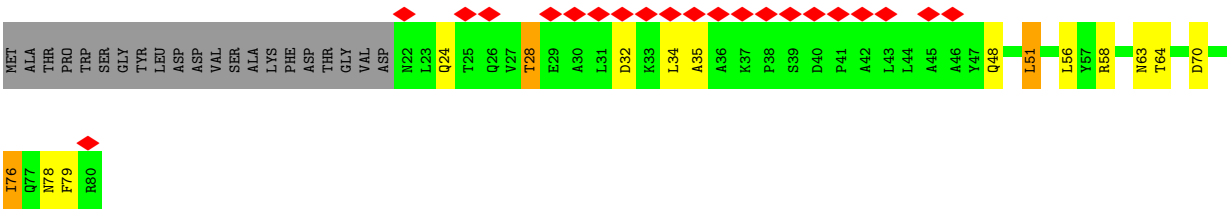
• Molecule 6: Protein PrgI

Chain AT:



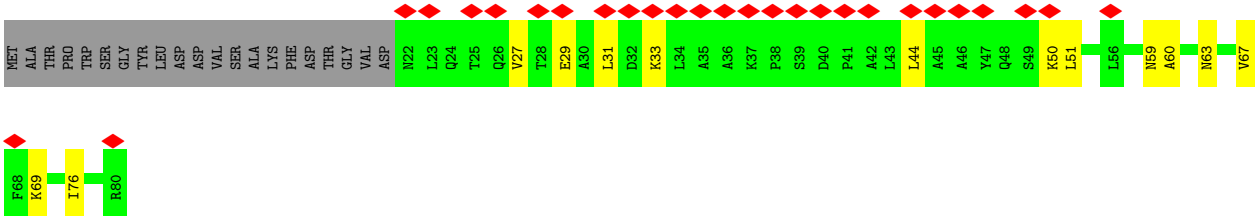
• Molecule 6: Protein PrgI

Chain AU:



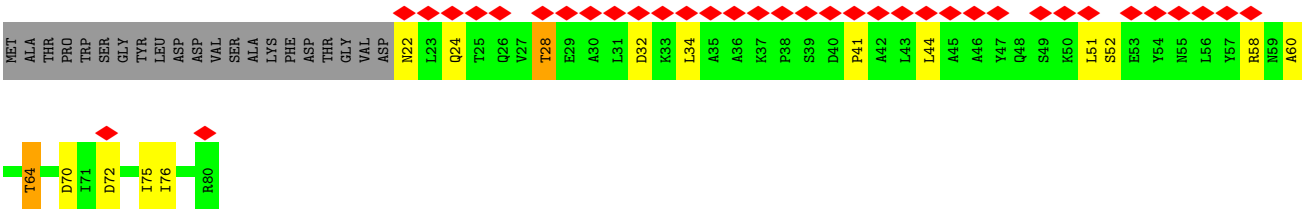
• Molecule 6: Protein PrgI

Chain AV:



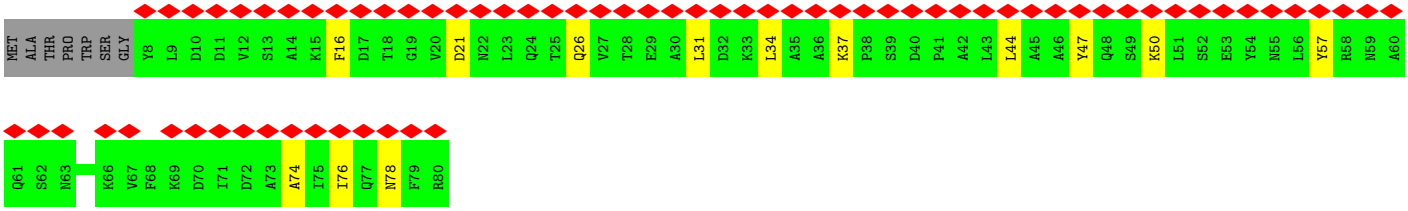
• Molecule 6: Protein PrgI

Chain AW:



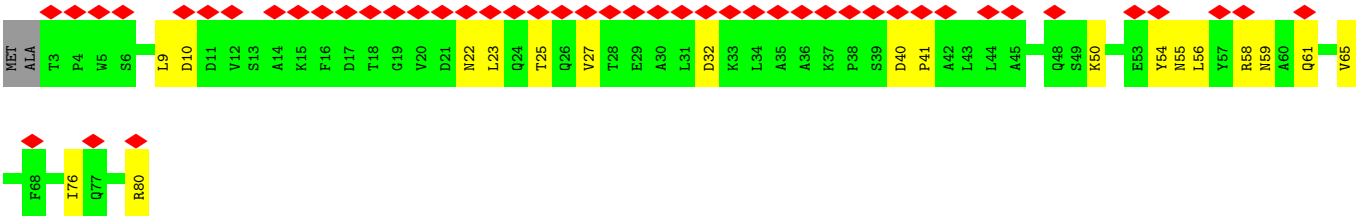
• Molecule 6: Protein PrgI

Chain AX:



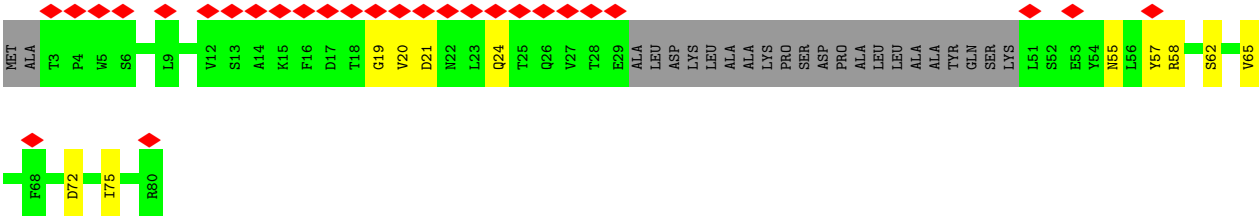
• Molecule 6: Protein PrgI

Chain AY:



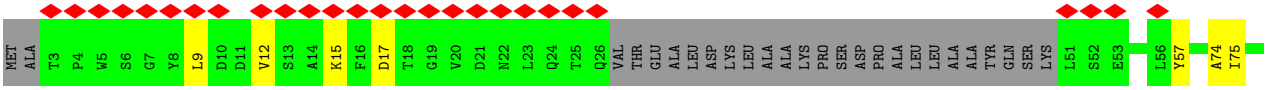
• Molecule 6: Protein PrgI

Chain AZ:



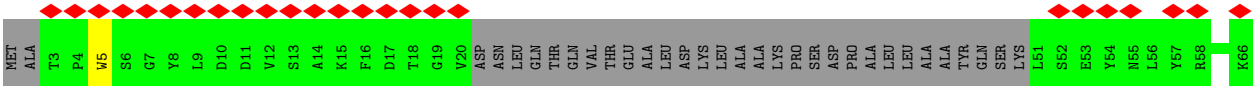
• Molecule 6: Protein PrgI

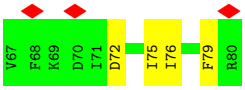
Chain BA:



• Molecule 6: Protein PrgI

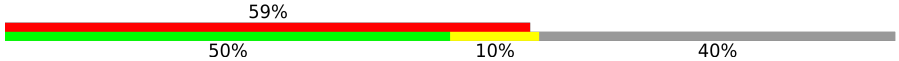
Chain BB:

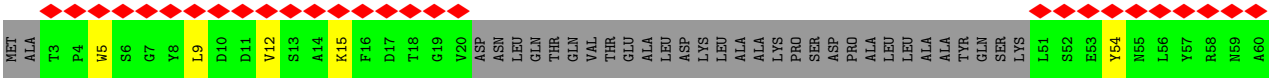


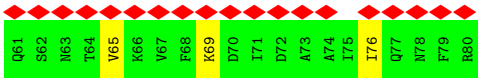


• Molecule 6: Protein PrgI

Chain BC:

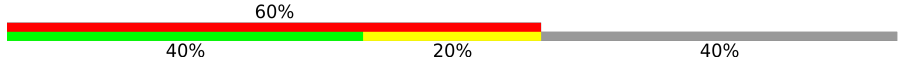


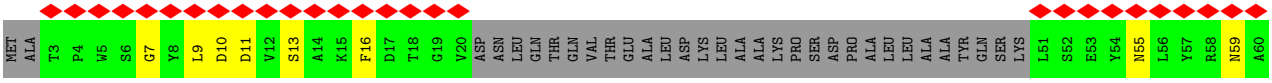


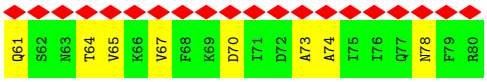


• Molecule 6: Protein PrgI

Chain BD:

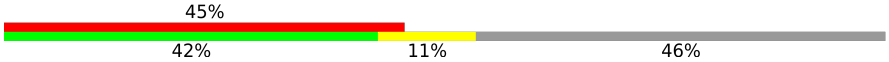


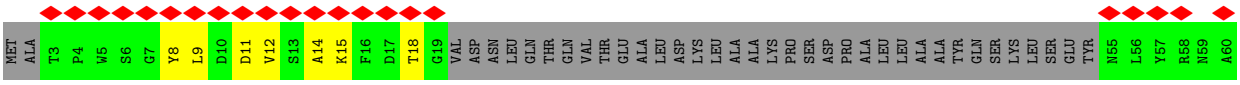


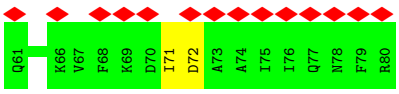


• Molecule 6: Protein PrgI

Chain BE:

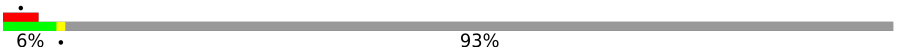


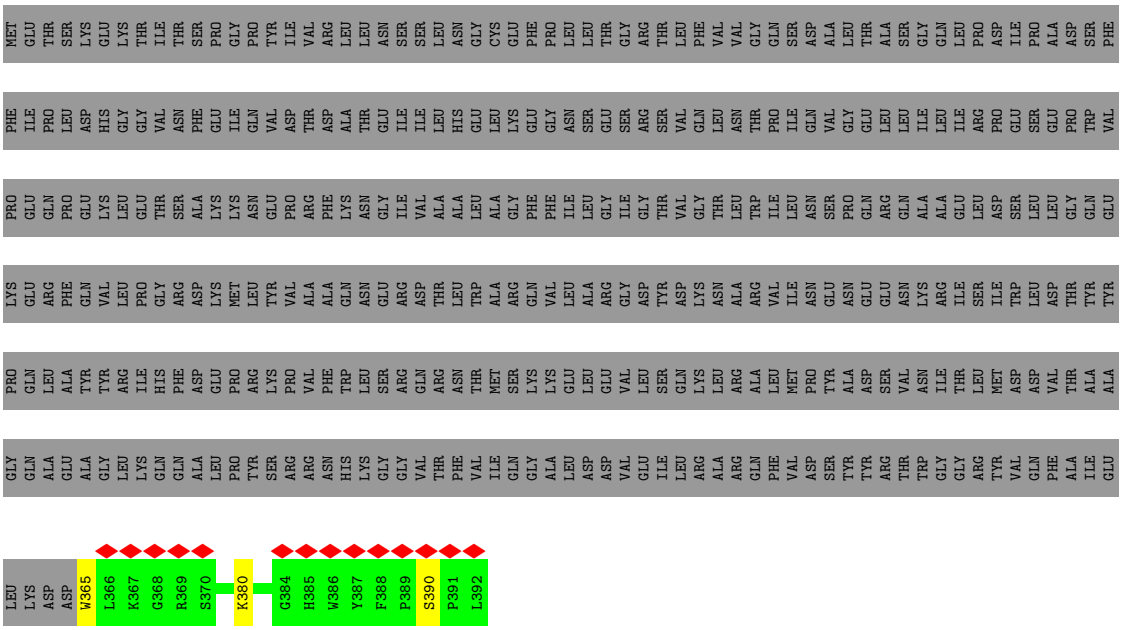




• Molecule 7: Protein PrgH

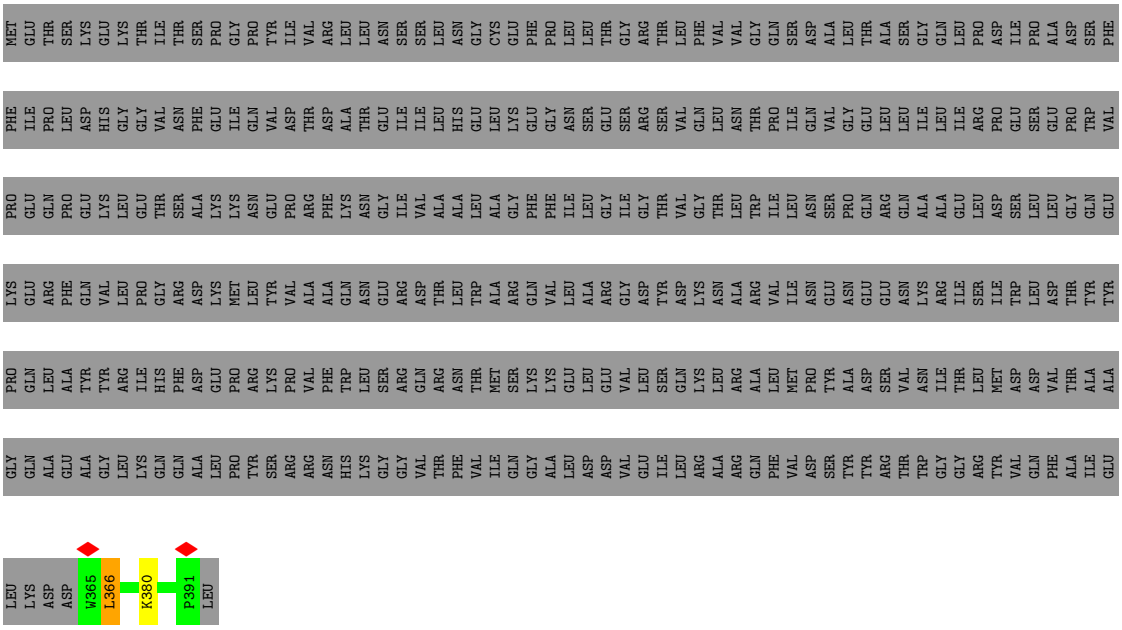
Chain E:





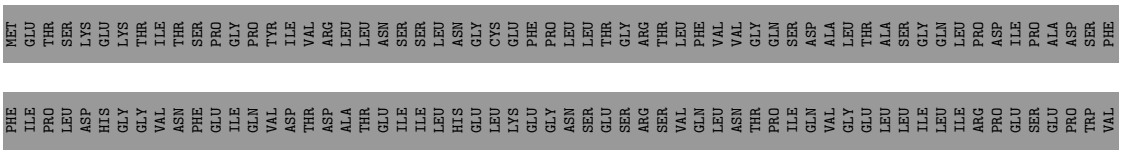
• Molecule 7: Protein PrgH

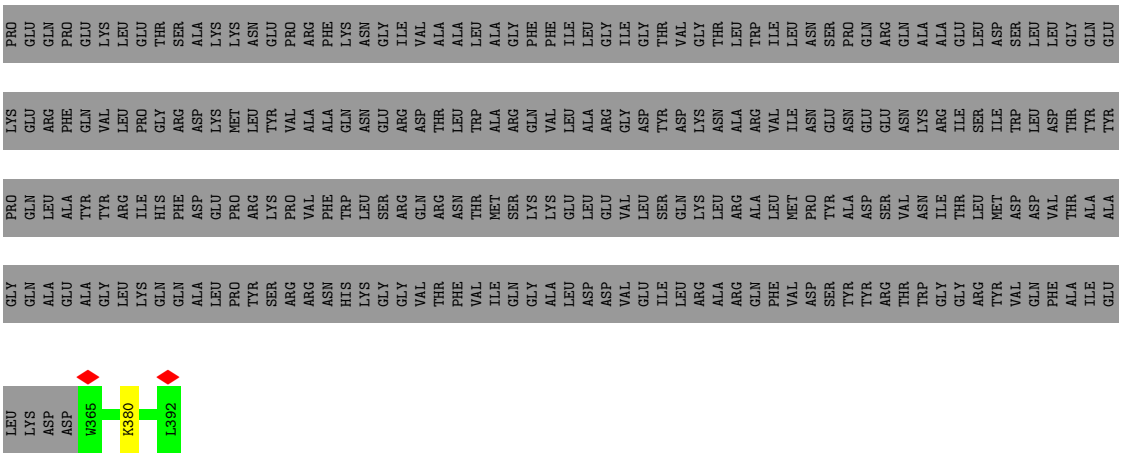
Chain R: 6% 93%



• Molecule 7: Protein PrgH

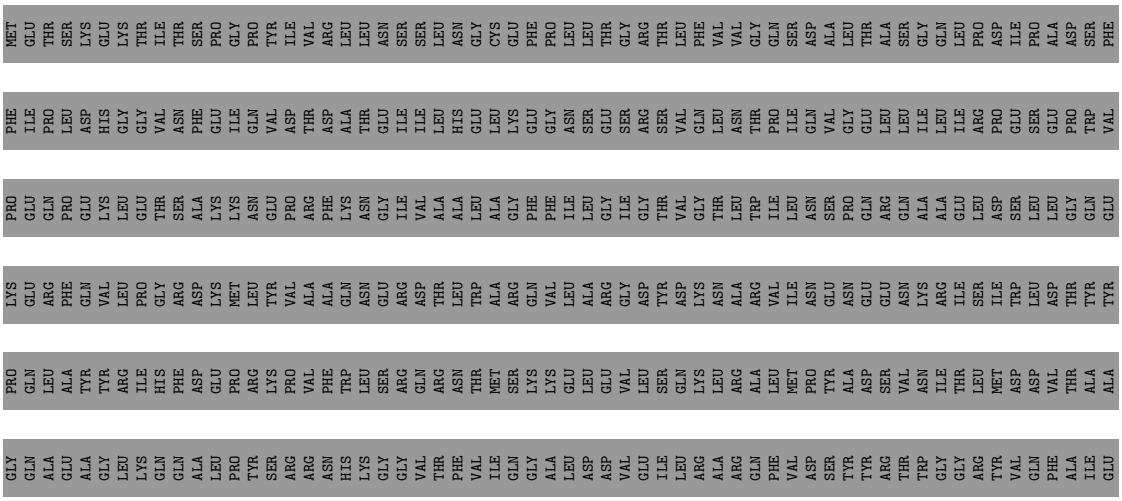
Chain S: 7% 93%





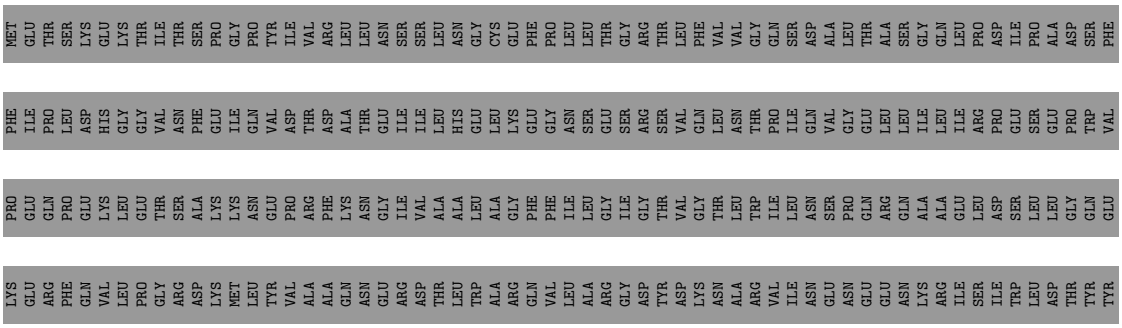
• Molecule 7: Protein PrgH

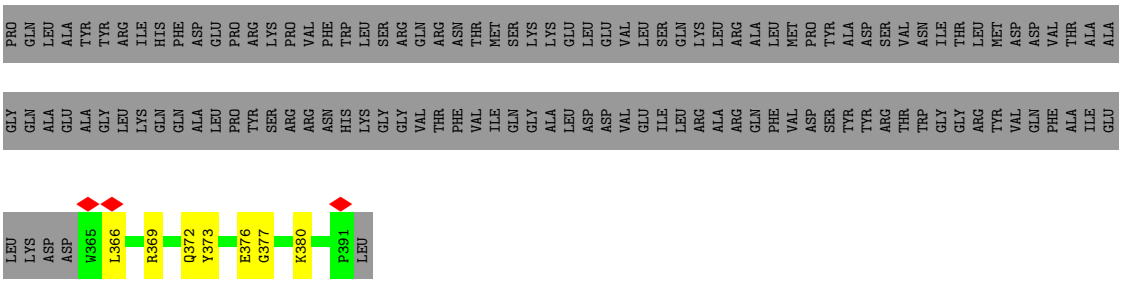
Chain T: 7% 93%



• Molecule 7: Protein PrgH

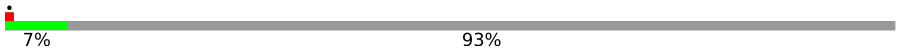
Chain U: 5% 93%

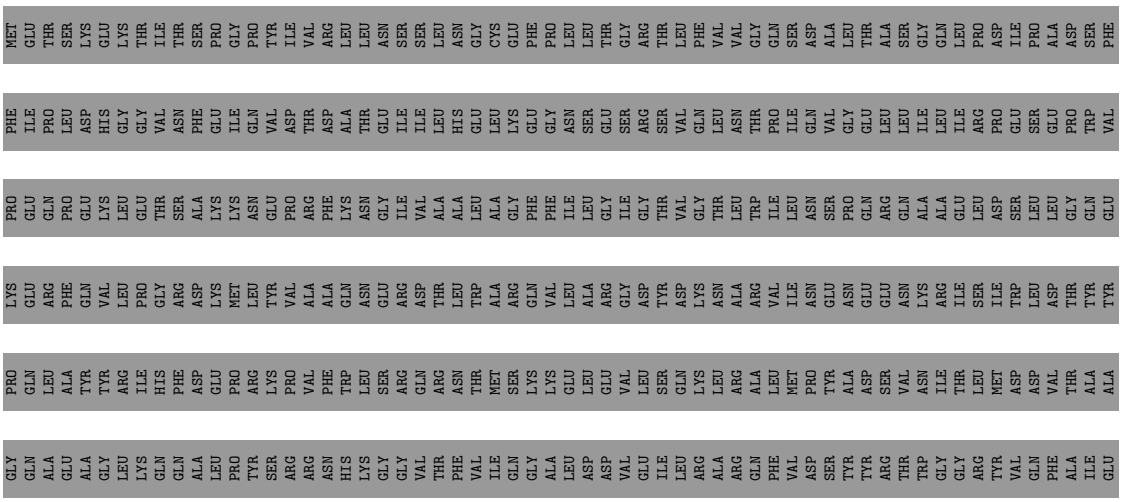


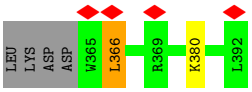


• Molecule 7: Protein PrgH

Chain V:

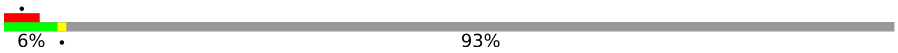


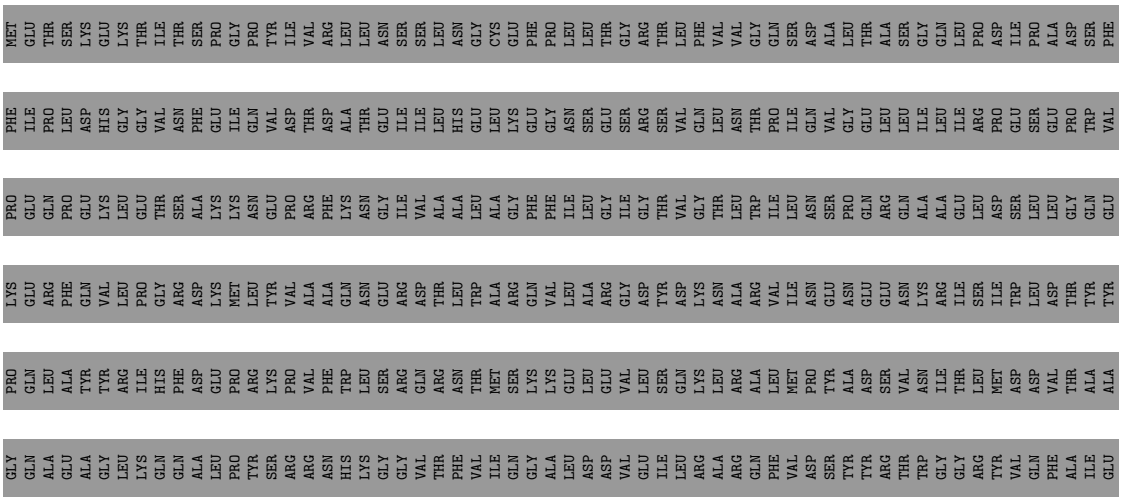


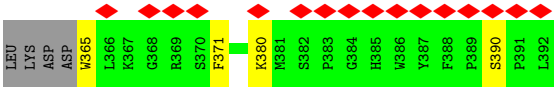


• Molecule 7: Protein PrgH

Chain W:

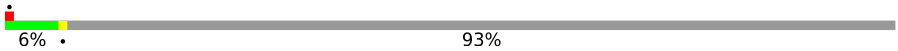


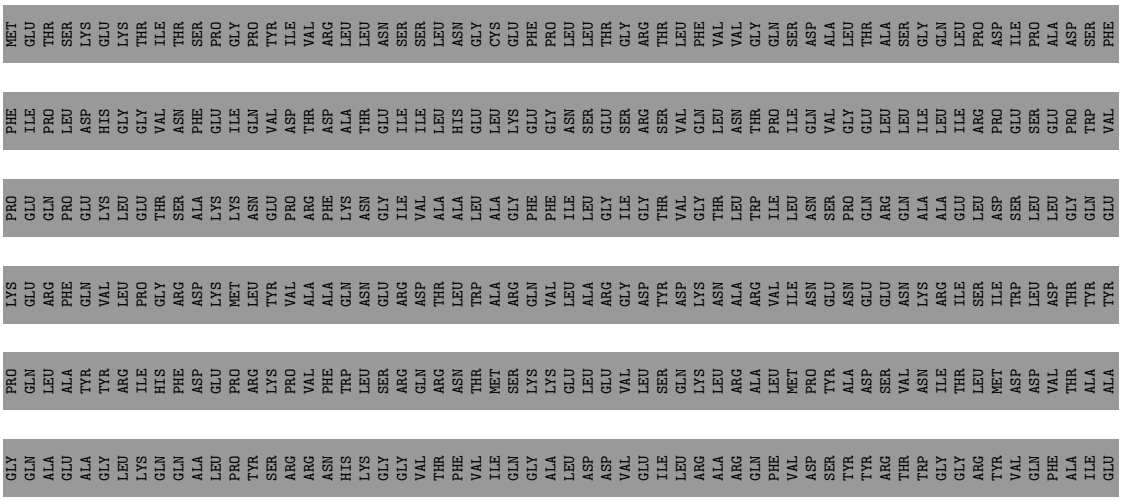




- Molecule 7: Protein PrgH

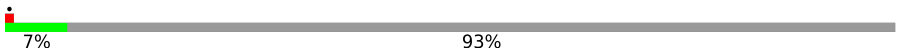
Chain X:

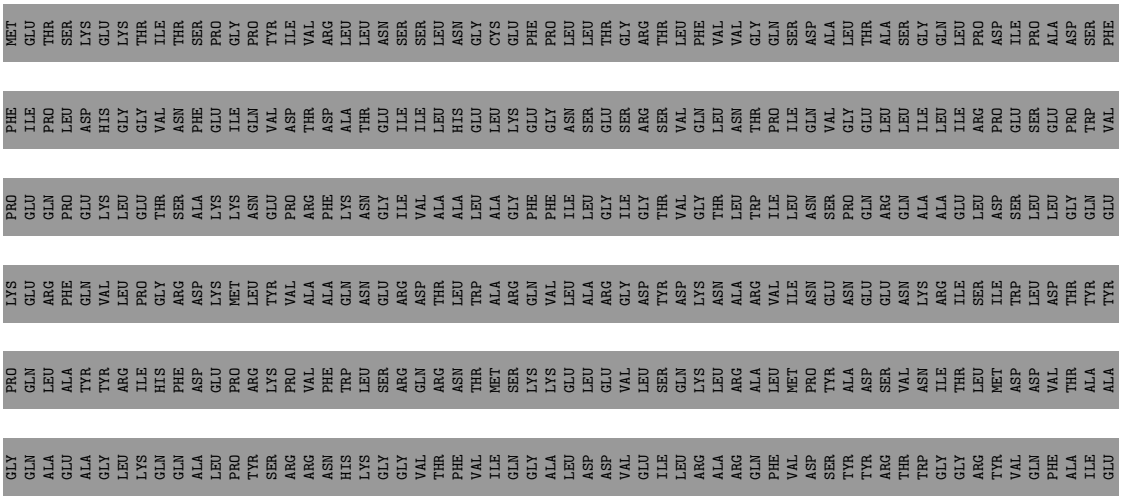


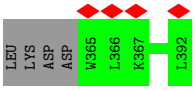


- Molecule 7: Protein PrgH

Chain Y:

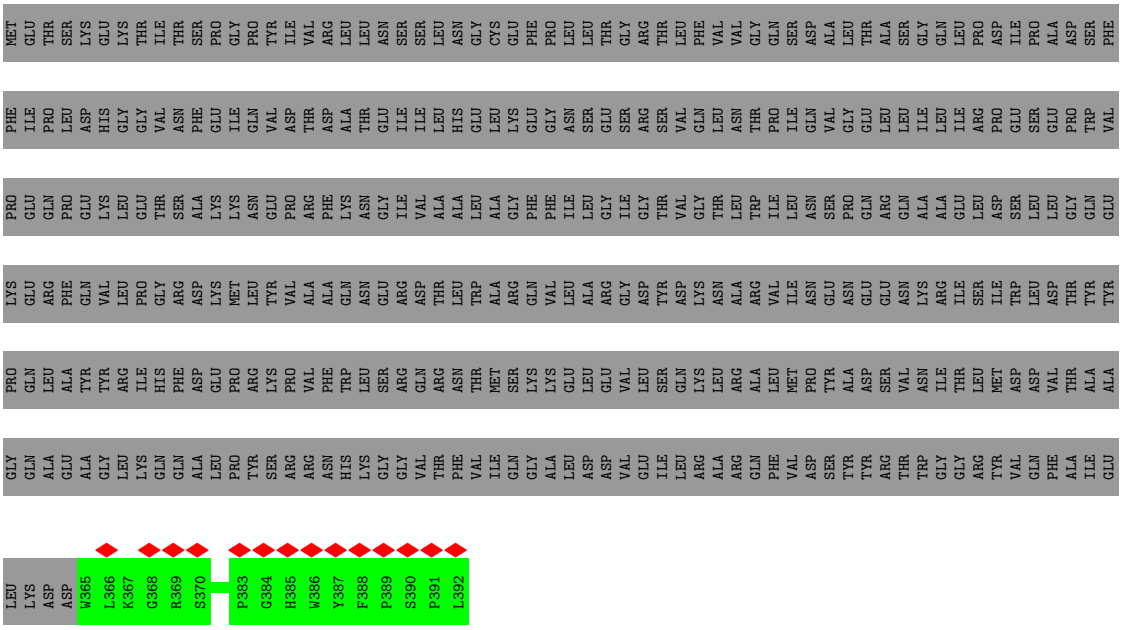






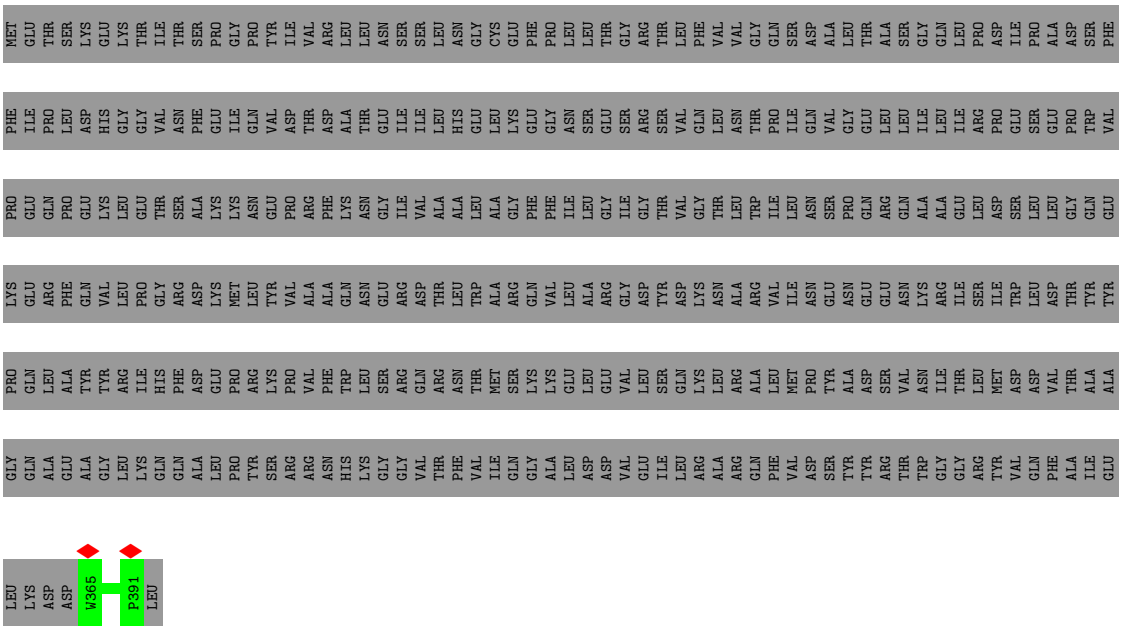
- Molecule 7: Protein PrgH

Chain Z: 7% 93%



- Molecule 7: Protein PrgH

Chain a: 7% 93%

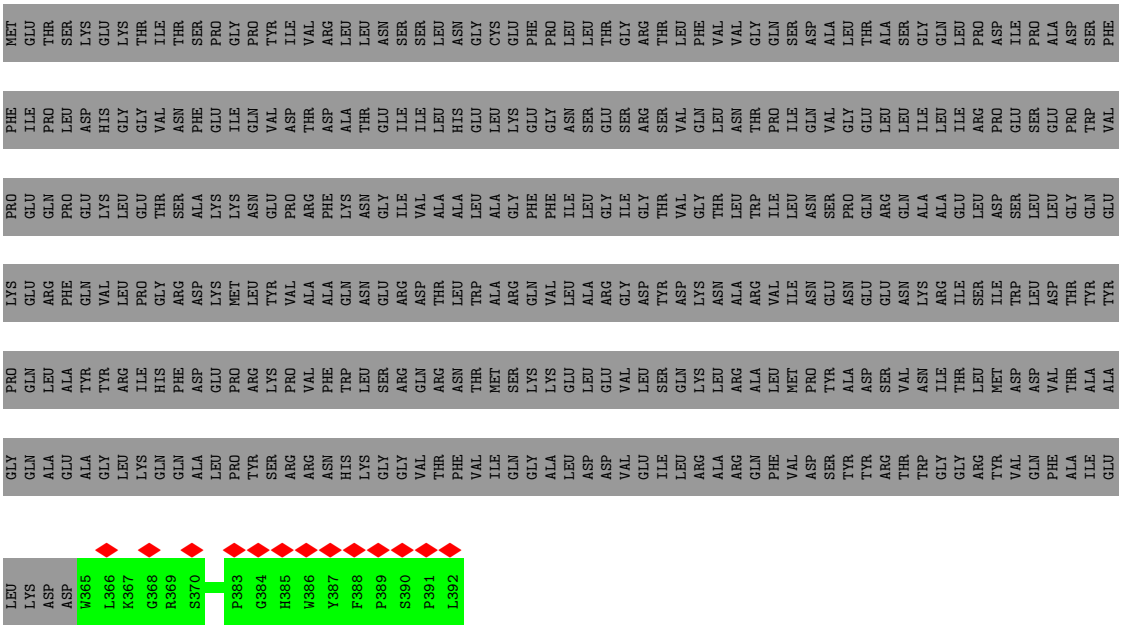


- Molecule 7: Protein PrgH

Chain b: 7% 93%

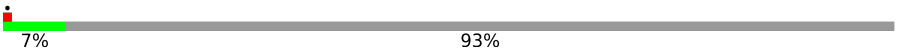
- Molecule 7: Protein PrgH

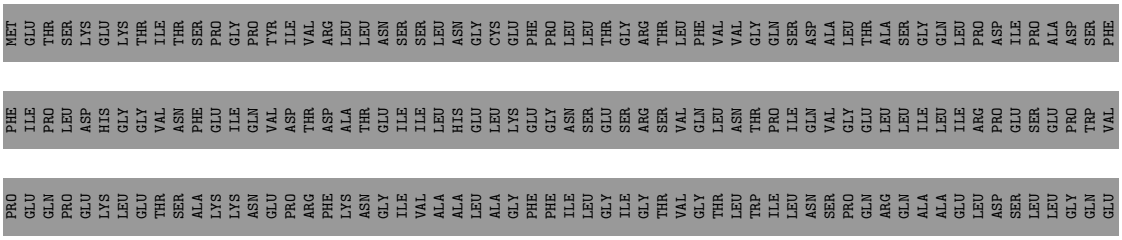
Chain c:

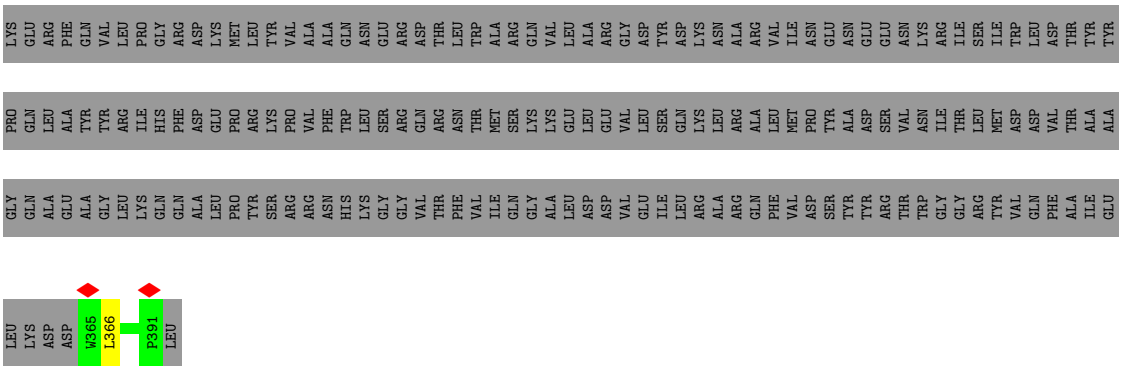


- Molecule 7: Protein PrgH

Chain d:

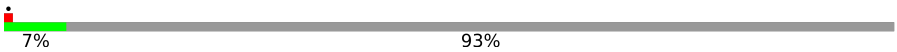


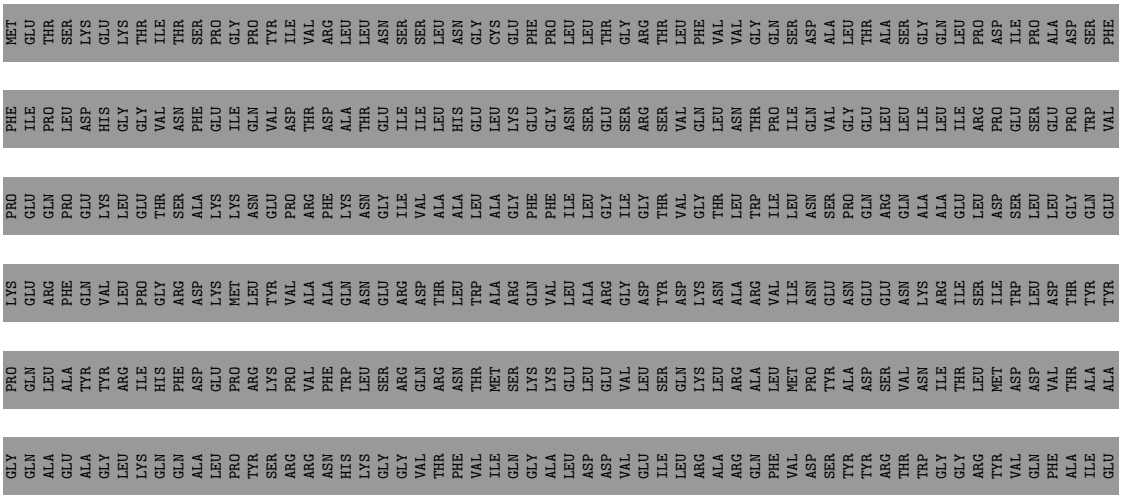




- Molecule 7: Protein PrgH

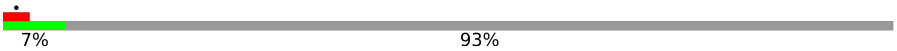
Chain e:

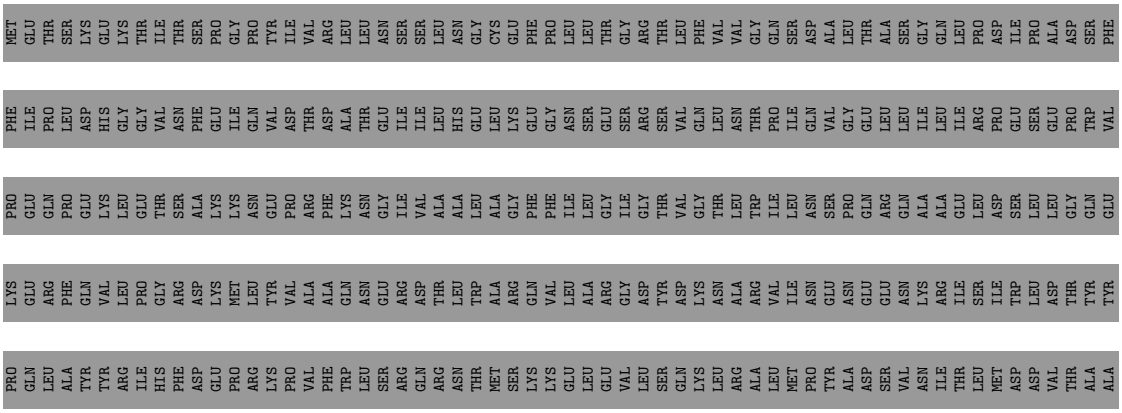


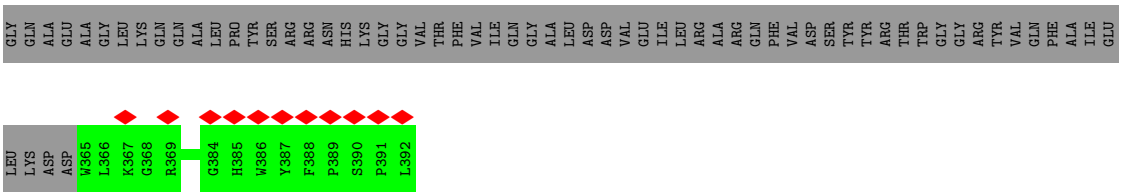


- Molecule 7: Protein PrgH

Chain f:

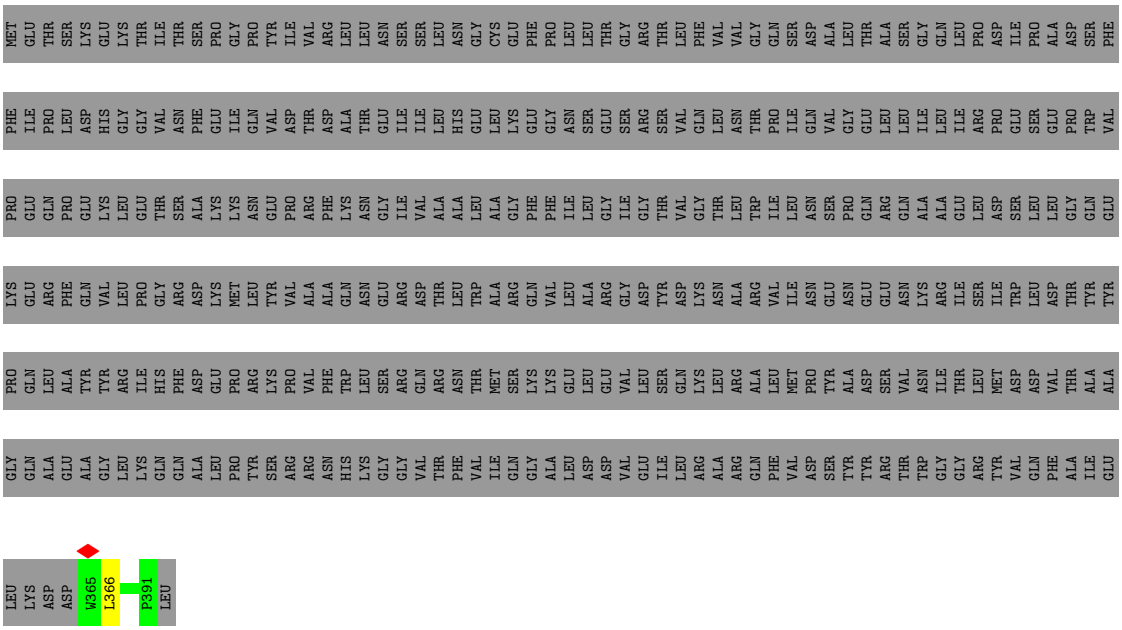






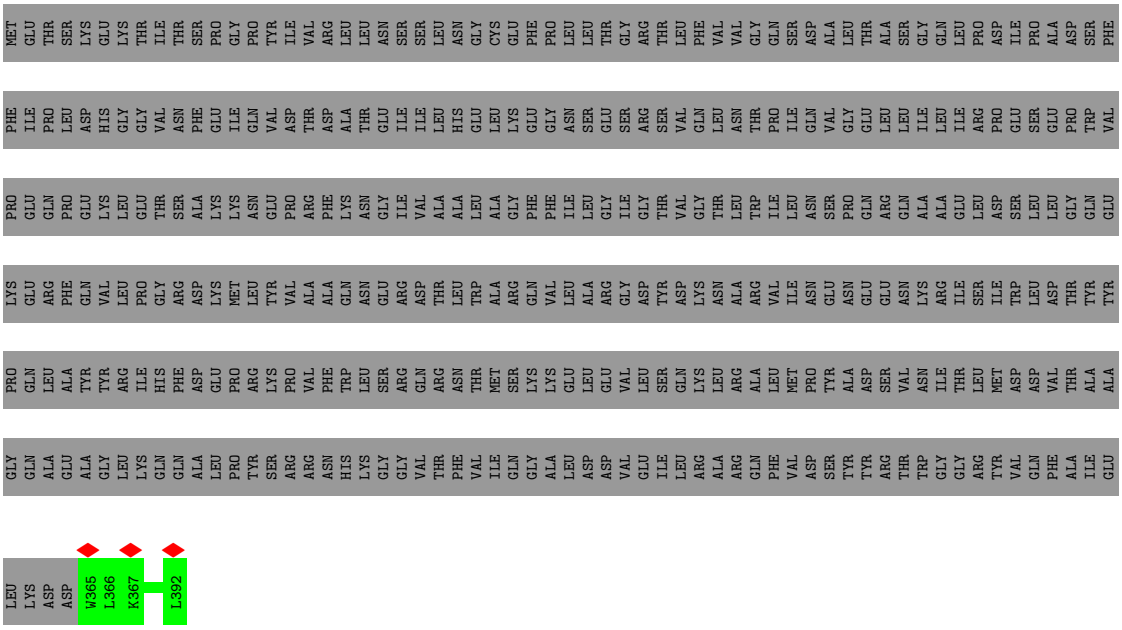
• Molecule 7: Protein PrgH

Chain g: 7% 93%



• Molecule 7: Protein PrgH

Chain h: 7% 93%



- Molecule 7: Protein PrgH

Chain i: 7% 93%

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

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

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

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

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

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

LEU LYS ASP ASP W365 L366 K367 G368 R369 P383 G384 H385 W386 Y387 F388 P389 S390 P391 L392

- Molecule 7: Protein PrgH

Chain j: 7% 93%

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

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

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

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

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

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

LEU LYS ASP ASP W365 S390 P391 LEU

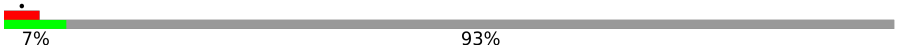
- Molecule 7: Protein PrgH

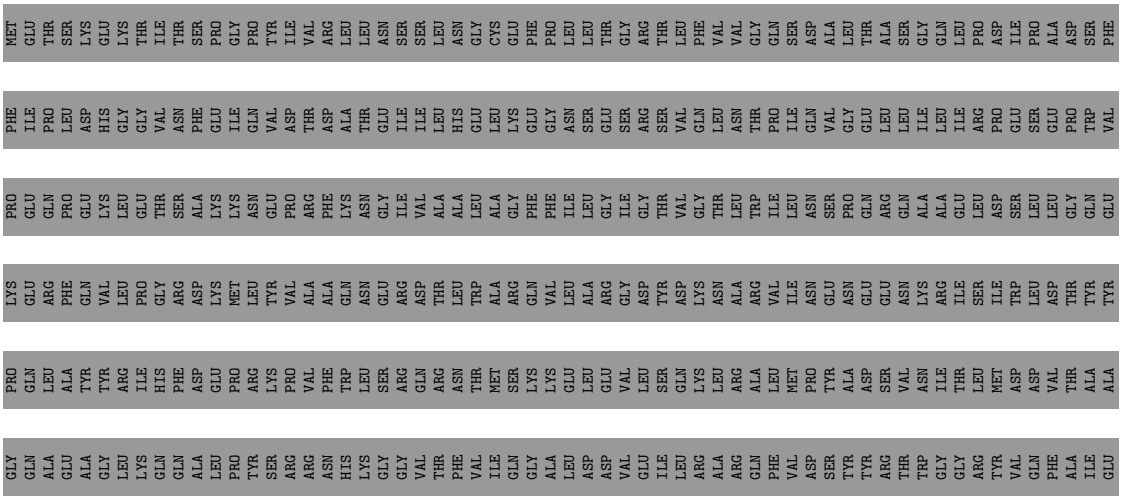
Chain k: 7% 93%

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

• Molecule 7: Protein PrgH

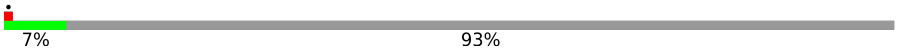
Chain l:

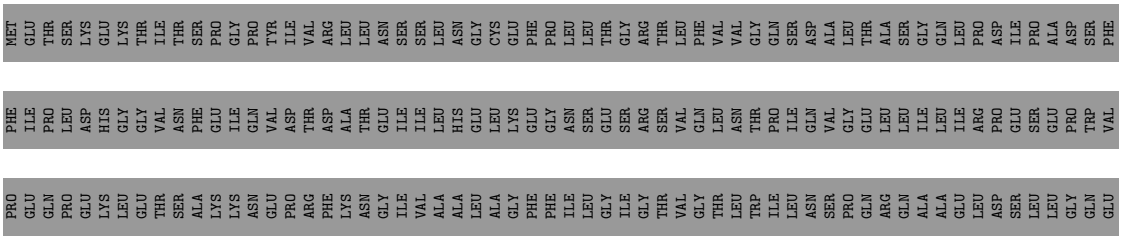


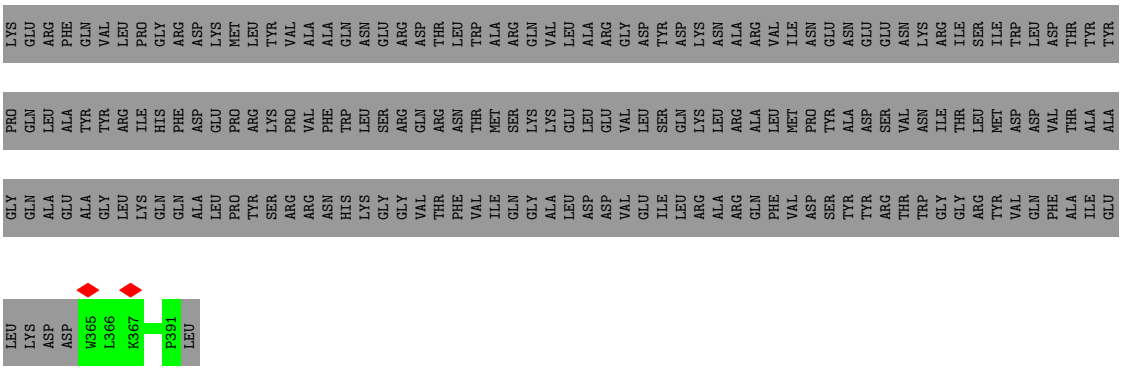


• Molecule 7: Protein PrgH

Chain m:

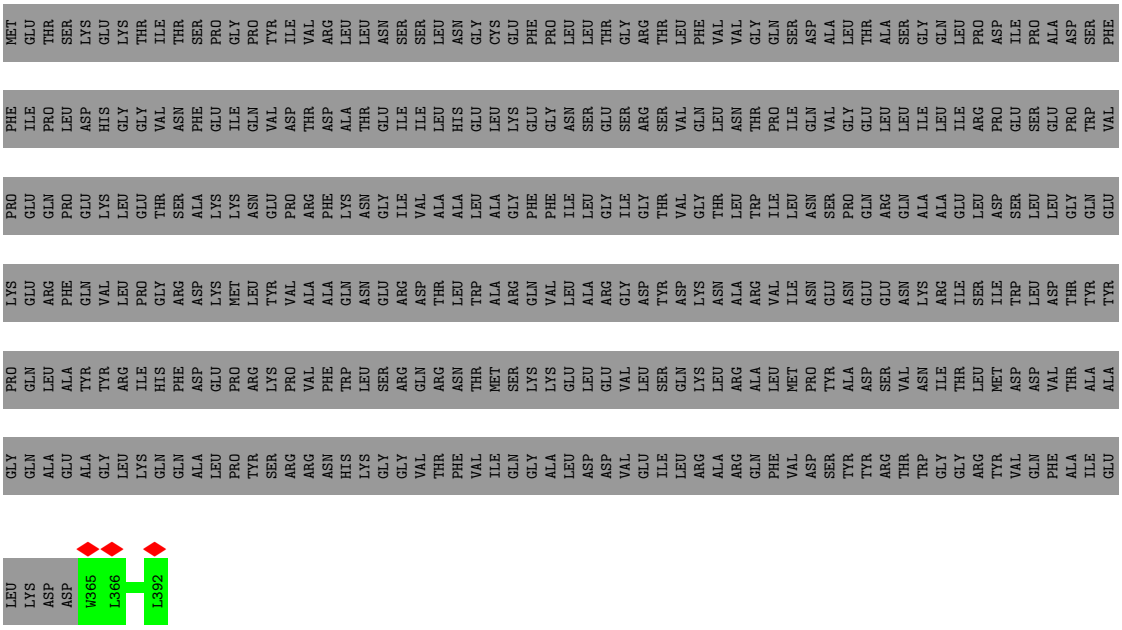






• Molecule 7: Protein PrgH

Chain n: 7% 93%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25666	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	5.972	Depositor
Minimum map value	-2.765	Depositor
Average map value	-0.012	Depositor
Map value standard deviation	0.211	Depositor
Recommended contour level	1.1	Depositor
Map size (Å)	427.5, 427.5, 427.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.71, 1.71, 1.71	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	0	0.40	0/1598	0.64	0/2172
1	1	0.37	0/1605	0.64	0/2181
1	2	0.36	0/1589	0.63	0/2159
1	3	0.38	0/1642	0.60	0/2230
1	4	0.39	0/1799	0.63	0/2441
2	5	0.39	0/1935	0.68	2/2647 (0.1%)
3	6	0.32	0/414	0.72	0/565
3	7	0.35	0/657	0.69	0/897
3	8	0.37	0/657	0.69	1/897 (0.1%)
3	9	0.38	0/660	0.64	0/900
4	A	0.39	0/1131	0.65	3/1525 (0.2%)
4	B	0.41	0/1181	0.65	1/1593 (0.1%)
4	C	0.40	0/1131	0.60	0/1525
4	D	0.41	0/1170	0.59	0/1579
4	F	0.41	0/1131	0.59	0/1525
4	G	0.40	0/1181	0.60	0/1593
4	H	0.45	0/1131	0.63	1/1525 (0.1%)
4	I	0.39	0/1181	0.59	0/1593
4	J	0.42	0/1131	0.58	0/1525
4	K	0.41	0/1181	0.61	0/1593
4	L	0.41	0/1131	0.59	0/1525
4	M	0.39	0/1170	0.61	1/1579 (0.1%)
4	N	0.42	0/1131	0.59	0/1525
4	O	0.40	0/1181	0.63	0/1593
4	P	0.41	0/1131	0.58	0/1525
4	Q	0.41	0/1181	0.62	0/1593
5	AM	0.40	0/300	0.78	1/403 (0.2%)
5	AN	0.35	0/646	0.59	0/870
5	AO	0.33	0/671	0.59	0/908
5	AP	0.36	0/679	0.64	0/919
5	AQ	0.32	0/679	0.63	1/919 (0.1%)
5	AR	0.33	0/671	0.62	0/908
6	AS	0.35	0/472	0.65	0/638
6	AT	0.35	0/472	0.59	0/638

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	AU	0.37	0/472	0.62	0/638
6	AV	0.39	0/472	0.70	1/638 (0.2%)
6	AW	0.35	0/472	0.56	0/638
6	AX	0.33	0/582	0.56	1/788 (0.1%)
6	AY	0.39	0/623	0.62	1/846 (0.1%)
6	AZ	0.31	0/467	0.50	0/632
6	BA	0.31	0/444	0.49	0/600
6	BB	0.33	0/395	0.66	0/533
6	BC	0.30	0/395	0.54	0/533
6	BD	0.32	0/395	0.61	1/533 (0.2%)
6	BE	0.32	0/352	0.59	0/474
7	E	0.39	0/248	0.54	0/334
7	R	0.41	0/239	0.71	2/323 (0.6%)
7	S	0.43	0/243	0.64	0/329
7	T	0.39	0/248	0.56	0/334
7	U	0.44	0/239	0.62	0/323
7	V	0.42	0/243	0.78	1/329 (0.3%)
7	W	0.40	0/248	0.52	0/334
7	X	0.42	0/239	0.61	0/323
7	Y	0.42	0/243	0.62	0/329
7	Z	0.38	0/248	0.53	0/334
7	a	0.44	0/239	0.62	0/323
7	b	0.43	0/243	0.60	0/329
7	c	0.40	0/248	0.56	0/334
7	d	0.40	0/239	0.53	0/323
7	e	0.46	0/243	0.69	0/329
7	f	0.41	0/248	0.61	0/334
7	g	0.39	0/239	0.57	0/323
7	h	0.42	0/243	0.67	0/329
7	i	0.39	0/248	0.52	0/334
7	j	0.43	0/239	0.56	0/323
7	k	0.42	0/243	0.63	0/329
7	l	0.41	0/248	0.57	0/334
7	m	0.43	0/239	0.65	0/323
7	n	0.43	0/243	0.64	0/329
All	All	0.39	0/46529	0.62	18/62949 (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	8	0	1
7	b	0	1
All	All	0	2

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	90	LEU	CA-CB-CG	8.54	134.93	115.30
4	B	47	ASP	CB-CG-OD1	8.49	125.94	118.30
5	AQ	47	ASP	CB-CG-OD2	7.27	124.84	118.30
2	5	158	ASP	CB-CG-OD2	7.17	124.75	118.30
6	AV	51	LEU	CA-CB-CG	6.98	131.35	115.30
2	5	5	LEU	CA-CB-CG	6.78	130.89	115.30
7	V	366	LEU	CA-CB-CG	6.38	129.97	115.30
7	R	366	LEU	CB-CG-CD2	5.93	121.07	111.00
5	AM	87	LEU	CA-CB-CG	5.82	128.69	115.30
7	R	366	LEU	CA-CB-CG	5.66	128.31	115.30
3	8	2	ASP	CB-CG-OD1	5.41	123.17	118.30
6	AY	32	ASP	CB-CG-OD1	5.36	123.12	118.30
6	AX	44	LEU	CA-CB-CG	5.29	127.46	115.30
4	M	126	LEU	CA-CB-CG	5.17	127.20	115.30
6	BD	11	ASP	CB-CG-OD2	5.10	122.89	118.30
4	A	126	LEU	CB-CG-CD1	5.04	119.58	111.00
4	H	143	ARG	CA-CB-CG	5.03	124.47	113.40
4	A	126	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1562	0	1597	14	0
1	1	1569	0	1613	8	0
1	2	1553	0	1598	23	0
1	3	1606	0	1649	21	0
1	4	1758	0	1806	17	0
2	5	1885	0	1931	27	0
3	6	405	0	418	2	0
3	7	644	0	685	8	0
3	8	644	0	685	9	0
3	9	647	0	692	13	0
4	A	1108	0	1103	10	0
4	B	1154	0	1163	7	0
4	C	1108	0	1103	10	0
4	D	1146	0	1150	6	0
4	F	1108	0	1103	10	0
4	G	1154	0	1163	7	0
4	H	1108	0	1103	6	0
4	I	1154	0	1163	6	0
4	J	1108	0	1103	8	0
4	K	1154	0	1163	8	0
4	L	1108	0	1103	13	0
4	M	1146	0	1150	9	0
4	N	1108	0	1103	10	0
4	O	1154	0	1163	7	0
4	P	1108	0	1103	13	0
4	Q	1154	0	1163	10	0
5	AM	298	0	307	1	0
5	AN	644	0	654	11	0
5	AO	667	0	672	6	0
5	AP	675	0	683	7	0
5	AQ	675	0	683	9	0
5	AR	667	0	672	8	0
6	AS	466	0	470	13	0
6	AT	466	0	470	5	0
6	AU	466	0	470	10	0
6	AV	466	0	470	6	0
6	AW	466	0	470	9	0
6	AX	574	0	566	8	0
6	AY	612	0	598	11	0
6	AZ	460	0	435	9	0
6	BA	437	0	413	6	0
6	BB	388	0	369	4	0
6	BC	388	0	369	7	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	BD	388	0	369	9	0
6	BE	346	0	329	7	0
7	E	236	0	219	2	0
7	R	227	0	208	1	0
7	S	231	0	207	1	0
7	T	236	0	219	0	0
7	U	227	0	208	5	0
7	V	231	0	207	1	0
7	W	236	0	219	2	0
7	X	227	0	208	2	0
7	Y	231	0	207	0	0
7	Z	236	0	219	0	0
7	a	227	0	208	0	0
7	b	231	0	207	0	0
7	c	236	0	219	0	0
7	d	227	0	208	0	0
7	e	231	0	207	0	0
7	f	236	0	219	0	0
7	g	227	0	208	0	0
7	h	231	0	207	0	0
7	i	236	0	219	0	0
7	j	227	0	208	0	0
7	k	231	0	207	0	0
7	l	236	0	219	0	0
7	m	227	0	208	0	0
7	n	231	0	207	0	0
All	All	45454	0	45317	372	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (372) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:39:ASP:H	4:Q:69:THR:HG22	1.55	0.72
4:I:169:GLN:HE22	4:J:115:ARG:HA	1.57	0.69
4:A:39:ASP:H	4:A:69:THR:HG22	1.59	0.68
1:0:46:ILE:HD12	2:5:97:ALA:HB1	1.77	0.65
6:AW:52:SER:HB2	6:BC:69:LYS:HD3	1.78	0.64
5:AP:31:ASP:O	5:AP:35:GLN:NE2	2.29	0.64
4:P:39:ASP:H	4:P:69:THR:HG22	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:149:VAL:HG21	4:J:159:VAL:HG11	1.79	0.64
4:N:149:VAL:HG21	4:N:159:VAL:HG21	1.80	0.63
6:BC:9:LEU:HD11	6:BC:65:VAL:HG23	1.79	0.63
2:5:13:VAL:HG13	5:AM:81:VAL:HG21	1.81	0.62
6:BC:12:VAL:HA	6:BC:15:LYS:HD2	1.80	0.62
4:A:137:PRO:HD2	4:Q:97:GLN:HE21	1.64	0.61
4:Q:149:VAL:HG21	4:Q:159:VAL:HG11	1.80	0.61
4:A:36:VAL:HG22	4:A:71:ASN:HD22	1.64	0.61
1:0:206:ASP:OD1	2:5:175:ASN:ND2	2.33	0.61
6:AZ:20:VAL:HG21	6:AZ:24:GLN:HE21	1.65	0.60
4:C:39:ASP:H	4:C:69:THR:HG22	1.66	0.60
5:AN:54:ARG:NH1	5:AN:66:GLU:OE2	2.35	0.60
3:9:29:ILE:HD12	3:9:51:ILE:HG22	1.84	0.60
4:A:149:VAL:HG11	4:A:159:VAL:HG21	1.84	0.59
1:2:214:GLY:HA3	3:7:83:LEU:HD13	1.84	0.59
1:3:15:THR:HG22	5:AP:90:LYS:HD2	1.85	0.59
4:D:97:GLN:HE21	4:F:137:PRO:HD2	1.68	0.59
6:AS:78:ASN:HA	6:AT:80:ARG:HH21	1.67	0.58
6:AY:55:ASN:O	6:AY:59:ASN:ND2	2.36	0.58
4:L:169:GLN:HE22	4:M:115:ARG:HA	1.67	0.58
6:AS:63:ASN:OD1	6:AY:80:ARG:NH1	2.36	0.57
1:0:97:ASP:OD2	1:0:100:ARG:NH1	2.36	0.57
3:8:60:LEU:O	3:8:64:SER:HB3	2.03	0.57
4:A:114:LEU:HD13	4:A:117:VAL:HG13	1.86	0.57
5:AQ:53:ASN:HA	5:AQ:56:GLU:HG3	1.85	0.57
1:2:25:THR:OG1	1:2:26:CYS:N	2.37	0.57
6:AX:26:GLN:OE1	6:AX:50:LYS:NZ	2.36	0.57
1:0:5:ILE:HD12	1:0:8:ILE:HD13	1.87	0.57
4:L:33:SER:OG	4:L:34:GLY:N	2.38	0.56
1:3:5:ILE:HG12	5:AQ:44:THR:HG21	1.87	0.56
6:AS:60:ALA:HB2	6:AY:76:ILE:HD13	1.87	0.56
4:A:115:ARG:HG2	4:Q:169:GLN:HE22	1.71	0.56
4:G:161:ASN:HA	4:G:164:THR:HG22	1.88	0.56
4:L:149:VAL:HG21	4:L:159:VAL:HG21	1.88	0.56
1:0:5:ILE:HG21	5:AN:41:ALA:HA	1.86	0.56
4:C:113:SER:HA	4:C:145:GLY:O	2.06	0.56
2:5:39:SER:OG	2:5:40:GLY:N	2.39	0.56
1:3:34:PHE:HB3	1:3:52:LEU:HD22	1.87	0.55
2:5:83:MET:HG2	2:5:165:PRO:HB3	1.89	0.55
2:5:206:ALA:HB1	3:9:38:THR:HG21	1.88	0.55
6:AX:16:PHE:HB3	6:AX:57:TYR:HE1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:97:GLN:HE22	4:H:139:ARG:HE	1.55	0.55
1:2:30:PHE:HB3	1:2:56:ALA:HB1	1.89	0.55
7:E:365:TRP:HD1	7:E:390:SER:HB2	1.71	0.55
5:AO:31:ASP:OD1	5:AO:31:ASP:N	2.38	0.55
5:AO:66:GLU:HA	5:AO:69:ILE:HG22	1.88	0.54
6:AT:39:SER:HB2	6:BE:9:LEU:HD23	1.87	0.54
6:AV:60:ALA:HB2	6:BB:76:ILE:HD11	1.88	0.54
4:O:38:LYS:NZ	7:U:369:ARG:O	2.36	0.54
6:AV:59:ASN:O	6:AV:63:ASN:ND2	2.36	0.54
6:AX:21:ASP:N	6:AX:21:ASP:OD1	2.41	0.54
6:AZ:24:GLN:NE2	6:AZ:57:TYR:OH	2.41	0.54
4:H:33:SER:OG	4:H:34:GLY:N	2.41	0.54
6:AZ:72:ASP:N	6:AZ:72:ASP:OD1	2.39	0.54
6:BD:13:SER:OG	6:BD:61:GLN:NE2	2.41	0.54
1:2:218:GLN:NE2	3:7:83:LEU:O	2.41	0.54
6:AY:27:VAL:HG12	6:AY:50:LYS:HB3	1.90	0.54
4:F:114:LEU:HD21	4:F:163:ALA:HB1	1.90	0.53
1:2:38:ARG:NH1	1:2:48:SER:O	2.42	0.53
2:5:176:GLN:OE1	2:5:179:GLN:NE2	2.41	0.53
4:B:114:LEU:HD21	4:B:163:ALA:HB1	1.91	0.53
1:4:147:LEU:HA	1:4:150:TYR:HB3	1.91	0.53
1:1:143:ILE:HD12	1:1:146:LEU:HD11	1.90	0.53
2:5:76:GLN:HE22	2:5:162:GLU:HG2	1.74	0.53
3:7:37:GLN:HB3	3:7:41:GLN:HA	1.90	0.53
1:3:84:ASP:OD1	1:3:87:SER:N	2.42	0.53
1:0:25:THR:OG1	1:0:26:CYS:N	2.42	0.53
4:O:39:ASP:H	4:O:69:THR:HB	1.74	0.53
6:BC:9:LEU:HA	6:BC:12:VAL:HG12	1.91	0.53
1:3:29:LYS:HG3	1:3:158:ALA:HB2	1.92	0.52
4:J:141:ASP:HB3	4:J:144:LYS:HB2	1.90	0.52
1:2:48:SER:OG	1:2:51:THR:N	2.38	0.52
6:AS:32:ASP:N	6:AS:32:ASP:OD1	2.38	0.52
6:AY:22:ASN:OD1	6:AY:25:THR:OG1	2.28	0.52
6:BD:55:ASN:O	6:BD:59:ASN:ND2	2.43	0.52
1:2:48:SER:HG	1:2:51:THR:H	1.57	0.52
1:0:16:LEU:HD11	5:AN:95:VAL:HG11	1.91	0.52
1:1:200:VAL:HA	1:1:203:VAL:HG12	1.91	0.52
3:7:79:ILE:HD12	3:7:82:ALA:HB3	1.92	0.52
4:Q:36:VAL:HG23	7:X:373:TYR:HE1	1.74	0.52
4:J:40:ASP:OD2	4:J:44:THR:OG1	2.24	0.52
4:P:149:VAL:HG21	4:P:159:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:176:VAL:HA	1:3:179:VAL:HG12	1.93	0.51
3:9:10:LYS:HE2	3:9:74:TYR:HE1	1.75	0.51
6:AY:58:ARG:HH11	6:AY:61:GLN:HE22	1.58	0.51
6:AS:24:GLN:O	6:AS:28:THR:OG1	2.21	0.51
6:AX:34:LEU:HD21	6:AX:47:TYR:HB2	1.92	0.51
7:W:371:PHE:HE1	7:W:380:LYS:HG2	1.76	0.51
4:G:60:SER:OG	4:G:61:LYS:N	2.44	0.51
3:8:10:LYS:NZ	3:8:77:GLN:OE1	2.37	0.51
6:AU:63:ASN:OD1	6:BA:80:ARG:NH1	2.43	0.51
6:BA:9:LEU:HA	6:BA:12:VAL:HG12	1.92	0.51
4:F:103:ASP:OD1	4:F:104:ALA:N	2.44	0.51
4:L:73:GLU:OE1	4:L:75:HIS:ND1	2.38	0.51
2:5:133:ALA:HA	2:5:136:VAL:HG12	1.93	0.50
3:9:3:ASP:OD1	3:9:3:ASP:N	2.43	0.50
4:I:118:SER:OG	4:I:119:LEU:N	2.44	0.50
6:BD:70:ASP:HA	6:BD:73:ALA:HB3	1.93	0.50
4:P:33:SER:OG	4:P:34:GLY:N	2.44	0.50
2:5:233:PRO:HG2	2:5:234:VAL:HG23	1.93	0.50
3:7:33:VAL:HG21	3:7:48:PRO:HB3	1.93	0.50
5:AP:89:ARG:O	5:AP:89:ARG:NH1	2.44	0.50
4:L:40:ASP:HB2	4:L:44:THR:HG23	1.94	0.50
4:P:57:VAL:HG12	4:P:99:ILE:HB	1.93	0.50
5:AO:64:PRO:HA	5:AO:67:LEU:HB2	1.93	0.50
4:H:57:VAL:HG12	4:H:99:ILE:HB	1.92	0.50
4:K:114:LEU:HD13	4:K:117:VAL:HB	1.93	0.49
4:D:60:SER:OG	4:D:61:LYS:N	2.44	0.49
4:I:41:SER:O	4:I:41:SER:OG	2.28	0.49
4:P:169:GLN:HE22	4:Q:115:ARG:HA	1.77	0.49
1:3:200:VAL:HA	1:3:203:VAL:HG22	1.95	0.49
3:9:14:LEU:HD23	3:9:17:ILE:HD11	1.95	0.49
6:AV:29:GLU:O	6:AV:33:LYS:NZ	2.46	0.49
1:4:97:ASP:OD1	1:4:140[A]:LYS:NZ	2.46	0.49
3:8:52:LYS:NZ	3:9:46:THR:OG1	2.44	0.49
5:AR:30:ASP:OD1	5:AR:30:ASP:N	2.45	0.49
4:M:114:LEU:HD11	4:M:147:PHE:HE1	1.78	0.49
4:N:44:THR:HB	7:S:380:LYS:HE2	1.95	0.49
6:AY:56:LEU:HD13	6:BE:72:ASP:HB2	1.94	0.49
4:F:57:VAL:HG12	4:F:99:ILE:HB	1.95	0.49
5:AR:47:ASP:HA	5:AR:50:THR:HG22	1.93	0.49
6:BB:76:ILE:HG13	6:BB:79:PHE:HE2	1.78	0.49
1:4:25:THR:OG1	1:4:26:CYS:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AO:63:ASP:HB3	5:AO:66:GLU:HG2	1.94	0.48
5:AQ:31:ASP:OD2	5:AQ:31:ASP:N	2.45	0.48
4:M:39:ASP:H	4:M:69:THR:HB	1.77	0.48
6:AY:23:LEU:HG	6:AY:54:TYR:HD1	1.77	0.48
3:9:6:PHE:O	3:9:10:LYS:NZ	2.46	0.48
5:AP:26:ILE:HG21	5:AP:32:ARG:HE	1.78	0.48
6:AZ:24:GLN:OE1	6:AZ:58:ARG:NH2	2.46	0.48
6:AV:27:VAL:HG13	6:AV:50:LYS:HE3	1.96	0.48
2:5:99:GLY:HA2	2:5:102:ILE:HG22	1.95	0.48
1:2:173:ASP:HA	1:2:176:VAL:HG22	1.94	0.48
3:8:3:ASP:HA	3:8:6:PHE:HB3	1.94	0.48
5:AR:55:ILE:HG13	6:AW:64:THR:HG21	1.95	0.48
1:4:25:THR:HG23	1:4:27:PHE:H	1.78	0.48
4:P:141:ASP:HB3	4:P:144:LYS:HB2	1.95	0.48
1:4:156:LYS:HG3	2:5:138:LEU:HG	1.96	0.48
1:4:191:VAL:O	1:4:195:THR:OG1	2.31	0.47
6:AX:31:LEU:HA	6:AX:34:LEU:HB2	1.96	0.47
4:F:149:VAL:HG21	4:F:159:VAL:HG11	1.95	0.47
1:2:93:ASP:OD1	1:2:93:ASP:N	2.46	0.47
1:3:35:VAL:HG13	1:3:38:ARG:HH21	1.79	0.47
6:AX:74:ALA:O	6:AX:78:ASN:ND2	2.47	0.47
6:BD:74:ALA:O	6:BD:78:ASN:ND2	2.47	0.47
6:AW:60:ALA:HA	6:BC:76:ILE:HD11	1.95	0.47
1:0:173:ASP:N	1:0:173:ASP:OD1	2.43	0.47
5:AQ:13:ILE:HG13	5:AQ:15:GLN:HE22	1.79	0.47
3:9:29:ILE:HD11	3:9:52:LYS:HA	1.97	0.47
1:1:180:LEU:HD12	1:1:190:PRO:HB3	1.95	0.47
4:A:97:GLN:HE21	4:B:137:PRO:HD2	1.78	0.47
5:AN:75:SER:HB3	6:AT:69:LYS:HD3	1.96	0.47
6:AS:48:GLN:NE2	6:BD:78:ASN:O	2.47	0.47
6:AU:32:ASP:OD2	6:AU:32:ASP:N	2.48	0.47
4:C:116:ASN:ND2	4:C:170:ASN:O	2.48	0.47
4:G:118:SER:OG	4:G:119:LEU:N	2.48	0.47
4:N:41:SER:O	4:N:41:SER:OG	2.30	0.47
4:Q:40:ASP:OD1	4:Q:44:THR:OG1	2.28	0.47
5:AO:49:GLN:HG3	5:AO:53:ASN:HD21	1.79	0.47
6:AW:32:ASP:N	6:AW:32:ASP:OD1	2.48	0.47
6:BE:8:TYR:HA	6:BE:11:ASP:HB2	1.97	0.47
4:P:51:LEU:HD22	4:Q:87:GLN:HG2	1.97	0.47
1:0:49:ASN:N	1:0:49:ASN:OD1	2.48	0.47
1:3:48:SER:OG	1:3:50:MET:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AY:9:LEU:HD21	6:AY:65:VAL:HG13	1.97	0.47
4:N:109:ASN:OD1	4:N:109:ASN:N	2.46	0.47
3:9:2:ASP:OD1	3:9:2:ASP:N	2.48	0.46
5:AO:90:LYS:NZ	6:AU:79:PHE:O	2.37	0.46
6:BD:13:SER:HA	6:BD:16:PHE:HD2	1.79	0.46
1:4:171:VAL:HG23	3:9:15:VAL:HG13	1.96	0.46
4:I:108:ARG:HH12	4:I:153:PRO:HB3	1.80	0.46
4:L:118:SER:OG	4:L:119:LEU:N	2.49	0.46
1:4:201:LEU:HD11	3:9:71:LEU:HB3	1.96	0.46
1:3:25:THR:OG1	1:3:26:CYS:N	2.48	0.46
1:2:191:VAL:O	1:2:195:THR:OG1	2.23	0.46
5:AQ:55:ILE:HD12	5:AQ:55:ILE:HA	1.88	0.46
6:AW:41:PRO:HG2	6:BC:54:TYR:HE2	1.81	0.46
2:5:102:ILE:HD11	2:5:223:ALA:HB1	1.97	0.46
2:5:224:VAL:HG13	3:9:16:LEU:HD12	1.97	0.46
1:4:5:ILE:HG22	1:4:8:ILE:HD12	1.97	0.46
5:AQ:24:THR:OG1	5:AQ:25:ASP:N	2.48	0.46
6:AU:24:GLN:O	6:AU:28:THR:OG1	2.29	0.46
4:B:141:ASP:HB3	4:B:144:LYS:HB2	1.97	0.46
6:BA:17:ASP:OD1	6:BA:57:TYR:OH	2.34	0.46
6:BA:74:ALA:O	6:BA:78:ASN:ND2	2.49	0.46
1:1:190:PRO:O	1:1:194:SER:HB3	2.15	0.45
4:K:169:GLN:HE22	4:L:115:ARG:HA	1.81	0.45
4:O:36:VAL:HG23	7:U:373:TYR:HE1	1.81	0.45
4:P:114:LEU:HD13	4:P:117:VAL:HB	1.98	0.45
4:P:116:ASN:OD1	4:P:116:ASN:N	2.50	0.45
1:3:113:GLN:O	1:3:117:ASN:ND2	2.48	0.45
1:4:10:LEU:HD21	5:AQ:87:LEU:HD21	1.98	0.45
4:A:108:ARG:HG3	4:A:156:VAL:HG21	1.98	0.45
6:AW:58:ARG:HA	6:AW:58:ARG:HD3	1.73	0.45
4:K:76:ASP:HA	4:K:77:PRO:HD3	1.86	0.45
1:0:213:LYS:HA	1:0:216:ILE:HG22	1.97	0.45
4:L:97:GLN:HE22	4:M:139:ARG:HE	1.65	0.45
3:8:25:VAL:HA	3:8:28:ILE:HG12	1.98	0.45
4:P:58:ILE:HD13	4:Q:105:SER:HA	1.97	0.45
1:3:192:THR:HG23	1:3:193:ILE:HG13	1.98	0.45
4:F:63:ALA:HB2	4:F:103:ASP:HB2	1.99	0.45
7:U:380:LYS:HE3	7:U:380:LYS:HB3	1.70	0.45
4:D:168:LYS:HA	4:D:168:LYS:HD3	1.76	0.45
4:F:60:SER:OG	4:F:61:LYS:N	2.48	0.45
2:5:52:LEU:HD23	2:5:52:LEU:HA	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:166:SER:O	2:5:166:SER:OG	2.32	0.45
6:AU:76:ILE:H	6:AU:76:ILE:HG12	1.42	0.45
4:N:76:ASP:OD1	4:N:76:ASP:N	2.49	0.45
4:A:76:ASP:OD1	4:A:76:ASP:N	2.50	0.45
6:AZ:55:ASN:HA	6:BE:71:ILE:HD11	1.99	0.45
6:AZ:72:ASP:HA	6:AZ:75:ILE:HD12	1.99	0.45
4:K:125:PHE:HD1	4:L:141:ASP:HB2	1.82	0.45
1:1:113:GLN:HA	1:1:116:GLU:HG3	1.99	0.44
1:3:82:PHE:HB2	1:3:88:LEU:HG	1.99	0.44
4:M:114:LEU:HD21	4:M:163:ALA:HB1	1.98	0.44
4:O:114:LEU:HD21	4:O:163:ALA:HB1	1.99	0.44
3:8:37:GLN:HE21	3:8:43:GLN:HA	1.82	0.44
4:N:114:LEU:HD13	4:N:117:VAL:HG13	2.00	0.44
1:0:86:SER:HA	1:0:89:SER:HB3	1.99	0.44
2:5:56:PRO:HD3	2:5:154:TYR:CD2	2.52	0.44
5:AN:63:ASP:OD1	5:AN:66:GLU:N	2.44	0.44
6:BD:9:LEU:HD11	6:BD:65:VAL:HG13	1.99	0.44
4:H:138:LEU:HD22	4:H:149:VAL:HG12	1.99	0.44
3:8:14:LEU:HA	3:8:17:ILE:HG22	1.99	0.44
4:C:40:ASP:HB3	4:C:44:THR:HG23	1.99	0.44
4:D:52:GLN:HG3	4:D:74:PHE:HB2	2.00	0.44
1:4:52:LEU:HA	1:4:55:VAL:HG12	2.00	0.44
4:N:57:VAL:HG12	4:N:99:ILE:HB	1.98	0.44
1:2:173:ASP:OD1	1:2:173:ASP:N	2.43	0.44
4:B:111:VAL:HG22	4:B:148:TYR:HD1	1.83	0.44
6:BD:64:THR:HA	6:BD:67:VAL:HG22	2.00	0.44
6:AS:26:GLN:HG3	6:AS:50:LYS:HZ1	1.83	0.44
6:AW:22:ASN:HD21	6:BC:5:TRP:HE1	1.63	0.44
4:P:87:GLN:HE22	7:U:376:GLU:HB3	1.83	0.44
1:2:48:SER:OG	1:2:50:MET:N	2.49	0.43
2:5:202:LEU:HD12	2:5:202:LEU:HA	1.91	0.43
6:BE:9:LEU:HA	6:BE:12:VAL:HG22	1.99	0.43
1:2:176:VAL:HA	1:2:179:VAL:HG22	2.00	0.43
4:J:38:LYS:HA	4:J:69:THR:HG23	1.99	0.43
5:AP:75:SER:HA	6:AV:69:LYS:HE3	2.00	0.43
4:J:97:GLN:HE22	4:K:139:ARG:HE	1.66	0.43
4:N:144:LYS:HD2	4:N:144:LYS:HA	1.89	0.43
3:7:66:TRP:HA	3:7:69:GLU:HG2	1.98	0.43
6:AZ:21:ASP:OD1	6:AZ:21:ASP:N	2.45	0.43
4:L:144:LYS:HD3	4:L:144:LYS:HA	1.87	0.43
4:P:50:ALA:HB2	4:P:57:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:52:LEU:HA	1:1:55:VAL:HG22	2.00	0.43
1:2:106:TYR:OH	1:2:218:GLN:O	2.31	0.43
4:G:63:ALA:HB2	4:G:103:ASP:HB2	1.99	0.43
4:H:42:LEU:HD22	4:H:66:LYS:HB2	2.00	0.43
4:I:76:ASP:HA	4:I:77:PRO:HD3	1.80	0.43
4:L:63:ALA:HB2	4:L:103:ASP:HB3	2.01	0.43
4:N:114:LEU:HD21	4:N:163:ALA:HB1	2.00	0.43
1:0:97:ASP:HA	1:0:100:ARG:HB3	2.01	0.43
1:3:27:PHE:O	1:3:31:SER:OG	2.27	0.43
5:AP:16:ALA:HB2	4:K:112:VAL:HG23	2.00	0.43
6:AT:58:ARG:HA	6:AT:58:ARG:HD3	1.75	0.43
5:AP:86:THR:HG22	6:AU:78:ASN:HD21	1.83	0.43
6:AS:58:ARG:HA	6:AS:58:ARG:HD3	1.87	0.43
4:M:44:THR:HB	7:R:380:LYS:HE2	2.00	0.43
3:6:6:PHE:HE1	3:6:77:GLN:HE22	1.66	0.43
5:AR:57:ASP:OD1	5:AR:60:LEU:N	2.52	0.43
6:BA:75:ILE:HA	6:BA:78:ASN:HB2	2.01	0.43
4:G:168:LYS:HE2	4:G:168:LYS:HB3	1.77	0.43
1:4:167:LEU:HD23	1:4:167:LEU:HA	1.85	0.42
2:5:89:SER:O	2:5:89:SER:OG	2.28	0.42
4:A:156:VAL:HA	4:A:159:VAL:HG22	2.01	0.42
5:AN:48:LYS:O	5:AN:52:THR:OG1	2.26	0.42
7:W:365:TRP:HD1	7:W:390:SER:HB2	1.84	0.42
1:3:172:VAL:HA	1:3:175:VAL:HG12	2.01	0.42
2:5:56:PRO:HG3	2:5:154:TYR:HB3	2.01	0.42
2:5:70:MET:HE3	2:5:70:MET:HB3	1.91	0.42
6:AS:56:LEU:HD13	6:AS:56:LEU:HA	1.87	0.42
1:0:59:LEU:HD23	1:0:59:LEU:HA	1.91	0.42
1:2:90:LYS:HE3	1:2:90:LYS:HB3	1.82	0.42
1:3:161:ILE:HG13	3:8:82:ALA:HB1	2.02	0.42
6:AS:76:ILE:H	6:AS:76:ILE:HG12	1.48	0.42
1:2:176:VAL:HG21	1:2:194:SER:HB2	2.01	0.42
6:AU:48:GLN:HA	6:AU:51:LEU:HD23	2.02	0.42
6:AU:58:ARG:HD3	6:AU:58:ARG:HA	1.78	0.42
4:M:120:ASN:O	4:M:124:ASN:ND2	2.48	0.42
1:2:163:PHE:HB2	1:3:199:LEU:HD11	2.02	0.42
1:3:97:ASP:OD1	1:3:100:ARG:NH1	2.52	0.42
1:4:152:LEU:HB3	2:5:143:LEU:HD13	2.01	0.42
1:1:96:LEU:HD11	1:1:100:ARG:HH21	1.85	0.42
4:F:116:ASN:OD1	4:F:116:ASN:N	2.53	0.42
2:5:51:ALA:HA	2:5:54:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:118:SER:OG	4:H:121:GLU:OE1	2.34	0.42
4:O:63:ALA:HB2	4:O:103:ASP:HB3	2.01	0.42
7:V:380:LYS:HE2	7:V:380:LYS:HB3	1.87	0.42
5:AQ:42:ILE:HD13	5:AQ:42:ILE:HA	1.92	0.42
4:B:76:ASP:HA	4:B:77:PRO:HD3	1.80	0.42
7:X:372:GLN:O	7:X:377:GLY:HA2	2.19	0.42
1:3:160:LYS:HB2	1:4:203:VAL:HG21	2.02	0.41
2:5:95:MET:HG3	2:5:129:LEU:HB3	2.02	0.41
6:AS:69:LYS:HD3	6:AS:69:LYS:HA	1.78	0.41
4:C:84:LEU:O	4:C:88:LEU:HB2	2.20	0.41
7:U:372:GLN:O	7:U:377:GLY:HA2	2.20	0.41
1:2:171:VAL:HG23	3:7:15:VAL:HG22	2.02	0.41
5:AR:25:ASP:OD1	4:C:61:LYS:NZ	2.49	0.41
6:AU:56:LEU:HD13	6:AU:56:LEU:HA	1.86	0.41
4:K:116:ASN:OD1	4:K:116:ASN:N	2.53	0.41
1:3:101:ASP:OD1	1:3:140:LYS:NZ	2.47	0.41
5:AR:85:SER:OG	5:AR:86:THR:N	2.53	0.41
6:AX:37:LYS:HA	6:AX:37:LYS:HD3	1.82	0.41
4:D:39:ASP:H	4:D:69:THR:HB	1.84	0.41
4:F:152:PRO:HA	4:F:153:PRO:HD3	1.96	0.41
1:0:111:LEU:HD23	1:0:115:PHE:HE2	1.85	0.41
6:BB:72:ASP:HA	6:BB:75:ILE:HG12	2.02	0.41
4:Q:141:ASP:HB3	4:Q:144:LYS:HB2	2.01	0.41
2:5:92:PHE:HB3	2:5:130:ASN:HD21	1.86	0.41
5:AN:67:LEU:HD23	5:AN:67:LEU:HA	1.90	0.41
6:AS:49:SER:OG	6:AY:10:ASP:OD1	2.30	0.41
6:AT:59:ASN:O	6:AT:63:ASN:ND2	2.43	0.41
4:B:109:ASN:OD1	4:B:109:ASN:N	2.54	0.41
6:BE:12:VAL:HA	6:BE:15:LYS:HE2	2.02	0.41
4:D:40:ASP:OD2	4:D:44:THR:OG1	2.31	0.41
1:2:186:MET:SD	1:2:186:MET:N	2.91	0.41
5:AR:83:MET:HG3	6:AX:76:ILE:HD12	2.02	0.41
4:C:141:ASP:HB3	4:C:144:LYS:HB2	2.03	0.41
4:I:144:LYS:HA	4:I:144:LYS:HD3	1.88	0.41
4:M:97:GLN:OE1	4:N:150:SER:OG	2.37	0.41
2:5:192:LEU:HD22	2:5:219:LYS:HG2	2.02	0.41
3:7:25:VAL:HA	3:7:28:ILE:HG22	2.02	0.41
6:AW:24:GLN:O	6:AW:28:THR:OG1	2.33	0.41
4:O:109:ASN:OD1	4:O:109:ASN:N	2.52	0.41
1:2:103:LEU:HD12	1:2:103:LEU:HA	1.89	0.41
5:AQ:58:PRO:HB2	6:BB:5:TRP:CZ2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BE:14:ALA:O	6:BE:18:THR:OG1	2.31	0.41
4:J:113:SER:HA	4:J:146:THR:HA	2.03	0.41
4:M:152:PRO:HA	4:M:153:PRO:HD3	1.96	0.41
3:8:35:LEU:HA	3:8:38:THR:HG22	2.03	0.41
5:AN:81:VAL:HA	5:AN:84:VAL:HG12	2.03	0.41
5:AR:19:ILE:HG22	4:C:161:ASN:HD22	1.84	0.41
6:AV:31:LEU:HD13	6:BA:15:LYS:HE3	2.03	0.41
6:AZ:62:SER:HA	6:AZ:65:VAL:HG12	2.01	0.41
7:E:380:LYS:HE3	7:E:380:LYS:HB3	4.39	0.41
4:L:116:ASN:OD1	4:L:116:ASN:N	2.54	0.41
4:P:113:SER:HB2	4:P:146:THR:HG22	2.03	0.41
1:1:171:VAL:HG13	3:6:15:VAL:HG12	2.02	0.41
1:4:8:ILE:HG12	6:AW:75:ILE:HG21	2.02	0.41
1:4:96:LEU:HD23	1:4:96:LEU:HA	1.92	0.41
1:4:132:LYS:HA	1:4:132:LYS:HD3	1.79	0.41
3:9:37:GLN:HE21	3:9:47:LEU:HD23	1.85	0.41
6:AS:59:ASN:O	6:AS:63:ASN:ND2	2.42	0.41
4:O:27:LYS:HB2	4:O:27:LYS:HE3	1.89	0.41
1:3:194:SER:O	1:3:198:LYS:N	2.54	0.40
4:K:109:ASN:N	4:K:109:ASN:OD1	2.53	0.40
1:2:20:ILE:HD13	1:2:20:ILE:HA	1.92	0.40
1:2:200:VAL:HA	1:2:203:VAL:HG12	2.02	0.40
6:AU:35:ALA:HB1	6:AZ:19:GLY:HA3	2.03	0.40
6:AY:40:ASP:HA	6:AY:41:PRO:HD3	1.94	0.40
6:BD:7:GLY:H	6:BD:10:ASP:HB2	1.85	0.40
4:C:60:SER:OG	4:C:61:LYS:N	2.54	0.40
4:F:109:ASN:OD1	4:F:109:ASN:N	2.54	0.40
1:2:113:GLN:HA	1:2:116:GLU:HG2	2.01	0.40
5:AN:51:ILE:HA	5:AN:54:ARG:HB3	2.03	0.40
5:AN:63:ASP:OD2	5:AN:65:LYS:NZ	2.55	0.40
4:B:114:LEU:HD13	4:B:117:VAL:HG13	2.03	0.40
4:J:112:VAL:HG11	4:J:160:VAL:HG23	2.03	0.40
4:G:40:ASP:HB3	4:G:44:THR:HG23	2.04	0.40
4:L:55:GLU:HG3	4:L:94:PHE:CE1	2.56	0.40
2:5:91:PRO:HA	2:5:94:VAL:HG12	2.04	0.40
5:AN:85:SER:OG	5:AN:86:THR:N	2.55	0.40
4:C:152:PRO:HA	4:C:153:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	195/224 (87%)	189 (97%)	5 (3%)	1 (0%)	29	66
1	1	195/224 (87%)	186 (95%)	8 (4%)	1 (0%)	29	66
1	2	193/224 (86%)	187 (97%)	5 (3%)	1 (0%)	29	66
1	3	200/224 (89%)	195 (98%)	5 (2%)	0	100	100
1	4	220/224 (98%)	209 (95%)	11 (5%)	0	100	100
2	5	243/263 (92%)	224 (92%)	19 (8%)	0	100	100
3	6	49/86 (57%)	46 (94%)	3 (6%)	0	100	100
3	7	82/86 (95%)	80 (98%)	2 (2%)	0	100	100
3	8	82/86 (95%)	80 (98%)	1 (1%)	1 (1%)	13	50
3	9	82/86 (95%)	81 (99%)	1 (1%)	0	100	100
4	A	137/562 (24%)	136 (99%)	1 (1%)	0	100	100
4	B	143/562 (25%)	139 (97%)	4 (3%)	0	100	100
4	C	137/562 (24%)	134 (98%)	3 (2%)	0	100	100
4	D	142/562 (25%)	138 (97%)	4 (3%)	0	100	100
4	F	137/562 (24%)	135 (98%)	2 (2%)	0	100	100
4	G	143/562 (25%)	137 (96%)	6 (4%)	0	100	100
4	H	137/562 (24%)	134 (98%)	3 (2%)	0	100	100
4	I	143/562 (25%)	141 (99%)	2 (1%)	0	100	100
4	J	137/562 (24%)	134 (98%)	3 (2%)	0	100	100
4	K	143/562 (25%)	139 (97%)	4 (3%)	0	100	100
4	L	137/562 (24%)	135 (98%)	2 (2%)	0	100	100
4	M	142/562 (25%)	137 (96%)	5 (4%)	0	100	100
4	N	137/562 (24%)	134 (98%)	3 (2%)	0	100	100
4	O	143/562 (25%)	140 (98%)	3 (2%)	0	100	100
4	P	137/562 (24%)	136 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	143/562 (25%)	139 (97%)	4 (3%)	0	100	100
5	AM	37/101 (37%)	37 (100%)	0	0	100	100
5	AN	79/101 (78%)	79 (100%)	0	0	100	100
5	AO	86/101 (85%)	84 (98%)	2 (2%)	0	100	100
5	AP	87/101 (86%)	87 (100%)	0	0	100	100
5	AQ	87/101 (86%)	87 (100%)	0	0	100	100
5	AR	86/101 (85%)	83 (96%)	3 (4%)	0	100	100
6	AS	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
6	AT	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
6	AU	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
6	AV	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
6	AW	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
6	AX	71/80 (89%)	68 (96%)	3 (4%)	0	100	100
6	AY	76/80 (95%)	73 (96%)	3 (4%)	0	100	100
6	AZ	53/80 (66%)	52 (98%)	1 (2%)	0	100	100
6	BA	50/80 (62%)	47 (94%)	3 (6%)	0	100	100
6	BB	44/80 (55%)	43 (98%)	1 (2%)	0	100	100
6	BC	44/80 (55%)	44 (100%)	0	0	100	100
6	BD	44/80 (55%)	43 (98%)	1 (2%)	0	100	100
6	BE	39/80 (49%)	37 (95%)	2 (5%)	0	100	100
7	E	26/392 (7%)	22 (85%)	4 (15%)	0	100	100
7	R	25/392 (6%)	25 (100%)	0	0	100	100
7	S	26/392 (7%)	20 (77%)	6 (23%)	0	100	100
7	T	26/392 (7%)	22 (85%)	4 (15%)	0	100	100
7	U	25/392 (6%)	24 (96%)	1 (4%)	0	100	100
7	V	26/392 (7%)	19 (73%)	7 (27%)	0	100	100
7	W	26/392 (7%)	23 (88%)	3 (12%)	0	100	100
7	X	25/392 (6%)	24 (96%)	1 (4%)	0	100	100
7	Y	26/392 (7%)	19 (73%)	7 (27%)	0	100	100
7	Z	26/392 (7%)	22 (85%)	4 (15%)	0	100	100
7	a	25/392 (6%)	24 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	b	26/392 (7%)	19 (73%)	7 (27%)	0	100	100
7	c	26/392 (7%)	22 (85%)	4 (15%)	0	100	100
7	d	25/392 (6%)	25 (100%)	0	0	100	100
7	e	26/392 (7%)	18 (69%)	8 (31%)	0	100	100
7	f	26/392 (7%)	22 (85%)	4 (15%)	0	100	100
7	g	25/392 (6%)	25 (100%)	0	0	100	100
7	h	26/392 (7%)	19 (73%)	7 (27%)	0	100	100
7	i	26/392 (7%)	22 (85%)	4 (15%)	0	100	100
7	j	25/392 (6%)	25 (100%)	0	0	100	100
7	k	26/392 (7%)	19 (73%)	7 (27%)	0	100	100
7	l	26/392 (7%)	22 (85%)	4 (15%)	0	100	100
7	m	25/392 (6%)	24 (96%)	1 (4%)	0	100	100
7	n	26/392 (7%)	19 (73%)	7 (27%)	0	100	100
All	All	5563/21773 (26%)	5329 (96%)	230 (4%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	8	42	LEU
1	0	49	ASN
1	1	49	ASN
1	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	0	175/199 (88%)	174 (99%)	1 (1%)	86	92
1	1	177/199 (89%)	177 (100%)	0	100	100
1	2	175/199 (88%)	174 (99%)	1 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	180/199 (90%)	179 (99%)	1 (1%)	86	92
1	4	197/199 (99%)	195 (99%)	2 (1%)	76	86
2	5	205/219 (94%)	204 (100%)	1 (0%)	88	94
3	6	41/71 (58%)	41 (100%)	0	100	100
3	7	69/71 (97%)	69 (100%)	0	100	100
3	8	69/71 (97%)	69 (100%)	0	100	100
3	9	70/71 (99%)	70 (100%)	0	100	100
4	A	119/477 (25%)	119 (100%)	0	100	100
4	B	125/477 (26%)	125 (100%)	0	100	100
4	C	119/477 (25%)	118 (99%)	1 (1%)	81	89
4	D	124/477 (26%)	123 (99%)	1 (1%)	81	89
4	F	119/477 (25%)	118 (99%)	1 (1%)	81	89
4	G	125/477 (26%)	124 (99%)	1 (1%)	81	89
4	H	119/477 (25%)	117 (98%)	2 (2%)	60	78
4	I	125/477 (26%)	124 (99%)	1 (1%)	81	89
4	J	119/477 (25%)	118 (99%)	1 (1%)	81	89
4	K	125/477 (26%)	124 (99%)	1 (1%)	81	89
4	L	119/477 (25%)	118 (99%)	1 (1%)	81	89
4	M	124/477 (26%)	123 (99%)	1 (1%)	81	89
4	N	119/477 (25%)	118 (99%)	1 (1%)	81	89
4	O	125/477 (26%)	124 (99%)	1 (1%)	81	89
4	P	119/477 (25%)	118 (99%)	1 (1%)	81	89
4	Q	125/477 (26%)	123 (98%)	2 (2%)	62	79
5	AM	34/88 (39%)	33 (97%)	1 (3%)	42	67
5	AN	71/88 (81%)	71 (100%)	0	100	100
5	AO	76/88 (86%)	75 (99%)	1 (1%)	69	82
5	AP	77/88 (88%)	75 (97%)	2 (3%)	46	69
5	AQ	77/88 (88%)	76 (99%)	1 (1%)	69	82
5	AR	76/88 (86%)	76 (100%)	0	100	100
6	AS	50/67 (75%)	47 (94%)	3 (6%)	19	50
6	AT	50/67 (75%)	44 (88%)	6 (12%)	5	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AU	50/67 (75%)	44 (88%)	6 (12%)	5	25
6	AV	50/67 (75%)	47 (94%)	3 (6%)	19	50
6	AW	50/67 (75%)	42 (84%)	8 (16%)	2	16
6	AX	62/67 (92%)	62 (100%)	0	100	100
6	AY	66/67 (98%)	66 (100%)	0	100	100
6	AZ	51/67 (76%)	51 (100%)	0	100	100
6	BA	48/67 (72%)	48 (100%)	0	100	100
6	BB	42/67 (63%)	42 (100%)	0	100	100
6	BC	42/67 (63%)	42 (100%)	0	100	100
6	BD	42/67 (63%)	42 (100%)	0	100	100
6	BE	37/67 (55%)	37 (100%)	0	100	100
7	E	23/337 (7%)	23 (100%)	0	100	100
7	R	22/337 (6%)	21 (96%)	1 (4%)	27	57
7	S	21/337 (6%)	21 (100%)	0	100	100
7	T	23/337 (7%)	23 (100%)	0	100	100
7	U	22/337 (6%)	21 (96%)	1 (4%)	27	57
7	V	21/337 (6%)	20 (95%)	1 (5%)	25	56
7	W	23/337 (7%)	23 (100%)	0	100	100
7	X	22/337 (6%)	21 (96%)	1 (4%)	27	57
7	Y	21/337 (6%)	21 (100%)	0	100	100
7	Z	23/337 (7%)	23 (100%)	0	100	100
7	a	22/337 (6%)	22 (100%)	0	100	100
7	b	21/337 (6%)	21 (100%)	0	100	100
7	c	23/337 (7%)	23 (100%)	0	100	100
7	d	22/337 (6%)	21 (96%)	1 (4%)	27	57
7	e	21/337 (6%)	21 (100%)	0	100	100
7	f	23/337 (7%)	23 (100%)	0	100	100
7	g	22/337 (6%)	21 (96%)	1 (4%)	27	57
7	h	21/337 (6%)	21 (100%)	0	100	100
7	i	23/337 (7%)	23 (100%)	0	100	100
7	j	22/337 (6%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	k	21/337 (6%)	21 (100%)	0	100	100
7	l	23/337 (7%)	23 (100%)	0	100	100
7	m	22/337 (6%)	22 (100%)	0	100	100
7	n	21/337 (6%)	21 (100%)	0	100	100
All	All	4887/18617 (26%)	4828 (99%)	59 (1%)	72	84

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	81	THR
1	2	84	ASP
1	3	211	LEU
1	4	133	ARG
1	4	135	LYS
2	5	163	CYS
5	AM	87	LEU
5	AO	100	ARG
5	AP	98	LEU
5	AP	100	ARG
5	AQ	32	ARG
6	AS	28	THR
6	AS	64	THR
6	AS	76	ILE
6	AT	28	THR
6	AT	44	LEU
6	AT	51	LEU
6	AT	64	THR
6	AT	72	ASP
6	AT	76	ILE
6	AU	28	THR
6	AU	34	LEU
6	AU	51	LEU
6	AU	64	THR
6	AU	70	ASP
6	AU	76	ILE
6	AV	44	LEU
6	AV	67	VAL
6	AV	76	ILE
6	AW	28	THR
6	AW	34	LEU
6	AW	44	LEU

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Mol	Chain	Res	Type
6	AW	51	LEU
6	AW	64	THR
6	AW	70	ASP
6	AW	72	ASP
6	AW	76	ILE
4	C	143	ARG
4	D	40	ASP
4	F	143	ARG
4	G	143	ARG
4	H	36	VAL
4	H	143	ARG
4	I	143	ARG
4	J	40	ASP
4	K	143	ARG
4	L	143	ARG
4	M	126	LEU
4	N	143	ARG
4	O	143	ARG
4	P	143	ARG
4	Q	40	ASP
4	Q	143	ARG
7	R	366	LEU
7	U	366	LEU
7	V	366	LEU
7	X	366	LEU
7	d	366	LEU
7	g	366	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	117	ASN
1	4	44	GLN
2	5	104	ASN
2	5	130	ASN
3	7	37	GLN
3	8	9	ASN
3	8	37	GLN
3	9	37	GLN
4	A	71	ASN
4	A	87	GLN
5	AN	78	ASN

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Mol	Chain	Res	Type
5	AO	53	ASN
5	AP	59	ASN
5	AQ	71	GLN
6	AS	26	GLN
6	AS	48	GLN
6	AT	26	GLN
6	AT	48	GLN
6	AU	55	ASN
6	AU	78	ASN
6	AV	22	ASN
6	AW	22	ASN
6	AW	63	ASN
6	AX	59	ASN
6	AX	78	ASN
6	AZ	26	GLN
6	AZ	78	ASN
4	B	87	GLN
4	B	170	ASN
6	BA	24	GLN
6	BA	26	GLN
6	BD	59	ASN
6	BD	61	GLN
6	BD	78	ASN
4	C	123	ASN
4	C	161	ASN
4	D	87	GLN
4	F	71	ASN
4	G	97	GLN
4	G	124	ASN
4	G	170	ASN
4	H	97	GLN
4	I	169	GLN
4	J	87	GLN
4	J	97	GLN
4	L	87	GLN
4	L	97	GLN
4	L	169	GLN
4	M	161	ASN
4	M	169	GLN
4	N	97	GLN
4	N	170	ASN
4	P	87	GLN

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Mol	Chain	Res	Type
4	P	169	GLN
4	Q	87	GLN
4	Q	97	GLN
4	Q	169	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

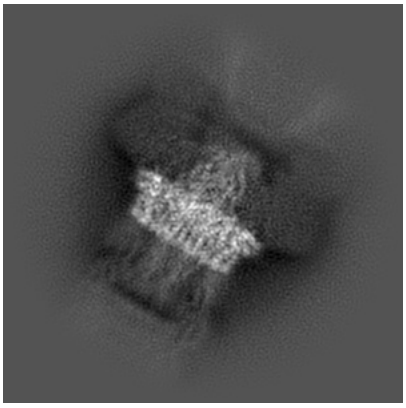
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20317. These allow visual inspection of the internal detail of the map and identification of artifacts.

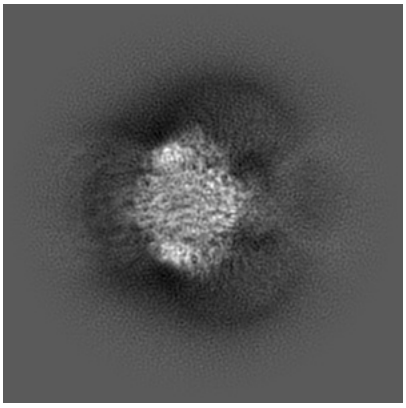
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

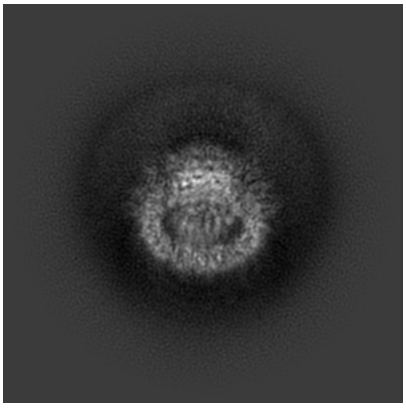
6.1.1 Primary map



X



Y

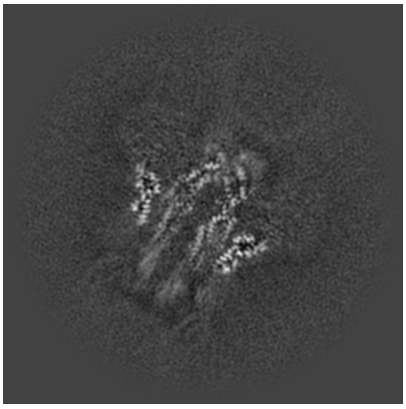


Z

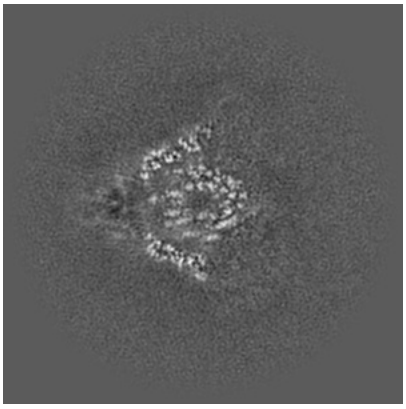
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

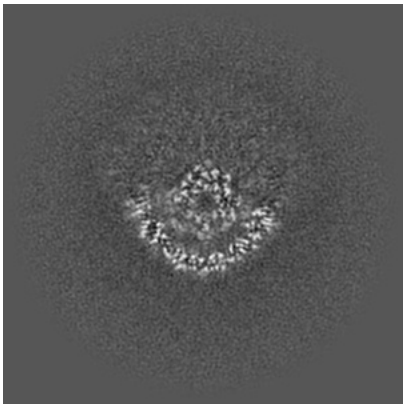
6.2.1 Primary map



X Index: 125



Y Index: 125

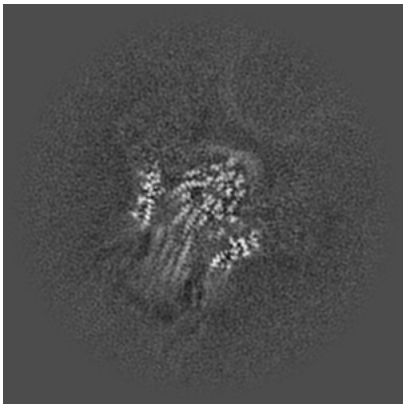


Z Index: 125

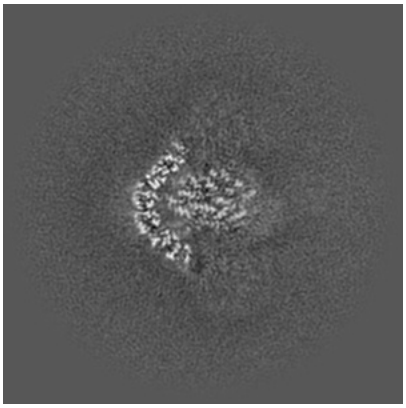
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

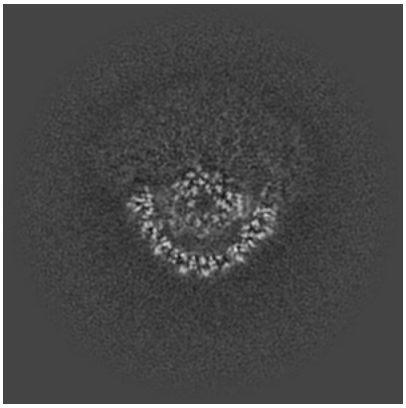
6.3.1 Primary map



X Index: 134



Y Index: 139



Z Index: 123

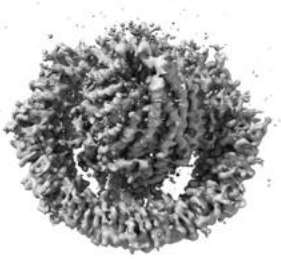
The images above show the largest variance slices of the map in three orthogonal directions.

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 1.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

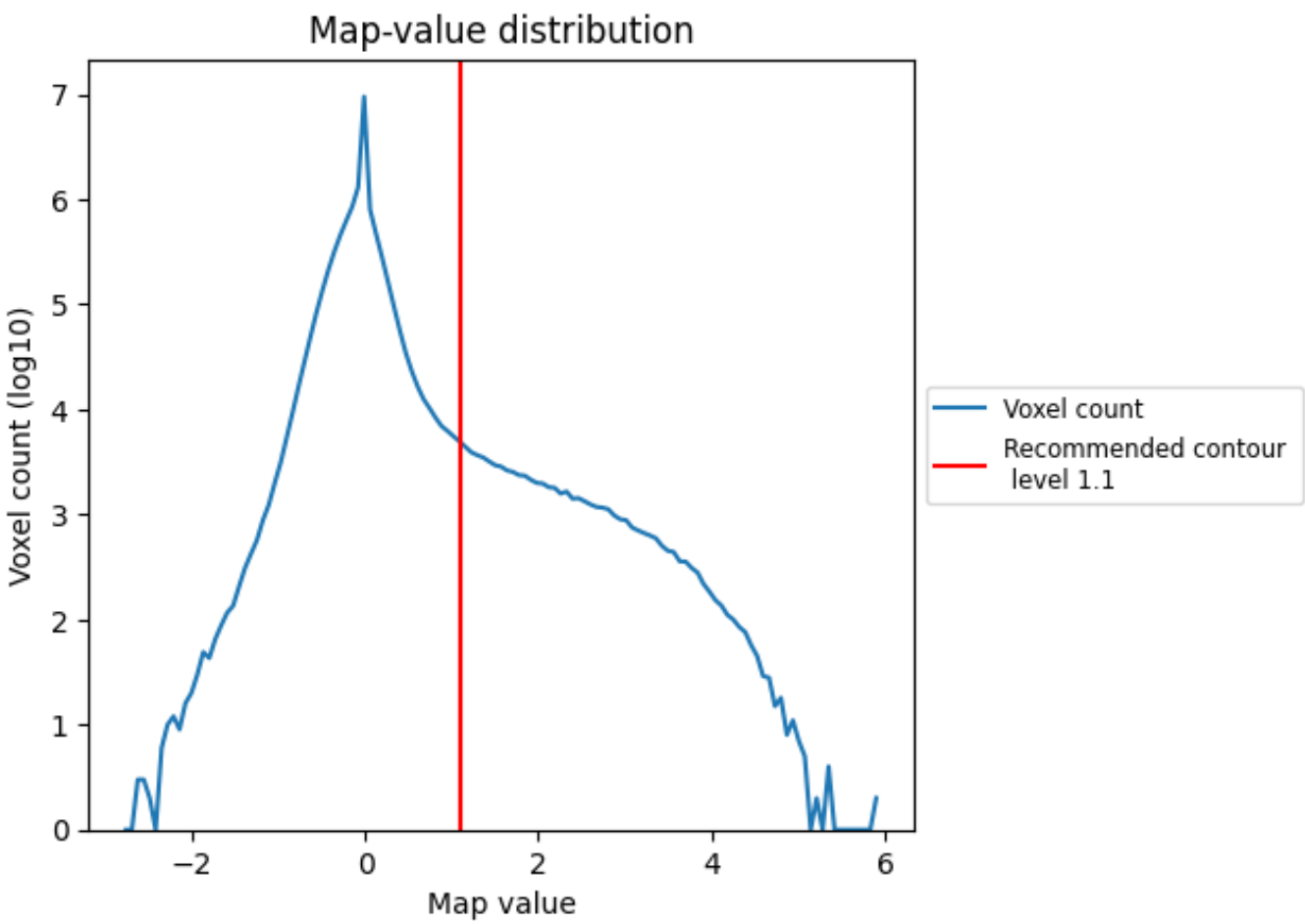
6.5 Mask visualisation (i)

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

7 Map analysis (i)

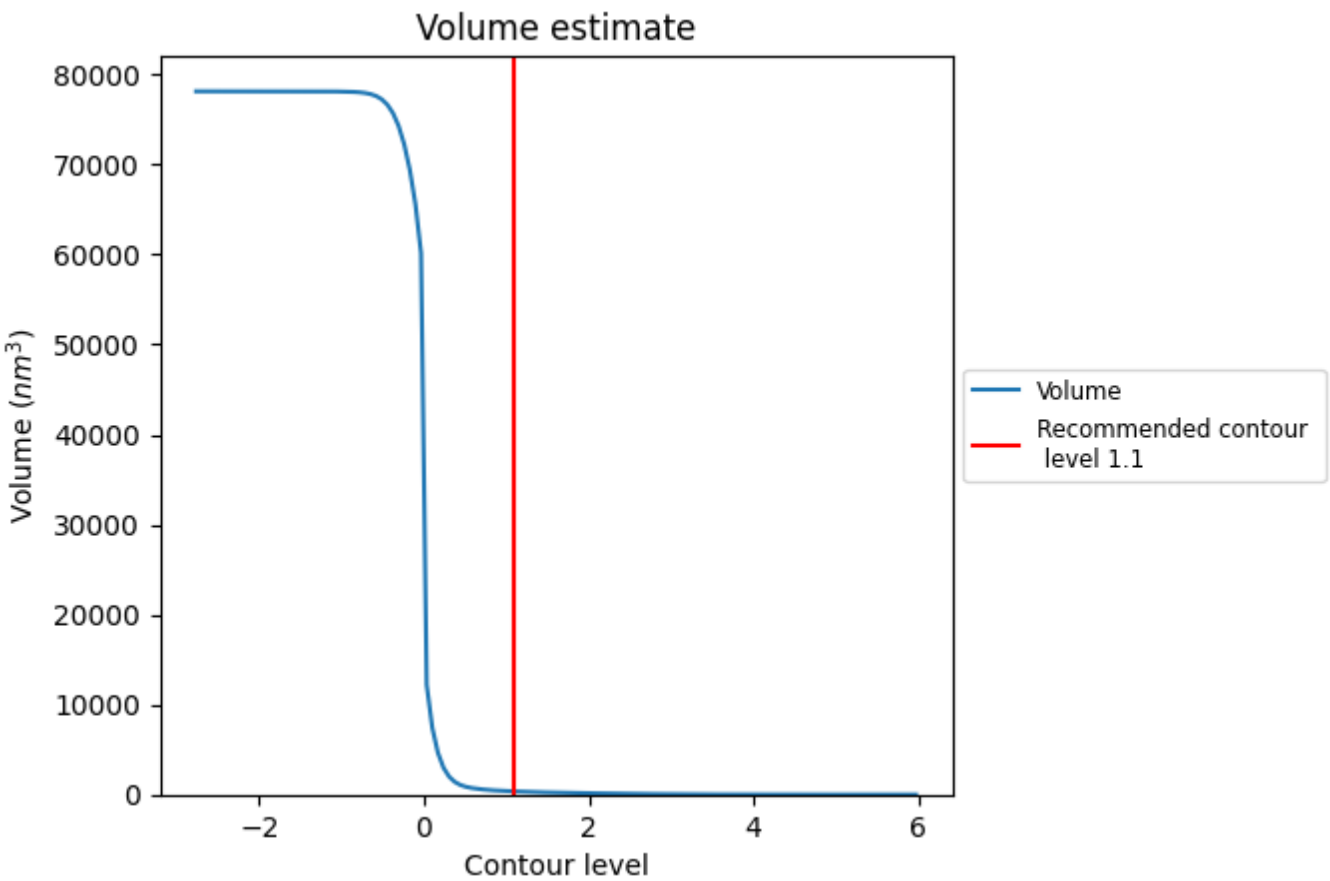
This section contains the results of statistical analysis of the map.

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.

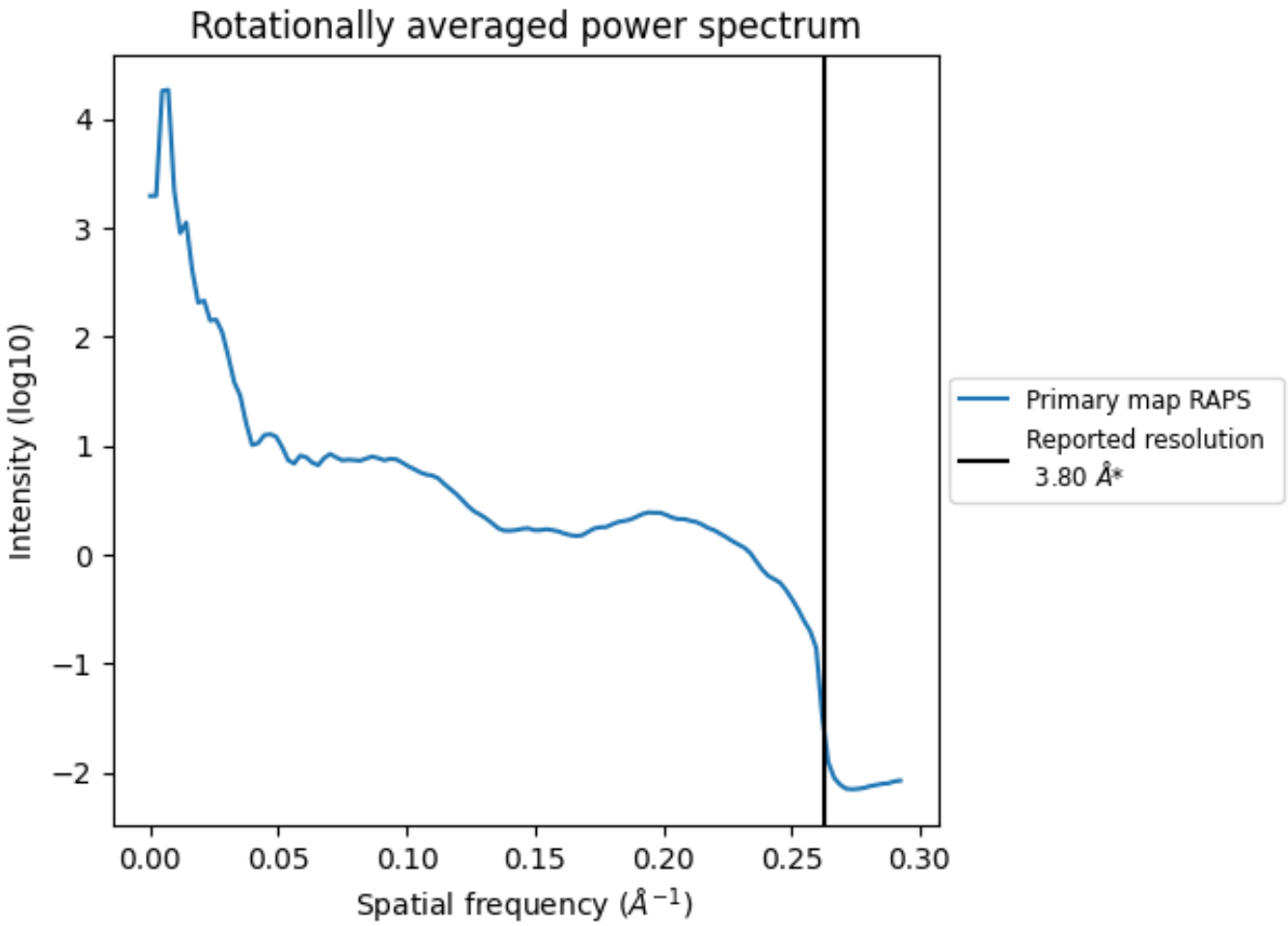
7.2 Volume estimate (i)



The volume at the recommended contour level is 352 nm^3; this corresponds to an approximate mass of 318 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

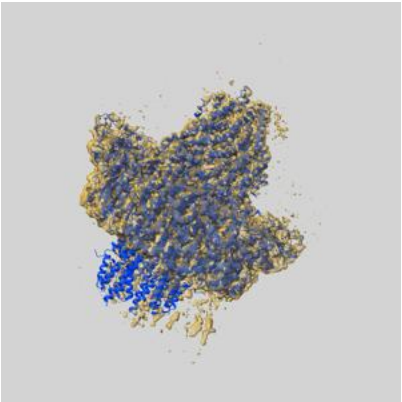
8 Fourier-Shell correlation (i)

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

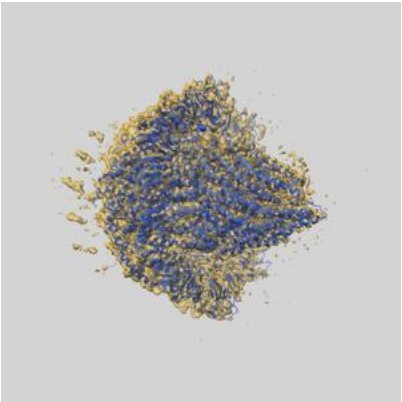
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20317 and PDB model 6PEP. Per-residue inclusion information can be found in section 3 on page 11.

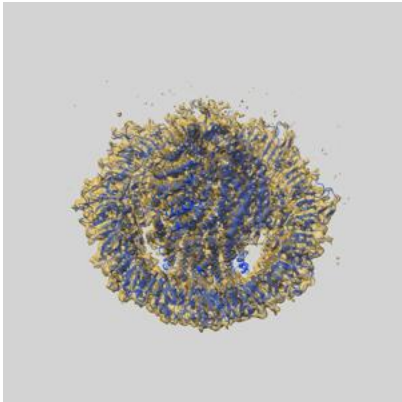
9.1 Map-model overlay (i)



X



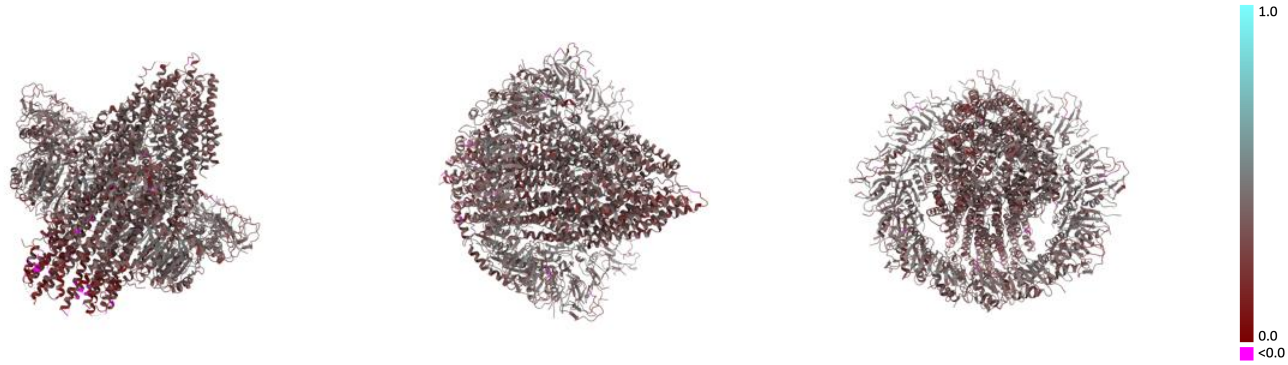
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.1 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.

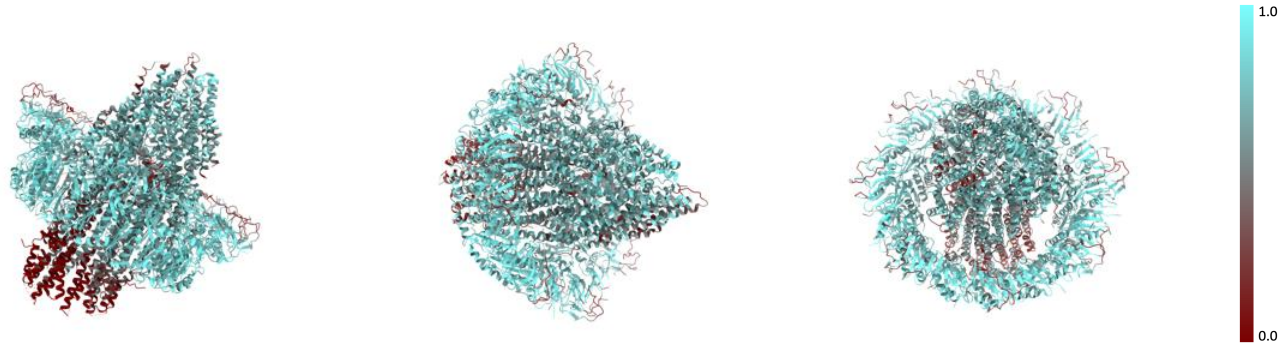
9.2 Q-score mapped to coordinate model (i)



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.

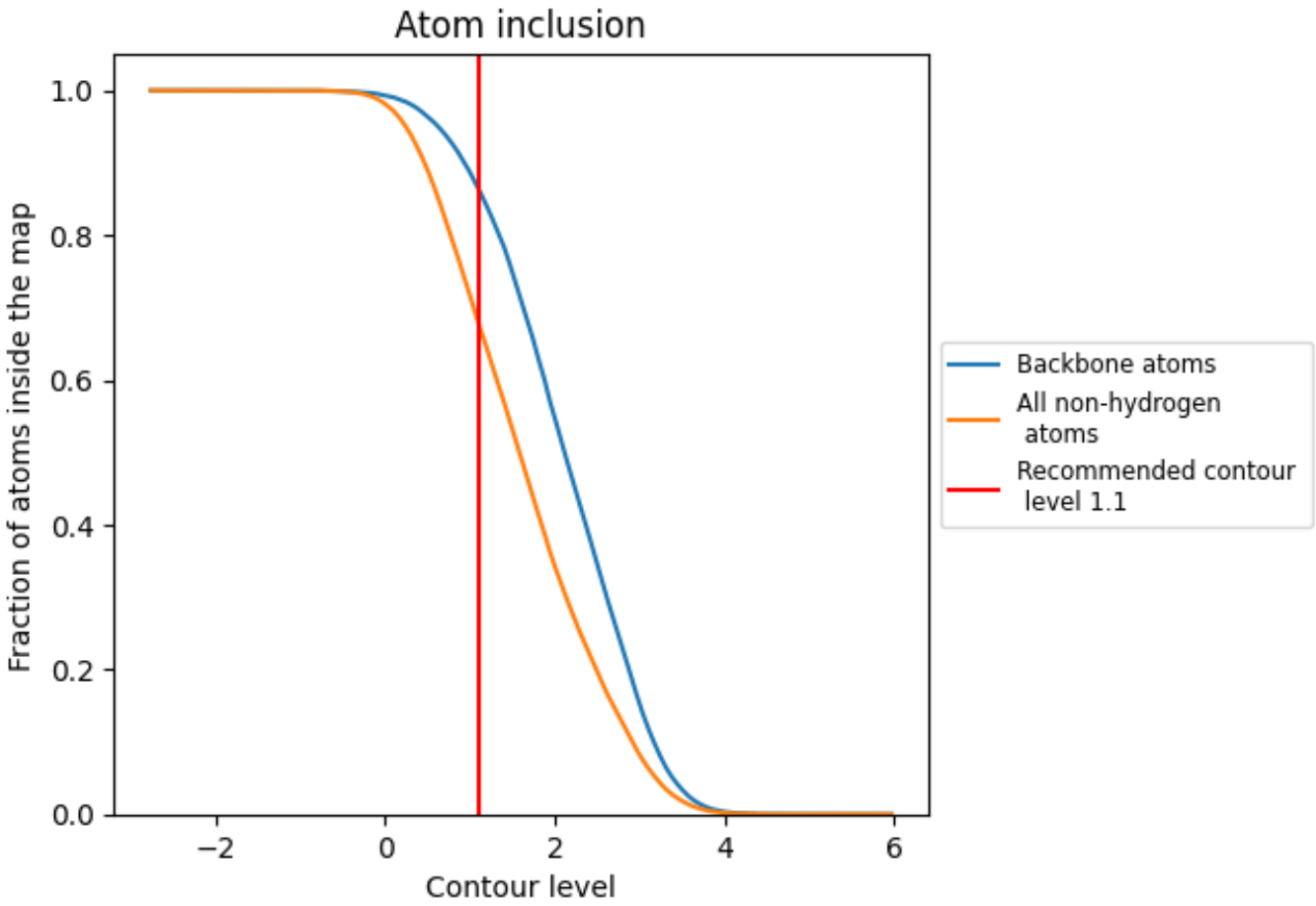
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.1).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6781	0.3540
0	0.6951	0.3510
1	0.6952	0.3290
2	0.7064	0.3440
3	0.7162	0.3590
4	0.7058	0.3560
5	0.7547	0.3840
6	0.2889	0.3300
7	0.4725	0.3090
8	0.6185	0.3280
9	0.6781	0.3490
A	0.8352	0.3860
AM	0.5993	0.3480
AN	0.6121	0.3240
AO	0.6122	0.3230
AP	0.5882	0.3370
AQ	0.6094	0.3310
AR	0.4977	0.3180
AS	0.4466	0.2930
AT	0.5316	0.2710
AU	0.4619	0.2840
AV	0.4379	0.2750
AW	0.3442	0.2710
AX	0.0760	0.2480
AY	0.2769	0.2410
AZ	0.3540	0.2470
B	0.8141	0.3820
BA	0.3287	0.2260
BB	0.3026	0.2240
BC	0.0316	0.2120
BD	0.0447	0.1870
BE	0.1386	0.1860
C	0.8343	0.3870
D	0.8167	0.3970
E	0.4279	0.3170

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Chain	Atom inclusion	Q-score
F	0.8333	0.3990
G	0.8114	0.3940
H	0.8343	0.4010
I	0.8052	0.3970
J	0.8416	0.4020
K	0.8283	0.3860
L	0.8416	0.3980
M	0.8230	0.3880
N	0.8481	0.3920
O	0.8176	0.3800
P	0.8416	0.3770
Q	0.8141	0.3840
R	0.7636	0.3900
S	0.7768	0.3880
T	0.3843	0.3150
U	0.7682	0.3880
V	0.7634	0.3920
W	0.3755	0.3230
X	0.7909	0.4040
Y	0.7902	0.4020
Z	0.4061	0.3170
a	0.7864	0.3920
b	0.8036	0.4070
c	0.4498	0.3230
d	0.7727	0.3920
e	0.7902	0.4030
f	0.4541	0.3210
g	0.7682	0.3970
h	0.7946	0.4130
i	0.4279	0.3170
j	0.8091	0.4170
k	0.8036	0.4220
l	0.4148	0.3190
m	0.7682	0.4210
n	0.7589	0.3930