Full wwPDB EM Validation Report (i)

May 7, 2026 – 03:18 PM JST

PDB ID	:	8Z5X / pdb_00008z5x
EMDB ID	:	EMD-39787
Title	:	Cryo-EM structure of the MS ring with the proximal rod and the export apparatus (C1) within the polar flagellar motor
Authors	:	Zhang, L.; Tan, J.X.; Zhou, Y.; Zhu, Y.Q.
Deposited on	:	2024-04-18
Resolution	:	3.64 Å(reported)
Based on initial model	:	.

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:

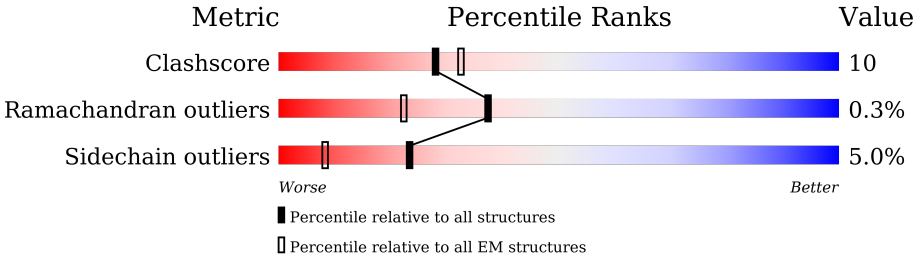
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

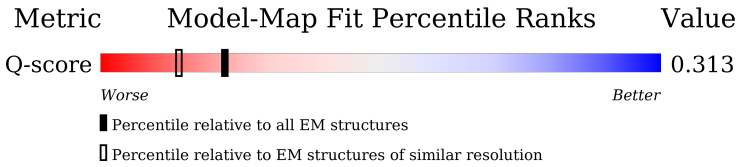
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.64 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11633 (3.14 - 4.14)

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	289	56% 15% • 28%
1	9	289	58% 13% 28%
1	AP	289	56% 15% 28%
1	Ak	289	57% 13% • 28%

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Mol	Chain	Length	Quality of chain
1	Al	289	54% 16% 28%
2	1	580	7% 22% 74%
2	2	580	6% 21% 74%
2	3	580	21% 5% 74%
2	4	580	5% 21% 74%
2	5	580	21% 74%
2	A	580	21% 74%
2	AA	580	97%
2	AB	580	97%
2	AC	580	97%
2	AD	580	97%
2	AE	580	97%
2	AF	580	96%
2	AG	580	98%
2	AH	580	98%
2	AI	580	98%
2	AJ	580	96%
2	AK	580	96%
2	AL	580	5% 94%
2	AM	580	5% 94%
2	AN	580	5% 94%
2	AO	580	94%
2	B	580	22% 74%
2	C	580	22% 74%
2	D	580	22% 74%

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Mol	Chain	Length	Quality of chain
2	E	580	21% • 74%
2	F	580	21% • 74%
2	G	580	21% • 74%
2	H	580	21% • 74%
2	I	580	21% • 74%
2	J	580	21% • 74%
2	K	580	22% • 74%
2	L	580	22% • 74%
2	M	580	21% • 74%
2	N	580	21% • 74%
2	O	580	5% 22% • 74%
2	P	580	22% • 74%
2	Q	580	21% • 74%
2	R	580	22% • 74%
2	S	580	11% 8% • 80%
2	T	580	10% 8% • 80%
2	U	580	12% 7% • 80%
2	V	580	12% 7% • 80%
2	W	580	11% 7% • 80%
2	X	580	12% 5% • 81%
2	Y	580	12% 6% • 80%
2	Z	580	12% 6% • 80%
2	a	580	13% 7% • 80%
2	b	580	11% 6% 84%
2	c	580	10% 7% • 82%

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Mol	Chain	Length	Quality of chain
2	d	580	9% 7% 82%
2	e	580	10% 7% 82%
2	f	580	9% 6% 85%
2	g	580	10% 5% 84%
2	h	580	10% 6% 84%
2	i	580	9% 6% 85%
2	j	580	10% 6% 84%
2	k	580	12% 7% 80%
2	l	580	12% 7% 80%
2	m	580	13% 6% 80%
2	n	580	11% 7% 82%
2	o	580	12% 6% 80%
2	p	580	22% 74%
2	q	580	21% 74%
2	r	580	22% 74%
2	s	580	21% 74%
2	t	580	22% 74%
2	u	580	22% 74%
2	v	580	6% 22% 74%
2	w	580	6% 21% 74%
2	x	580	5% 21% 5% 74%
2	y	580	5% 21% 74%
2	z	580	6% 22% 74%
3	6	89	69% 29%
3	7	89	78% 22%

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Mol	Chain	Length	Quality of chain
3	AQ	89	71% 28%
3	AR	89	71% 26%
4	8	260	69% 22% 7%
5	AS	131	69% 13% 17%
5	AT	131	66% 16% 18%
5	AU	131	69% 14% 17%
5	AV	131	68% 15% 18%
5	AW	131	70% 12% 18%
6	AX	137	15% 79% 16% 5%
6	AY	137	42% 77% 18% 5%
6	AZ	137	46% 70% 22% 5%
6	Aa	137	36% 83% 11% 5%
6	Ab	137	28% 77% 18% 5%
6	Ac	137	20% 80% 14% 5%
7	Ad	103	54% 16% 30%
7	Ae	103	66% 11% 22%
7	Af	103	63% 15% 22%
7	Ag	103	60% 10% 30%
7	Ah	103	59% 11% 30%
7	Ai	103	29% 10% 61%
8	Aj	376	14% 5% 81%
9	Am	13	8% 46% 38% 8% 8%
9	An	13	15% 15% 38% 15% 31%
9	Ao	13	38% 31% 8% 23%
9	Ap	13	38% 23% 15% 23%

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Mol	Chain	Length	Quality of chain
9	Aq	13	38% 54% 8%
10	Ar	17	6% 88% 12%
10	As	17	6% 82% 18%
10	At	17	18% 88% 12%
10	Au	17	59% 94% 6%
10	Av	17	18% 88% 12%
10	Aw	17	94% 6%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 88315 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 Flagellar biosynthetic protein FliP.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	208	1608	1060	244	285	19	0	0
1	9	207	1599	1055	243	282	19	0	0
1	AP	208	1608	1060	244	285	19	0	0
1	Ak	208	1608	1060	244	285	19	0	0
1	Al	208	1608	1060	244	285	19	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	26	SER	THR	conflict	UNP A0A1W6TTE6
0	204	ASP	GLU	conflict	UNP A0A1W6TTE6
9	26	SER	THR	conflict	UNP A0A1W6TTE6
9	204	ASP	GLU	conflict	UNP A0A1W6TTE6
AP	26	SER	THR	conflict	UNP A0A1W6TTE6
AP	204	ASP	GLU	conflict	UNP A0A1W6TTE6
Ak	26	SER	THR	conflict	UNP A0A1W6TTE6
Ak	204	ASP	GLU	conflict	UNP A0A1W6TTE6
Al	26	SER	THR	conflict	UNP A0A1W6TTE6
Al	204	ASP	GLU	conflict	UNP A0A1W6TTE6

- Molecule 2 is a protein called Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	148	1171	719	215	235	2	0	0
2	2	148	1171	719	215	235	2	0	0
2	3	148	1171	719	215	235	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	4	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	5	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	A	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	AA	19	135	82	23	29	1	0	0
			Total	C	N	O	S		
2	AB	19	135	82	23	29	1	0	0
			Total	C	N	O	S		
2	AC	20	139	84	24	30	1	0	0
			Total	C	N	O	S		
2	AD	19	135	82	23	29	1	0	0
			Total	C	N	O	S		
2	AE	19	135	82	23	29	1	0	0
			Total	C	N	O	S		
2	AF	23	158	97	27	33	1	0	0
			Total	C	N	O			
2	AG	11	73	46	13	14		0	0
			Total	C	N	O			
2	AH	11	73	46	13	14		0	0
			Total	C	N	O			
2	AI	11	73	46	13	14		0	0
			Total	C	N	O	S		
2	AJ	24	163	100	28	34	1	0	0
			Total	C	N	O	S		
2	AK	25	169	104	29	35	1	0	0
			Total	C	N	O	S		
2	AL	32	220	134	38	46	2	0	0
			Total	C	N	O	S		
2	AM	33	224	136	39	47	2	0	0
			Total	C	N	O	S		
2	AN	33	224	136	39	47	2	0	0
			Total	C	N	O	S		
2	AO	32	220	134	38	46	2	0	0
			Total	C	N	O	S		
2	B	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	C	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	D	148	1171	719	215	235	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	F	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	G	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	H	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	I	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	J	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	K	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	L	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	M	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	N	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	O	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	P	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	Q	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	R	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	S	114	881	543	165	169	4	0	0
			Total	C	N	O	S		
2	T	114	881	543	165	169	4	0	0
			Total	C	N	O	S		
2	U	114	881	543	165	169	4	0	0
			Total	C	N	O	S		
2	V	114	881	543	165	169	4	0	0
			Total	C	N	O	S		
2	W	114	881	543	165	169	4	0	0
			Total	C	N	O	S		
2	X	109	839	515	157	163	4	0	0
			Total	C	N	O	S		
2	Y	114	881	543	165	169	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Z	114	881	543	165	169	4	0	0
			Total	C	N	O	S		
2	a	114	881	543	165	169	4	0	0
			Total	C	N	O	S		
2	b	94	724	446	135	140	3	0	0
			Total	C	N	O	S		
2	c	103	803	496	153	151	3	0	0
			Total	C	N	O	S		
2	d	103	803	496	153	151	3	0	0
			Total	C	N	O	S		
2	e	103	803	496	153	151	3	0	0
			Total	C	N	O	S		
2	f	85	660	405	125	127	3	0	0
			Total	C	N	O	S		
2	g	92	704	432	132	137	3	0	0
			Total	C	N	O	S		
2	h	91	695	427	131	134	3	0	0
			Total	C	N	O	S		
2	i	89	684	420	129	132	3	0	0
			Total	C	N	O	S		
2	j	92	704	432	132	137	3	0	0
			Total	C	N	O	S		
2	k	114	881	543	165	169	4	0	0
			Total	C	N	O	S		
2	l	114	881	543	165	169	4	0	0
			Total	C	N	O	S		
2	m	114	881	543	165	169	4	0	0
			Total	C	N	O	S		
2	n	105	802	494	147	157	4	0	0
			Total	C	N	O	S		
2	o	114	881	543	165	169	4	0	0
			Total	C	N	O	S		
2	p	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	q	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	r	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	s	148	1171	719	215	235	2	0	0
			Total	C	N	O	S		
2	t	148	1171	719	215	235	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	u	148	1171	719	215	235	2	0	0
2	v	148	1171	719	215	235	2	0	0
2	w	148	1171	719	215	235	2	0	0
2	x	148	1171	719	215	235	2	0	0
2	y	148	1171	719	215	235	2	0	0
2	z	148	1171	719	215	235	2	0	0

- Molecule 3 is a protein called Flagellar biosynthetic protein FliQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	6	89	722	489	107	117	9	0	0
3	7	89	722	489	107	117	9	0	0
3	AQ	89	722	489	107	117	9	0	0
3	AR	89	722	489	107	117	9	0	0

- Molecule 4 is a protein called Flagellar biosynthetic protein FliR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	8	242	1896	1265	295	315	21	0	0

- Molecule 5 is a protein called Flagellar basal body rod protein FlgB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AS	109	845	523	155	166	1	0	0
5	AT	107	835	518	153	163	1	0	0
5	AU	109	845	523	155	166	1	0	0
5	AV	108	837	519	154	163	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AW	108	837	519	154	163	1	0	0

- Molecule 6 is a protein called Flagellar basal-body rod protein FlgC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AX	130	983	605	168	203	7	0	0
6	AY	130	983	605	168	203	7	0	0
6	AZ	130	983	605	168	203	7	0	0
6	Aa	130	983	605	168	203	7	0	0
6	Ab	130	983	605	168	203	7	0	0
6	Ac	130	983	605	168	203	7	0	0

- Molecule 7 is a protein called Flagellar hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Ad	72	560	345	99	113	3	0	0
7	Ae	80	605	372	108	122	3	0	0
7	Af	80	605	372	108	122	3	0	0
7	Ag	72	560	345	99	113	3	0	0
7	Ah	72	560	345	99	113	3	0	0
7	Ai	40	311	194	53	61	3	0	0

- Molecule 8 is a protein called Flagellar biosynthetic protein FlhB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Aj	71	552	370	83	95	4	0	0

- Molecule 9 is a protein called Alanine-modelled FlgB-Dc loop.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	Am	12	58	34	12	12	0	0
			Total	C	N	O		
9	An	9	44	26	9	9	0	0
			Total	C	N	O		
9	Ao	10	49	29	10	10	0	0
			Total	C	N	O		
9	Ap	10	49	29	10	10	0	0
			Total	C	N	O		
9	Aq	13	63	37	13	13	0	0

- Molecule 10 is a protein called FliE-helix 1.

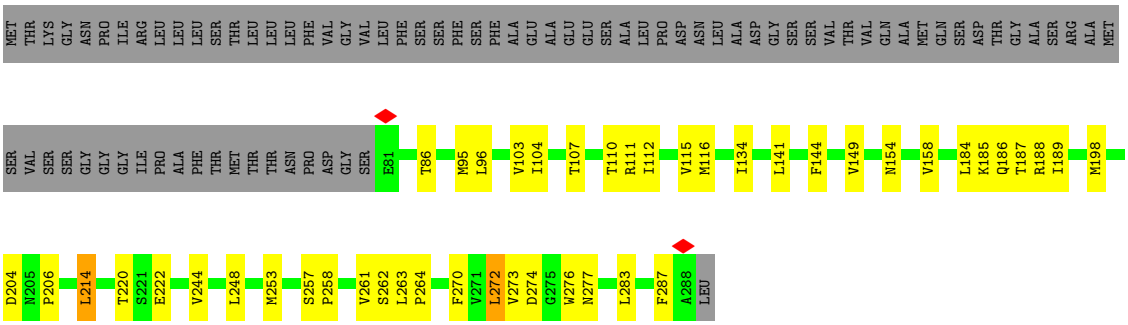
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	Ar	17	84	50	17	17	0	0
			Total	C	N	O		
10	As	17	84	50	17	17	0	0
			Total	C	N	O		
10	At	17	84	50	17	17	0	0
			Total	C	N	O		
10	Au	17	84	50	17	17	0	0
			Total	C	N	O		
10	Av	17	84	50	17	17	0	0
			Total	C	N	O		
10	Aw	17	84	50	17	17	0	0

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.

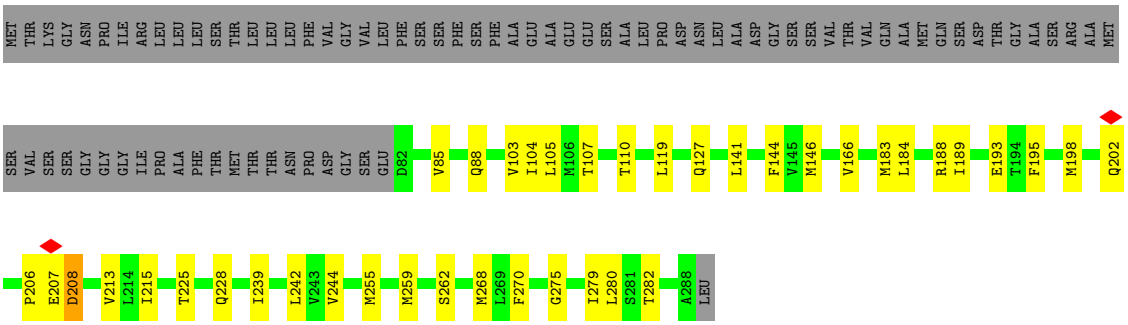
- Molecule 1: Flagellar biosynthetic protein FliP

Chain 0:



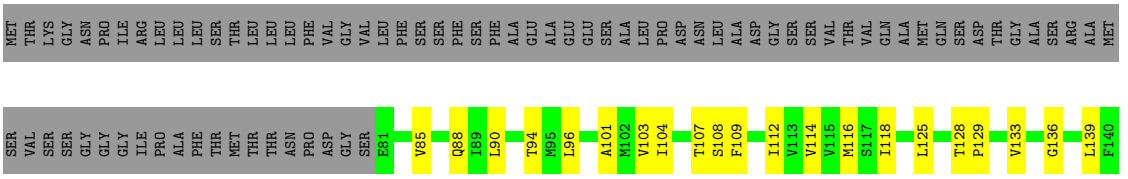
- Molecule 1: Flagellar biosynthetic protein FliP

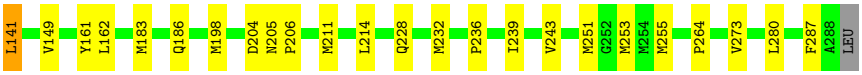
Chain 9:



- Molecule 1: Flagellar biosynthetic protein FliP

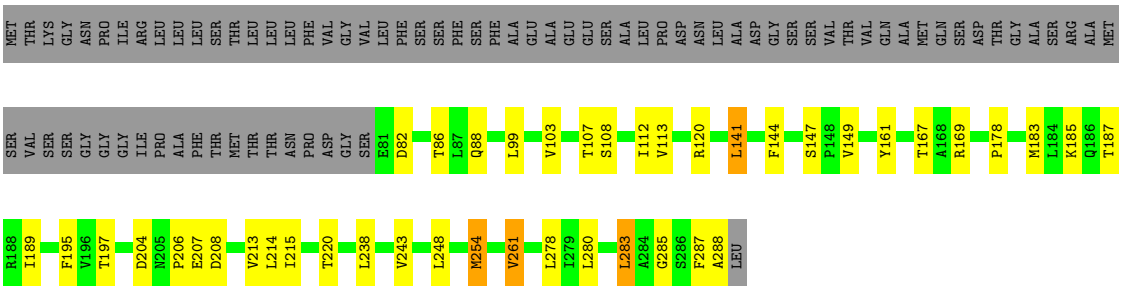
Chain AP:





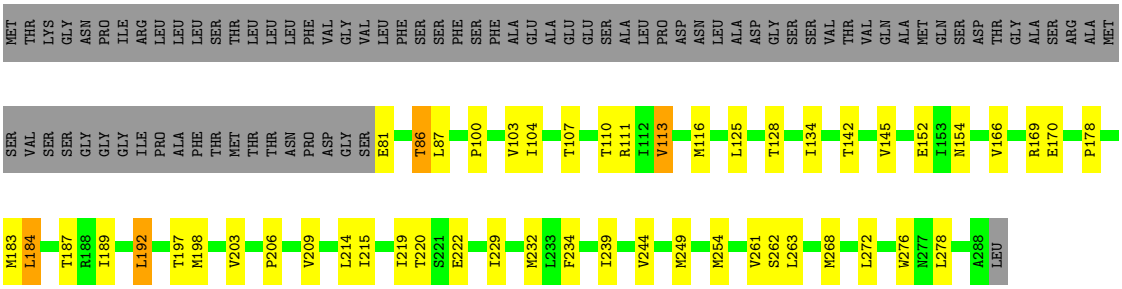
• Molecule 1: Flagellar biosynthetic protein FliP

Chain Ak:



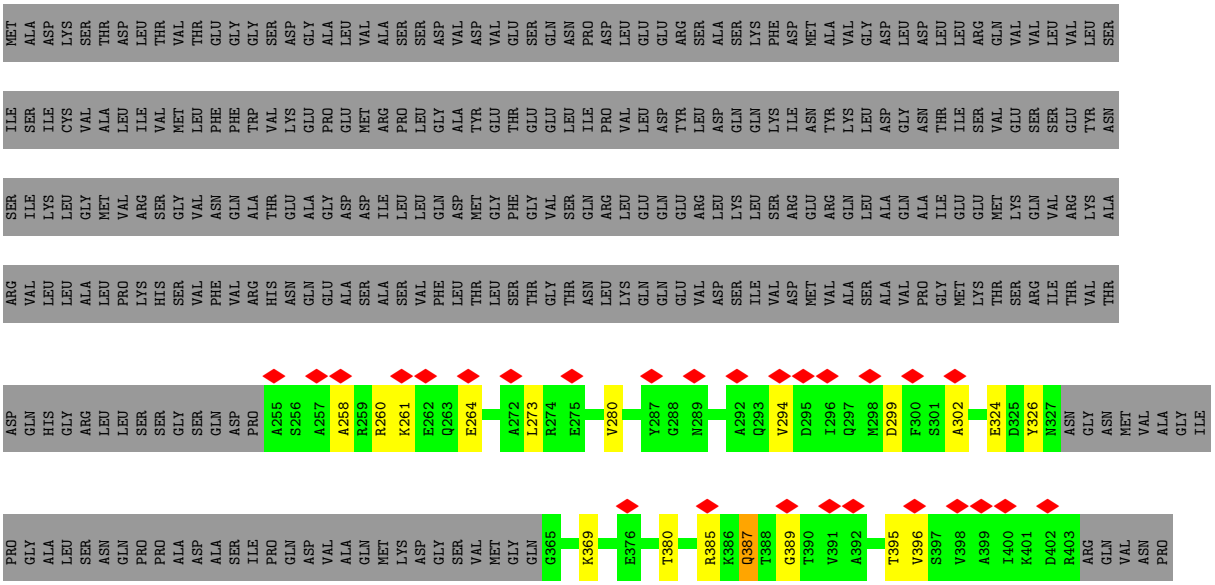
• Molecule 1: Flagellar biosynthetic protein FliP

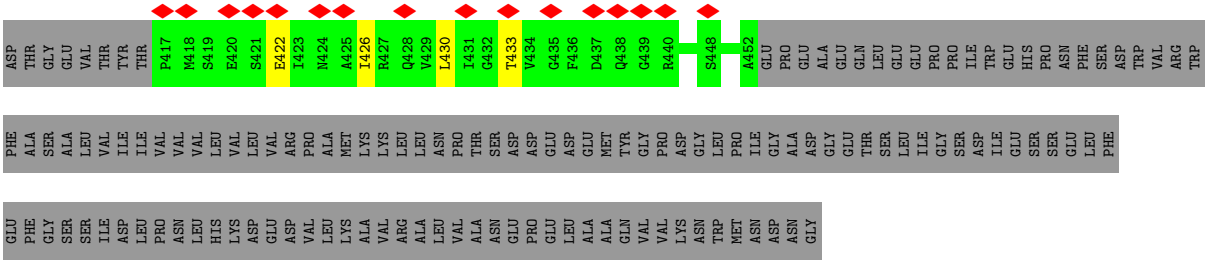
Chain Al:



• Molecule 2: Flagellar M-ring protein

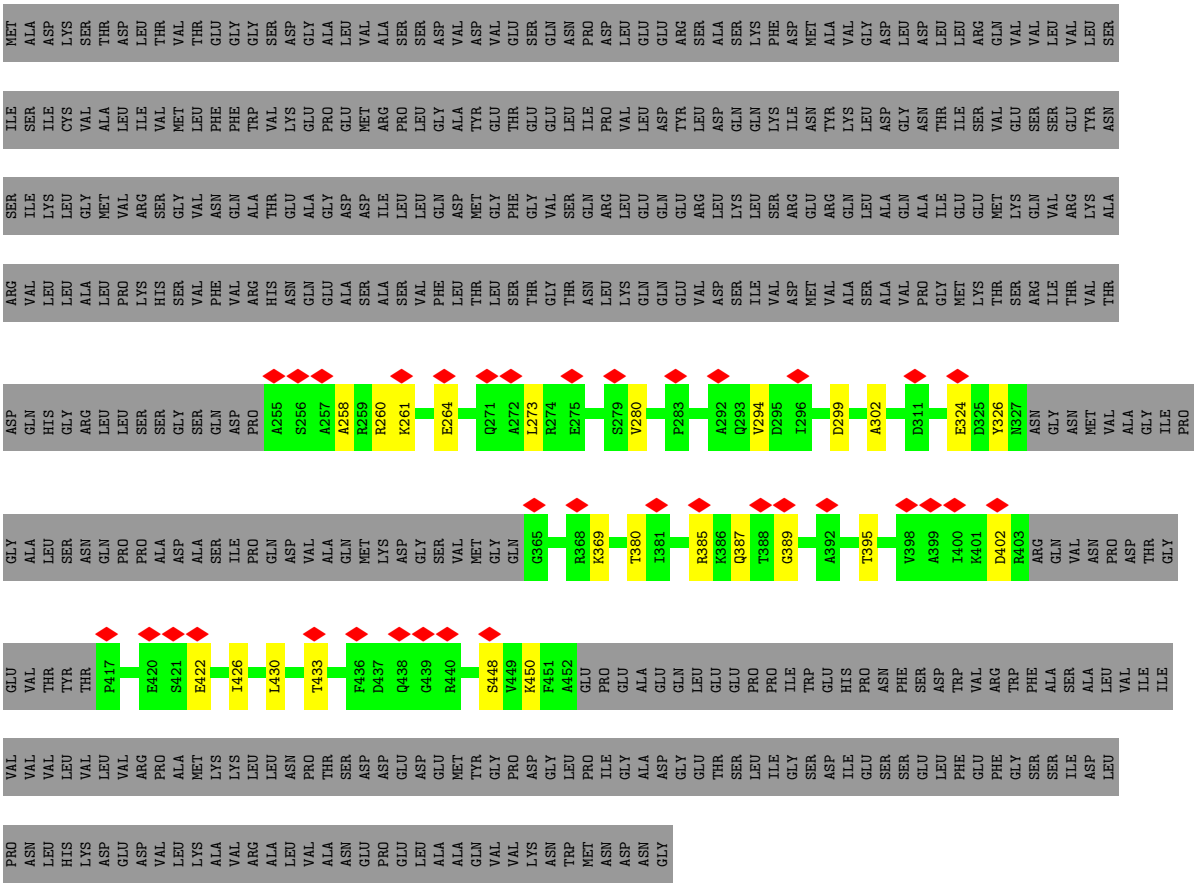
Chain 1:





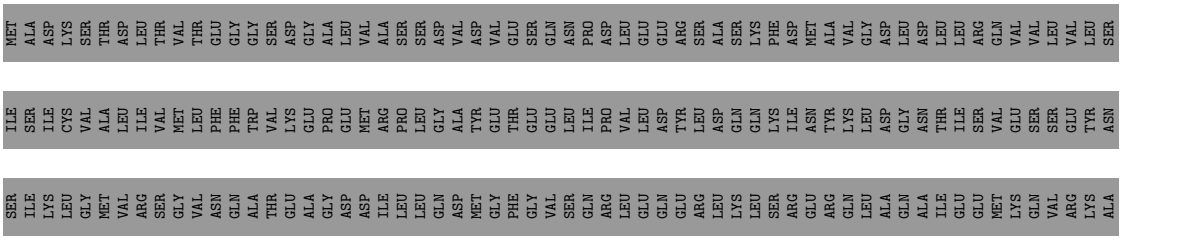
• Molecule 2: Flagellar M-ring protein

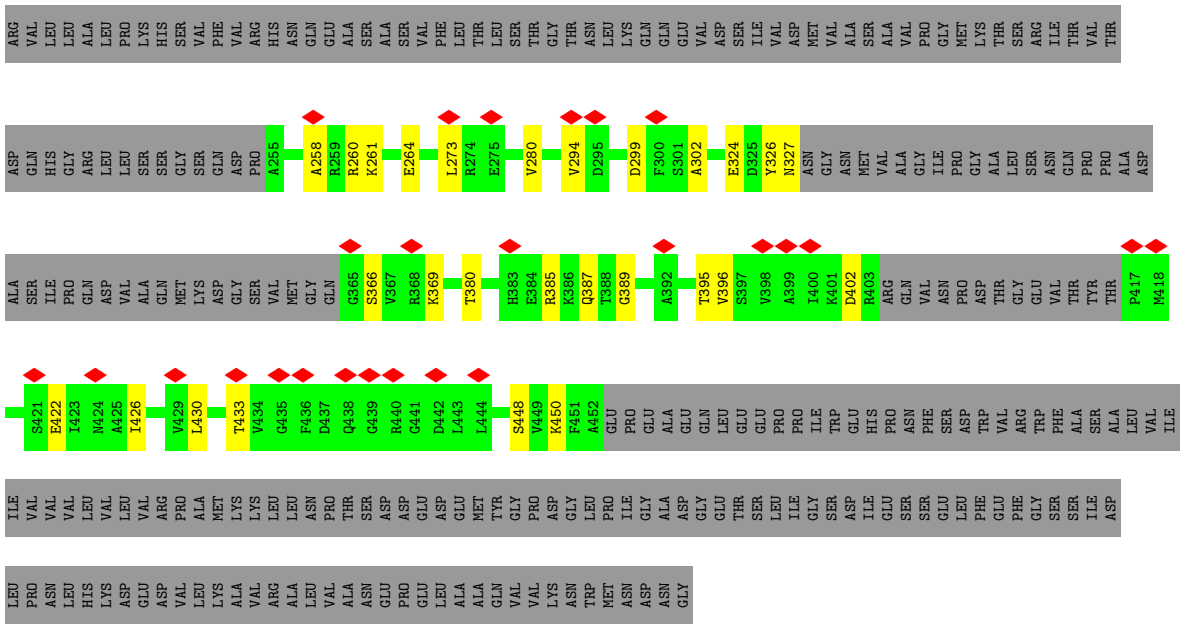
Chain 2:



• Molecule 2: Flagellar M-ring protein

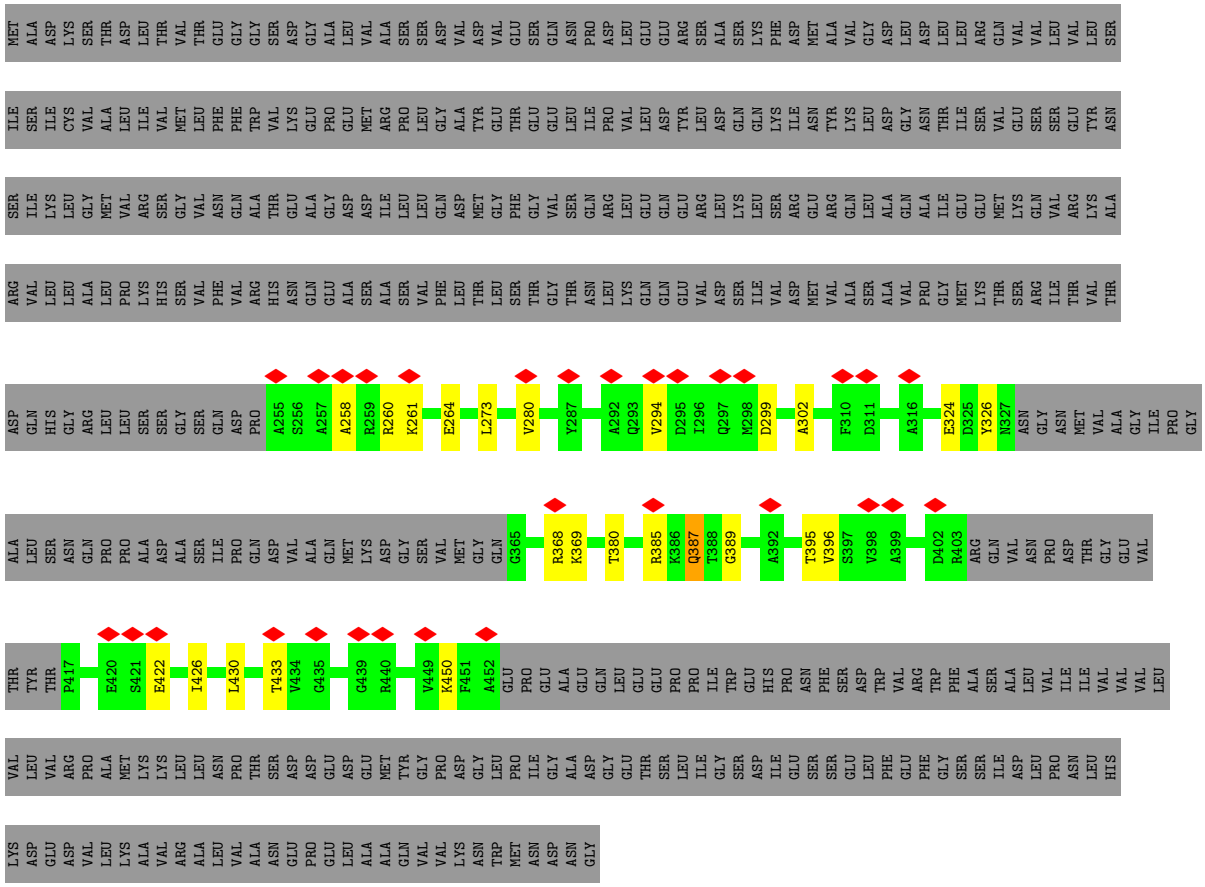
Chain 3:





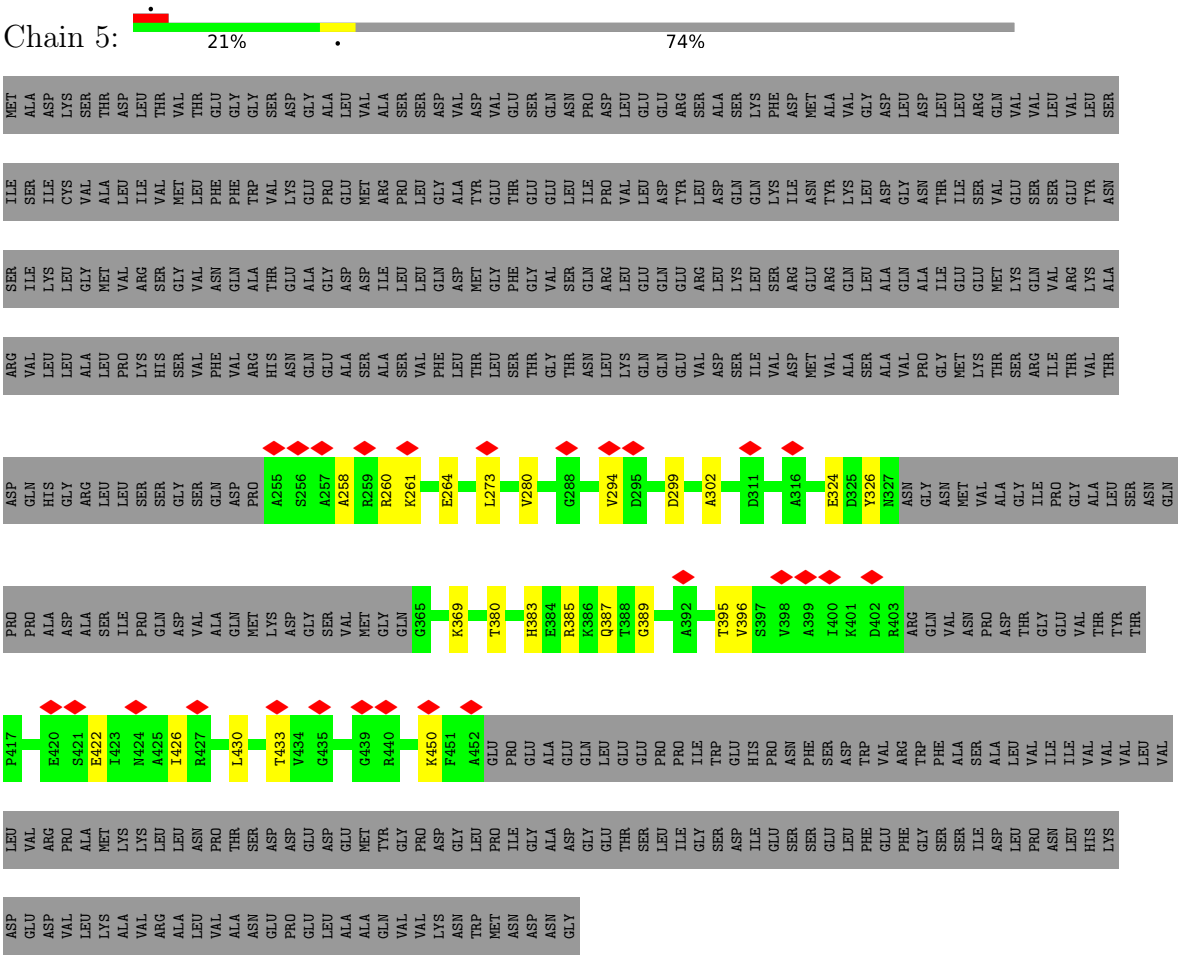
- Molecule 2: Flagellar M-ring protein

Chain 4:



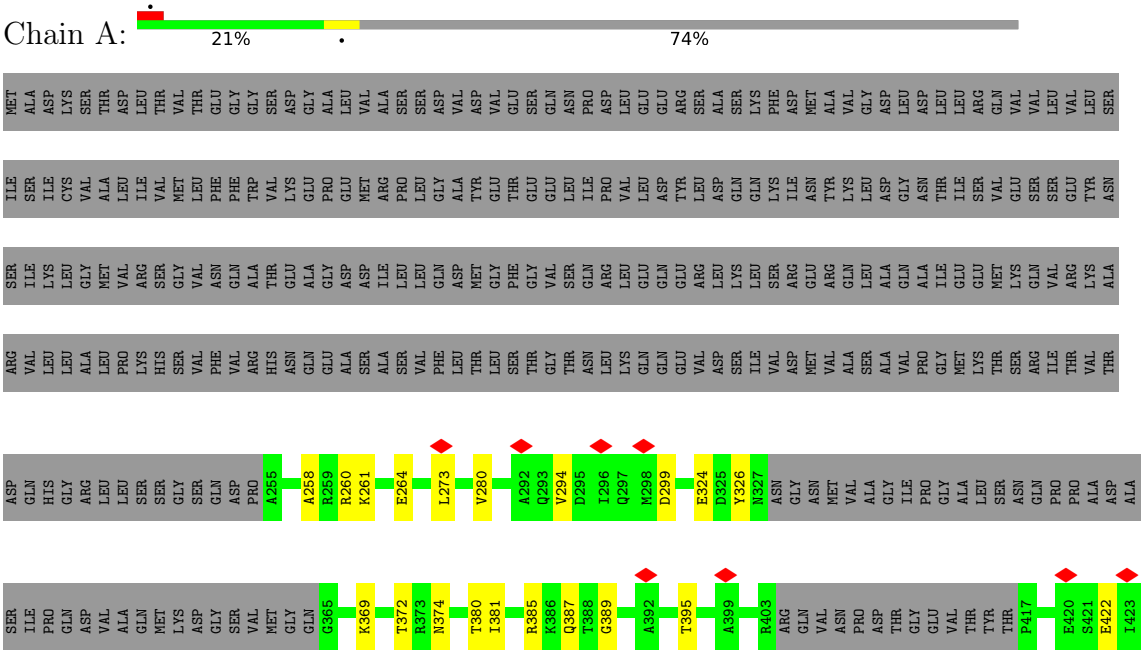
- Molecule 2: Flagellar M-ring protein

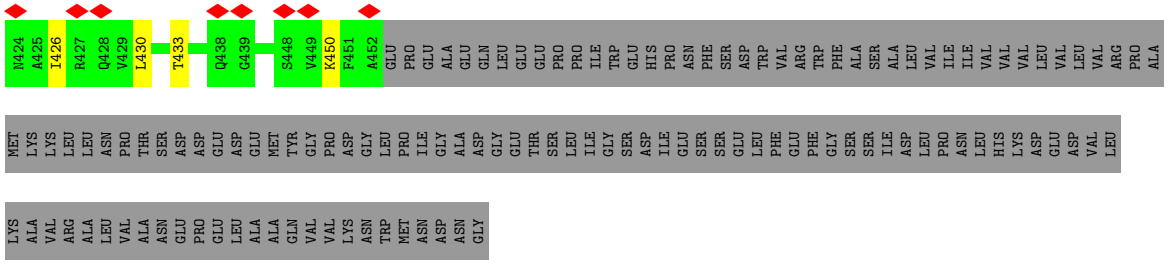
Chain 5:



• Molecule 2: Flagellar M-ring protein

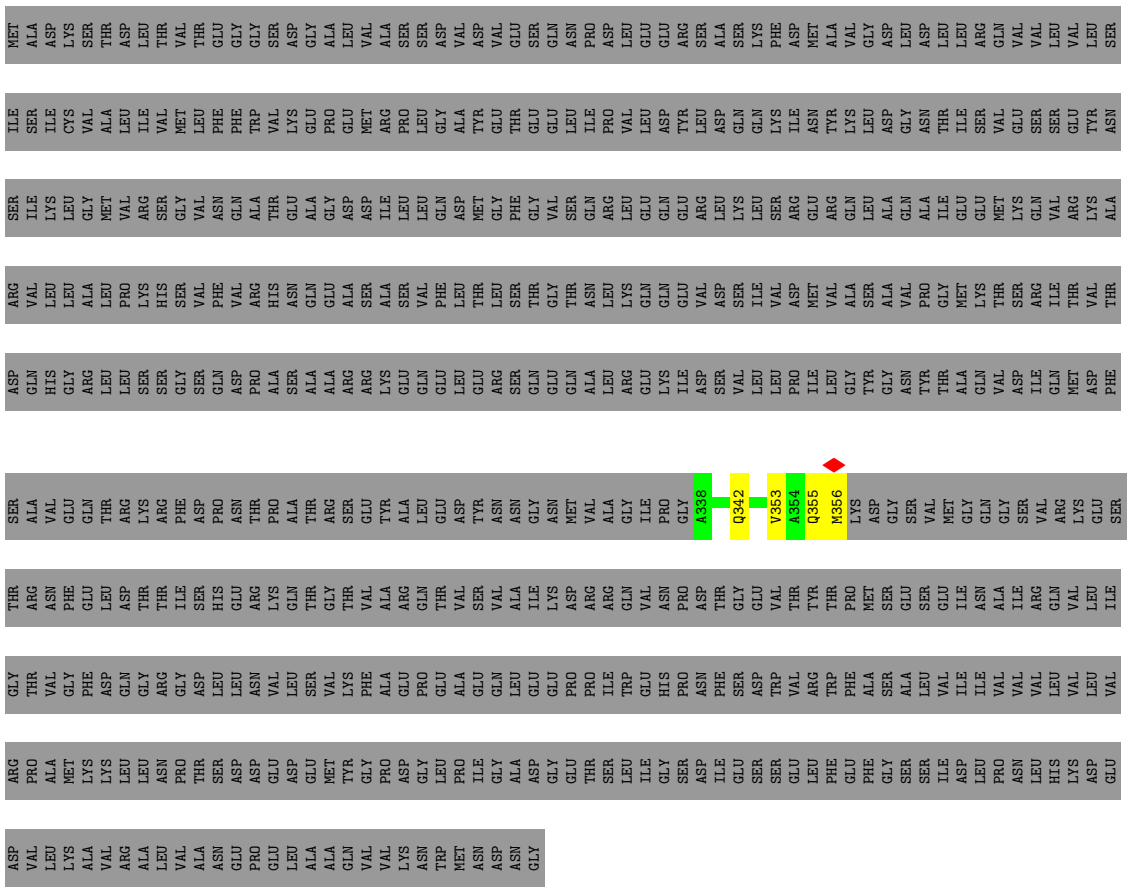
Chain A:





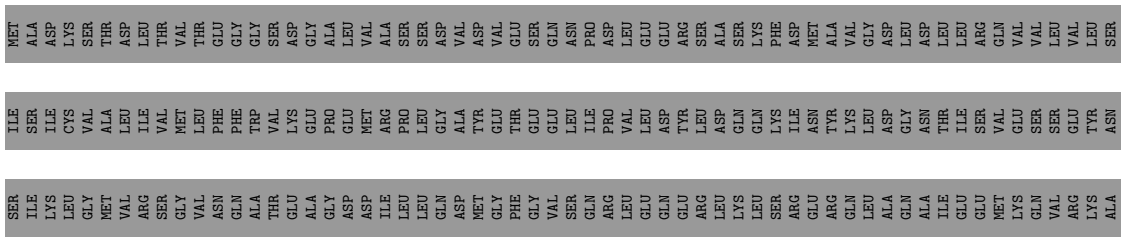
• Molecule 2: Flagellar M-ring protein

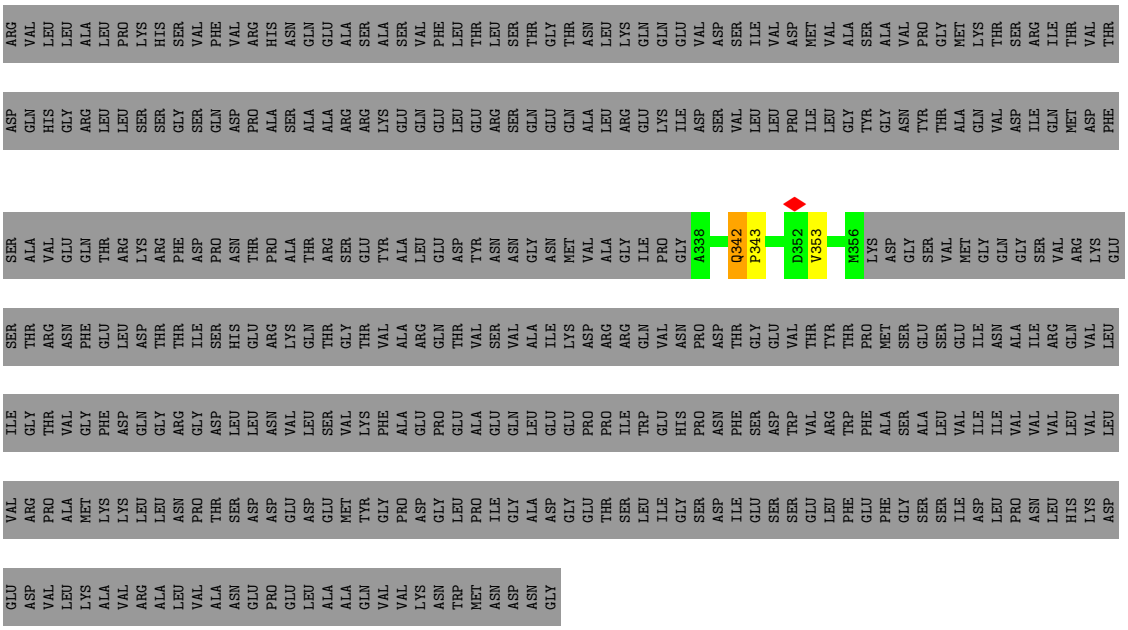
Chain AA: 97%



• Molecule 2: Flagellar M-ring protein

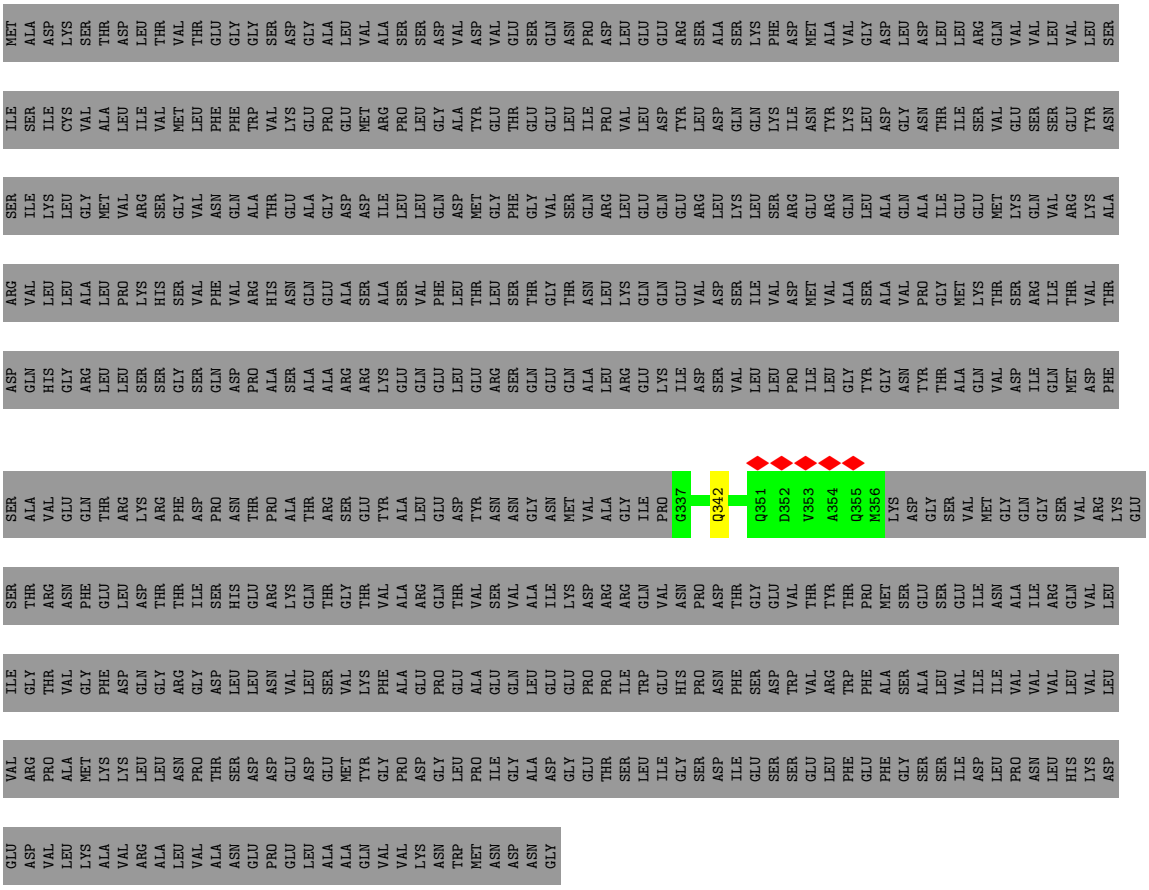
Chain AB: 97%





• Molecule 2: Flagellar M-ring protein

Chain AC: 97%



• Molecule 2: Flagellar M-ring protein

Chain AD: 97%

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

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

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

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

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

SER ALA VAL GLU GLN THR ARG LYS ARG PHE ASP PRO ASN THR PRO ALA THR ARG SER GLU TYR ALA LEU GLU ASP TYR ASN ASN GLY ASN MET VAL ALA GLY ILE PRO GLY A338 N341 D346 A347 S348 I349 P350 Q351 D352 V353 A354 Q355 M356 LYS ASP GLY SER VAL MET GLY GLN

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

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

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

PRO ASN LEU HIS LYS ASP GLU ASP VAL LEU LYS ALA VAL ARG ALA LEU VAL ALA ASN GLU PRO GLU LEU ALA ALA GLN VAL VAL LYS ASN TRP MET ASN ASP ASN GLY

- Molecule 2: Flagellar M-ring protein

Chain AE: 97%

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

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

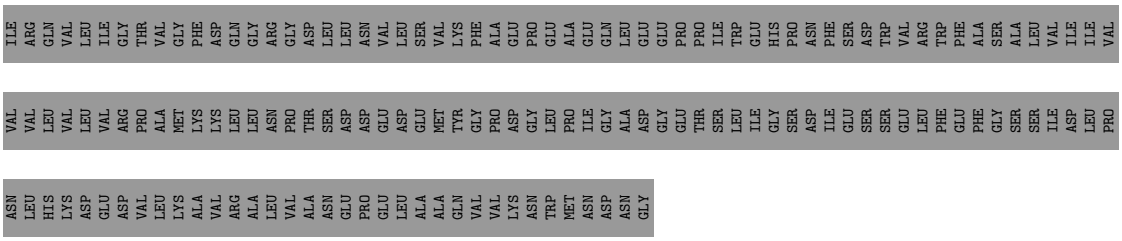
SER ILE LYS LEU GLY MET VAL ARG SER GLY VAL ASN GLN ALA THR GLU ALA GLY ASP ASP ILE LEU LEU GLN ASP MET GLY PHE GLY VAL SER GLN ARG LEU GLU GLU GLN GLU ARG LEU LYS LEU SER ARG GLU ARG GLN LEU ALA GLN ALA ILE GLU GLU GLU MET LYS GLN VAL ARG LYS ALA

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

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

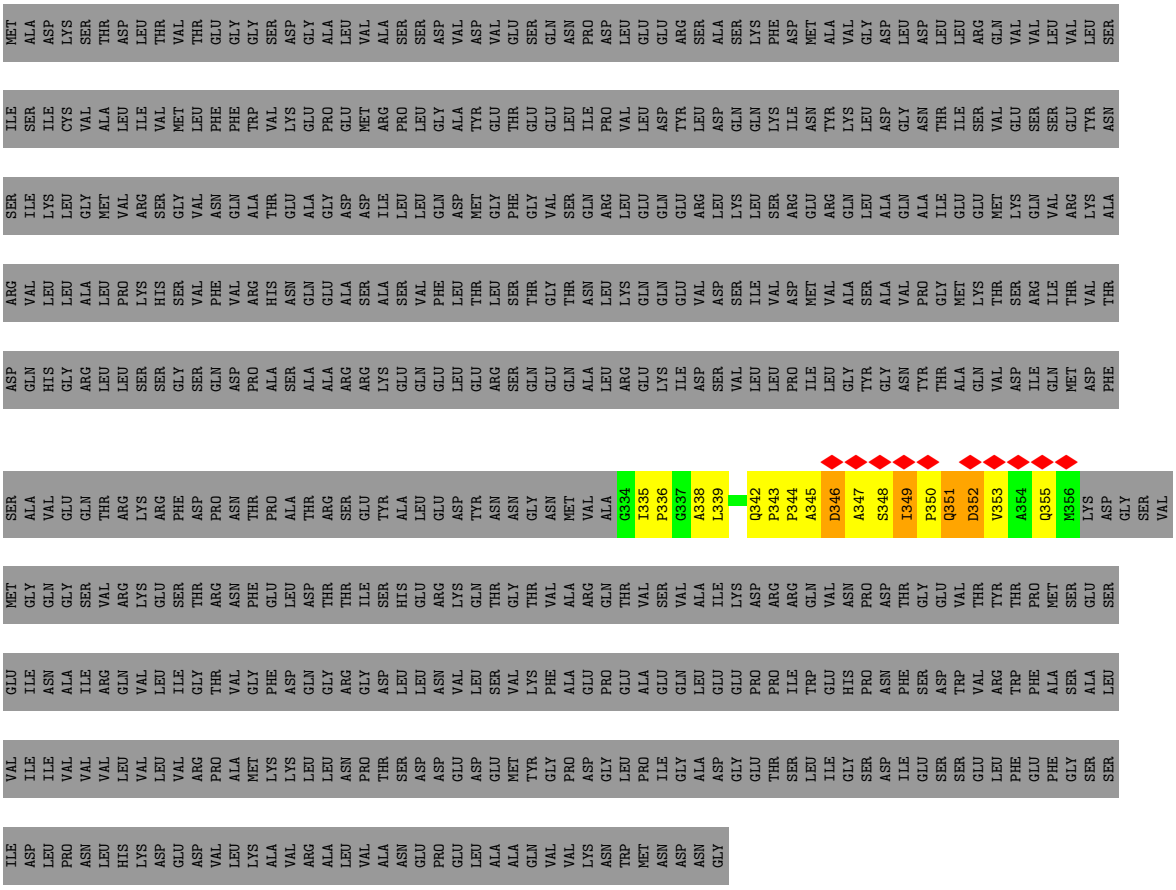
SER ALA VAL GLU GLN THR ARG LYS ARG PHE ASP PRO ASN THR PRO ALA THR ARG SER GLU TYR ALA LEU GLU ASP TYR ASN ASN GLY ASN MET VAL ALA GLY ILE PRO GLY A338 P343 A347 S348 I349 P350 Q351 D352 V353 A354 Q355 M356 LYS ASP GLY SER VAL MET GLY GLN GLY

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



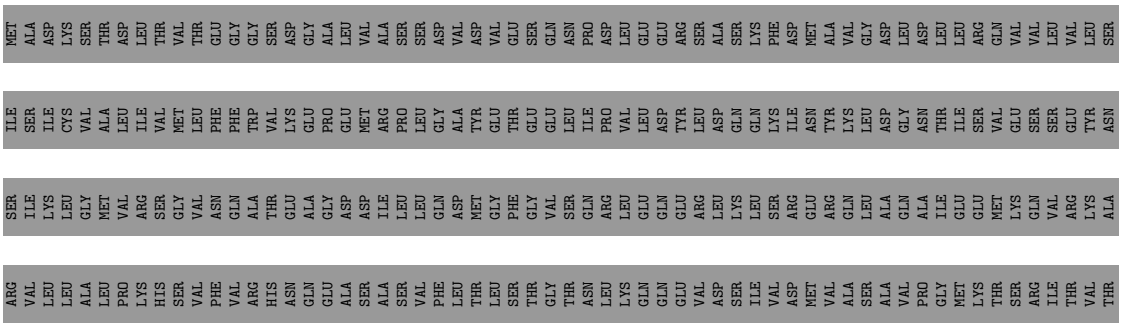
• Molecule 2: Flagellar M-ring protein

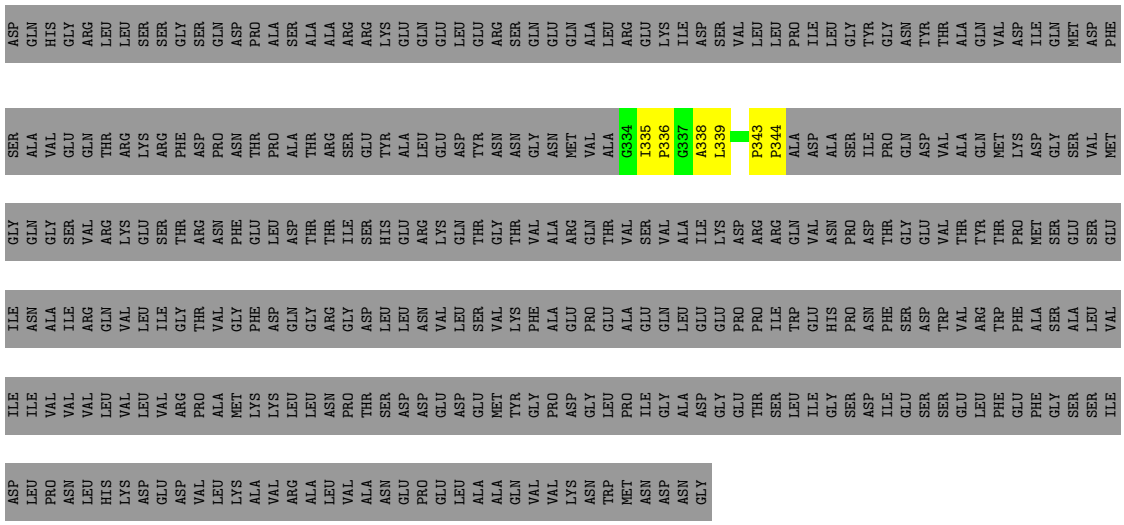
Chain AF: 96%



• Molecule 2: Flagellar M-ring protein

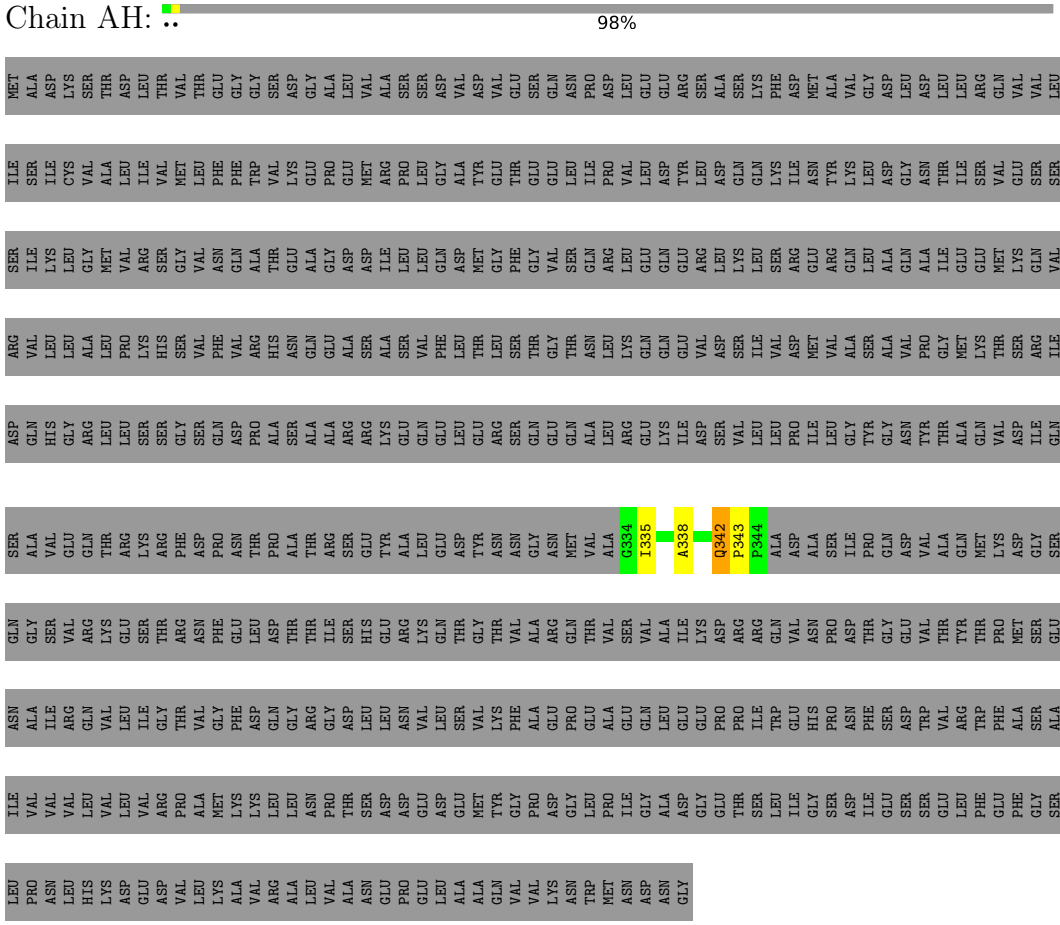
Chain AG: 98%





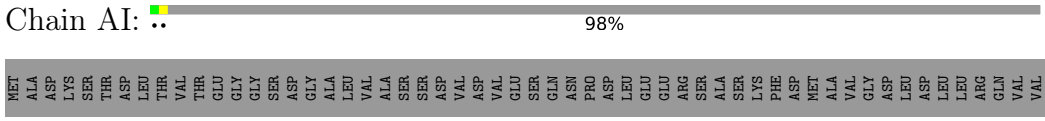
• Molecule 2: Flagellar M-ring protein

Chain AH:



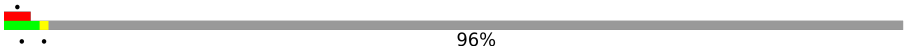
• Molecule 2: Flagellar M-ring protein

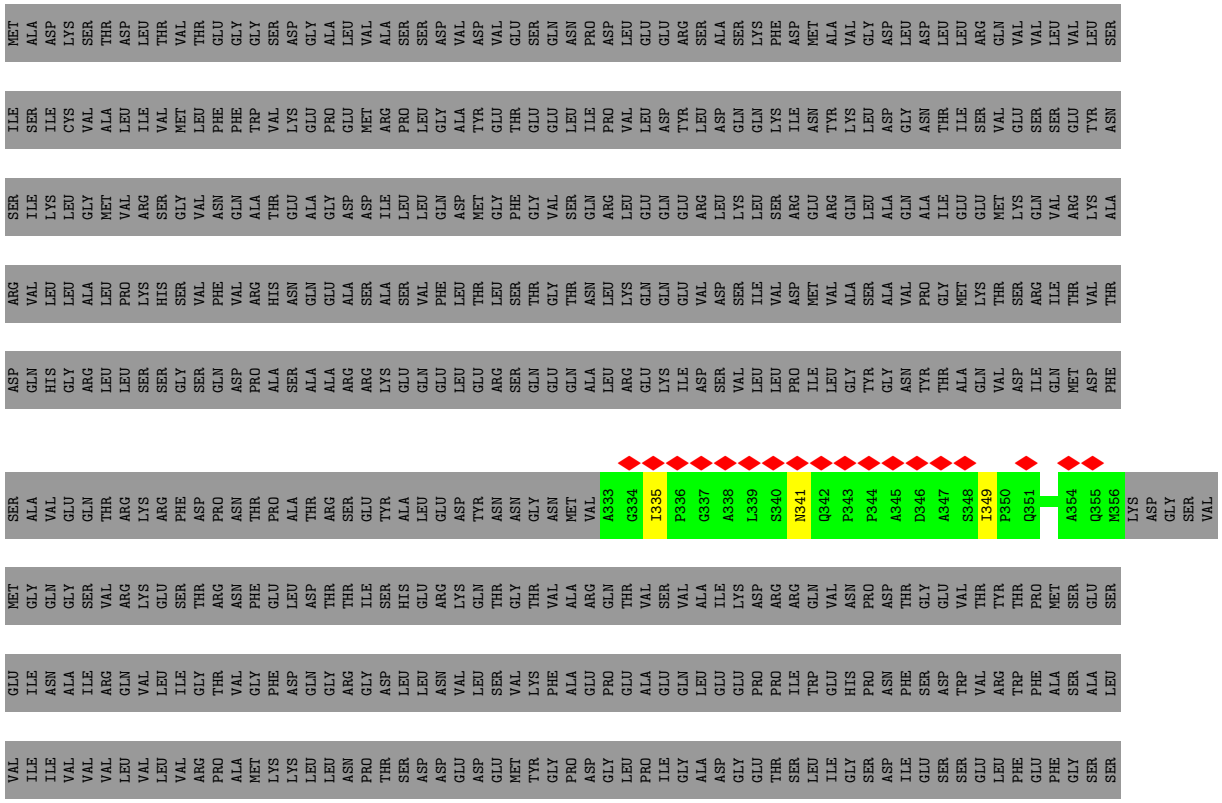
Chain AI:

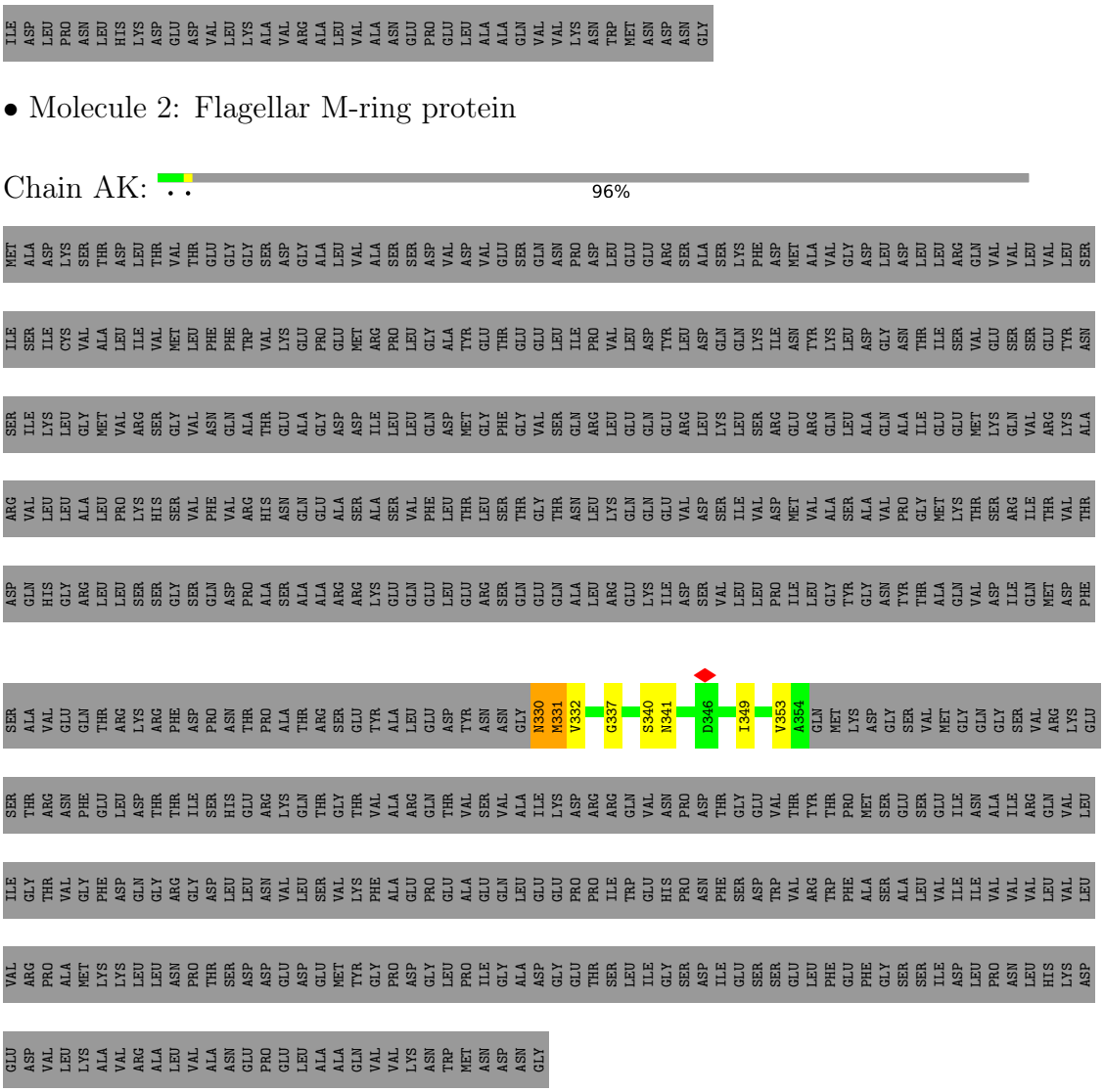


- Molecule 2: Flagellar M-ring protein

Chain AJ:





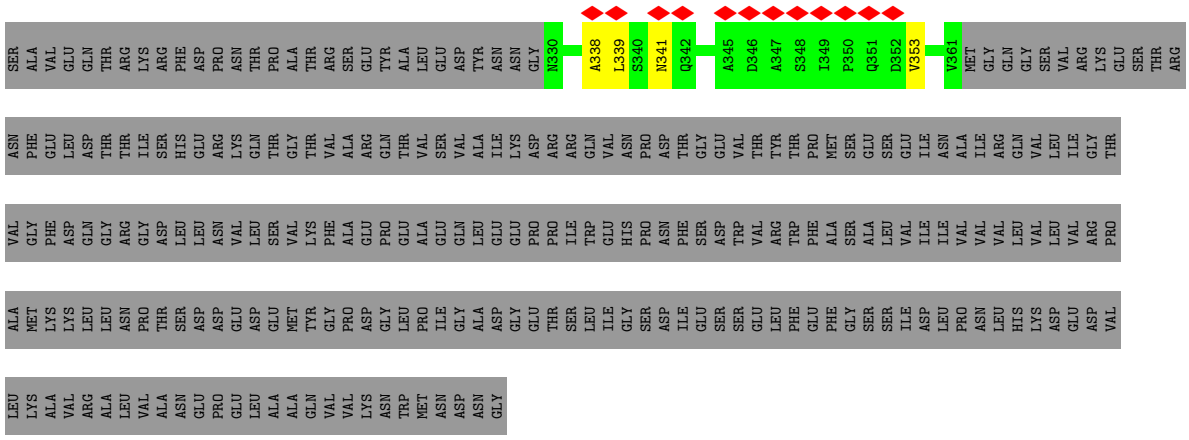


• Molecule 2: Flagellar M-ring protein

Chain AK: 96%

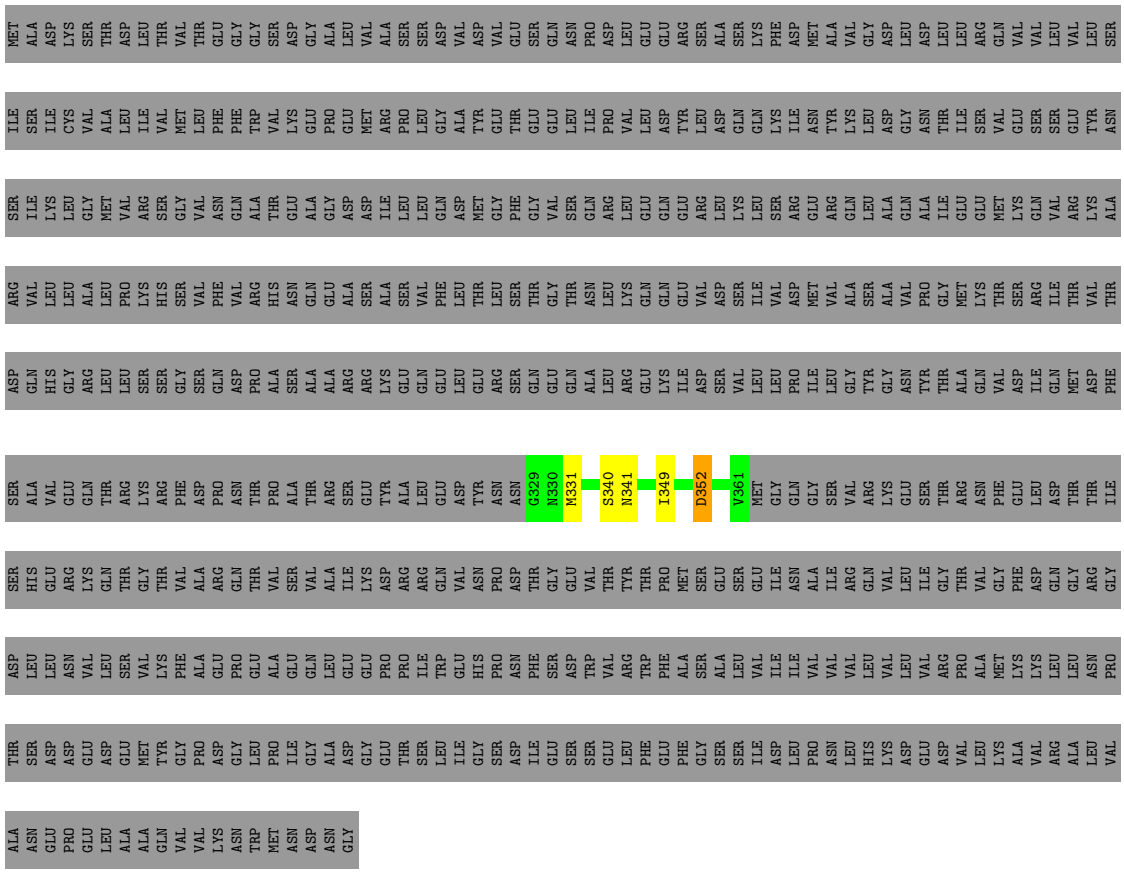
• Molecule 2: Flagellar M-ring protein

Chain AL: 5% 94%



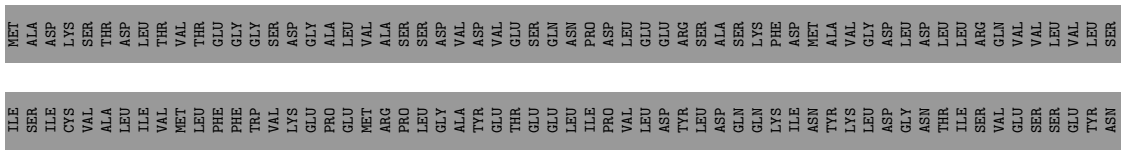
• Molecule 2: Flagellar M-ring protein

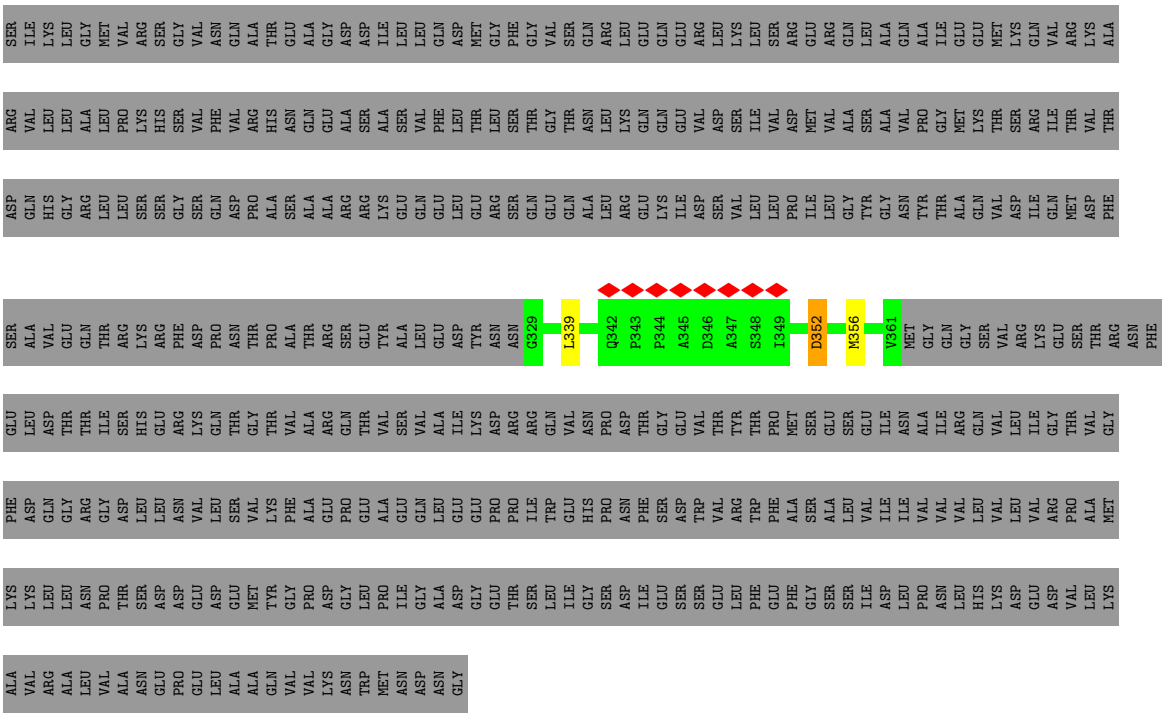
Chain AM: 5% 94%



• Molecule 2: Flagellar M-ring protein

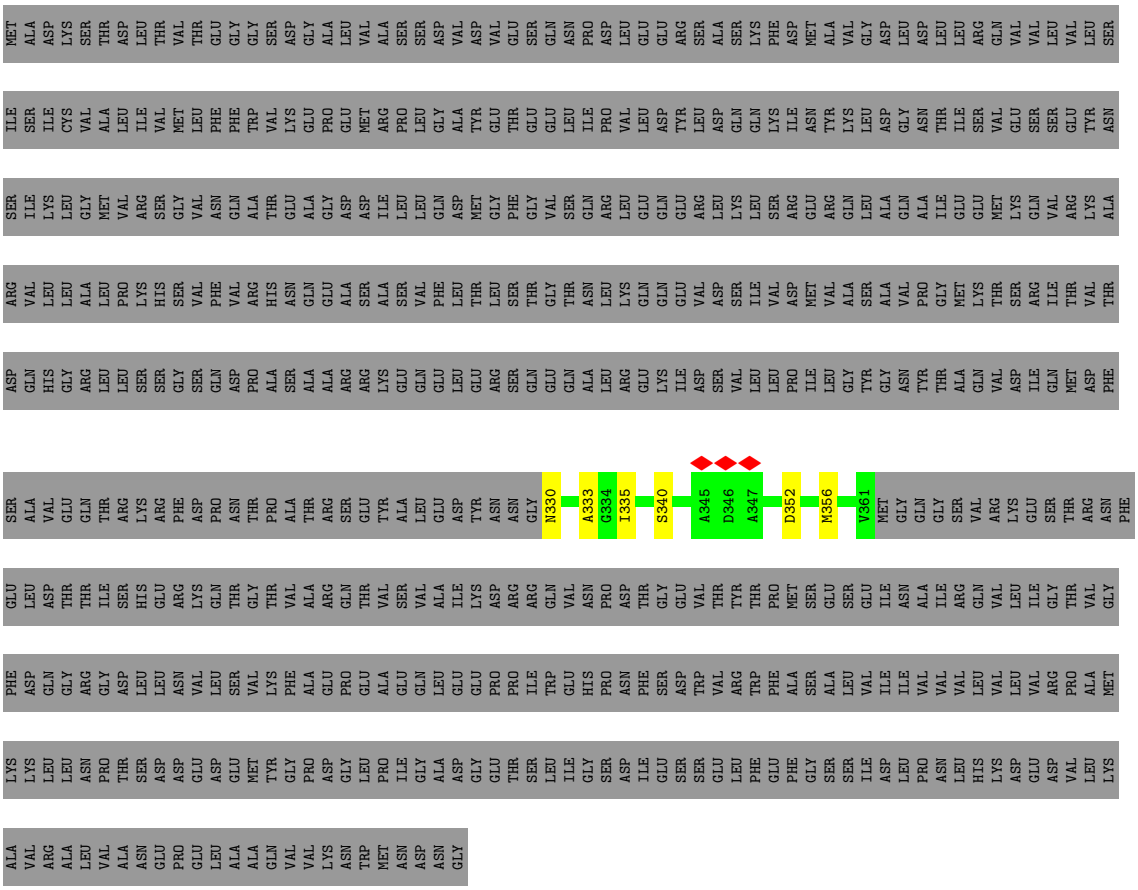
Chain AN: 5% 94%





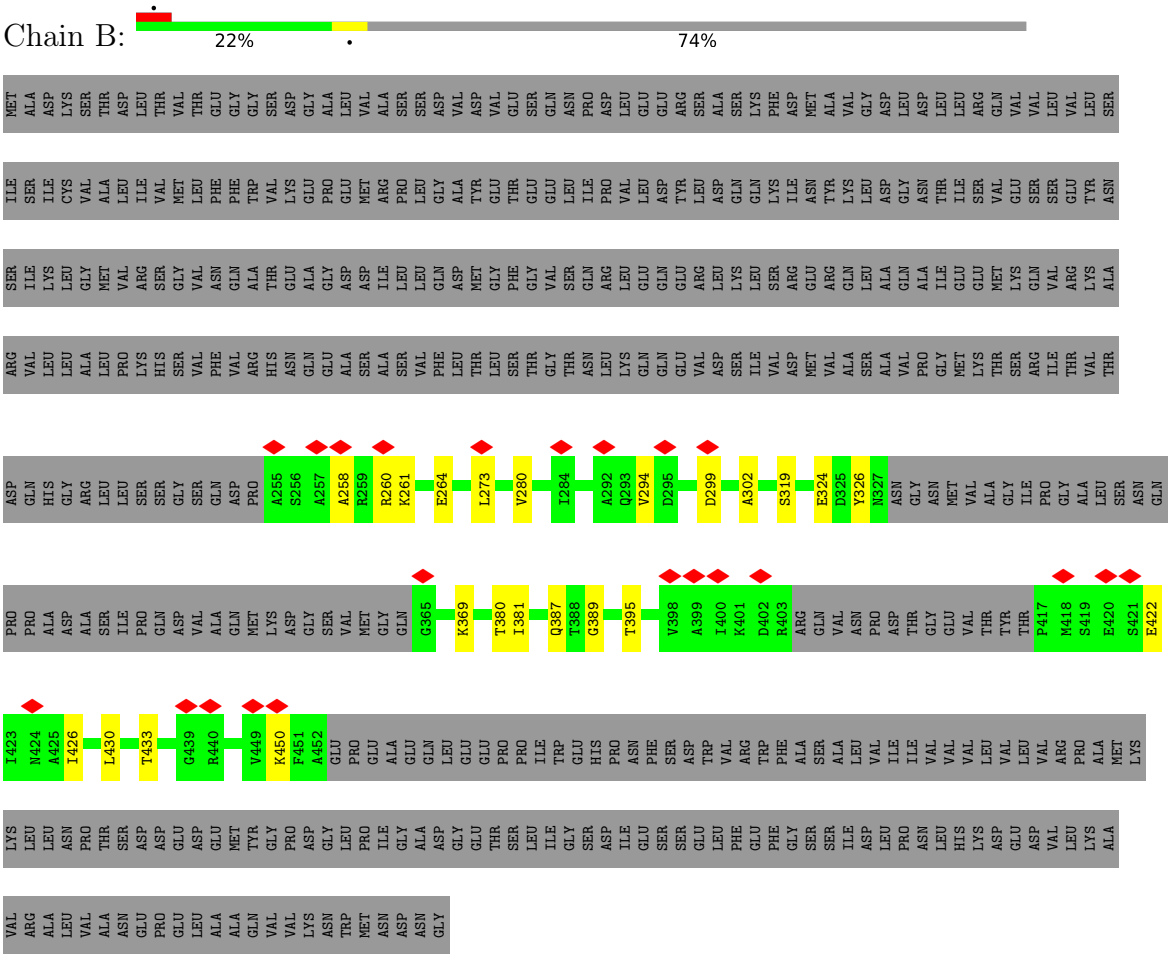
• Molecule 2: Flagellar M-ring protein

Chain AO: 94%



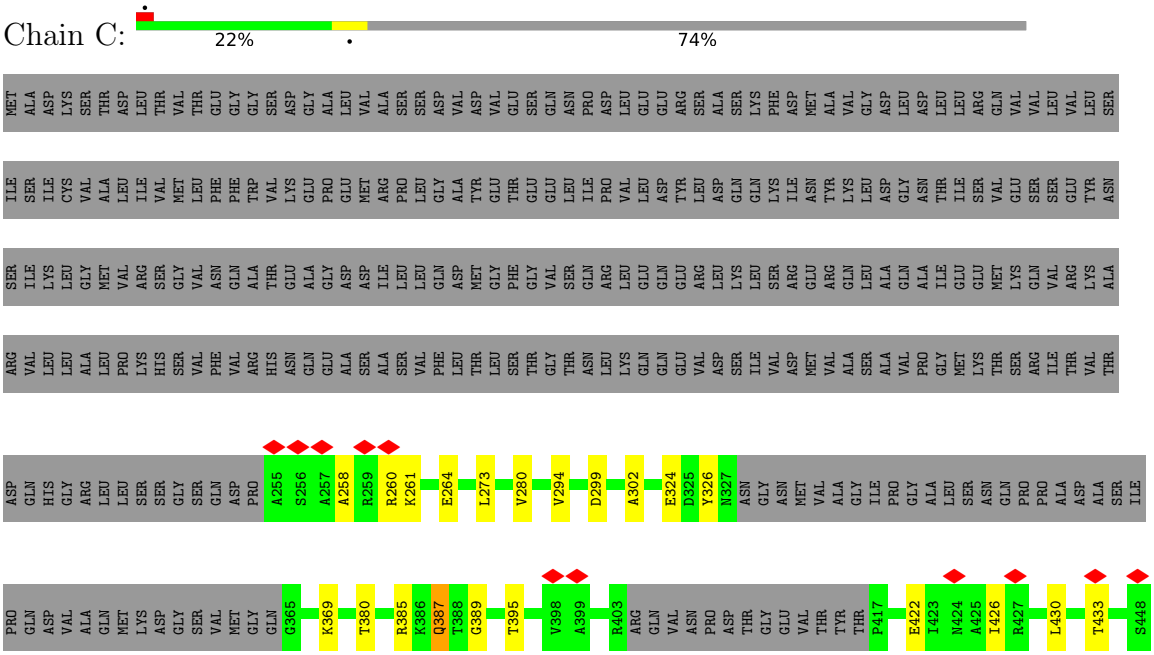
• Molecule 2: Flagellar M-ring protein

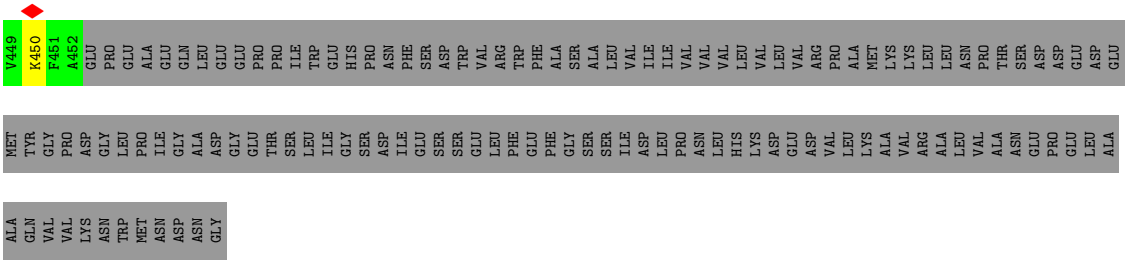
Chain B:



• Molecule 2: Flagellar M-ring protein

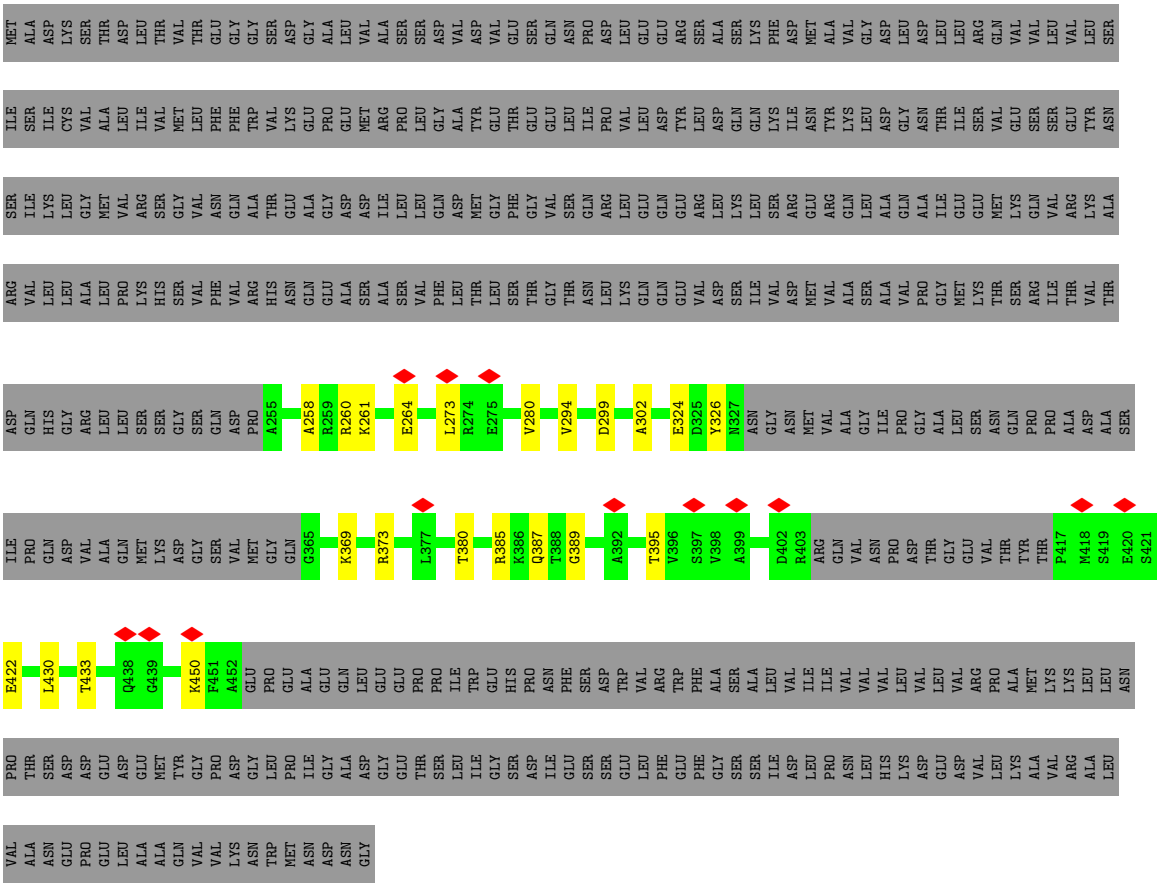
Chain C:





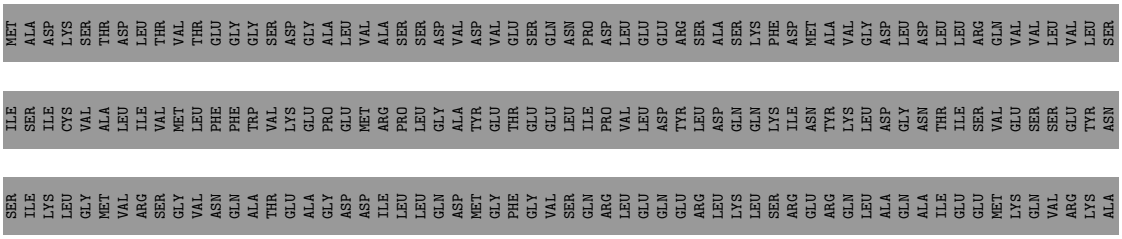
• Molecule 2: Flagellar M-ring protein

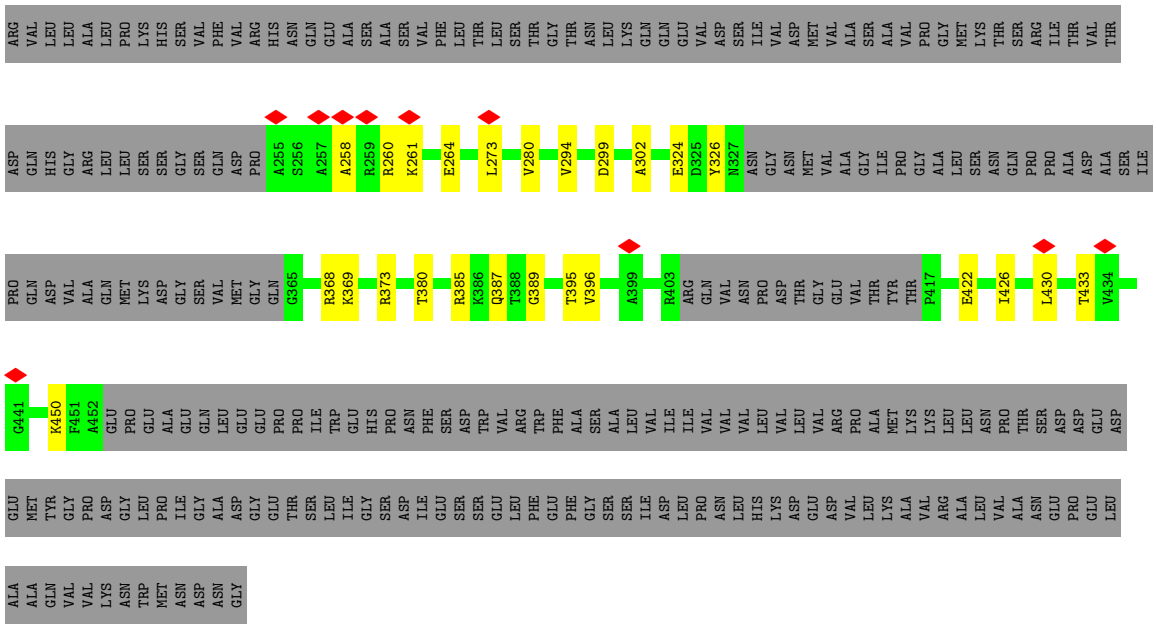
Chain D:



• Molecule 2: Flagellar M-ring protein

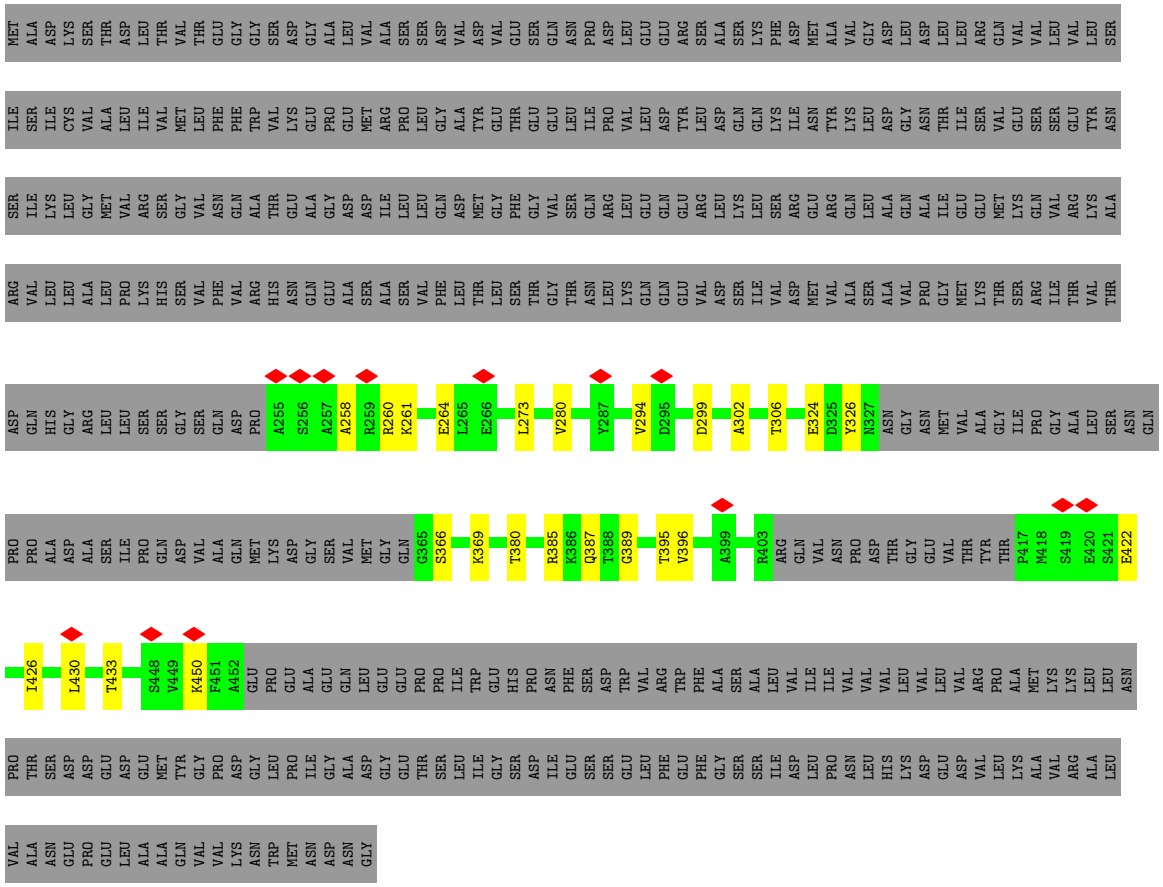
Chain E:





- Molecule 2: Flagellar M-ring protein

Chain F:



- Molecule 2: Flagellar M-ring protein

Chain G: 21% 74%

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

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

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

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

ASP GLN HIS GLY ARG LEU LEU SER SER GLY SER GLN ASP PRO A255 S256 A257 A258 R259 R260 K261 E264 L273 V280 Y287 V294 D295 D299 A302 T306 E324 D325 Y326 N327 ASN GLY ASN MET VAL ALA GLY ILE PRO GLY ALA LEU SER ASN GLN PRO PRO

ALA ASP ALA SER ILE PRO GLN ASP VAL ALA GLN MET LYS ASP GLY SER VAL MET GLY GLN G365 K369 R373 N374 T380 R385 K386 Q387 T388 G389 T395 V396 S397 V398 A399 D402 R403 ARG GLN VAL ASN PRO ASP THR GLY GLU VAL THR TYR THR P417 E422

I426 L430 T433 S448 V449 K450 F451 A452 GLU PRO GLU ALA GLU GLN LEU GLU GLU PRO PRO ILE TRP GLU HIS PRO ASN PHE SER ASP TRP VAL ARG TRP PHE ALA SER ALA LEU VAL ILE ILE VAL VAL VAL LEU VAL LEU VAL ARG PRO ALA MET LYS LYS LEU LEU ASN PRO

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

ALA ASN GLU PRO GLU LEU ALA ALA GLN VAL VAL LYS ASN TRP MET ASN ASP ASN GLY

- Molecule 2: Flagellar M-ring protein

Chain H: 21% 74%

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

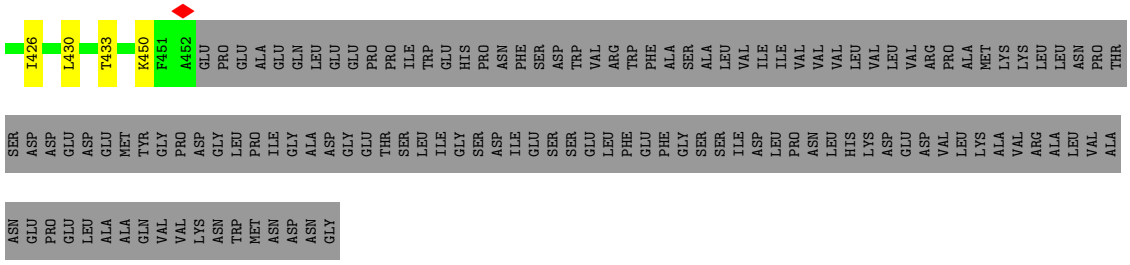
ILE SER ILE CYS VAL ALA LEU ILE VAL MET MET LEU PHE PHE TRP VAL LYS GLU PRO GLU MET ARG PRO LEU GLY ALA TYR GLU THR GLU GLU LEU ILE PRO VAL LEU ASP TYR LEU ASP GLN GLN LYS ILE ASN TYR LYS LEU ASP GLY ASN THR ILE SER VAL GLU SER SER GLU TYR ASN

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

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

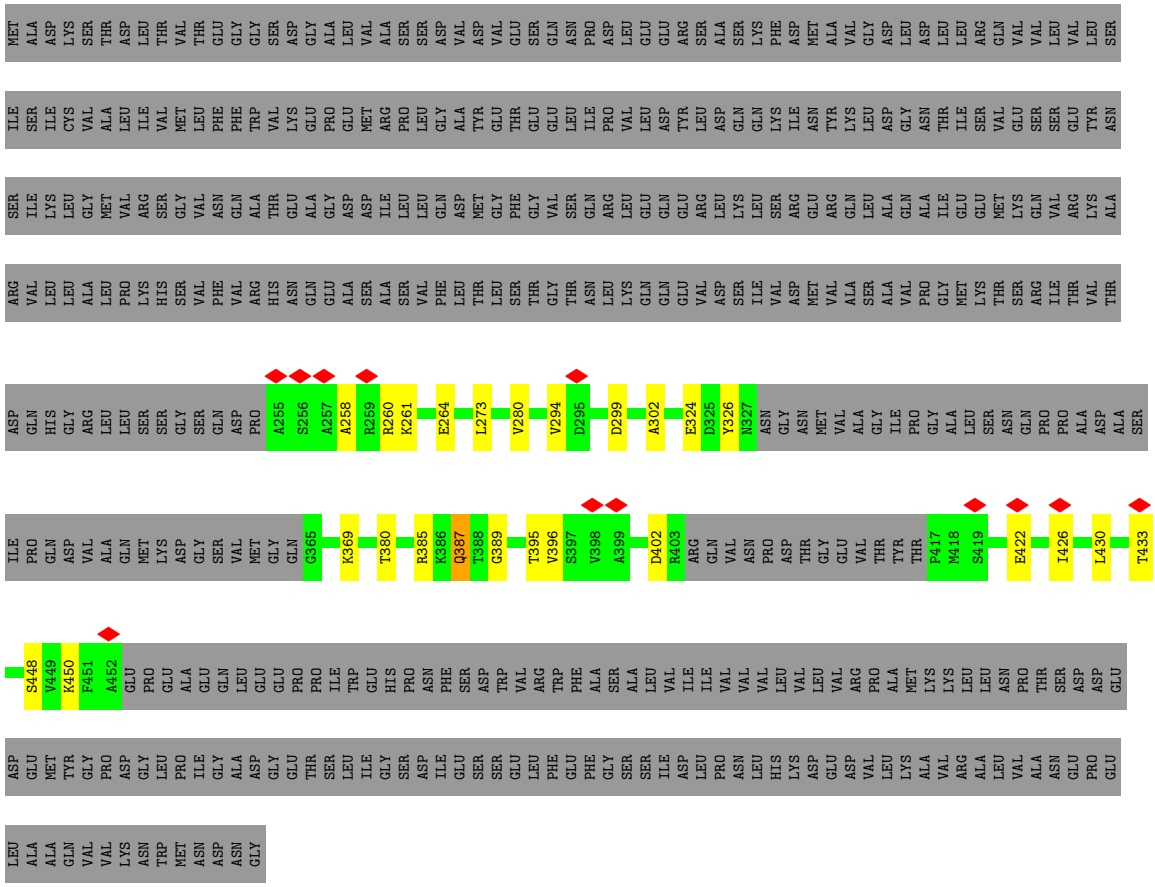
ASP GLN HIS GLY ARG LEU LEU SER SER GLY SER GLN ASP PRO A255 S256 A257 A258 R259 R260 K261 E264 L273 V280 Y287 V294 D295 I296 D299 A302 R318 S319 E324 D325 Y326 N327 ASN GLY ASN MET VAL ALA GLY ILE PRO GLY ALA LEU SER ASN GLN

PRO PRO ALA ASP ALA SER ILE PRO GLN ASP VAL ALA GLN MET LYS ASP GLY SER VAL MET MET GLY GLN G365 K369 T372 R373 N374 T380 R385 K386 Q387 T388 G389 A392 R393 Q394 T395 R403 ARG GLN VAL ASN PRO ASP THR GLY GLU VAL THR TYR THR P417 E422



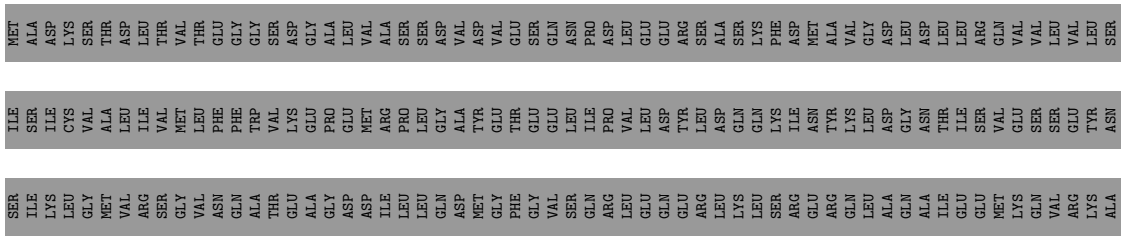
• Molecule 2: Flagellar M-ring protein

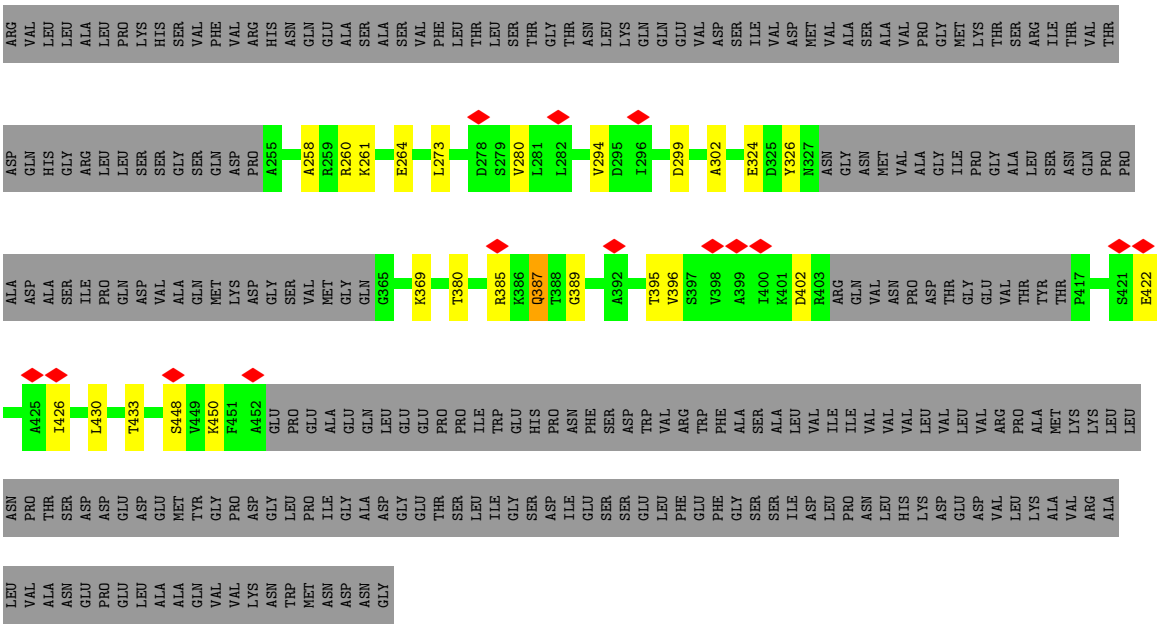
Chain I:



• Molecule 2: Flagellar M-ring protein

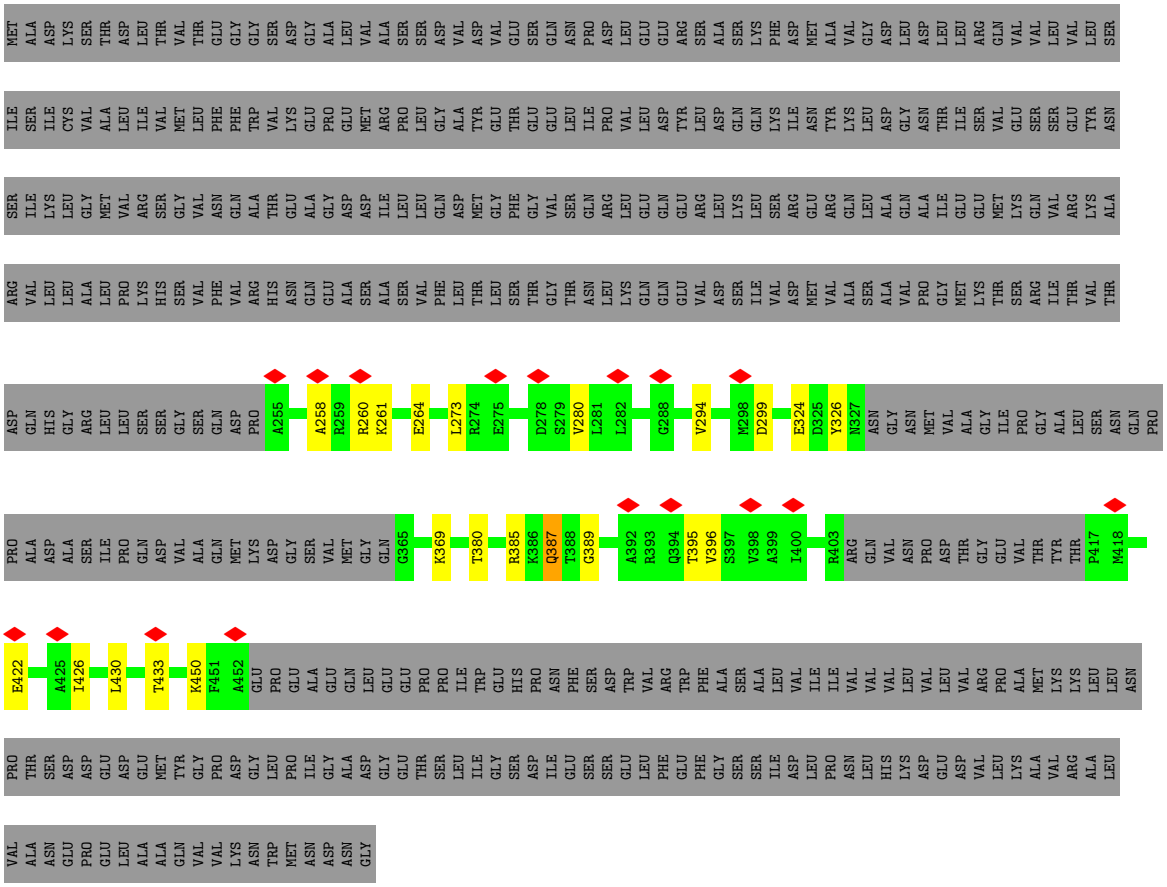
Chain J:





- Molecule 2: Flagellar M-ring protein

Chain K:



- Molecule 2: Flagellar M-ring protein

Chain L: 22% 74%

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

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

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

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

ASP GLN HIS GLY ARG LEU LEU SER SER GLY SER GLN ASP PRO A255 S256 A257 A258 R259 R260 K261 E264 L273 R274 E275 S279 V280 L281 L282 V294 D295 I296 Q297 M298 D299 A302 E324 D325 Y326 N327 ASN GLY ASN MET VAL ALA GLY ILE PRO GLY ALA LEU SER ASN

GLN PRO PRO ALA ASP ALA SER ILE PRO GLN ASP VAL ALA GLN MET LYS ASP GLY SER VAL MET GLY GLN G365 K369 T380 Q387 T388 G389 T395 V398 A399 I400 K401 D402 R403 ARG GLN VAL ASN PRO ASP THR GLY GLU VAL THR TYR THR P417 M418 E422 A425

I426 L430 T433 R440 G441 D442 L443 S448 A452 GLU PRO GLU ALA GLU GLN LEU GLU GLU PRO PRO ILE TRP GLU HIS PRO ASN PHE SER ASP TRP VAL ARG TRP PHE ALA SER ALA LEU VAL ILE ILE VAL VAL VAL LEU VAL LEU VAL ARG PRO ALA MET LYS LYS LEU

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

ALA LEU VAL ALA ASN GLU PRO GLU LEU ALA ALA GLN VAL VAL LYS ASN TRP MET ASN ASP ASN GLY

- Molecule 2: Flagellar M-ring protein

Chain M: 21% 74%

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

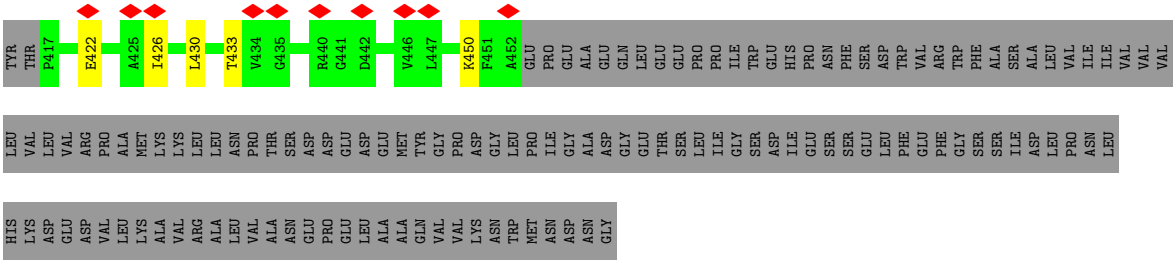
ILE SER ILE CYS VAL ALA LEU ILE VAL MET MET LEU PHE PHE TRP VAL LYS GLU PRO GLU MET ARG PRO LEU GLY ALA TYR GLU THR GLU GLU LEU ILE PRO VAL LEU ASP TYR LEU ASP GLN GLN LYS ILE ASN TYR LYS LEU ASP GLY ASN THR ILE SER VAL GLU SER SER GLU TYR ASN

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

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

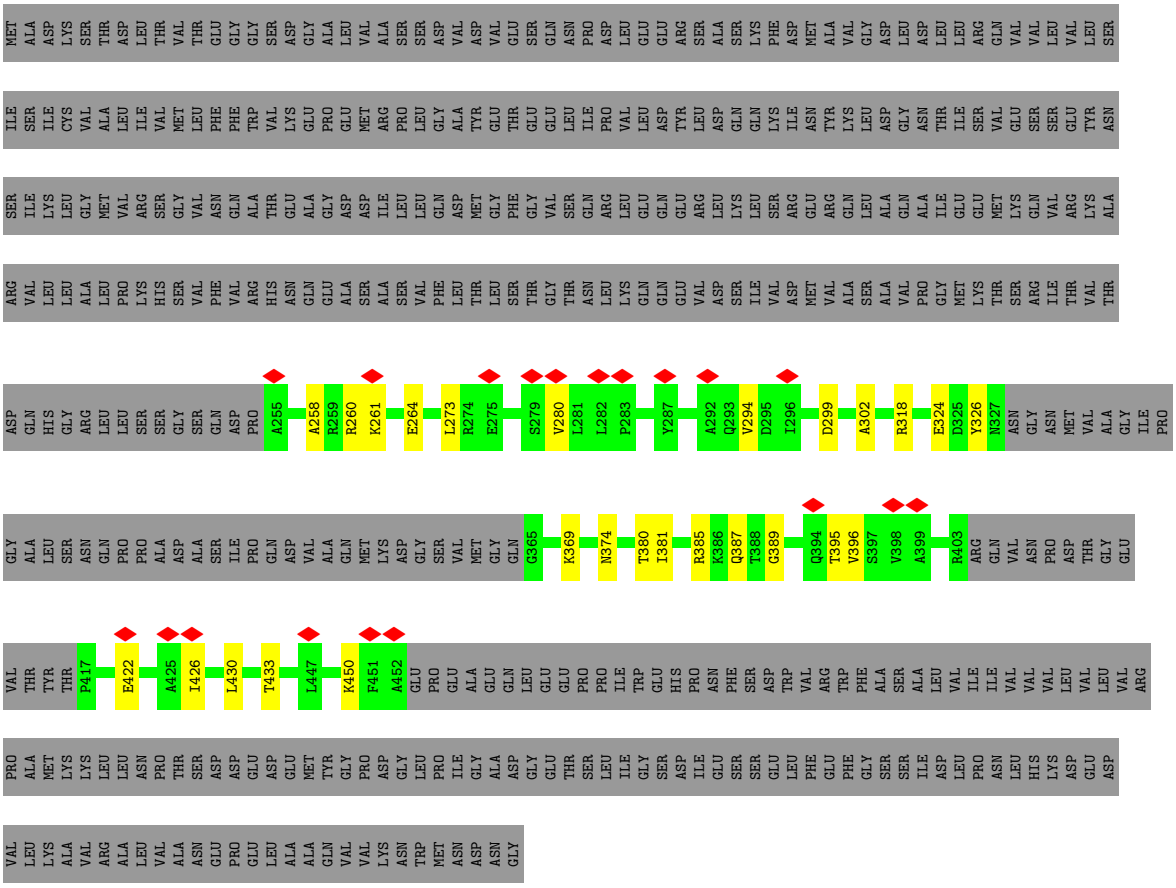
ASP GLN HIS GLY ARG LEU LEU SER SER GLY SER GLN ASP PRO A255 A258 R259 R260 K261 E262 Q263 E264 L273 R274 E275 S279 V280 L281 L282 P283 A292 Q293 V294 D295 I296 Q297 M298 D299 A302 E324 D325 Y326 N327 ASN GLY ASN MET VAL ALA GLY ILE PRO GLY ALA

LEU SER ASN GLN PRO PRO ALA ASP ALA SER ILE PRO GLN ASP VAL ALA GLN MET LYS ASP GLY SER VAL MET GLY GLN G365 K369 T380 R385 K386 Q387 T388 G389 A392 T395 V396 S397 V398 A399 I400 K401 D402 R403 ARG GLN VAL ASN PRO ASP THR GLY GLU VAL THR



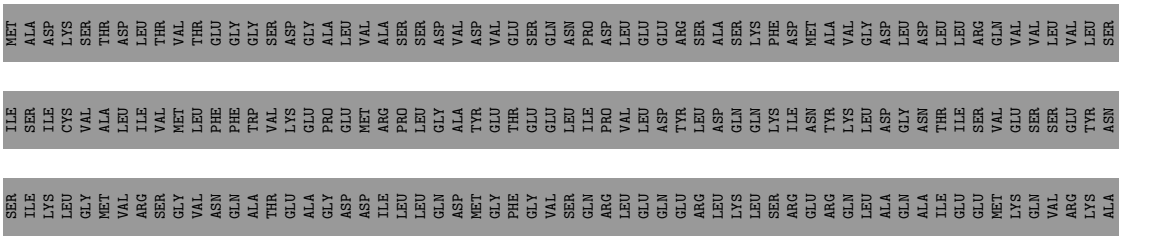
• Molecule 2: Flagellar M-ring protein

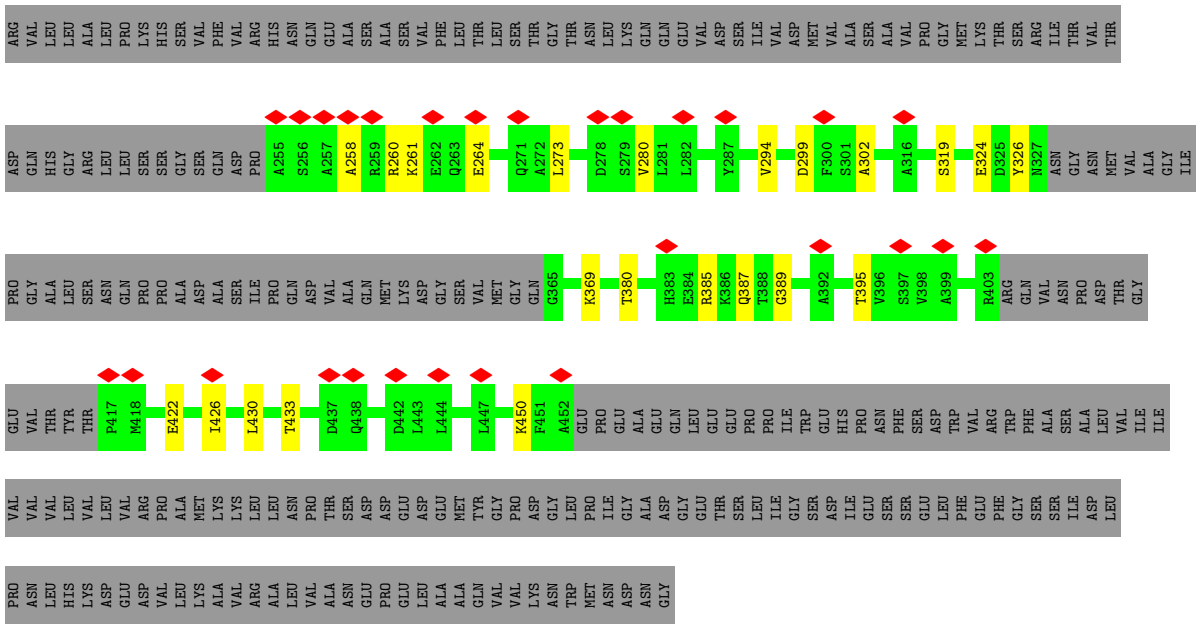
Chain N:



• Molecule 2: Flagellar M-ring protein

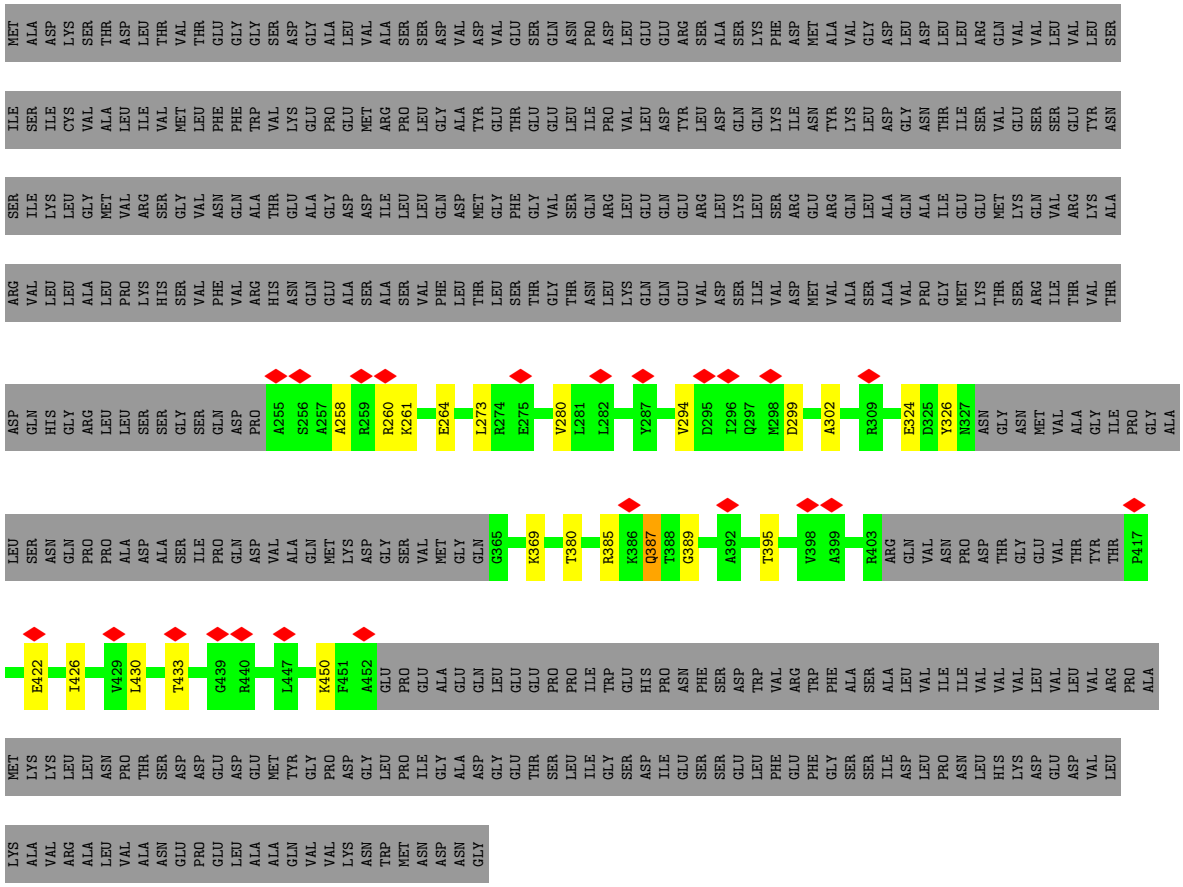
Chain O:





- Molecule 2: Flagellar M-ring protein

Chain P: 22% 74%



- Molecule 2: Flagellar M-ring protein

Chain Q: 21% 74%

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

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

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

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

ASP GLN HIS GLY ARG LEU LEU SER SER GLY SER GLN ASP PRO A255 A258 R259 R260 K261 E264 A272 L273 V280 L281 L282 A292 Q293 V294 D295 D299 A302 N313 E324 D325 Y326 N327 ASN GLY ASN MET VAL ALA GLY ILE PRO GLY ALA LEU SER ASN GLN

PRO PRO ALA ASP ALA SER ILE PRO GLN ASP VAL ALA GLN MET LYS ASP GLY SER VAL MET GLY GLN G365 S366 K369 T380 R385 K386 Q387 T388 G389 A392 T395 V398 A399 R403 ARG GLN VAL ASN PRO ASP THR GLY GLU VAL THR TYR THR P417 E422

I426 L430 T433 D437 Q438 G439 R440 L447 S448 V449 K450 F451 A452 GLU PRO GLU ALA GLU GLN LEU GLU GLU PRO PRO ILE TRP GLU HIS PRO ASN PHE SER ASP TRP VAL ARG TRP PHE ALA SER ALA LEU VAL ILE ILE VAL VAL VAL LEU VAL LEU VAL ARG PRO ALA MET

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

ALA VAL ARG ALA LEU VAL ALA ASN GLU PRO GLU LEU ALA ALA GLN VAL VAL LYS ASN TRP MET ASN ASP ASN GLY

- Molecule 2: Flagellar M-ring protein

Chain R: 22% 74%

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

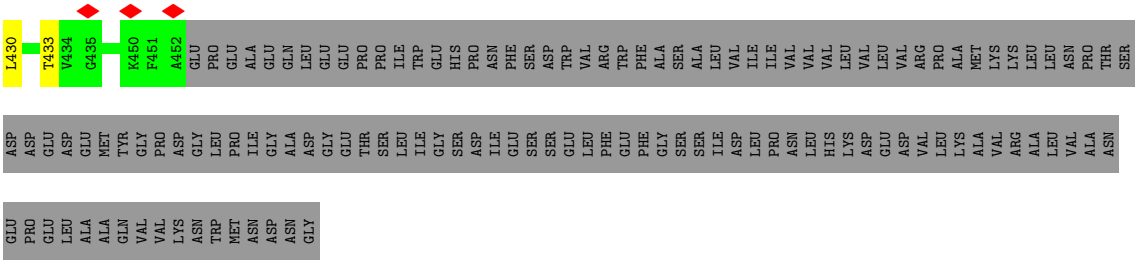
ILE SER ILE CYS VAL ALA LEU ILE VAL MET LEU PHE PHE TRP VAL LYS GLU PRO GLU MET ARG PRO LEU GLY ALA TYR GLU THR GLU GLU LEU ILE PRO VAL LEU ASP TYR LEU ASP GLN GLN LYS ILE ASN TYR LYS LEU ASP GLY ASN THR ILE SER VAL GLU SER SER GLU TYR ASN

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

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

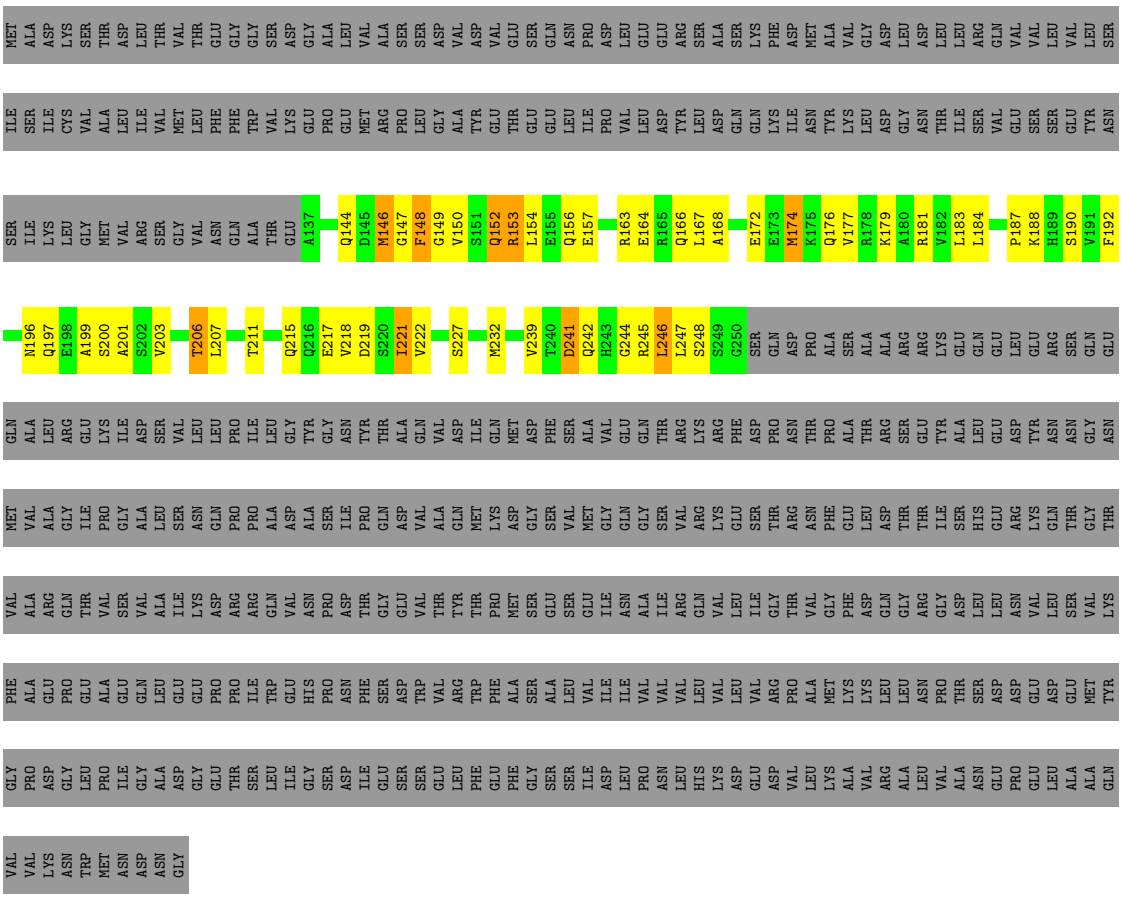
ASP GLN HIS GLY ARG LEU LEU SER SER GLY SER GLN ASP PRO A255 S256 A257 A258 R259 R260 K261 E262 Q263 E264 L273 V280 L281 L282 Y287 V294 D295 D299 A302 E324 D325 Y326 N327 ASN GLY ASN MET VAL ALA GLY ILE PRO GLY ALA LEU SER ASN GLN PRO

PRO ALA ASP ALA SER ILE PRO GLN ASP VAL ALA GLN MET LYS ASP GLY SER VAL MET GLY GLN G365 R368 K369 T380 R385 K386 Q387 T388 G389 T395 V398 A399 R403 ARG GLN VAL ASN PRO ASP THR GLY GLU VAL THR TYR THR P417 M418 E422 I426



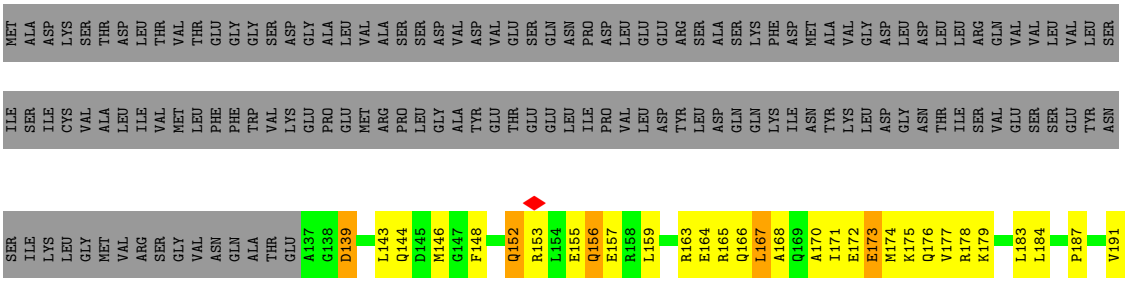
• Molecule 2: Flagellar M-ring protein

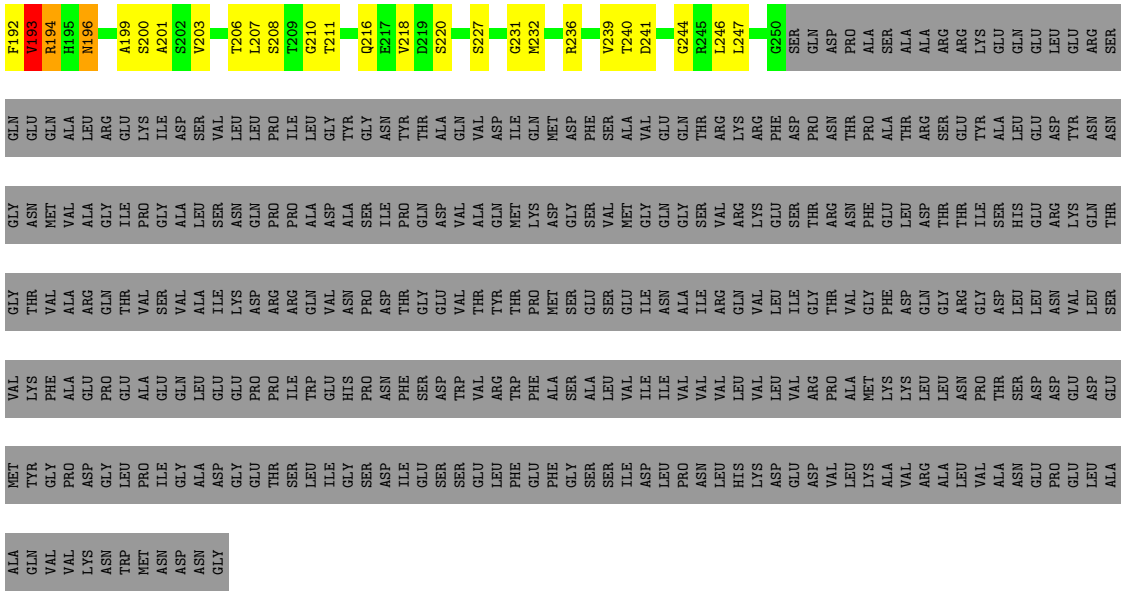
Chain S: 11% 8% • 80%



• Molecule 2: Flagellar M-ring protein

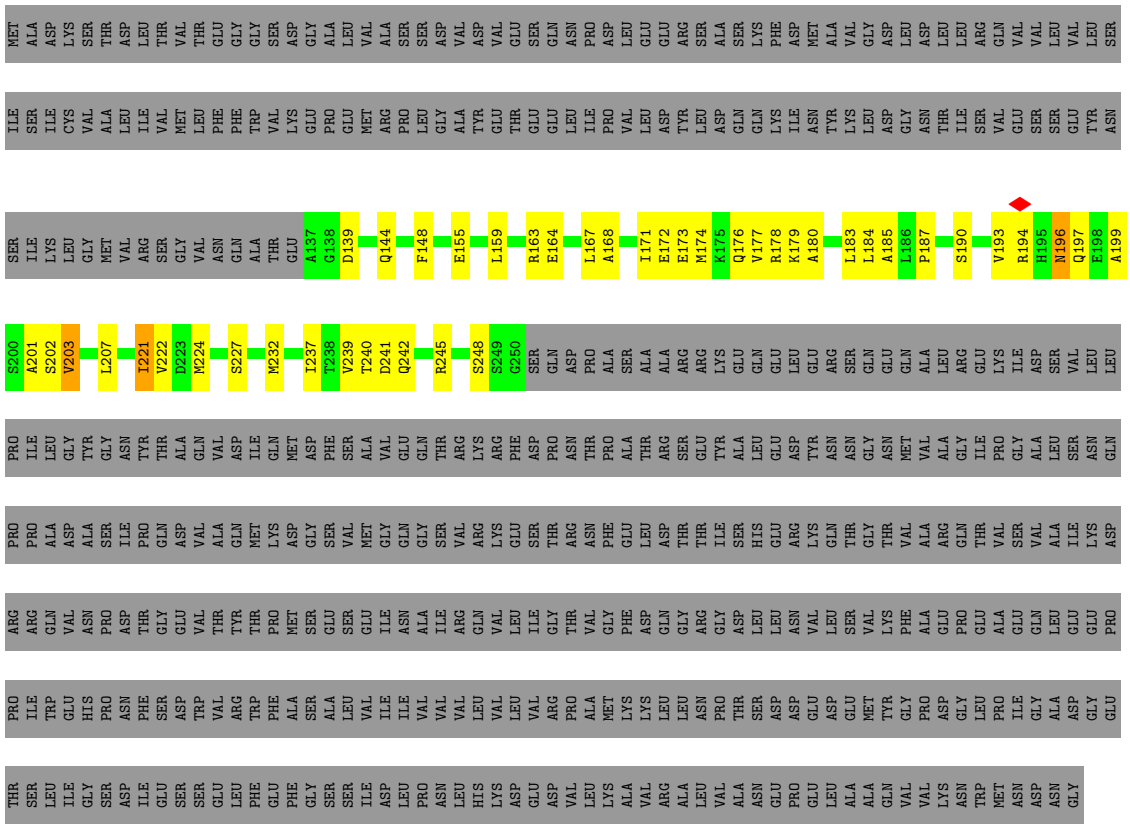
Chain T: 10% 8% • 80%





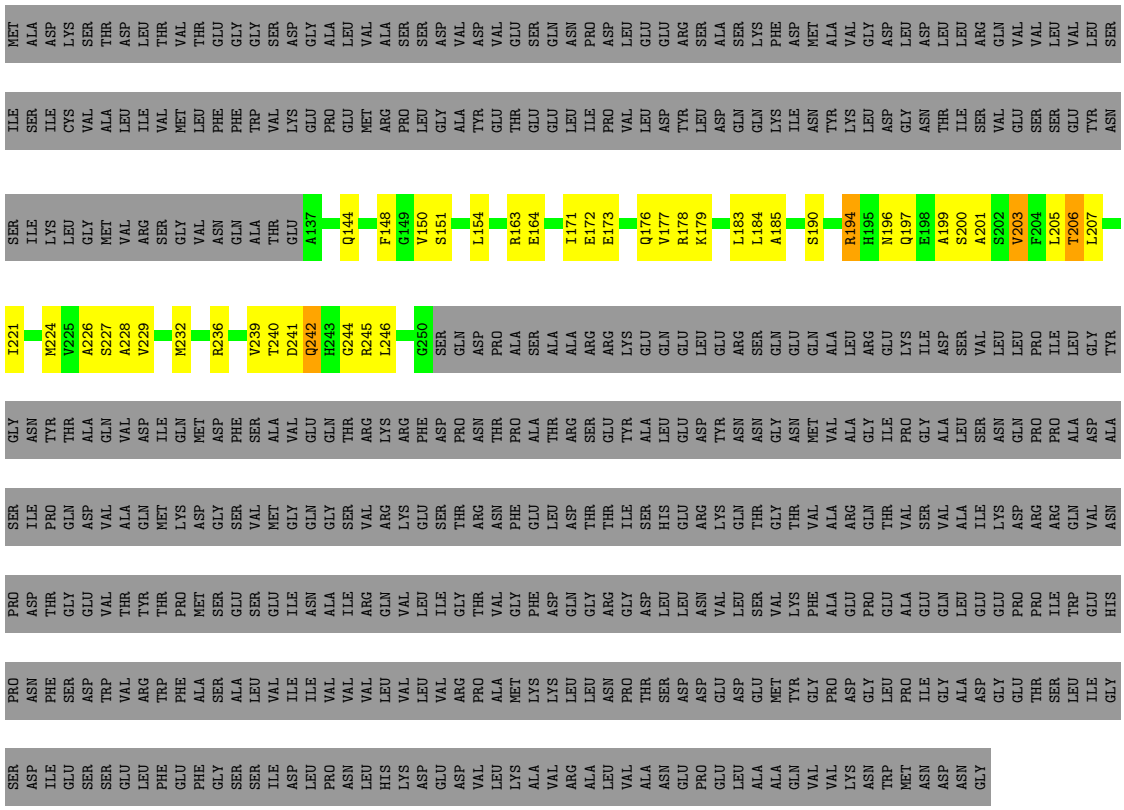
• Molecule 2: Flagellar M-ring protein

Chain U: 12% 7% • 80%



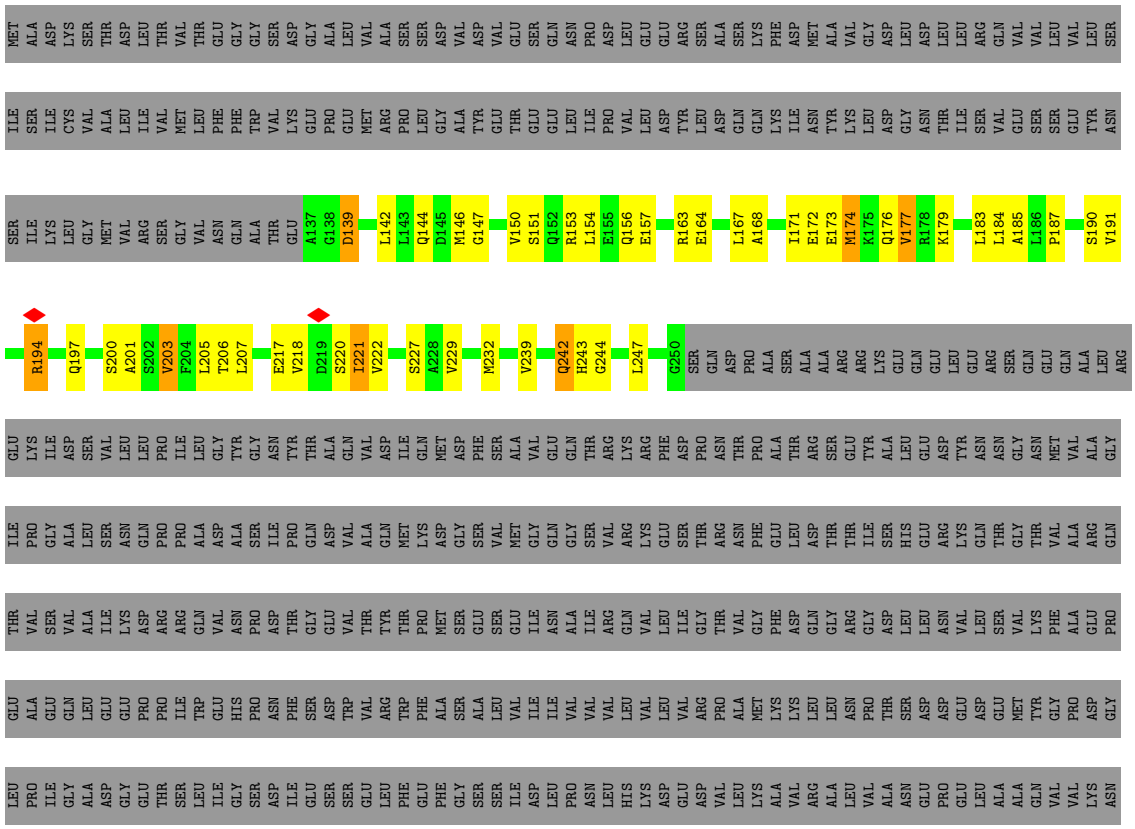
• Molecule 2: Flagellar M-ring protein

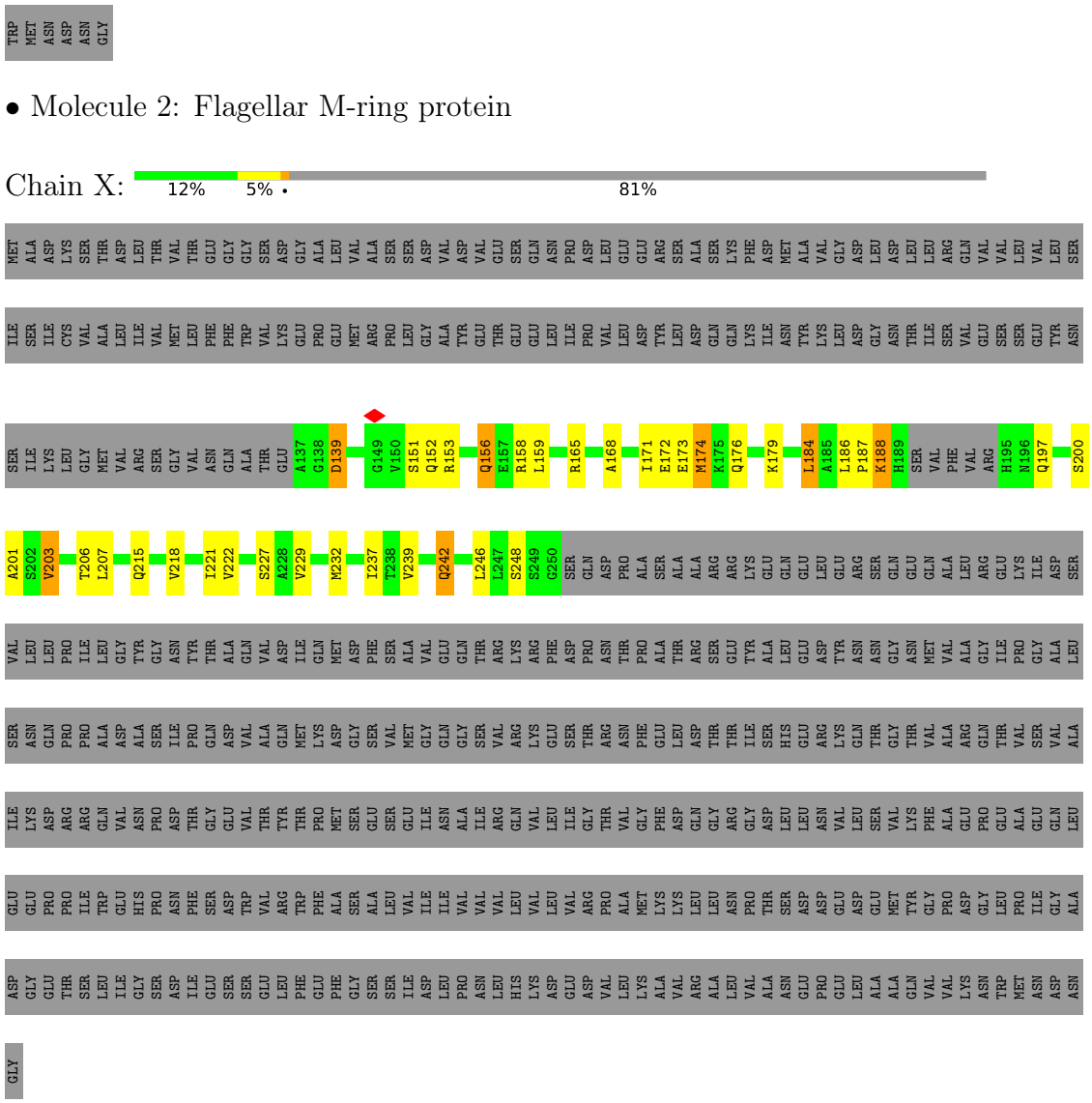
Chain V: 12% 7% • 80%

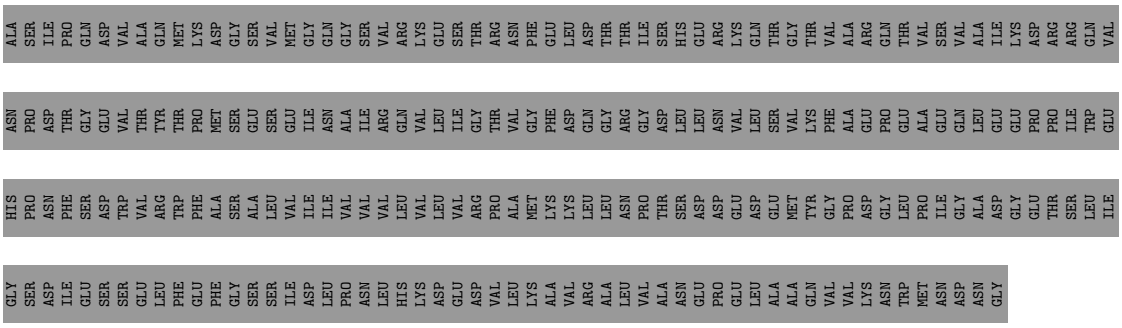


- Molecule 2: Flagellar M-ring protein

Chain W: 11% 7% • 80%

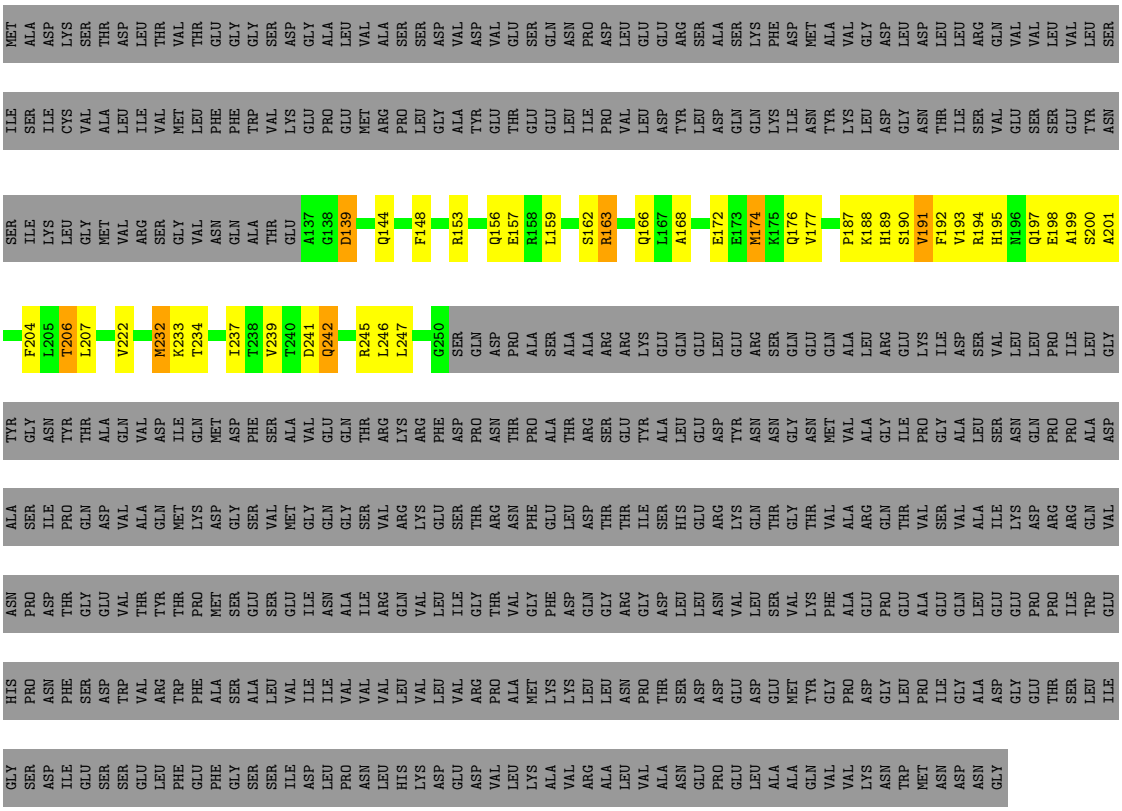



TRP MET ASN ASP ASN GLY
• Molecule 2: Flagellar M-ring protein
Chain X:
12%
5%
81%
MET ALA ASP LYS SER THR ASP LEU THR VAL THR GLU GLY GLY SER ASP GLY ALA LEU VAL ALA SER SER ASP VAL ASP VAL GLU SER GLN ASN PRO ASP LEU GLU GLU ARG SER ALA SER LYS PHE ASP MET ALA VAL GLY ASP LEU ASP LEU LEU ARG GLN VAL VAL LEU VAL LEU SER
ILE SER ILE CYS VAL ALA LEU ILE VAL MET LEU PHE PHE TRP VAL LYS GLU PRO GLU MET ARG PRO LEU GLY ALA TYR GLU THR GLU GLU LEU ILE PRO VAL LEU ASP TYR LEU ASP GLN GLN LYS ILE ASN TYR LYS LEU ASP GLY ASN THR ILE SER VAL GLU SER SER GLU TYR ASN
SER ILE LYS LEU GLY MET VAL ARG SER GLY VAL ASN GLN ALA THR GLU A137 G138 D139 G149 V150 S151 Q152 R153 Q156 E157 R158 L159 R165 A168 I171 E172 E173 M174 K175 Q176 K179 L184 A185 L186 P187 K188 H189 SER VAL PHE VAL ARG H195 N196 Q197 S200
A201 S202 V203 T206 L207 Q215 V218 I221 V222 S227 A228 V229 M232 I237 T238 V239 Q242 L246 L247 S248 S249 G250 SER GLN ASP PRO ALA SER ALA ALA ARG ARG LYS GLU GLN GLU LEU GLU ARG SER GLN GLU GLN ALA LEU ARG GLU LYS ILE ASP SER
VAL LEU LEU PRO ILE LEU GLY TYR GLY ASN TYR THR ALA GLN VAL ASP ILE GLN MET ASP PHE SER ALA VAL GLU GLN THR ARG LYS ARG PHE ASP PRO ASN THR PRO ALA THR ARG SER GLU TYR ALA LEU GLU ASP TYR ASN ASN GLY ASN MET VAL ALA GLY ILE PRO GLY ALA LEU
SER ASN GLN PRO PRO ALA ASP ALA SER ILE PRO GLN ASP VAL ALA GLN MET LYS ASP GLY SER VAL MET GLY GLN GLY SER VAL ARG LYS GLU SER THR ARG ASN PHE GLU LEU ASP THR THR ILE SER HIS GLU ARG LYS GLN THR GLY THR VAL ALA ARG GLN THR VAL SER VAL ALA
ILE LYS ASP ARG ARG GLN VAL ASN PRO ASP THR GLY GLU VAL THR TYR THR PRO MET SER SER GLU SER GLU ILE ASN ALA ILE ARG GLN VAL LEU ILE GLY THR VAL GLY PHE ASP GLN GLY ARG GLY ASP LEU LEU ASN VAL LEU SER VAL LYS PHE ALA GLU PRO GLU ALA GLU GLN LEU
GLU GLU PRO PRO ILE TRP GLU HIS PRO ASN PHE SER ASP TRP VAL ARG TRP PHE ALA SER ALA LEU VAL ILE ILE VAL VAL VAL LEU LEU VAL LEU VAL ARG PRO ALA MET LYS LYS LEU LEU ASN PRO THR SER ASP ASP VAL LEU ASP GLU MET TYR GLY PRO ASP GLY LEU PRO ILE GLY ALA
ASP GLY GLU THR SER LEU ILE GLY SER ASP ILE GLU SER SER GLU LEU PHE GLU PHE GLY SER SER ILE ASP LEU PRO ASN LEU HIS LYS ASP GLU ASP VAL LEU LYS ALA VAL ARG ALA LEU VAL ALA ASN GLU PRO GLU LEU ALA ALA GLN VAL VAL LYS ASN TRP MET ASN ASP ASN
GLY
• Molecule 2: Flagellar M-ring protein
Chain Y:
12%
6%
80%
MET ALA ASP LYS SER THR ASP LEU THR VAL THR GLU GLY GLY SER ASP GLY ALA LEU VAL ALA SER SER SER ASP VAL ASP VAL GLU SER GLN ASN PRO ASP LEU GLU GLU ARG SER ALA SER LYS PHE ASP MET ALA VAL GLY ASP LEU ASP LEU LEU ARG GLN VAL VAL LEU VAL LEU SER
ILE SER ILE CYS VAL ALA LEU ILE VAL MET LEU PHE PHE TRP VAL LYS GLU PRO GLU MET ARG PRO LEU GLY ALA TYR GLU THR GLU GLU LEU ILE PRO VAL LEU ASP TYR LEU ASP GLN GLN LYS ILE ASN TYR LYS LEU ASP GLY ASN THR ILE SER VAL GLU SER SER GLU TYR ASN
SER ILE LYS LEU GLY MET VAL ARG SER GLY VAL ASN GLN ALA THR GLU A137 G138 D139 Q144 S151 Q152 R153 E157 R158 L159 S162 R163 E164 R165 Q166 L167 A168 I171 E172 E173 M174 K175 L184 K188 H189 S190 V191 F192 V193 R194 H195 N196 S200 A201 S202 V203
T206 V218 I221 S227 G231 M232 S235 R236 D241 Q242 R245 L246 L247 S248 S249 G250 SER GLN ASP PRO ALA SER ALA ALA ARG ARG LYS GLU GLN GLU LEU GLU ARG SER GLN GLU GLN ALA LEU ARG GLU LYS ILE ASP SER VAL LEU LEU PRO ILE LEU GLY
TYR GLY ASN TYR THR ALA GLN VAL ASP ILE GLN MET ASP PHE SER ALA VAL GLU GLN THR ARG LYS ARG PHE ASP PRO ASN THR PRO ALA THR ARG SER GLU TYR ALA LEU GLU ASP TYR ASN ASN GLY ASN MET VAL ALA GLY ILE PRO GLY ALA LEU SER ASN GLN PRO PRO ALA ASP



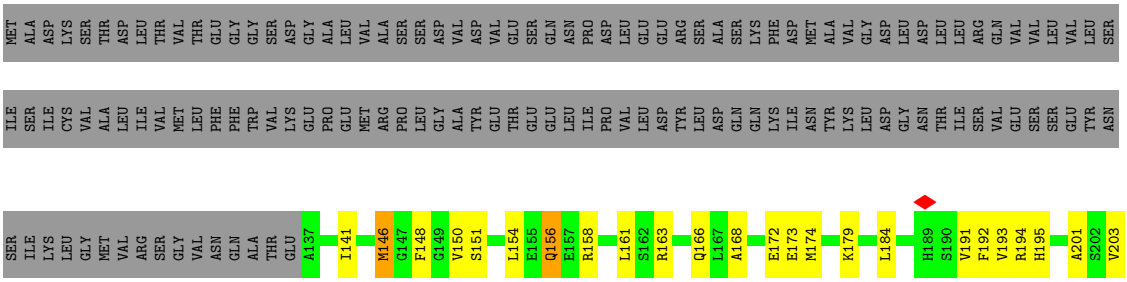
• Molecule 2: Flagellar M-ring protein

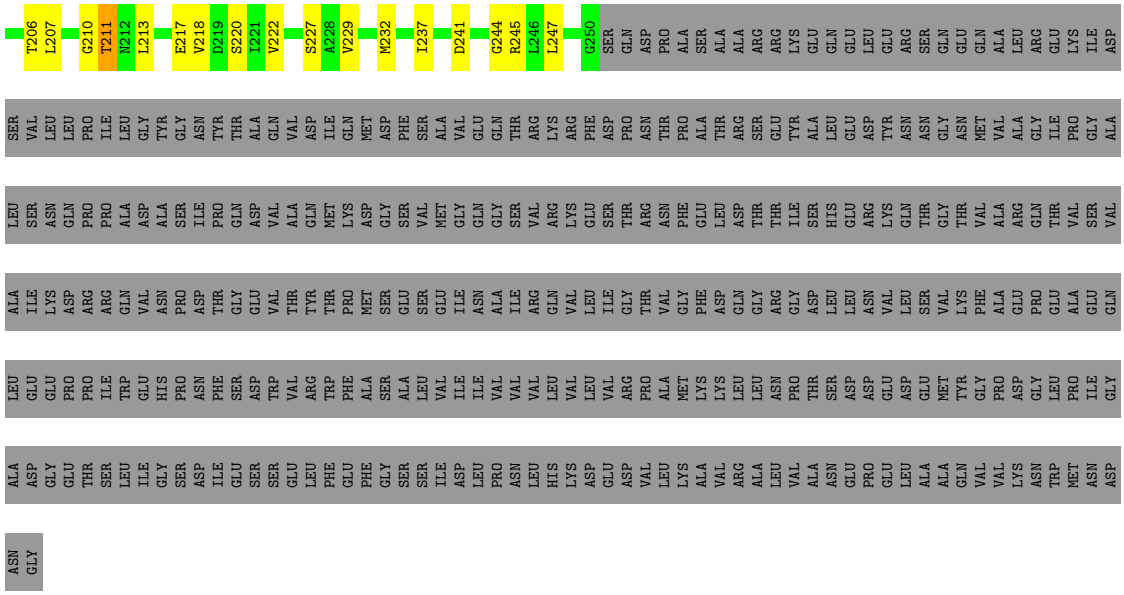
Chain Z: 12% 6% • 80%



• Molecule 2: Flagellar M-ring protein

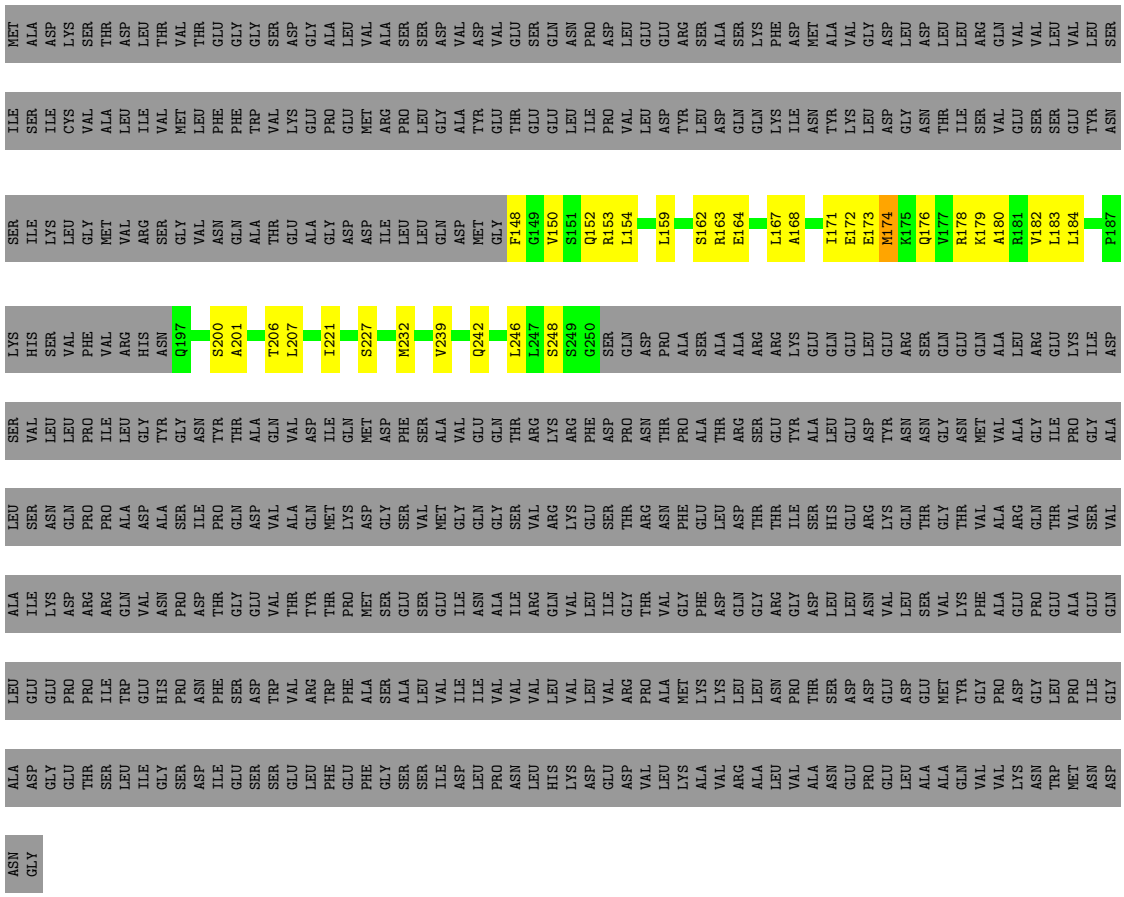
Chain a: 13% 7% • 80%





- Molecule 2: Flagellar M-ring protein

Chain b: 11% 6% 84%



- Molecule 2: Flagellar M-ring protein

Chain c: 10% 7% • 82%

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

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

SER ILE LYS LEU GLY MET VAL ARG SER GLY VAL ASN GLN ALA THR GLU ALA GLY ASP ASP ILE LEU LEU GLN ASP MET GLY F148 G149 V150 S151 Q152 R153 L154 E157 R163 L167 I171 E172 E173 M174 K175 Q176 V177 R178 K179 A180 L183 L184 F192 V193 R194 S200

A201 S202 V203 T206 L207 S208 L213 K214 Q215 V218 D219 S220 I221 V222 V229 M232 I237 D241 G244 R245 L246 L247 G250 SER GLN ASP PRO ALA SER ALA ALA ARG ARG LYS GLU GLN GLU LEU GLU ARG SER GLN GLU GLN GLN ALA LEU ARG GLU LYS ILE ASP

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

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

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

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

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

ASN GLY

• Molecule 2: Flagellar M-ring protein

Chain d: 9% 7% • 82%

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

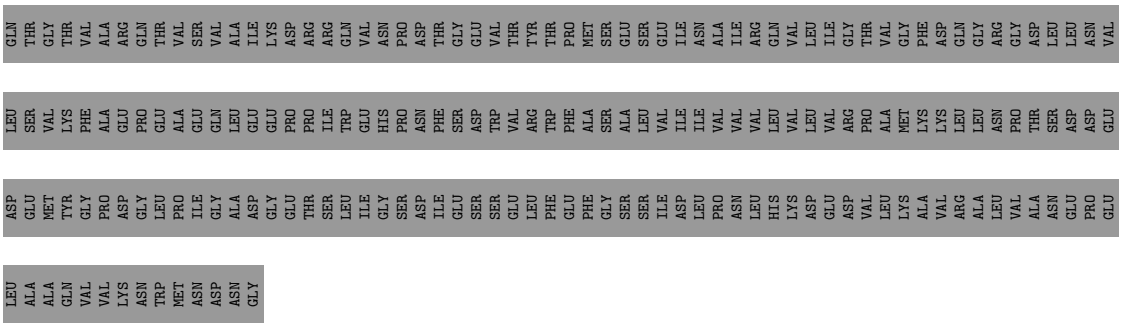
ILE SER ILE CYS VAL ALA LEU ILE VAL MET MET LEU PHE PHE TRP VAL LYS GLU PRO GLU MET ARG PRO LEU GLY ALA TYR GLU THR GLU GLU LEU ILE PRO VAL LEU ASP TYR LEU ASP GLN GLN LYS ILE ASN TYR LYS LEU ASP GLY ASN THR ILE SER VAL GLU SER SER GLU TYR ASN

SER ILE LYS LEU GLY MET VAL ARG SER GLY VAL ASN GLN ALA THR GLU ALA GLY ASP ASP ILE LEU LEU GLN ASP MET GLY F148 Q152 R153 Q156 E157 R163 L167 A168 G169 A170 I171 E172 E173 M174 K175 Q176 V177 R178 K179 A180 R181 V182 L183 L184 A185 K188 H189 S190

V191 F192 E198 A199 S200 A201 T206 L207 G210 T211 Q216 D219 S220 I221 V222 D223 S227 A228 V229 M232 K233 T234 S235 R236 I237 T238 V239 T240 D241 Q242 H243 G244 R245 L246 L247 G250 SER GLN ASP PRO ALA SER ALA ALA ARG ARG LYS GLU GLN GLU LEU GLU

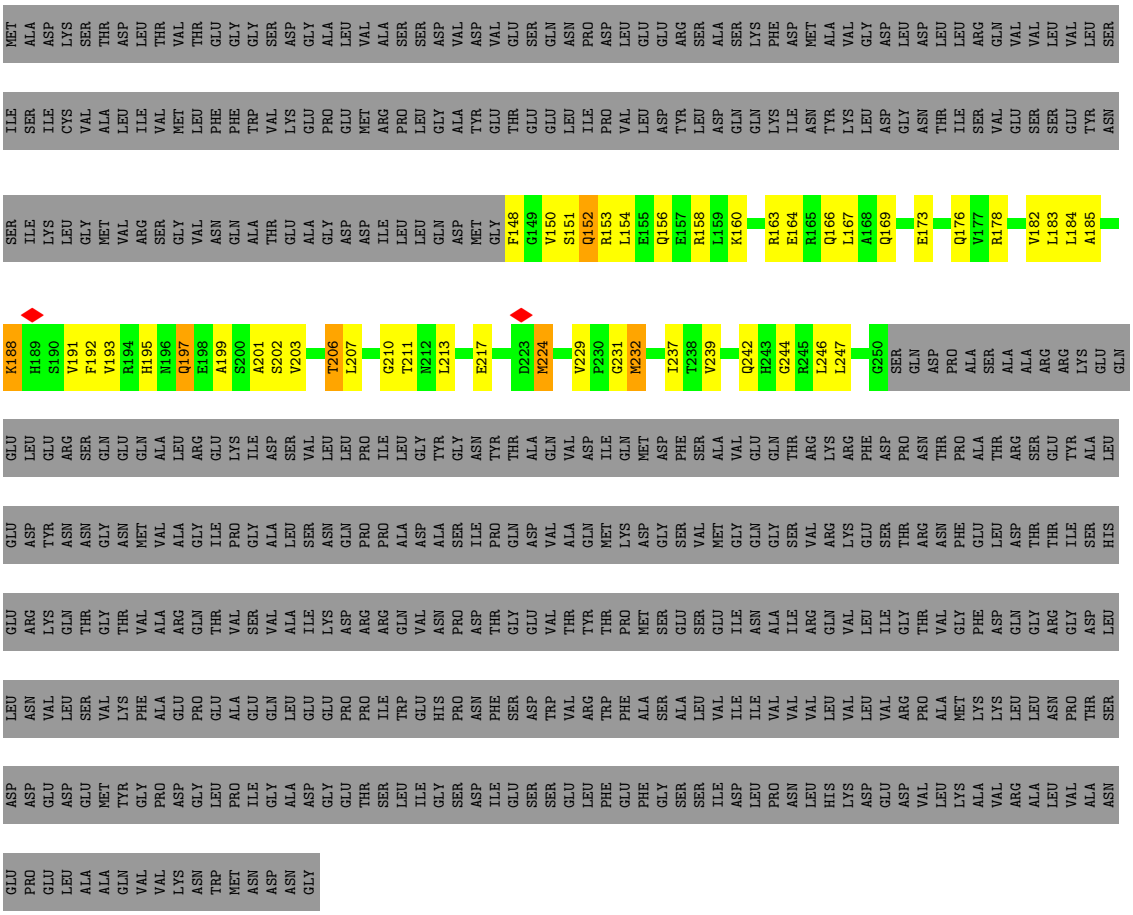
ARG SER GLN GLU GLN ALA LEU ARG GLU LYS ILE ASP SER VAL LEU LEU PRO ILE LEU GLY TYR GLY ASN TYR THR ALA GLN VAL ASP ILE GLN MET ASP PHE SER ALA VAL GLU GLN THR ARG LYS ARG PHE ASP PRO ASN THR PRO ALA THR ARG SER GLU TYR ALA LEU GLU TYR

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



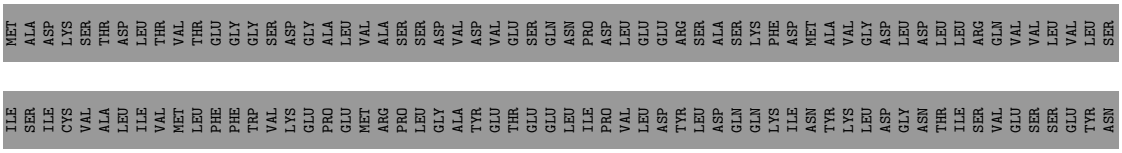
• Molecule 2: Flagellar M-ring protein

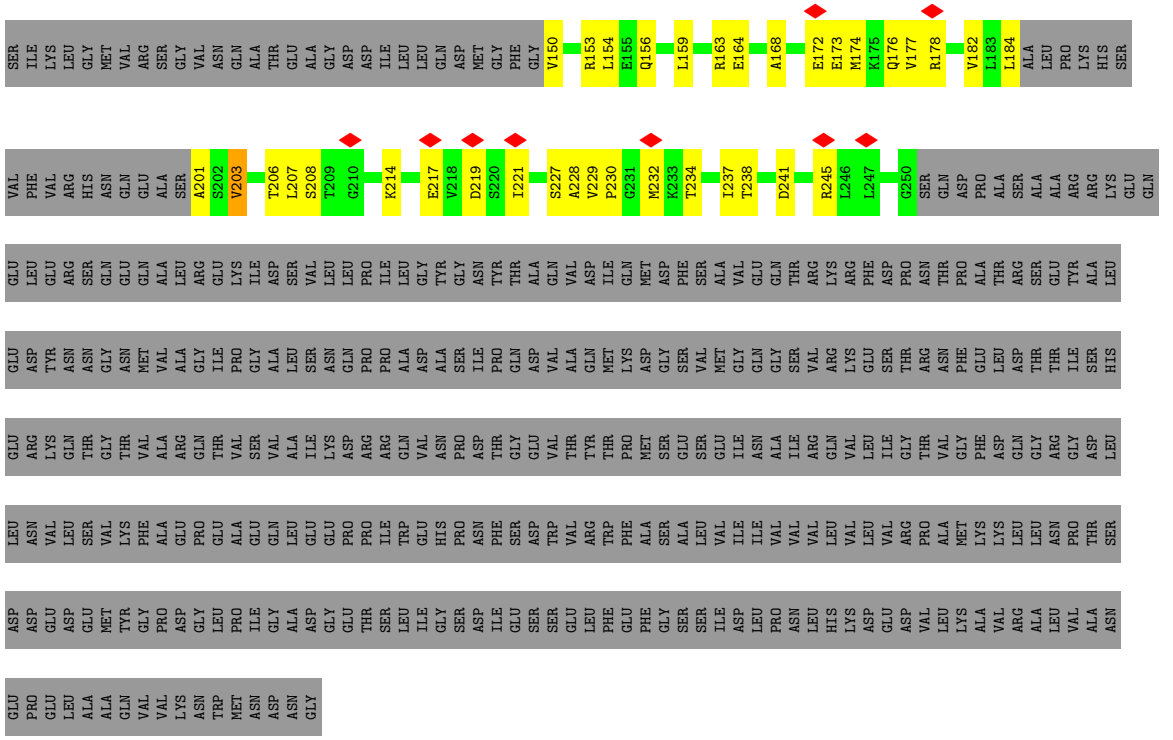
Chain e: 10% 7% • 82%



• Molecule 2: Flagellar M-ring protein

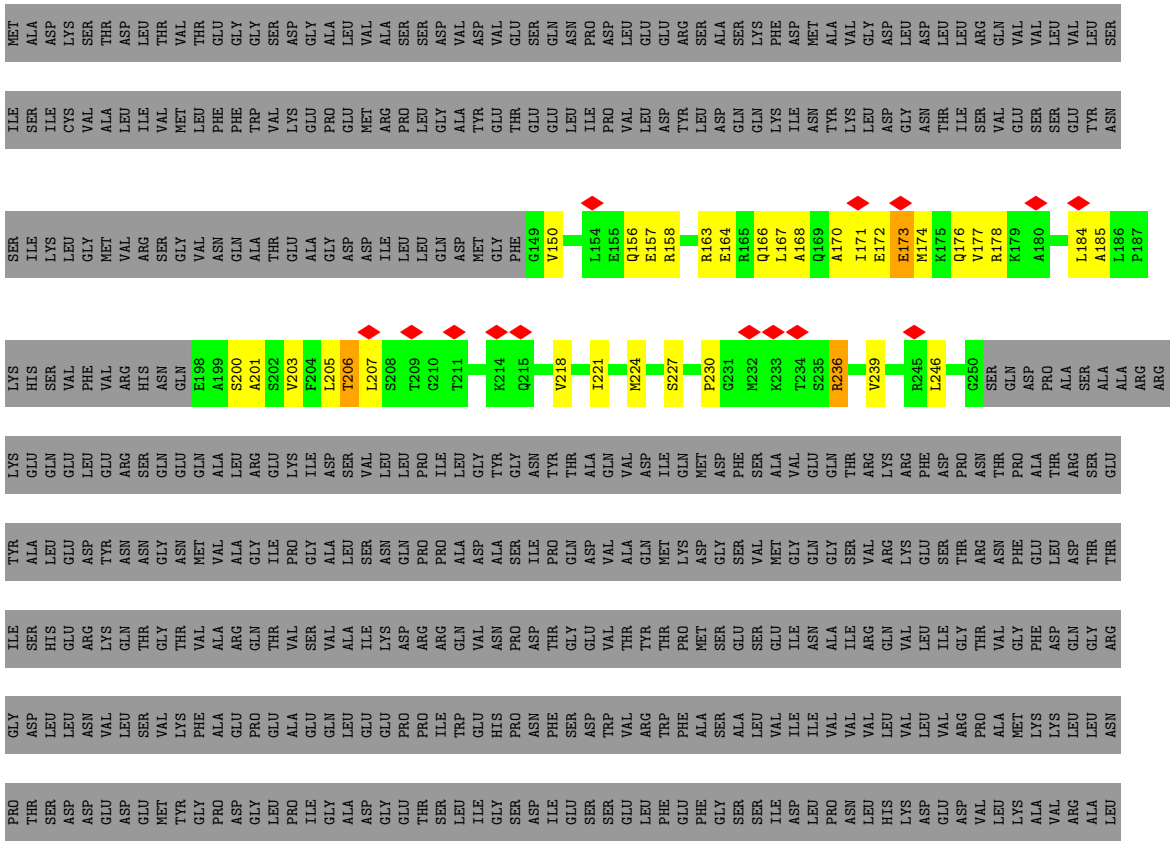
Chain f: • 9% 6% 85%





- Molecule 2: Flagellar M-ring protein

Chain g:



VAL ALA ASN GLU PRO GLU LEU ALA ALA GLN VAL VAL LYS ASN TRP MET ASN ASP ASN GLY

• Molecule 2: Flagellar M-ring protein

Chain h: 10% 6% • 84%

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

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

SER ILE LYS LEU GLY MET VAL ARG SER GLY VAL ASN GLN ALA THR GLU ALA GLY ASP ASP ILE LEU LEU GLN ASP MET GLY PHE G149 R153 Q156 E157 R163 L167 A168 I171 E172 E173 M174 K179 A180 R181 V182 L183 L184 A185 L186 P187 LYS HIS SER VAL PHE VAL

ARG HIS ASN GLN GLU A199 S200 A201 S202 V203 T206 L207 G210 Q215 Q216 E217 V218 D219 S220 I221 M224 S227 A228 V229 P230 G231 M232 K233 T238 L246 L247 S248 S249 G250 SER GLN ASP PRO ALA SER ALA ALA ARG ARG LYS GLU GLN GLU LEU GLU ARG SER GLN

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

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

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

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

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

GLN VAL VAL LYS ASN TRP MET ASN ASP ASN GLY

• Molecule 2: Flagellar M-ring protein

Chain i: 9% 6% 85%

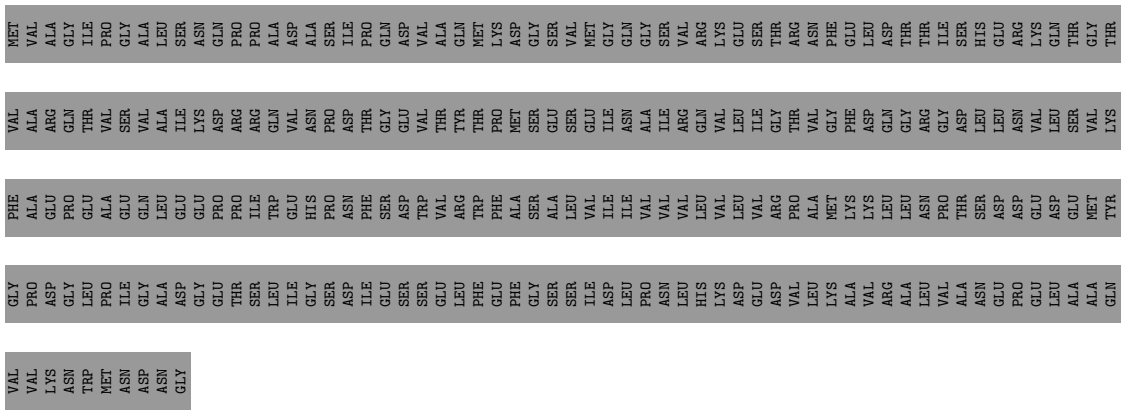
MET ALA ASP LYS SER THR ASP LEU THR VAL THR GLU GLY GLY SER ASP GLY ALA LEU VAL ALA SER SER ASP VAL ASP VAL GLU SER GLN ASN PRO ASP LEU GLU GLU ARG SER ALA SER LYS PHE ASP MET ALA VAL GLY ASP LEU ASP LEU LEU ARG GLN VAL VAL LEU VAL LEU SER

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

SER ILE LYS LEU GLY MET VAL ARG SER GLY VAL ASN GLN ALA THR GLU ALA GLY ASP ASP ILE LEU LEU GLN ASP MET GLY PHE GLY V150 S151 Q152 R153 E157 R163 E164 R165 Q166 L167 A168 E172 E173 M174 K175 Q176 V177 R178 K179 V182 L183 L184 A185 L186 PRO LYS HIS

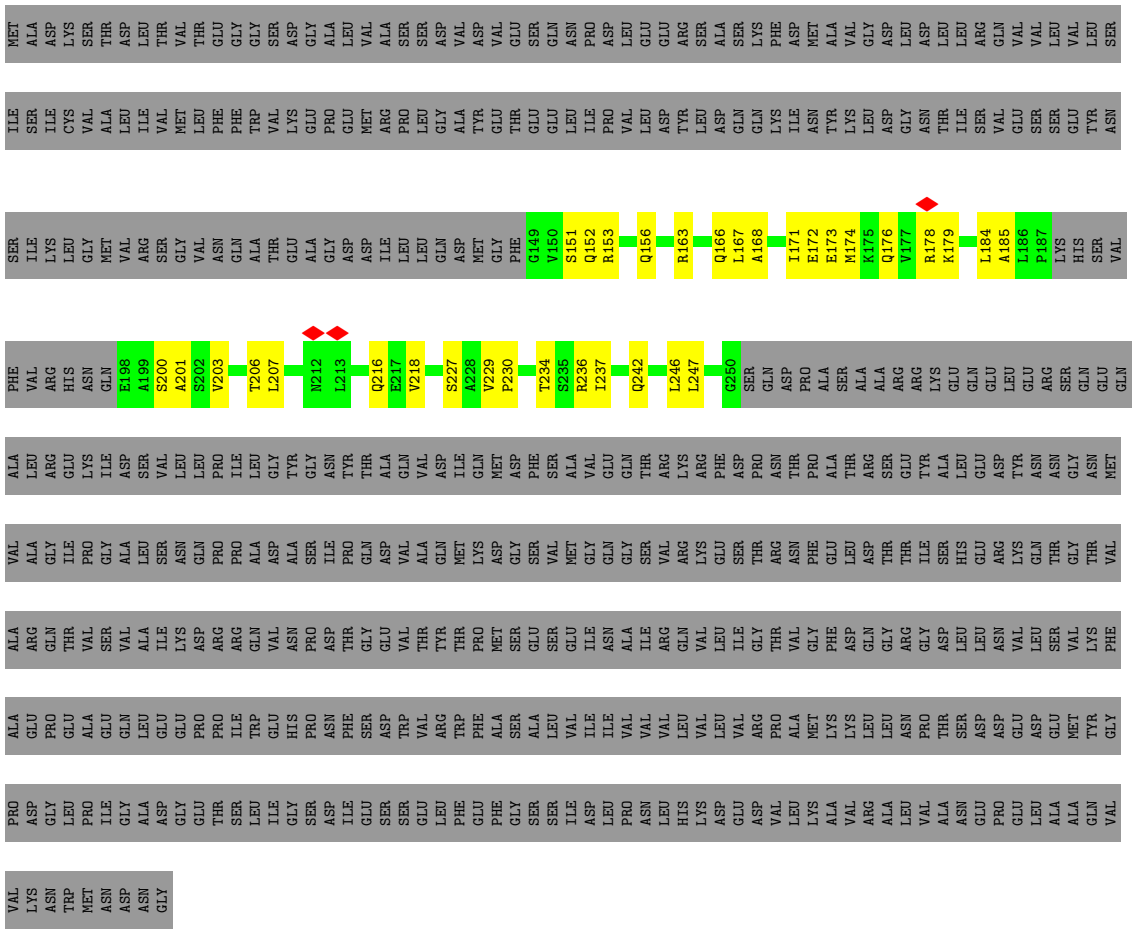
SER VAL PHE VAL ARG HIS ASN GLN GLU A199 S200 V203 F204 L205 T206 L207 G210 T211 Q215 D219 S220 S227 P230 G231 M232 D241 Q242 H243 G244 R245 L246 G250 SER GLN ASP PRO ALA SER ALA ALA ARG ARG LYS GLU GLN GLU LEU GLU ARG SER GLN GLU

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



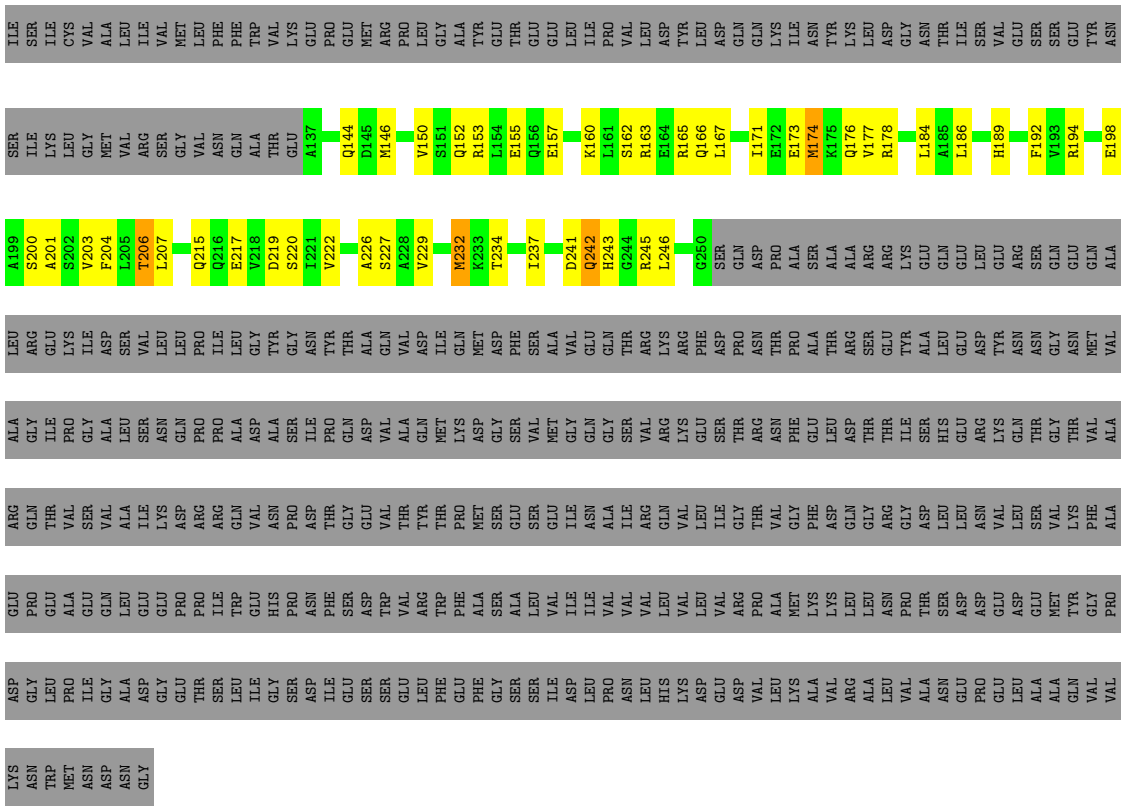
• Molecule 2: Flagellar M-ring protein

Chain j:



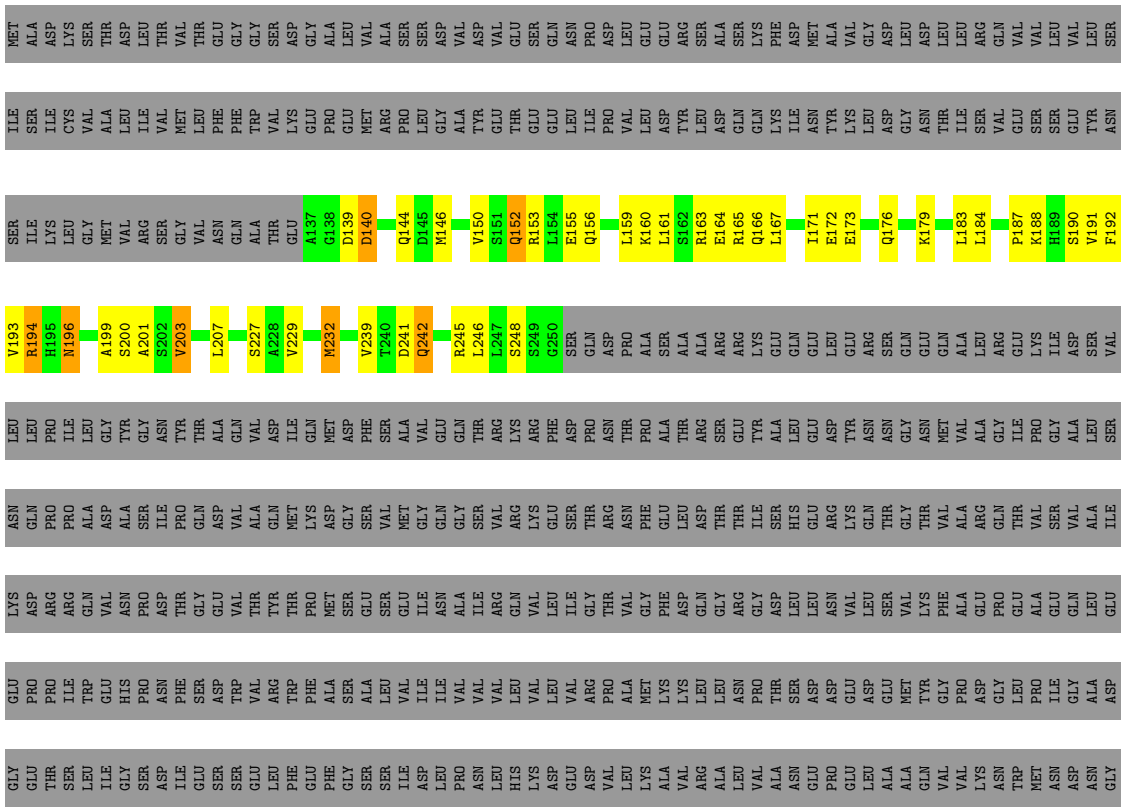
• Molecule 2: Flagellar M-ring protein

Chain k:



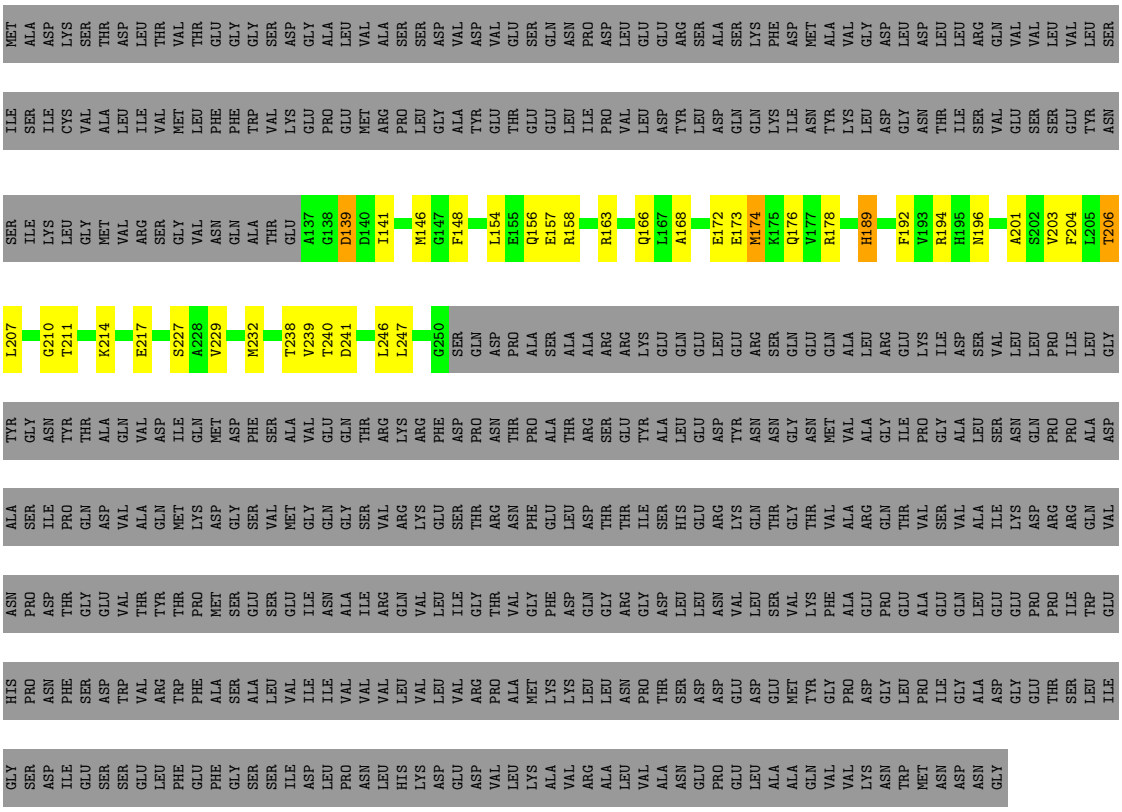
• Molecule 2: Flagellar M-ring protein

Chain l: 12% 7% • 80%



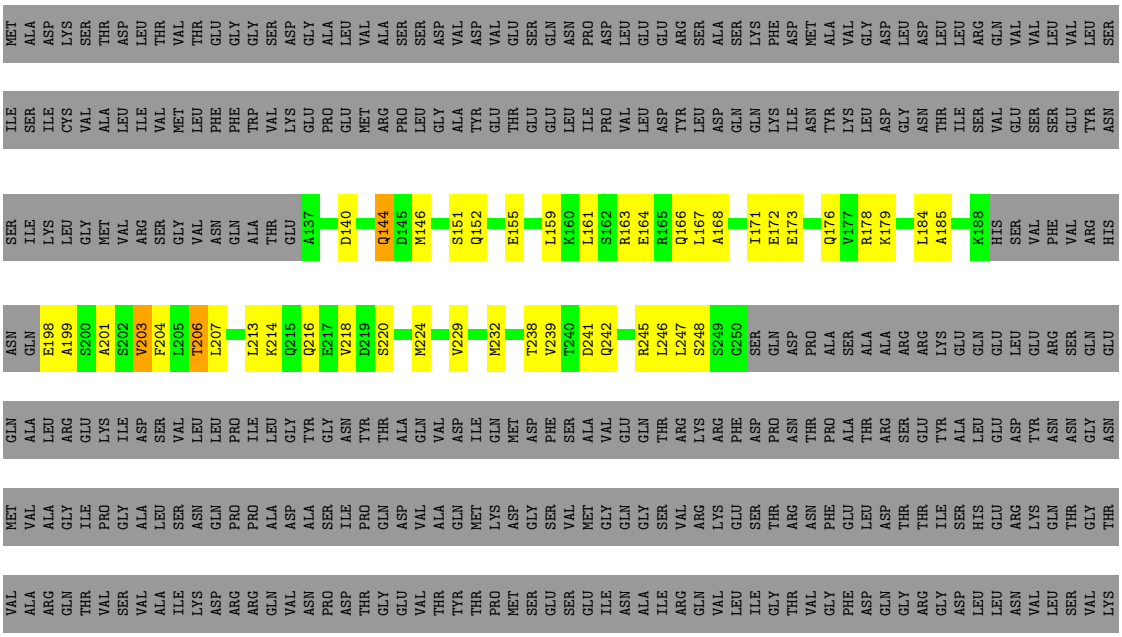
• Molecule 2: Flagellar M-ring protein

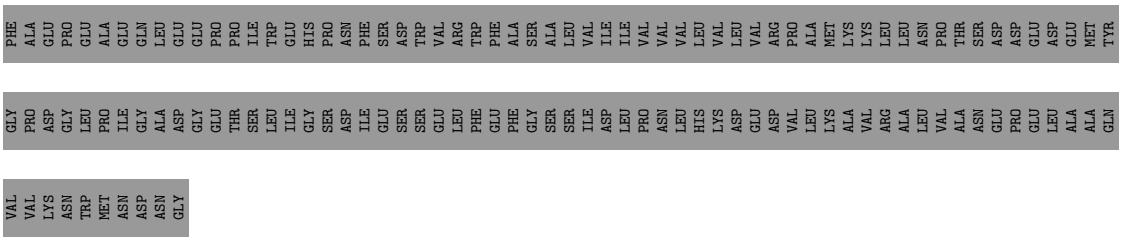
Chain m: 13% 6% • 80%



• Molecule 2: Flagellar M-ring protein

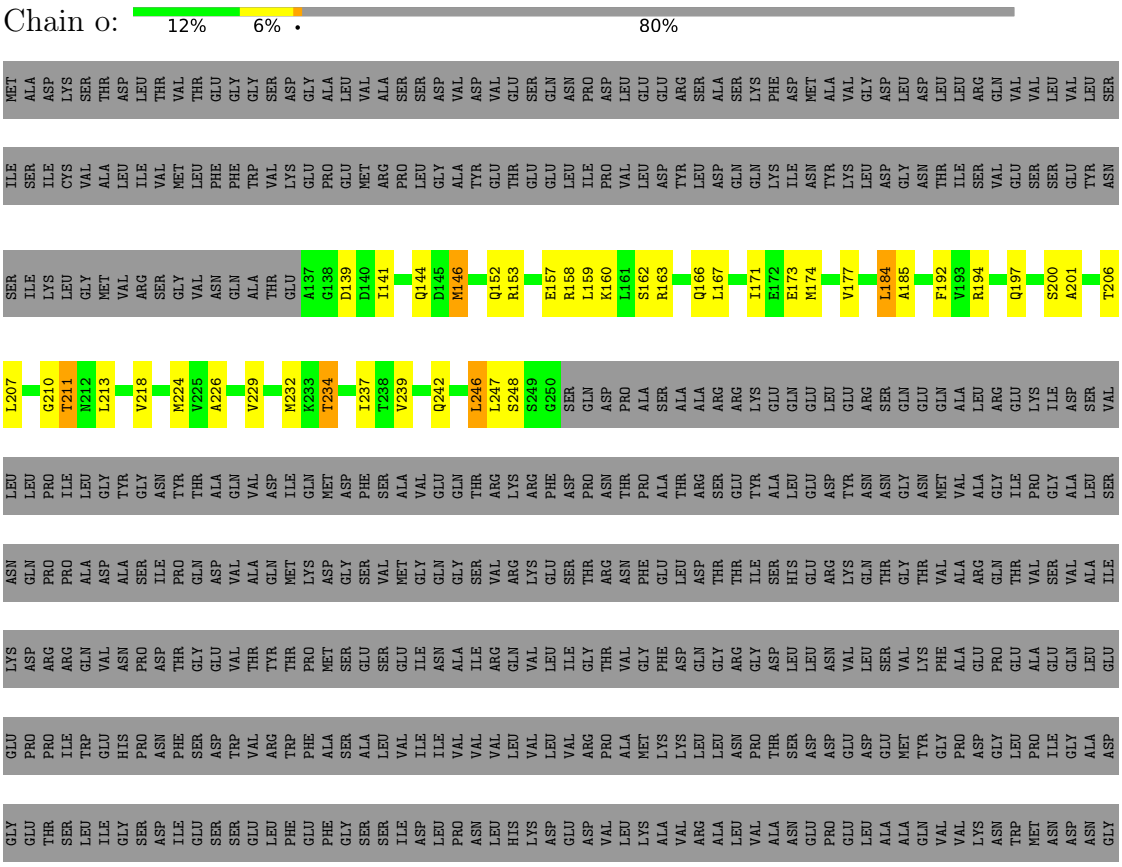
Chain n: 11% 7% • 82%





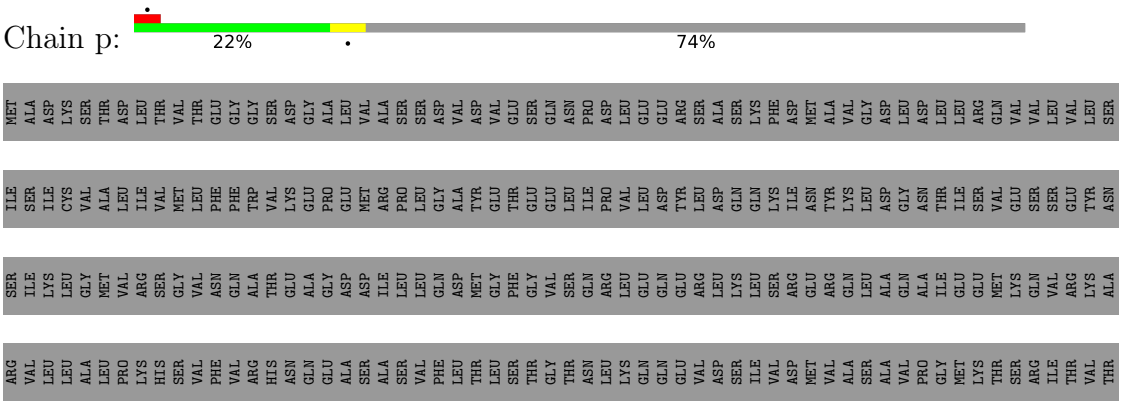
• Molecule 2: Flagellar M-ring protein

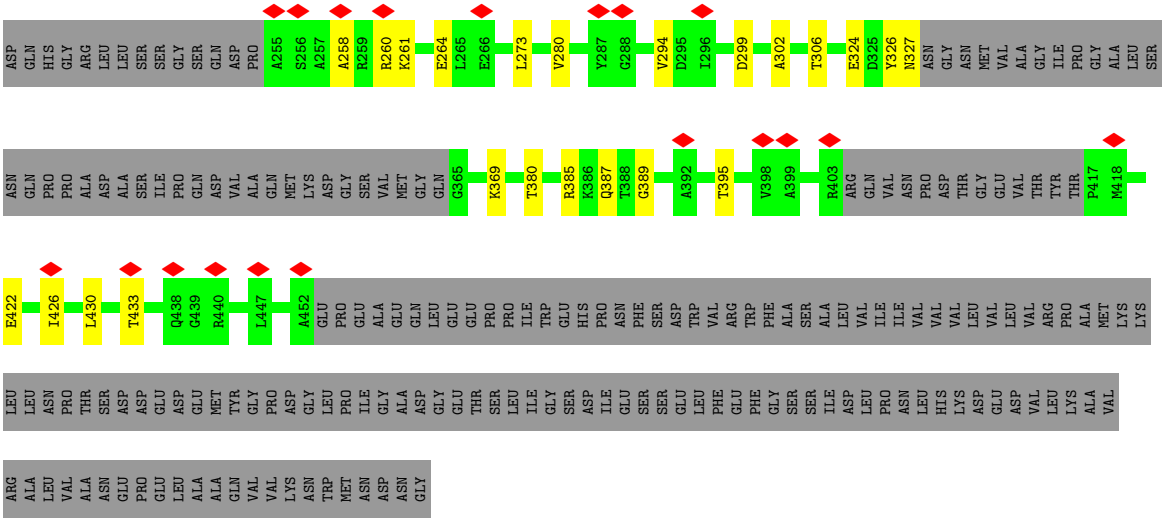
Chain o:



• Molecule 2: Flagellar M-ring protein

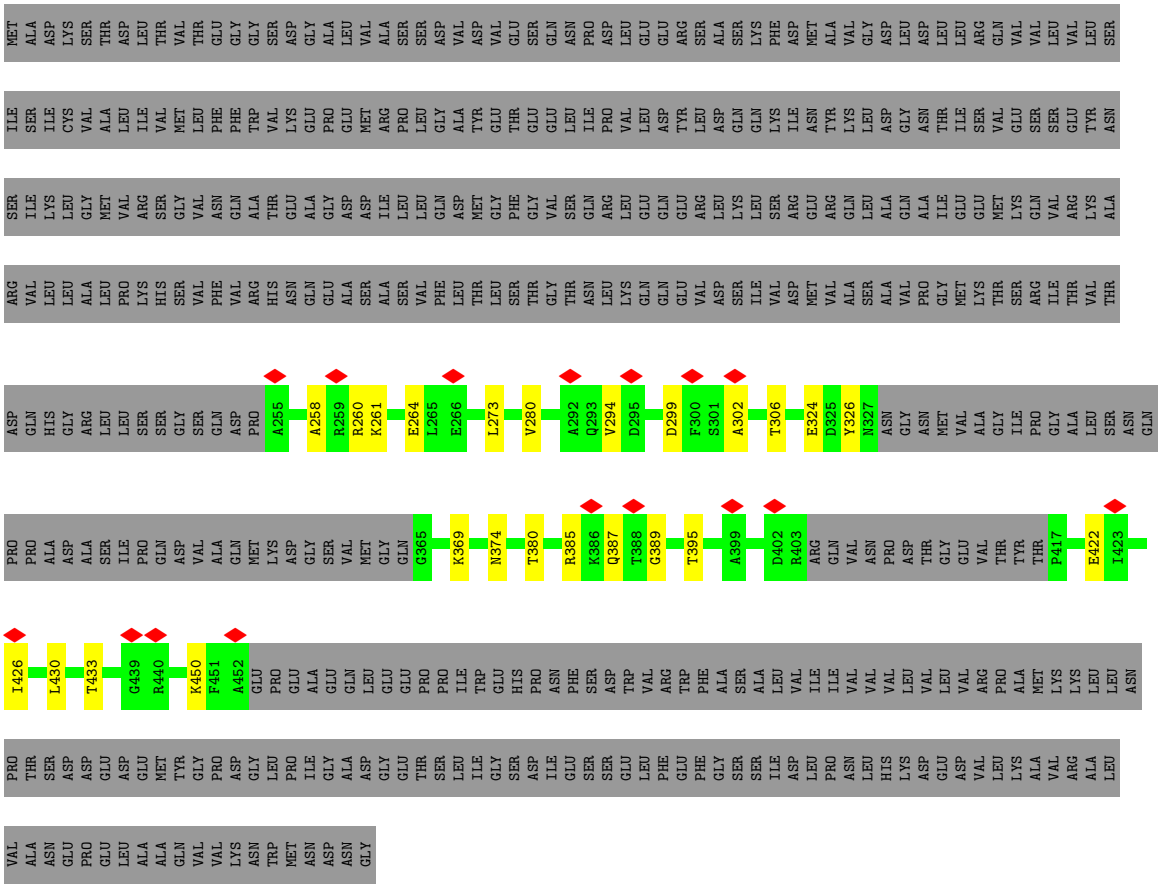
Chain p:





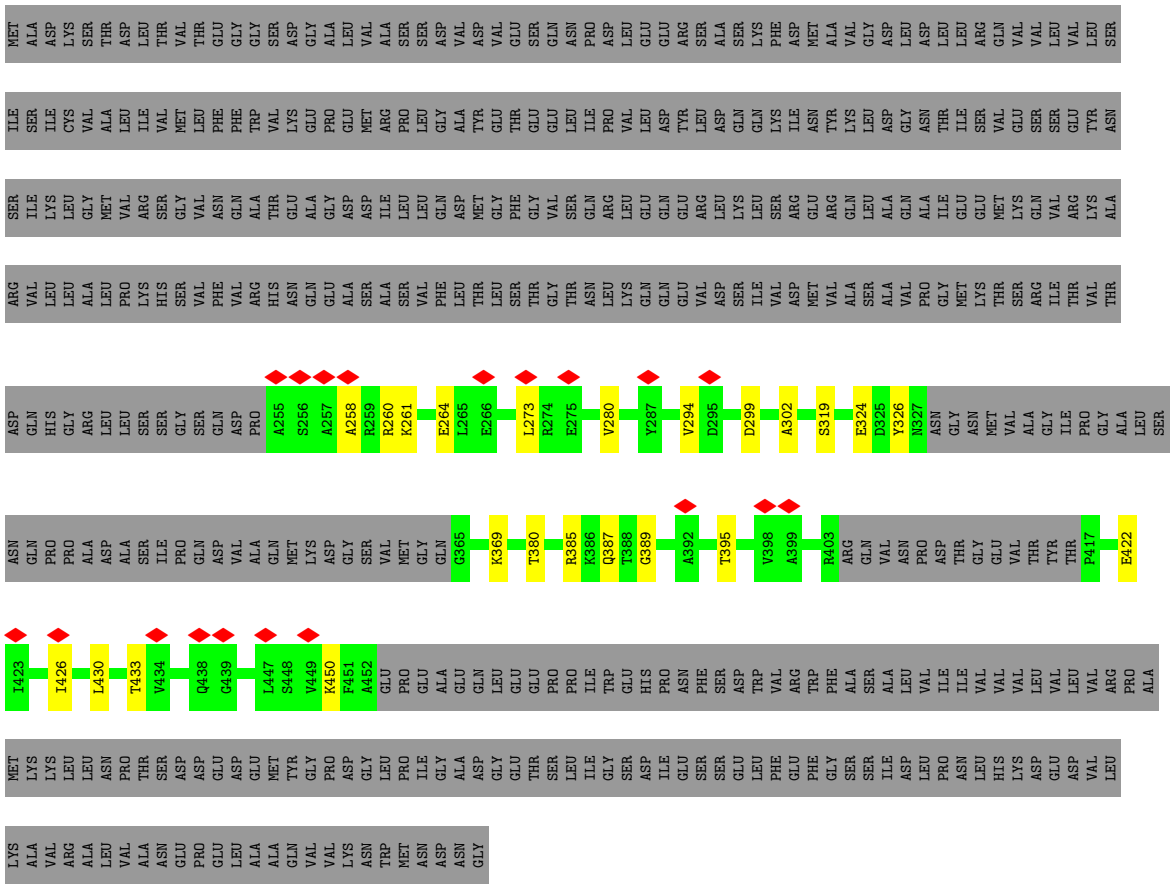
• Molecule 2: Flagellar M-ring protein

Chain q:



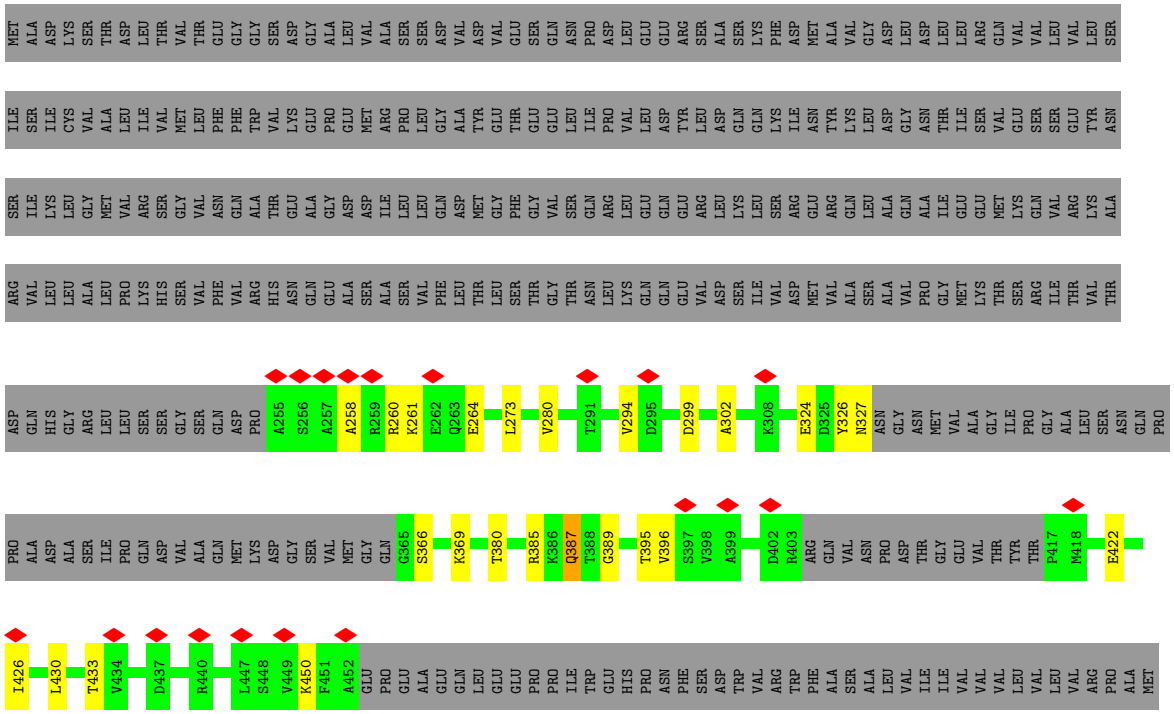
• Molecule 2: Flagellar M-ring protein

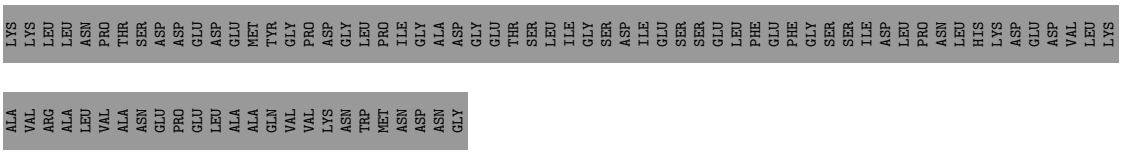
Chain r:



• Molecule 2: Flagellar M-ring protein

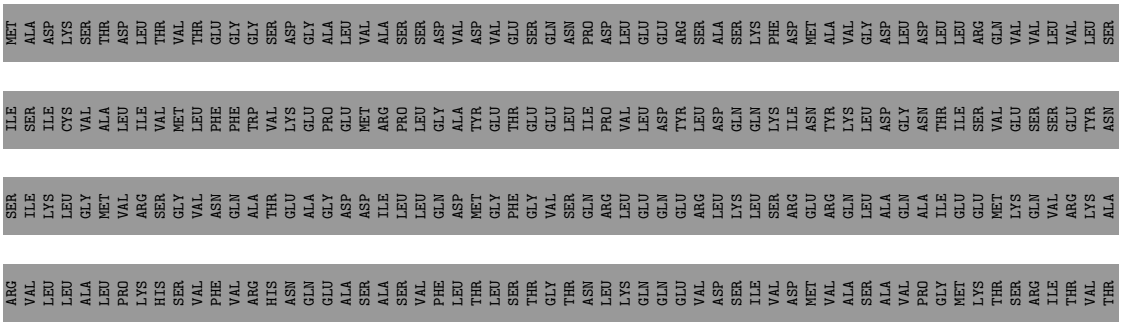
Chain s: 21% 74%





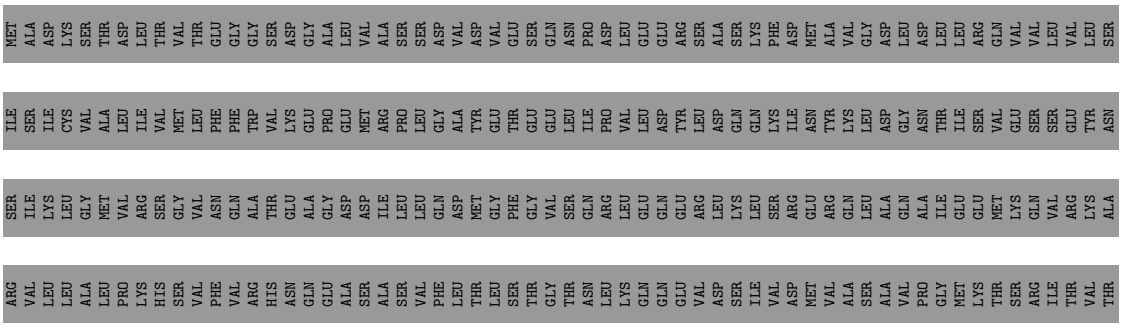
- Molecule 2: Flagellar M-ring protein

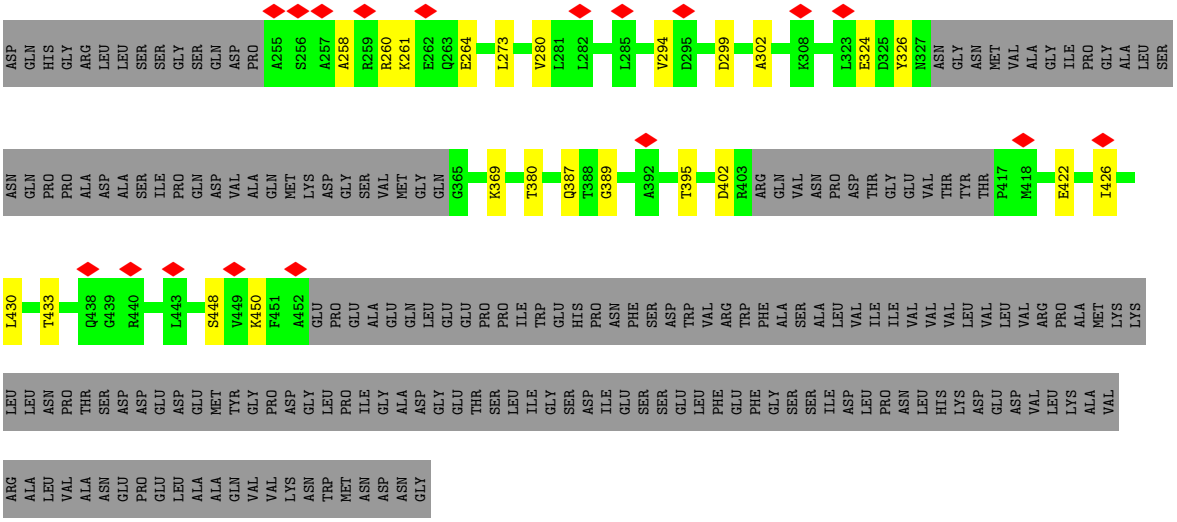
Chain t:



- Molecule 2: Flagellar M-ring protein

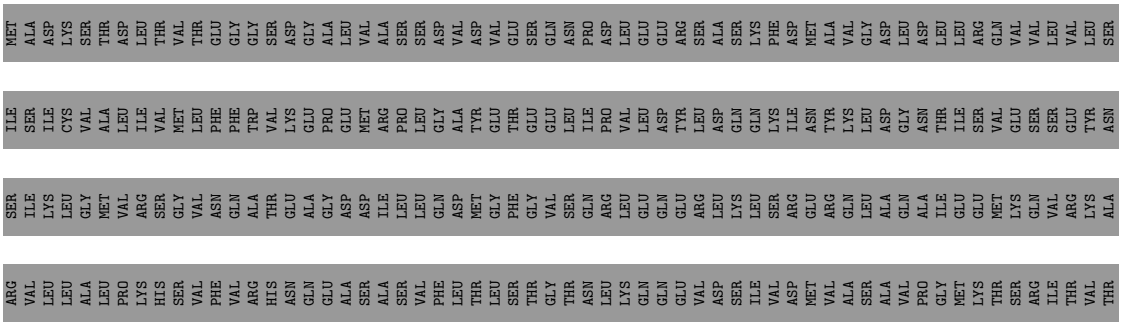
Chain u:

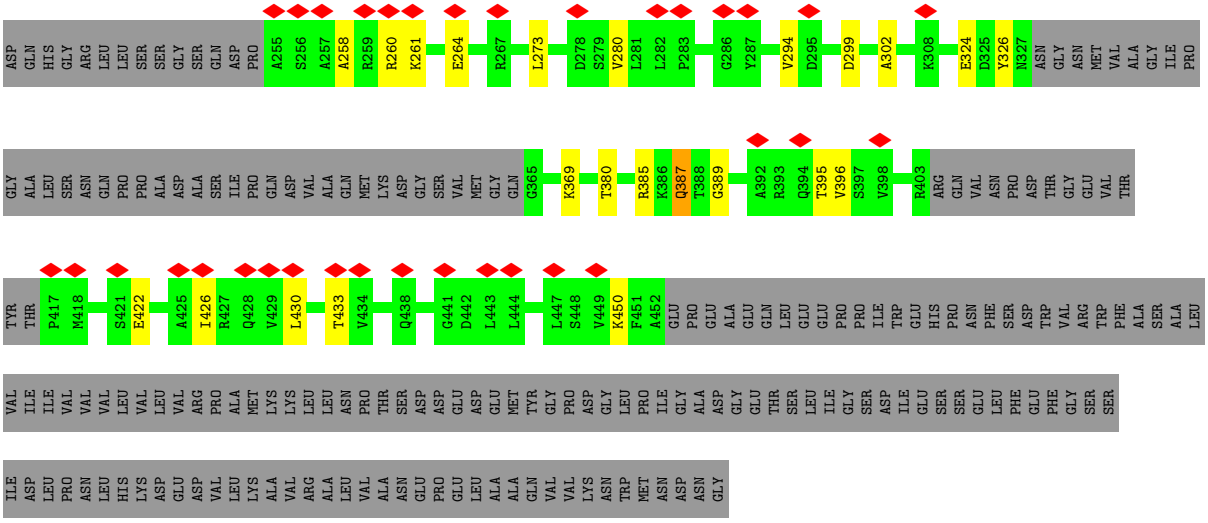




• Molecule 2: Flagellar M-ring protein

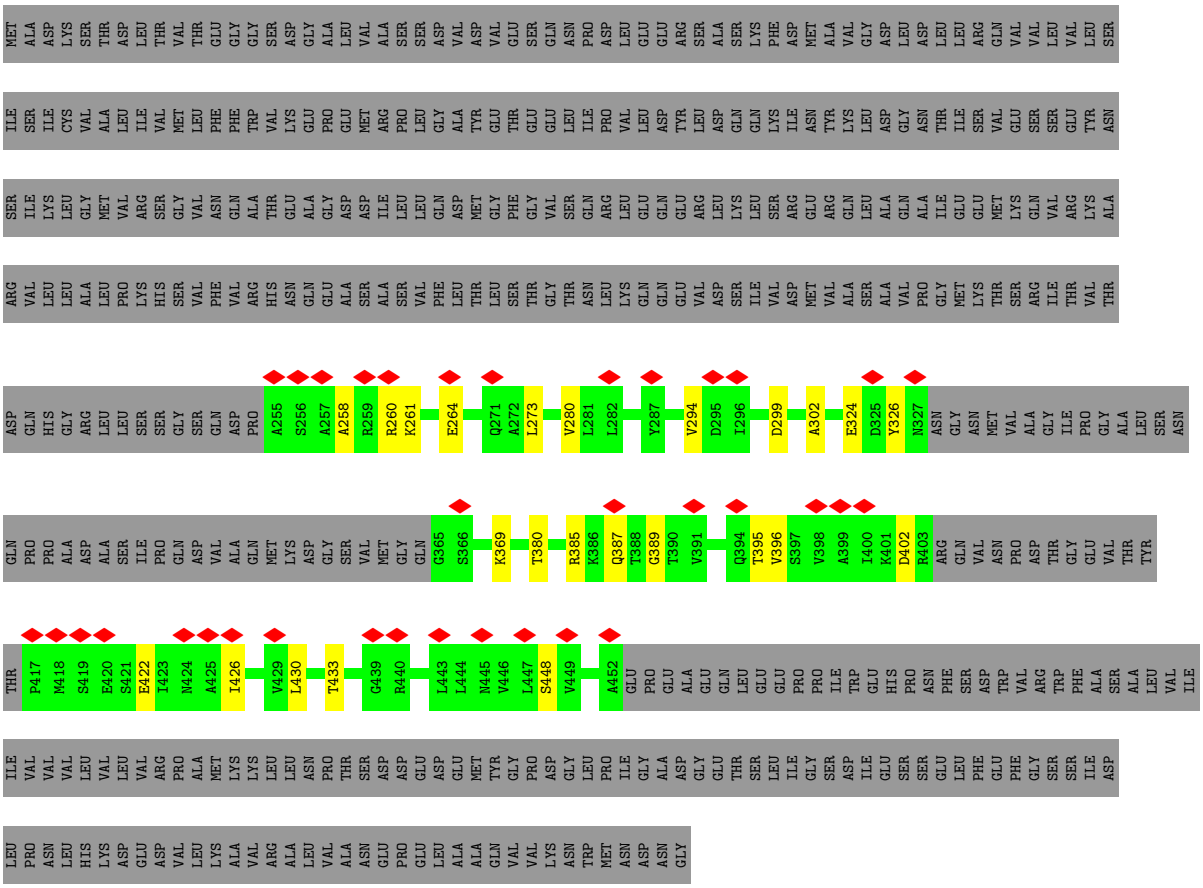
Chain v:





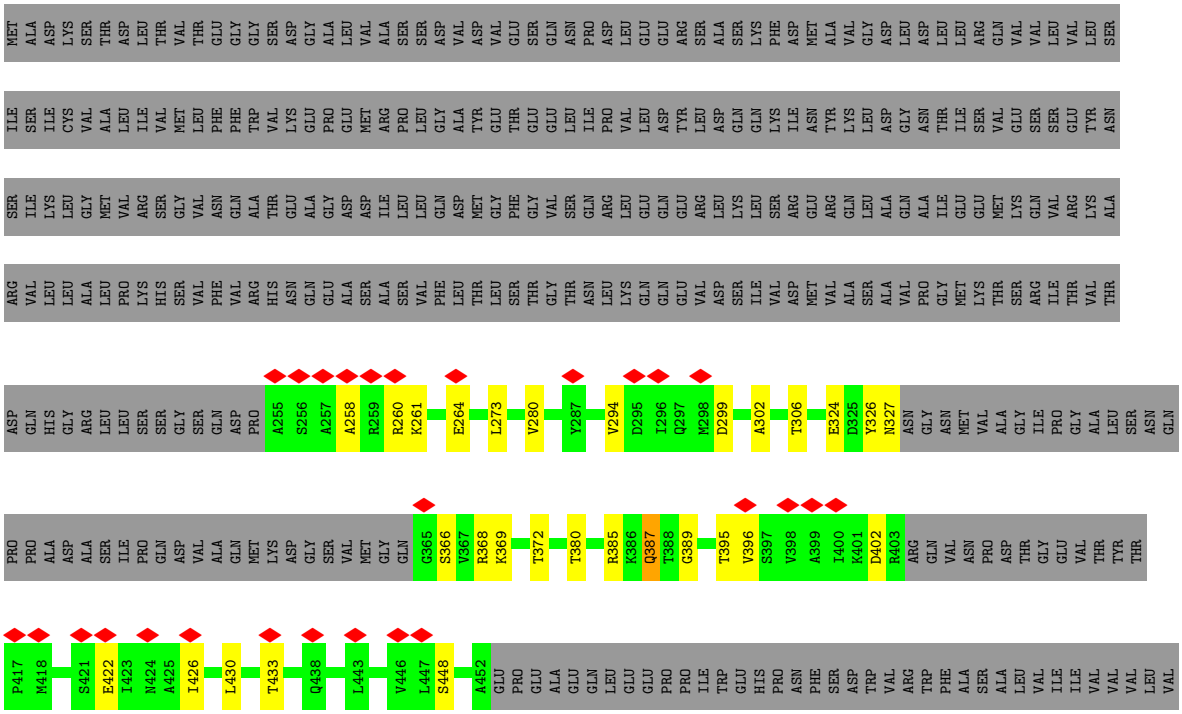
• Molecule 2: Flagellar M-ring protein

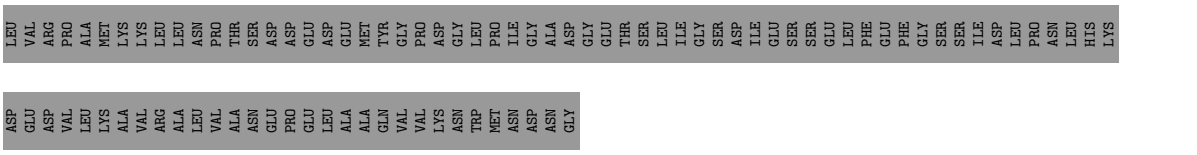
Chain w:



• Molecule 2: Flagellar M-ring protein

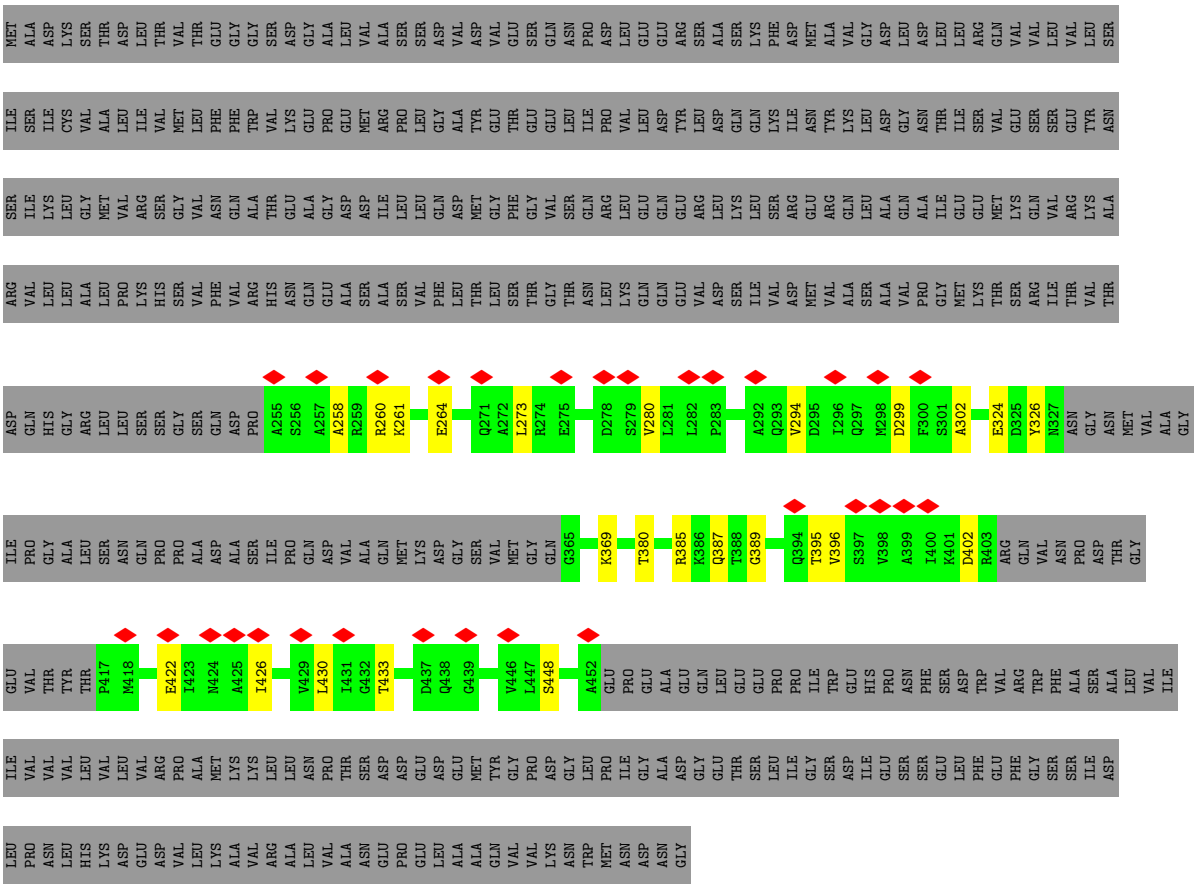
Chain x: 5% 21% 5% 74%





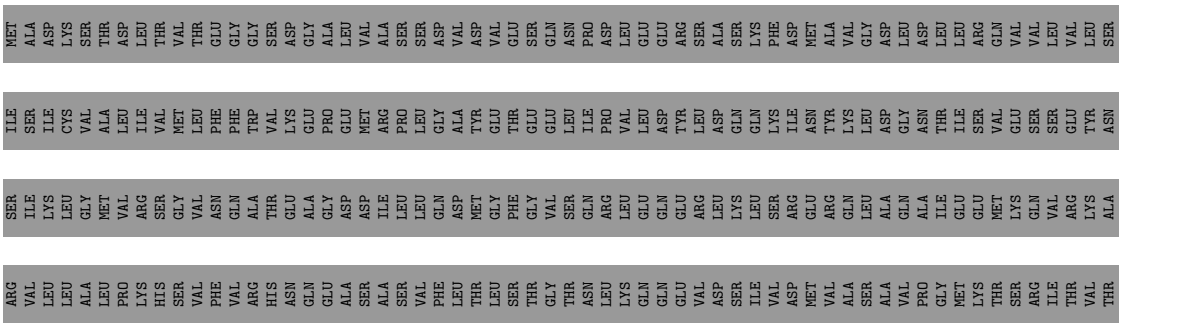
• Molecule 2: Flagellar M-ring protein

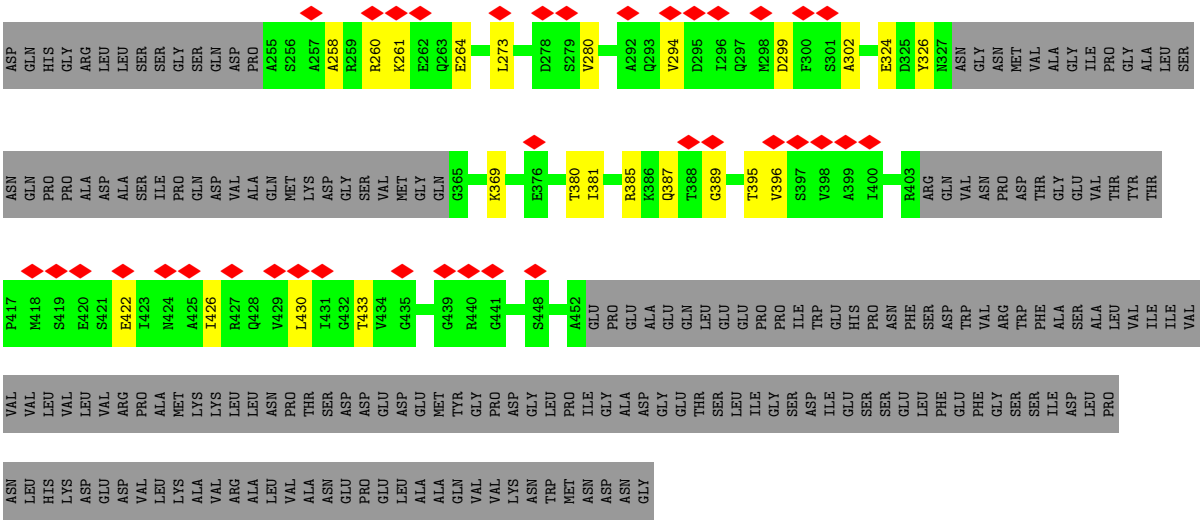
Chain y:



• Molecule 2: Flagellar M-ring protein

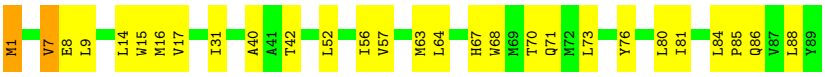
Chain z:





- Molecule 3: Flagellar biosynthetic protein FliQ

Chain 6:



- Molecule 3: Flagellar biosynthetic protein FliQ

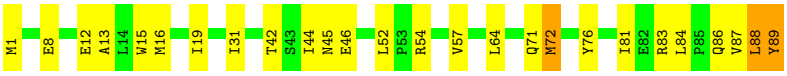
Chain 7:

- Molecule 3: Flagellar biosynthetic protein FliQ

Chain AQ:

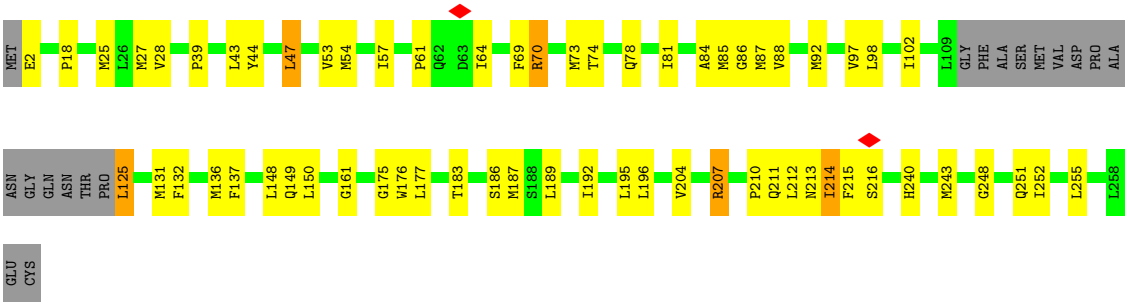
- Molecule 3: Flagellar biosynthetic protein FliQ

Chain AR:



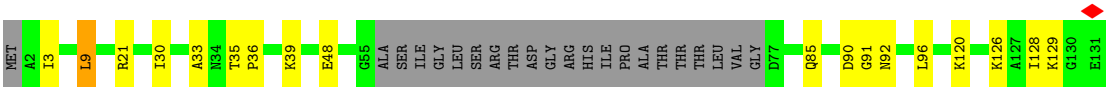
- Molecule 4: Flagellar biosynthetic protein FliR

Chain 8:



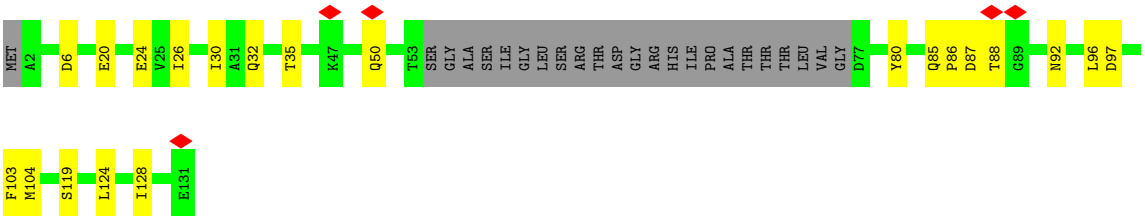
- Molecule 5: Flagellar basal body rod protein FlgB

Chain AS:



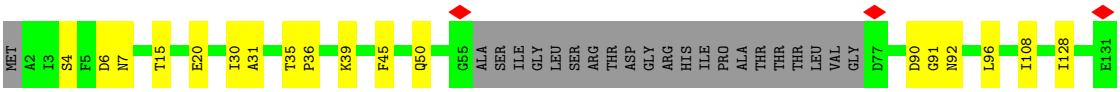
- Molecule 5: Flagellar basal body rod protein FlgB

Chain AT:



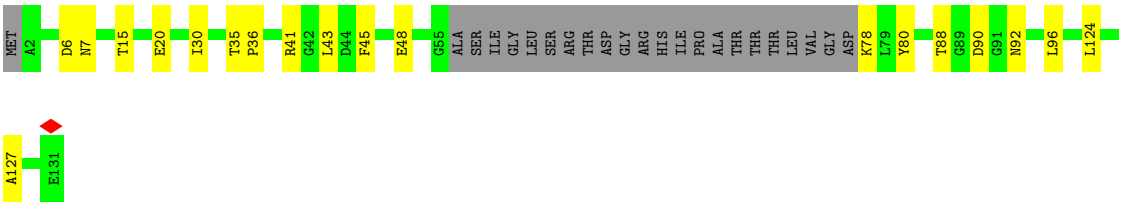
- Molecule 5: Flagellar basal body rod protein FlgB

Chain AU:



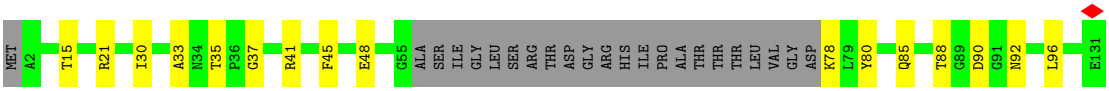
- Molecule 5: Flagellar basal body rod protein FlgB

Chain AV:



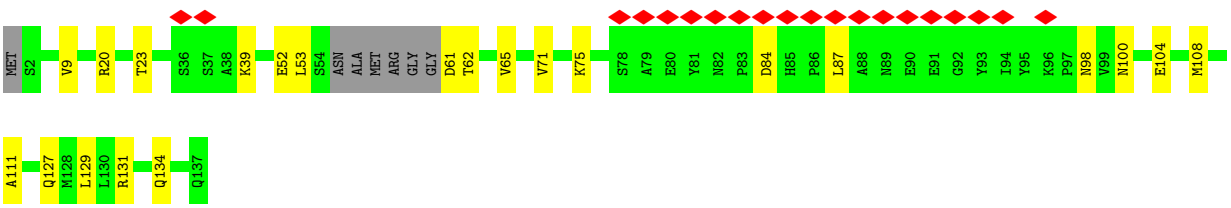
- Molecule 5: Flagellar basal body rod protein FlgB

Chain AW:



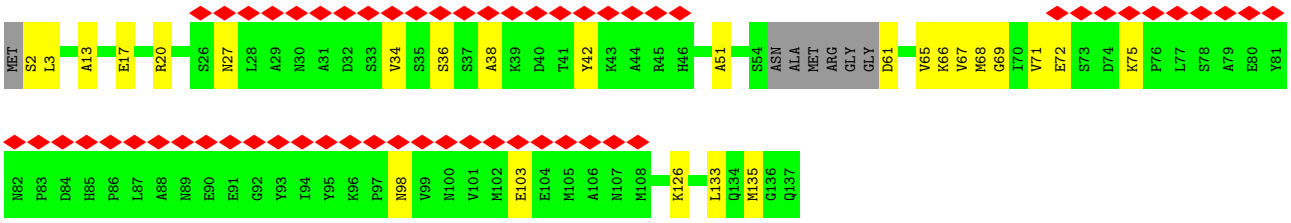
• Molecule 6: Flagellar basal-body rod protein FlgC

Chain AX:



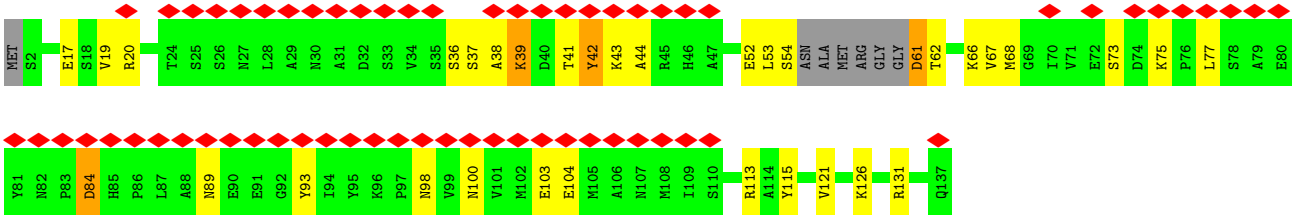
• Molecule 6: Flagellar basal-body rod protein FlgC

Chain AY:



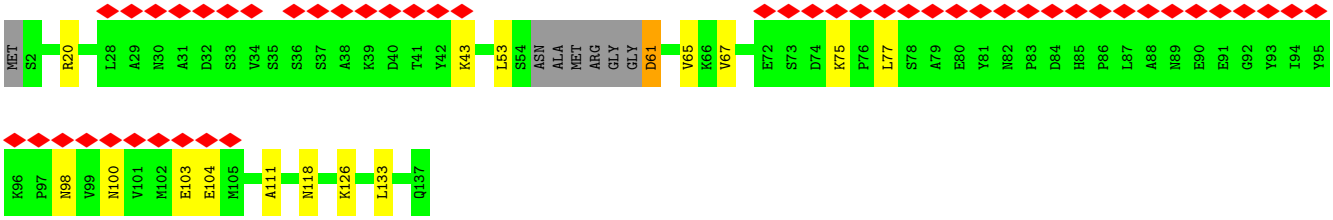
• Molecule 6: Flagellar basal-body rod protein FlgC

Chain AZ:



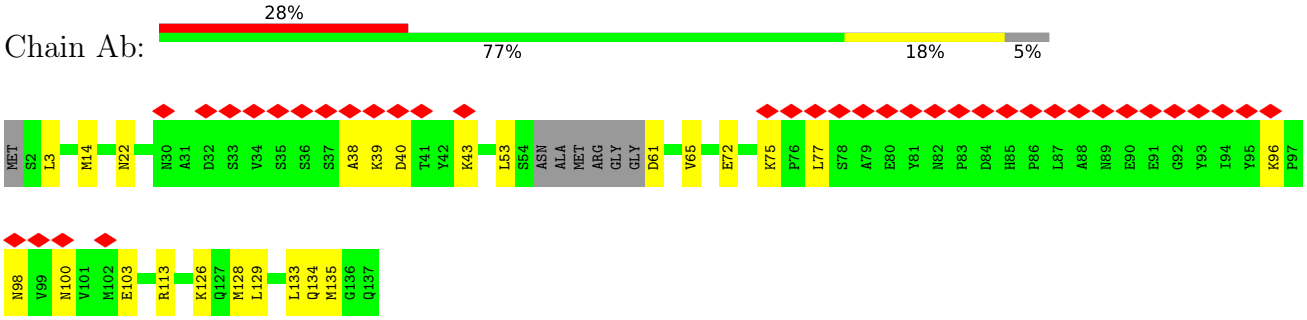
• Molecule 6: Flagellar basal-body rod protein FlgC

Chain Aa:



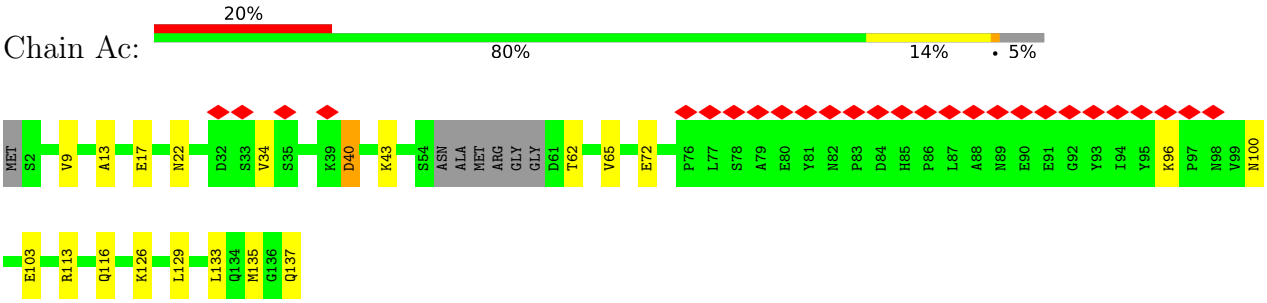
• Molecule 6: Flagellar basal-body rod protein FlgC

Chain Ab:



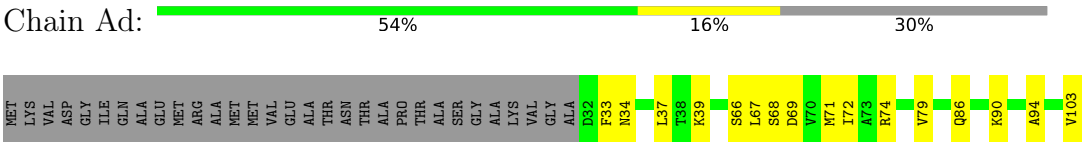
- Molecule 6: Flagellar basal-body rod protein FlgC

Chain Ac:



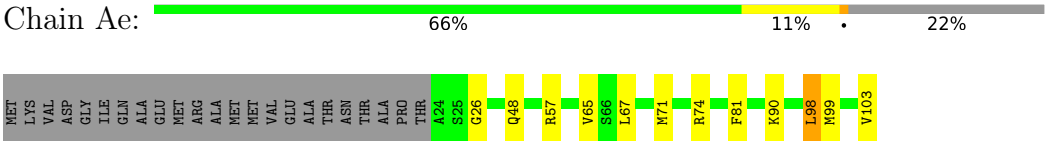
- Molecule 7: Flagellar hook-basal body complex protein FliE

Chain Ad:



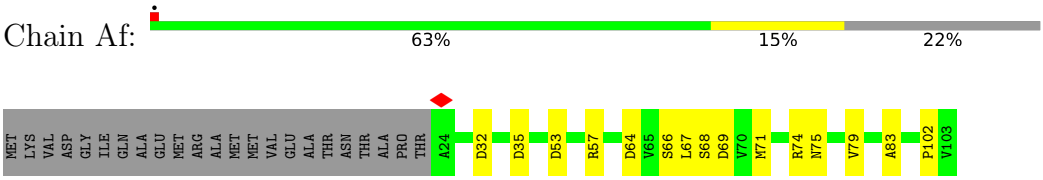
- Molecule 7: Flagellar hook-basal body complex protein FliE

Chain Ae:



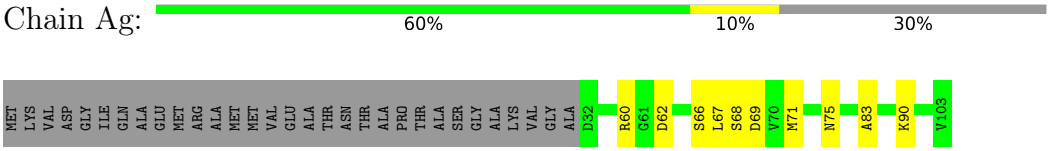
- Molecule 7: Flagellar hook-basal body complex protein FliE

Chain Af:



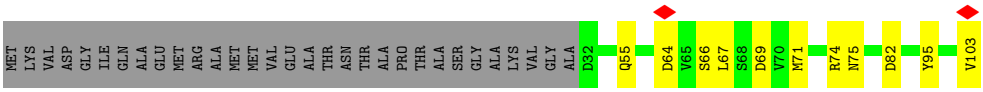
- Molecule 7: Flagellar hook-basal body complex protein FliE

Chain Ag:



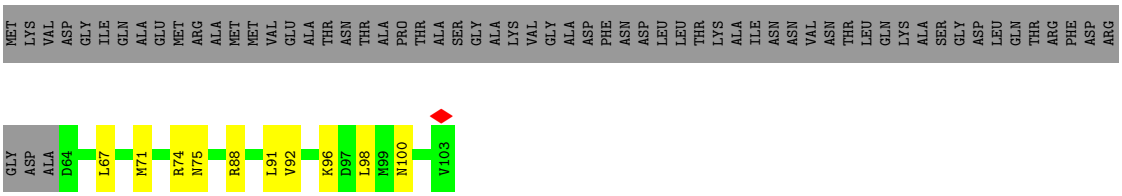
- Molecule 7: Flagellar hook-basal body complex protein FliE

Chain Ah:



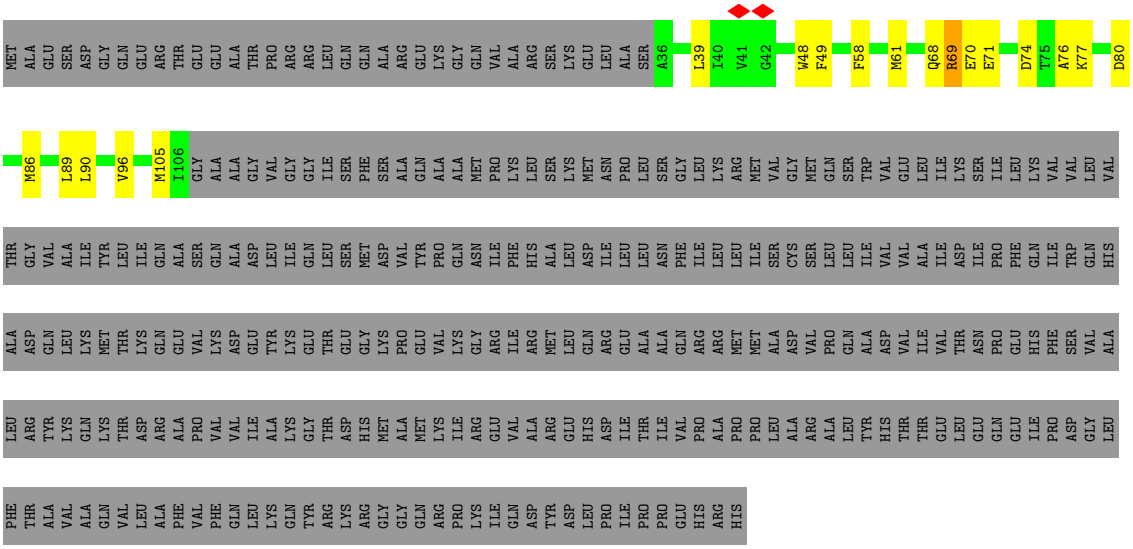
• Molecule 7: Flagellar hook-basal body complex protein FliE

Chain Ai:



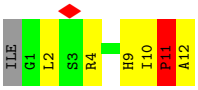
• Molecule 8: Flagellar biosynthetic protein FlhB

Chain Aj:



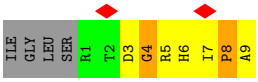
• Molecule 9: Alanine-modelled FlgB-Dc loop

Chain Am:



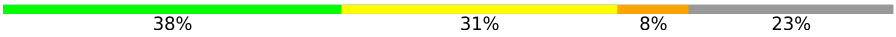
• Molecule 9: Alanine-modelled FlgB-Dc loop

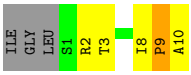
Chain An:



- Molecule 9: Alanine-modelled FlgB-Dc loop

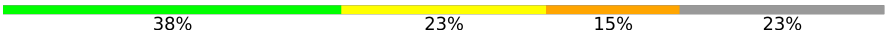
Chain Ao:

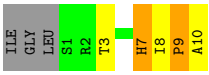




- Molecule 9: Alanine-modelled FlgB-Dc loop

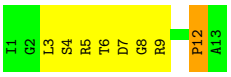
Chain Ap:





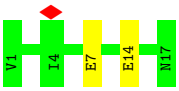
- Molecule 9: Alanine-modelled FlgB-Dc loop

Chain Aq:



- Molecule 10: FliE-helix 1

Chain Ar:

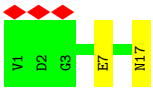


- Molecule 10: FliE-helix 1

Chain As:

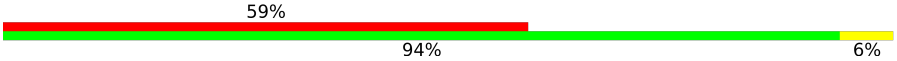
- Molecule 10: FliE-helix 1

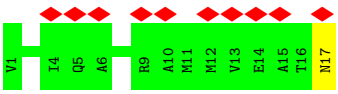
Chain At:



- Molecule 10: FliE-helix 1

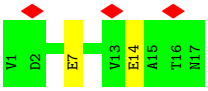
Chain Au:



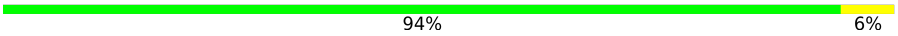


• Molecule 10: FliE-helix 1

Chain Av:



• Molecule 10: FliE-helix 1

Chain Aw: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58418	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.065	Depositor
Minimum map value	-0.657	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	744.0, 744.0, 744.0	wwPDB
Map dimensions	620, 620, 620	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	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	0.16	0/1637	0.33	0/2221
1	9	0.14	0/1628	0.30	0/2209
1	AP	0.10	0/1637	0.26	0/2221
1	Ak	0.11	0/1637	0.27	0/2221
1	Al	0.12	0/1637	0.28	0/2221
2	1	0.16	0/1182	0.27	0/1588
2	2	0.16	0/1182	0.27	0/1588
2	3	0.16	0/1182	0.27	0/1588
2	4	0.16	0/1182	0.27	0/1588
2	5	0.16	0/1182	0.27	0/1588
2	A	0.16	0/1182	0.27	0/1588
2	AA	0.35	0/137	0.45	0/188
2	AB	0.29	0/137	0.43	0/188
2	AC	0.14	0/141	0.31	0/193
2	AD	0.31	0/137	0.46	0/188
2	AE	0.13	0/137	0.28	0/188
2	AF	0.92	0/161	1.23	0/221
2	AG	0.16	0/75	0.32	0/103
2	AH	0.20	0/75	0.41	0/103
2	AI	0.95	0/75	1.34	0/103
2	AJ	0.37	0/166	0.57	0/228
2	AK	0.32	0/172	0.70	0/237
2	AL	0.39	0/223	0.61	0/304
2	AM	0.20	0/227	0.44	0/309
2	AN	0.24	0/227	0.49	0/309
2	AO	0.17	0/223	0.40	0/304
2	B	0.16	0/1182	0.27	0/1588
2	C	0.16	0/1182	0.27	0/1588
2	D	0.16	0/1182	0.27	0/1588
2	E	0.16	0/1182	0.27	0/1588
2	F	0.16	0/1182	0.27	0/1588
2	G	0.16	0/1182	0.27	0/1588
2	H	0.16	0/1182	0.27	0/1588
2	I	0.16	0/1182	0.27	0/1588

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	J	0.16	0/1182	0.27	0/1588
2	K	0.16	0/1182	0.27	0/1588
2	L	0.16	0/1182	0.27	0/1588
2	M	0.16	0/1182	0.27	0/1588
2	N	0.16	0/1182	0.27	0/1588
2	O	0.16	0/1182	0.27	0/1588
2	P	0.16	0/1182	0.27	0/1588
2	Q	0.16	0/1182	0.27	0/1588
2	R	0.16	0/1182	0.27	0/1588
2	S	0.33	0/888	0.56	0/1192
2	T	0.30	0/888	0.44	0/1192
2	U	0.21	0/888	0.37	0/1192
2	V	0.22	0/888	0.40	0/1192
2	W	0.21	0/888	0.41	0/1192
2	X	0.23	0/844	0.41	0/1131
2	Y	0.29	0/888	0.48	0/1192
2	Z	0.29	0/888	0.44	0/1192
2	a	0.21	0/888	0.40	0/1192
2	b	0.22	0/727	0.40	0/974
2	c	0.26	0/810	0.44	0/1087
2	d	0.27	0/810	0.44	0/1087
2	e	0.16	0/810	0.38	0/1087
2	f	0.13	0/661	0.31	0/884
2	g	0.14	0/706	0.35	0/946
2	h	0.14	0/697	0.34	0/934
2	i	0.14	0/685	0.33	0/917
2	j	0.16	0/706	0.35	0/946
2	k	0.22	0/888	0.38	0/1192
2	l	0.24	0/888	0.45	0/1192
2	m	0.20	0/888	0.35	0/1192
2	n	0.19	0/805	0.37	0/1078
2	o	0.20	0/888	0.40	0/1192
2	p	0.16	0/1182	0.27	0/1588
2	q	0.16	0/1182	0.27	0/1588
2	r	0.16	0/1182	0.27	0/1588
2	s	0.16	0/1182	0.27	0/1588
2	t	0.16	0/1182	0.27	0/1588
2	u	0.16	0/1182	0.27	0/1588
2	v	0.16	0/1182	0.27	0/1588
2	w	0.16	0/1182	0.27	0/1588
2	x	0.16	0/1182	0.27	0/1588
2	y	0.16	0/1182	0.27	0/1588
2	z	0.16	0/1182	0.27	0/1588

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	6	0.28	0/739	0.49	0/1005
3	7	0.16	0/739	0.33	0/1005
3	AQ	0.12	0/739	0.31	0/1005
3	AR	0.17	0/739	0.34	0/1005
4	8	0.09	0/1941	0.25	0/2631
5	AS	0.23	0/856	0.36	0/1151
5	AT	0.22	0/846	0.30	0/1138
5	AU	0.24	0/856	0.31	0/1151
5	AV	0.19	0/848	0.31	0/1140
5	AW	0.22	0/848	0.35	0/1140
6	AX	0.11	0/996	0.27	0/1348
6	AY	0.11	0/996	0.26	0/1348
6	AZ	0.30	0/996	0.46	0/1348
6	Aa	0.10	0/996	0.24	0/1348
6	Ab	0.11	0/996	0.28	0/1348
6	Ac	0.14	0/996	0.30	0/1348
7	Ad	0.32	0/564	0.43	0/759
7	Ae	0.08	0/609	0.20	0/819
7	Af	0.08	0/609	0.17	0/819
7	Ag	0.08	0/564	0.16	0/759
7	Ah	0.08	0/564	0.18	0/759
7	Ai	0.10	0/313	0.19	0/420
8	Aj	0.08	0/562	0.19	0/760
9	Am	1.13	0/57	1.46	1/77 (1.3%)
9	An	1.26	0/43	1.85	1/58 (1.7%)
9	Ao	1.22	0/48	1.61	1/65 (1.5%)
9	Ap	1.09	0/48	1.55	1/65 (1.5%)
9	Aq	1.19	0/62	1.42	1/84 (1.2%)
10	Ar	1.12	0/83	1.44	0/114
10	As	1.11	0/83	1.44	0/114
10	At	1.12	0/83	1.45	0/114
10	Au	1.11	0/83	1.45	0/114
10	Av	1.11	0/83	1.45	0/114
10	Aw	1.11	0/83	1.44	0/114
All	All	0.21	0/89262	0.35	5/120213 (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
1	0	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	T	0	1
2	c	0	1
2	d	0	1
2	l	0	1
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	An	8	PRO	N-CA-CB	10.53	109.83	102.35
9	Ap	9	PRO	N-CA-CB	6.81	109.66	103.33
9	Am	11	PRO	N-CA-CB	6.73	110.31	103.25
9	Ao	9	PRO	N-CA-CB	6.10	109.75	103.23
9	Aq	12	PRO	N-CA-CB	5.81	109.35	103.25

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	188	ARG	Sidechain
2	T	194	ARG	Sidechain
2	c	194	ARG	Sidechain
2	d	236	ARG	Sidechain
2	l	194	ARG	Sidechain

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	1608	0	1691	45	0
1	9	1599	0	1685	42	0
1	AP	1608	0	1691	37	0
1	Ak	1608	0	1691	66	0
1	Al	1608	0	1691	55	0
2	1	1171	0	1164	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	1171	0	1164	13	0
2	3	1171	0	1164	15	0
2	4	1171	0	1164	16	0
2	5	1171	0	1164	14	0
2	A	1171	0	1164	20	0
2	AA	135	0	128	2	0
2	AB	135	0	128	3	0
2	AC	139	0	131	4	0
2	AD	135	0	128	7	0
2	AE	135	0	128	1	0
2	AF	158	0	152	13	0
2	AG	73	0	72	4	0
2	AH	73	0	72	3	0
2	AI	73	0	72	8	0
2	AJ	163	0	157	3	0
2	AK	169	0	164	6	0
2	AL	220	0	215	3	0
2	AM	224	0	218	4	0
2	AN	224	0	218	2	0
2	AO	220	0	215	3	0
2	B	1171	0	1164	15	0
2	C	1171	0	1164	13	0
2	D	1171	0	1164	12	0
2	E	1171	0	1164	15	0
2	F	1171	0	1164	23	0
2	G	1171	0	1164	20	0
2	H	1171	0	1164	23	0
2	I	1171	0	1164	15	0
2	J	1171	0	1164	16	0
2	K	1171	0	1164	13	0
2	L	1171	0	1164	11	0
2	M	1171	0	1164	18	0
2	N	1171	0	1164	22	0
2	O	1171	0	1164	14	0
2	P	1171	0	1164	14	0
2	Q	1171	0	1164	14	0
2	R	1171	0	1164	11	0
2	S	881	0	910	59	0
2	T	881	0	910	62	0
2	U	881	0	910	35	0
2	V	881	0	910	35	0
2	W	881	0	910	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	839	0	864	30	0
2	Y	881	0	910	56	0
2	Z	881	0	910	38	0
2	a	881	0	910	40	0
2	b	724	0	758	33	0
2	c	803	0	837	45	0
2	d	803	0	837	40	0
2	e	803	0	837	35	0
2	f	660	0	699	22	0
2	g	704	0	741	27	0
2	h	695	0	735	29	0
2	i	684	0	725	31	0
2	j	704	0	741	28	0
2	k	881	0	910	60	0
2	l	881	0	910	39	0
2	m	881	0	910	39	0
2	n	802	0	836	36	0
2	o	881	0	910	37	0
2	p	1171	0	1164	13	0
2	q	1171	0	1164	16	0
2	r	1171	0	1164	14	0
2	s	1171	0	1164	16	0
2	t	1171	0	1164	15	0
2	u	1171	0	1164	13	0
2	v	1171	0	1164	15	0
2	w	1171	0	1164	14	0
2	x	1171	0	1164	22	0
2	y	1171	0	1164	13	0
2	z	1171	0	1164	14	0
3	6	722	0	768	36	0
3	7	722	0	768	40	0
3	AQ	722	0	768	29	0
3	AR	722	0	768	31	0
4	8	1896	0	1968	49	0
5	AS	845	0	833	11	0
5	AT	835	0	825	18	0
5	AU	845	0	833	11	0
5	AV	837	0	829	10	0
5	AW	837	0	829	10	0
6	AX	983	0	958	12	0
6	AY	983	0	958	18	0
6	AZ	983	0	958	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Aa	983	0	958	8	0
6	Ab	983	0	958	15	0
6	Ac	983	0	958	11	0
7	Ad	560	0	561	11	0
7	Ae	605	0	609	10	0
7	Af	605	0	609	10	0
7	Ag	560	0	561	7	0
7	Ah	560	0	561	10	0
7	Ai	311	0	320	8	0
8	Aj	552	0	577	22	0
9	Am	58	0	30	7	0
9	An	44	0	23	12	0
9	Ao	49	0	25	14	0
9	Ap	49	0	25	7	0
9	Aq	63	0	32	5	0
10	Ar	84	0	46	6	0
10	As	84	0	46	3	0
10	At	84	0	46	4	0
10	Au	84	0	46	1	0
10	Av	84	0	46	2	0
10	Aw	84	0	46	4	0
All	All	88315	0	88899	1692	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 10.

All (1692) 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)
3:7:64:LEU:HD11	2:T:148:PHE:CE1	1.54	1.42
3:AQ:15:TRP:CD1	2:m:148:PHE:HE2	1.51	1.27
1:Ak:288:ALA:CB	2:m:192:PHE:HA	1.63	1.26
2:x:306:THR:HG21	10:At:17:ASN:CB	1.66	1.25
1:9:189:ILE:HD11	2:c:192:PHE:C	1.59	1.25
1:9:189:ILE:CD1	2:c:192:PHE:C	2.09	1.25
1:Ak:206:PRO:HA	2:k:192:PHE:HE2	1.10	1.13
1:9:189:ILE:HD11	2:c:192:PHE:O	1.51	1.11
1:Ak:206:PRO:CA	2:k:192:PHE:CE2	2.35	1.10
1:0:185:LYS:CD	2:Y:194:ARG:NH1	2.14	1.10
3:AQ:15:TRP:CD1	2:m:148:PHE:CE2	2.41	1.09
1:0:189:ILE:HD13	2:Y:193:VAL:HG22	1.36	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:306:THR:HG21	10:Ar:7:GLU:CB	1.82	1.08
1:Ak:206:PRO:HA	2:k:192:PHE:CE2	1.89	1.07
8:Aj:74:ASP:OD2	2:j:152:GLN:HG2	1.55	1.07
1:Ak:206:PRO:HB3	2:k:192:PHE:CE2	1.89	1.06
6:AZ:52:GLU:HG3	6:AZ:52:GLU:O	1.47	1.06
3:7:64:LEU:HD11	2:T:148:PHE:CD1	1.89	1.06
1:Ak:206:PRO:HB3	2:k:192:PHE:CD2	1.91	1.06
1:0:185:LYS:CD	2:Y:194:ARG:HH12	1.69	1.05
3:6:15:TRP:CZ2	2:b:148:PHE:HE2	1.74	1.04
2:N:381:ILE:HG21	10:Aw:3:GLY:HA2	1.36	1.03
3:7:64:LEU:HD11	2:T:148:PHE:CZ	1.96	1.01
8:Aj:76:ALA:HB3	2:j:152:GLN:HE21	1.26	1.01
1:0:189:ILE:CD1	2:Y:193:VAL:HG22	1.89	1.00
1:9:206:PRO:HG3	2:d:192:PHE:CD2	1.95	1.00
1:Ak:197:THR:HG21	2:V:194:ARG:HG2	1.39	1.00
3:6:15:TRP:CZ2	2:b:148:PHE:CE2	2.51	0.99
1:Ak:206:PRO:CB	2:k:192:PHE:CE2	2.46	0.98
3:AR:71:GLN:NE2	2:V:151:SER:HB2	1.76	0.98
1:0:185:LYS:HD2	2:Y:194:ARG:NH1	1.78	0.97
3:6:68:TRP:CZ2	2:a:148:PHE:HZ	1.81	0.97
1:Al:206:PRO:HG3	2:S:192:PHE:CG	2.00	0.96
1:Ak:288:ALA:HB3	2:m:192:PHE:CD1	2.00	0.96
3:AQ:89:TYR:HE2	2:l:188:LYS:HB2	1.28	0.95
1:Ak:288:ALA:HB3	2:m:192:PHE:HA	1.44	0.94
6:AZ:52:GLU:O	6:AZ:52:GLU:CG	2.15	0.94
3:7:64:LEU:CD1	2:T:148:PHE:CD1	2.50	0.94
2:N:381:ILE:HG21	10:Aw:3:GLY:CA	1.96	0.94
1:AP:205:ASN:HD22	2:o:194:ARG:HH12	1.12	0.94
3:AQ:15:TRP:CG	2:m:148:PHE:CE2	2.56	0.94
2:F:306:THR:HG21	10:Ar:14:GLU:CB	1.97	0.94
1:Ak:288:ALA:HB3	2:m:192:PHE:HD1	1.29	0.94
1:Ak:288:ALA:HB1	2:m:192:PHE:HA	1.46	0.94
2:G:374:ASN:OD1	9:Ao:3:THR:N	2.01	0.94
3:7:64:LEU:CD1	2:T:148:PHE:CE1	2.49	0.93
1:9:189:ILE:HD11	2:c:193:VAL:N	1.85	0.92
1:0:185:LYS:HD3	2:Y:194:ARG:NH1	1.80	0.92
2:H:374:ASN:OD1	9:Ao:8:ILE:CB	2.17	0.91
1:Ak:206:PRO:CB	2:k:192:PHE:CD2	2.52	0.91
3:AQ:15:TRP:CG	2:m:148:PHE:HE2	1.88	0.90
1:AP:205:ASN:HD22	2:o:194:ARG:NH1	1.69	0.90
1:Ak:189:ILE:HD11	2:k:192:PHE:CD1	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AD:341:ASN:ND2	2:F:366:SER:H	1.69	0.88
2:x:372:THR:CG2	9:Am:10:ILE:CB	2.50	0.88
3:7:89:TYR:CD2	2:Y:190:SER:HB2	2.09	0.88
1:9:189:ILE:HD11	2:c:193:VAL:CA	2.03	0.87
1:9:189:ILE:CD1	2:c:192:PHE:O	2.18	0.87
2:A:374:ASN:ND2	9:An:7:ILE:CB	2.38	0.87
1:9:189:ILE:CD1	2:c:193:VAL:N	2.38	0.86
3:7:71:GLN:NE2	2:W:151:SER:HB2	1.89	0.86
3:7:71:GLN:HG2	2:S:152:GLN:OE1	1.74	0.85
3:AQ:71:GLN:OE1	2:n:151:SER:CB	2.25	0.84
3:AQ:89:TYR:CE2	2:l:188:LYS:HB2	2.12	0.84
2:H:319:SER:HB3	9:Ao:3:THR:CB	2.08	0.84
1:9:206:PRO:HG3	2:d:192:PHE:CE2	2.11	0.83
2:H:374:ASN:OD1	9:Ao:8:ILE:HA	1.77	0.83
3:6:85:PRO:HD3	2:a:192:PHE:CZ	2.14	0.82
8:Aj:68:GLN:OE1	2:i:152:GLN:HG2	1.79	0.82
1:9:189:ILE:HD11	2:c:193:VAL:HA	1.59	0.82
1:Al:197:THR:CB	2:W:194:ARG:HG2	2.11	0.81
3:6:68:TRP:CZ2	2:a:148:PHE:CZ	2.67	0.81
2:AC:342:GLN:NE2	2:M:327:ASN:ND2	2.29	0.81
2:x:372:THR:HG21	9:Am:10:ILE:CB	2.09	0.81
3:6:88:LEU:O	2:c:192:PHE:CE1	2.34	0.80
1:Ak:82:ASP:HB3	1:Ak:167:THR:HG23	1.62	0.80
8:Aj:76:ALA:CB	2:j:152:GLN:HE21	1.95	0.80
3:6:85:PRO:HD3	2:a:192:PHE:CE2	2.18	0.79
2:AC:342:GLN:NE2	2:M:327:ASN:HD22	1.80	0.79
1:Ak:207:GLU:OE2	2:k:194:ARG:NH1	2.15	0.79
2:H:374:ASN:OD1	9:Ao:8:ILE:CA	2.30	0.78
2:S:146:MET:HB2	2:S:150:VAL:HG21	1.66	0.78
2:i:163:ARG:NH2	2:j:184:LEU:O	2.17	0.78
1:Ak:206:PRO:CA	2:k:192:PHE:HE2	1.80	0.77
2:AC:342:GLN:HE22	2:M:327:ASN:ND2	1.83	0.77
1:9:189:ILE:HD12	2:c:192:PHE:C	2.06	0.77
1:Al:189:ILE:HD11	2:S:190:SER:HB2	1.65	0.77
2:G:374:ASN:OD1	9:Ao:2:ARG:C	2.28	0.77
2:Z:206:THR:HA	2:Z:242:GLN:HG2	1.66	0.77
1:Al:206:PRO:HD3	2:S:192:PHE:HB3	1.67	0.76
2:A:372:THR:HG21	9:An:7:ILE:H	1.50	0.75
2:S:163:ARG:NH2	2:W:184:LEU:O	2.19	0.75
3:6:64:LEU:HD21	2:Z:148:PHE:HE2	1.51	0.75
3:AR:71:GLN:HE22	2:V:151:SER:HB2	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:206:PRO:N	2:k:192:PHE:CD2	2.55	0.74
3:7:71:GLN:HE22	2:W:151:SER:HB2	1.52	0.74
2:T:201:ALA:HB2	2:T:232:MET:HE1	1.70	0.74
1:Ak:197:THR:CG2	2:V:194:ARG:HG2	2.17	0.74
2:f:163:ARG:NH2	2:f:228:ALA:O	2.20	0.74
1:0:206:PRO:HG2	2:Z:194:ARG:HH11	1.51	0.74
2:A:374:ASN:OD1	9:An:5:ARG:CB	2.36	0.73
2:P:258:ALA:HA	2:P:261:LYS:HD2	1.70	0.73
2:w:258:ALA:HA	2:w:261:LYS:HD2	1.70	0.73
2:z:258:ALA:HA	2:z:261:LYS:HD2	1.70	0.73
2:p:258:ALA:HA	2:p:261:LYS:HD2	1.70	0.73
2:t:258:ALA:HA	2:t:261:LYS:HD2	1.70	0.73
2:F:258:ALA:HA	2:F:261:LYS:HD2	1.70	0.73
2:Q:258:ALA:HA	2:Q:261:LYS:HD2	1.70	0.73
2:s:258:ALA:HA	2:s:261:LYS:HD2	1.70	0.73
2:i:220:SER:HA	2:j:246:LEU:HD12	1.71	0.73
2:q:258:ALA:HA	2:q:261:LYS:HD2	1.70	0.73
2:v:258:ALA:HA	2:v:261:LYS:HD2	1.70	0.73
2:3:258:ALA:HA	2:3:261:LYS:HD2	1.70	0.73
2:y:258:ALA:HA	2:y:261:LYS:HD2	1.70	0.73
2:a:163:ARG:HA	2:a:166:GLN:HE21	1.53	0.73
2:d:171:ILE:HG22	2:d:177:VAL:HG11	1.68	0.73
2:H:258:ALA:HA	2:H:261:LYS:HD2	1.70	0.72
2:M:258:ALA:HA	2:M:261:LYS:HD2	1.70	0.72
2:C:258:ALA:HA	2:C:261:LYS:HD2	1.70	0.72
2:D:258:ALA:HA	2:D:261:LYS:HD2	1.70	0.72
2:E:258:ALA:HA	2:E:261:LYS:HD2	1.70	0.72
2:N:258:ALA:HA	2:N:261:LYS:HD2	1.70	0.72
2:x:258:ALA:HA	2:x:261:LYS:HD2	1.70	0.72
2:j:218:VAL:HG21	2:j:247:LEU:HB3	1.71	0.72
2:2:258:ALA:HA	2:2:261:LYS:HD2	1.70	0.72
2:G:258:ALA:HA	2:G:261:LYS:HD2	1.71	0.72
2:I:258:ALA:HA	2:I:261:LYS:HD2	1.70	0.72
2:R:258:ALA:HA	2:R:261:LYS:HD2	1.70	0.72
2:1:258:ALA:HA	2:1:261:LYS:HD2	1.71	0.72
1:Ak:206:PRO:CD	2:k:192:PHE:HD2	2.03	0.72
2:O:258:ALA:HA	2:O:261:LYS:HD2	1.70	0.72
2:m:139:ASP:OD1	2:m:139:ASP:N	2.20	0.72
2:B:258:ALA:HA	2:B:261:LYS:HD2	1.70	0.72
2:u:258:ALA:HA	2:u:261:LYS:HD2	1.70	0.72
2:A:258:ALA:HA	2:A:261:LYS:HD2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:89:TYR:O	2:Y:192:PHE:CE2	2.43	0.71
2:AK:330:ASN:N	2:x:368:ARG:HD2	2.05	0.71
2:z:381:ILE:HG21	10:At:7:GLU:CB	2.19	0.71
2:r:258:ALA:HA	2:r:261:LYS:HD2	1.70	0.71
2:5:258:ALA:HA	2:5:261:LYS:HD2	1.70	0.71
2:K:258:ALA:HA	2:K:261:LYS:HD2	1.70	0.71
2:J:258:ALA:HA	2:J:261:LYS:HD2	1.70	0.71
2:n:201:ALA:HB2	2:n:232:MET:HE1	1.72	0.71
3:AQ:25:ILE:HG13	3:AR:52:LEU:HD12	1.73	0.71
2:p:306:THR:HG21	10:Av:14:GLU:CB	2.21	0.71
3:6:15:TRP:HZ2	2:b:148:PHE:HE2	1.35	0.70
2:L:258:ALA:HA	2:L:261:LYS:HD2	1.70	0.70
2:a:163:ARG:HH22	2:b:183:LEU:HB3	1.56	0.70
2:4:258:ALA:HA	2:4:261:LYS:HD2	1.70	0.70
3:AR:19:ILE:HD13	2:V:148:PHE:CZ	2.25	0.70
2:A:374:ASN:HD21	9:An:7:ILE:CB	2.05	0.70
1:Ak:206:PRO:CA	2:k:192:PHE:CD2	2.73	0.70
3:7:64:LEU:HD12	2:T:148:PHE:CG	2.26	0.70
1:Al:197:THR:HB	2:W:194:ARG:HG2	1.72	0.70
2:l:201:ALA:HB2	2:l:232:MET:HE1	1.74	0.70
1:Ak:187:THR:O	2:l:192:PHE:HA	1.92	0.70
1:Ak:288:ALA:CB	2:m:192:PHE:CA	2.58	0.70
4:8:243:MET:CE	2:e:151:SER:HB2	2.21	0.70
1:Ak:206:PRO:N	2:k:192:PHE:HD2	1.89	0.70
3:6:68:TRP:CE2	2:a:148:PHE:HZ	2.09	0.69
1:Al:189:ILE:HD11	2:S:190:SER:CB	2.22	0.69
2:W:146:MET:N	2:W:146:MET:SD	2.64	0.69
2:j:163:ARG:HA	2:j:166:GLN:HE21	1.57	0.69
1:0:185:LYS:CD	2:Y:194:ARG:HH11	2.05	0.69
4:8:47:LEU:HD21	7:Ae:98:LEU:HD21	1.72	0.69
7:Ah:103:VAL:O	1:Ak:120:ARG:NH2	2.25	0.69
2:m:163:ARG:HA	2:m:166:GLN:HE21	1.57	0.68
6:Ac:40:ASP:OD1	6:Ac:40:ASP:N	2.26	0.68
2:W:220:SER:HA	2:X:246:LEU:HD12	1.76	0.68
2:AL:341:ASN:ND2	5:AT:88:THR:OG1	2.27	0.68
2:V:199:ALA:O	2:V:236:ARG:NE	2.25	0.68
1:Ak:197:THR:HG21	2:V:194:ARG:CG	2.22	0.68
2:o:146:MET:N	2:o:146:MET:SD	2.67	0.68
7:Ad:103:VAL:HG23	1:Al:113:VAL:HG13	1.76	0.68
2:U:187:PRO:HB3	2:U:197:GLN:HB2	1.76	0.68
3:6:71:GLN:HE22	2:a:151:SER:CB	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AD:341:ASN:HD21	2:F:366:SER:H	1.39	0.68
2:AF:335:ILE:HG13	2:AF:338:ALA:HB2	1.74	0.68
1:Ak:185:LYS:O	2:l:194:ARG:NH1	2.27	0.68
2:e:213:LEU:HD22	2:e:217:GLU:HG3	1.76	0.68
4:8:92:MET:HE2	4:8:248:GLY:HA3	1.76	0.67
1:9:189:ILE:CD1	2:c:193:VAL:CA	2.72	0.67
2:T:152:GLN:NE2	2:T:156:GLN:OE1	2.27	0.67
2:Z:201:ALA:HB2	2:Z:232:MET:HE1	1.74	0.67
3:7:64:LEU:CD1	2:T:148:PHE:CG	2.77	0.67
3:7:64:LEU:CD1	2:T:148:PHE:CZ	2.74	0.67
2:C:324:GLU:HG3	2:C:369:LYS:HD2	1.77	0.67
2:U:178:ARG:NH1	2:U:207:LEU:O	2.27	0.67
2:c:178:ARG:NH1	2:c:207:LEU:O	2.28	0.67
2:F:324:GLU:HG3	2:F:369:LYS:HD2	1.77	0.67
2:P:324:GLU:HG3	2:P:369:LYS:HD2	1.77	0.67
2:W:163:ARG:NH2	2:X:184:LEU:O	2.28	0.67
2:M:324:GLU:HG3	2:M:369:LYS:HD2	1.77	0.67
2:N:324:GLU:HG3	2:N:369:LYS:HD2	1.77	0.67
1:0:189:ILE:HD13	2:Y:193:VAL:CG2	2.20	0.67
2:B:324:GLU:HG3	2:B:369:LYS:HD2	1.77	0.67
2:D:324:GLU:HG3	2:D:369:LYS:HD2	1.77	0.67
2:E:324:GLU:HG3	2:E:369:LYS:HD2	1.77	0.67
2:Q:324:GLU:HG3	2:Q:369:LYS:HD2	1.77	0.67
2:n:218:VAL:HG21	2:n:247:LEU:HB3	1.77	0.67
1:9:189:ILE:CD1	2:c:193:VAL:HA	2.25	0.67
1:Ak:206:PRO:CD	2:k:192:PHE:CD2	2.78	0.67
1:Al:197:THR:HG21	2:W:194:ARG:HG2	1.77	0.67
2:I:324:GLU:HG3	2:I:369:LYS:HD2	1.77	0.67
1:0:244:VAL:HG11	1:0:262:SER:HB2	1.77	0.66
3:7:48:THR:OG1	3:AR:54:ARG:NH1	2.28	0.66
1:Al:197:THR:CG2	2:W:194:ARG:HG2	2.25	0.66
2:G:324:GLU:HG3	2:G:369:LYS:HD2	1.77	0.66
2:J:324:GLU:HG3	2:J:369:LYS:HD2	1.77	0.66
2:K:324:GLU:HG3	2:K:369:LYS:HD2	1.77	0.66
2:L:324:GLU:HG3	2:L:369:LYS:HD2	1.77	0.66
2:O:324:GLU:HG3	2:O:369:LYS:HD2	1.77	0.66
2:R:324:GLU:HG3	2:R:369:LYS:HD2	1.77	0.66
2:X:139:ASP:OD2	2:Y:165:ARG:NH2	2.28	0.66
2:i:220:SER:HB3	2:j:246:LEU:HB2	1.76	0.66
2:5:324:GLU:HG3	2:5:369:LYS:HD2	1.77	0.66
2:T:241:ASP:OD1	2:T:244:GLY:N	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:324:GLU:HG3	2:x:369:LYS:HD2	1.77	0.66
2:AA:355:GLN:O	2:AA:356:MET:HB3	1.94	0.66
2:q:306:THR:HG21	10:Av:7:GLU:CB	2.25	0.66
1:0:141:LEU:HG	1:Al:198:MET:HE1	1.78	0.66
2:A:324:GLU:HG3	2:A:369:LYS:HD2	1.77	0.66
2:H:324:GLU:HG3	2:H:369:LYS:HD2	1.77	0.66
2:m:201:ALA:HB2	2:m:232:MET:HE1	1.78	0.66
2:w:324:GLU:HG3	2:w:369:LYS:HD2	1.77	0.66
2:4:324:GLU:HG3	2:4:369:LYS:HD2	1.77	0.66
2:p:324:GLU:HG3	2:p:369:LYS:HD2	1.77	0.66
2:x:306:THR:CG2	10:At:17:ASN:CB	2.61	0.66
2:q:324:GLU:HG3	2:q:369:LYS:HD2	1.77	0.66
2:X:176:GLN:OE1	2:X:176:GLN:N	2.27	0.66
2:c:184:LEU:HD21	2:c:229:VAL:HG21	1.76	0.66
2:u:324:GLU:HG3	2:u:369:LYS:HD2	1.77	0.66
2:S:163:ARG:HD3	2:S:166:GLN:HE21	1.61	0.66
2:y:324:GLU:HG3	2:y:369:LYS:HD2	1.77	0.66
1:Al:197:THR:HG21	2:W:194:ARG:CG	2.26	0.66
2:k:165:ARG:NH2	2:l:139:ASP:OD2	2.28	0.66
2:t:324:GLU:HG3	2:t:369:LYS:HD2	1.77	0.66
2:z:324:GLU:HG3	2:z:369:LYS:HD2	1.77	0.66
2:1:324:GLU:HG3	2:1:369:LYS:HD2	1.77	0.65
1:AP:205:ASN:ND2	2:o:194:ARG:NH1	2.43	0.65
1:Ak:285:GLY:O	2:m:192:PHE:HB3	1.95	0.65
2:v:324:GLU:HG3	2:v:369:LYS:HD2	1.77	0.65
6:AZ:53:LEU:O	6:AZ:54:SER:C	2.38	0.65
6:Aa:75:LYS:O	6:Aa:98:ASN:ND2	2.29	0.65
2:d:241:ASP:OD2	2:d:245:ARG:NH1	2.29	0.65
3:7:89:TYR:O	2:Y:192:PHE:CD2	2.49	0.65
2:o:157:GLU:HA	2:o:160:LYS:HE2	1.78	0.65
2:3:324:GLU:HG3	2:3:369:LYS:HD2	1.77	0.65
2:e:176:GLN:OE1	2:e:176:GLN:N	2.29	0.65
2:r:324:GLU:HG3	2:r:369:LYS:HD2	1.77	0.65
2:s:324:GLU:HG3	2:s:369:LYS:HD2	1.77	0.65
2:2:324:GLU:HG3	2:2:369:LYS:HD2	1.77	0.65
1:Ak:103:VAL:O	1:Ak:107:THR:OG1	2.15	0.65
2:Y:241:ASP:OD1	2:Y:245:ARG:N	2.30	0.65
1:Ak:88:GLN:OE1	1:Ak:161:TYR:OH	2.14	0.65
1:0:185:LYS:CG	2:Y:194:ARG:HH12	2.10	0.65
2:T:239:VAL:HB	2:T:247:LEU:HB2	1.78	0.65
2:j:184:LEU:HD21	2:j:229:VAL:HG21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:185:ALA:O	2:n:199:ALA:HA	1.97	0.65
2:a:146:MET:N	2:a:146:MET:SD	2.70	0.64
3:AQ:89:TYR:CE2	2:l:190:SER:HB2	2.33	0.64
3:6:17:VAL:HG12	1:9:239:ILE:HG23	1.79	0.64
1:AP:198:MET:HE2	1:Ak:144:PHE:HB2	1.80	0.64
3:6:9:LEU:HD21	3:6:80:LEU:HD21	1.80	0.64
1:Al:244:VAL:HG11	1:Al:262:SER:HB3	1.79	0.64
2:V:178:ARG:NH1	2:V:207:LEU:O	2.31	0.64
2:W:194:ARG:H	2:W:194:ARG:HE	1.43	0.64
2:H:319:SER:HB3	9:Ao:3:THR:H	1.62	0.64
9:Ao:9:PRO:O	9:Ao:10:ALA:C	2.41	0.64
4:8:186:SER:HA	4:8:189:LEU:HD23	1.80	0.63
2:AI:335:ILE:HG13	2:AI:338:ALA:HB2	1.78	0.63
1:Ak:204:ASP:O	2:k:192:PHE:HA	1.97	0.63
1:Al:187:THR:O	2:T:192:PHE:HB3	1.98	0.63
3:7:50:SER:O	3:7:54:ARG:NH1	2.31	0.63
1:0:184:LEU:HG	1:0:214:LEU:HD11	1.81	0.63
3:6:71:GLN:HE22	2:a:151:SER:HB3	1.62	0.63
2:d:178:ARG:NH1	2:d:207:LEU:O	2.30	0.63
2:t:306:THR:HG21	10:Au:17:ASN:CB	2.28	0.63
1:9:85:VAL:HA	1:9:88:GLN:HE21	1.63	0.63
1:9:183:MET:HE1	1:9:215:ILE:HG12	1.80	0.63
2:F:306:THR:CG2	10:Ar:14:GLU:CB	2.74	0.63
2:b:164:GLU:HG2	2:b:184:LEU:HD13	1.80	0.63
2:m:246:LEU:HD12	2:n:220:SER:HA	1.80	0.63
2:o:153:ARG:HA	2:o:153:ARG:HE	1.64	0.63
6:AZ:43:LYS:HG2	6:AZ:77:LEU:HD21	1.80	0.62
1:Ak:288:ALA:HB3	2:m:192:PHE:CA	2.24	0.62
2:X:201:ALA:HB2	2:X:232:MET:HE1	1.80	0.62
2:Y:139:ASP:N	2:Y:139:ASP:OD1	2.31	0.62
2:a:217:GLU:O	2:a:220:SER:OG	2.15	0.62
8:Aj:76:ALA:HB3	2:j:152:GLN:NE2	2.06	0.62
2:U:241:ASP:OD1	2:U:245:ARG:N	2.32	0.62
2:l:176:GLN:OE1	2:l:176:GLN:N	2.33	0.62
5:AW:30:ILE:HG23	5:AW:96:LEU:HD11	1.80	0.62
2:k:200:SER:OG	2:l:227:SER:OG	2.18	0.62
2:W:164:GLU:OE2	2:W:184:LEU:N	2.33	0.62
2:h:218:VAL:HG21	2:h:247:LEU:HB3	1.81	0.62
1:0:103:VAL:O	1:0:107:THR:OG1	2.18	0.62
2:AI:334:GLY:O	2:AI:335:ILE:C	2.40	0.62
6:AZ:61:ASP:OD1	6:AZ:61:ASP:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Al:103:VAL:O	1:Al:107:THR:OG1	2.17	0.61
2:m:176:GLN:N	2:m:176:GLN:OE1	2.32	0.61
2:G:306:THR:CG2	10:Ar:7:GLU:CB	2.71	0.61
5:AU:35:THR:O	5:AU:92:ASN:ND2	2.33	0.61
2:c:241:ASP:OD1	2:c:244:GLY:N	2.33	0.61
2:f:241:ASP:OD2	2:f:245:ARG:NH1	2.33	0.61
2:S:181:ARG:NH1	2:T:173:GLU:OE2	2.32	0.61
1:0:189:ILE:HD11	2:Y:193:VAL:HA	1.82	0.61
3:AR:15:TRP:NE1	2:U:148:PHE:HB3	2.15	0.61
2:T:218:VAL:HG21	2:T:247:LEU:HB3	1.81	0.61
2:j:178:ARG:NH1	2:j:207:LEU:O	2.33	0.61
3:AQ:59:LEU:HD13	8:Aj:90:LEU:HD22	1.82	0.61
7:Ai:71:MET:O	7:Ai:75:ASN:ND2	2.30	0.61
1:Al:206:PRO:HG3	2:S:192:PHE:CD2	2.35	0.61
2:d:163:ARG:HH12	2:e:183:LEU:HB3	1.65	0.61
2:AH:335:ILE:HB	2:AH:338:ALA:HB2	1.82	0.61
1:9:141:LEU:HD11	1:9:280:LEU:HD22	1.82	0.61
2:e:207:LEU:N	2:e:242:GLN:OE1	2.34	0.61
1:9:104:ILE:O	1:9:110:THR:OG1	2.19	0.61
6:AY:17:GLU:OE1	6:AY:20:ARG:NH2	2.32	0.61
2:e:201:ALA:HB2	2:e:232:MET:HE1	1.83	0.61
2:h:215:GLN:NE2	2:h:219:ASP:OD2	2.34	0.61
1:9:244:VAL:HG11	1:9:262:SER:HB3	1.81	0.61
2:T:176:GLN:OE1	2:T:176:GLN:N	2.31	0.61
2:AD:341:ASN:HD22	2:F:366:SER:HB2	1.65	0.60
3:AQ:1:MET:N	3:AQ:1:MET:SD	2.73	0.60
3:AQ:71:GLN:OE1	2:n:151:SER:HB3	1.99	0.60
2:H:318:ARG:HG3	9:Ao:3:THR:CB	2.31	0.60
2:AD:341:ASN:ND2	2:F:366:SER:N	2.44	0.60
2:B:319:SER:HB3	9:An:5:ARG:CB	2.30	0.60
2:i:168:ALA:O	2:i:172:GLU:HG2	2.01	0.60
2:n:176:GLN:OE1	2:n:176:GLN:N	2.33	0.60
9:Am:2:LEU:C	9:Am:4:ARG:H	2.09	0.60
3:AQ:71:GLN:OE1	2:n:151:SER:OG	2.17	0.60
2:V:206:THR:OG1	2:V:242:GLN:NE2	2.34	0.60
3:7:31:ILE:HG13	3:7:57:VAL:HG11	1.82	0.60
3:7:89:TYR:CD2	2:Y:190:SER:CB	2.83	0.60
2:AI:335:ILE:HD12	6:AY:71:VAL:HG23	1.82	0.60
5:AV:15:THR:HG23	5:AV:45:PHE:HZ	1.67	0.60
6:Ab:75:LYS:O	6:Ab:98:ASN:ND2	2.34	0.60
2:n:163:ARG:HA	2:n:166:GLN:HE21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AY:135:MET:HE2	7:Af:75:ASN:HD22	1.66	0.60
6:AZ:100:ASN:HD22	6:AZ:103:GLU:H	1.49	0.60
2:n:204:PHE:HE1	2:n:206:THR:HG22	1.66	0.60
4:8:243:MET:HE1	2:e:151:SER:HB2	1.82	0.60
1:Ak:112:ILE:HG23	1:Ak:283:LEU:HD23	1.84	0.60
1:Ak:206:PRO:HD2	2:k:194:ARG:HH12	1.66	0.60
2:d:206:THR:HA	2:d:242:GLN:HG2	1.84	0.60
2:S:163:ARG:HA	2:S:166:GLN:HE21	1.64	0.60
2:Y:241:ASP:OD2	2:Y:245:ARG:NH1	2.34	0.60
3:7:64:LEU:HD12	2:T:148:PHE:CD2	2.37	0.59
2:k:184:LEU:HD21	2:k:229:VAL:HG21	1.84	0.59
2:Y:164:GLU:HG2	2:Y:184:LEU:HD13	1.84	0.59
6:Aa:133:LEU:HD23	7:Ag:71:MET:HE3	1.83	0.59
2:S:146:MET:HB2	2:S:150:VAL:CG2	2.32	0.59
2:U:201:ALA:O	2:V:227:SER:OG	2.20	0.59
2:a:156:GLN:HE22	2:b:153:ARG:HG3	1.67	0.59
2:a:220:SER:HA	2:b:246:LEU:HD12	1.85	0.59
2:i:176:GLN:OE1	2:i:176:GLN:N	2.33	0.59
3:6:71:GLN:NE2	2:a:151:SER:CB	2.65	0.59
6:Ac:113:ARG:NH2	6:Ac:116:GLN:OE1	2.36	0.59
2:f:177:VAL:HA	2:f:207:LEU:HA	1.85	0.59
2:i:230:PRO:HD3	2:j:185:ALA:HB1	1.83	0.59
2:N:381:ILE:CG2	10:Aw:3:GLY:CA	2.78	0.59
9:An:8:PRO:O	9:An:9:ALA:C	2.45	0.59
1:9:189:ILE:HD12	2:c:193:VAL:N	2.12	0.59
3:AR:86:GLN:HE21	2:T:153:ARG:CZ	2.16	0.59
2:o:218:VAL:HG21	2:o:247:LEU:HB3	1.84	0.59
2:AC:342:GLN:HE22	2:M:327:ASN:HD22	1.41	0.59
2:AF:350:PRO:HA	2:AF:353:VAL:HG22	1.83	0.59
2:b:239:VAL:N	2:b:248:SER:OG	2.34	0.59
2:k:201:ALA:O	2:l:227:SER:OG	2.19	0.59
5:AU:108:ILE:HD11	6:AY:126:LYS:HG3	1.85	0.58
5:AW:35:THR:O	5:AW:92:ASN:ND2	2.37	0.58
2:W:220:SER:HB3	2:X:246:LEU:HB2	1.85	0.58
3:AQ:31:ILE:HG13	3:AQ:57:VAL:HG21	1.86	0.58
6:Aa:61:ASP:N	6:Aa:61:ASP:OD1	2.35	0.58
2:f:150:VAL:HG12	2:f:154:LEU:HD23	1.86	0.58
2:f:164:GLU:HG2	2:f:184:LEU:HD13	1.84	0.58
2:j:200:SER:HB2	2:j:236:ARG:HH21	1.68	0.58
3:7:68:TRP:HB2	2:S:148:PHE:HB3	1.84	0.58
2:S:246:LEU:H	2:T:216:GLN:HE21	1.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:151:SER:O	2:c:153:ARG:N	2.36	0.58
2:o:207:LEU:N	2:o:242:GLN:OE1	2.36	0.58
2:n:164:GLU:HG2	2:n:184:LEU:HD13	1.85	0.58
5:AW:41:ARG:HG2	5:AW:78:LYS:HE2	1.85	0.58
7:Ae:90:LYS:HE3	7:Ai:74:ARG:HH21	1.69	0.58
1:Al:183:MET:HE1	1:Al:215:ILE:HG12	1.86	0.58
2:V:184:LEU:HD21	2:V:229:VAL:HG21	1.86	0.58
2:b:176:GLN:N	2:b:176:GLN:OE1	2.35	0.58
1:Ak:189:ILE:HD11	2:k:192:PHE:HD1	1.67	0.57
2:B:381:ILE:HD12	10:As:3:GLY:HA3	1.86	0.57
2:AG:335:ILE:HB	2:AG:338:ALA:HB2	1.86	0.57
3:AQ:54:ARG:NH1	3:AR:46:GLU:OE2	2.38	0.57
1:Ak:206:PRO:HD3	2:k:192:PHE:HD2	1.69	0.57
1:Ak:248:LEU:HD11	1:Ak:261:VAL:HG11	1.86	0.57
2:f:227:SER:OG	2:g:201:ALA:O	2.22	0.57
4:8:70:ARG:HA	4:8:73:MET:HE2	1.85	0.57
2:m:238:THR:HG21	2:n:224:MET:HA	1.85	0.57
2:n:168:ALA:O	2:n:172:GLU:HG2	2.03	0.57
2:A:381:ILE:HD12	10:As:10:ALA:CB	2.35	0.57
3:AR:86:GLN:NE2	2:T:153:ARG:CZ	2.67	0.57
2:g:163:ARG:HH22	2:h:183:LEU:HB3	1.69	0.57
3:7:65:PHE:HE1	2:S:148:PHE:CD2	2.23	0.57
2:AO:335:ILE:O	2:AO:340:SER:OG	2.14	0.57
2:U:176:GLN:OE1	2:U:176:GLN:N	2.30	0.57
3:7:71:GLN:CG	2:S:152:GLN:OE1	2.51	0.57
7:Ah:66:SER:OG	7:Ah:69:ASP:OD1	2.23	0.57
2:Y:171:ILE:HD12	2:Y:221:ILE:HD12	1.87	0.57
3:7:85:PRO:HG2	2:W:191:VAL:HG21	1.86	0.57
4:8:187:MET:HE2	4:8:240:HIS:HB3	1.85	0.57
5:AU:20:GLU:OE2	7:Ag:68:SER:OG	2.20	0.57
2:T:146:MET:N	2:T:146:MET:SD	2.78	0.57
6:Ab:61:ASP:OD1	6:Ab:61:ASP:N	2.38	0.57
2:AK:331:MET:HE3	6:AX:52:GLU:HB2	1.87	0.57
2:AN:352:ASP:OD1	2:AN:352:ASP:N	2.38	0.57
6:AX:75:LYS:O	6:AX:98:ASN:ND2	2.33	0.57
6:Ac:34:VAL:HG12	6:Ac:96:LYS:HG2	1.87	0.57
1:AP:239:ILE:HG23	8:Aj:89:LEU:HD22	1.87	0.56
6:AY:61:ASP:N	6:AY:61:ASP:OD1	2.36	0.56
1:Ak:207:GLU:OE2	2:k:194:ARG:CZ	2.54	0.56
3:6:15:TRP:CE2	2:b:148:PHE:CZ	2.93	0.56
4:8:87:MET:HE2	1:AP:136:GLY:HA3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:8:136:MET:HE1	1:9:228:GLN:HA	1.85	0.56
2:AI:335:ILE:HD11	6:AY:69:GLY:HA3	1.86	0.56
2:S:168:ALA:O	2:S:172:GLU:HG2	2.06	0.56
2:S:176:GLN:OE1	2:S:176:GLN:N	2.39	0.56
2:U:201:ALA:HB2	2:U:232:MET:HE1	1.86	0.56
2:k:215:GLN:NE2	2:k:219:ASP:OD1	2.38	0.56
3:AR:31:ILE:HG13	3:AR:57:VAL:HG21	1.88	0.56
6:AZ:17:GLU:OE1	6:AZ:20:ARG:NH2	2.34	0.56
2:b:227:SER:OG	2:c:200:SER:OG	2.15	0.56
2:g:177:VAL:HG13	2:g:207:LEU:HD23	1.86	0.56
2:V:203:VAL:HG13	2:V:239:VAL:HG22	1.87	0.56
2:B:319:SER:CB	9:An:5:ARG:HA	2.36	0.56
2:V:201:ALA:O	2:k:227:SER:OG	2.24	0.56
1:0:144:PHE:HB2	1:Al:198:MET:HE2	1.86	0.56
2:X:207:LEU:N	2:X:242:GLN:OE1	2.39	0.56
2:Y:227:SER:OG	2:Z:201:ALA:O	2.24	0.56
2:b:178:ARG:NH1	2:b:207:LEU:O	2.37	0.56
1:0:206:PRO:CG	2:Z:194:ARG:HH11	2.16	0.56
2:AB:342:GLN:OE1	2:p:327:ASN:ND2	2.39	0.56
2:V:241:ASP:OD1	2:V:244:GLY:N	2.39	0.56
2:4:368:ARG:HH22	5:AT:50:GLN:HE22	1.52	0.56
2:S:227:SER:OG	2:W:201:ALA:O	2.23	0.56
2:f:168:ALA:O	2:f:172:GLU:HG2	2.06	0.56
3:AQ:89:TYR:HE2	2:l:188:LYS:CB	2.08	0.56
2:j:153:ARG:HA	2:j:153:ARG:HE	1.69	0.56
2:n:184:LEU:HD21	2:n:229:VAL:HG21	1.88	0.56
2:A:372:THR:CG2	9:An:7:ILE:H	2.20	0.55
5:AT:20:GLU:OE2	7:Af:68:SER:OG	2.24	0.55
1:Ak:220:THR:HG23	1:Al:276:TRP:HB3	1.88	0.55
2:Y:218:VAL:HG21	2:Y:247:LEU:HB3	1.87	0.55
2:Z:241:ASP:OD1	2:Z:245:ARG:N	2.39	0.55
2:j:227:SER:OG	2:o:201:ALA:O	2.18	0.55
3:6:15:TRP:CE2	2:b:148:PHE:HZ	2.25	0.55
2:AH:335:ILE:HD12	2:AN:356:MET:HE1	1.88	0.55
3:AR:15:TRP:CE2	2:U:148:PHE:CB	2.90	0.55
2:N:374:ASN:OD1	9:Ap:7:HIS:CB	2.54	0.55
2:i:163:ARG:O	2:i:166:GLN:HG2	2.06	0.55
2:i:206:THR:HA	2:i:242:GLN:HB3	1.89	0.55
2:l:201:ALA:O	2:m:227:SER:OG	2.25	0.55
2:AF:350:PRO:O	2:AF:351:GLN:C	2.50	0.55
1:Al:197:THR:HG21	2:W:194:ARG:CD	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:201:ALA:O	2:T:227:SER:OG	2.24	0.55
2:Y:168:ALA:O	2:Y:172:GLU:HG2	2.07	0.55
2:Y:246:LEU:HD22	2:Y:248:SER:O	2.06	0.55
2:Z:153:ARG:HA	2:Z:153:ARG:HE	1.70	0.55
2:W:207:LEU:N	2:W:242:GLN:OE1	2.38	0.55
6:AX:20:ARG:HH21	6:AX:111:ALA:HA	1.71	0.55
2:f:214:LYS:NZ	2:f:217:GLU:OE2	2.37	0.55
2:g:177:VAL:HA	2:g:207:LEU:HA	1.87	0.55
2:o:159:LEU:O	2:o:162:SER:OG	2.19	0.55
3:6:64:LEU:HD21	2:Z:148:PHE:CE2	2.38	0.55
1:9:103:VAL:O	1:9:107:THR:HG22	2.06	0.55
3:AR:13:ALA:HB1	1:Al:239:ILE:HD11	1.89	0.55
1:Ak:187:THR:O	2:l:192:PHE:CD1	2.59	0.55
2:U:187:PRO:HD3	2:U:199:ALA:HA	1.88	0.55
3:6:40:ALA:HA	4:8:211:GLN:HG3	1.87	0.55
3:AR:86:GLN:HE21	2:T:153:ARG:NH1	2.05	0.55
6:Ab:135:MET:HE1	7:Ad:72:ILE:HG12	1.89	0.55
2:U:168:ALA:O	2:U:172:GLU:HG2	2.07	0.55
2:Z:207:LEU:N	2:Z:242:GLN:OE1	2.40	0.55
2:o:163:ARG:HA	2:o:166:GLN:HE21	1.72	0.55
3:7:1:MET:HG3	1:9:268:MET:HE1	1.88	0.55
6:AX:129:LEU:HD22	7:Ai:67:LEU:HD12	1.88	0.55
6:Ab:3:LEU:HD21	6:Ab:128:MET:HE3	1.89	0.55
2:V:241:ASP:OD1	2:V:245:ARG:N	2.38	0.55
1:0:115:VAL:HG11	1:0:283:LEU:HD11	1.87	0.55
3:7:4:GLU:HB2	2:Y:152:GLN:NE2	2.20	0.55
1:Al:104:ILE:O	1:Al:110:THR:OG1	2.24	0.55
2:e:164:GLU:HG2	2:e:184:LEU:HD13	1.88	0.55
2:l:191:VAL:HG22	2:l:192:PHE:H	1.72	0.55
3:6:8:GLU:OE2	2:c:152:GLN:HB2	2.06	0.54
3:6:84:LEU:N	3:6:85:PRO:HD2	2.21	0.54
2:T:187:PRO:HD2	2:T:199:ALA:HB2	1.90	0.54
2:a:146:MET:HG3	2:a:158:ARG:HH11	1.71	0.54
1:AP:103:VAL:O	1:AP:107:THR:OG1	2.23	0.54
1:AP:112:ILE:HD13	1:AP:141:LEU:HB3	1.89	0.54
2:h:163:ARG:NH2	2:h:228:ALA:O	2.39	0.54
2:h:220:SER:HA	2:i:246:LEU:HD12	1.89	0.54
2:o:201:ALA:HB2	2:o:232:MET:HE1	1.89	0.54
2:AD:348:SER:HB2	2:AD:356:MET:HE3	1.89	0.54
2:Y:201:ALA:HB2	2:Y:232:MET:HE1	1.88	0.54
2:h:227:SER:OG	2:i:200:SER:OG	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Ag:66:SER:OG	7:Ag:69:ASP:OD1	2.25	0.54
2:B:319:SER:OG	9:An:5:ARG:HA	2.07	0.54
2:T:165:ARG:NH2	2:U:139:ASP:OD2	2.40	0.54
2:4:368:ARG:HH22	5:AT:50:GLN:NE2	2.04	0.54
2:AF:352:ASP:O	2:AF:353:VAL:C	2.51	0.54
6:AX:108:MET:HE2	6:AZ:121:VAL:HG22	1.89	0.54
6:Ab:3:LEU:HB3	6:Ab:129:LEU:HD21	1.89	0.54
6:Ab:43:LYS:HG2	6:Ab:77:LEU:HD21	1.90	0.54
2:F:324:GLU:OE2	2:F:326:TYR:OH	2.26	0.54
2:G:324:GLU:OE2	2:G:326:TYR:OH	2.26	0.54
2:S:245:ARG:HG3	2:S:247:LEU:HD21	1.90	0.54
2:g:227:SER:O	2:h:200:SER:OG	2.23	0.54
2:i:241:ASP:OD1	2:i:244:GLY:N	2.41	0.54
2:l:164:GLU:HG2	2:l:184:LEU:HD13	1.89	0.54
2:n:146:MET:N	2:n:146:MET:SD	2.81	0.54
3:AQ:6:PHE:HB2	1:Al:268:MET:HE2	1.89	0.54
5:AT:30:ILE:HG23	5:AT:96:LEU:HD11	1.89	0.54
1:Al:206:PRO:CD	2:S:192:PHE:HB3	2.38	0.54
2:E:324:GLU:OE2	2:E:326:TYR:OH	2.26	0.54
2:u:324:GLU:OE2	2:u:326:TYR:OH	2.26	0.54
1:0:185:LYS:HD2	2:Y:194:ARG:HH11	1.65	0.54
2:H:324:GLU:OE2	2:H:326:TYR:OH	2.26	0.54
2:b:227:SER:OG	2:c:201:ALA:O	2.25	0.54
2:h:238:THR:HG23	2:h:246:LEU:HD21	1.89	0.54
2:m:168:ALA:O	2:m:172:GLU:HG2	2.08	0.54
1:AP:198:MET:HE1	1:Ak:141:LEU:HD22	1.90	0.54
1:AP:239:ILE:HD12	8:Aj:89:LEU:HD22	1.90	0.54
2:Z:176:GLN:N	2:Z:176:GLN:OE1	2.41	0.54
2:g:227:SER:OG	2:h:201:ALA:O	2.26	0.54
2:x:324:GLU:OE2	2:x:326:TYR:OH	2.26	0.54
3:7:89:TYR:CE2	2:Y:190:SER:HB2	2.43	0.54
2:I:324:GLU:OE2	2:I:326:TYR:OH	2.26	0.54
2:y:324:GLU:OE2	2:y:326:TYR:OH	2.26	0.54
6:AX:9:VAL:HG21	6:AX:62:THR:HB	1.90	0.53
2:S:239:VAL:N	2:S:248:SER:OG	2.41	0.53
2:c:172:GLU:OE2	2:c:180:ALA:N	2.42	0.53
9:Ap:9:PRO:O	9:Ap:10:ALA:C	2.51	0.53
7:Af:66:SER:OG	7:Af:69:ASP:OD1	2.26	0.53
2:J:324:GLU:OE2	2:J:326:TYR:OH	2.26	0.53
2:X:151:SER:O	2:X:153:ARG:N	2.42	0.53
2:z:324:GLU:OE2	2:z:326:TYR:OH	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AI:339:LEU:HD11	6:AY:72:GLU:HG3	1.91	0.53
6:AY:133:LEU:HA	7:Af:71:MET:HE3	1.89	0.53
2:R:324:GLU:OE2	2:R:326:TYR:OH	2.26	0.53
2:5:273:LEU:HD23	2:5:294:VAL:HG11	1.91	0.53
2:A:273:LEU:HD23	2:A:294:VAL:HG11	1.91	0.53
7:Ad:94:ALA:HA	1:Al:100:PRO:HG3	1.90	0.53
2:N:273:LEU:HD23	2:N:294:VAL:HG11	1.91	0.53
2:O:273:LEU:HD23	2:O:294:VAL:HG11	1.91	0.53
2:b:159:LEU:HD13	2:c:157:GLU:HG3	1.91	0.53
2:c:178:ARG:NH2	2:c:206:THR:OG1	2.42	0.53
2:k:207:LEU:N	2:k:242:GLN:OE1	2.42	0.53
2:1:324:GLU:OE2	2:1:326:TYR:OH	2.26	0.53
3:7:4:GLU:CB	2:Y:152:GLN:NE2	2.71	0.53
4:8:54:MET:HE2	7:Ae:26:GLY:HA3	1.90	0.53
2:AJ:335:ILE:HG22	6:AX:87:LEU:HD11	1.89	0.53
1:Al:197:THR:HG21	2:W:194:ARG:HD2	1.90	0.53
2:D:273:LEU:HD23	2:D:294:VAL:HG11	1.91	0.53
2:L:273:LEU:HD23	2:L:294:VAL:HG11	1.91	0.53
2:P:273:LEU:HD23	2:P:294:VAL:HG11	1.91	0.53
2:V:150:VAL:HG12	2:V:154:LEU:HD23	1.90	0.53
2:V:171:ILE:HD12	2:V:221:ILE:HD12	1.91	0.53
2:m:204:PHE:HE1	2:m:206:THR:HG22	1.73	0.53
2:B:273:LEU:HD23	2:B:294:VAL:HG11	1.91	0.53
2:K:324:GLU:OE2	2:K:326:TYR:OH	2.26	0.53
2:S:147:GLY:O	2:S:148:PHE:C	2.51	0.53
2:h:199:ALA:HB3	2:h:232:MET:HB3	1.91	0.53
2:i:178:ARG:NH1	2:i:207:LEU:O	2.41	0.53
2:C:273:LEU:HD23	2:C:294:VAL:HG11	1.91	0.53
2:H:273:LEU:HD23	2:H:294:VAL:HG11	1.91	0.53
2:K:273:LEU:HD23	2:K:294:VAL:HG11	1.91	0.53
2:M:273:LEU:HD23	2:M:294:VAL:HG11	1.91	0.53
2:S:174:MET:SD	2:S:221:ILE:HD11	2.49	0.53
2:V:176:GLN:OE1	2:V:176:GLN:N	2.40	0.53
2:q:324:GLU:OE2	2:q:326:TYR:OH	2.26	0.53
9:Aq:8:GLY:O	9:Aq:9:ARG:C	2.52	0.53
2:3:273:LEU:HD23	2:3:294:VAL:HG11	1.91	0.53
5:AT:85:GLN:HE21	6:AZ:19:VAL:HG22	1.73	0.53
5:AU:31:ALA:HA	6:Aa:118:ASN:HD21	1.73	0.53
2:F:273:LEU:HD23	2:F:294:VAL:HG11	1.91	0.53
2:J:273:LEU:HD23	2:J:294:VAL:HG11	1.91	0.53
2:Y:196:ASN:OD1	2:Y:196:ASN:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:178:ARG:NH1	2:n:207:LEU:O	2.41	0.53
2:4:273:LEU:HD23	2:4:294:VAL:HG11	1.91	0.53
4:8:64:ILE:HG22	4:8:70:ARG:HG2	1.91	0.53
3:AR:81:ILE:HG13	1:Al:278:LEU:HD21	1.91	0.53
5:AV:36:PRO:HB3	5:AV:90:ASP:HB2	1.91	0.53
5:AW:37:GLY:N	5:AW:90:ASP:O	2.42	0.53
2:E:273:LEU:HD23	2:E:294:VAL:HG11	1.91	0.53
2:L:324:GLU:OE2	2:L:326:TYR:OH	2.26	0.53
2:U:207:LEU:N	2:U:242:GLN:OE1	2.40	0.53
2:Z:168:ALA:O	2:Z:172:GLU:HG2	2.09	0.53
2:p:324:GLU:OE2	2:p:326:TYR:OH	2.26	0.53
2:q:374:ASN:HD21	9:Aq:3:LEU:HA	1.74	0.53
2:2:324:GLU:OE2	2:2:326:TYR:OH	2.26	0.52
1:AP:85:VAL:HG13	5:AS:3:ILE:HA	1.90	0.52
6:Ac:133:LEU:HD23	7:Ah:71:MET:HE3	1.91	0.52
2:S:241:ASP:OD1	2:S:244:GLY:N	2.42	0.52
2:Z:139:ASP:HB3	2:a:161:LEU:HD21	1.90	0.52
2:h:173:GLU:HB2	2:i:204:PHE:CZ	2.43	0.52
2:h:184:LEU:HD21	2:h:229:VAL:HG21	1.91	0.52
2:l:207:LEU:N	2:l:242:GLN:OE1	2.43	0.52
3:6:15:TRP:CZ2	2:b:148:PHE:CZ	2.96	0.52
4:8:97:VAL:HG22	4:8:131:MET:HB2	1.90	0.52
5:AS:128:ILE:HG13	5:AS:129:LYS:HG3	1.91	0.52
2:R:273:LEU:HD23	2:R:294:VAL:HG11	1.91	0.52
2:X:179:LYS:HB3	2:X:206:THR:OG1	2.09	0.52
2:c:174:MET:HB2	2:c:177:VAL:HB	1.91	0.52
2:k:241:ASP:OD1	2:k:245:ARG:N	2.43	0.52
2:3:324:GLU:OE2	2:3:326:TYR:OH	2.26	0.52
2:AM:340:SER:HA	2:AM:349:ILE:HD11	1.90	0.52
5:AV:41:ARG:NH2	5:AV:80:TYR:OH	2.38	0.52
2:Q:273:LEU:HD23	2:Q:294:VAL:HG11	1.91	0.52
1:AP:125:LEU:HB3	1:AP:128:THR:HB	1.91	0.52
2:I:273:LEU:HD23	2:I:294:VAL:HG11	1.91	0.52
2:M:324:GLU:OE2	2:M:326:TYR:OH	2.26	0.52
2:v:273:LEU:HD23	2:v:294:VAL:HG11	1.91	0.52
2:w:273:LEU:HD23	2:w:294:VAL:HG11	1.91	0.52
2:1:273:LEU:HD23	2:1:294:VAL:HG11	1.91	0.52
2:2:273:LEU:HD23	2:2:294:VAL:HG11	1.91	0.52
4:8:150:LEU:HD13	4:8:252:ILE:HG21	1.92	0.52
2:j:227:SER:O	2:o:200:SER:OG	2.20	0.52
2:G:273:LEU:HD23	2:G:294:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:176:GLN:OE1	2:k:176:GLN:N	2.42	0.52
2:l:184:LEU:HD21	2:l:229:VAL:HG21	1.91	0.52
2:4:324:GLU:OE2	2:4:326:TYR:OH	2.26	0.52
3:AR:81:ILE:HG21	1:Al:278:LEU:HD11	1.91	0.52
1:Ak:189:ILE:CD1	2:k:192:PHE:CD1	2.87	0.52
2:T:196:ASN:OD1	2:T:196:ASN:N	2.43	0.52
9:Am:11:PRO:O	9:Am:12:ALA:C	2.53	0.52
1:Al:187:THR:O	2:T:192:PHE:CB	2.57	0.52
2:V:229:VAL:HB	2:V:232:MET:SD	2.50	0.52
2:Y:248:SER:O	2:Y:249:SER:HB2	2.10	0.52
2:d:241:ASP:OD1	2:d:245:ARG:N	2.43	0.52
2:k:229:VAL:HB	2:k:232:MET:SD	2.49	0.52
2:q:273:LEU:HD23	2:q:294:VAL:HG11	1.91	0.52
2:r:273:LEU:HD23	2:r:294:VAL:HG11	1.91	0.52
2:r:324:GLU:OE2	2:r:326:TYR:OH	2.26	0.52
1:0:248:LEU:HD11	1:0:261:VAL:HG11	1.92	0.52
4:8:28:VAL:HB	4:8:86:GLY:HA3	1.91	0.52
2:H:319:SER:CB	9:Ao:3:THR:H	2.22	0.52
2:s:273:LEU:HD23	2:s:294:VAL:HG11	1.91	0.52
2:N:324:GLU:OE2	2:N:326:TYR:OH	2.26	0.51
2:W:139:ASP:OD1	2:W:139:ASP:N	2.43	0.51
2:d:227:SER:OG	2:e:201:ALA:O	2.21	0.51
2:g:174:MET:SD	2:g:221:ILE:HD11	2.49	0.51
2:j:230:PRO:HB2	2:o:197:GLN:HE21	1.74	0.51
2:o:184:LEU:HD21	2:o:229:VAL:HG21	1.93	0.51
2:p:273:LEU:HD23	2:p:294:VAL:HG11	1.91	0.51
1:0:112:ILE:HD13	1:0:141:LEU:HB3	1.92	0.51
6:AX:84:ASP:OD1	6:AZ:73:SER:OG	2.23	0.51
2:a:184:LEU:HD21	2:a:229:VAL:HG21	1.91	0.51
2:x:273:LEU:HD23	2:x:294:VAL:HG11	1.91	0.51
2:B:324:GLU:OE2	2:B:326:TYR:OH	2.26	0.51
2:Q:324:GLU:OE2	2:Q:326:TYR:OH	2.26	0.51
2:S:246:LEU:H	2:T:216:GLN:NE2	2.08	0.51
2:d:176:GLN:OE1	2:d:176:GLN:N	2.40	0.51
2:u:273:LEU:HD23	2:u:294:VAL:HG11	1.91	0.51
2:5:324:GLU:OE2	2:5:326:TYR:OH	2.26	0.51
2:AF:347:ALA:O	2:AF:353:VAL:HG13	2.10	0.51
1:AP:139:LEU:HD21	7:Ai:98:LEU:HD13	1.92	0.51
6:Ac:9:VAL:HG21	6:Ac:62:THR:HB	1.92	0.51
2:a:168:ALA:O	2:a:172:GLU:HG2	2.10	0.51
4:8:53:VAL:HG11	1:9:198:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AT:119:SER:OG	7:Ae:74:ARG:NH2	2.44	0.51
2:l:187:PRO:HD2	2:l:199:ALA:HB2	1.93	0.51
4:8:214:ILE:HG12	1:AP:255:MET:HB2	1.93	0.51
1:Al:192:LEU:HB3	2:S:192:PHE:CZ	2.46	0.51
2:O:324:GLU:OE2	2:O:326:TYR:OH	2.26	0.51
2:d:168:ALA:O	2:d:172:GLU:HG2	2.10	0.51
2:g:224:MET:HG3	2:h:202:SER:HB3	1.91	0.51
2:h:174:MET:HE3	2:i:204:PHE:HE1	1.75	0.51
2:y:273:LEU:HD23	2:y:294:VAL:HG11	1.91	0.51
2:AI:339:LEU:HD11	6:AY:72:GLU:CG	2.41	0.51
2:d:207:LEU:N	2:d:242:GLN:OE1	2.43	0.51
2:f:178:ARG:N	2:f:206:THR:O	2.39	0.51
2:m:154:LEU:O	2:m:158:ARG:HG3	2.11	0.51
2:m:246:LEU:H	2:n:216:GLN:HE21	1.58	0.51
2:s:324:GLU:OE2	2:s:326:TYR:OH	2.26	0.51
2:z:273:LEU:HD23	2:z:294:VAL:HG11	1.91	0.51
1:9:206:PRO:CG	2:d:192:PHE:CE2	2.89	0.51
2:C:324:GLU:OE2	2:C:326:TYR:OH	2.26	0.51
2:e:185:ALA:O	2:e:199:ALA:HA	2.11	0.51
2:g:163:ARG:HA	2:g:166:GLN:HE21	1.76	0.51
2:j:167:LEU:O	2:j:171:ILE:HG12	2.10	0.51
2:t:273:LEU:HD23	2:t:294:VAL:HG11	1.91	0.51
1:0:112:ILE:HG22	1:0:116:MET:HE2	1.93	0.51
3:6:81:ILE:HG23	1:9:282:THR:HG21	1.93	0.51
2:P:324:GLU:OE2	2:P:326:TYR:OH	2.26	0.51
2:n:207:LEU:HD21	2:n:213:LEU:HD11	1.91	0.51
2:A:324:GLU:OE2	2:A:326:TYR:OH	2.26	0.51
2:X:227:SER:OG	2:Y:201:ALA:O	2.21	0.51
2:Z:174:MET:HB2	2:Z:177:VAL:HB	1.93	0.51
1:0:189:ILE:HG12	2:Y:191:VAL:O	2.10	0.50
2:S:227:SER:O	2:W:200:SER:OG	2.21	0.50
2:W:168:ALA:O	2:W:172:GLU:HG2	2.11	0.50
2:e:229:VAL:HB	2:e:232:MET:SD	2.51	0.50
2:k:160:LYS:HD3	2:k:186:LEU:HG	1.93	0.50
3:6:52:LEU:HB2	3:7:25:ILE:HG21	1.94	0.50
4:8:81:ILE:HG22	4:8:85:MET:HE1	1.94	0.50
5:AS:35:THR:O	5:AS:92:ASN:ND2	2.44	0.50
2:U:241:ASP:CG	2:U:245:ARG:HG2	2.37	0.50
2:Z:199:ALA:HB3	2:Z:232:MET:HB3	1.94	0.50
2:c:179:LYS:HB3	2:c:206:THR:HG23	1.93	0.50
2:c:241:ASP:OD2	2:c:245:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:174:MET:SD	2:f:221:ILE:HD11	2.51	0.50
2:m:239:VAL:HG12	2:m:247:LEU:HD12	1.93	0.50
4:8:204:VAL:HG23	8:Aj:39:LEU:HD22	1.93	0.50
2:A:374:ASN:HD22	9:An:7:ILE:CB	2.21	0.50
2:AD:341:ASN:HD22	2:F:366:SER:CB	2.24	0.50
2:AG:336:PRO:HG2	2:AO:352:ASP:HB3	1.92	0.50
2:F:306:THR:OG1	10:Ar:14:GLU:CB	2.59	0.50
2:G:374:ASN:OD1	9:Ao:3:THR:CA	2.59	0.50
2:d:239:VAL:HG12	2:d:247:LEU:HD12	1.92	0.50
2:t:324:GLU:OE2	2:t:326:TYR:OH	2.26	0.50
9:Am:2:LEU:C	9:Am:4:ARG:N	2.70	0.50
9:Am:9:HIS:O	9:Am:10:ILE:C	2.53	0.50
2:AH:342:GLN:HG3	2:AH:343:PRO:HD2	1.93	0.50
2:V:179:LYS:HB3	2:V:206:THR:HG23	1.92	0.50
2:V:200:SER:HB2	2:V:236:ARG:HH21	1.76	0.50
4:8:149:GLN:HE22	2:e:192:PHE:HB3	1.77	0.50
2:AK:330:ASN:N	2:AK:330:ASN:HD22	2.10	0.50
2:Z:193:VAL:O	2:Z:195:HIS:N	2.44	0.50
2:f:229:VAL:HB	2:f:232:MET:HE2	1.93	0.50
5:AT:104:MET:SD	6:AZ:126:LYS:NZ	2.80	0.50
6:AZ:37:SER:O	6:AZ:38:ALA:HB3	2.11	0.50
2:X:153:ARG:HH22	2:X:188:LYS:HD3	1.76	0.50
2:a:218:VAL:HG21	2:a:247:LEU:HB3	1.93	0.50
2:a:227:SER:OG	2:b:200:SER:OG	2.28	0.50
2:g:178:ARG:NH1	2:g:207:LEU:O	2.45	0.50
2:j:216:GLN:HE21	2:o:246:LEU:H	1.60	0.50
2:q:430:LEU:HA	2:q:433:THR:HB	1.94	0.50
2:AF:347:ALA:HA	2:AF:353:VAL:CG1	2.42	0.50
2:E:430:LEU:HA	2:E:433:THR:HB	1.94	0.50
2:G:430:LEU:HA	2:G:433:THR:HB	1.94	0.50
2:R:430:LEU:HA	2:R:433:THR:HB	1.94	0.50
2:U:203:VAL:HG13	2:U:239:VAL:HG22	1.93	0.50
2:AK:353:VAL:HG21	6:AX:71:VAL:HG11	1.94	0.50
1:AP:183:MET:HE1	1:AP:211:MET:HG3	1.92	0.50
5:AU:128:ILE:HD13	7:Ag:83:ALA:HB2	1.94	0.50
2:D:324:GLU:OE2	2:D:326:TYR:OH	2.26	0.50
2:H:430:LEU:HA	2:H:433:THR:HB	1.94	0.50
2:J:430:LEU:HA	2:J:433:THR:HB	1.94	0.50
2:O:430:LEU:HA	2:O:433:THR:HB	1.94	0.50
2:Q:430:LEU:HA	2:Q:433:THR:HB	1.94	0.50
2:c:171:ILE:HD12	2:c:221:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:173:GLU:OE2	2:h:181:ARG:NH1	2.38	0.50
2:h:182:VAL:HG13	2:h:203:VAL:HB	1.92	0.50
2:i:241:ASP:OD2	2:i:245:ARG:NH1	2.45	0.50
2:k:178:ARG:NH1	2:k:207:LEU:O	2.45	0.50
2:k:204:PHE:HE1	2:k:206:THR:HG22	1.76	0.50
1:0:276:TRP:HB3	1:Al:220:THR:HG23	1.93	0.50
2:L:430:LEU:HA	2:L:433:THR:HB	1.94	0.50
2:S:164:GLU:HG2	2:S:184:LEU:HD13	1.93	0.50
2:Z:139:ASP:OD1	2:Z:139:ASP:N	2.45	0.50
2:Z:222:VAL:HG23	2:Z:237:ILE:HB	1.93	0.50
2:m:246:LEU:H	2:n:216:GLN:NE2	2.09	0.50
2:n:238:THR:HG21	2:o:224:MET:HA	1.94	0.50
2:p:430:LEU:HA	2:p:433:THR:HB	1.94	0.50
2:s:430:LEU:HA	2:s:433:THR:HB	1.94	0.50
4:8:43:LEU:HD21	7:Ae:99:MET:HA	1.94	0.49
4:8:44:TYR:HE2	1:9:104:ILE:HD12	1.77	0.49
7:Ag:60:ARG:NH1	7:Ag:62:ASP:OD1	2.45	0.49
1:Al:142:THR:HA	1:Al:145:VAL:HG22	1.93	0.49
2:F:430:LEU:HA	2:F:433:THR:HB	1.94	0.49
2:K:430:LEU:HA	2:K:433:THR:HB	1.94	0.49
2:P:430:LEU:HA	2:P:433:THR:HB	1.94	0.49
2:S:150:VAL:HG12	2:S:154:LEU:HD23	1.94	0.49
2:W:187:PRO:HB3	2:W:197:GLN:HB2	1.93	0.49
2:d:245:ARG:HG3	2:d:247:LEU:HD21	1.94	0.49
2:j:168:ALA:O	2:j:172:GLU:HG2	2.12	0.49
2:l:161:LEU:HD21	2:l:165:ARG:HH21	1.77	0.49
3:AQ:5:MET:SD	3:AQ:83:ARG:NH2	2.85	0.49
3:AR:15:TRP:CE2	2:U:148:PHE:HB3	2.47	0.49
2:I:430:LEU:HA	2:I:433:THR:HB	1.94	0.49
2:M:430:LEU:HA	2:M:433:THR:HB	1.94	0.49
2:e:201:ALA:HB3	2:e:237:ILE:HG13	1.93	0.49
2:e:231:GLY:O	2:e:232:MET:HG3	2.12	0.49
2:j:176:GLN:N	2:j:176:GLN:OE1	2.45	0.49
2:S:217:GLU:OE1	2:W:244:GLY:HA3	2.12	0.49
2:Y:235:SER:O	2:Y:250:GLY:HA2	2.13	0.49
2:r:430:LEU:HA	2:r:433:THR:HB	1.94	0.49
1:0:112:ILE:HG23	1:0:283:LEU:HD23	1.94	0.49
2:C:430:LEU:HA	2:C:433:THR:HB	1.94	0.49
2:D:430:LEU:HA	2:D:433:THR:HB	1.94	0.49
2:a:222:VAL:HG23	2:a:237:ILE:HB	1.95	0.49
2:b:171:ILE:HD12	2:b:221:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:220:SER:HB2	2:d:240:THR:HG21	1.93	0.49
1:Ak:144:PHE:O	1:Ak:147:SER:OG	2.27	0.49
2:N:430:LEU:HA	2:N:433:THR:HB	1.94	0.49
2:U:172:GLU:OE2	2:U:179:LYS:HA	2.12	0.49
2:W:203:VAL:HG13	2:W:239:VAL:HG22	1.93	0.49
2:b:172:GLU:OE2	2:b:180:ALA:N	2.42	0.49
1:0:116:MET:HE3	1:0:134:ILE:HG23	1.93	0.49
2:2:430:LEU:HA	2:2:433:THR:HB	1.94	0.49
1:9:195:PHE:HB3	1:9:213:VAL:HG22	1.95	0.49
2:g:168:ALA:O	2:g:172:GLU:HG2	2.12	0.49
2:l:196:ASN:OD1	2:l:196:ASN:N	2.44	0.49
2:3:430:LEU:HA	2:3:433:THR:HB	1.94	0.49
2:U:222:VAL:HG23	2:U:237:ILE:HB	1.95	0.49
2:W:218:VAL:HG21	2:W:247:LEU:HB3	1.94	0.49
2:X:239:VAL:N	2:X:248:SER:OG	2.44	0.49
2:a:210:GLY:O	2:a:211:THR:OG1	2.30	0.49
2:w:324:GLU:OE2	2:w:326:TYR:OH	2.26	0.49
2:y:430:LEU:HA	2:y:433:THR:HB	1.94	0.49
2:z:430:LEU:HA	2:z:433:THR:HB	1.94	0.49
6:Ab:133:LEU:HD23	7:Ad:71:MET:HE3	1.95	0.49
2:C:299:ASP:O	2:C:389:GLY:HA2	2.13	0.49
2:P:299:ASP:O	2:P:389:GLY:HA2	2.13	0.49
2:W:146:MET:HB3	2:W:150:VAL:HG21	1.94	0.49
2:X:187:PRO:HB3	2:X:197:GLN:HB2	1.94	0.49
2:c:176:GLN:O	2:c:208:SER:N	2.45	0.49
2:t:430:LEU:HA	2:t:433:THR:HB	1.94	0.49
2:v:324:GLU:OE2	2:v:326:TYR:OH	2.26	0.49
2:z:299:ASP:O	2:z:389:GLY:HA2	2.13	0.49
5:AW:33:ALA:O	5:AW:92:ASN:ND2	2.45	0.49
6:AY:75:LYS:O	6:AY:98:ASN:ND2	2.43	0.49
2:n:207:LEU:N	2:n:242:GLN:OE1	2.46	0.49
2:n:241:ASP:OD2	2:n:245:ARG:NH1	2.45	0.49
2:v:299:ASP:O	2:v:389:GLY:HA2	2.13	0.49
2:x:299:ASP:O	2:x:389:GLY:HA2	2.13	0.49
1:0:253:MET:HA	1:Al:249:MET:HE3	1.95	0.49
2:J:299:ASP:O	2:J:389:GLY:HA2	2.13	0.49
2:S:246:LEU:HG	2:T:220:SER:HA	1.95	0.49
2:h:173:GLU:HB2	2:i:204:PHE:HZ	1.76	0.49
2:t:299:ASP:O	2:t:389:GLY:HA2	2.13	0.49
2:2:299:ASP:O	2:2:389:GLY:HA2	2.13	0.48
2:5:299:ASP:O	2:5:389:GLY:HA2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:1:MET:SD	3:6:1:MET:N	2.70	0.48
1:Ak:206:PRO:HD2	2:k:194:ARG:NH1	2.27	0.48
2:M:299:ASP:O	2:M:389:GLY:HA2	2.13	0.48
2:T:201:ALA:O	2:U:227:SER:OG	2.21	0.48
2:s:299:ASP:O	2:s:389:GLY:HA2	2.13	0.48
2:u:430:LEU:HA	2:u:433:THR:HB	1.94	0.48
1:0:185:LYS:HG3	2:Y:194:ARG:HH12	1.78	0.48
1:9:184:LEU:HD11	1:9:207:GLU:HA	1.95	0.48
2:H:299:ASP:O	2:H:389:GLY:HA2	2.13	0.48
2:T:200:SER:OG	2:T:201:ALA:N	2.45	0.48
2:g:218:VAL:HG23	2:g:239:VAL:HG11	1.95	0.48
2:A:430:LEU:HA	2:A:433:THR:HB	1.94	0.48
5:AT:97:ASP:OD1	6:AZ:115:TYR:OH	2.32	0.48
8:Aj:49:PHE:HB3	8:Aj:96:VAL:HG22	1.95	0.48
2:B:299:ASP:O	2:B:389:GLY:HA2	2.13	0.48
2:B:430:LEU:HA	2:B:433:THR:HB	1.94	0.48
2:E:299:ASP:O	2:E:389:GLY:HA2	2.13	0.48
2:S:218:VAL:HG21	2:S:247:LEU:HB3	1.96	0.48
2:q:299:ASP:O	2:q:389:GLY:HA2	2.13	0.48
2:3:299:ASP:O	2:3:389:GLY:HA2	2.13	0.48
2:F:299:ASP:O	2:F:389:GLY:HA2	2.13	0.48
2:K:299:ASP:O	2:K:389:GLY:HA2	2.13	0.48
2:N:299:ASP:O	2:N:389:GLY:HA2	2.13	0.48
2:R:299:ASP:O	2:R:389:GLY:HA2	2.13	0.48
2:T:177:VAL:HA	2:T:207:LEU:HA	1.95	0.48
2:a:163:ARG:NH2	2:b:183:LEU:HB3	2.27	0.48
2:b:159:LEU:O	2:b:162:SER:OG	2.27	0.48
2:f:176:GLN:O	2:f:208:SER:N	2.47	0.48
2:k:171:ILE:HG22	2:k:177:VAL:HG11	1.95	0.48
2:l:163:ARG:HA	2:l:166:GLN:HE21	1.78	0.48
2:p:299:ASP:O	2:p:389:GLY:HA2	2.13	0.48
2:v:430:LEU:HA	2:v:433:THR:HB	1.94	0.48
2:1:299:ASP:O	2:1:389:GLY:HA2	2.13	0.48
2:AL:353:VAL:HG21	6:AY:71:VAL:HG11	1.94	0.48
2:Q:299:ASP:O	2:Q:389:GLY:HA2	2.13	0.48
2:T:172:GLU:OE2	2:T:179:LYS:HA	2.14	0.48
2:l:203:VAL:HG13	2:l:239:VAL:HG22	1.95	0.48
2:o:173:GLU:OE1	2:o:173:GLU:N	2.46	0.48
2:y:299:ASP:O	2:y:389:GLY:HA2	2.13	0.48
2:5:430:LEU:HA	2:5:433:THR:HB	1.94	0.48
4:8:183:THR:HG22	4:8:187:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:299:ASP:O	2:A:389:GLY:HA2	2.13	0.48
1:AP:206:PRO:HG3	2:o:192:PHE:CD1	2.48	0.48
1:AP:236:PRO:HB2	8:Aj:61:MET:HG2	1.95	0.48
6:AX:61:ASP:OD1	6:AX:61:ASP:N	2.45	0.48
1:Ak:183:MET:HE1	1:Ak:215:ILE:HG12	1.95	0.48
2:H:372:THR:HG21	9:Ao:10:ALA:HA	1.96	0.48
2:L:299:ASP:O	2:L:389:GLY:HA2	2.13	0.48
2:S:196:ASN:OD1	2:S:197:GLN:N	2.46	0.48
2:e:163:ARG:NH2	2:f:184:LEU:O	2.45	0.48
2:j:174:MET:HE2	2:j:174:MET:HB3	1.80	0.48
2:n:161:LEU:HD21	2:o:139:ASP:HB3	1.96	0.48
2:u:299:ASP:O	2:u:389:GLY:HA2	2.13	0.48
2:w:430:LEU:HA	2:w:433:THR:HB	1.94	0.48
2:4:299:ASP:O	2:4:389:GLY:HA2	2.13	0.48
1:Ak:82:ASP:OD1	1:Ak:82:ASP:N	2.45	0.48
2:N:381:ILE:CG2	10:Aw:3:GLY:HA3	2.44	0.48
2:O:299:ASP:O	2:O:389:GLY:HA2	2.13	0.48
2:Y:159:LEU:O	2:Y:162:SER:OG	2.28	0.48
2:d:153:ARG:O	2:d:157:GLU:HG2	2.13	0.48
2:g:178:ARG:NH2	2:g:206:THR:OG1	2.47	0.48
2:r:299:ASP:O	2:r:389:GLY:HA2	2.13	0.48
2:h:167:LEU:O	2:h:171:ILE:HG12	2.13	0.48
2:o:207:LEU:HD21	2:o:213:LEU:HD11	1.96	0.48
4:8:243:MET:HE2	2:e:152:GLN:HB2	1.96	0.48
1:Al:111:ARG:NE	1:Al:222:GLU:OE1	2.44	0.48
2:G:299:ASP:O	2:G:389:GLY:HA2	2.13	0.48
2:k:201:ALA:HB2	2:k:232:MET:HE1	1.96	0.48
3:AR:8:GLU:HG2	3:AR:83:ARG:NH2	2.29	0.48
5:AU:39:LYS:NZ	5:AU:91:GLY:O	2.40	0.48
2:U:174:MET:SD	2:U:221:ILE:HD11	2.54	0.48
2:h:187:PRO:HD3	2:h:199:ALA:HB2	1.96	0.48
1:9:119:LEU:HD21	1:9:270:PHE:CE1	2.49	0.47
2:S:200:SER:OG	2:T:227:SER:O	2.24	0.47
2:w:299:ASP:O	2:w:389:GLY:HA2	2.13	0.47
2:x:430:LEU:HA	2:x:433:THR:HB	1.94	0.47
2:4:430:LEU:HA	2:4:433:THR:HB	1.94	0.47
1:Ak:149:VAL:HG23	1:Ak:178:PRO:HB2	1.96	0.47
2:Z:193:VAL:C	2:Z:195:HIS:N	2.70	0.47
2:b:168:ALA:O	2:b:172:GLU:HG2	2.14	0.47
2:m:157:GLU:HG3	2:n:159:LEU:HD22	1.97	0.47
2:1:430:LEU:HA	2:1:433:THR:HB	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:68:TRP:CE2	2:a:148:PHE:CZ	2.98	0.47
1:9:189:ILE:CG1	2:c:193:VAL:HA	2.44	0.47
3:AR:42:THR:HG23	3:AR:44:ILE:HG12	1.96	0.47
6:AY:13:ALA:O	6:AY:17:GLU:HG2	2.14	0.47
2:D:299:ASP:O	2:D:389:GLY:HA2	2.13	0.47
2:I:299:ASP:O	2:I:389:GLY:HA2	2.13	0.47
2:Q:260:ARG:O	2:Q:264:GLU:HG2	2.15	0.47
2:T:178:ARG:NH1	2:T:207:LEU:O	2.47	0.47
2:V:241:ASP:CG	2:V:245:ARG:HG2	2.39	0.47
2:X:174:MET:SD	2:X:221:ILE:HD11	2.54	0.47
2:Y:227:SER:O	2:Z:200:SER:OG	2.29	0.47
2:i:227:SER:OG	2:j:201:ALA:O	2.33	0.47
7:Ag:71:MET:O	7:Ag:75:ASN:ND2	2.29	0.47
2:T:236:ARG:HD3	2:T:236:ARG:HA	1.65	0.47
2:a:220:SER:HB3	2:b:246:LEU:HB2	1.96	0.47
2:e:160:LYS:HD3	2:e:184:LEU:HB2	1.97	0.47
2:m:214:LYS:NZ	2:m:217:GLU:OE2	2.47	0.47
2:u:260:ARG:O	2:u:264:GLU:HG2	2.15	0.47
2:x:372:THR:HG22	9:Am:10:ILE:CB	2.40	0.47
3:6:71:GLN:NE2	2:a:151:SER:HB3	2.27	0.47
4:8:27:MET:HE1	7:Ai:92:VAL:HG13	1.96	0.47
5:AW:85:GLN:OE1	6:Ab:22:ASN:ND2	2.47	0.47
7:Ae:71:MET:SD	7:Ae:74:ARG:NH1	2.85	0.47
2:B:260:ARG:O	2:B:264:GLU:HG2	2.15	0.47
2:H:260:ARG:O	2:H:264:GLU:HG2	2.15	0.47
2:K:260:ARG:O	2:K:264:GLU:HG2	2.15	0.47
2:f:227:SER:O	2:g:200:SER:OG	2.31	0.47
2:z:260:ARG:O	2:z:264:GLU:HG2	2.15	0.47
1:0:154:ASN:HA	1:0:158:VAL:HB	1.95	0.47
2:2:260:ARG:O	2:2:264:GLU:HG2	2.15	0.47
5:AS:9:LEU:HD12	5:AS:120:LYS:HB3	1.97	0.47
5:AS:30:ILE:HG23	5:AS:96:LEU:HD11	1.96	0.47
5:AU:30:ILE:HG23	5:AU:96:LEU:HD11	1.97	0.47
7:Ai:88:ARG:HH11	7:Ai:92:VAL:HG21	1.80	0.47
2:O:260:ARG:O	2:O:264:GLU:HG2	2.15	0.47
2:d:201:ALA:HB3	2:d:237:ILE:HG23	1.95	0.47
2:p:260:ARG:O	2:p:264:GLU:HG2	2.15	0.47
2:3:260:ARG:O	2:3:264:GLU:HG2	2.15	0.47
2:5:260:ARG:O	2:5:264:GLU:HG2	2.15	0.47
5:AT:24:GLU:OE2	6:AY:2:SER:N	2.47	0.47
1:Ak:207:GLU:OE2	2:k:194:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:260:ARG:O	2:J:264:GLU:HG2	2.15	0.47
2:Y:206:THR:HA	2:Y:242:GLN:HB3	1.97	0.47
2:g:164:GLU:OE2	2:g:184:LEU:N	2.47	0.47
2:l:152:GLN:HG3	2:l:153:ARG:HE	1.80	0.47
2:r:260:ARG:O	2:r:264:GLU:HG2	2.15	0.47
2:s:260:ARG:O	2:s:264:GLU:HG2	2.15	0.47
2:w:260:ARG:O	2:w:264:GLU:HG2	2.15	0.47
1:0:264:PRO:HG3	1:Al:234:PHE:CG	2.50	0.47
2:E:260:ARG:O	2:E:264:GLU:HG2	2.15	0.47
2:M:260:ARG:O	2:M:264:GLU:HG2	2.15	0.47
2:h:163:ARG:HE	2:h:229:VAL:HG22	1.79	0.47
2:l:161:LEU:HD21	2:l:165:ARG:NH2	2.30	0.47
2:m:141:ILE:HG22	2:m:146:MET:HE1	1.97	0.47
2:m:210:GLY:O	2:m:211:THR:OG1	2.31	0.47
2:y:260:ARG:O	2:y:264:GLU:HG2	2.15	0.47
4:8:44:TYR:HB3	1:9:105:LEU:HD23	1.97	0.47
6:AZ:84:ASP:OD1	6:AZ:84:ASP:N	2.32	0.47
1:Ak:206:PRO:HG2	2:k:194:ARG:HH22	1.80	0.47
2:G:260:ARG:O	2:G:264:GLU:HG2	2.15	0.47
2:U:171:ILE:HG22	2:U:177:VAL:HG11	1.95	0.47
2:q:260:ARG:O	2:q:264:GLU:HG2	2.15	0.47
3:7:64:LEU:CD1	2:T:148:PHE:CD2	2.98	0.47
1:9:206:PRO:CG	2:d:192:PHE:CD2	2.82	0.47
5:AW:21:ARG:NH1	5:AW:48:GLU:OE1	2.48	0.47
2:T:139:ASP:OD1	2:T:139:ASP:N	2.48	0.47
2:W:194:ARG:HE	2:W:194:ARG:N	2.13	0.47
2:n:172:GLU:OE2	2:n:179:LYS:HA	2.15	0.47
2:o:171:ILE:HG22	2:o:177:VAL:HG11	1.97	0.47
1:0:258:PRO:HA	1:0:261:VAL:HG12	1.98	0.46
2:C:260:ARG:O	2:C:264:GLU:HG2	2.15	0.46
2:S:179:LYS:HB3	2:S:206:THR:HG23	1.96	0.46
2:d:182:VAL:O	2:d:183:LEU:HD13	2.15	0.46
2:t:260:ARG:O	2:t:264:GLU:HG2	2.15	0.46
9:Aq:5:ARG:O	9:Aq:6:THR:C	2.58	0.46
2:AF:349:ILE:O	2:AF:350:PRO:C	2.58	0.46
2:AM:341:ASN:ND2	5:AW:88:THR:OG1	2.48	0.46
3:AR:87:VAL:C	3:AR:89:TYR:H	2.23	0.46
2:D:260:ARG:O	2:D:264:GLU:HG2	2.15	0.46
2:N:260:ARG:O	2:N:264:GLU:HG2	2.15	0.46
2:Z:193:VAL:C	2:Z:195:HIS:H	2.22	0.46
2:b:163:ARG:HH12	2:c:183:LEU:HD12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:179:LYS:HB3	2:n:206:THR:OG1	2.15	0.46
2:AK:340:SER:HA	2:AK:349:ILE:HD11	1.97	0.46
5:AV:43:LEU:HG	5:AV:48:GLU:HG3	1.96	0.46
2:F:260:ARG:O	2:F:264:GLU:HG2	2.15	0.46
2:P:260:ARG:O	2:P:264:GLU:HG2	2.15	0.46
2:U:202:SER:HB3	2:V:224:MET:HG3	1.96	0.46
2:d:188:LYS:HA	2:d:188:LYS:HD3	1.75	0.46
2:e:150:VAL:HG12	2:e:154:LEU:HD23	1.98	0.46
2:n:140:ASP:O	2:n:144:GLN:HB2	2.16	0.46
2:z:381:ILE:CG2	10:At:7:GLU:CB	2.91	0.46
2:4:260:ARG:O	2:4:264:GLU:HG2	2.15	0.46
4:8:196:LEU:HD11	1:AP:264:PRO:HG2	1.98	0.46
6:AY:66:LYS:HE3	6:AY:68:MET:SD	2.56	0.46
6:Aa:20:ARG:HH21	6:Aa:111:ALA:HA	1.79	0.46
6:Aa:100:ASN:O	6:Aa:104:GLU:HG2	2.16	0.46
1:Al:81:GLU:O	1:Al:169:ARG:NH2	2.49	0.46
2:I:260:ARG:O	2:I:264:GLU:HG2	2.15	0.46
2:v:260:ARG:O	2:v:264:GLU:HG2	2.15	0.46
1:0:206:PRO:CD	2:Z:194:ARG:HH11	2.28	0.46
3:7:64:LEU:CD1	2:T:148:PHE:CE2	2.98	0.46
4:8:43:LEU:HB2	7:Ae:103:VAL:HG11	1.98	0.46
5:AT:35:THR:O	5:AT:92:ASN:ND2	2.48	0.46
6:Aa:100:ASN:HB3	6:Aa:103:GLU:HG2	1.97	0.46
7:Ae:90:LYS:HG3	7:Ai:74:ARG:HE	1.80	0.46
2:U:224:MET:HE3	2:U:224:MET:HB3	1.77	0.46
2:a:201:ALA:HB2	2:a:232:MET:HE1	1.98	0.46
4:8:85:MET:HG3	4:8:252:ILE:HG23	1.98	0.46
2:A:260:ARG:O	2:A:264:GLU:HG2	2.15	0.46
2:S:146:MET:CB	2:S:150:VAL:HG21	2.40	0.46
2:S:167:LEU:HA	2:S:167:LEU:HD23	1.66	0.46
2:Z:190:SER:O	2:Z:191:VAL:C	2.57	0.46
2:1:260:ARG:O	2:1:264:GLU:HG2	2.15	0.46
1:9:208:ASP:OD1	1:9:208:ASP:N	2.49	0.46
5:AU:15:THR:HG23	5:AU:45:PHE:HZ	1.81	0.46
6:AY:36:SER:OG	6:AY:38:ALA:O	2.27	0.46
1:Ak:141:LEU:HD11	1:Ak:280:LEU:HD22	1.98	0.46
2:L:260:ARG:O	2:L:264:GLU:HG2	2.15	0.46
2:R:260:ARG:O	2:R:264:GLU:HG2	2.15	0.46
2:W:167:LEU:O	2:W:171:ILE:HG12	2.15	0.46
2:c:163:ARG:NH2	2:d:184:LEU:O	2.49	0.46
2:f:182:VAL:HG13	2:f:203:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:234:THR:HA	2:f:237:ILE:HD13	1.98	0.46
2:i:164:GLU:HG2	2:i:184:LEU:HD13	1.96	0.46
1:0:186:GLN:NE2	1:0:287:PHE:O	2.49	0.46
3:6:16:MET:HE1	3:6:76:TYR:HB2	1.97	0.46
2:X:227:SER:O	2:Y:200:SER:OG	2.33	0.46
2:b:167:LEU:O	2:b:171:ILE:HG12	2.16	0.46
2:d:184:LEU:HD21	2:d:229:VAL:HG21	1.98	0.46
2:AI:342:GLN:O	2:AI:343:PRO:C	2.59	0.46
1:Ak:208:ASP:OD1	1:Ak:208:ASP:N	2.42	0.46
2:T:153:ARG:O	2:T:157:GLU:HG2	2.15	0.46
2:j:163:ARG:HA	2:j:166:GLN:NE2	2.29	0.46
2:n:239:VAL:N	2:n:248:SER:OG	2.48	0.46
4:8:98:LEU:HG	1:AP:128:THR:HG22	1.98	0.45
1:Al:192:LEU:HB3	2:S:192:PHE:CE2	2.51	0.45
2:T:174:MET:HB3	2:T:174:MET:HE2	1.67	0.45
2:e:210:GLY:O	2:e:211:THR:OG1	2.31	0.45
2:h:182:VAL:O	2:h:183:LEU:HD13	2.16	0.45
2:x:260:ARG:O	2:x:264:GLU:HG2	2.15	0.45
4:8:25:MET:HE1	4:8:148:LEU:HD23	1.98	0.45
2:S:199:ALA:HB3	2:S:232:MET:H	1.81	0.45
2:c:167:LEU:O	2:c:171:ILE:HG12	2.16	0.45
2:AF:344:PRO:O	2:AF:345:ALA:C	2.57	0.45
5:AV:30:ILE:HG23	5:AV:96:LEU:HD11	1.98	0.45
7:Af:53:ASP:OD2	7:Af:57:ARG:NH1	2.50	0.45
8:Aj:76:ALA:CB	2:j:152:GLN:NE2	2.71	0.45
2:a:150:VAL:HG12	2:a:154:LEU:HD23	1.98	0.45
2:i:153:ARG:O	2:i:157:GLU:HG2	2.17	0.45
1:0:263:LEU:HD23	1:Al:234:PHE:HE2	1.80	0.45
5:AS:39:LYS:NZ	5:AS:91:GLY:O	2.42	0.45
1:Ak:183:MET:HE2	1:Ak:214:LEU:HG	1.98	0.45
2:U:185:ALA:HB2	2:V:228:ALA:O	2.16	0.45
2:X:242:GLN:H	2:X:242:GLN:HG2	1.53	0.45
2:c:245:ARG:HG3	2:c:247:LEU:HD21	1.98	0.45
2:n:204:PHE:CE1	2:n:206:THR:HG22	2.50	0.45
2:o:229:VAL:HB	2:o:232:MET:SD	2.57	0.45
5:AS:126:LYS:HE2	7:Ah:82:ASP:OD1	2.16	0.45
2:V:172:GLU:OE2	2:V:179:LYS:HA	2.17	0.45
2:X:171:ILE:HD12	2:X:221:ILE:HD12	1.97	0.45
2:a:194:ARG:HA	2:a:194:ARG:CZ	2.46	0.45
2:c:241:ASP:CG	2:c:245:ARG:HG2	2.41	0.45
2:d:189:HIS:NE2	2:e:197:GLN:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:178:ARG:NH1	2:e:207:LEU:O	2.49	0.45
9:An:3:ASP:O	9:An:4:GLY:C	2.59	0.45
1:9:193:GLU:HG3	2:d:191:VAL:HB	1.99	0.45
3:AR:19:ILE:HG21	3:AR:72:MET:HE1	1.98	0.45
6:AZ:52:GLU:O	6:AZ:53:LEU:C	2.59	0.45
2:W:167:LEU:HD23	2:W:167:LEU:HA	1.74	0.45
2:i:163:ARG:HG3	2:i:166:GLN:HE21	1.82	0.45
4:8:74:THR:O	4:8:78:GLN:HG2	2.17	0.45
2:S:197:GLN:HE21	2:T:231:GLY:N	2.15	0.45
2:b:167:LEU:HD23	2:b:167:LEU:HA	1.77	0.45
2:e:239:VAL:HB	2:e:247:LEU:HB2	1.97	0.45
2:k:206:THR:HA	2:k:242:GLN:HG2	1.99	0.45
2:n:167:LEU:O	2:n:171:ILE:HG12	2.17	0.45
1:0:204:ASP:OD1	1:0:204:ASP:N	2.49	0.45
2:AF:336:PRO:HG2	2:AM:352:ASP:HB3	1.98	0.45
1:AP:90:LEU:O	1:AP:94:THR:OG1	2.34	0.45
1:Ak:206:PRO:CG	2:k:192:PHE:CD2	3.00	0.45
2:a:191:VAL:HA	2:a:195:HIS:HE1	1.81	0.45
9:Ap:7:HIS:O	9:Ap:9:PRO:N	2.50	0.45
4:8:177:LEU:HD22	1:AP:116:MET:HE3	1.98	0.45
1:9:184:LEU:O	2:c:193:VAL:HG11	2.17	0.45
5:AV:20:GLU:OE2	7:Ad:68:SER:OG	2.34	0.45
8:Aj:70:GLU:OE1	2:i:152:GLN:OE1	2.34	0.45
2:T:200:SER:OG	2:U:227:SER:OG	2.35	0.45
2:X:172:GLU:OE2	2:X:179:LYS:HA	2.17	0.45
2:X:227:SER:OG	2:Y:200:SER:OG	2.26	0.45
2:Y:151:SER:O	2:Y:153:ARG:N	2.50	0.45
2:Z:239:VAL:HG12	2:Z:247:LEU:HD12	1.99	0.45
2:g:167:LEU:HD23	2:g:167:LEU:HA	1.80	0.45
3:6:31:ILE:HG13	3:6:57:VAL:HG11	1.99	0.45
2:AJ:341:ASN:HD21	5:AT:86:PRO:HG3	1.82	0.45
5:AT:26:ILE:HG21	5:AT:103:PHE:HB2	1.99	0.45
7:Ad:86:GLN:O	7:Ad:90:LYS:HG2	2.17	0.45
2:T:167:LEU:HD23	2:T:167:LEU:HA	1.73	0.45
2:U:174:MET:HE2	2:U:174:MET:HB3	1.76	0.45
2:W:174:MET:HE2	2:W:174:MET:HB3	1.89	0.45
1:0:198:MET:HE3	1:9:144:PHE:HD2	1.82	0.44
2:5:383:HIS:HB2	10:As:14:GLU:CB	2.47	0.44
1:AP:108:SER:HB2	1:AP:287:PHE:CZ	2.51	0.44
6:AY:27:ASN:OD1	6:AY:42:TYR:OH	2.27	0.44
2:S:176:GLN:NE2	2:W:243:HIS:O	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:176:GLN:OE1	2:f:176:GLN:N	2.47	0.44
2:4:450:LYS:HE2	2:4:450:LYS:HB2	1.85	0.44
2:AM:331:MET:HE2	2:AM:331:MET:HB3	1.87	0.44
1:AP:251:MET:HE2	8:Aj:39:LEU:HD23	1.99	0.44
3:AR:1:MET:HE2	3:AR:87:VAL:HG11	1.98	0.44
1:Al:116:MET:SD	1:Al:134:ILE:HG23	2.57	0.44
2:P:258:ALA:O	2:P:261:LYS:HG2	2.18	0.44
2:W:185:ALA:HB3	2:W:200:SER:HB3	1.99	0.44
2:d:167:LEU:O	2:d:171:ILE:HG12	2.17	0.44
2:l:140:ASP:N	2:l:140:ASP:OD1	2.50	0.44
4:8:18:PRO:HB3	4:8:57:ILE:HD13	2.00	0.44
4:8:215:PHE:HD2	4:8:216:SER:H	1.66	0.44
3:AR:87:VAL:C	3:AR:89:TYR:N	2.74	0.44
2:H:258:ALA:O	2:H:261:LYS:HG2	2.18	0.44
2:Q:258:ALA:O	2:Q:261:LYS:HG2	2.18	0.44
2:W:150:VAL:HG12	2:W:154:LEU:HD23	1.99	0.44
2:f:153:ARG:NE	2:f:153:ARG:HA	2.32	0.44
2:A:258:ALA:O	2:A:261:LYS:HG2	2.18	0.44
2:AF:339:LEU:HD11	6:Ac:72:GLU:HG3	1.99	0.44
3:AQ:89:TYR:CE2	2:l:188:LYS:CB	2.90	0.44
1:Al:125:LEU:HD22	1:Al:263:LEU:HD11	1.98	0.44
1:Al:187:THR:CG2	2:T:193:VAL:HG23	2.47	0.44
1:Al:206:PRO:HG3	2:S:192:PHE:CB	2.46	0.44
2:E:258:ALA:O	2:E:261:LYS:HG2	2.18	0.44
2:K:258:ALA:O	2:K:261:LYS:HG2	2.18	0.44
2:Y:241:ASP:CG	2:Y:245:ARG:HG2	2.41	0.44
2:d:242:GLN:H	2:d:242:GLN:HG3	1.53	0.44
2:h:220:SER:HB3	2:i:246:LEU:HB2	1.99	0.44
2:l:232:MET:HE2	2:l:232:MET:HB2	1.73	0.44
2:o:141:ILE:HG23	2:o:158:ARG:HH21	1.83	0.44
2:z:258:ALA:O	2:z:261:LYS:HG2	2.18	0.44
3:7:89:TYR:CE2	2:Y:188:LYS:HB2	2.53	0.44
5:AS:85:GLN:OE1	6:Ac:22:ASN:ND2	2.51	0.44
7:Ai:96:LYS:O	7:Ai:100:ASN:ND2	2.45	0.44
2:D:258:ALA:O	2:D:261:LYS:HG2	2.18	0.44
2:J:258:ALA:O	2:J:261:LYS:HG2	2.18	0.44
2:S:153:ARG:NE	2:S:153:ARG:HA	2.31	0.44
2:S:183:LEU:HB3	2:T:163:ARG:HH22	1.82	0.44
2:S:241:ASP:OD2	2:S:245:ARG:NH1	2.50	0.44
2:i:215:GLN:O	2:i:219:ASP:HB2	2.17	0.44
2:l:241:ASP:OD1	2:l:245:ARG:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:258:ALA:O	2:r:261:LYS:HG2	2.18	0.44
2:u:258:ALA:O	2:u:261:LYS:HG2	2.18	0.44
2:v:258:ALA:O	2:v:261:LYS:HG2	2.17	0.44
2:y:258:ALA:O	2:y:261:LYS:HG2	2.18	0.44
2:1:258:ALA:O	2:1:261:LYS:HG2	2.18	0.44
6:Ac:129:LEU:HD22	7:Ah:67:LEU:HD12	1.99	0.44
2:G:258:ALA:O	2:G:261:LYS:HG2	2.18	0.44
2:I:402:ASP:OD1	2:I:448:SER:OG	2.33	0.44
2:Z:153:ARG:O	2:Z:157:GLU:HG2	2.17	0.44
2:n:203:VAL:HG13	2:n:239:VAL:HG22	1.99	0.44
2:o:234:THR:HA	2:o:237:ILE:HD13	1.99	0.44
2:x:258:ALA:O	2:x:261:LYS:HG2	2.18	0.44
3:6:63:MET:HG2	3:7:11:ARG:HA	1.99	0.44
7:Ae:48:GLN:HE21	7:Ae:81:PHE:HB2	1.81	0.44
8:Aj:71:GLU:HA	8:Aj:77:LYS:HD2	1.99	0.44
2:C:387:GLN:HE21	2:C:387:GLN:HB2	1.63	0.44
2:J:402:ASP:OD1	2:J:448:SER:OG	2.33	0.44
2:J:450:LYS:HE2	2:J:450:LYS:HB2	1.85	0.44
2:M:369:LYS:HE3	2:M:369:LYS:HB3	1.85	0.44
2:a:241:ASP:OD2	2:a:245:ARG:NH1	2.51	0.44
2:d:216:GLN:HE21	2:e:246:LEU:H	1.65	0.44
2:d:229:VAL:HB	2:d:232:MET:SD	2.57	0.44
2:e:166:GLN:O	2:e:169:GLN:HB3	2.18	0.44
2:F:258:ALA:O	2:F:261:LYS:HG2	2.18	0.44
2:U:164:GLU:HG2	2:U:184:LEU:HD13	2.00	0.44
2:V:171:ILE:HG22	2:V:177:VAL:HG11	1.99	0.44
2:Z:198:GLU:HG2	2:Z:233:LYS:HE2	2.00	0.44
2:m:204:PHE:CE1	2:m:206:THR:HG22	2.51	0.44
2:o:226:ALA:HA	2:o:232:MET:SD	2.58	0.44
2:AF:348:SER:O	2:AF:349:ILE:HB	2.17	0.44
6:AZ:66:LYS:HE3	6:AZ:68:MET:HG2	1.99	0.44
2:B:258:ALA:O	2:B:261:LYS:HG2	2.18	0.44
2:M:450:LYS:HE2	2:M:450:LYS:HB2	1.85	0.44
2:N:258:ALA:O	2:N:261:LYS:HG2	2.18	0.44
2:R:258:ALA:O	2:R:261:LYS:HG2	2.18	0.44
2:S:181:ARG:HD2	2:T:170:ALA:HB2	2.00	0.44
2:W:142:LEU:O	2:X:158:ARG:NH1	2.50	0.44
2:W:229:VAL:HG11	2:W:232:MET:HE3	2.00	0.44
2:Z:153:ARG:HH21	2:Z:156:GLN:CD	2.24	0.44
2:Z:163:ARG:HA	2:Z:166:GLN:HE21	1.83	0.44
2:k:146:MET:HB3	2:k:150:VAL:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:258:ALA:O	2:s:261:LYS:HG2	2.18	0.44
2:v:387:GLN:HE21	2:v:387:GLN:HB2	1.63	0.44
1:0:187:THR:O	2:Y:192:PHE:CD1	2.71	0.43
2:AA:353:VAL:O	2:AA:356:MET:HG2	2.18	0.43
3:AQ:20:MET:HE1	3:AQ:69:MET:HB3	2.00	0.43
7:Ah:64:ASP:OD1	7:Ah:64:ASP:N	2.48	0.43
8:Aj:68:GLN:CD	2:i:152:GLN:HG2	2.39	0.43
2:N:374:ASN:OD1	9:Ap:7:HIS:HA	2.17	0.43
2:S:153:ARG:HG3	2:T:156:GLN:HE22	1.82	0.43
2:S:187:PRO:HB3	2:S:199:ALA:N	2.32	0.43
2:c:215:GLN:HA	2:c:218:VAL:HG12	2.00	0.43
2:e:206:THR:HA	2:e:242:GLN:HG2	2.00	0.43
2:k:174:MET:HE2	2:k:174:MET:HA	2.00	0.43
2:o:206:THR:O	2:o:206:THR:OG1	2.36	0.43
2:t:258:ALA:O	2:t:261:LYS:HG2	2.18	0.43
2:4:258:ALA:O	2:4:261:LYS:HG2	2.18	0.43
2:5:258:ALA:O	2:5:261:LYS:HG2	2.18	0.43
3:6:67:HIS:HD2	3:7:11:ARG:HH22	1.65	0.43
3:AR:8:GLU:HG2	3:AR:83:ARG:HH22	1.82	0.43
3:AR:12:GLU:OE1	3:AR:83:ARG:NH1	2.50	0.43
5:AS:21:ARG:NH1	5:AS:48:GLU:OE1	2.51	0.43
6:Ab:39:LYS:HD2	6:Ab:39:LYS:HA	1.85	0.43
2:H:374:ASN:HD21	9:Ao:10:ALA:HB2	1.83	0.43
2:O:258:ALA:O	2:O:261:LYS:HG2	2.18	0.43
2:W:177:VAL:HG11	2:W:205:LEU:HD23	2.00	0.43
2:Z:206:THR:O	2:Z:206:THR:OG1	2.32	0.43
2:h:174:MET:HE2	2:h:174:MET:HA	2.00	0.43
2:5:450:LYS:HB2	2:5:450:LYS:HE2	1.85	0.43
6:AX:100:ASN:O	6:AX:104:GLU:HG2	2.18	0.43
1:Ak:238:LEU:HD11	1:Al:261:VAL:HG13	2.00	0.43
2:I:258:ALA:O	2:I:261:LYS:HG2	2.18	0.43
2:I:387:GLN:HE21	2:I:387:GLN:HB2	1.63	0.43
2:O:369:LYS:HE3	2:O:369:LYS:HB3	1.85	0.43
2:l:167:LEU:O	2:l:171:ILE:HG12	2.18	0.43
2:l:183:LEU:HD12	2:m:163:ARG:HH21	1.83	0.43
2:3:258:ALA:O	2:3:261:LYS:HG2	2.18	0.43
1:Ak:108:SER:HB2	1:Ak:287:PHE:CZ	2.53	0.43
1:Ak:204:ASP:OD1	1:Ak:204:ASP:N	2.46	0.43
1:Ak:206:PRO:HD3	2:k:192:PHE:CD2	2.49	0.43
2:H:319:SER:HB3	9:Ao:3:THR:N	2.32	0.43
2:L:258:ALA:O	2:L:261:LYS:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:227:SER:O	2:X:200:SER:OG	2.24	0.43
2:Y:173:GLU:HB3	2:Z:204:PHE:CE1	2.53	0.43
2:c:184:LEU:HG	2:c:232:MET:HE1	1.99	0.43
2:k:200:SER:OG	2:k:201:ALA:N	2.51	0.43
2:o:239:VAL:N	2:o:248:SER:OG	2.51	0.43
2:q:258:ALA:O	2:q:261:LYS:HG2	2.18	0.43
2:2:258:ALA:O	2:2:261:LYS:HG2	2.18	0.43
3:AR:15:TRP:CZ2	2:U:148:PHE:HB2	2.53	0.43
5:AV:35:THR:O	5:AV:92:ASN:ND2	2.52	0.43
5:AV:41:ARG:HD3	5:AV:78:LYS:HD2	2.00	0.43
7:Ah:55:GLN:NE2	7:Ah:74:ARG:HE	2.16	0.43
2:C:258:ALA:O	2:C:261:LYS:HG2	2.18	0.43
2:J:369:LYS:HE3	2:J:369:LYS:HB3	1.85	0.43
2:M:258:ALA:O	2:M:261:LYS:HG2	2.18	0.43
2:X:156:GLN:HE22	2:Y:153:ARG:HD2	1.83	0.43
2:X:168:ALA:O	2:X:172:GLU:HG2	2.18	0.43
2:Y:175:LYS:HB2	2:Y:175:LYS:HE2	1.79	0.43
2:Y:231:GLY:N	2:Z:197:GLN:HE21	2.16	0.43
2:Z:163:ARG:HA	2:Z:166:GLN:NE2	2.33	0.43
2:Z:191:VAL:O	2:Z:192:PHE:C	2.60	0.43
2:g:176:GLN:OE1	2:g:176:GLN:N	2.39	0.43
2:k:146:MET:HG2	2:k:155:GLU:OE1	2.18	0.43
2:k:153:ARG:O	2:k:157:GLU:HG2	2.18	0.43
2:o:185:ALA:HB3	2:o:200:SER:HB3	2.00	0.43
2:r:450:LYS:HE2	2:r:450:LYS:HB2	1.85	0.43
5:AS:36:PRO:HB3	5:AS:90:ASP:HB2	2.01	0.43
2:T:176:GLN:O	2:T:208:SER:N	2.50	0.43
2:a:174:MET:HE2	2:a:174:MET:HB3	1.78	0.43
2:p:258:ALA:O	2:p:261:LYS:HG2	2.18	0.43
2:v:450:LYS:HE2	2:v:450:LYS:HB2	1.85	0.43
5:AS:33:ALA:O	5:AS:92:ASN:ND2	2.51	0.43
5:AW:15:THR:HG23	5:AW:45:PHE:HZ	1.84	0.43
6:Ab:100:ASN:HB3	6:Ab:103:GLU:HG2	1.99	0.43
1:Al:187:THR:CG2	2:T:193:VAL:CG2	2.96	0.43
1:Al:203:VAL:HG11	1:Al:209:VAL:HG12	1.99	0.43
2:H:387:GLN:HE21	2:H:387:GLN:HB2	1.63	0.43
2:I:450:LYS:HE2	2:I:450:LYS:HB2	1.85	0.43
2:L:402:ASP:OD1	2:L:448:SER:OG	2.33	0.43
2:n:146:MET:HG2	2:n:155:GLU:OE1	2.19	0.43
2:o:174:MET:HE2	2:o:174:MET:HA	1.99	0.43
2:q:374:ASN:OD1	9:Aq:4:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:257:SER:HA	1:9:255:MET:HG2	2.01	0.43
2:AE:343:PRO:HG3	5:AT:80:TYR:CZ	2.54	0.43
1:AP:114:VAL:O	1:AP:118:ILE:HG12	2.17	0.43
2:J:387:GLN:HE21	2:J:387:GLN:HB2	1.63	0.43
2:N:374:ASN:OD1	9:Ap:7:HIS:CA	2.67	0.43
2:d:243:HIS:HB2	2:d:245:ARG:NH1	2.34	0.43
2:g:150:VAL:HG11	2:g:158:ARG:NH1	2.33	0.43
2:k:163:ARG:HA	2:k:166:GLN:HE21	1.83	0.43
2:k:176:GLN:NE2	2:k:217:GLU:OE1	2.51	0.43
2:m:178:ARG:NH1	2:m:207:LEU:O	2.52	0.43
2:o:210:GLY:O	2:o:211:THR:OG1	2.28	0.43
4:8:132:PHE:O	4:8:136:MET:HG2	2.19	0.43
3:AQ:81:ILE:HG13	1:Ak:278:LEU:HD21	2.01	0.43
3:AR:84:LEU:HD11	1:Al:229:ILE:HG12	2.01	0.43
6:AZ:75:LYS:HB2	6:AZ:98:ASN:HD22	1.84	0.43
7:Af:64:ASP:OD1	7:Af:64:ASP:N	2.46	0.43
1:Ak:195:PHE:HB3	1:Ak:213:VAL:HG13	2.01	0.43
2:d:233:LYS:O	2:d:234:THR:C	2.61	0.43
2:g:163:ARG:HA	2:g:166:GLN:NE2	2.34	0.43
2:w:258:ALA:O	2:w:261:LYS:HG2	2.18	0.43
5:AU:36:PRO:HB3	5:AU:90:ASP:HB2	2.01	0.43
6:Ac:13:ALA:O	6:Ac:17:GLU:HG2	2.19	0.43
2:N:318:ARG:HG2	9:Ap:3:THR:CB	2.49	0.43
2:W:217:GLU:O	2:W:220:SER:OG	2.31	0.43
2:W:242:GLN:H	2:W:242:GLN:HG2	1.64	0.43
2:1:387:GLN:HE21	2:1:387:GLN:HB2	1.63	0.42
3:7:16:MET:HE1	3:7:76:TYR:HB2	2.01	0.42
1:9:275:GLY:O	1:9:279:ILE:HG12	2.19	0.42
1:AP:204:ASP:OD1	1:AP:204:ASP:N	2.52	0.42
2:U:221:ILE:HA	2:U:221:ILE:HD13	1.67	0.42
2:Z:159:LEU:O	2:Z:162:SER:OG	2.29	0.42
2:c:174:MET:SD	2:c:221:ILE:HD11	2.59	0.42
2:g:167:LEU:O	2:g:171:ILE:HG12	2.19	0.42
2:g:170:ALA:HA	2:h:181:ARG:NH1	2.34	0.42
2:i:172:GLU:OE2	2:i:179:LYS:HA	2.18	0.42
4:8:207:ARG:HH12	4:8:210:PRO:HA	1.84	0.42
2:A:450:LYS:HE2	2:A:450:LYS:HB2	1.85	0.42
1:AP:243:VAL:HG21	8:Aj:89:LEU:HD11	2.01	0.42
3:AQ:49:LEU:HD23	3:AQ:49:LEU:H	1.84	0.42
6:AZ:100:ASN:O	6:AZ:104:GLU:HG2	2.19	0.42
6:Ab:126:LYS:HE2	6:Ab:126:LYS:HB3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:164:GLU:HG2	2:T:184:LEU:HD13	2.00	0.42
2:T:175:LYS:HB2	2:T:175:LYS:HE2	1.78	0.42
2:U:179:LYS:HD3	2:U:180:ALA:H	1.84	0.42
2:e:193:VAL:HG12	2:e:195:HIS:H	1.83	0.42
4:8:176:TRP:HE1	4:8:251:GLN:HG2	1.83	0.42
1:AP:228:GLN:O	1:AP:232:MET:HG2	2.18	0.42
6:AZ:44:ALA:O	6:AZ:73:SER:N	2.46	0.42
1:Ak:204:ASP:O	2:k:192:PHE:CD2	2.72	0.42
2:H:450:LYS:HE2	2:H:450:LYS:HB2	1.85	0.42
2:N:450:LYS:HE2	2:N:450:LYS:HB2	1.85	0.42
2:V:246:LEU:HD12	2:k:220:SER:HA	2.00	0.42
2:Y:246:LEU:O	2:Y:247:LEU:HD23	2.18	0.42
2:b:174:MET:SD	2:b:221:ILE:HD11	2.59	0.42
2:h:168:ALA:O	2:h:172:GLU:HG2	2.19	0.42
2:h:179:LYS:HB3	2:h:206:THR:OG1	2.19	0.42
2:o:153:ARG:HA	2:o:153:ARG:NE	2.33	0.42
2:AL:338:ALA:HB1	6:AY:103:GLU:HB2	2.02	0.42
2:F:306:THR:CB	10:Ar:14:GLU:CB	2.97	0.42
2:S:153:ARG:O	2:S:157:GLU:HG2	2.20	0.42
2:V:226:ALA:HA	2:V:232:MET:SD	2.59	0.42
2:W:172:GLU:OE2	2:W:179:LYS:HA	2.19	0.42
2:X:222:VAL:HG23	2:X:237:ILE:HB	2.01	0.42
2:c:150:VAL:HG12	2:c:154:LEU:HD23	2.01	0.42
2:e:224:MET:HA	2:f:238:THR:HG21	2.01	0.42
2:k:157:GLU:HG3	2:l:159:LEU:HD22	2.02	0.42
2:k:222:VAL:HG23	2:k:237:ILE:HB	2.01	0.42
2:l:246:LEU:HD23	2:l:248:SER:H	1.84	0.42
2:m:229:VAL:HB	2:m:232:MET:SD	2.59	0.42
2:4:387:GLN:HE21	2:4:387:GLN:HB2	1.63	0.42
3:6:70:THR:O	3:6:71:GLN:C	2.63	0.42
4:8:84:ALA:HB1	4:8:255:LEU:HD13	2.01	0.42
1:Al:110:THR:HG21	1:Al:219:ILE:HD11	2.01	0.42
2:T:210:GLY:O	2:T:211:THR:OG1	2.34	0.42
2:W:147:GLY:O	2:W:150:VAL:HG22	2.20	0.42
2:Y:236:ARG:HD3	2:Y:250:GLY:HA3	2.01	0.42
2:d:174:MET:HB2	2:d:177:VAL:HB	2.01	0.42
2:i:186:LEU:HD23	2:i:199:ALA:HA	2.01	0.42
2:m:174:MET:HB3	2:m:174:MET:HE2	1.78	0.42
2:m:206:THR:O	2:m:206:THR:OG1	2.35	0.42
2:2:402:ASP:OD1	2:2:448:SER:OG	2.33	0.42
1:AP:101:ALA:HB2	7:Ah:95:TYR:OH	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AU:50:GLN:OE1	2:E:368:ARG:NH2	2.52	0.42
6:Ab:133:LEU:HA	7:Ad:71:MET:HE3	2.01	0.42
2:F:369:LYS:HE3	2:F:369:LYS:HB3	1.85	0.42
2:P:369:LYS:HE3	2:P:369:LYS:HB3	1.85	0.42
2:P:387:GLN:HE21	2:P:387:GLN:HB2	1.63	0.42
2:d:152:GLN:HE21	2:d:152:GLN:HB2	1.69	0.42
2:g:170:ALA:HA	2:h:181:ARG:HH11	1.83	0.42
2:l:146:MET:HG2	2:l:155:GLU:OE1	2.20	0.42
2:l:165:ARG:NH2	2:m:139:ASP:OD2	2.52	0.42
2:m:241:ASP:OD1	2:m:241:ASP:N	2.51	0.42
3:7:63:MET:HE1	3:AR:15:TRP:HE3	1.85	0.42
2:AO:333:ALA:HB3	2:AO:356:MET:HB3	2.02	0.42
6:AX:127:GLN:O	6:AX:131:ARG:HG2	2.20	0.42
6:AZ:41:THR:O	6:AZ:42:TYR:C	2.62	0.42
7:Ad:33:PHE:HE1	1:Al:154:ASN:HB2	1.84	0.42
7:Ad:71:MET:HA	7:Ad:74:ARG:HG2	2.02	0.42
1:Ak:167:THR:HG22	1:Ak:169:ARG:H	1.84	0.42
1:Al:166:VAL:HB	1:Al:170:GLU:HB2	2.00	0.42
2:N:302:ALA:HB3	2:O:385:ARG:HB3	2.02	0.42
2:T:163:ARG:HA	2:T:166:GLN:NE2	2.34	0.42
2:V:201:ALA:HB2	2:V:232:MET:HE1	2.02	0.42
2:a:141:ILE:O	2:a:146:MET:HE1	2.20	0.42
2:a:207:LEU:HD21	2:a:213:LEU:HD11	2.02	0.42
2:i:175:LYS:HE2	2:i:175:LYS:HB2	1.90	0.42
2:j:172:GLU:OE2	2:j:179:LYS:HA	2.20	0.42
2:k:243:HIS:O	2:l:176:GLN:NE2	2.41	0.42
2:x:387:GLN:HE21	2:x:387:GLN:HB2	1.63	0.42
2:AF:342:GLN:O	2:AF:343:PRO:C	2.61	0.42
2:AK:337:GLY:O	2:AK:341:ASN:ND2	2.53	0.42
3:AQ:17:VAL:HG23	1:Ak:243:VAL:HG23	2.01	0.42
8:Aj:105:MET:HE2	8:Aj:105:MET:HB3	1.98	0.42
2:U:190:SER:HB2	2:U:196:ASN:ND2	2.35	0.42
2:W:218:VAL:HG21	2:W:247:LEU:CB	2.49	0.42
2:b:201:ALA:HB2	2:b:232:MET:HE1	2.01	0.42
2:c:241:ASP:OD1	2:c:245:ARG:HG2	2.20	0.42
2:i:177:VAL:HG11	2:i:205:LEU:HD23	2.01	0.42
2:m:189:HIS:O	2:m:196:ASN:ND2	2.52	0.42
2:u:369:LYS:HE3	2:u:369:LYS:HB3	1.85	0.42
2:x:302:ALA:HB3	2:y:385:ARG:HB3	2.02	0.42
1:0:272:LEU:HD12	1:0:273:VAL:HG23	2.02	0.42
4:8:175:GLY:HA2	1:AP:280:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AQ:21:VAL:O	3:AQ:25:ILE:HG12	2.20	0.42
3:AR:16:MET:HE2	3:AR:76:TYR:HB2	2.02	0.42
7:Ad:66:SER:OG	7:Ad:69:ASP:OD1	2.38	0.42
2:O:302:ALA:HB3	2:P:385:ARG:HB3	2.02	0.42
2:X:203:VAL:HG13	2:X:239:VAL:HG13	2.02	0.42
2:c:153:ARG:O	2:c:157:GLU:HG2	2.20	0.42
2:e:167:LEU:HA	2:e:167:LEU:HD23	1.84	0.42
2:l:172:GLU:OE2	2:l:179:LYS:HA	2.20	0.42
2:m:240:THR:HG21	2:n:224:MET:HE2	2.02	0.42
2:o:206:THR:HA	2:o:242:GLN:CG	2.50	0.42
2:2:302:ALA:HB3	2:3:385:ARG:HB3	2.02	0.42
4:8:69:PHE:HB3	1:AP:162:LEU:HD21	2.02	0.42
3:AQ:80:LEU:HA	3:AQ:83:ARG:HG2	2.01	0.42
6:AZ:39:LYS:HA	6:AZ:39:LYS:HD3	1.74	0.42
2:M:302:ALA:HB3	2:N:385:ARG:HB3	2.02	0.42
2:N:369:LYS:HE3	2:N:369:LYS:HB3	1.85	0.42
2:W:221:ILE:HD13	2:W:221:ILE:HA	1.76	0.42
2:X:215:GLN:HA	2:X:218:VAL:HG12	2.02	0.42
2:a:146:MET:HB3	2:a:150:VAL:HG21	2.02	0.42
2:b:150:VAL:HG12	2:b:154:LEU:HD23	2.02	0.42
2:d:210:GLY:O	2:d:211:THR:OG1	2.30	0.42
2:d:243:HIS:HB2	2:d:245:ARG:HH12	1.84	0.42
2:e:188:LYS:H	2:e:188:LYS:HD2	1.85	0.42
2:k:226:ALA:HA	2:k:232:MET:SD	2.60	0.42
2:r:319:SER:HB3	9:Aq:4:SER:O	2.20	0.42
2:t:369:LYS:HE3	2:t:369:LYS:HB3	1.85	0.42
2:u:450:LYS:HE2	2:u:450:LYS:HB2	1.85	0.42
2:v:369:LYS:HE3	2:v:369:LYS:HB3	1.85	0.42
2:x:426:ILE:O	2:x:430:LEU:HG	2.20	0.42
2:3:302:ALA:HB3	2:4:385:ARG:HB3	2.02	0.41
4:8:214:ILE:HG12	1:AP:255:MET:HE3	2.01	0.41
3:AQ:4:GLU:OE2	2:k:152:GLN:HB3	2.20	0.41
5:AT:128:ILE:HD13	7:Af:83:ALA:HB2	2.02	0.41
6:Ac:100:ASN:HB3	6:Ac:103:GLU:HG2	2.01	0.41
1:Ak:197:THR:CB	2:V:194:ARG:HG2	2.49	0.41
1:Al:183:MET:HB2	1:Al:214:LEU:HD21	2.02	0.41
2:B:450:LYS:HE2	2:B:450:LYS:HB2	1.85	0.41
2:G:387:GLN:HE21	2:G:387:GLN:HB2	1.63	0.41
2:S:188:LYS:HD3	2:S:188:LYS:HA	1.85	0.41
2:S:219:ASP:HA	2:S:222:VAL:HG12	2.01	0.41
2:T:168:ALA:O	2:T:172:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:139:ASP:OD2	2:X:165:ARG:NH2	2.52	0.41
2:b:172:GLU:OE1	2:b:179:LYS:HA	2.20	0.41
2:n:198:GLU:OE2	2:n:199:ALA:N	2.53	0.41
2:q:450:LYS:HE2	2:q:450:LYS:HB2	1.85	0.41
2:w:302:ALA:HB3	2:x:385:ARG:HB3	2.02	0.41
4:8:207:ARG:O	4:8:207:ARG:HD3	2.20	0.41
2:A:426:ILE:O	2:A:430:LEU:HG	2.20	0.41
2:AB:343:PRO:HG3	5:AW:80:TYR:CZ	2.55	0.41
2:AD:346:ASP:OD1	5:AU:39:LYS:NZ	2.44	0.41
3:AQ:8:GLU:OE1	3:AQ:83:ARG:NH2	2.53	0.41
8:Aj:77:LYS:HE3	8:Aj:77:LYS:HB2	1.89	0.41
2:C:450:LYS:HE2	2:C:450:LYS:HB2	1.85	0.41
2:G:450:LYS:HE2	2:G:450:LYS:HB2	1.85	0.41
2:J:426:ILE:O	2:J:430:LEU:HG	2.21	0.41
2:K:387:GLN:HE21	2:K:387:GLN:HB2	1.63	0.41
2:M:426:ILE:O	2:M:430:LEU:HG	2.20	0.41
2:S:163:ARG:HH12	2:W:183:LEU:HB3	1.85	0.41
2:W:229:VAL:HB	2:W:232:MET:SD	2.59	0.41
2:o:162:SER:O	2:o:166:GLN:HG2	2.20	0.41
2:p:302:ALA:HB3	2:q:385:ARG:HB3	2.02	0.41
2:y:302:ALA:HB3	2:z:385:ARG:HB3	2.02	0.41
1:0:206:PRO:HG2	2:Z:194:ARG:NH1	2.26	0.41
1:0:274:ASP:OD2	1:0:277:ASN:ND2	2.52	0.41
2:5:426:ILE:O	2:5:430:LEU:HG	2.20	0.41
2:AB:353:VAL:HG21	6:Ab:38:ALA:HB2	2.01	0.41
2:R:302:ALA:HB3	2:p:385:ARG:HB3	2.02	0.41
2:c:222:VAL:HG23	2:c:237:ILE:HB	2.02	0.41
2:q:302:ALA:HB3	2:r:385:ARG:HB3	2.02	0.41
2:q:426:ILE:O	2:q:430:LEU:HG	2.20	0.41
2:s:369:LYS:HE3	2:s:369:LYS:HB3	1.85	0.41
2:s:450:LYS:HE2	2:s:450:LYS:HB2	1.85	0.41
2:w:402:ASP:OD1	2:w:448:SER:OG	2.33	0.41
2:2:426:ILE:O	2:2:430:LEU:HG	2.20	0.41
2:4:302:ALA:HB3	2:5:385:ARG:HB3	2.02	0.41
3:7:4:GLU:HB3	2:Y:152:GLN:HE21	1.85	0.41
4:8:88:VAL:HG12	4:8:92:MET:HE3	2.02	0.41
1:AP:88:GLN:OE1	1:AP:161:TYR:OH	2.29	0.41
1:AP:253:MET:H	1:AP:253:MET:HG2	1.69	0.41
2:F:450:LYS:HE2	2:F:450:LYS:HB2	1.85	0.41
2:I:426:ILE:O	2:I:430:LEU:HG	2.20	0.41
2:J:294:VAL:HG22	2:J:396:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:153:ARG:O	2:W:157:GLU:HG2	2.20	0.41
2:b:227:SER:HG	2:c:200:SER:HG	1.58	0.41
2:e:150:VAL:HG11	2:e:158:ARG:HH11	1.84	0.41
2:l:160:LYS:O	2:l:164:GLU:HG3	2.20	0.41
2:o:174:MET:HB2	2:o:177:VAL:HB	2.02	0.41
2:p:426:ILE:O	2:p:430:LEU:HG	2.21	0.41
2:w:426:ILE:O	2:w:430:LEU:HG	2.20	0.41
2:1:302:ALA:HB3	2:2:385:ARG:HB3	2.02	0.41
4:8:61:PRO:HG3	4:8:161:GLY:HA3	2.03	0.41
2:AF:346:ASP:HB3	2:AF:347:ALA:H	1.61	0.41
6:Aa:43:LYS:HG2	6:Aa:77:LEU:HD21	2.02	0.41
6:Ab:96:LYS:HE3	6:Ab:96:LYS:HB3	1.89	0.41
2:L:426:ILE:O	2:L:430:LEU:HG	2.21	0.41
2:O:450:LYS:HE2	2:O:450:LYS:HB2	1.85	0.41
2:V:185:ALA:HB3	2:V:200:SER:HB3	2.02	0.41
2:Y:166:GLN:H	2:Y:166:GLN:HG2	1.71	0.41
2:l:191:VAL:O	2:l:192:PHE:HB2	2.21	0.41
2:r:426:ILE:O	2:r:430:LEU:HG	2.20	0.41
2:t:387:GLN:HE21	2:t:387:GLN:HB2	1.63	0.41
2:v:302:ALA:HB3	2:w:385:ARG:HB3	2.02	0.41
2:w:369:LYS:HE3	2:w:369:LYS:HB3	1.85	0.41
2:y:426:ILE:O	2:y:430:LEU:HG	2.21	0.41
2:1:294:VAL:HG22	2:1:396:VAL:HG22	2.03	0.41
2:1:426:ILE:O	2:1:430:LEU:HG	2.20	0.41
1:AP:104:ILE:HG22	1:AP:109:PHE:CD2	2.56	0.41
1:AP:273:VAL:HG22	8:Aj:58:PHE:CE2	2.56	0.41
5:AT:32:GLN:NE2	6:AY:51:ALA:HB2	2.35	0.41
8:Aj:80:ASP:OD2	2:j:151:SER:HA	2.20	0.41
2:B:426:ILE:O	2:B:430:LEU:HG	2.21	0.41
2:D:450:LYS:HE2	2:D:450:LYS:HB2	1.85	0.41
2:G:402:ASP:OD1	2:G:448:SER:OG	2.33	0.41
2:G:426:ILE:O	2:G:430:LEU:HG	2.20	0.41
2:N:426:ILE:O	2:N:430:LEU:HG	2.21	0.41
2:R:426:ILE:O	2:R:430:LEU:HG	2.21	0.41
2:S:177:VAL:HG13	2:S:207:LEU:HD23	2.02	0.41
2:U:155:GLU:O	2:U:159:LEU:HG	2.21	0.41
2:U:183:LEU:HB3	2:V:163:ARG:NH2	2.36	0.41
2:X:159:LEU:HD13	2:Y:157:GLU:OE2	2.21	0.41
2:a:150:VAL:HG11	2:a:158:ARG:NH1	2.36	0.41
2:a:163:ARG:HA	2:a:166:GLN:NE2	2.30	0.41
2:d:185:ALA:O	2:d:199:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:174:MET:HE2	2:i:174:MET:HB3	2.00	0.41
2:j:201:ALA:HB3	2:j:237:ILE:HG23	2.02	0.41
2:k:162:SER:O	2:k:166:GLN:HG2	2.21	0.41
2:v:426:ILE:O	2:v:430:LEU:HG	2.20	0.41
2:w:294:VAL:HG22	2:w:396:VAL:HG22	2.03	0.41
4:8:39:PRO:HD2	7:Af:102:PRO:HG2	2.02	0.41
4:8:213:ASN:HB2	4:8:215:PHE:CE1	2.56	0.41
1:9:188:ARG:NH1	1:9:225:THR:OG1	2.46	0.41
1:Al:184:LEU:O	1:Al:187:THR:HG22	2.21	0.41
2:E:450:LYS:HE2	2:E:450:LYS:HB2	1.85	0.41
2:F:426:ILE:O	2:F:430:LEU:HG	2.21	0.41
2:K:426:ILE:O	2:K:430:LEU:HG	2.21	0.41
2:L:302:ALA:HB3	2:M:385:ARG:HB3	2.02	0.41
2:S:163:ARG:HD3	2:S:163:ARG:HA	1.74	0.41
2:S:215:GLN:NE2	2:S:219:ASP:OD2	2.54	0.41
2:T:143:LEU:HA	2:T:143:LEU:HD23	1.74	0.41
2:T:167:LEU:O	2:T:171:ILE:HG12	2.21	0.41
2:V:244:GLY:HA2	2:k:174:MET:HE1	2.03	0.41
2:X:186:LEU:HD21	2:X:229:VAL:HG11	2.02	0.41
2:Y:174:MET:SD	2:Y:221:ILE:HD11	2.60	0.41
2:f:230:PRO:HD3	2:g:185:ALA:HB1	2.03	0.41
2:l:200:SER:OG	2:l:201:ALA:N	2.53	0.41
2:r:302:ALA:HB3	2:s:385:ARG:HB3	2.02	0.41
2:r:369:LYS:HE3	2:r:369:LYS:HB3	1.85	0.41
2:4:426:ILE:O	2:4:430:LEU:HG	2.20	0.41
3:6:73:LEU:HD13	3:6:73:LEU:HA	1.97	0.41
3:AQ:44:ILE:HG22	3:AQ:46:GLU:H	1.86	0.41
2:I:294:VAL:HG22	2:I:396:VAL:HG22	2.03	0.41
2:M:294:VAL:HG22	2:M:396:VAL:HG22	2.03	0.41
2:N:294:VAL:HG22	2:N:396:VAL:HG22	2.03	0.41
2:P:302:ALA:HB3	2:Q:385:ARG:HB3	2.02	0.41
2:Q:369:LYS:HE3	2:Q:369:LYS:HB3	1.85	0.41
2:X:174:MET:HE2	2:X:174:MET:HB3	1.79	0.41
2:Z:174:MET:HE1	2:a:244:GLY:CA	2.50	0.41
2:d:216:GLN:NE2	2:e:246:LEU:H	2.19	0.41
2:d:219:ASP:HA	2:d:222:VAL:HG12	2.03	0.41
2:e:213:LEU:HD13	2:e:217:GLU:HB2	2.02	0.41
2:f:201:ALA:HB2	2:f:232:MET:SD	2.60	0.41
2:o:166:GLN:HG2	2:o:166:GLN:H	1.70	0.41
2:s:294:VAL:HG22	2:s:396:VAL:HG22	2.03	0.41
2:u:426:ILE:O	2:u:430:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:v:294:VAL:HG22	2:v:396:VAL:HG22	2.03	0.41
2:z:294:VAL:HG22	2:z:396:VAL:HG22	2.03	0.41
2:3:426:ILE:O	2:3:430:LEU:HG	2.20	0.41
2:3:450:LYS:HB2	2:3:450:LYS:HE2	1.85	0.41
2:4:294:VAL:HG22	2:4:396:VAL:HG22	2.03	0.41
3:7:64:LEU:CG	2:T:148:PHE:CD1	3.04	0.41
2:AI:335:ILE:O	2:AI:336:PRO:C	2.61	0.41
2:AJ:341:ASN:ND2	5:AT:86:PRO:HG3	2.36	0.41
1:AP:128:THR:HB	1:AP:129:PRO:HD3	2.03	0.41
3:AR:15:TRP:CE2	2:U:148:PHE:HB2	2.56	0.41
5:AT:124:LEU:HD23	7:Af:79:VAL:HG11	2.03	0.41
5:AV:124:LEU:HD23	7:Ad:79:VAL:HG11	2.03	0.41
6:AZ:89:ASN:OD1	6:AZ:93:TYR:N	2.51	0.41
6:Ac:135:MET:HE2	7:Ah:75:ASN:HD22	1.85	0.41
7:Ah:71:MET:SD	7:Ah:74:ARG:HD3	2.61	0.41
1:Al:187:THR:O	2:T:192:PHE:HA	2.20	0.41
2:D:302:ALA:HB3	2:E:385:ARG:HB3	2.02	0.41
2:E:302:ALA:HB3	2:F:385:ARG:HB3	2.02	0.41
2:E:426:ILE:O	2:E:430:LEU:HG	2.21	0.41
2:G:373:ARG:HE	2:G:373:ARG:HB2	1.77	0.41
2:K:450:LYS:HB2	2:K:450:LYS:HE2	1.85	0.41
2:Q:302:ALA:HB3	2:R:385:ARG:HB3	2.02	0.41
2:Q:426:ILE:O	2:Q:430:LEU:HG	2.20	0.41
2:T:183:LEU:HB3	2:U:163:ARG:HH22	1.86	0.41
2:U:239:VAL:N	2:U:248:SER:OG	2.52	0.41
2:V:197:GLN:OE1	2:k:189:HIS:NE2	2.53	0.41
2:b:242:GLN:H	2:b:242:GLN:HG2	1.72	0.41
2:d:221:ILE:HD13	2:d:221:ILE:HA	1.91	0.41
2:e:152:GLN:HG3	2:e:153:ARG:HE	1.86	0.41
2:k:153:ARG:NE	2:k:153:ARG:HA	2.36	0.41
2:n:241:ASP:CG	2:n:245:ARG:HG2	2.46	0.41
2:o:167:LEU:HD23	2:o:167:LEU:HA	1.78	0.41
2:s:387:GLN:HE21	2:s:387:GLN:HB2	1.63	0.41
2:s:426:ILE:O	2:s:430:LEU:HG	2.21	0.41
2:t:450:LYS:HE2	2:t:450:LYS:HB2	1.85	0.41
2:u:402:ASP:OD1	2:u:448:SER:OG	2.33	0.41
2:1:385:ARG:HB3	2:z:302:ALA:HB3	2.02	0.41
3:6:81:ILE:HA	3:6:84:LEU:HD13	2.02	0.41
1:9:189:ILE:HD12	1:9:189:ILE:H	1.85	0.41
2:A:372:THR:CG2	9:An:6:HIS:CB	2.99	0.41
2:AG:339:LEU:HD11	6:Ab:72:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:426:ILE:O	2:C:430:LEU:HG	2.20	0.41
2:D:373:ARG:HE	2:D:373:ARG:HB2	1.77	0.41
2:E:294:VAL:HG22	2:E:396:VAL:HG22	2.03	0.41
2:F:294:VAL:HG22	2:F:396:VAL:HG22	2.03	0.41
2:G:302:ALA:HB3	2:H:385:ARG:HB3	2.02	0.41
2:I:302:ALA:HB3	2:J:385:ARG:HB3	2.02	0.41
2:O:426:ILE:O	2:O:430:LEU:HG	2.20	0.41
2:W:171:ILE:HD12	2:W:221:ILE:HD12	2.03	0.41
2:g:236:ARG:HD3	2:g:236:ARG:HA	1.84	0.41
2:t:294:VAL:HG22	2:t:396:VAL:HG22	2.03	0.41
2:u:302:ALA:HB3	2:v:385:ARG:HB3	2.02	0.41
2:x:294:VAL:HG22	2:x:396:VAL:HG22	2.03	0.41
1:0:104:ILE:O	1:0:110:THR:OG1	2.38	0.40
1:0:270:PHE:HE2	1:0:276:TRP:CD1	2.38	0.40
2:3:402:ASP:OD1	2:3:448:SER:OG	2.33	0.40
1:AP:186:GLN:HE22	1:AP:287:PHE:HA	1.86	0.40
3:AR:88:LEU:O	2:T:192:PHE:CE2	2.74	0.40
2:O:319:SER:HB3	9:Ap:7:HIS:HA	2.03	0.40
2:S:147:GLY:O	2:S:149:GLY:N	2.54	0.40
2:Y:167:LEU:HA	2:Y:167:LEU:HD23	1.75	0.40
2:Z:188:LYS:HD3	2:Z:188:LYS:HA	1.82	0.40
2:a:163:ARG:HA	2:a:166:GLN:HG2	2.02	0.40
2:a:179:LYS:HB3	2:a:206:THR:OG1	2.21	0.40
2:n:167:LEU:HA	2:n:167:LEU:HD23	1.87	0.40
2:s:302:ALA:HB3	2:t:385:ARG:HB3	2.02	0.40
2:t:426:ILE:O	2:t:430:LEU:HG	2.21	0.40
1:0:96:LEU:HB3	7:Ag:90:LYS:HB3	2.03	0.40
1:0:111:ARG:NE	1:0:222:GLU:OE1	2.50	0.40
2:2:450:LYS:HB2	2:2:450:LYS:HE2	1.85	0.40
2:3:294:VAL:HG22	2:3:396:VAL:HG22	2.03	0.40
2:3:327:ASN:HB2	2:3:366:SER:HB3	2.04	0.40
3:7:68:TRP:CD1	2:S:148:PHE:CD1	3.09	0.40
4:8:125:LEU:HD12	1:9:242:LEU:HD13	2.01	0.40
2:AG:343:PRO:HA	2:AG:344:PRO:HD3	1.92	0.40
3:AR:84:LEU:HD13	1:Al:232:MET:HG3	2.04	0.40
6:AZ:53:LEU:N	6:AZ:53:LEU:HD23	2.36	0.40
1:Ak:254:MET:HB2	1:Al:254:MET:SD	2.61	0.40
2:F:302:ALA:HB3	2:G:385:ARG:HB3	2.02	0.40
2:H:302:ALA:HB3	2:I:385:ARG:HB3	2.02	0.40
2:K:294:VAL:HG22	2:K:396:VAL:HG22	2.03	0.40
2:Q:450:LYS:HB2	2:Q:450:LYS:HE2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:164:GLU:HG2	2:V:184:LEU:HD13	2.02	0.40
2:b:182:VAL:O	2:b:183:LEU:HD13	2.21	0.40
2:q:369:LYS:HE3	2:q:369:LYS:HB3	1.85	0.40
2:5:302:ALA:HB3	2:A:385:ARG:HB3	2.02	0.40
2:A:369:LYS:HE3	2:A:369:LYS:HB3	1.85	0.40
3:AQ:14:LEU:HA	3:AQ:17:VAL:HG12	2.03	0.40
7:Af:71:MET:SD	7:Af:74:ARG:HD3	2.61	0.40
8:Aj:69:ARG:H	8:Aj:69:ARG:CZ	2.34	0.40
1:Al:152:GLU:CD	1:Al:178:PRO:HB3	2.46	0.40
2:C:302:ALA:HB3	2:D:385:ARG:HB3	2.02	0.40
2:J:302:ALA:HB3	2:K:385:ARG:HB3	2.02	0.40
2:P:426:ILE:O	2:P:430:LEU:HG	2.20	0.40
2:T:155:GLU:O	2:T:159:LEU:HG	2.21	0.40
2:Z:187:PRO:HB2	2:Z:189:HIS:CD2	2.57	0.40
2:e:197:GLN:CD	2:e:197:GLN:H	2.29	0.40
2:i:210:GLY:O	2:i:211:THR:OG1	2.34	0.40
2:x:402:ASP:OD1	2:x:448:SER:OG	2.33	0.40
2:z:426:ILE:O	2:z:430:LEU:HG	2.20	0.40
2:5:294:VAL:HG22	2:5:396:VAL:HG22	2.03	0.40
3:6:56:ILE:HG12	3:7:18:LEU:HD11	2.04	0.40
3:7:4:GLU:HB2	2:Y:152:GLN:HE22	1.83	0.40
2:B:302:ALA:HB3	2:C:385:ARG:HB3	2.02	0.40
2:E:373:ARG:HE	2:E:373:ARG:HB2	1.77	0.40
2:P:450:LYS:HE2	2:P:450:LYS:HB2	1.85	0.40
2:Q:327:ASN:HB2	2:Q:366:SER:HB3	2.04	0.40
2:g:230:PRO:HD3	2:h:185:ALA:HB1	2.03	0.40
2:x:327:ASN:HB2	2:x:366:SER:HB3	2.04	0.40
2:y:294:VAL:HG22	2:y:396:VAL:HG22	2.03	0.40
3:6:7:VAL:HG23	4:8:137:PHE:HZ	1.87	0.40
5:AV:127:ALA:HB2	1:Al:86:THR:HG22	2.02	0.40
7:Ae:57:ARG:HB3	7:Ae:65:VAL:HG21	2.02	0.40
2:H:426:ILE:O	2:H:430:LEU:HG	2.21	0.40
2:W:176:GLN:N	2:W:176:GLN:OE1	2.54	0.40
2:c:175:LYS:HE2	2:c:175:LYS:HB2	1.84	0.40
2:d:174:MET:HE1	2:e:244:GLY:CA	2.51	0.40
2:f:159:LEU:HD22	2:g:157:GLU:HG3	2.02	0.40
2:h:217:GLU:O	2:h:221:ILE:HG12	2.22	0.40
2:s:327:ASN:HB2	2:s:366:SER:HB3	2.04	0.40
2:x:369:LYS:HE3	2:x:369:LYS:HB3	1.85	0.40
2:y:402:ASP:OD1	2:y:448:SER:OG	2.33	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	206/289 (71%)	203 (98%)	3 (2%)	0	100	100
1	9	205/289 (71%)	202 (98%)	3 (2%)	0	100	100
1	AP	206/289 (71%)	204 (99%)	2 (1%)	0	100	100
1	Ak	206/289 (71%)	202 (98%)	4 (2%)	0	100	100
1	Al	206/289 (71%)	202 (98%)	4 (2%)	0	100	100
2	1	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	2	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	3	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	4	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	5	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	A	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	AA	17/580 (3%)	17 (100%)	0	0	100	100
2	AB	17/580 (3%)	15 (88%)	2 (12%)	0	100	100
2	AC	18/580 (3%)	18 (100%)	0	0	100	100
2	AD	17/580 (3%)	17 (100%)	0	0	100	100
2	AE	17/580 (3%)	17 (100%)	0	0	100	100
2	AF	21/580 (4%)	14 (67%)	6 (29%)	1 (5%)	2	14
2	AG	9/580 (2%)	7 (78%)	2 (22%)	0	100	100
2	AH	9/580 (2%)	9 (100%)	0	0	100	100
2	AI	9/580 (2%)	8 (89%)	1 (11%)	0	100	100
2	AJ	22/580 (4%)	18 (82%)	4 (18%)	0	100	100
2	AK	23/580 (4%)	23 (100%)	0	0	100	100
2	AL	30/580 (5%)	26 (87%)	4 (13%)	0	100	100
2	AM	31/580 (5%)	31 (100%)	0	0	100	100
2	AN	31/580 (5%)	31 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AO	30/580 (5%)	30 (100%)	0	0	100	100
2	B	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	C	142/580 (24%)	139 (98%)	3 (2%)	0	100	100
2	D	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	E	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	F	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	G	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	H	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	I	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	J	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	K	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	L	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	M	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	N	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	O	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	P	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	Q	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	R	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	S	112/580 (19%)	100 (89%)	10 (9%)	2 (2%)	6	30
2	T	112/580 (19%)	99 (88%)	12 (11%)	1 (1%)	14	43
2	U	112/580 (19%)	102 (91%)	10 (9%)	0	100	100
2	V	112/580 (19%)	102 (91%)	9 (8%)	1 (1%)	14	43
2	W	112/580 (19%)	104 (93%)	7 (6%)	1 (1%)	14	43
2	X	105/580 (18%)	97 (92%)	7 (7%)	1 (1%)	12	41
2	Y	112/580 (19%)	99 (88%)	11 (10%)	2 (2%)	6	30
2	Z	112/580 (19%)	99 (88%)	12 (11%)	1 (1%)	14	43
2	a	112/580 (19%)	102 (91%)	9 (8%)	1 (1%)	14	43
2	b	90/580 (16%)	83 (92%)	6 (7%)	1 (1%)	11	40
2	c	101/580 (17%)	93 (92%)	7 (7%)	1 (1%)	12	41
2	d	101/580 (17%)	93 (92%)	8 (8%)	0	100	100
2	e	101/580 (17%)	90 (89%)	10 (10%)	1 (1%)	12	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	f	81/580 (14%)	74 (91%)	7 (9%)	0	100	100
2	g	88/580 (15%)	83 (94%)	5 (6%)	0	100	100
2	h	87/580 (15%)	82 (94%)	5 (6%)	0	100	100
2	i	85/580 (15%)	81 (95%)	4 (5%)	0	100	100
2	j	88/580 (15%)	80 (91%)	8 (9%)	0	100	100
2	k	112/580 (19%)	106 (95%)	5 (4%)	1 (1%)	14	43
2	l	112/580 (19%)	98 (88%)	13 (12%)	1 (1%)	14	43
2	m	112/580 (19%)	103 (92%)	8 (7%)	1 (1%)	14	43
2	n	101/580 (17%)	95 (94%)	5 (5%)	1 (1%)	12	41
2	o	112/580 (19%)	104 (93%)	6 (5%)	2 (2%)	6	30
2	p	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	q	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	r	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	s	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	t	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	u	142/580 (24%)	139 (98%)	3 (2%)	0	100	100
2	v	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	w	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	x	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	y	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
2	z	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
3	6	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
3	7	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
3	AQ	87/89 (98%)	87 (100%)	0	0	100	100
3	AR	87/89 (98%)	86 (99%)	0	1 (1%)	11	40
4	8	238/260 (92%)	232 (98%)	6 (2%)	0	100	100
5	AS	105/131 (80%)	104 (99%)	1 (1%)	0	100	100
5	AT	103/131 (79%)	102 (99%)	1 (1%)	0	100	100
5	AU	105/131 (80%)	103 (98%)	2 (2%)	0	100	100
5	AV	104/131 (79%)	104 (100%)	0	0	100	100
5	AW	104/131 (79%)	103 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AX	126/137 (92%)	122 (97%)	4 (3%)	0	100	100
6	AY	126/137 (92%)	123 (98%)	3 (2%)	0	100	100
6	AZ	126/137 (92%)	122 (97%)	3 (2%)	1 (1%)	16	45
6	Aa	126/137 (92%)	125 (99%)	1 (1%)	0	100	100
6	Ab	126/137 (92%)	120 (95%)	6 (5%)	0	100	100
6	Ac	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
7	Ad	70/103 (68%)	70 (100%)	0	0	100	100
7	Ae	78/103 (76%)	78 (100%)	0	0	100	100
7	Af	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
7	Ag	70/103 (68%)	69 (99%)	1 (1%)	0	100	100
7	Ah	70/103 (68%)	69 (99%)	1 (1%)	0	100	100
7	Ai	38/103 (37%)	38 (100%)	0	0	100	100
8	Aj	69/376 (18%)	69 (100%)	0	0	100	100
9	Am	10/13 (77%)	5 (50%)	4 (40%)	1 (10%)	0	4
9	An	7/13 (54%)	2 (29%)	4 (57%)	1 (14%)	0	2
9	Ao	8/13 (62%)	8 (100%)	0	0	100	100
9	Ap	8/13 (62%)	2 (25%)	4 (50%)	2 (25%)	0	0
9	Aq	11/13 (85%)	6 (54%)	3 (27%)	2 (18%)	0	1
10	Ar	15/17 (88%)	15 (100%)	0	0	100	100
10	As	15/17 (88%)	15 (100%)	0	0	100	100
10	At	15/17 (88%)	15 (100%)	0	0	100	100
10	Au	15/17 (88%)	15 (100%)	0	0	100	100
10	Av	15/17 (88%)	15 (100%)	0	0	100	100
10	Aw	15/17 (88%)	15 (100%)	0	0	100	100
All	All	11000/46459 (24%)	10564 (96%)	408 (4%)	28 (0%)	37	64

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	c	152	GLN
9	Am	11	PRO
9	Ap	7	HIS
9	Aq	7	ASP
2	T	193	VAL

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Mol	Chain	Res	Type
2	X	152	GLN
2	Y	152	GLN
2	n	152	GLN
9	Ap	8	ILE
3	AR	88	LEU
2	W	190	SER
2	l	152	GLN
2	o	152	GLN
9	Aq	12	PRO
6	AZ	42	TYR
2	S	148	PHE
2	V	190	SER
2	Y	249	SER
2	e	152	GLN
2	S	211	THR
2	b	152	GLN
2	a	211	THR
2	k	198	GLU
2	m	189	HIS
2	o	211	THR
2	Z	191	VAL
9	An	4	GLY
2	AF	349	ILE

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	182/247 (74%)	176 (97%)	6 (3%)	33	54
1	9	181/247 (73%)	175 (97%)	6 (3%)	33	54
1	AP	182/247 (74%)	177 (97%)	5 (3%)	39	57
1	Ak	182/247 (74%)	175 (96%)	7 (4%)	29	51
1	Al	182/247 (74%)	175 (96%)	7 (4%)	29	51
2	1	128/500 (26%)	123 (96%)	5 (4%)	28	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	3	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	4	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	5	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	A	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	AA	15/500 (3%)	14 (93%)	1 (7%)	15	40
2	AB	15/500 (3%)	14 (93%)	1 (7%)	15	40
2	AC	15/500 (3%)	15 (100%)	0	100	100
2	AD	15/500 (3%)	14 (93%)	1 (7%)	15	40
2	AE	15/500 (3%)	15 (100%)	0	100	100
2	AF	17/500 (3%)	13 (76%)	4 (24%)	1	5
2	AG	8/500 (2%)	8 (100%)	0	100	100
2	AH	8/500 (2%)	7 (88%)	1 (12%)	4	20
2	AI	8/500 (2%)	8 (100%)	0	100	100
2	AJ	17/500 (3%)	16 (94%)	1 (6%)	18	42
2	AK	18/500 (4%)	15 (83%)	3 (17%)	2	12
2	AL	24/500 (5%)	23 (96%)	1 (4%)	26	49
2	AM	24/500 (5%)	23 (96%)	1 (4%)	26	49
2	AN	24/500 (5%)	22 (92%)	2 (8%)	10	33
2	AO	24/500 (5%)	23 (96%)	1 (4%)	26	49
2	B	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	C	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	D	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	E	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	F	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	G	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	H	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	I	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	J	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	K	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	L	128/500 (26%)	123 (96%)	5 (4%)	28	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	N	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	O	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	P	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	Q	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	R	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	S	98/500 (20%)	86 (88%)	12 (12%)	5	20
2	T	98/500 (20%)	84 (86%)	14 (14%)	3	16
2	U	98/500 (20%)	89 (91%)	9 (9%)	8	30
2	V	98/500 (20%)	88 (90%)	10 (10%)	7	27
2	W	98/500 (20%)	86 (88%)	12 (12%)	5	20
2	X	93/500 (19%)	85 (91%)	8 (9%)	10	32
2	Y	98/500 (20%)	89 (91%)	9 (9%)	8	30
2	Z	98/500 (20%)	89 (91%)	9 (9%)	8	30
2	a	98/500 (20%)	93 (95%)	5 (5%)	21	45
2	b	81/500 (16%)	78 (96%)	3 (4%)	30	52
2	c	90/500 (18%)	84 (93%)	6 (7%)	15	40
2	d	90/500 (18%)	81 (90%)	9 (10%)	7	28
2	e	90/500 (18%)	78 (87%)	12 (13%)	4	18
2	f	75/500 (15%)	71 (95%)	4 (5%)	20	44
2	g	79/500 (16%)	72 (91%)	7 (9%)	9	31
2	h	78/500 (16%)	73 (94%)	5 (6%)	16	40
2	i	77/500 (15%)	72 (94%)	5 (6%)	15	40
2	j	79/500 (16%)	73 (92%)	6 (8%)	12	36
2	k	98/500 (20%)	88 (90%)	10 (10%)	7	27
2	l	98/500 (20%)	88 (90%)	10 (10%)	7	27
2	m	98/500 (20%)	91 (93%)	7 (7%)	13	38
2	n	89/500 (18%)	83 (93%)	6 (7%)	15	40
2	o	98/500 (20%)	93 (95%)	5 (5%)	21	45
2	p	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	q	128/500 (26%)	123 (96%)	5 (4%)	28	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	r	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	s	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	t	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	u	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	v	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	w	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	x	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	y	128/500 (26%)	123 (96%)	5 (4%)	28	51
2	z	128/500 (26%)	123 (96%)	5 (4%)	28	51
3	6	80/80 (100%)	75 (94%)	5 (6%)	16	41
3	7	80/80 (100%)	79 (99%)	1 (1%)	61	69
3	AQ	80/80 (100%)	77 (96%)	3 (4%)	29	51
3	AR	80/80 (100%)	76 (95%)	4 (5%)	22	46
4	8	204/218 (94%)	194 (95%)	10 (5%)	22	46
5	AS	89/106 (84%)	88 (99%)	1 (1%)	65	71
5	AT	88/106 (83%)	86 (98%)	2 (2%)	44	61
5	AU	89/106 (84%)	86 (97%)	3 (3%)	32	53
5	AV	88/106 (83%)	85 (97%)	3 (3%)	32	53
5	AW	88/106 (83%)	88 (100%)	0	100	100
6	AX	111/115 (96%)	106 (96%)	5 (4%)	24	48
6	AY	111/115 (96%)	107 (96%)	4 (4%)	31	52
6	AZ	111/115 (96%)	103 (93%)	8 (7%)	13	37
6	Aa	111/115 (96%)	106 (96%)	5 (4%)	24	48
6	Ab	111/115 (96%)	105 (95%)	6 (5%)	20	44
6	Ac	111/115 (96%)	106 (96%)	5 (4%)	24	48
7	Ad	63/84 (75%)	59 (94%)	4 (6%)	16	41
7	Ae	66/84 (79%)	64 (97%)	2 (3%)	36	55
7	Af	66/84 (79%)	63 (96%)	3 (4%)	24	48
7	Ag	63/84 (75%)	62 (98%)	1 (2%)	55	65
7	Ah	63/84 (75%)	63 (100%)	0	100	100
7	Ai	36/84 (43%)	35 (97%)	1 (3%)	38	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Aj	58/317 (18%)	55 (95%)	3 (5%)	21	45
All	All	9652/39814 (24%)	9172 (95%)	480 (5%)	23	46

All (480) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	86	THR
1	0	95	MET
1	0	149	VAL
1	0	214	LEU
1	0	220	THR
1	0	272	LEU
2	1	280	VAL
2	1	380	THR
2	1	387	GLN
2	1	395	THR
2	1	422	GLU
2	2	280	VAL
2	2	380	THR
2	2	387	GLN
2	2	395	THR
2	2	422	GLU
2	3	280	VAL
2	3	380	THR
2	3	387	GLN
2	3	395	THR
2	3	422	GLU
2	4	280	VAL
2	4	380	THR
2	4	387	GLN
2	4	395	THR
2	4	422	GLU
2	5	280	VAL
2	5	380	THR
2	5	387	GLN
2	5	395	THR
2	5	422	GLU
3	6	1	MET
3	6	7	VAL
3	6	14	LEU
3	6	42	THR
3	6	86	GLN

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Mol	Chain	Res	Type
3	7	88	LEU
4	8	2	GLU
4	8	47	LEU
4	8	70	ARG
4	8	102	ILE
4	8	125	LEU
4	8	192	ILE
4	8	195	LEU
4	8	207	ARG
4	8	212	LEU
4	8	214	ILE
1	9	127	GLN
1	9	146	MET
1	9	166	VAL
1	9	202	GLN
1	9	208	ASP
1	9	259	MET
2	A	280	VAL
2	A	380	THR
2	A	387	GLN
2	A	395	THR
2	A	422	GLU
2	AA	342	GLN
2	AB	342	GLN
2	AD	349	ILE
2	AF	346	ASP
2	AF	351	GLN
2	AF	352	ASP
2	AF	355	GLN
2	AH	342	GLN
2	AJ	349	ILE
2	AK	330	ASN
2	AK	331	MET
2	AK	332	VAL
2	AL	339	LEU
2	AM	352	ASP
2	AN	339	LEU
2	AN	352	ASP
2	AO	330	ASN
1	AP	96	LEU
1	AP	133	VAL
1	AP	141	LEU

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Mol	Chain	Res	Type
1	AP	149	VAL
1	AP	214	LEU
3	AQ	1	MET
3	AQ	16	MET
3	AQ	55	LEU
3	AR	45	ASN
3	AR	64	LEU
3	AR	72	MET
3	AR	89	TYR
5	AS	9	LEU
5	AT	6	ASP
5	AT	87	ASP
5	AU	4	SER
5	AU	6	ASP
5	AU	7	ASN
5	AV	6	ASP
5	AV	7	ASN
5	AV	88	THR
6	AX	23	THR
6	AX	39	LYS
6	AX	53	LEU
6	AX	65	VAL
6	AX	134	GLN
6	AY	3	LEU
6	AY	34	VAL
6	AY	65	VAL
6	AY	67	VAL
6	AZ	36	SER
6	AZ	39	LYS
6	AZ	61	ASP
6	AZ	62	THR
6	AZ	67	VAL
6	AZ	84	ASP
6	AZ	113	ARG
6	AZ	131	ARG
6	Aa	53	LEU
6	Aa	61	ASP
6	Aa	65	VAL
6	Aa	67	VAL
6	Aa	126	LYS
6	Ab	14	MET
6	Ab	40	ASP

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Mol	Chain	Res	Type
6	Ab	53	LEU
6	Ab	65	VAL
6	Ab	113	ARG
6	Ab	134	GLN
6	Ac	40	ASP
6	Ac	43	LYS
6	Ac	65	VAL
6	Ac	126	LYS
6	Ac	137	GLN
7	Ad	34	ASN
7	Ad	37	LEU
7	Ad	39	LYS
7	Ad	67	LEU
7	Ae	67	LEU
7	Ae	98	LEU
7	Af	32	ASP
7	Af	35	ASP
7	Af	67	LEU
7	Ag	67	LEU
7	Ai	91	LEU
8	Aj	48	TRP
8	Aj	69	ARG
8	Aj	86	MET
1	Ak	86	THR
1	Ak	99	LEU
1	Ak	113	VAL
1	Ak	141	LEU
1	Ak	254	MET
1	Ak	261	VAL
1	Ak	283	LEU
1	Al	86	THR
1	Al	87	LEU
1	Al	113	VAL
1	Al	128	THR
1	Al	184	LEU
1	Al	192	LEU
1	Al	272	LEU
2	B	280	VAL
2	B	380	THR
2	B	387	GLN
2	B	395	THR
2	B	422	GLU

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Mol	Chain	Res	Type
2	C	280	VAL
2	C	380	THR
2	C	387	GLN
2	C	395	THR
2	C	422	GLU
2	D	280	VAL
2	D	380	THR
2	D	387	GLN
2	D	395	THR
2	D	422	GLU
2	E	280	VAL
2	E	380	THR
2	E	387	GLN
2	E	395	THR
2	E	422	GLU
2	F	280	VAL
2	F	380	THR
2	F	387	GLN
2	F	395	THR
2	F	422	GLU
2	G	280	VAL
2	G	380	THR
2	G	387	GLN
2	G	395	THR
2	G	422	GLU
2	H	280	VAL
2	H	380	THR
2	H	387	GLN
2	H	395	THR
2	H	422	GLU
2	I	280	VAL
2	I	380	THR
2	I	387	GLN
2	I	395	THR
2	I	422	GLU
2	J	280	VAL
2	J	380	THR
2	J	387	GLN
2	J	395	THR
2	J	422	GLU
2	K	280	VAL
2	K	380	THR

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Mol	Chain	Res	Type
2	K	387	GLN
2	K	395	THR
2	K	422	GLU
2	L	280	VAL
2	L	380	THR
2	L	387	GLN
2	L	395	THR
2	L	422	GLU
2	M	280	VAL
2	M	380	THR
2	M	387	GLN
2	M	395	THR
2	M	422	GLU
2	N	280	VAL
2	N	380	THR
2	N	387	GLN
2	N	395	THR
2	N	422	GLU
2	O	280	VAL
2	O	380	THR
2	O	387	GLN
2	O	395	THR
2	O	422	GLU
2	P	280	VAL
2	P	380	THR
2	P	387	GLN
2	P	395	THR
2	P	422	GLU
2	Q	280	VAL
2	Q	380	THR
2	Q	387	GLN
2	Q	395	THR
2	Q	422	GLU
2	R	280	VAL
2	R	380	THR
2	R	387	GLN
2	R	395	THR
2	R	422	GLU
2	S	144	GLN
2	S	146	MET
2	S	152	GLN
2	S	153	ARG

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Mol	Chain	Res	Type
2	S	156	GLN
2	S	174	MET
2	S	203	VAL
2	S	206	THR
2	S	221	ILE
2	S	241	ASP
2	S	242	GLN
2	S	246	LEU
2	T	139	ASP
2	T	144	GLN
2	T	152	GLN
2	T	156	GLN
2	T	167	LEU
2	T	173	GLU
2	T	191	VAL
2	T	193	VAL
2	T	194	ARG
2	T	196	ASN
2	T	203	VAL
2	T	206	THR
2	T	240	THR
2	T	246	LEU
2	U	144	GLN
2	U	167	LEU
2	U	173	GLU
2	U	193	VAL
2	U	194	ARG
2	U	196	ASN
2	U	203	VAL
2	U	221	ILE
2	U	240	THR
2	V	144	GLN
2	V	173	GLU
2	V	183	LEU
2	V	194	ARG
2	V	196	ASN
2	V	203	VAL
2	V	205	LEU
2	V	206	THR
2	V	240	THR
2	V	242	GLN
2	W	139	ASP

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Mol	Chain	Res	Type
2	W	144	GLN
2	W	156	GLN
2	W	173	GLU
2	W	174	MET
2	W	177	VAL
2	W	194	ARG
2	W	203	VAL
2	W	206	THR
2	W	221	ILE
2	W	222	VAL
2	W	242	GLN
2	X	139	ASP
2	X	156	GLN
2	X	173	GLU
2	X	174	MET
2	X	184	LEU
2	X	188	LYS
2	X	203	VAL
2	X	242	GLN
2	Y	139	ASP
2	Y	144	GLN
2	Y	173	GLU
2	Y	196	ASN
2	Y	200	SER
2	Y	203	VAL
2	Y	206	THR
2	Y	236	ARG
2	Y	246	LEU
2	Z	139	ASP
2	Z	144	GLN
2	Z	163	ARG
2	Z	174	MET
2	Z	206	THR
2	Z	232	MET
2	Z	234	THR
2	Z	242	GLN
2	Z	246	LEU
2	a	146	MET
2	a	156	GLN
2	a	173	GLU
2	a	193	VAL
2	a	203	VAL

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Mol	Chain	Res	Type
2	b	173	GLU
2	b	174	MET
2	b	206	THR
2	c	148	PHE
2	c	173	GLU
2	c	203	VAL
2	c	206	THR
2	c	241	ASP
2	c	246	LEU
2	d	156	GLN
2	d	169	GLN
2	d	173	GLU
2	d	174	MET
2	d	206	THR
2	d	236	ARG
2	d	237	ILE
2	d	242	GLN
2	d	246	LEU
2	e	148	PHE
2	e	156	GLN
2	e	173	GLU
2	e	182	VAL
2	e	188	LYS
2	e	191	VAL
2	e	197	GLN
2	e	202	SER
2	e	203	VAL
2	e	206	THR
2	e	224	MET
2	e	232	MET
2	f	156	GLN
2	f	173	GLU
2	f	203	VAL
2	f	219	ASP
2	g	156	GLN
2	g	173	GLU
2	g	203	VAL
2	g	205	LEU
2	g	206	THR
2	g	236	ARG
2	g	246	LEU
2	h	156	GLN

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Mol	Chain	Res	Type
2	h	173	GLU
2	h	182	VAL
2	h	224	MET
2	h	246	LEU
2	i	152	GLN
2	i	173	GLU
2	i	182	VAL
2	i	203	VAL
2	i	206	THR
2	j	156	GLN
2	j	173	GLU
2	j	203	VAL
2	j	206	THR
2	j	234	THR
2	j	242	GLN
2	k	144	GLN
2	k	167	LEU
2	k	173	GLU
2	k	174	MET
2	k	203	VAL
2	k	206	THR
2	k	232	MET
2	k	234	THR
2	k	242	GLN
2	k	246	LEU
2	l	140	ASP
2	l	144	GLN
2	l	150	VAL
2	l	156	GLN
2	l	173	GLU
2	l	193	VAL
2	l	196	ASN
2	l	203	VAL
2	l	232	MET
2	l	242	GLN
2	m	139	ASP
2	m	156	GLN
2	m	173	GLU
2	m	174	MET
2	m	194	ARG
2	m	203	VAL
2	m	206	THR

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Mol	Chain	Res	Type
2	n	144	GLN
2	n	173	GLU
2	n	203	VAL
2	n	206	THR
2	n	214	LYS
2	n	246	LEU
2	o	144	GLN
2	o	146	MET
2	o	184	LEU
2	o	234	THR
2	o	246	LEU
2	p	280	VAL
2	p	380	THR
2	p	387	GLN
2	p	395	THR
2	p	422	GLU
2	q	280	VAL
2	q	380	THR
2	q	387	GLN
2	q	395	THR
2	q	422	GLU
2	r	280	VAL
2	r	380	THR
2	r	387	GLN
2	r	395	THR
2	r	422	GLU
2	s	280	VAL
2	s	380	THR
2	s	387	GLN
2	s	395	THR
2	s	422	GLU
2	t	280	VAL
2	t	380	THR
2	t	387	GLN
2	t	395	THR
2	t	422	GLU
2	u	280	VAL
2	u	380	THR
2	u	387	GLN
2	u	395	THR
2	u	422	GLU
2	v	280	VAL

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Mol	Chain	Res	Type
2	v	380	THR
2	v	387	GLN
2	v	395	THR
2	v	422	GLU
2	w	280	VAL
2	w	380	THR
2	w	387	GLN
2	w	395	THR
2	w	422	GLU
2	x	280	VAL
2	x	380	THR
2	x	387	GLN
2	x	395	THR
2	x	422	GLU
2	y	280	VAL
2	y	380	THR
2	y	387	GLN
2	y	395	THR
2	y	422	GLU
2	z	280	VAL
2	z	380	THR
2	z	387	GLN
2	z	395	THR
2	z	422	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (242) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	127	GLN
2	1	305	GLN
2	1	387	GLN
2	1	445	ASN
2	2	305	GLN
2	2	387	GLN
2	2	445	ASN
2	3	305	GLN
2	3	387	GLN
2	3	445	ASN
2	4	305	GLN
2	4	387	GLN
2	4	445	ASN
2	5	305	GLN

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Mol	Chain	Res	Type
2	5	387	GLN
2	5	445	ASN
3	6	47	GLN
3	6	67	HIS
3	6	71	GLN
3	7	39	GLN
3	7	67	HIS
4	8	90	GLN
4	8	106	GLN
4	8	149	GLN
4	8	182	GLN
4	8	199	ASN
4	8	211	GLN
1	9	88	GLN
1	9	127	GLN
1	9	228	GLN
2	A	305	GLN
2	A	387	GLN
2	A	445	ASN
2	AD	341	ASN
2	AH	342	GLN
2	AK	330	ASN
2	AL	341	ASN
2	AL	351	GLN
2	AM	341	ASN
2	AN	341	ASN
2	AN	342	GLN
2	AO	330	ASN
2	AO	355	GLN
1	AP	186	GLN
1	AP	205	ASN
3	AQ	47	GLN
3	AR	86	GLN
5	AS	50	GLN
5	AT	32	GLN
5	AT	50	GLN
5	AT	85	GLN
5	AT	106	ASN
5	AT	110	HIS
5	AU	14	HIS
5	AU	105	GLN
5	AU	106	ASN

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Mol	Chain	Res	Type
5	AU	107	GLN
5	AU	110	HIS
5	AV	85	GLN
5	AV	101	ASN
5	AV	107	GLN
5	AV	110	HIS
5	AW	14	HIS
5	AW	34	ASN
5	AW	50	GLN
5	AW	110	HIS
6	AX	100	ASN
6	AX	118	ASN
6	AX	134	GLN
6	AZ	22	ASN
6	AZ	30	ASN
6	AZ	46	HIS
6	AZ	100	ASN
6	AZ	118	ASN
6	Aa	118	ASN
6	Ab	100	ASN
6	Ac	100	ASN
7	Ad	42	ASN
7	Ad	86	GLN
7	Ae	45	ASN
7	Ae	86	GLN
7	Ae	89	ASN
7	Af	45	ASN
7	Af	75	ASN
7	Af	86	GLN
7	Ag	86	GLN
7	Ah	55	GLN
7	Ah	75	ASN
1	Ak	186	GLN
1	Al	126	GLN
1	Al	127	GLN
1	Al	165	GLN
2	B	305	GLN
2	B	387	GLN
2	B	445	ASN
2	C	305	GLN
2	C	387	GLN
2	C	445	ASN

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Mol	Chain	Res	Type
2	D	305	GLN
2	D	387	GLN
2	D	445	ASN
2	E	305	GLN
2	E	387	GLN
2	E	445	ASN
2	F	305	GLN
2	F	387	GLN
2	F	445	ASN
2	G	305	GLN
2	G	387	GLN
2	G	445	ASN
2	H	305	GLN
2	H	387	GLN
2	H	445	ASN
2	I	305	GLN
2	I	387	GLN
2	I	445	ASN
2	J	305	GLN
2	J	387	GLN
2	J	445	ASN
2	K	305	GLN
2	K	387	GLN
2	K	445	ASN
2	L	305	GLN
2	L	327	ASN
2	L	387	GLN
2	L	445	ASN
2	M	305	GLN
2	M	327	ASN
2	M	387	GLN
2	M	445	ASN
2	N	305	GLN
2	N	387	GLN
2	N	445	ASN
2	O	305	GLN
2	O	387	GLN
2	O	445	ASN
2	P	305	GLN
2	P	387	GLN
2	P	445	ASN
2	Q	305	GLN

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Mol	Chain	Res	Type
2	Q	387	GLN
2	Q	445	ASN
2	R	305	GLN
2	R	327	ASN
2	R	387	GLN
2	R	445	ASN
2	S	166	GLN
2	S	197	GLN
2	T	152	GLN
2	T	156	GLN
2	T	212	ASN
2	T	216	GLN
2	T	243	HIS
2	U	144	GLN
2	U	152	GLN
2	U	196	ASN
2	U	197	GLN
2	U	215	GLN
2	V	242	GLN
2	W	144	GLN
2	W	212	ASN
2	X	152	GLN
2	X	156	GLN
2	X	166	GLN
2	X	212	ASN
2	Y	152	GLN
2	Y	212	ASN
2	Z	197	GLN
2	a	152	GLN
2	a	156	GLN
2	a	166	GLN
2	a	195	HIS
2	b	152	GLN
2	b	212	ASN
2	c	152	GLN
2	c	156	GLN
2	c	189	HIS
2	c	196	ASN
2	d	152	GLN
2	d	216	GLN
2	d	243	HIS
2	e	166	GLN

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Mol	Chain	Res	Type
2	e	212	ASN
2	f	152	GLN
2	f	212	ASN
2	f	216	GLN
2	f	242	GLN
2	g	152	GLN
2	g	166	GLN
2	g	242	GLN
2	h	152	GLN
2	h	242	GLN
2	j	152	GLN
2	j	166	GLN
2	j	212	ASN
2	j	216	GLN
2	k	144	GLN
2	k	152	GLN
2	l	144	GLN
2	l	166	GLN
2	l	197	GLN
2	m	166	GLN
2	m	189	HIS
2	m	196	ASN
2	m	197	GLN
2	m	242	GLN
2	n	166	GLN
2	n	216	GLN
2	o	144	GLN
2	p	305	GLN
2	p	387	GLN
2	p	445	ASN
2	q	305	GLN
2	q	387	GLN
2	q	445	ASN
2	r	305	GLN
2	r	387	GLN
2	r	445	ASN
2	s	305	GLN
2	s	387	GLN
2	s	445	ASN
2	t	305	GLN
2	t	387	GLN
2	t	445	ASN

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Mol	Chain	Res	Type
2	u	305	GLN
2	u	387	GLN
2	u	445	ASN
2	v	305	GLN
2	v	387	GLN
2	v	445	ASN
2	w	305	GLN
2	w	387	GLN
2	w	445	ASN
2	x	305	GLN
2	x	387	GLN
2	x	445	ASN
2	y	305	GLN
2	y	387	GLN
2	y	445	ASN
2	z	305	GLN
2	z	387	GLN
2	z	445	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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

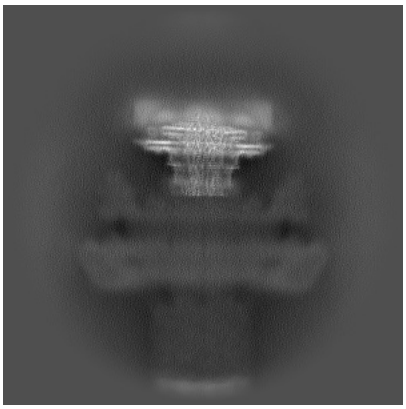
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-39787. These allow visual inspection of the internal detail of the map and identification of artifacts.

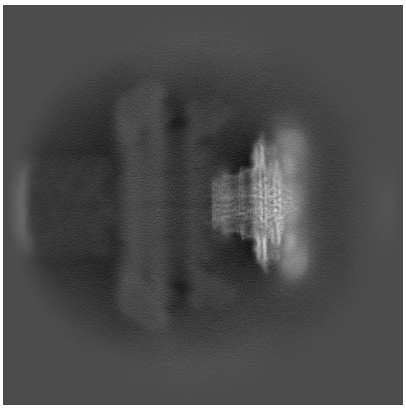
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

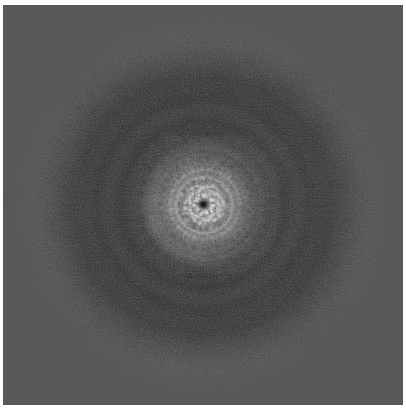
6.1.1 Primary map



X

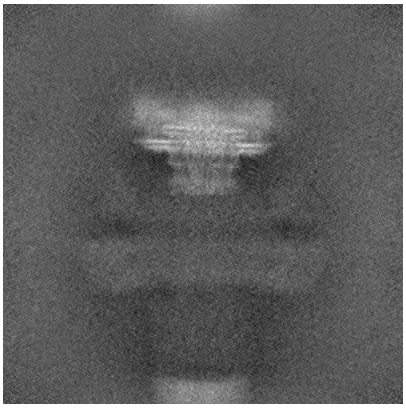


Y

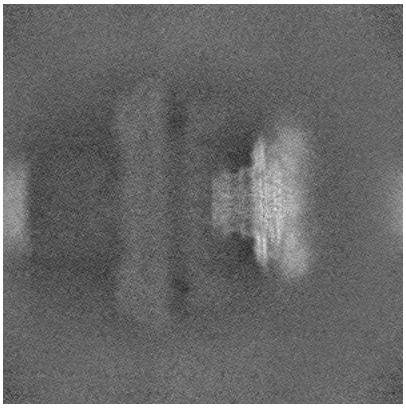


Z

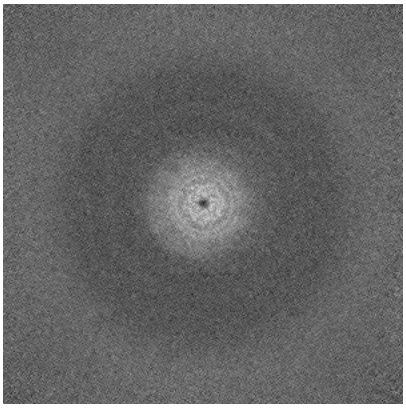
6.1.2 Raw map



X



Y

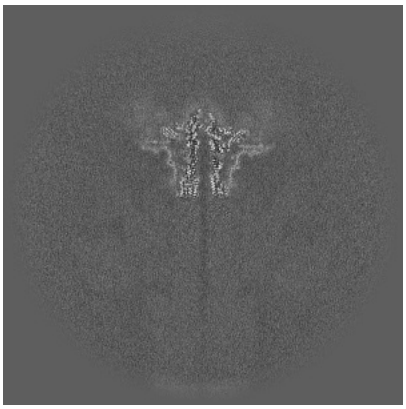


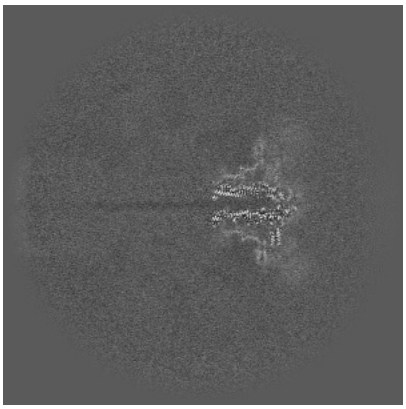
Z

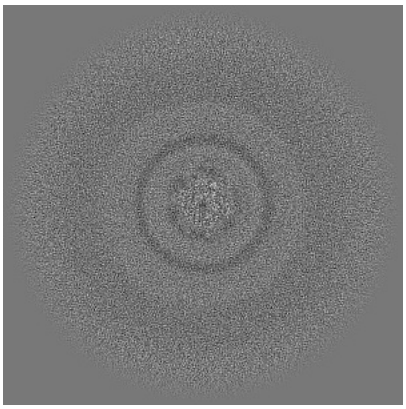
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

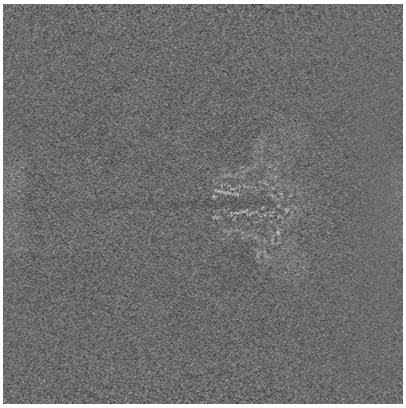

X Index: 310

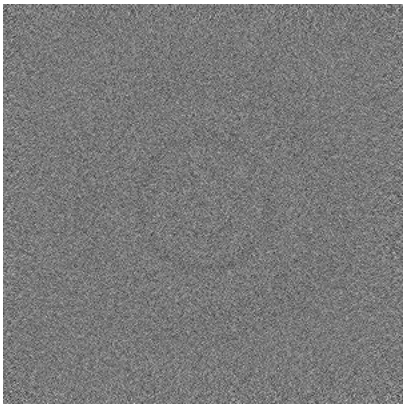

Y Index: 310


Z Index: 310

6.2.2 Raw map

X Index: 310


Y Index: 310

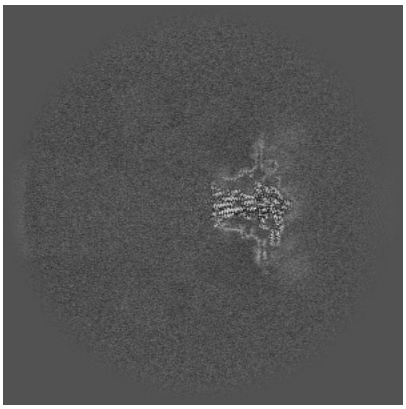

Z Index: 310

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

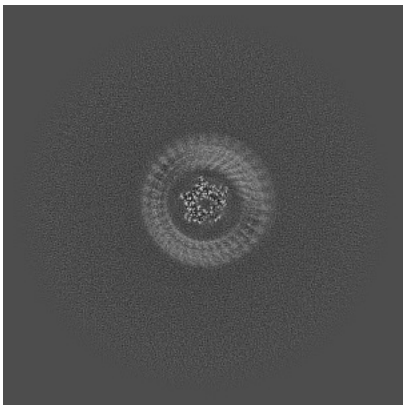
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 301

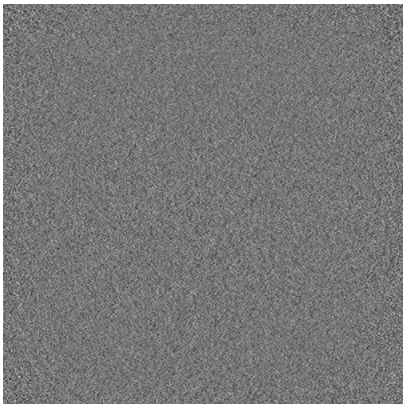


Y Index: 325

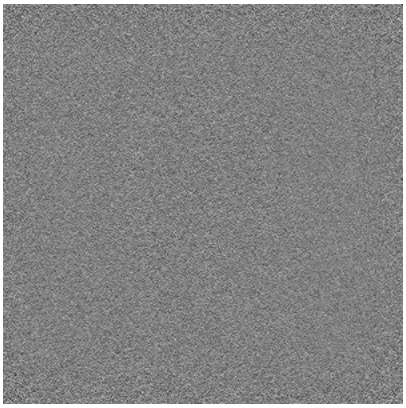


Z Index: 399

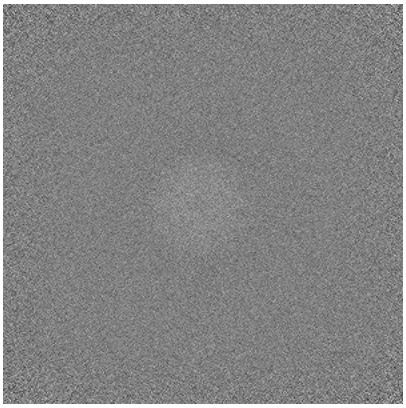
6.3.2 Raw map



X Index: 0



Y Index: 0

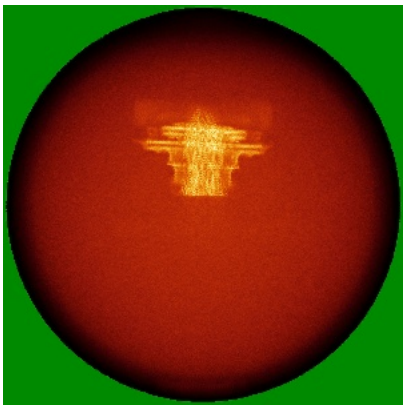


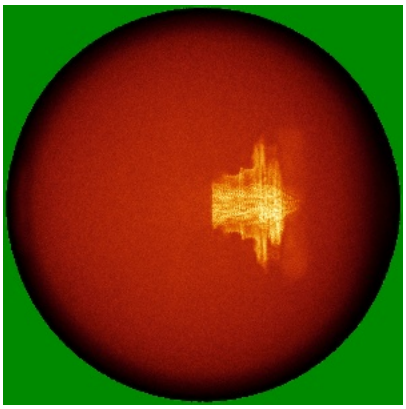
Z Index: 0

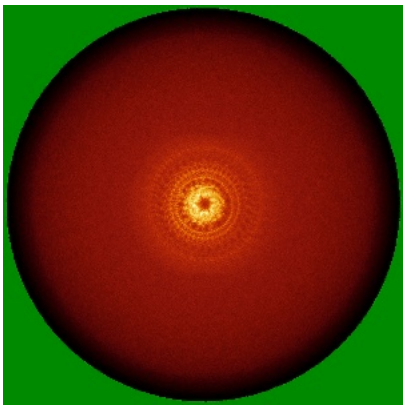
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

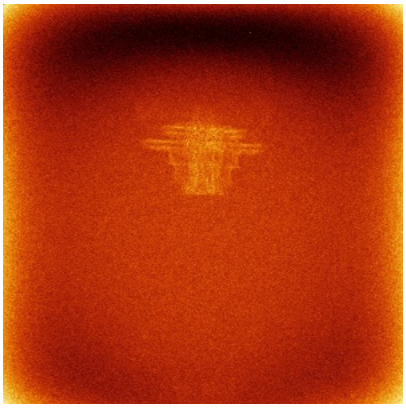
6.4.1 Primary map

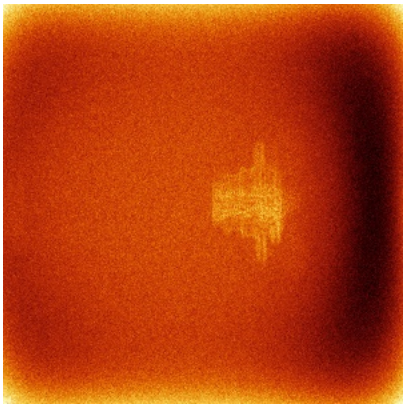

X

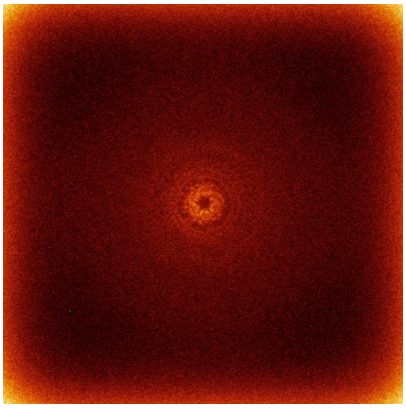

Y


Z

6.4.2 Raw map


X

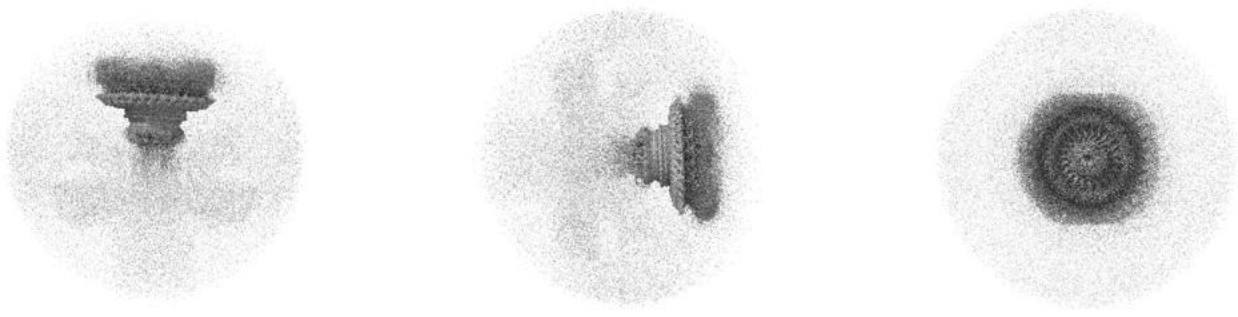

Y


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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

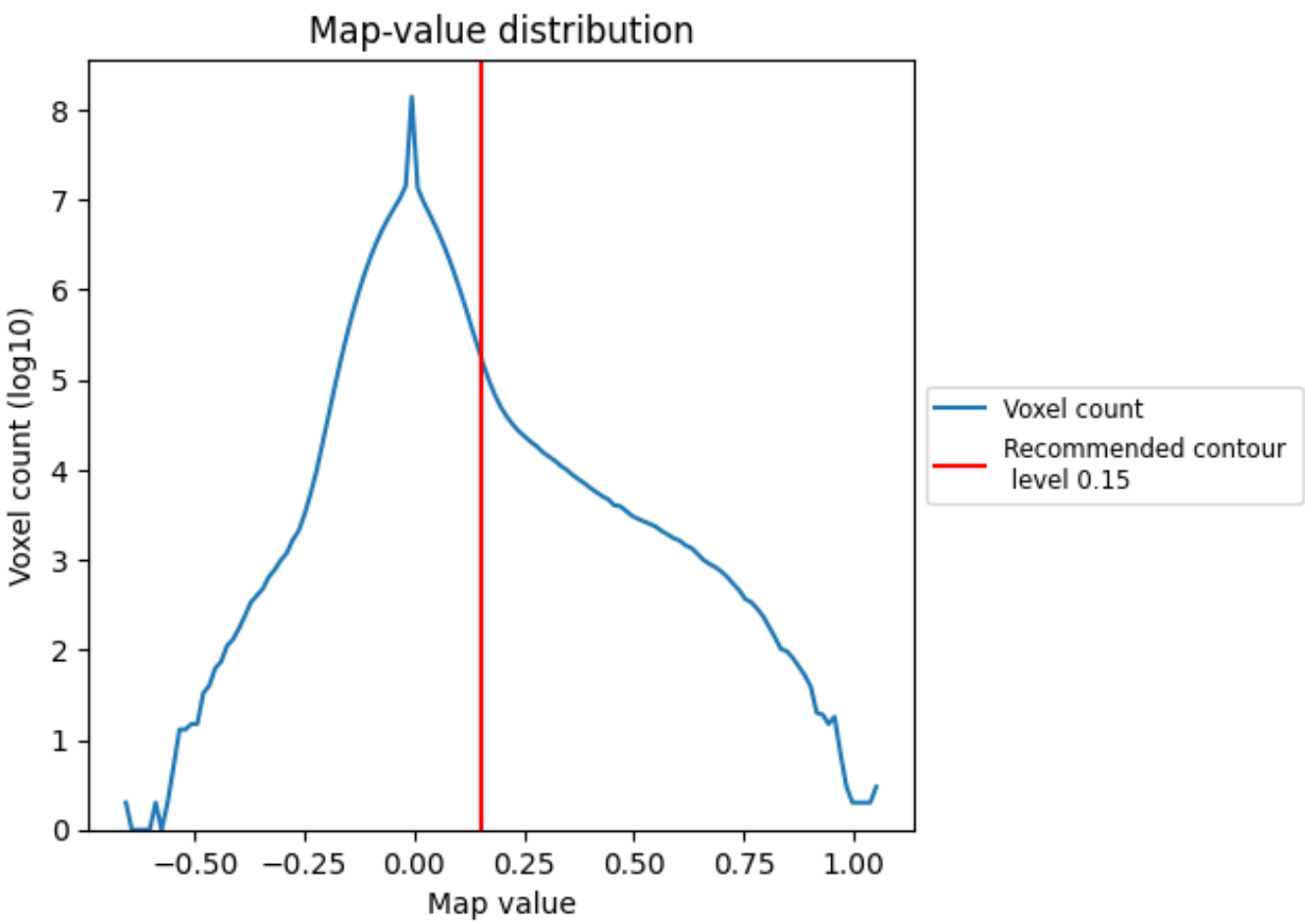
6.6 Mask visualisation (i)

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

7 Map analysis (i)

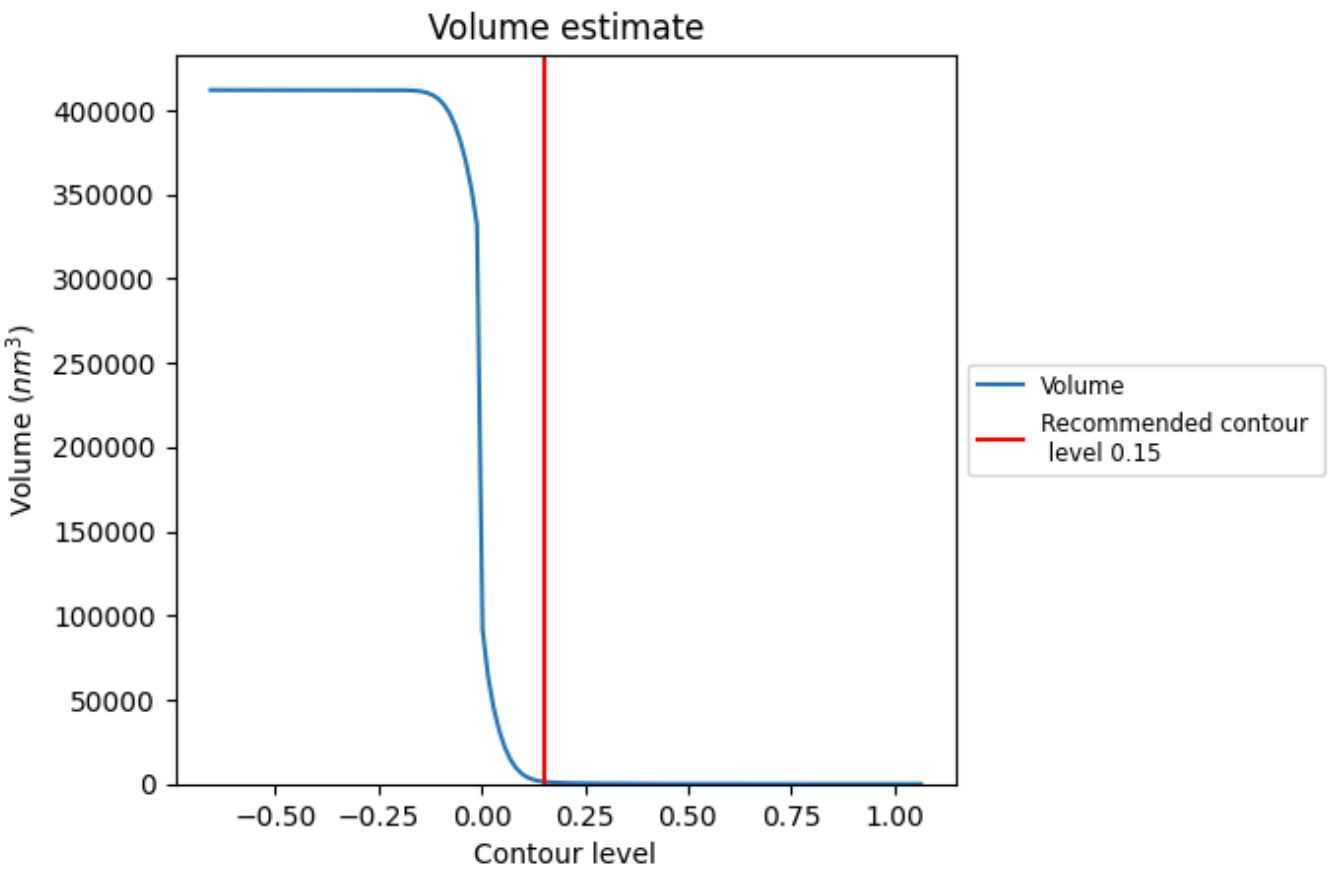
This section contains the results of statistical analysis of the map.

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.

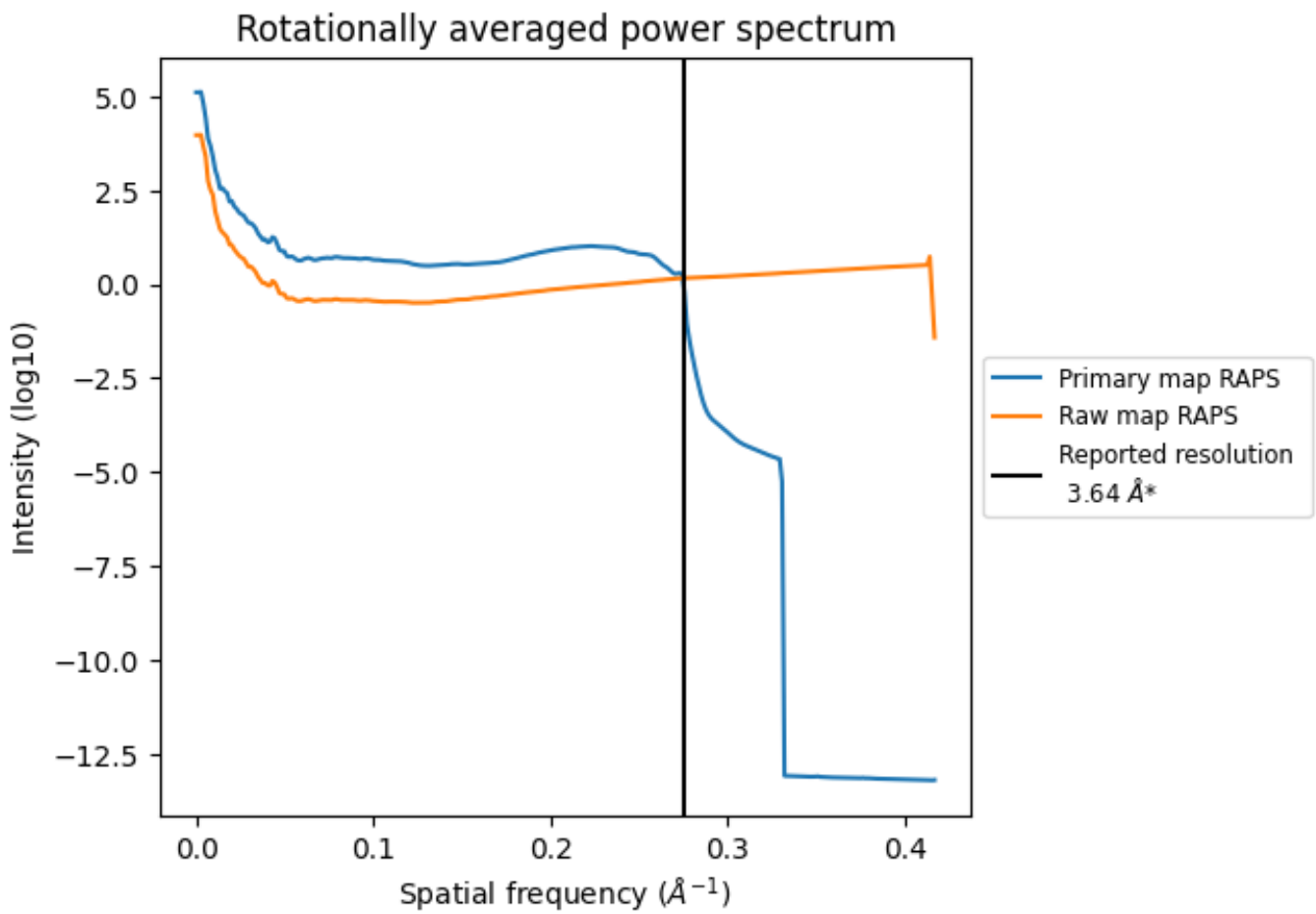
7.2 Volume estimate (i)



The volume at the recommended contour level is 1347 nm^3; this corresponds to an approximate mass of 1217 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)

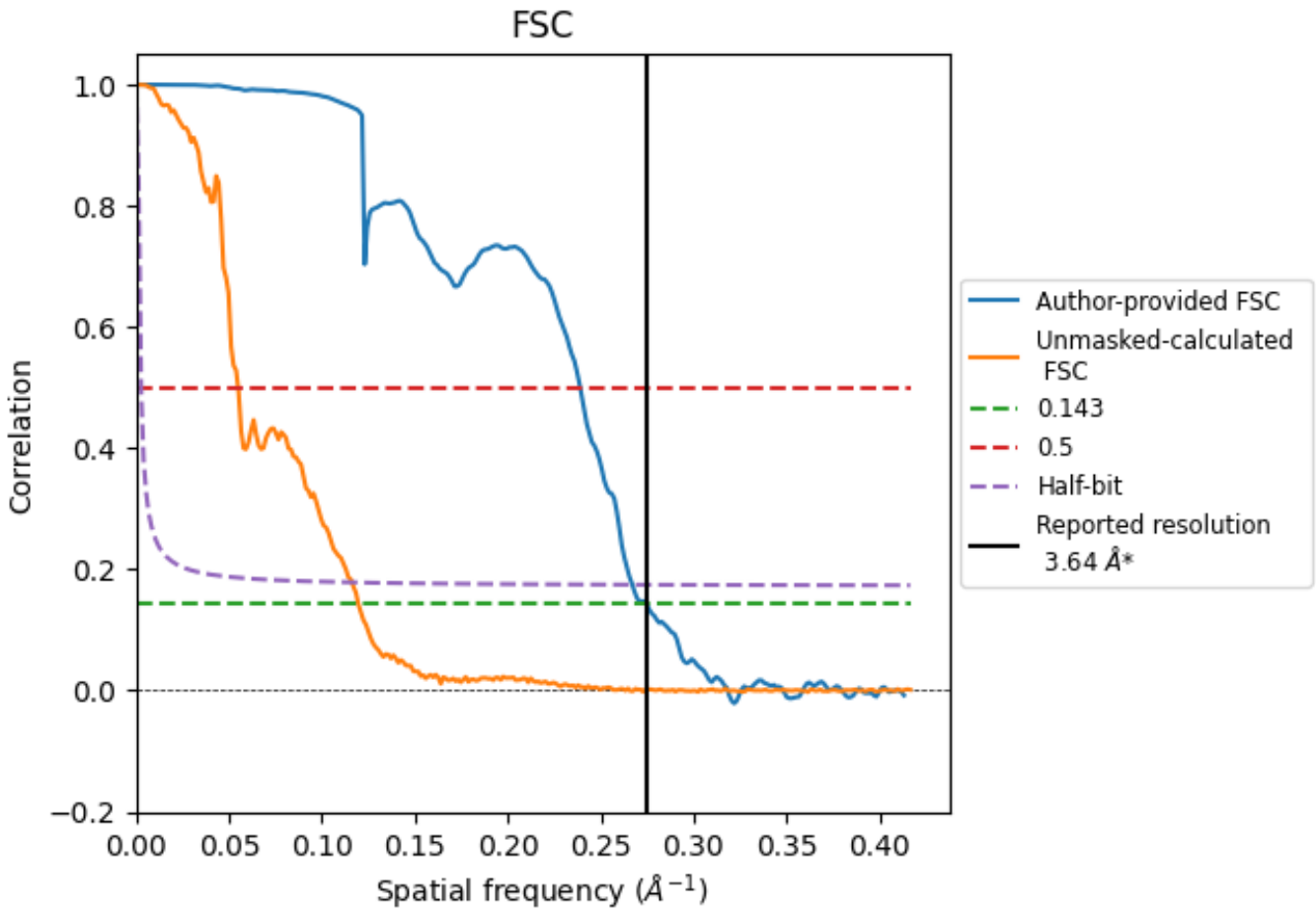


*Reported resolution corresponds to spatial frequency of 0.275 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.275 Å^{-1}

8.2 Resolution estimates (i)

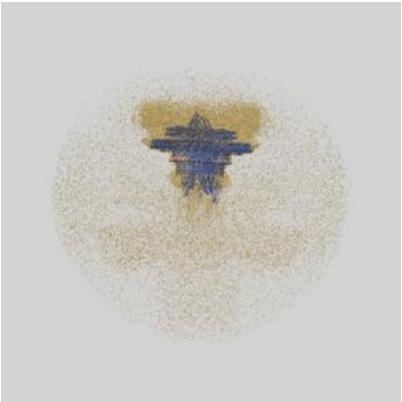
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	3.64	4.18	3.74
Unmasked-calculated*	8.36	18.25	8.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.36 differs from the reported value 3.64 by more than 10 %

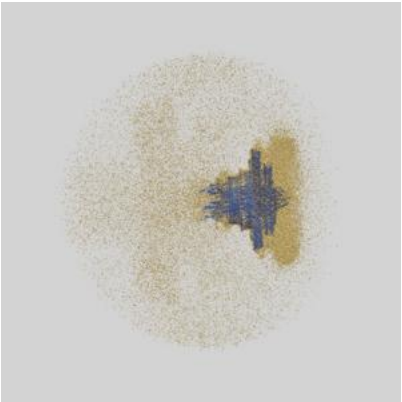
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-39787 and PDB model 8Z5X. Per-residue inclusion information can be found in section 3 on page 15.

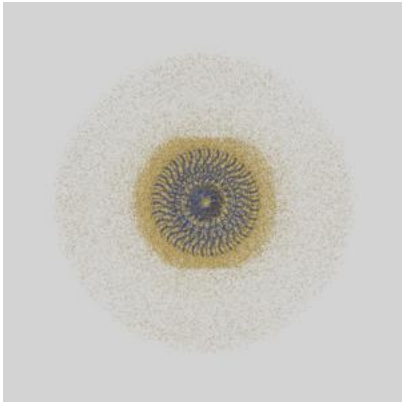
9.1 Map-model overlay (i)



X



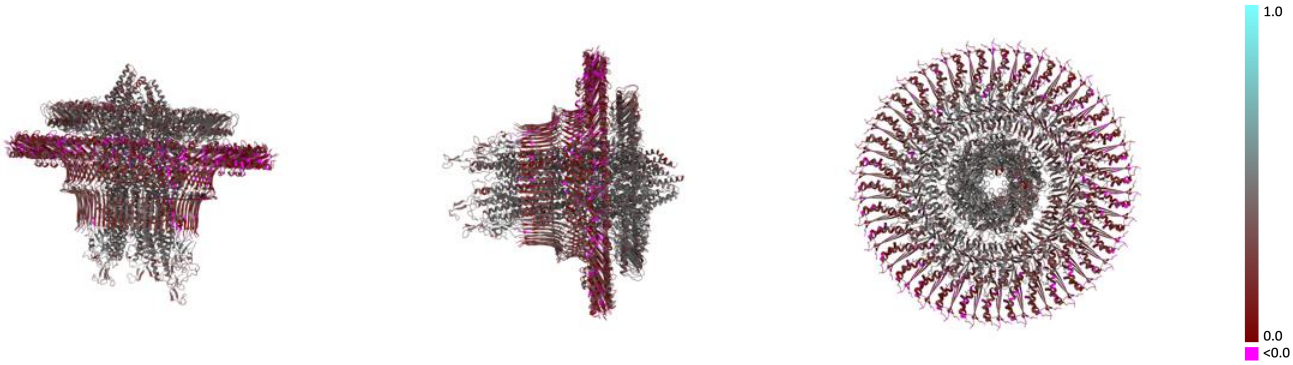
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

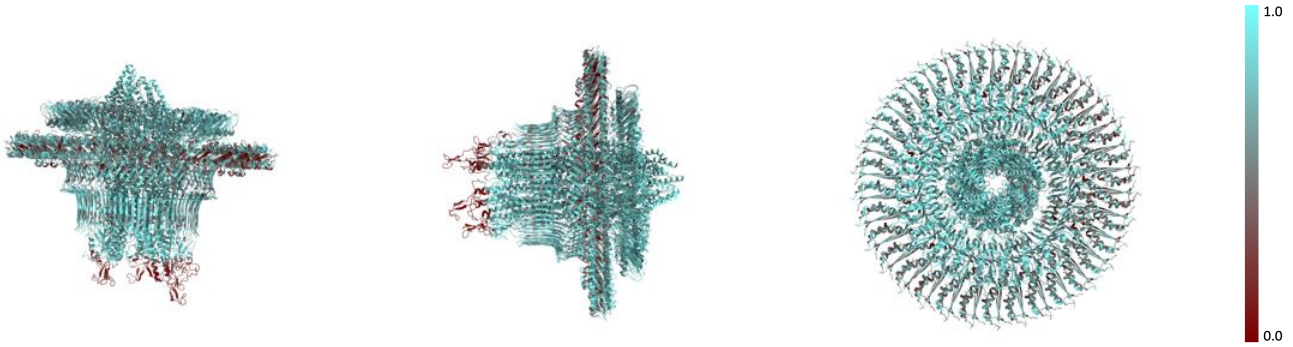
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

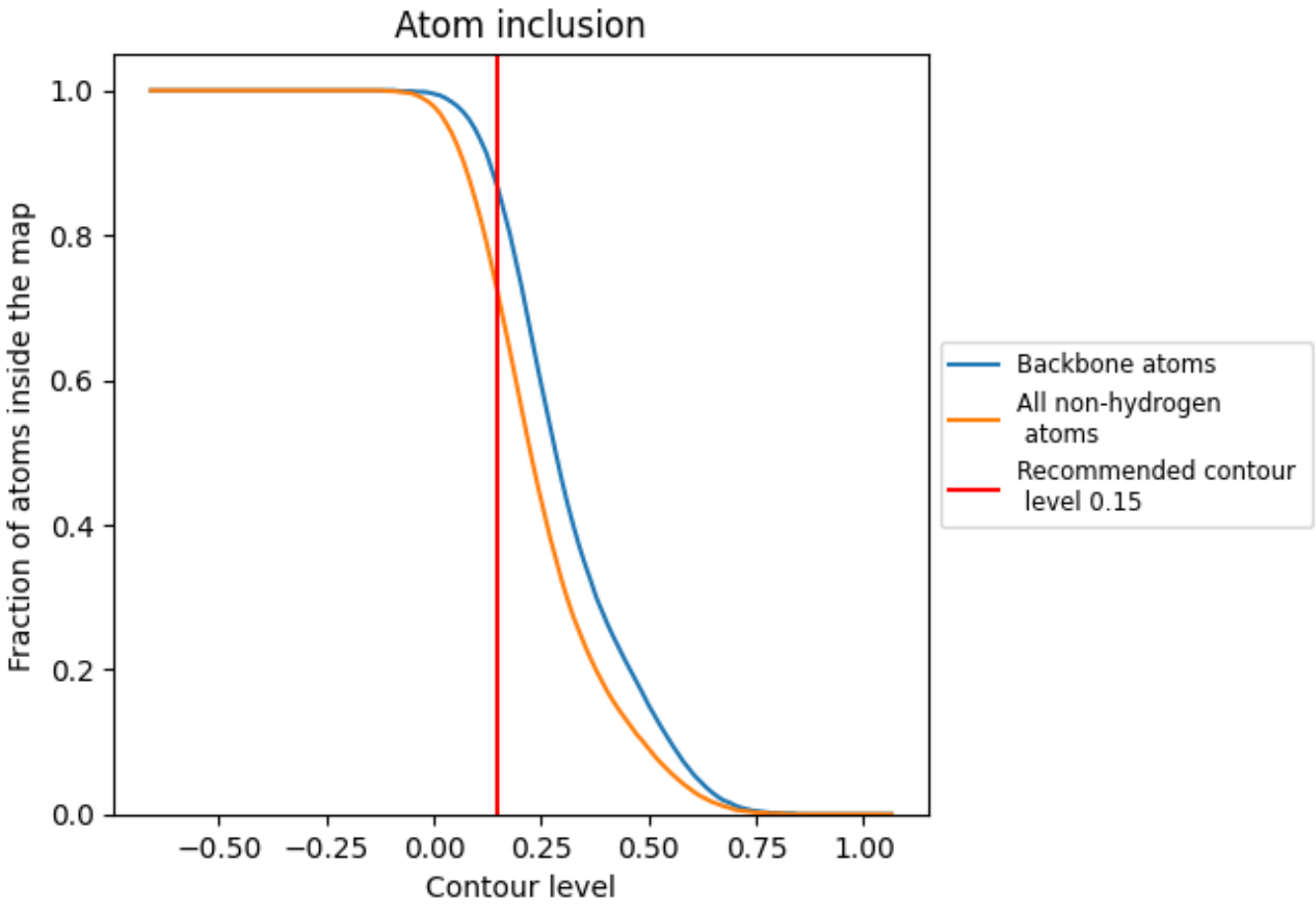
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 72% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7190	0.3130
0	0.8340	0.4560
1	0.5490	0.1320
2	0.5810	0.1440
3	0.5950	0.1420
4	0.6080	0.1490
5	0.6270	0.1720
6	0.8260	0.4330
7	0.8380	0.4440
8	0.8250	0.4280
9	0.8130	0.4360
A	0.6660	0.1800
AA	0.7330	0.4000
AB	0.8220	0.4370
AC	0.5830	0.3990
AD	0.4960	0.4030
AE	0.4370	0.3600
AF	0.4870	0.3450
AG	0.9040	0.4450
AH	0.8630	0.4310
AI	0.7120	0.4150
AJ	0.2090	0.2870
AK	0.7570	0.3960
AL	0.4860	0.3860
AM	0.8210	0.4250
AN	0.6470	0.4030
AO	0.7540	0.4190
AP	0.8290	0.4360
AQ	0.8230	0.4190
AR	0.8550	0.4520
AS	0.8350	0.4550
AT	0.8230	0.4250
AU	0.8510	0.4530
AV	0.8590	0.4660
AW	0.8690	0.4640

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Chain	Atom inclusion	Q-score
AX	0.7080	0.4220
AY	0.4880	0.4020
AZ	0.4640	0.4000
Aa	0.5470	0.4250
Ab	0.6300	0.4300
Ac	0.6800	0.4300
Ad	0.8440	0.4550
Ae	0.8220	0.4310
Af	0.8310	0.4280
Ag	0.8440	0.4410
Ah	0.8480	0.4420
Ai	0.8430	0.4390
Aj	0.7250	0.3240
Ak	0.8450	0.4520
Al	0.8550	0.4620
Am	0.7930	0.3750
An	0.6820	0.3520
Ao	0.8980	0.4520
Ap	0.9800	0.4690
Aq	0.9210	0.4960
Ar	0.8090	0.2940
As	0.8210	0.2520
At	0.7620	0.3190
Au	0.4640	0.2320
Av	0.7140	0.2490
Aw	0.8570	0.2880
B	0.6490	0.1720
C	0.7020	0.2210
D	0.6900	0.2250
E	0.6970	0.2200
F	0.6960	0.2260
G	0.7180	0.2320
H	0.6960	0.2070
I	0.7080	0.2190
J	0.7050	0.2240
K	0.6590	0.1990
L	0.6510	0.1890
M	0.6670	0.1870
N	0.6510	0.1690
O	0.6400	0.1550
P	0.6490	0.1560
Q	0.6450	0.1840

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Chain	Atom inclusion	Q-score
R	0.6620	0.1890
S	0.8370	0.4330
T	0.8490	0.4330
U	0.8130	0.4140
V	0.8380	0.4280
W	0.8120	0.4110
X	0.8210	0.4340
Y	0.8340	0.4440
Z	0.8360	0.4340
a	0.7880	0.4320
b	0.7910	0.4060
c	0.7830	0.4040
d	0.7440	0.3840
e	0.7070	0.3480
f	0.6490	0.3160
g	0.6160	0.3140
h	0.6700	0.3140
i	0.7190	0.3300
j	0.7540	0.3610
k	0.8530	0.4330
l	0.8390	0.4400
m	0.8080	0.4170
n	0.8130	0.4120
o	0.7880	0.3920
p	0.6650	0.2010
q	0.6670	0.2000
r	0.6460	0.1900
s	0.6630	0.2040
t	0.6420	0.1830
u	0.6540	0.1960
v	0.5910	0.1520
w	0.5960	0.1680
x	0.6250	0.1830
y	0.6050	0.1790
z	0.6000	0.1520