Full wwPDB EM Validation Report (i)

May 6, 2025 – 02:51 PM EDT

PDB ID	:	8VKR / pdb_00008vkr
EMDB ID	:	EMD-43328
Title	:	CW Flagellar Switch Complex with extra density - FliF, FliG, FliM, and FliN forming the C-ring from Salmonella
Authors	:	Singh, P.K.; Iverson, T.M.
Deposited on	:	2024-01-09
Resolution	:	5.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

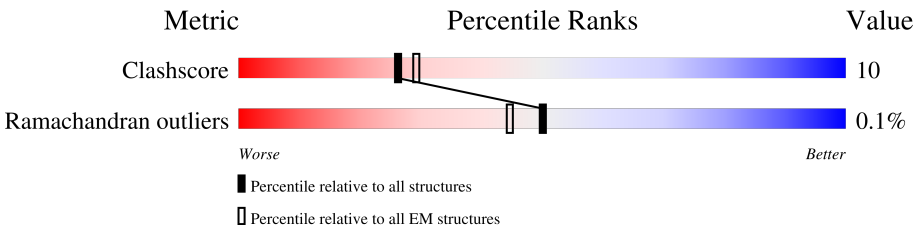
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 5.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835

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	A	560	7% 8% 92%
1	BC	560	7% 8% 92%
1	BF	560	7% 8% 92%
1	DB	560	7% 8% 92%
1	DE	560	7% 8% 92%
1	F	560	7% 8% 92%
1	FA	560	7% 8% 92%
1	FD	560	7% 8% 92%
1	FG	560	7% 8% 92%

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Mol	Chain	Length	Quality of chain
1	HC	560	7% 8% 92%
1	HF	560	7% 8% 92%
1	I	560	7% 8% 92%
1	JB	560	7% 8% 92%
1	JE	560	7% 8% 92%
1	LA	560	7% 8% 92%
1	LD	560	7% 8% 92%
1	LG	560	7% 8% 92%
1	NC	560	7% 8% 92%
1	NF	560	7% 8% 92%
1	PB	560	7% 8% 92%
1	PE	560	7% 8% 92%
1	RA	560	7% 8% 92%
1	RD	560	7% 8% 92%
1	RG	560	7% 8% 92%
1	S	560	7% 8% 92%
1	TC	560	7% 8% 92%
1	TF	560	7% 8% 92%
1	VB	560	7% 8% 92%
1	VE	560	7% 8% 92%
1	XA	560	7% 8% 92%
1	XD	560	7% 8% 92%
1	Z	560	7% 8% 92%
1	ZC	560	7% 8% 92%
1	ZF	560	7% 8% 92%

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Mol	Chain	Length	Quality of chain
2	AA	331	25% 86% 10%
2	AD	331	25% 85% 11%
2	AG	331	25% 86% 10%
2	B	331	25% 86% 10%
2	CC	331	25% 86% 10%
2	CF	331	25% 86% 10%
2	EB	331	25% 86% 10%
2	EE	331	25% 86% 10%
2	G	331	25% 86% 10%
2	GA	331	25% 85% 11%
2	GD	331	25% 85% 11%
2	GG	331	25% 86% 10%
2	IC	331	25% 86% 10%
2	IF	331	25% 86% 10%
2	J	331	25% 86% 10%
2	KB	331	25% 85% 11%
2	KE	331	25% 85% 11%
2	MA	331	25% 85% 11%
2	MD	331	25% 86% 10%
2	MG	331	25% 86% 10%
2	OC	331	25% 85% 11%
2	OF	331	25% 86% 10%
2	QB	331	25% 85% 11%
2	QE	331	26% 85% 11%
2	SA	331	25% 86% 10%

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Mol	Chain	Length	Quality of chain
2	SD	331	25% 86% 10% •
2	SG	331	25% 86% 10% •
2	T	331	25% 86% 10% •
2	UC	331	25% 85% 11% •
2	UF	331	25% 86% 10% •
2	WB	331	25% 86% 10% •
2	WE	331	25% 86% 10% •
2	YA	331	25% 86% 10% •
2	YD	331	25% 86% 10% •
3	BA	334	23% 78% 8% 14%
3	BD	334	23% 78% 8% 14%
3	BG	334	23% 78% 8% 14%
3	C	334	23% 78% 8% 14%
3	DC	334	23% 78% 8% 14%
3	DF	334	23% 78% 8% 14%
3	FB	334	23% 78% 8% 14%
3	FE	334	23% 78% 8% 14%
3	HA	334	23% 78% 8% 14%
3	HD	334	23% 78% 8% 14%
3	HG	334	23% 78% 8% 14%
3	JC	334	23% 78% 8% 14%
3	JF	334	23% 78% 8% 14%
3	K	334	23% 78% 8% 14%
3	LB	334	23% 78% 8% 14%
3	LE	334	23% 78% 8% 14%

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Mol	Chain	Length	Quality of chain
3	M	334	23% 78% 8% 14%
3	NA	334	23% 78% 8% 14%
3	ND	334	23% 78% 8% 14%
3	NG	334	23% 78% 8% 14%
3	PC	334	23% 78% 8% 14%
3	PF	334	23% 78% 8% 14%
3	RB	334	23% 78% 8% 14%
3	RE	334	23% 78% 8% 14%
3	TA	334	23% 78% 8% 14%
3	TD	334	23% 78% 8% 14%
3	TG	334	23% 78% 8% 14%
3	V	334	23% 78% 8% 14%
3	VC	334	23% 78% 8% 14%
3	VF	334	23% 78% 8% 14%
3	XB	334	23% 78% 8% 14%
3	XE	334	23% 78% 8% 14%
3	ZA	334	23% 78% 8% 14%
3	ZD	334	23% 78% 8% 14%
4	AB	137	36% 63% 5% 32%
4	AC	137	50% 9% 41%
4	AE	137	36% 61% 7% 32%
4	AF	137	50% 9% 41%
4	BB	137	55% 6% 39%
4	BE	137	53% 7% 39%
4	CA	137	36% 61% 7% 32%

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Mol	Chain	Length	Quality of chain
4	CB	137	49% 10% 41%
4	CD	137	35% 61% 7% 32%
4	CE	137	50% 9% 41%
4	CG	137	35% 61% 7% 32%
4	D	137	35% 61% 7% 32%
4	DA	137	55% 6% 39%
4	DD	137	53% 7% 39%
4	DG	137	55% 6% 39%
4	E	137	55% 6% 39%
4	EA	137	50% 9% 41%
4	EC	137	35% 61% 7% 32%
4	ED	137	49% 10% 41%
4	EF	137	35% 61% 7% 32%
4	EG	137	49% 10% 41%
4	FC	137	55% 6% 39%
4	FF	137	53% 7% 39%
4	GB	137	35% 63% 5% 32%
4	GC	137	50% 9% 41%
4	GE	137	35% 61% 7% 32%
4	GF	137	50% 9% 41%
4	H	137	49% 10% 41%
4	HB	137	55% 6% 39%
4	HE	137	53% 7% 39%
4	IA	137	35% 63% 5% 32%
4	IB	137	49% 10% 41%

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Mol	Chain	Length	Quality of chain
4	ID	137	35% 61% 7% 32%
4	IE	137	50% 9% 41%
4	IG	137	35% 61% 7% 32%
4	JA	137	55% 6% 39%
4	JD	137	55% 6% 39%
4	JG	137	55% 6% 39%
4	KA	137	49% 10% 41%
4	KC	137	34% 61% 7% 32%
4	KD	137	49% 10% 41%
4	KF	137	35% 61% 7% 32%
4	KG	137	49% 10% 41%
4	L	137	36% 61% 7% 32%
4	LC	137	55% 6% 39%
4	LF	137	53% 7% 39%
4	MB	137	35% 63% 5% 32%
4	MC	137	50% 9% 41%
4	ME	137	35% 61% 7% 32%
4	MF	137	50% 9% 41%
4	N	137	35% 61% 7% 32%
4	NB	137	55% 6% 39%
4	NE	137	53% 7% 39%
4	O	137	53% 7% 39%
4	OA	137	35% 61% 7% 32%
4	OB	137	49% 10% 41%
4	OD	137	35% 60% 8% 32%

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Mol	Chain	Length	Quality of chain
4	OE	137	50% 9% 41%
4	OG	137	35% 61% 7% 32%
4	P	137	55% 6% 39%
4	PA	137	53% 7% 39%
4	PD	137	55% 6% 39%
4	PG	137	55% 6% 39%
4	Q	137	49% 10% 41%
4	QA	137	49% 10% 41%
4	QC	137	35% 61% 7% 32%
4	QD	137	49% 10% 41%
4	QF	137	35% 61% 7% 32%
4	QG	137	49% 10% 41%
4	R	137	50% 9% 41%
4	RC	137	53% 7% 39%
4	RF	137	53% 7% 39%
4	SB	137	35% 61% 7% 32%
4	SC	137	50% 9% 41%
4	SE	137	35% 61% 7% 32%
4	SF	137	50% 9% 41%
4	TB	137	53% 7% 39%
4	TE	137	55% 6% 39%
4	UA	137	36% 63% 5% 32%
4	UB	137	49% 10% 41%
4	UD	137	35% 60% 8% 32%
4	UE	137	49% 10% 41%

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Mol	Chain	Length	Quality of chain
4	UG	137	35% 61% 7% 32%
4	VA	137	55% 6% 39%
4	VD	137	53% 7% 39%
4	VG	137	53% 7% 39%
4	W	137	35% 61% 7% 32%
4	WA	137	49% 10% 41%
4	WC	137	35% 61% 7% 32%
4	WD	137	49% 10% 41%
4	WF	137	35% 61% 7% 32%
4	WG	137	49% 10% 41%
4	X	137	53% 7% 39%
4	XC	137	53% 7% 39%
4	XF	137	55% 6% 39%
4	Y	137	50% 9% 41%
4	YB	137	35% 61% 7% 32%
4	YC	137	50% 9% 41%
4	YE	137	35% 61% 7% 32%
4	YF	137	49% 10% 41%
4	ZB	137	53% 7% 39%
4	ZE	137	55% 6% 39%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 152898 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 M-ring protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	F	47	234	140	47	47	0	0
1	A	47	234	140	47	47	0	0
1	I	47	234	140	47	47	0	0
1	S	47	234	140	47	47	0	0
1	Z	47	234	140	47	47	0	0
1	FA	47	234	140	47	47	0	0
1	LA	47	234	140	47	47	0	0
1	RA	47	234	140	47	47	0	0
1	XA	47	234	140	47	47	0	0
1	DB	47	234	140	47	47	0	0
1	JB	47	234	140	47	47	0	0
1	PB	47	234	140	47	47	0	0
1	VB	47	234	140	47	47	0	0
1	BC	47	234	140	47	47	0	0
1	HC	47	234	140	47	47	0	0
1	NC	47	234	140	47	47	0	0
1	TC	47	234	140	47	47	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	ZC	47	234	140	47	47	0	0
1	FD	47	234	140	47	47	0	0
1	LD	47	234	140	47	47	0	0
1	RD	47	234	140	47	47	0	0
1	XD	47	234	140	47	47	0	0
1	DE	47	234	140	47	47	0	0
1	JE	47	234	140	47	47	0	0
1	PE	47	234	140	47	47	0	0
1	VE	47	234	140	47	47	0	0
1	BF	47	234	140	47	47	0	0
1	HF	47	234	140	47	47	0	0
1	NF	47	234	140	47	47	0	0
1	TF	47	234	140	47	47	0	0
1	ZF	47	234	140	47	47	0	0
1	FG	47	234	140	47	47	0	0
1	LG	47	234	140	47	47	0	0
1	RG	47	234	140	47	47	0	0

- Molecule 2 is a protein called Flagellar motor switch protein FliG.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	G	319	1579	941	319	319	0	0
2	B	319	1579	941	319	319	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	J	319	1579	941	319	319	0	0
2	T	319	1579	941	319	319	0	0
2	AA	319	1579	941	319	319	0	0
2	GA	319	1579	941	319	319	0	0
2	MA	319	1579	941	319	319	0	0
2	SA	319	1579	941	319	319	0	0
2	YA	319	1579	941	319	319	0	0
2	EB	319	1579	941	319	319	0	0
2	KB	319	1579	941	319	319	0	0
2	QB	319	1579	941	319	319	0	0
2	WB	319	1579	941	319	319	0	0
2	CC	319	1579	941	319	319	0	0
2	IC	319	1579	941	319	319	0	0
2	OC	319	1579	941	319	319	0	0
2	UC	319	1579	941	319	319	0	0
2	AD	319	1579	941	319	319	0	0
2	GD	319	1579	941	319	319	0	0
2	MD	319	1579	941	319	319	0	0
2	SD	319	1579	941	319	319	0	0
2	YD	319	1579	941	319	319	0	0
2	EE	319	1579	941	319	319	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	KE	319	1579	941	319	319	0	0
2	QE	319	1579	941	319	319	0	0
2	WE	319	1579	941	319	319	0	0
2	CF	319	1579	941	319	319	0	0
2	IF	319	1579	941	319	319	0	0
2	OF	319	1579	941	319	319	0	0
2	UF	319	1579	941	319	319	0	0
2	AG	319	1579	941	319	319	0	0
2	GG	319	1579	941	319	319	0	0
2	MG	319	1579	941	319	319	0	0
2	SG	319	1579	941	319	319	0	0

- Molecule 3 is a protein called Flagellar motor switch protein FliM.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	M	287	1420	846	287	287	0	0
3	C	287	1420	846	287	287	0	0
3	K	287	1420	846	287	287	0	0
3	V	287	1420	846	287	287	0	0
3	BA	287	1420	846	287	287	0	0
3	HA	287	1420	846	287	287	0	0
3	NA	287	1420	846	287	287	0	0
3	TA	287	1420	846	287	287	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	ZA	287	1420	846	287	287	0	0
3	FB	287	1420	846	287	287	0	0
3	LB	287	1420	846	287	287	0	0
3	RB	287	1420	846	287	287	0	0
3	XB	287	1420	846	287	287	0	0
3	DC	287	1420	846	287	287	0	0
3	JC	287	1420	846	287	287	0	0
3	PC	287	1420	846	287	287	0	0
3	VC	287	1420	846	287	287	0	0
3	BD	287	1420	846	287	287	0	0
3	HD	287	1420	846	287	287	0	0
3	ND	287	1420	846	287	287	0	0
3	TD	287	1420	846	287	287	0	0
3	ZD	287	1420	846	287	287	0	0
3	FE	287	1420	846	287	287	0	0
3	LE	287	1420	846	287	287	0	0
3	RE	287	1420	846	287	287	0	0
3	XE	287	1420	846	287	287	0	0
3	DF	287	1420	846	287	287	0	0
3	JF	287	1420	846	287	287	0	0
3	PF	287	1420	846	287	287	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	VF	287	1420	846	287	287	0	0
3	BG	287	1420	846	287	287	0	0
3	HG	287	1420	846	287	287	0	0
3	NG	287	1420	846	287	287	0	0
3	TG	287	1420	846	287	287	0	0

- Molecule 4 is a protein called Flagellar motor switch protein FliN.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	N	93	456	270	93	93	0	0
4	P	83	409	242	83	84	0	0
4	Q	81	399	236	81	82	0	0
4	D	93	456	270	93	93	0	0
4	E	83	409	242	83	84	0	0
4	H	81	399	236	81	82	0	0
4	L	93	456	270	93	93	0	0
4	O	83	409	242	83	84	0	0
4	R	81	399	236	81	82	0	0
4	W	93	456	270	93	93	0	0
4	X	83	409	242	83	84	0	0
4	Y	81	399	236	81	82	0	0
4	CA	93	456	270	93	93	0	0
4	DA	83	409	242	83	84	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	EA	81	399	236	81	82	0	0
			Total	C	N	O		
4	IA	93	456	270	93	93	0	0
			Total	C	N	O		
4	JA	83	409	242	83	84	0	0
			Total	C	N	O		
4	KA	81	399	236	81	82	0	0
			Total	C	N	O		
4	OA	93	456	270	93	93	0	0
			Total	C	N	O		
4	PA	83	409	242	83	84	0	0
			Total	C	N	O		
4	QA	81	399	236	81	82	0	0
			Total	C	N	O		
4	UA	93	456	270	93	93	0	0
			Total	C	N	O		
4	VA	83	409	242	83	84	0	0
			Total	C	N	O		
4	WA	81	399	236	81	82	0	0
			Total	C	N	O		
4	AB	93	456	270	93	93	0	0
			Total	C	N	O		
4	BB	83	409	242	83	84	0	0
			Total	C	N	O		
4	CB	81	399	236	81	82	0	0
			Total	C	N	O		
4	GB	93	456	270	93	93	0	0
			Total	C	N	O		
4	HB	83	409	242	83	84	0	0
			Total	C	N	O		
4	IB	81	399	236	81	82	0	0
			Total	C	N	O		
4	MB	93	456	270	93	93	0	0
			Total	C	N	O		
4	NB	83	409	242	83	84	0	0
			Total	C	N	O		
4	OB	81	399	236	81	82	0	0
			Total	C	N	O		
4	SB	93	456	270	93	93	0	0
			Total	C	N	O		
4	TB	83	409	242	83	84	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	UB	81	399	236	81	82	0	0
			Total	C	N	O		
4	YB	93	456	270	93	93	0	0
			Total	C	N	O		
4	ZB	83	409	242	83	84	0	0
			Total	C	N	O		
4	AC	81	399	236	81	82	0	0
			Total	C	N	O		
4	EC	93	456	270	93	93	0	0
			Total	C	N	O		
4	FC	83	409	242	83	84	0	0
			Total	C	N	O		
4	GC	81	399	236	81	82	0	0
			Total	C	N	O		
4	KC	93	456	270	93	93	0	0
			Total	C	N	O		
4	LC	83	409	242	83	84	0	0
			Total	C	N	O		
4	MC	81	399	236	81	82	0	0
			Total	C	N	O		
4	QC	93	456	270	93	93	0	0
			Total	C	N	O		
4	RC	83	409	242	83	84	0	0
			Total	C	N	O		
4	SC	81	399	236	81	82	0	0
			Total	C	N	O		
4	WC	93	456	270	93	93	0	0
			Total	C	N	O		
4	XC	83	409	242	83	84	0	0
			Total	C	N	O		
4	YC	81	399	236	81	82	0	0
			Total	C	N	O		
4	CD	93	456	270	93	93	0	0
			Total	C	N	O		
4	DD	83	409	242	83	84	0	0
			Total	C	N	O		
4	ED	81	399	236	81	82	0	0
			Total	C	N	O		
4	ID	93	456	270	93	93	0	0
			Total	C	N	O		
4	JD	83	409	242	83	84	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	KD	81	399	236	81	82	0	0
			Total	C	N	O		
4	OD	93	456	270	93	93	0	0
			Total	C	N	O		
4	PD	83	409	242	83	84	0	0
			Total	C	N	O		
4	QD	81	399	236	81	82	0	0
			Total	C	N	O		
4	UD	93	456	270	93	93	0	0
			Total	C	N	O		
4	VD	83	409	242	83	84	0	0
			Total	C	N	O		
4	WD	81	399	236	81	82	0	0
			Total	C	N	O		
4	AE	93	456	270	93	93	0	0
			Total	C	N	O		
4	BE	83	409	242	83	84	0	0
			Total	C	N	O		
4	CE	81	399	236	81	82	0	0
			Total	C	N	O		
4	GE	93	456	270	93	93	0	0
			Total	C	N	O		
4	HE	83	409	242	83	84	0	0
			Total	C	N	O		
4	IE	81	399	236	81	82	0	0
			Total	C	N	O		
4	ME	93	456	270	93	93	0	0
			Total	C	N	O		
4	NE	83	409	242	83	84	0	0
			Total	C	N	O		
4	OE	81	399	236	81	82	0	0
			Total	C	N	O		
4	SE	93	456	270	93	93	0	0
			Total	C	N	O		
4	TE	83	409	242	83	84	0	0
			Total	C	N	O		
4	UE	81	399	236	81	82	0	0
			Total	C	N	O		
4	YE	93	456	270	93	93	0	0
			Total	C	N	O		
4	ZE	83	409	242	83	84	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	AF	81	399	236	81	82	0	0
			Total	C	N	O		
4	EF	93	456	270	93	93	0	0
			Total	C	N	O		
4	FF	83	409	242	83	84	0	0
			Total	C	N	O		
4	GF	81	399	236	81	82	0	0
			Total	C	N	O		
4	KF	93	456	270	93	93	0	0
			Total	C	N	O		
4	LF	83	409	242	83	84	0	0
			Total	C	N	O		
4	MF	81	399	236	81	82	0	0
			Total	C	N	O		
4	QF	93	456	270	93	93	0	0
			Total	C	N	O		
4	RF	83	409	242	83	84	0	0
			Total	C	N	O		
4	SF	81	399	236	81	82	0	0
			Total	C	N	O		
4	WF	93	456	270	93	93	0	0
			Total	C	N	O		
4	XF	83	409	242	83	84	0	0
			Total	C	N	O		
4	YF	81	399	236	81	82	0	0
			Total	C	N	O		
4	CG	93	456	270	93	93	0	0
			Total	C	N	O		
4	DG	83	409	242	83	84	0	0
			Total	C	N	O		
4	EG	81	399	236	81	82	0	0
			Total	C	N	O		
4	IG	93	456	270	93	93	0	0
			Total	C	N	O		
4	JG	83	409	242	83	84	0	0
			Total	C	N	O		
4	KG	81	399	236	81	82	0	0
			Total	C	N	O		
4	OG	93	456	270	93	93	0	0
			Total	C	N	O		
4	PG	83	409	242	83	84	0	0

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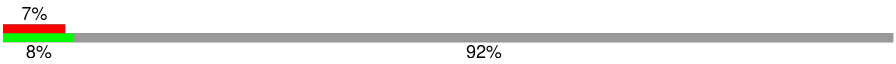
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	QG	81	399	236	81	82	0	0
			Total	C	N	O		
4	UG	93	456	270	93	93	0	0
			Total	C	N	O		
4	VG	83	409	242	83	84	0	0
			Total	C	N	O		
4	WG	81	399	236	81	82	0	0

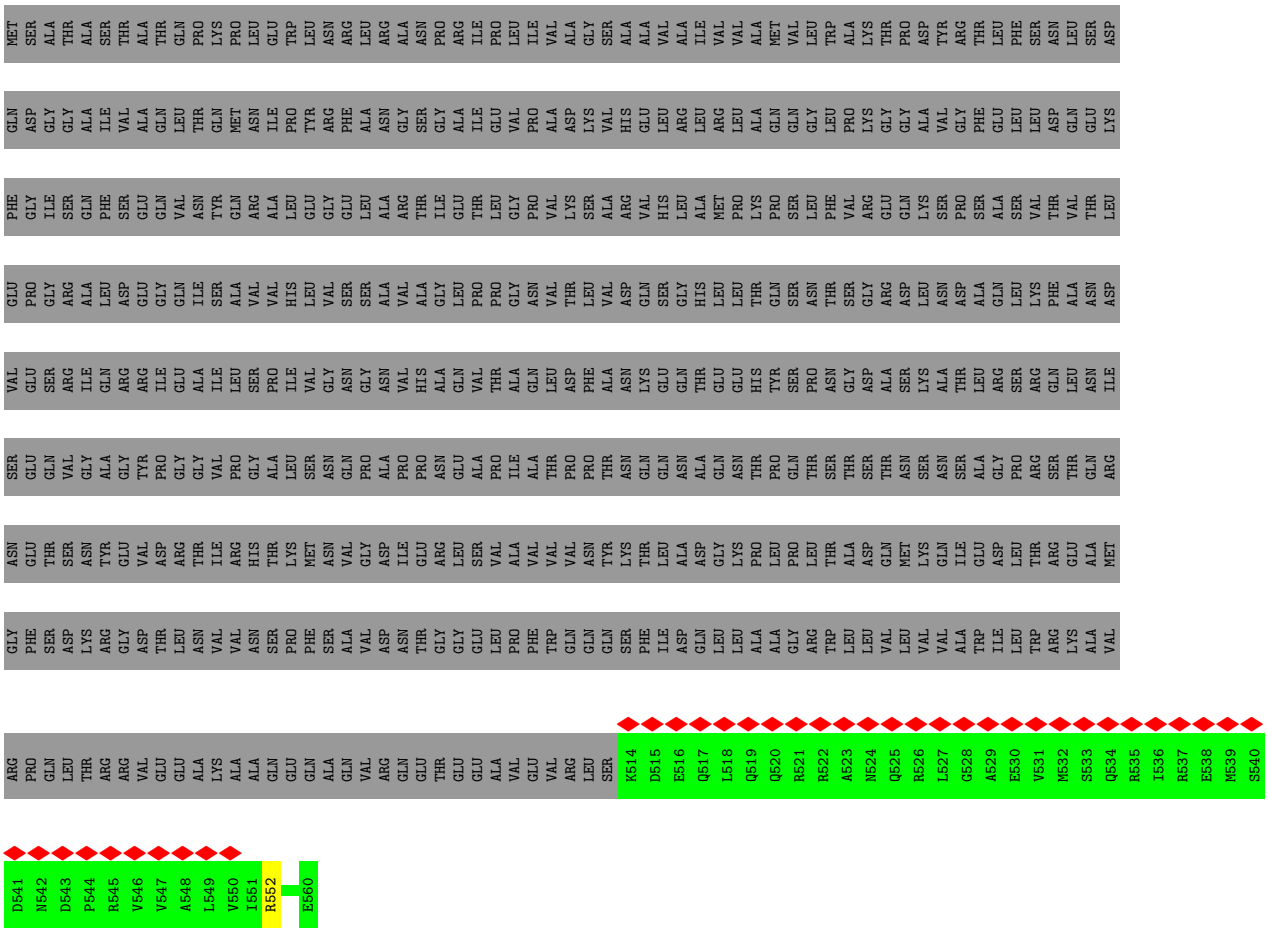
3 Residue-property plots (i)

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 M-ring protein

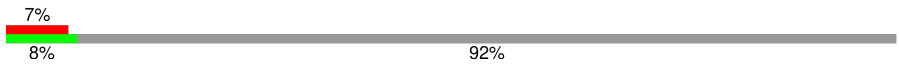
Chain F:

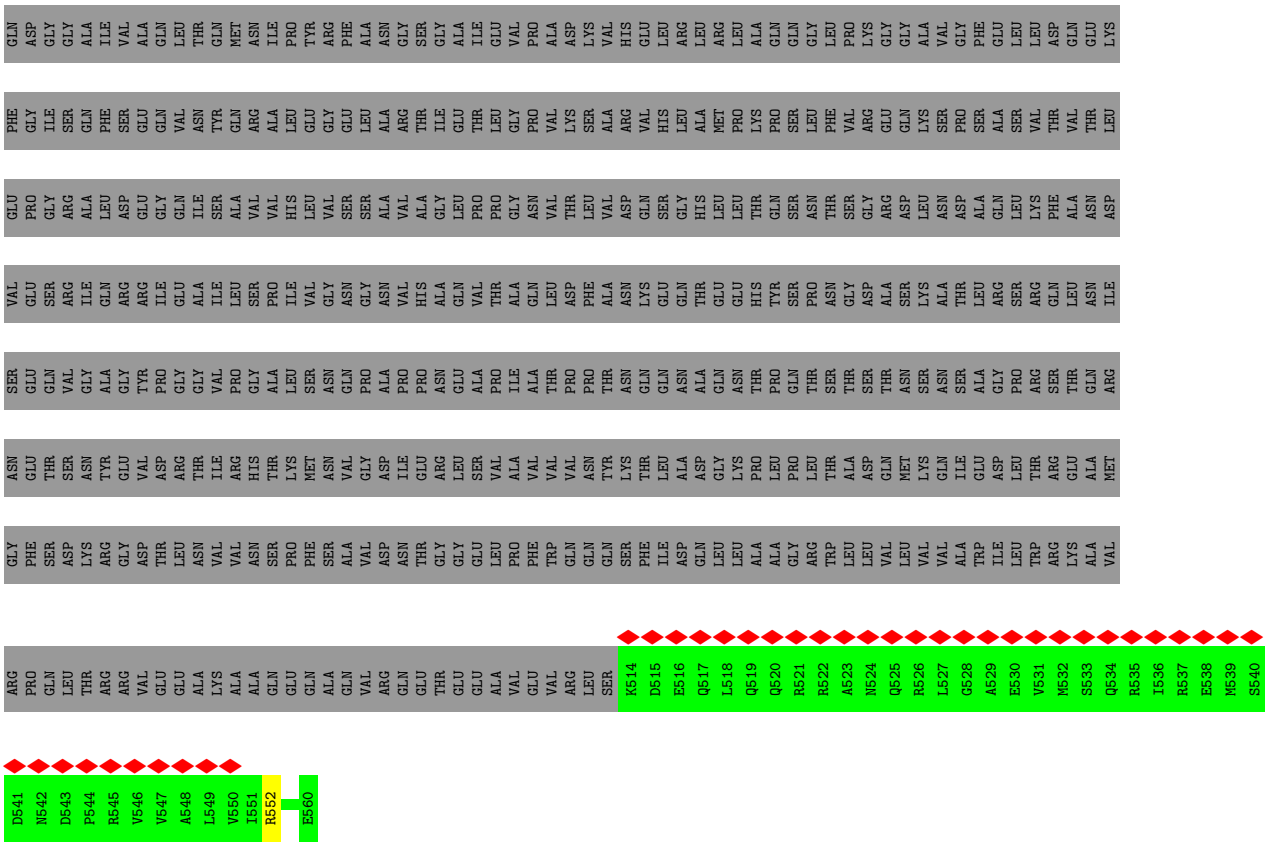




- Molecule 1: Flagellar M-ring protein

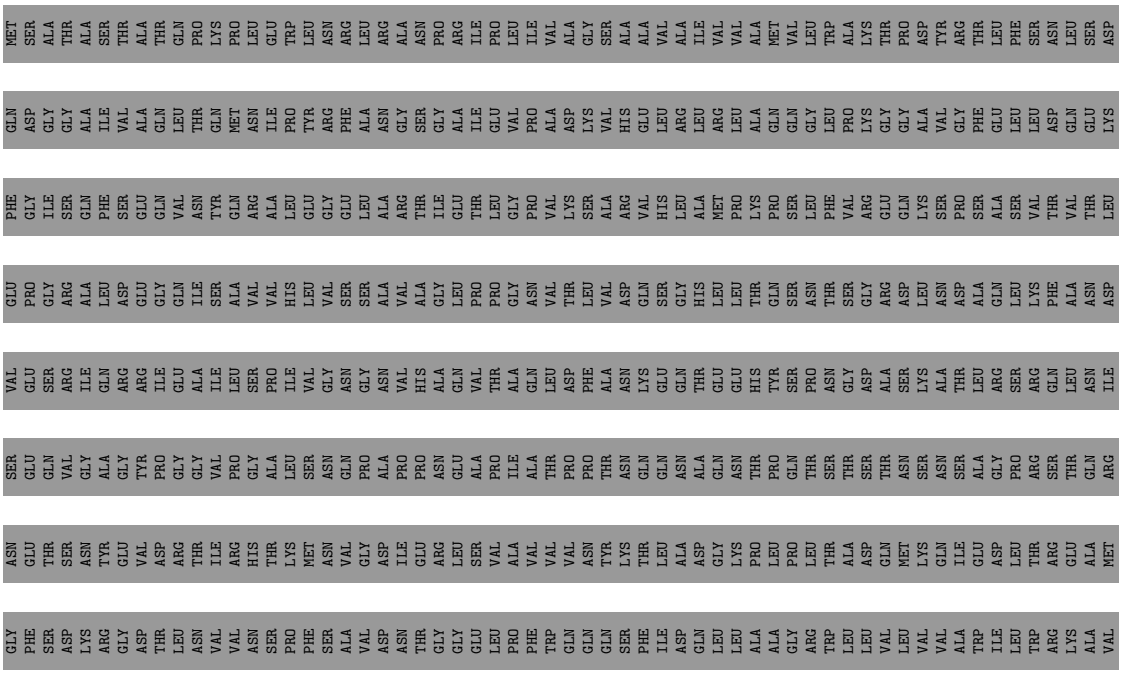
Chain A:

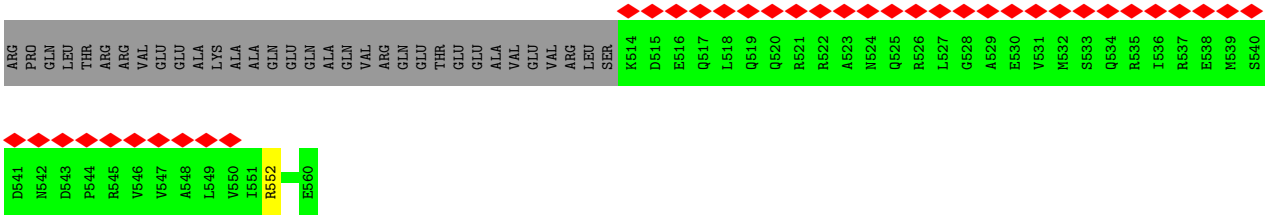




- Molecule 1: Flagellar M-ring protein

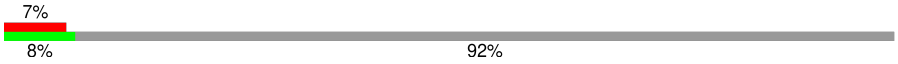
Chain I: 7% 8% 92%

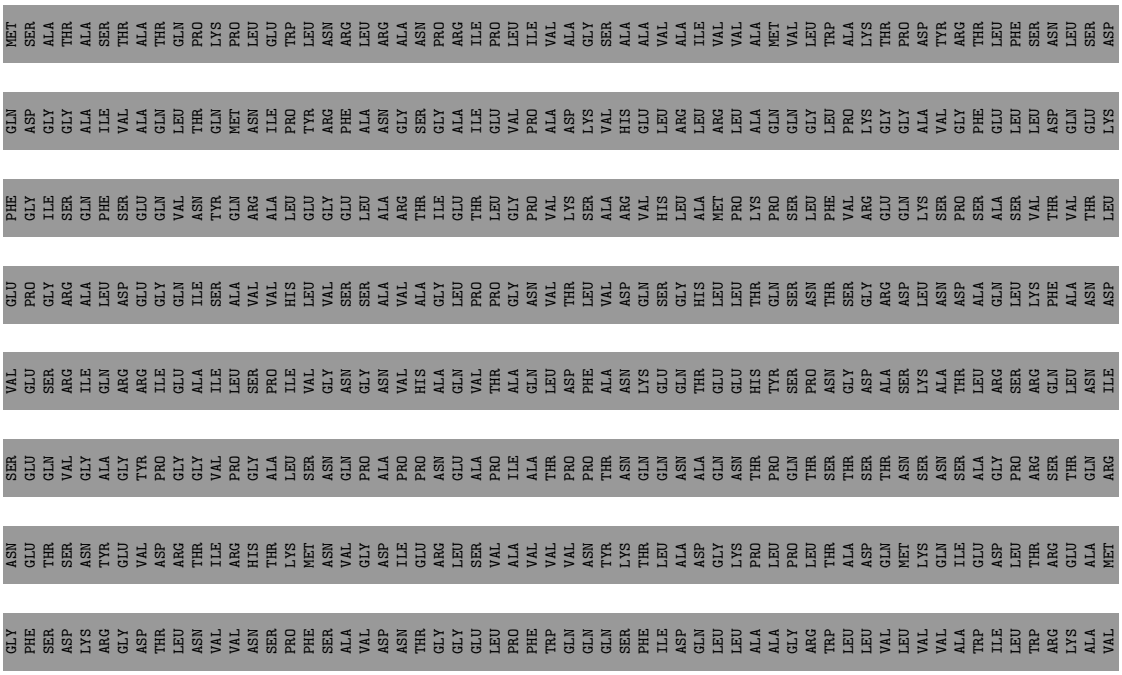


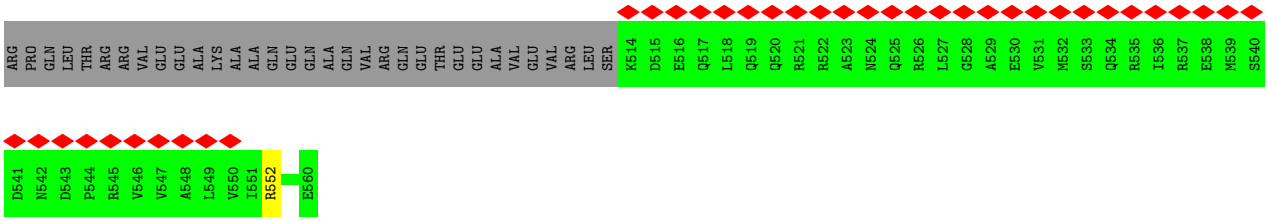


• Molecule 1: Flagellar M-ring protein

Chain S:

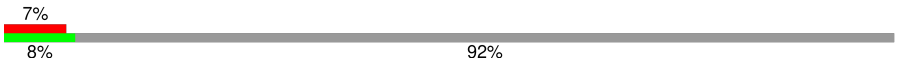


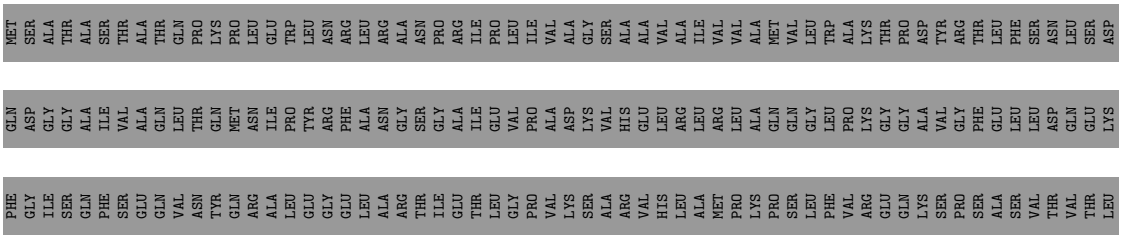


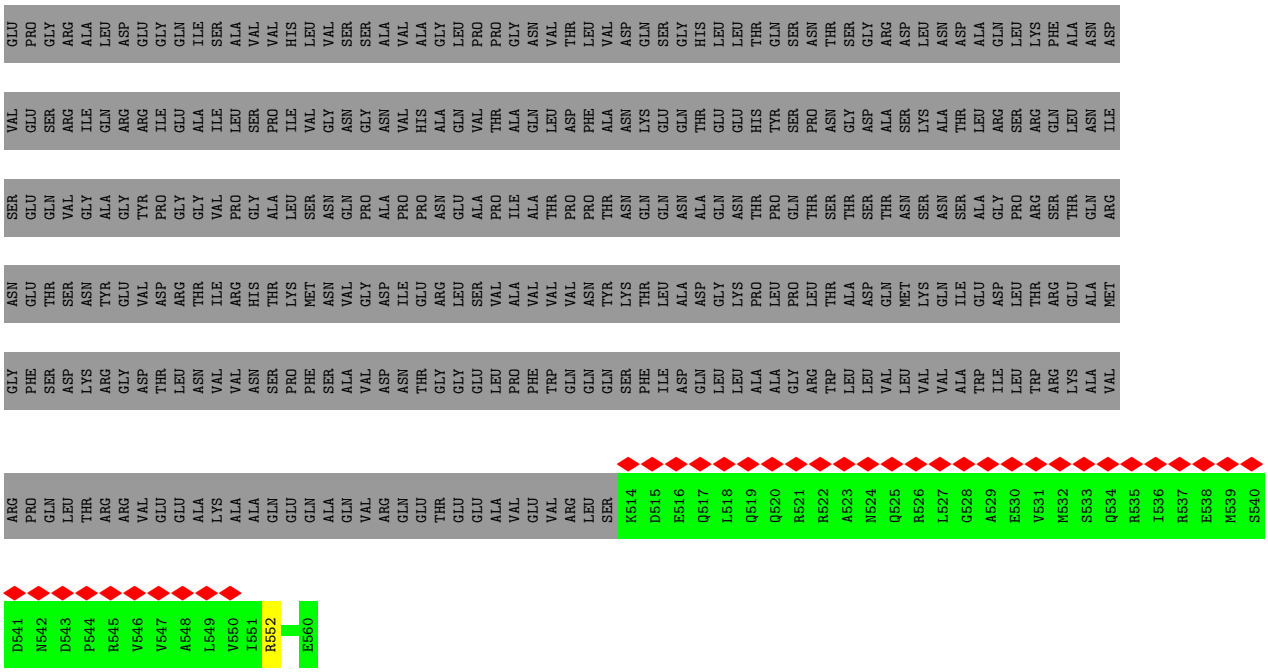


• Molecule 1: Flagellar M-ring protein

Chain Z:

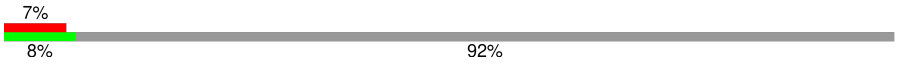


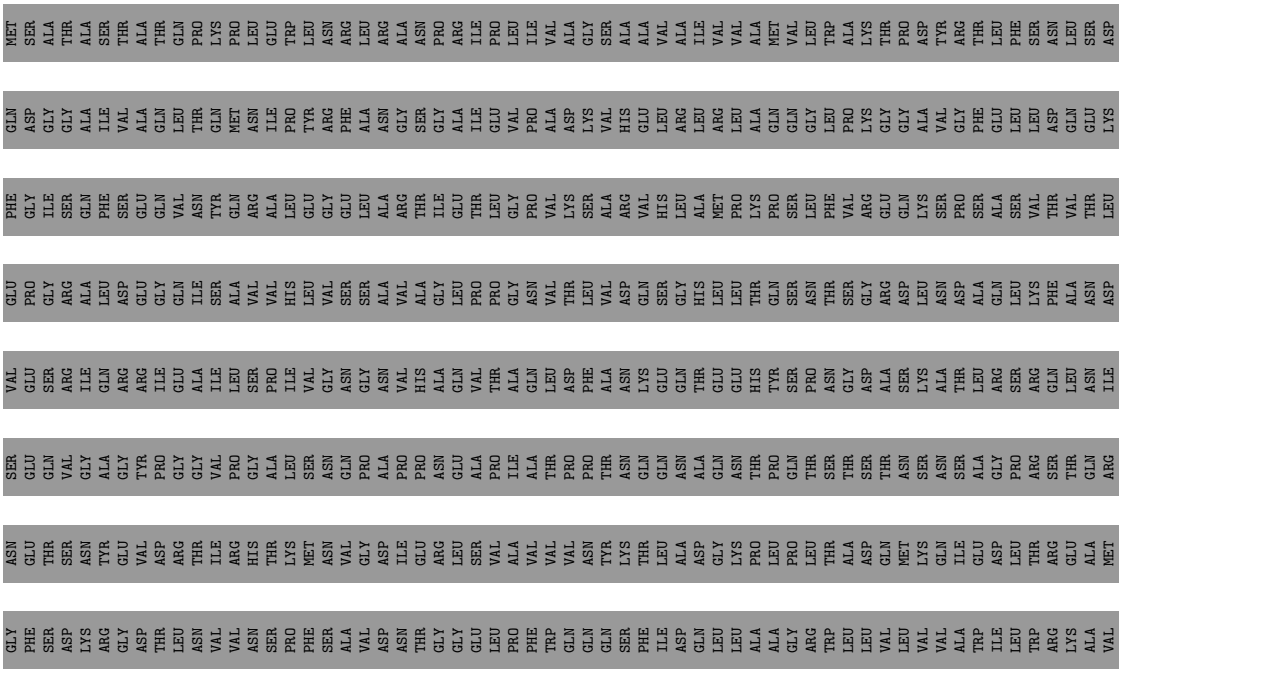




- Molecule 1: Flagellar M-ring protein

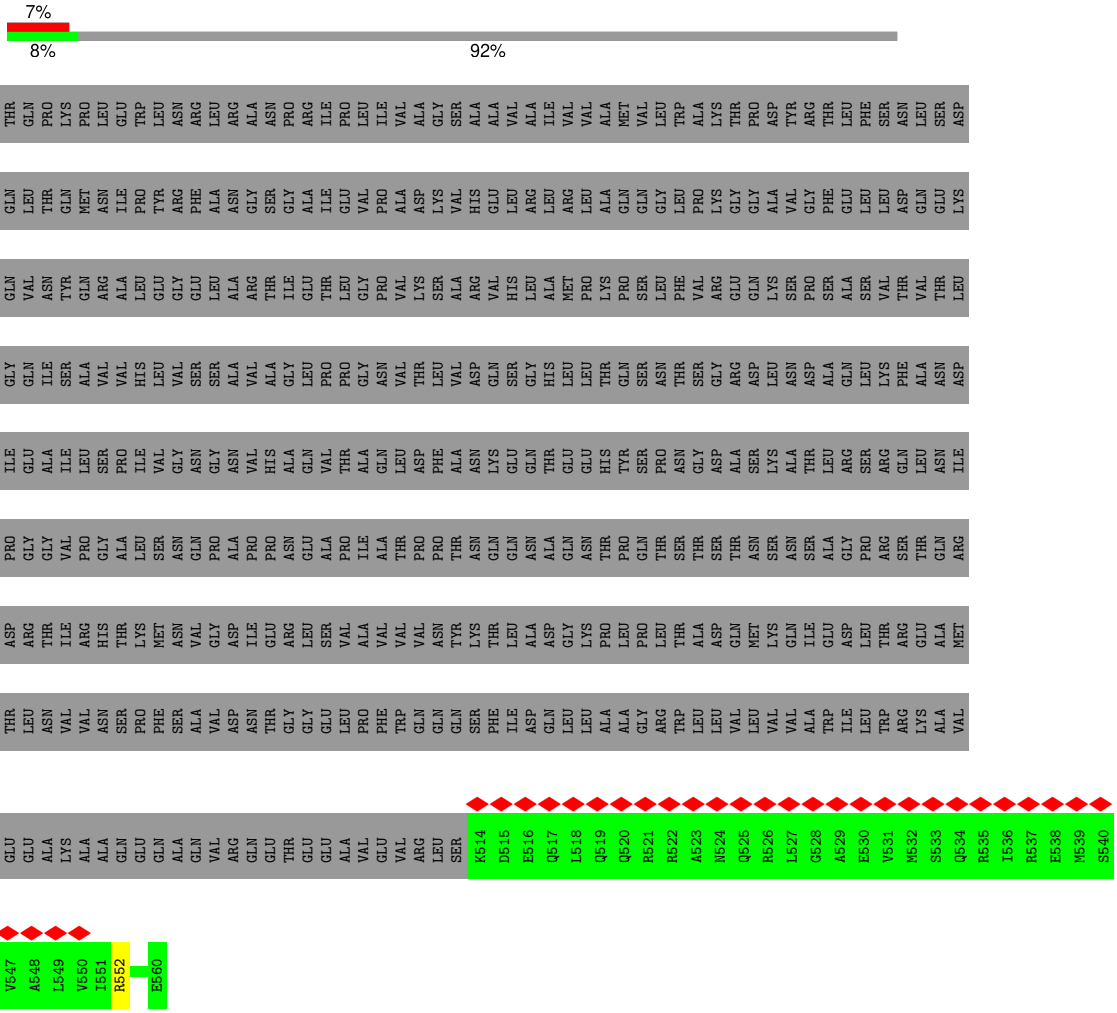
Chain FA:





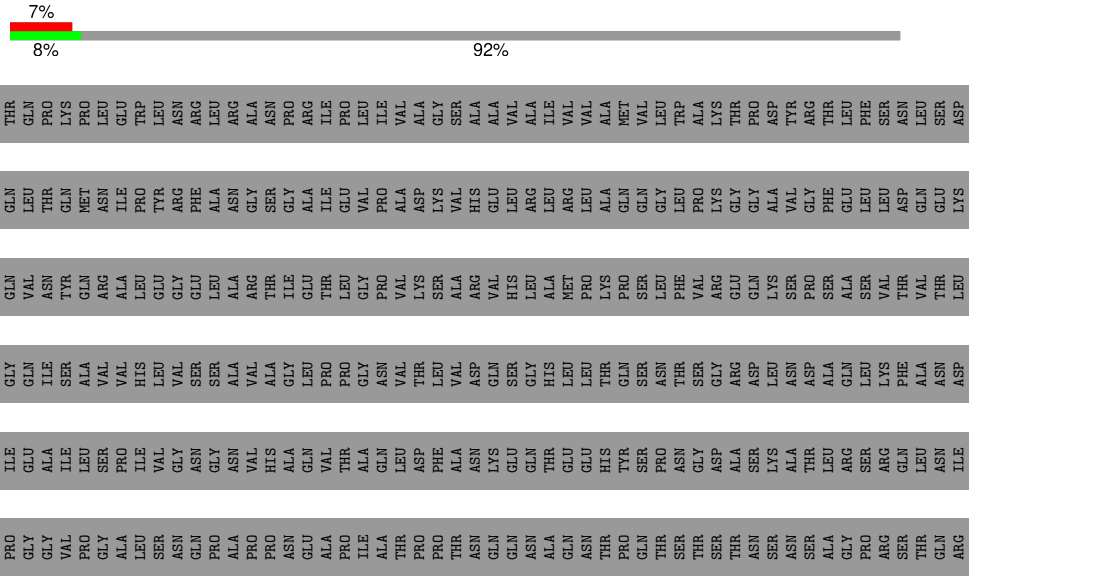
• Molecule 1: Flagellar M-ring protein

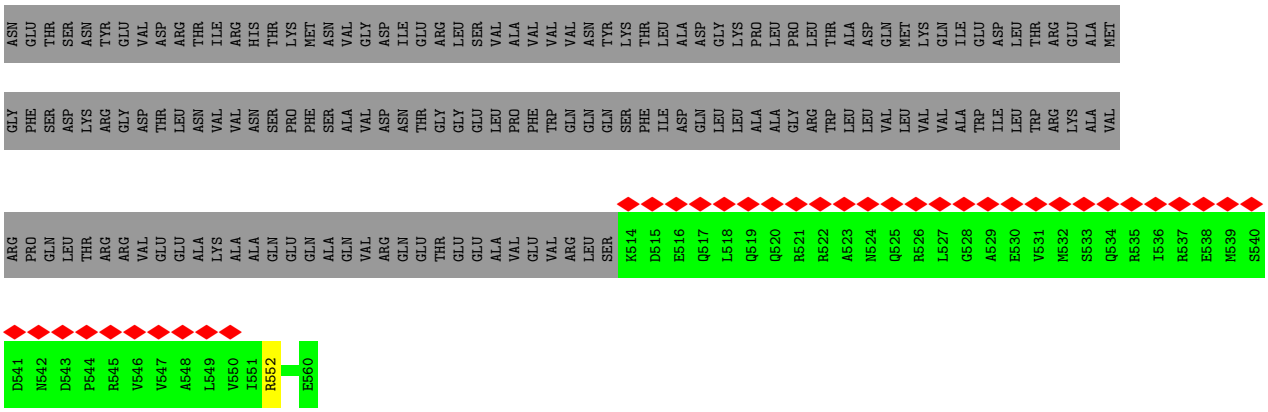
Chain LA:



• Molecule 1: Flagellar M-ring protein

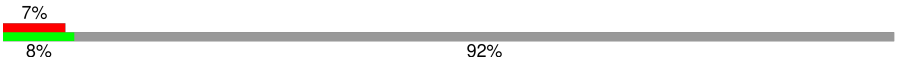
Chain RA:

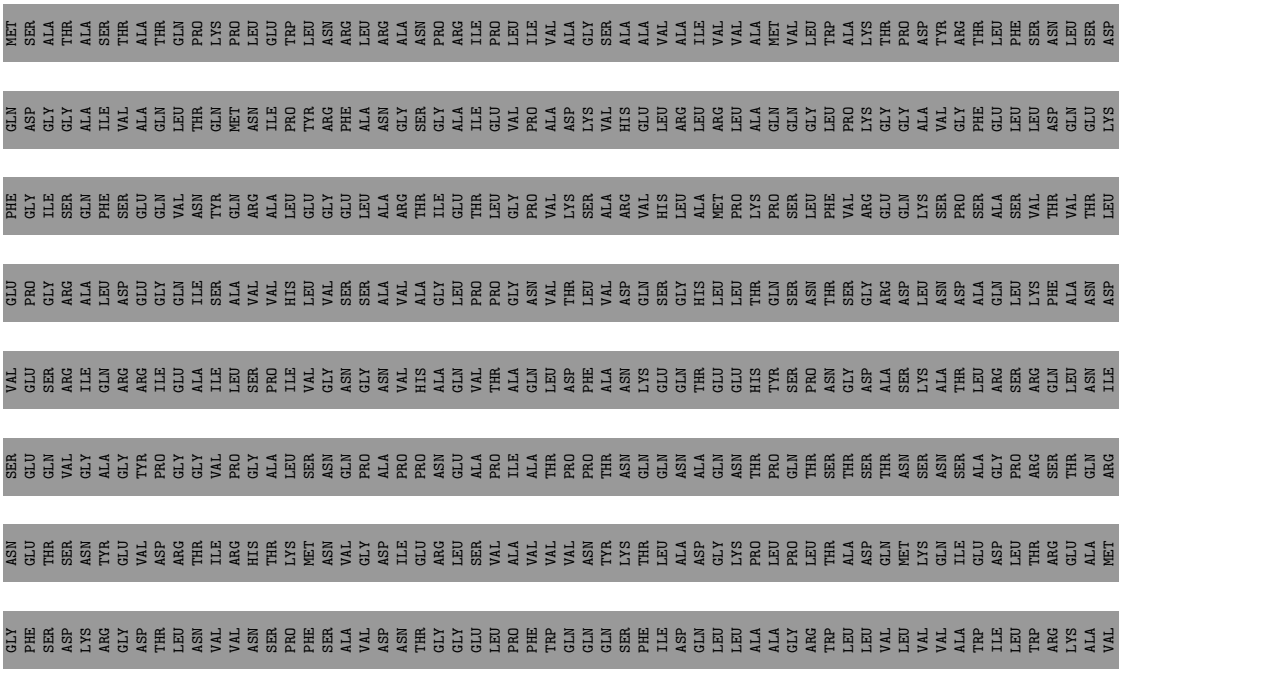




• Molecule 1: Flagellar M-ring protein

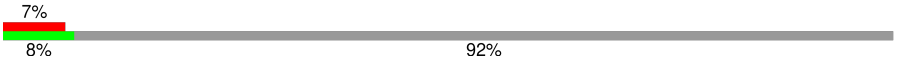
Chain XA:

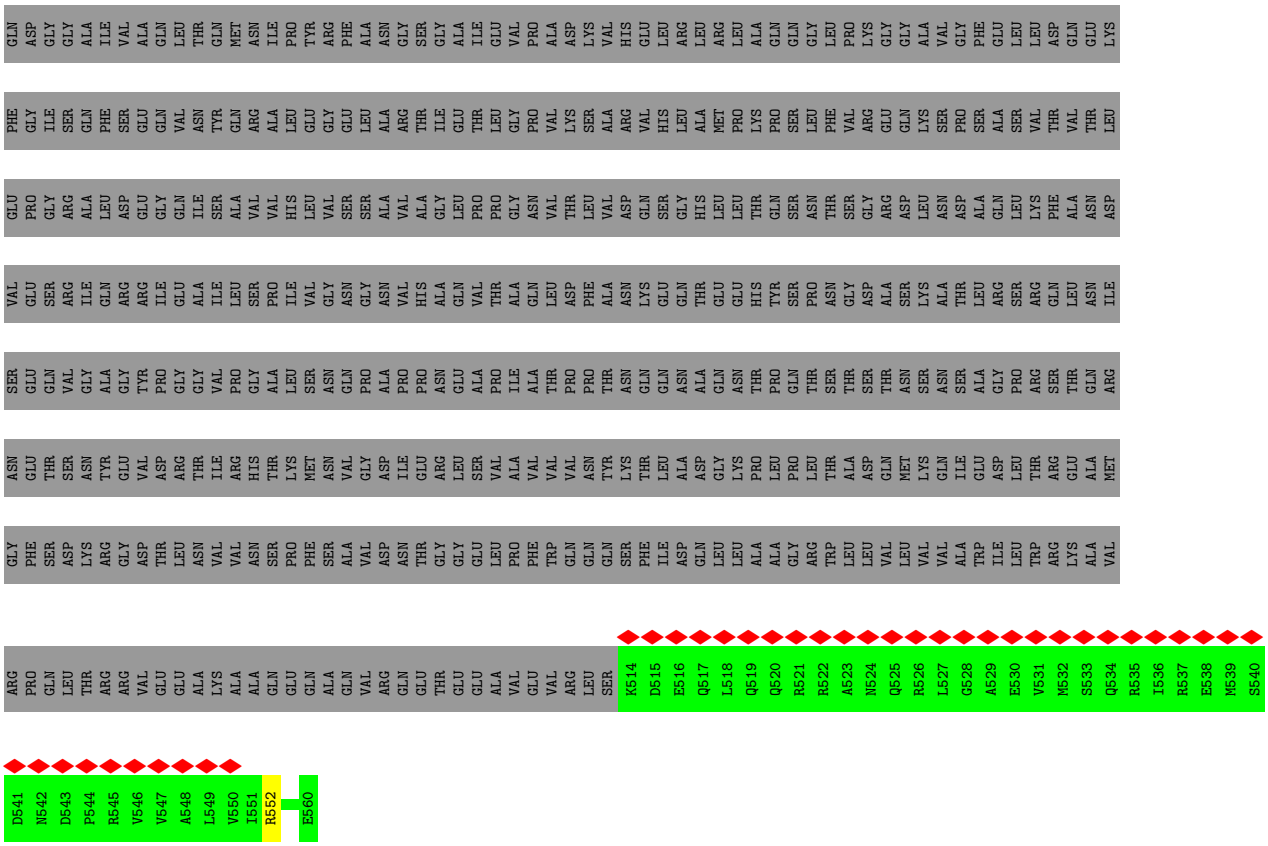




• Molecule 1: Flagellar M-ring protein

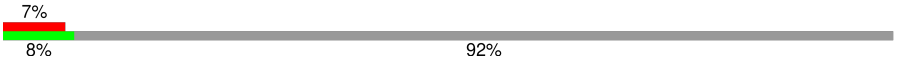
Chain DB:

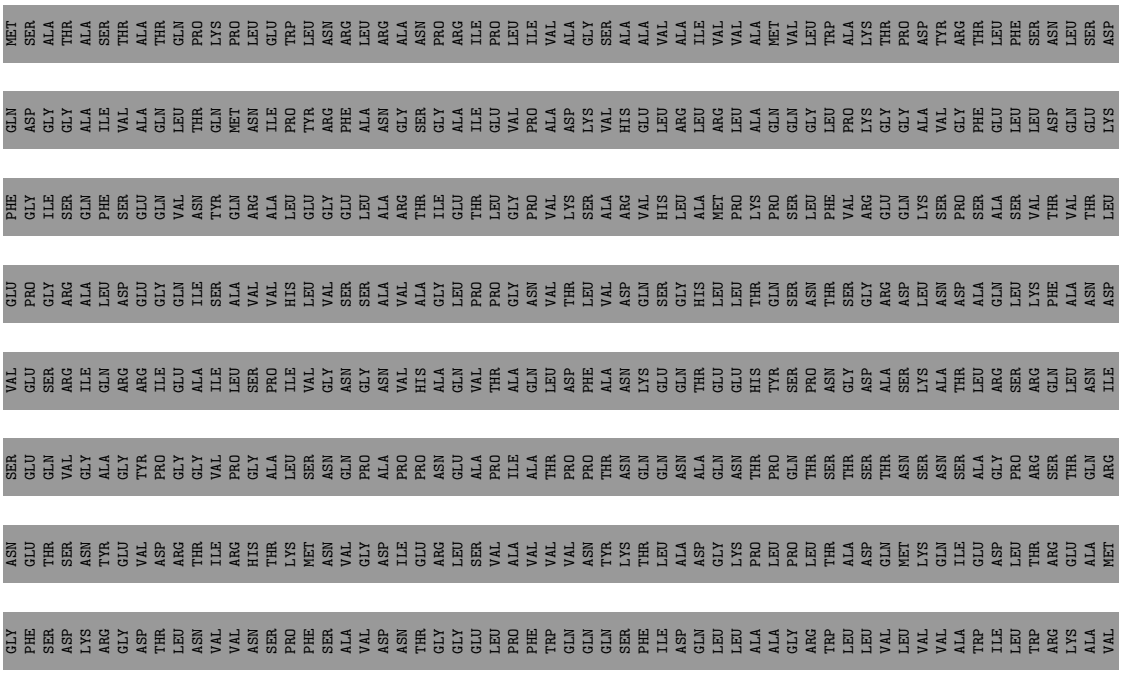


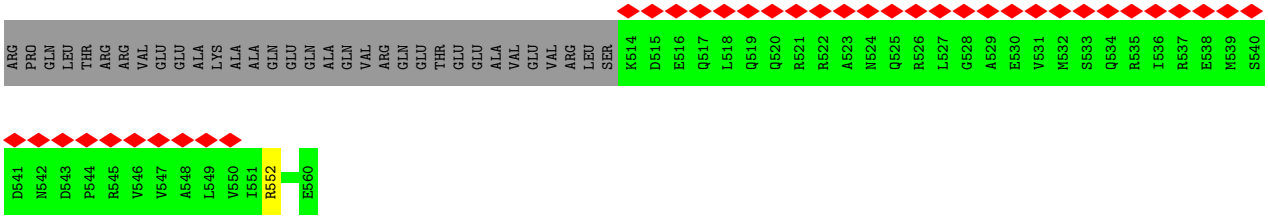


- Molecule 1: Flagellar M-ring protein

Chain JB:

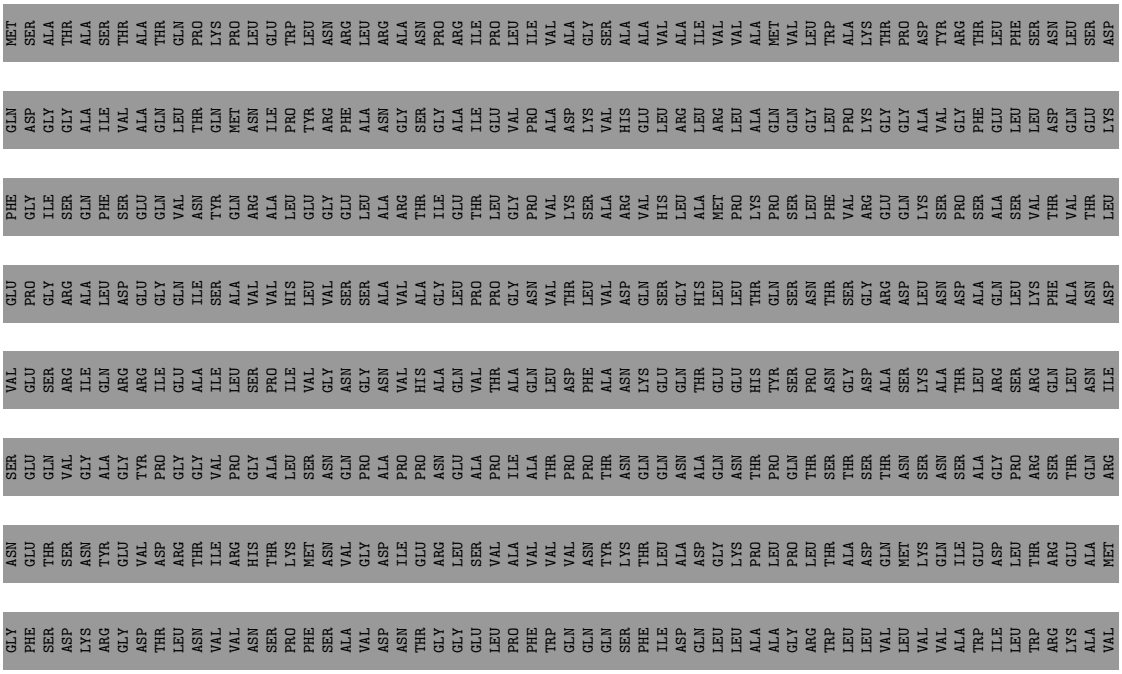






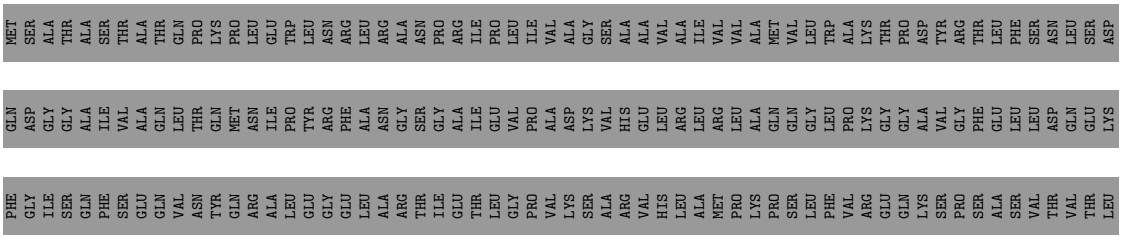
• Molecule 1: Flagellar M-ring protein

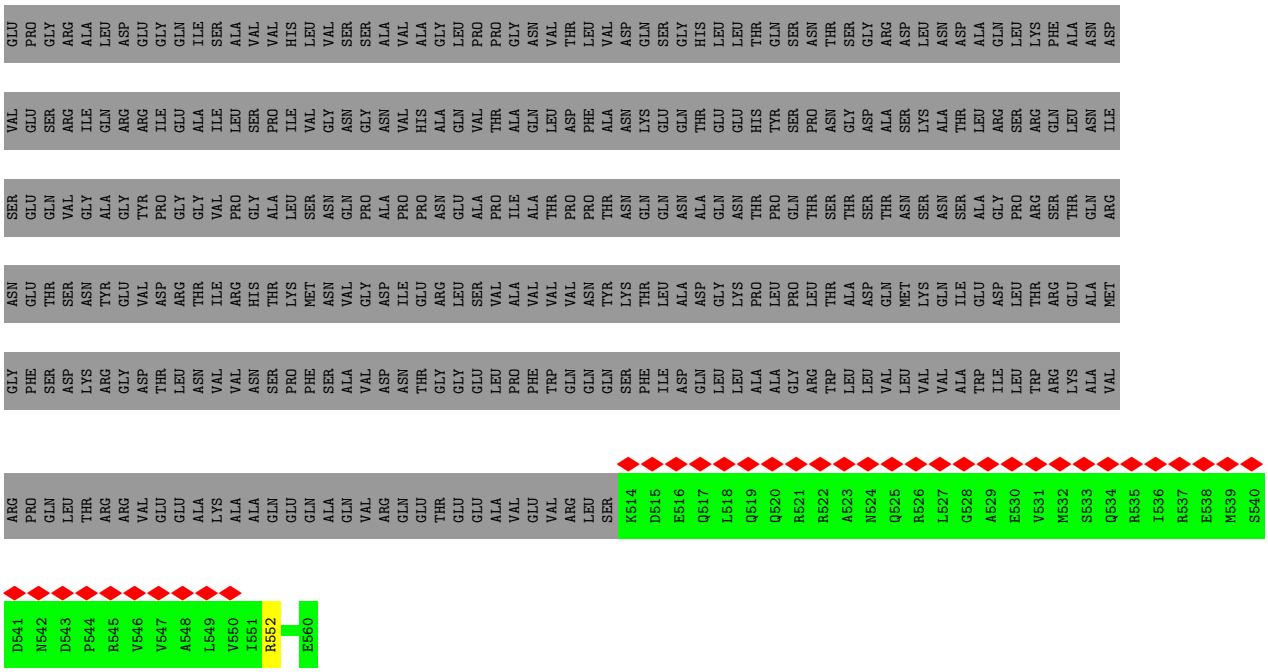
Chain PB: 7% 8% 92%



• Molecule 1: Flagellar M-ring protein

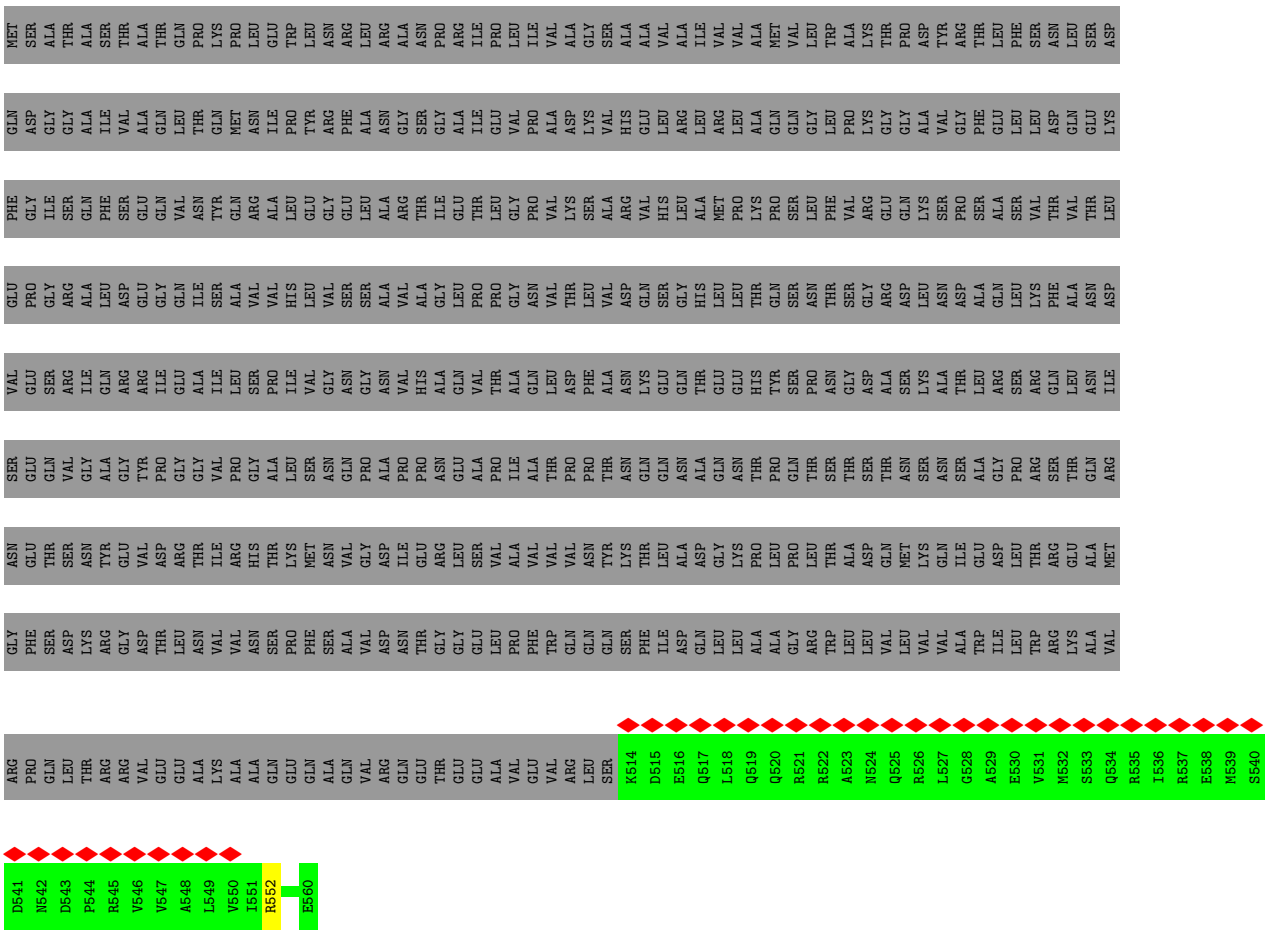
Chain VB: 7% 8% 92%





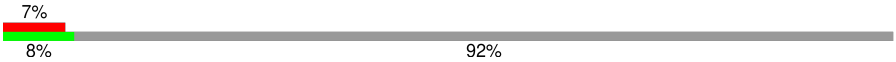
• Molecule 1: Flagellar M-ring protein

Chain BC: 7% 8% 92%



• Molecule 1: Flagellar M-ring protein

Chain HC:



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

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

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

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

SER GLU GLN VAL GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ALA GLY PRO ARG SER THR GLN ARG

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

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

ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU GLN ALA GLN VAL ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER K514 D515 E516 Q517 L518 Q519 Q520 R521 R522 A523 N524 Q525 R526 L527 G528 A529 E530 V531 M532 S533 Q534 R535 I536 R537 E538 M539 S540

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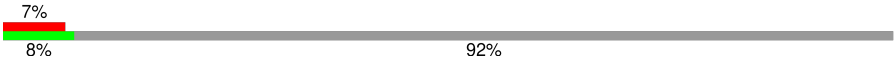
• Molecule 1: Flagellar M-ring protein

Chain NC:



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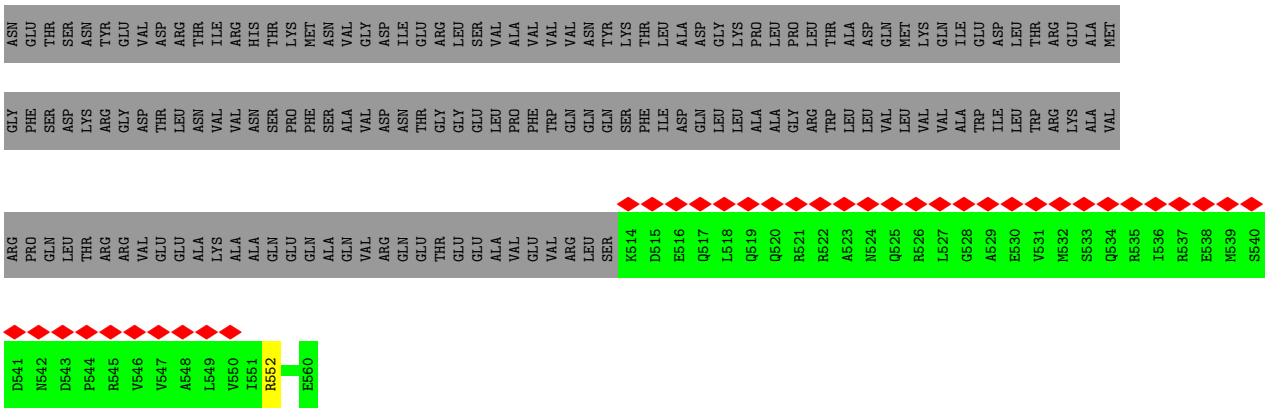
GLN ASP GLY GLY ALA ILE VAL ALA GLN LEU THR GLN MET ASN ILE PRO TYR ARG PHE ALA ASN GLY SER GLY ALA ILE GLU VAL PRO ALA ASP LYS VAL HIS GLU LEU ARG LEU ARG LEU ALA GLN GLN GLY LEU PRO LYS GLY GLY ALA VAL GLY PHE GLU LEU LEU ASP GLN GLU LYS

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

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

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

SER GLU GLN VAL GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ALA GLY PRO ARG SER THR GLN ARG



• Molecule 1: Flagellar M-ring protein

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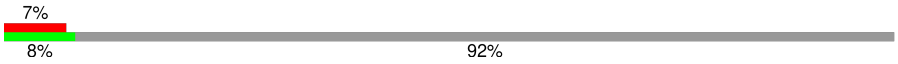
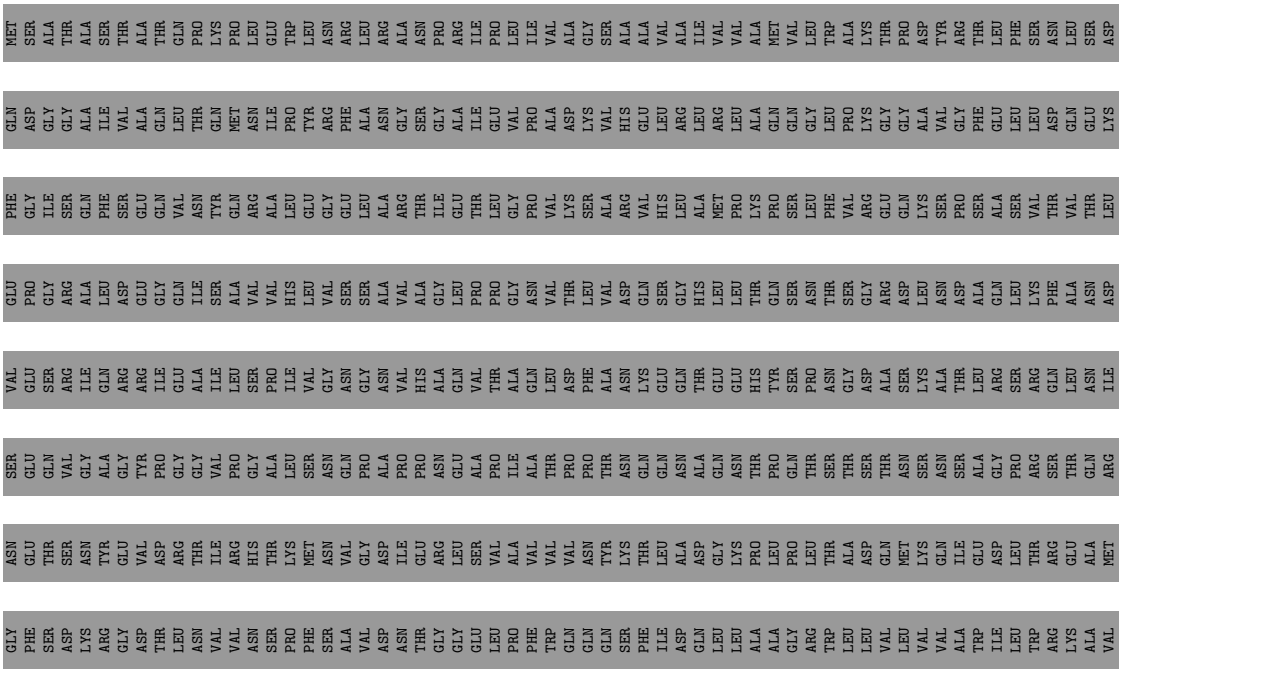
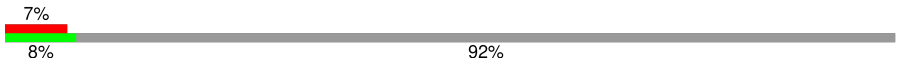
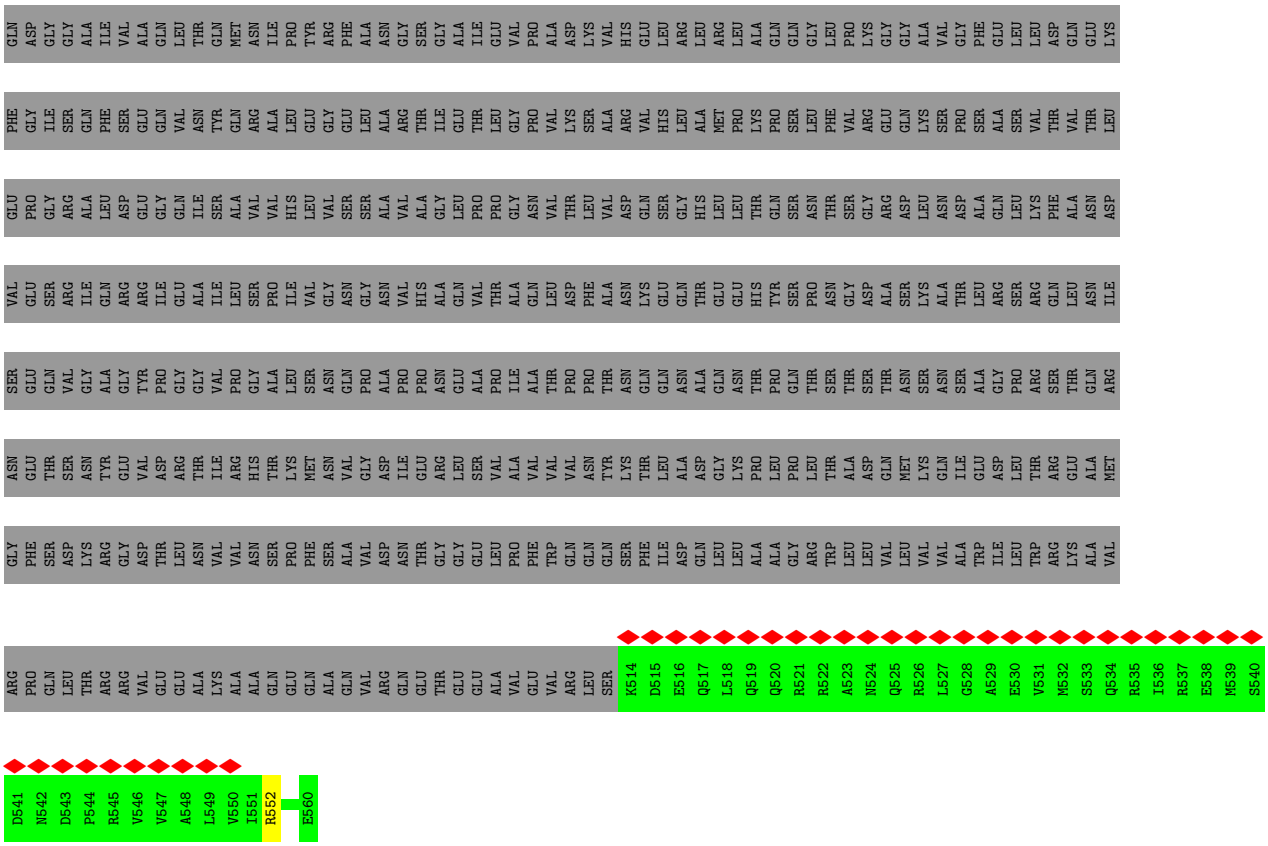




• Molecule 1: Flagellar M-ring protein

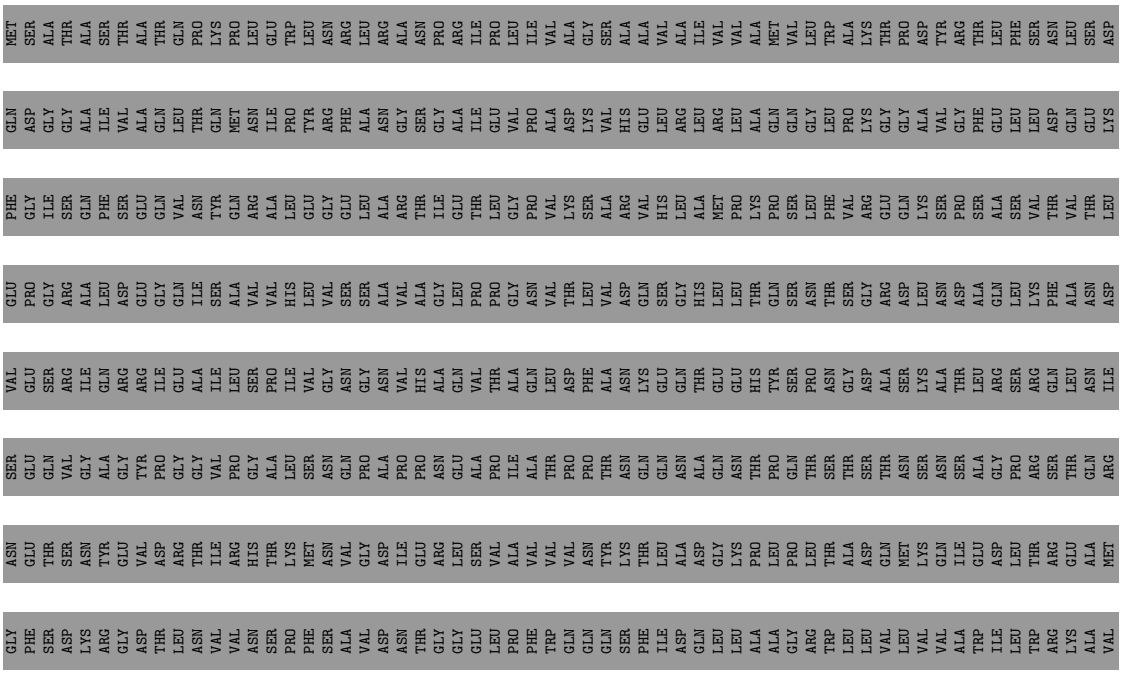
Chain ZC:

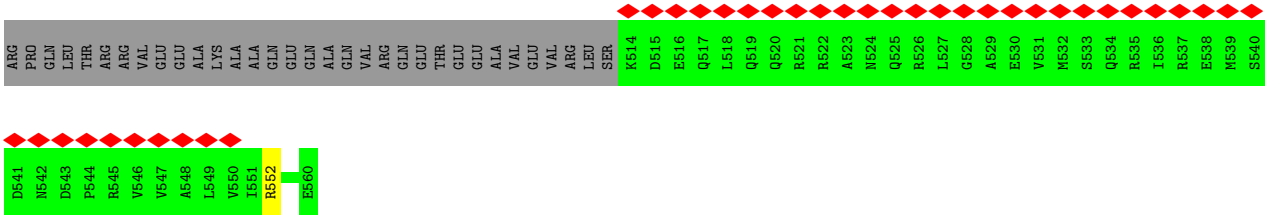




- Molecule 1: Flagellar M-ring protein

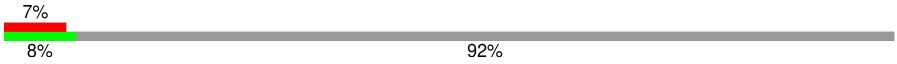
Chain FD: 7% 8% 92%

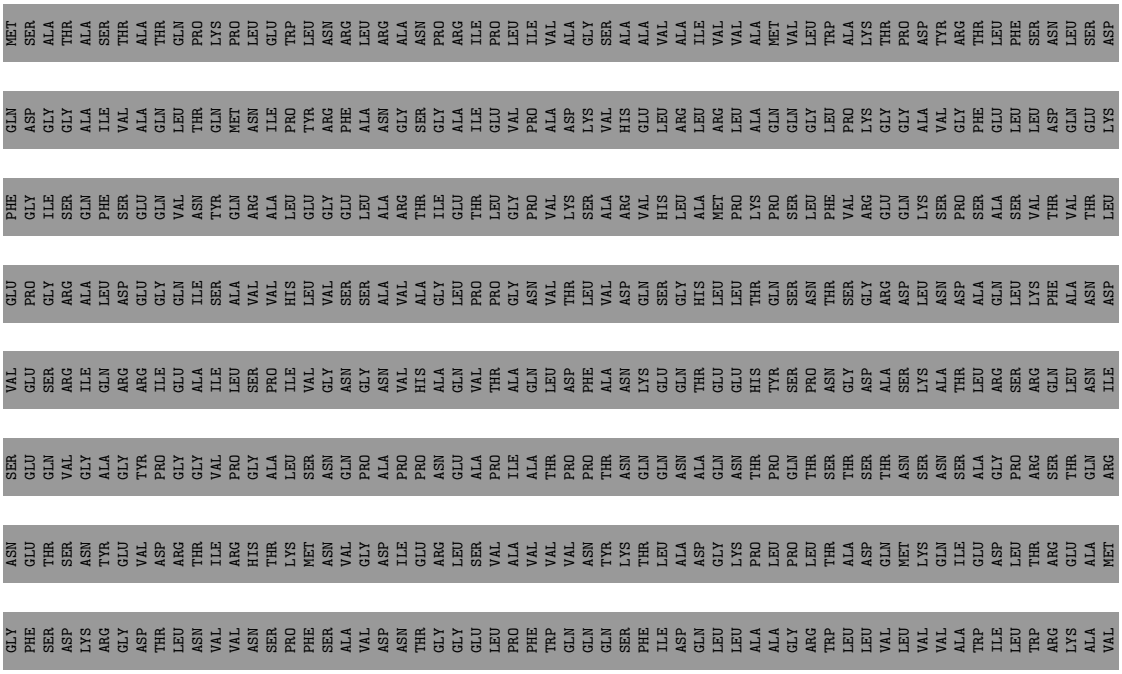


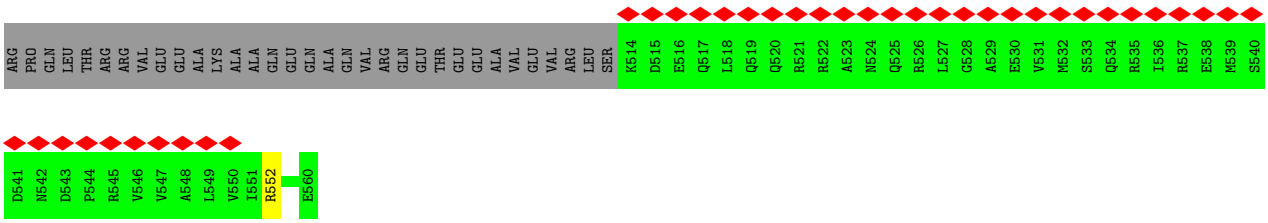


• Molecule 1: Flagellar M-ring protein

Chain LD:

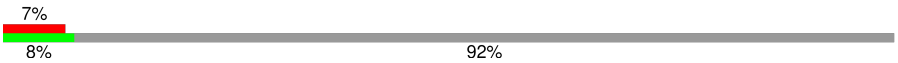


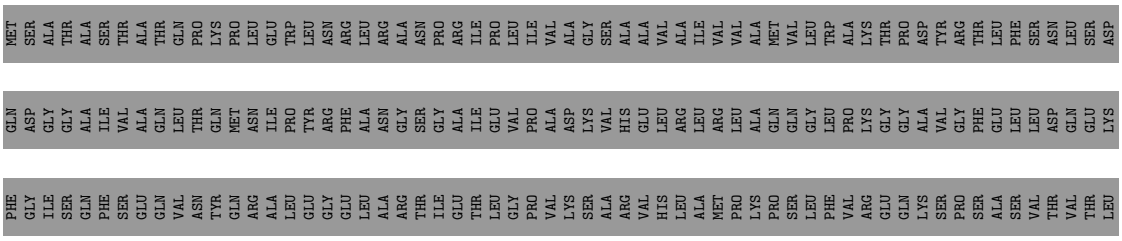


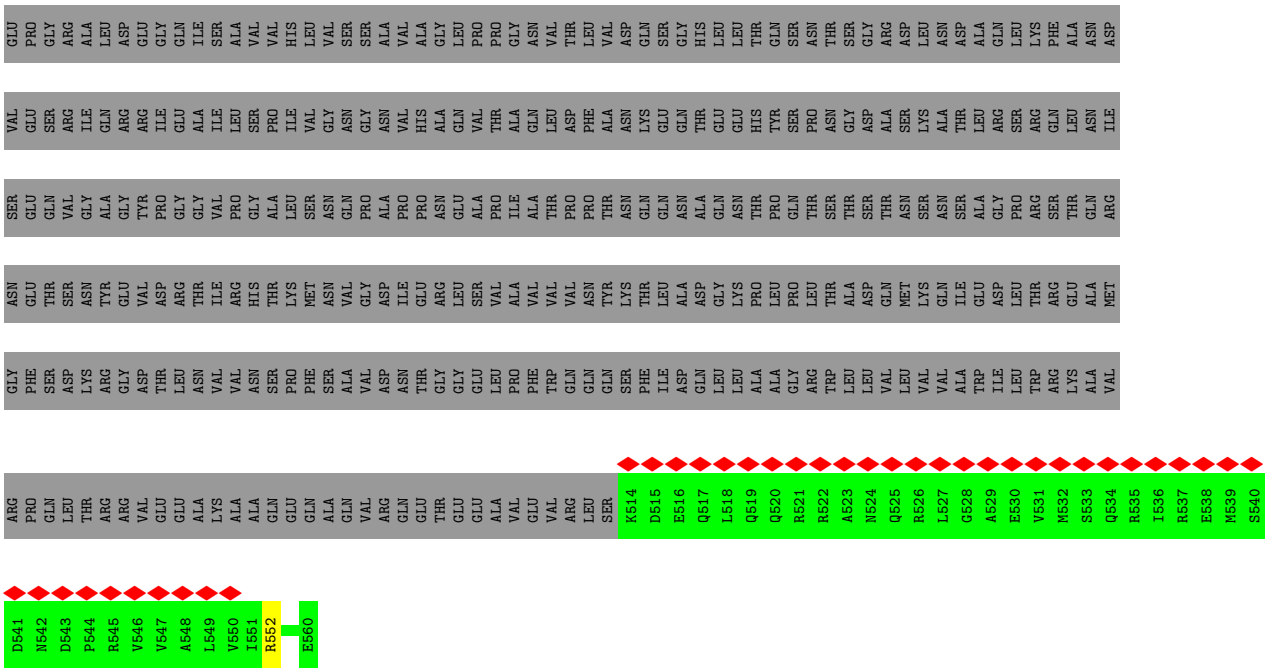


• Molecule 1: Flagellar M-ring protein

Chain RD:

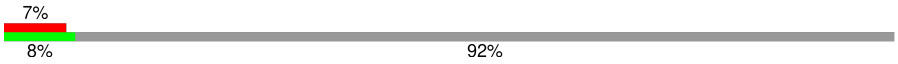


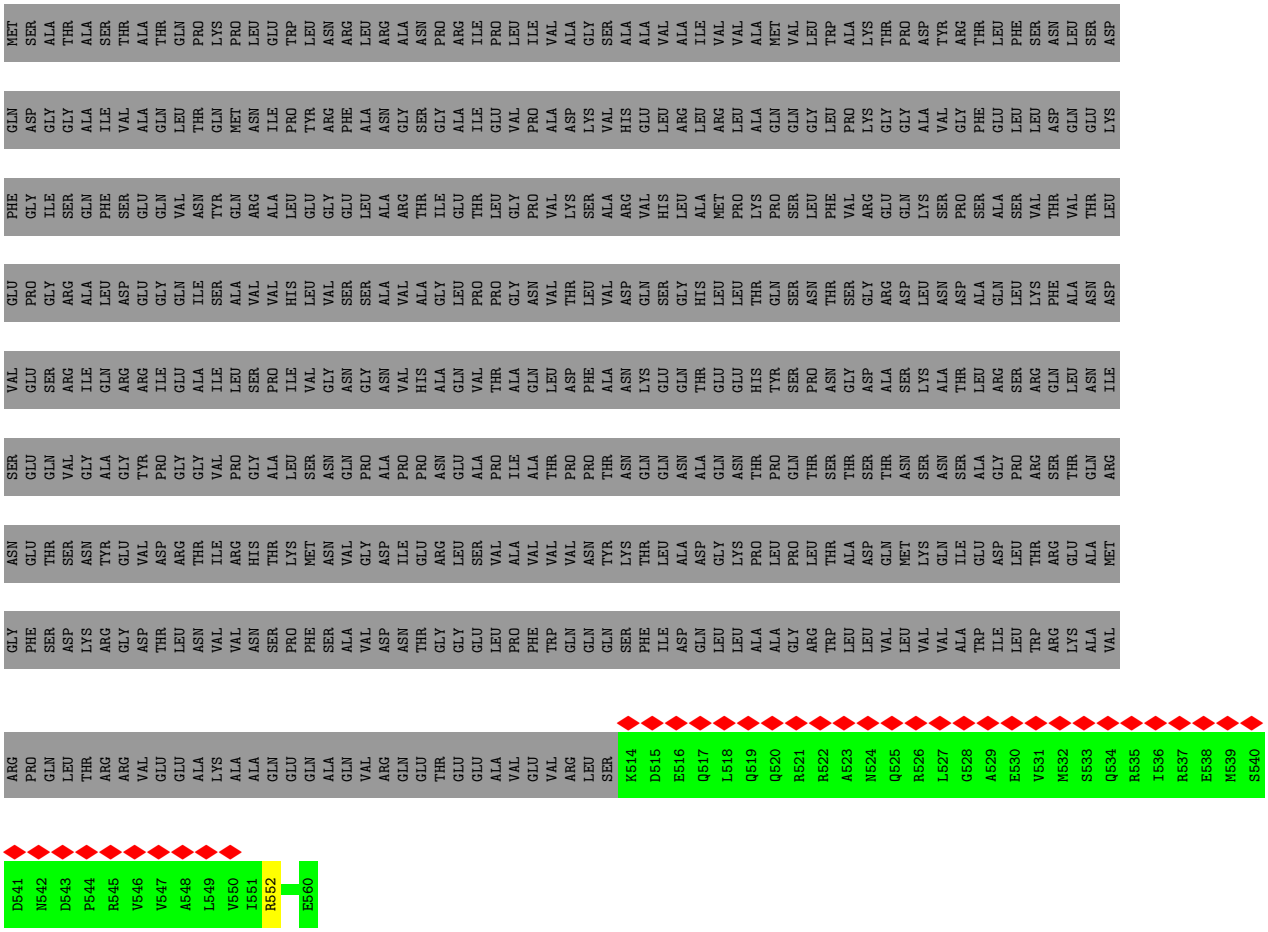




- Molecule 1: Flagellar M-ring protein

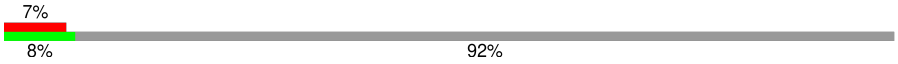
Chain XD:





• Molecule 1: Flagellar M-ring protein

Chain DE:



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

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

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

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

SER GLU GLN VAL GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ALA GLY PRO ARG SER THR GLN ARG

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

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

ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU GLN ALA GLN VAL ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER K514 D515 E516 Q517 L518 Q519 Q520 R521 R522 A523 N524 Q525 R526 L527 G528 A529 E530 V531 M532 S533 Q534 R535 I536 R537 E538 M539 S540

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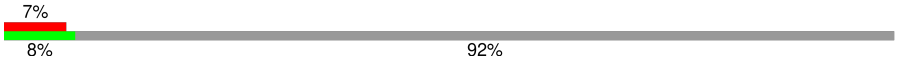
• Molecule 1: Flagellar M-ring protein

Chain JE:



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

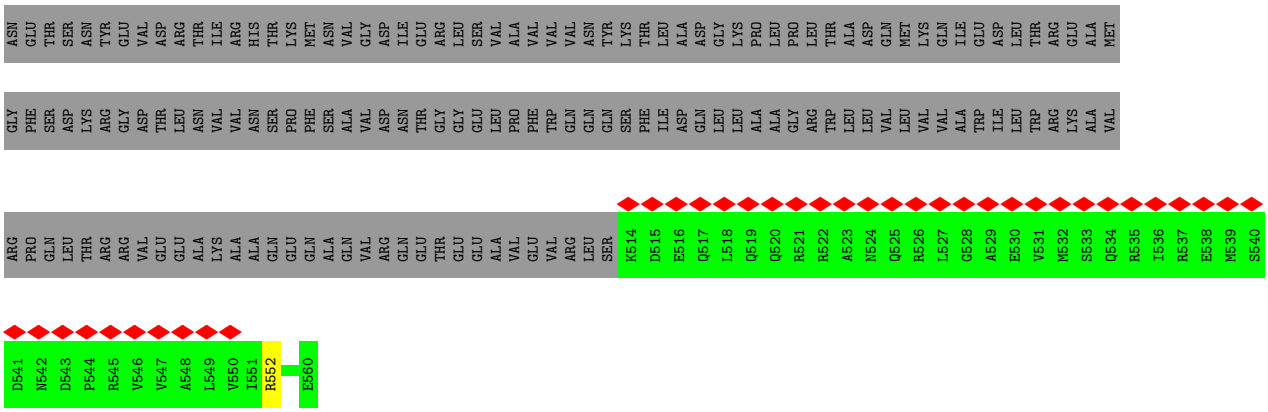
GLN ASP GLY GLY ALA ILE VAL ALA GLN LEU THR GLN MET ASN ILE PRO TYR ARG PHE ALA ASN GLY SER GLY ALA ILE GLU VAL PRO ALA ASP LYS VAL HIS GLU LEU ARG LEU ARG LEU ALA GLN GLN GLY LEU PRO LYS GLY GLY ALA VAL GLY PHE GLU LEU LEU ASP GLN GLU LYS

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

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

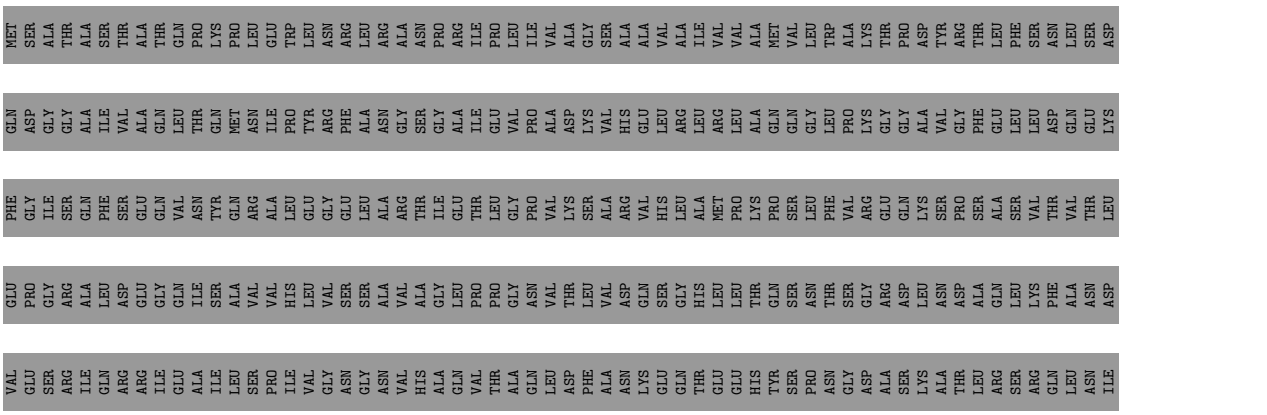
VAL GLU SER ARG ILE GLN ARG ARG ILE GLU ALA ILE LEU SER PRO ILE VAL GLY ASN GLY ASN VAL HIS ALA GLN VAL THR ALA GLN LEU ASP PHE ALA ASN LYS GLU GLN THR GLU GLU HIS TYR SER PRO ASN GLY ASP ALA SER LYS ALA THR LEU ARG SER ARG GLN LEU ASN ILE

SER GLU GLN VAL GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ALA GLY PRO ARG SER THR GLN ARG



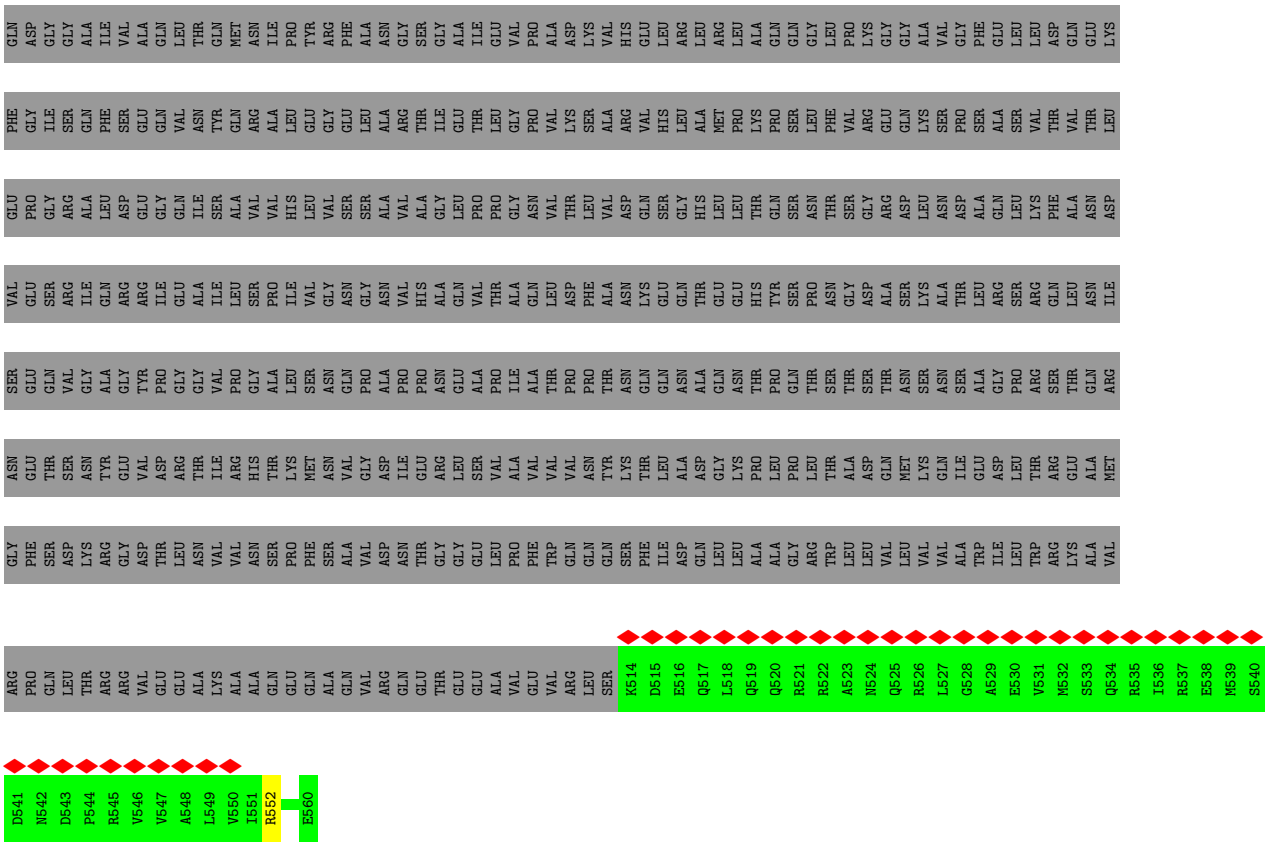
- Molecule 1: Flagellar M-ring protein

Chain PE: 7% 8% 92%



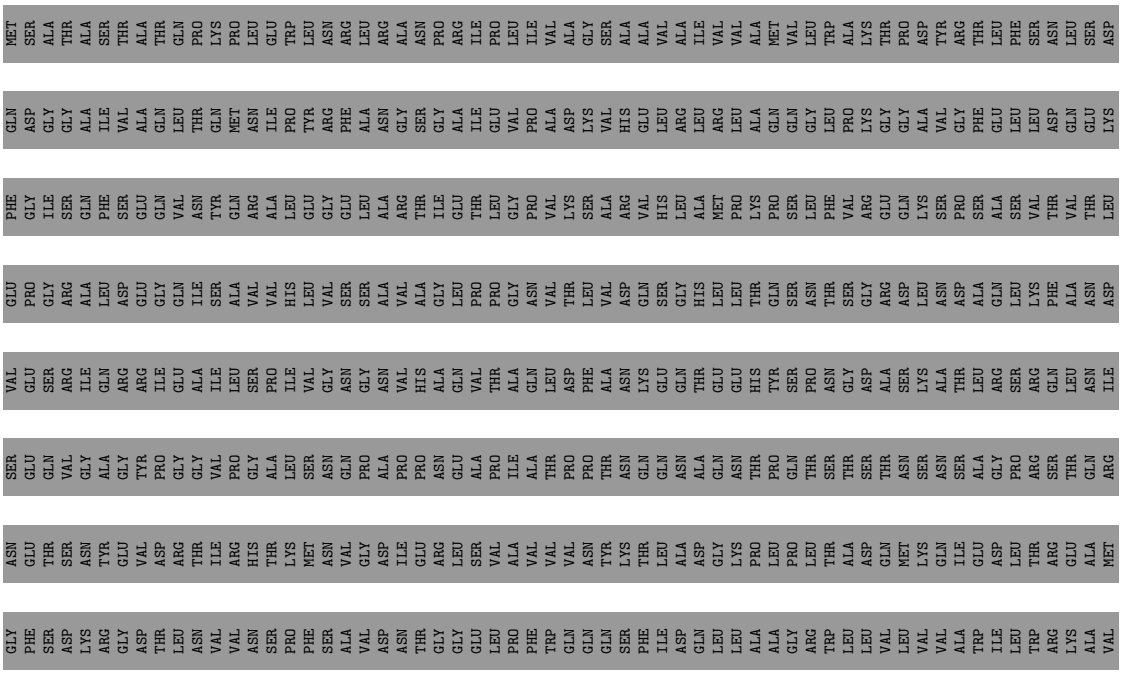
- Molecule 1: Flagellar M-ring protein

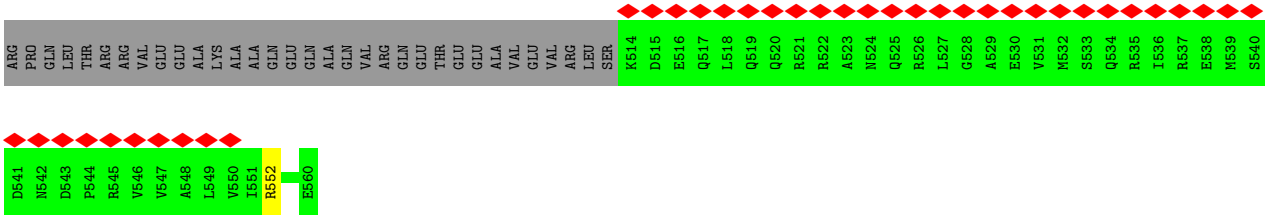
Chain VE: 7% 8% 92%



- Molecule 1: Flagellar M-ring protein

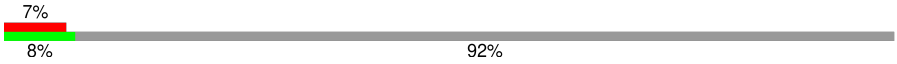
Chain BF: 7% 8% 92%

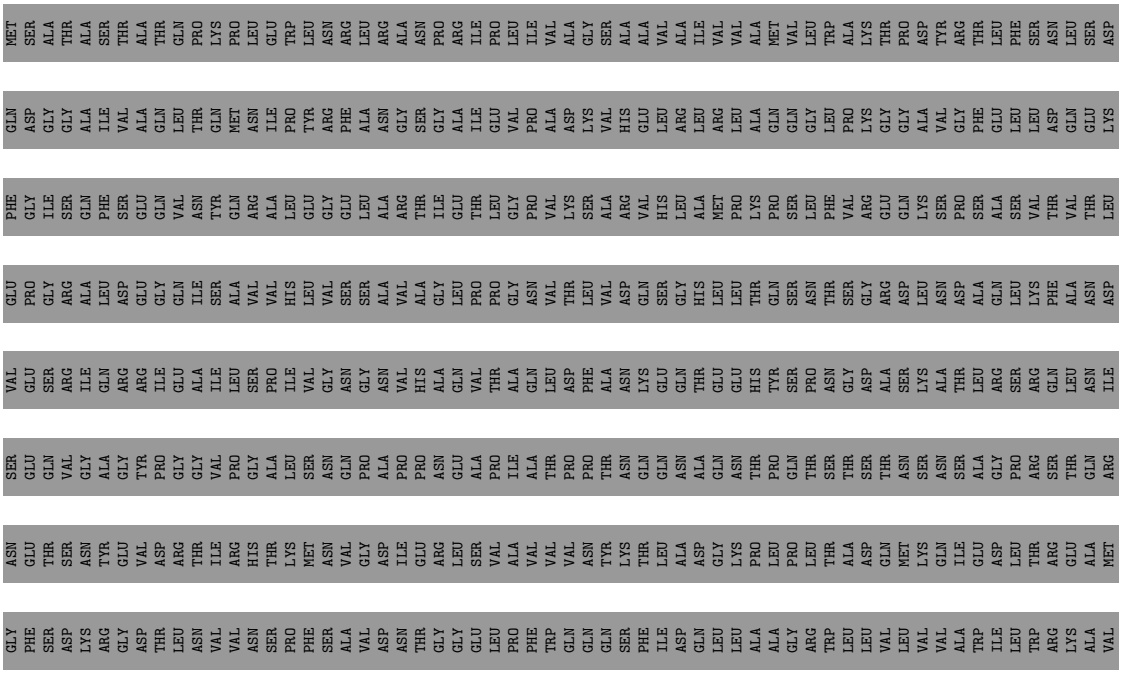


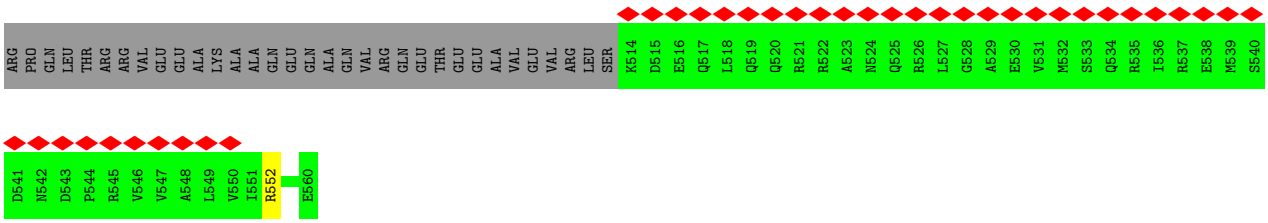


• Molecule 1: Flagellar M-ring protein

Chain HF:

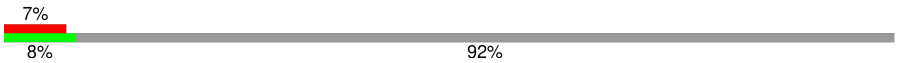


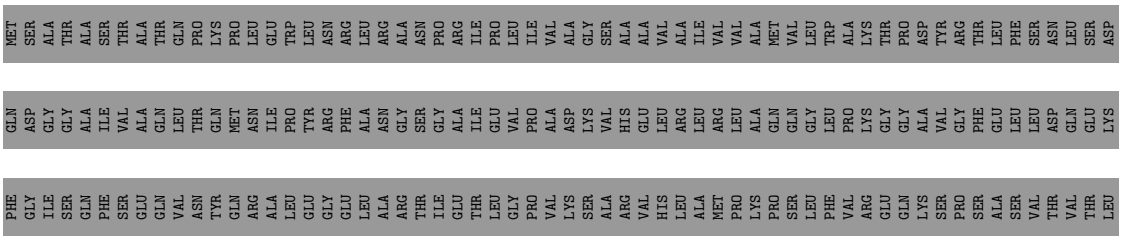


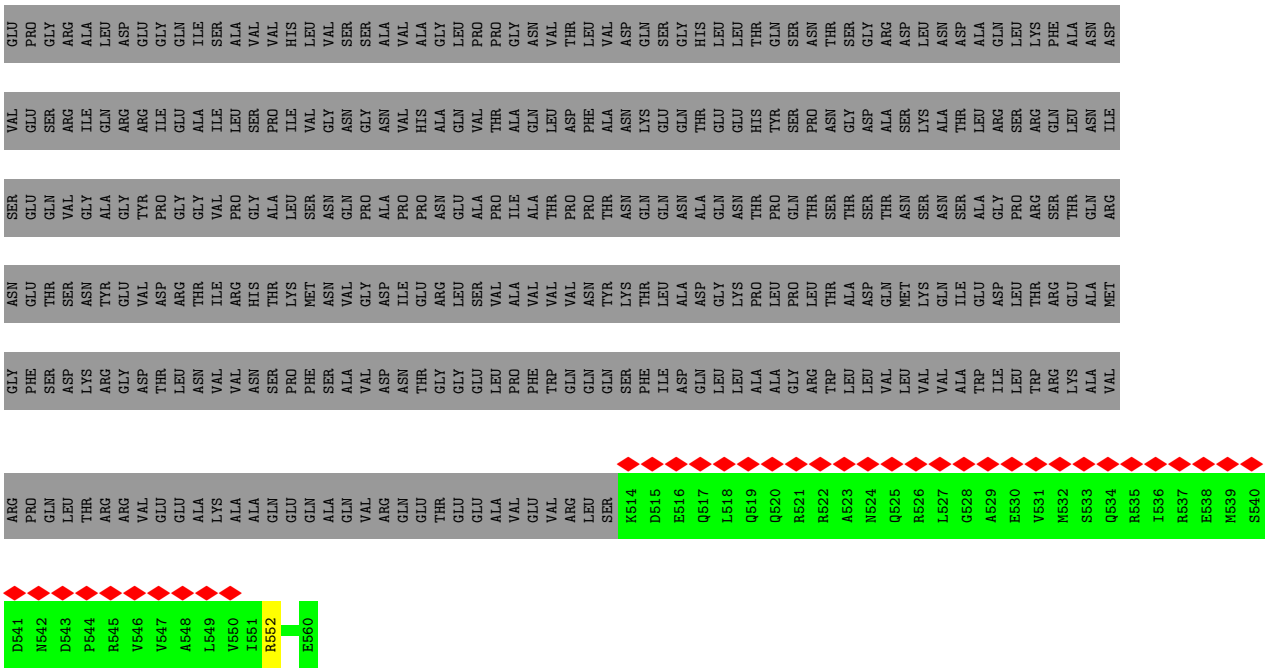


• Molecule 1: Flagellar M-ring protein

Chain NF:

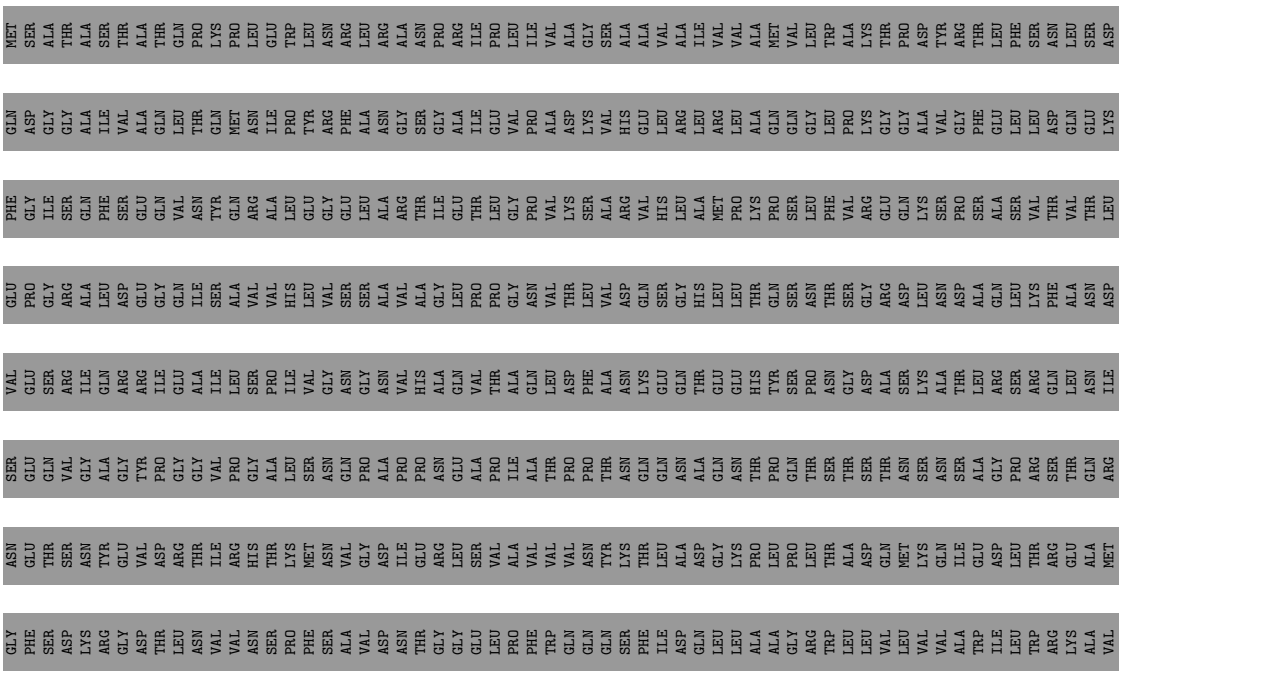






• Molecule 1: Flagellar M-ring protein

Chain TF: 7% 8% 92%



• Molecule 1: Flagellar M-ring protein

Chain ZF: 7% 8% 92%

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

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

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

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

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

SER GLU GLN VAL GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ALA GLY PRO ARG SER THR GLN ARG

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

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

ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU GLN ALA GLN VAL ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER K514 D515 E516 Q517 L518 Q519 Q520 R521 R522 A523 N524 Q525 R526 L527 G528 A529 E530 V531 M532 S533 Q534 R535 I536 R537 E538 M539 S540

D541 N542 D543 P544 R545 V546 V547 A548 L549 V550 I551 R552 E560

• Molecule 1: Flagellar M-ring protein

Chain FG: 7% 8% 92%

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

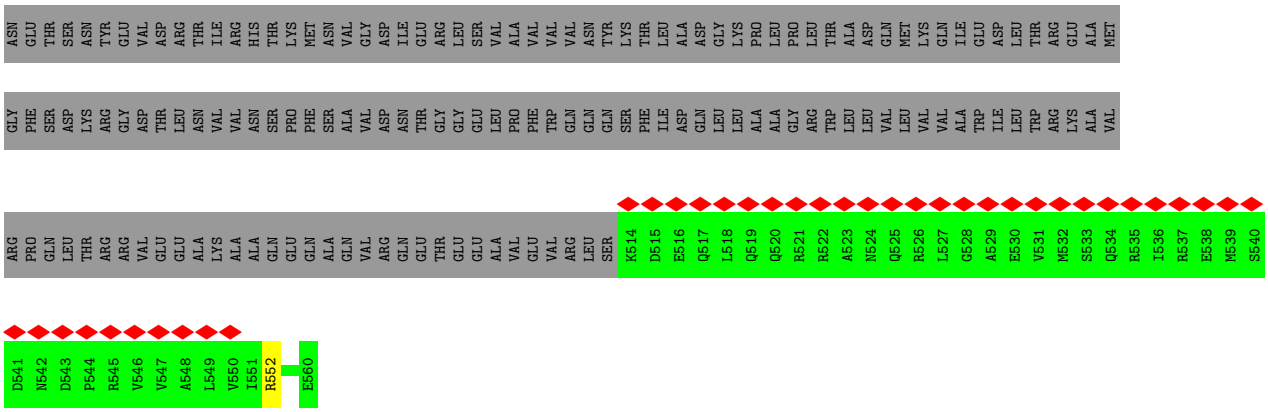
GLN ASP GLY GLY ALA ILE VAL ALA GLN LEU THR GLN MET ASN ILE PRO TYR ARG PHE ALA ASN GLY SER GLY ALA ILE GLU VAL PRO ALA ASP LYS VAL HIS GLU LEU ARG LEU ARG LEU ALA GLN GLN GLY LEU PRO LYS GLY GLY ALA VAL GLY PHE GLU LEU LEU ASP GLN GLU LYS

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

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

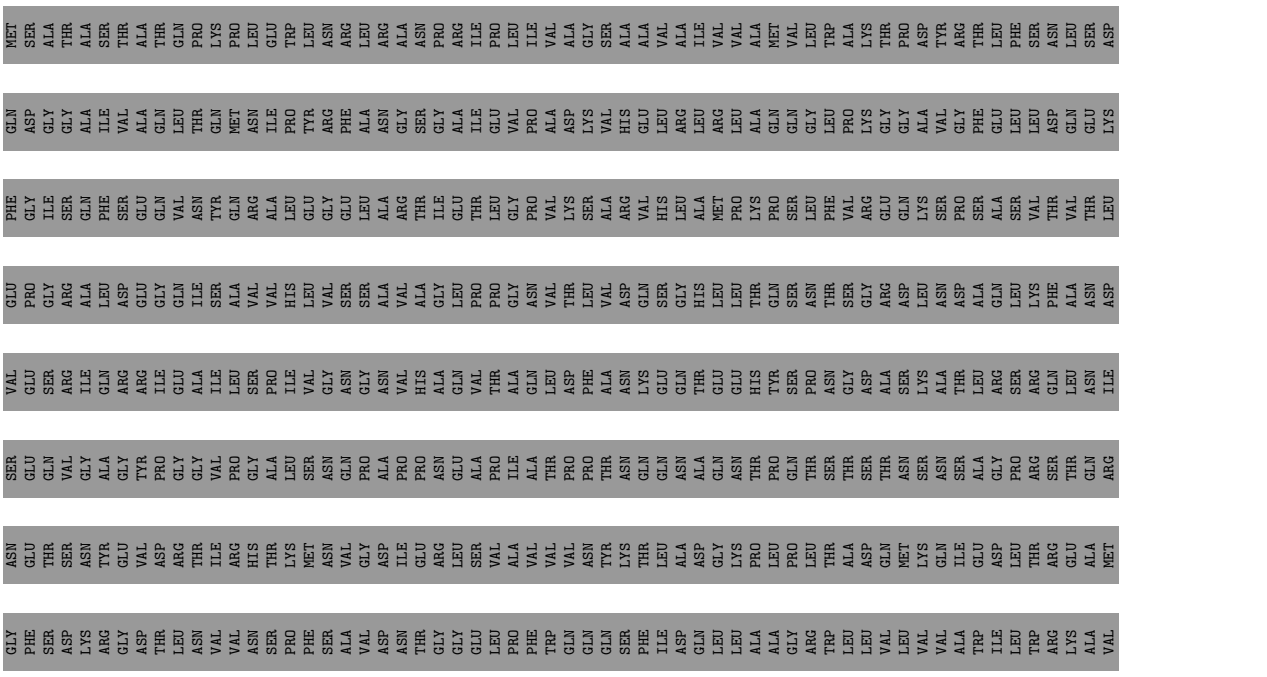
VAL GLU SER ARG ILE GLN ARG ARG ILE GLU ALA ILE LEU SER PRO ILE VAL GLY ASN GLY ASN VAL HIS ALA GLN VAL THR ALA GLN LEU ASP PHE ALA ASN LYS GLU GLN THR GLU GLU HIS TYR SER PRO ASN GLY ASP ALA SER LYS ALA THR LEU ARG SER ARG GLN LEU ASN ILE

SER GLU GLN VAL GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ALA GLY PRO ARG SER THR GLN ARG



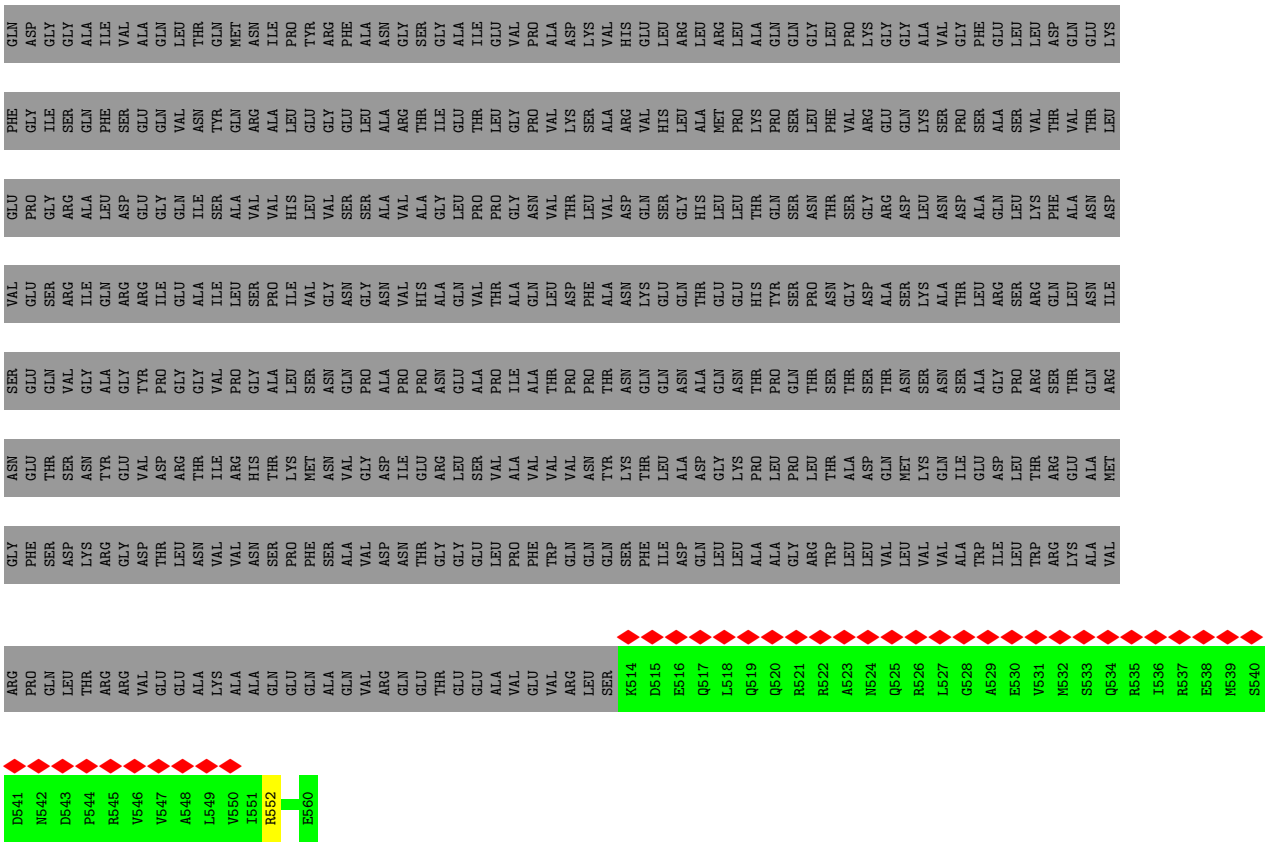
- Molecule 1: Flagellar M-ring protein

Chain LG: 7% 8% 92%



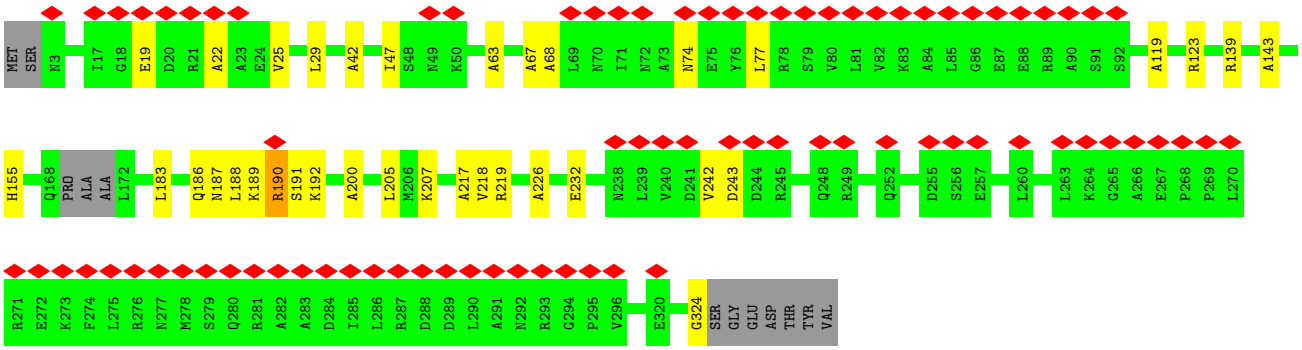
- Molecule 1: Flagellar M-ring protein

Chain RG: 7% 8% 92%



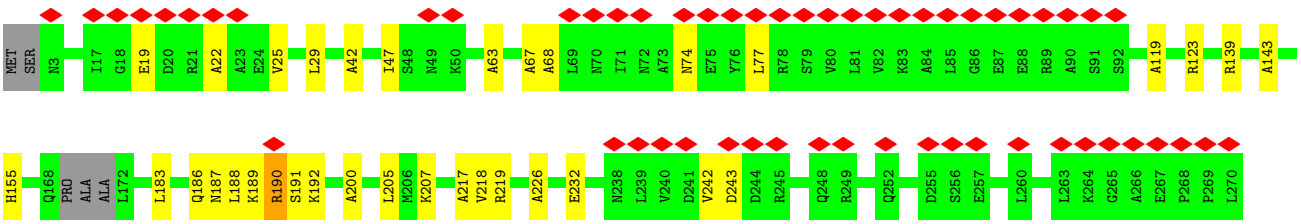
• Molecule 2: Flagellar motor switch protein FliG

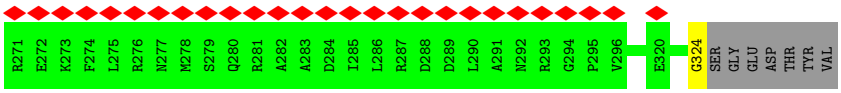
Chain G:



• Molecule 2: Flagellar motor switch protein FliG

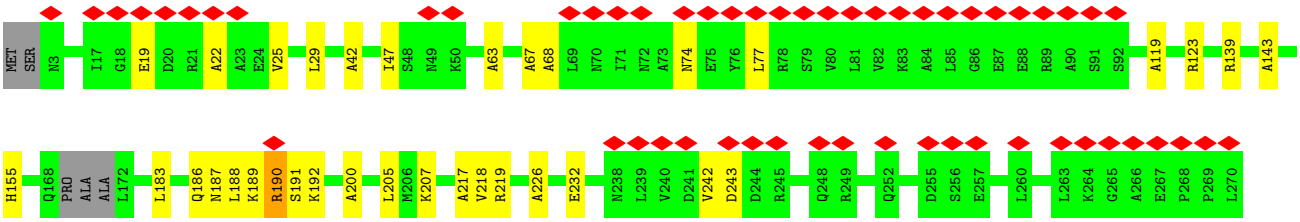
Chain B:

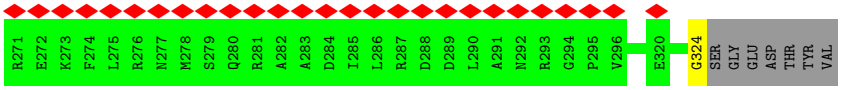




• Molecule 2: Flagellar motor switch protein FliG

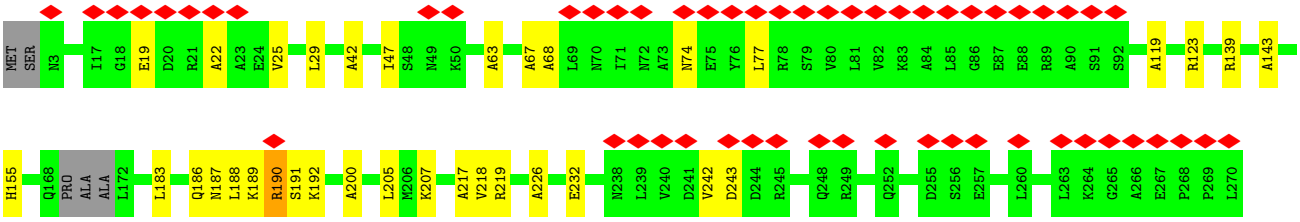
Chain J:

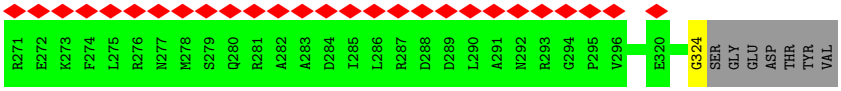




• Molecule 2: Flagellar motor switch protein FliG

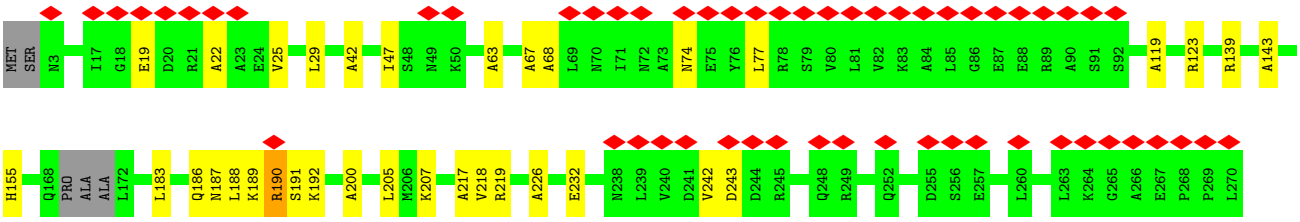
Chain T:

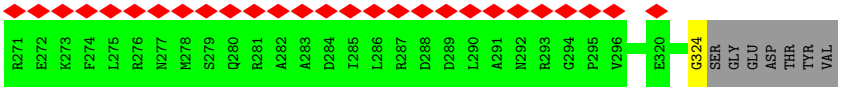




• Molecule 2: Flagellar motor switch protein FliG

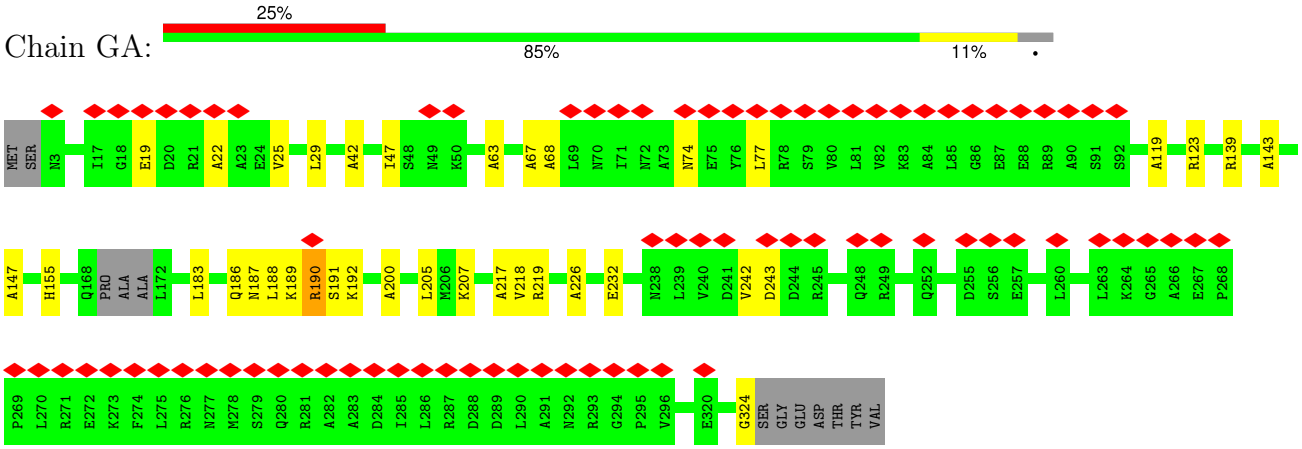
Chain AA:





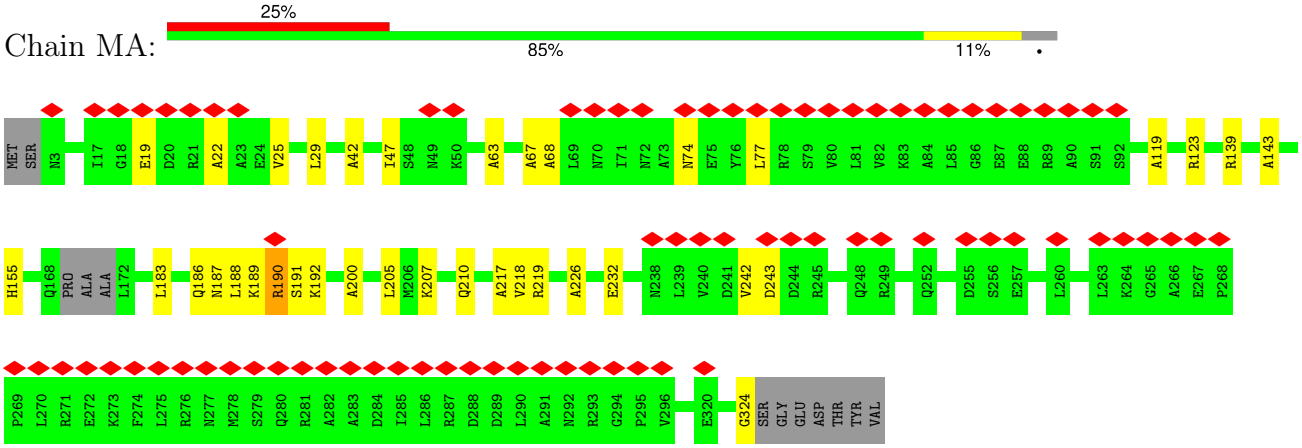
• Molecule 2: Flagellar motor switch protein FliG

Chain GA:



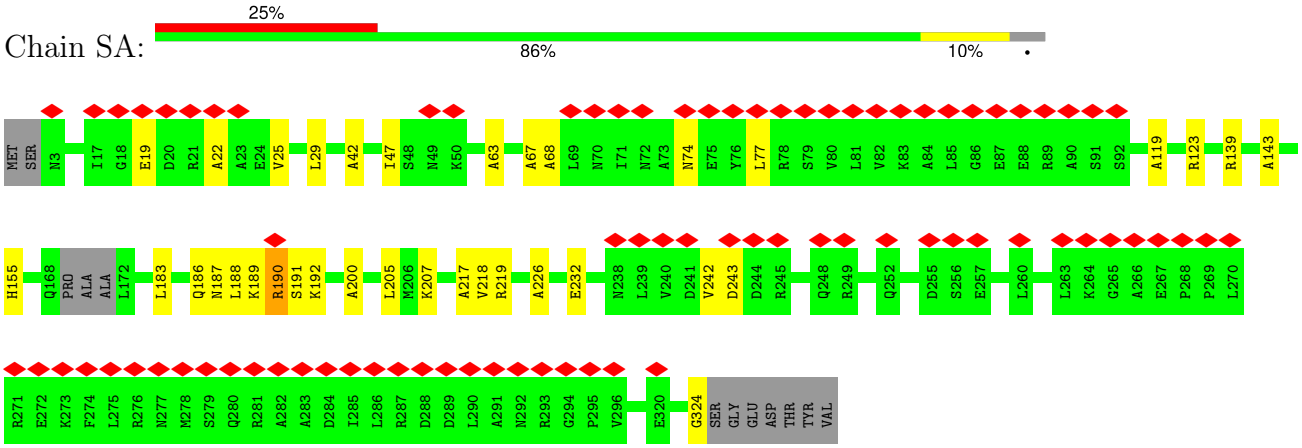
• Molecule 2: Flagellar motor switch protein FliG

Chain MA:



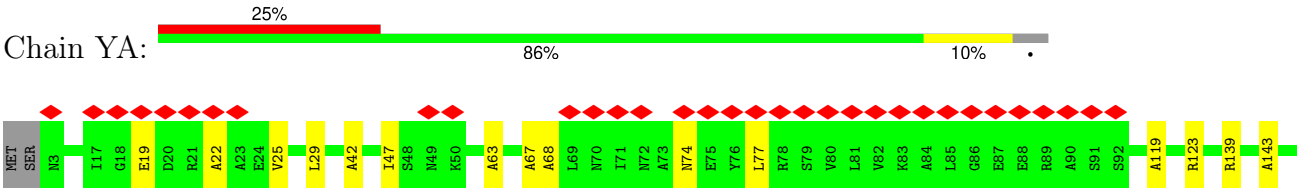
• Molecule 2: Flagellar motor switch protein FliG

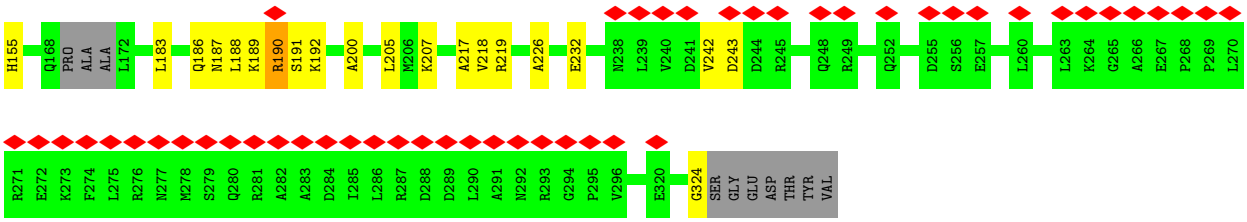
Chain SA:



• Molecule 2: Flagellar motor switch protein FliG

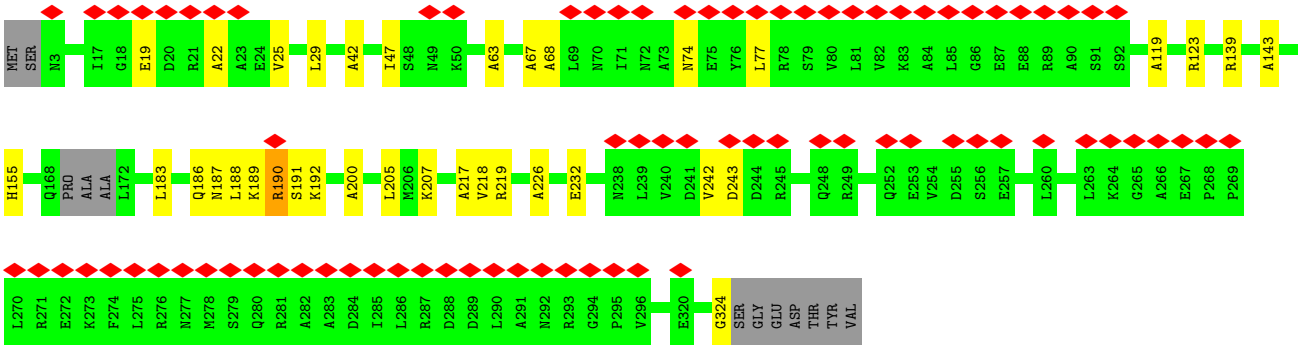
Chain YA:





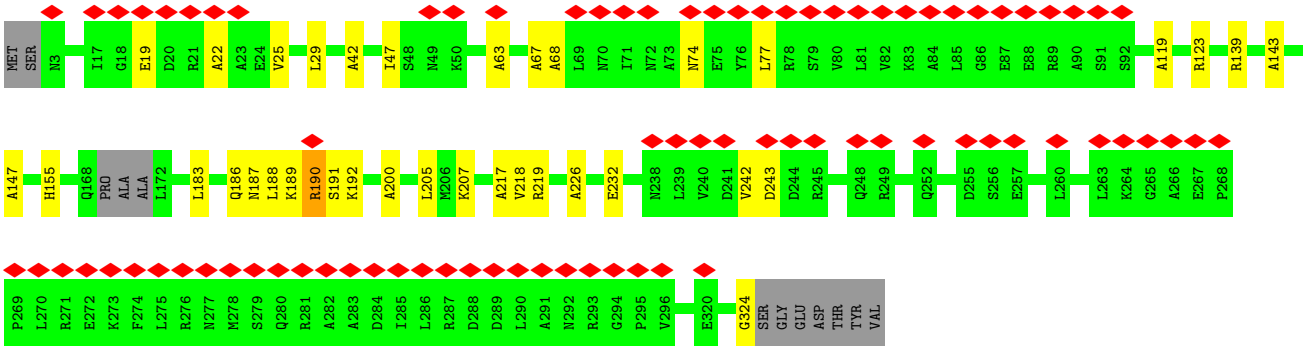
• Molecule 2: Flagellar motor switch protein FliG

Chain EB:



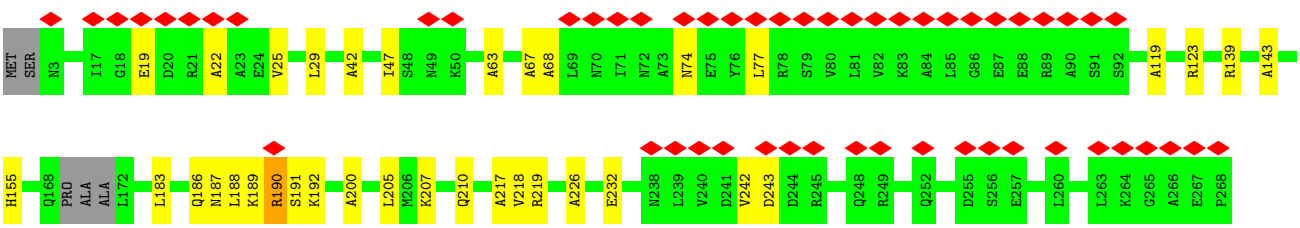
• Molecule 2: Flagellar motor switch protein FliG

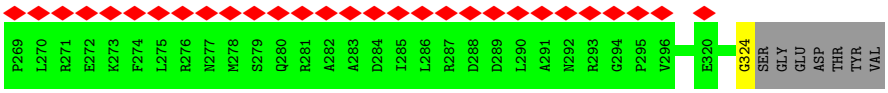
Chain KB:



• Molecule 2: Flagellar motor switch protein FliG

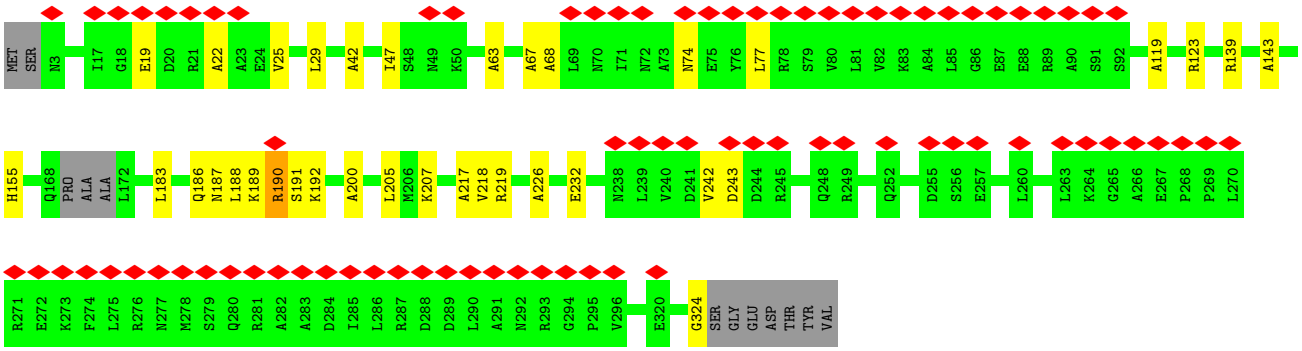
Chain QB:





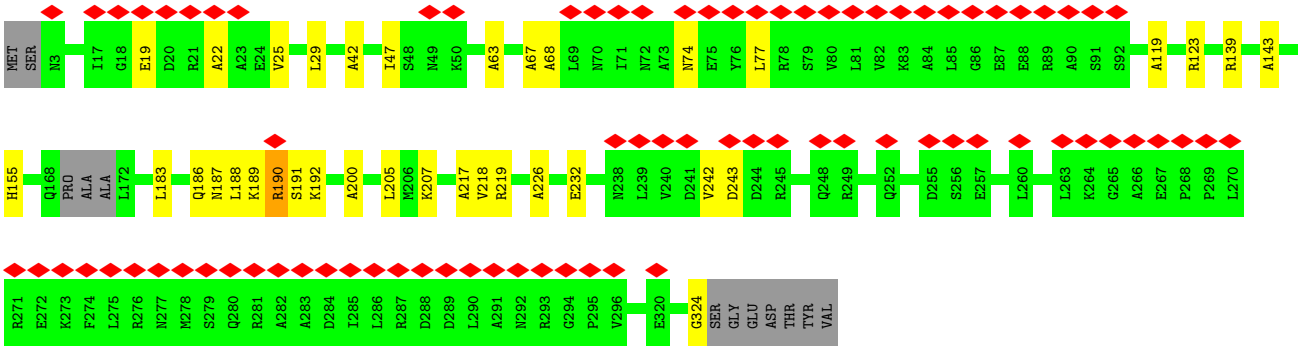
• Molecule 2: Flagellar motor switch protein FliG

Chain WB:



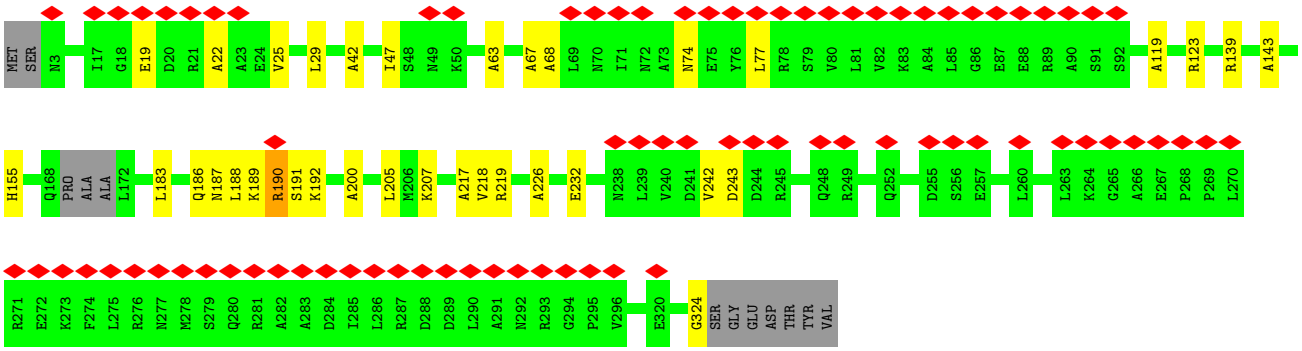
• Molecule 2: Flagellar motor switch protein FliG

Chain CC:



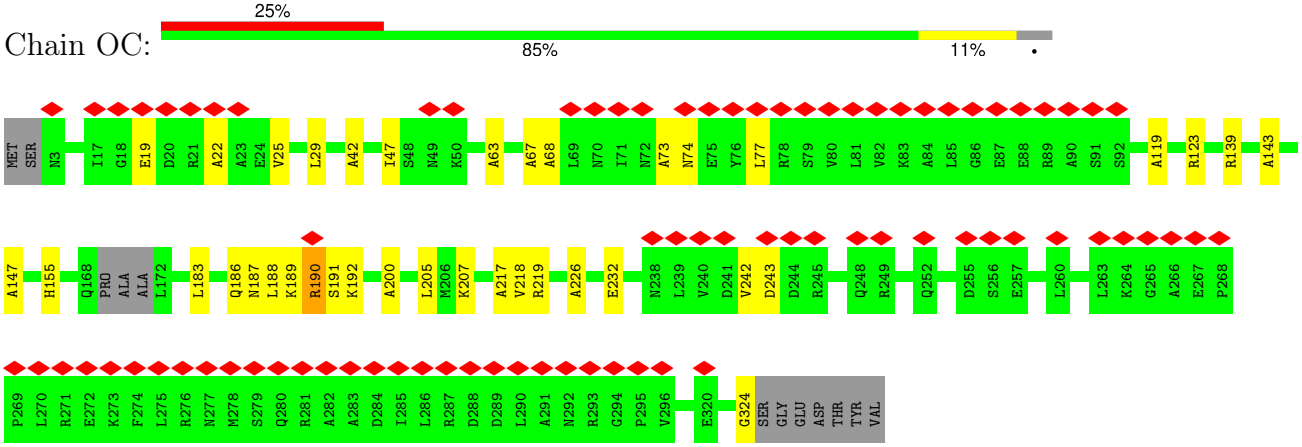
• Molecule 2: Flagellar motor switch protein FliG

Chain IC:



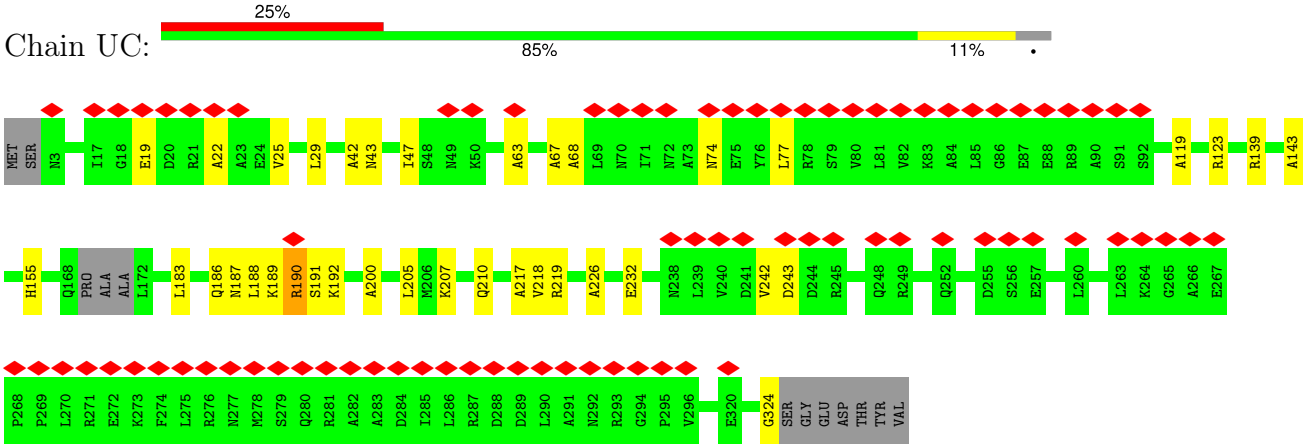
• Molecule 2: Flagellar motor switch protein FliG

Chain OC:



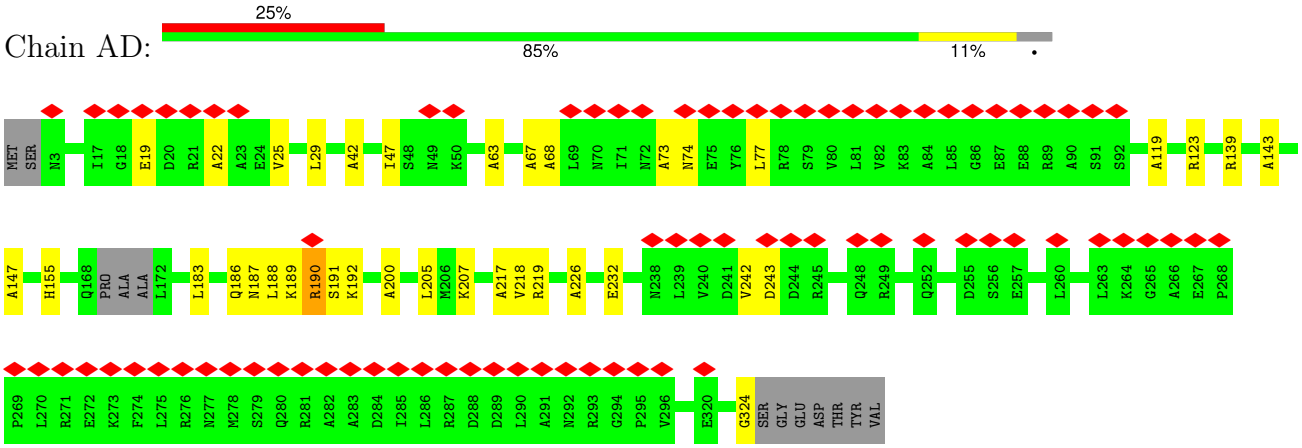
• Molecule 2: Flagellar motor switch protein FliG

Chain UC:



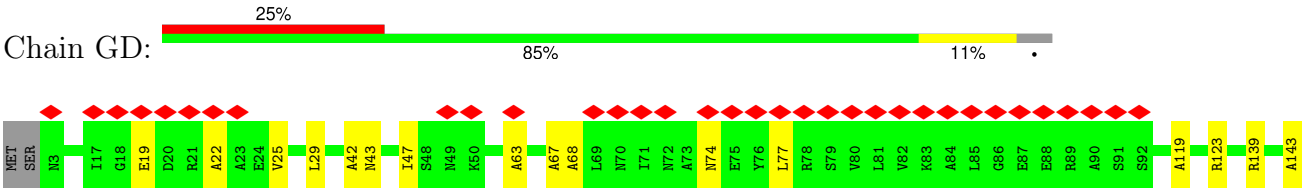
• Molecule 2: Flagellar motor switch protein FliG

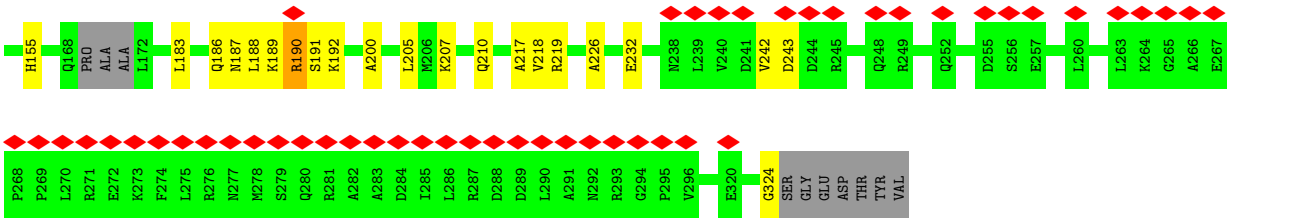
Chain AD:



• Molecule 2: Flagellar motor switch protein FliG

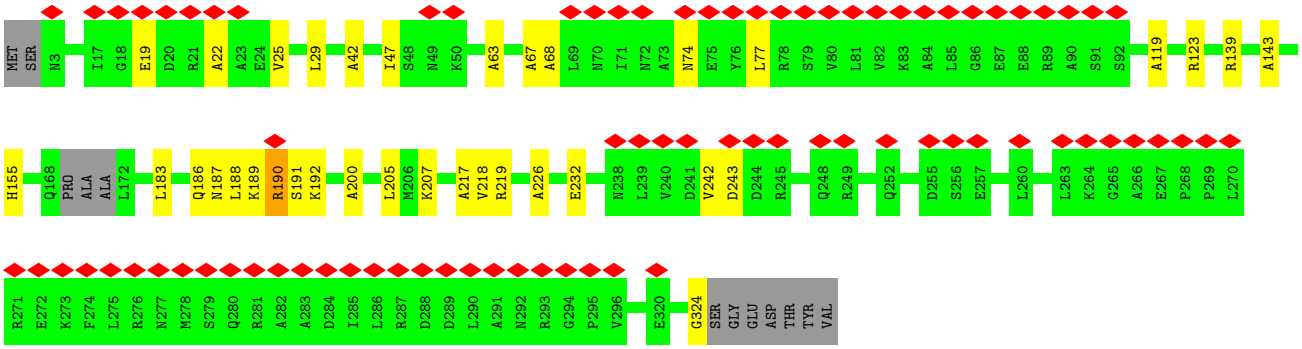
Chain GD:





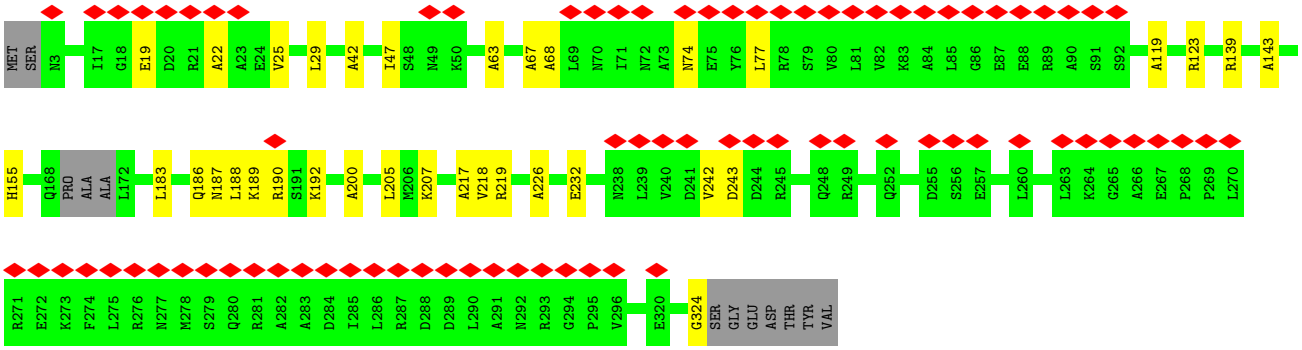
- Molecule 2: Flagellar motor switch protein FliG

Chain MD:



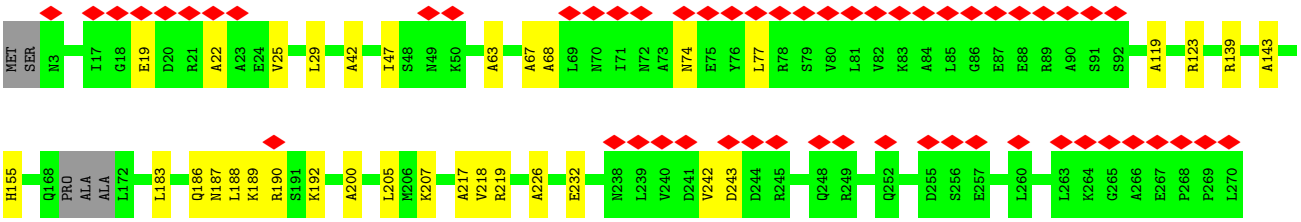
- Molecule 2: Flagellar motor switch protein FliG

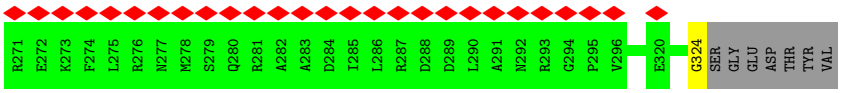
Chain SD:



- Molecule 2: Flagellar motor switch protein FliG

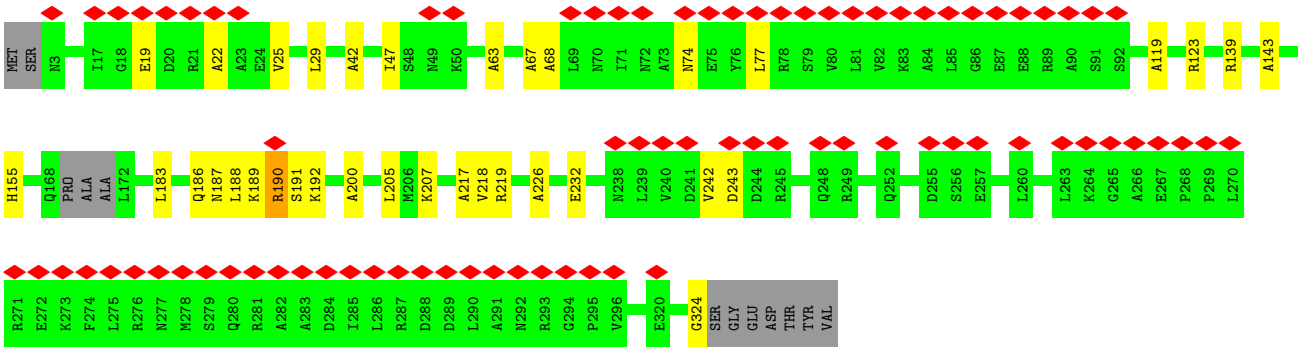
Chain YD:





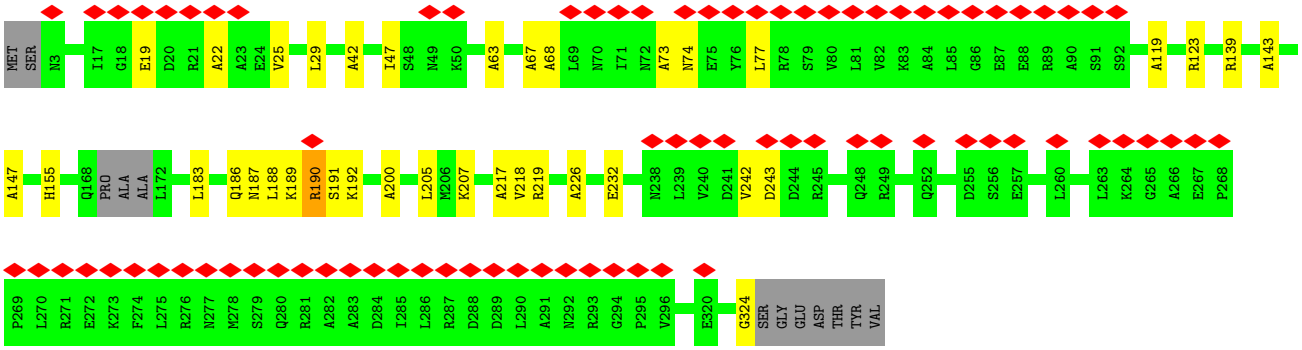
• Molecule 2: Flagellar motor switch protein FliG

Chain EE:



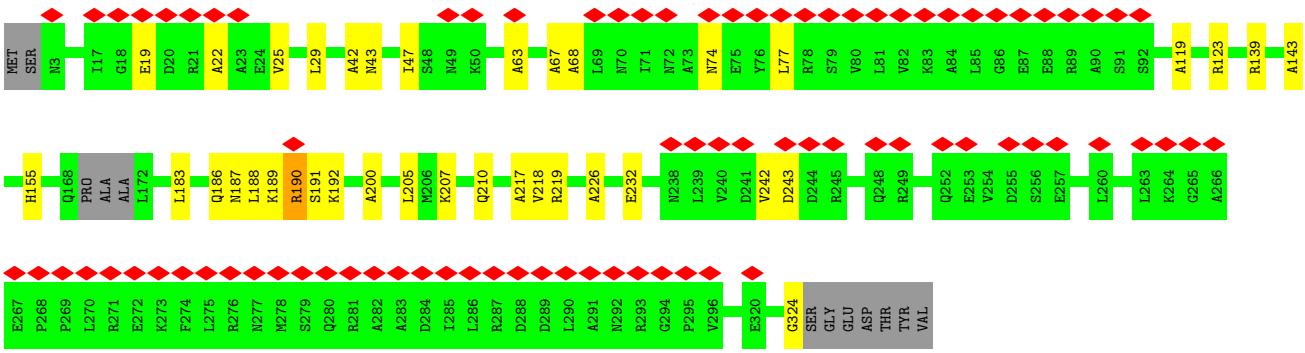
• Molecule 2: Flagellar motor switch protein FliG

Chain KE:



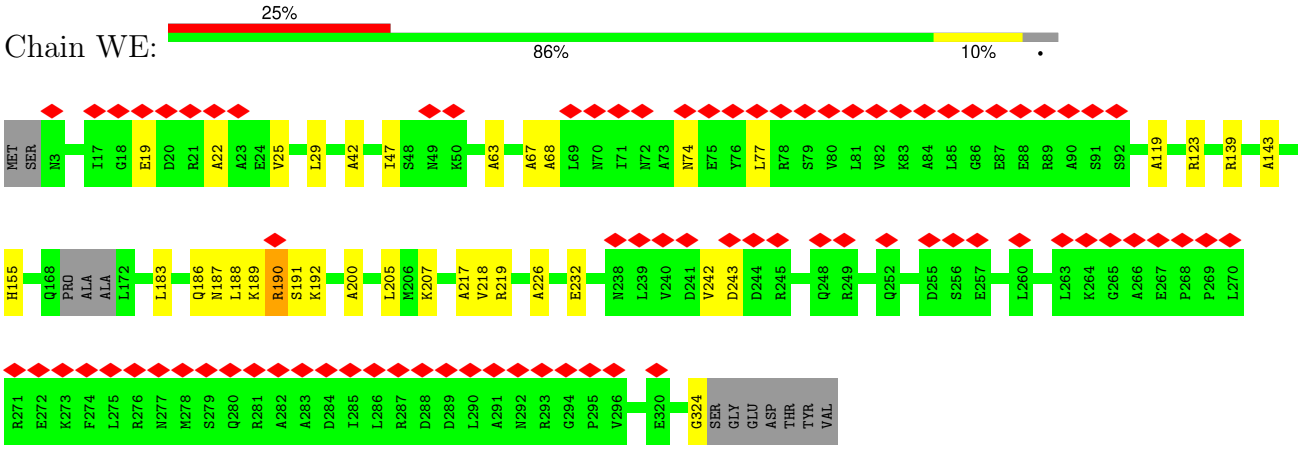
• Molecule 2: Flagellar motor switch protein FliG

Chain QE:



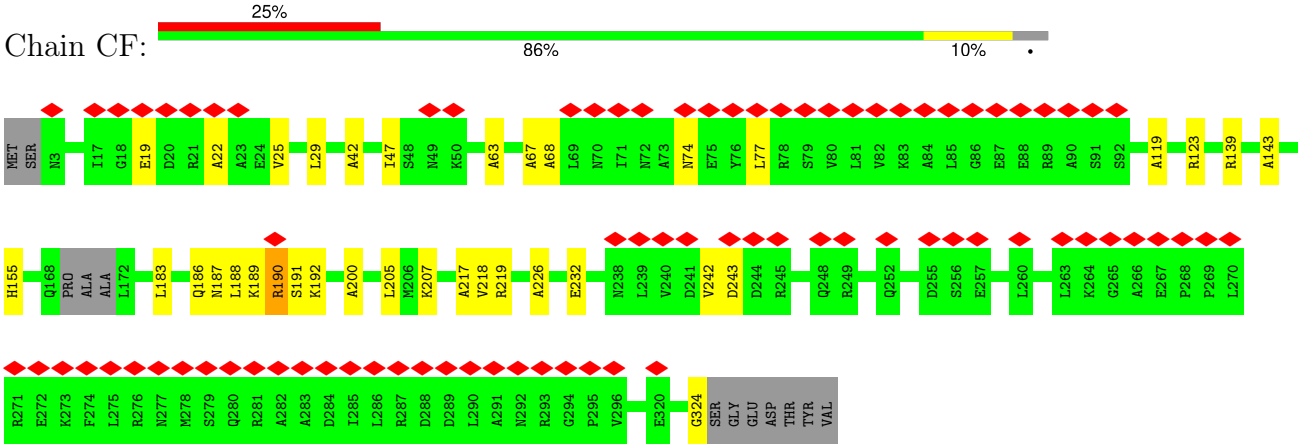
• Molecule 2: Flagellar motor switch protein FliG

Chain WE:



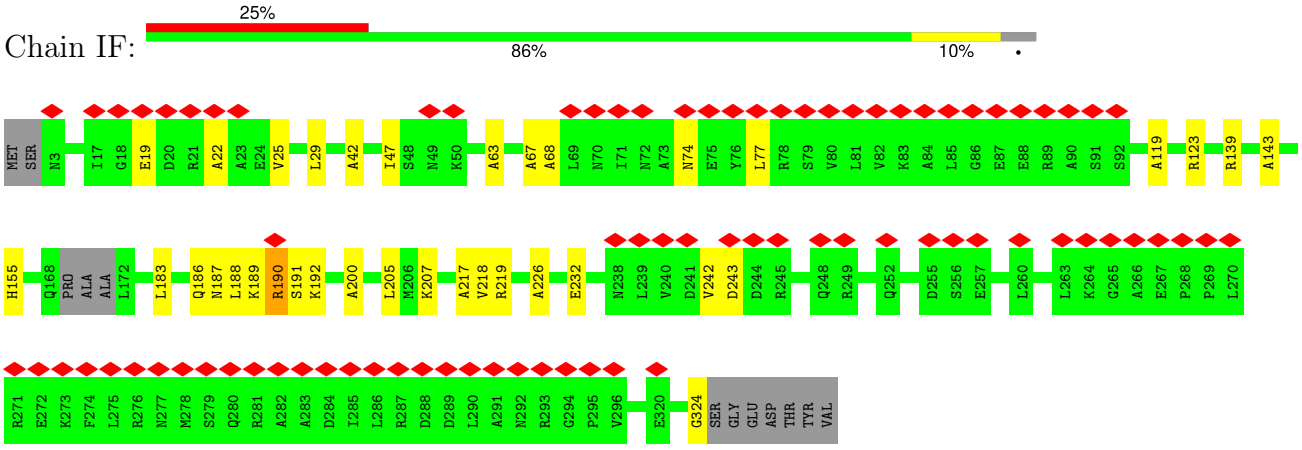
• Molecule 2: Flagellar motor switch protein FliG

Chain CF:



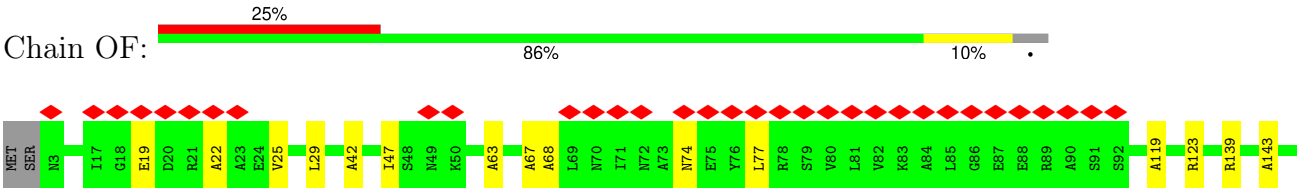
• Molecule 2: Flagellar motor switch protein FliG

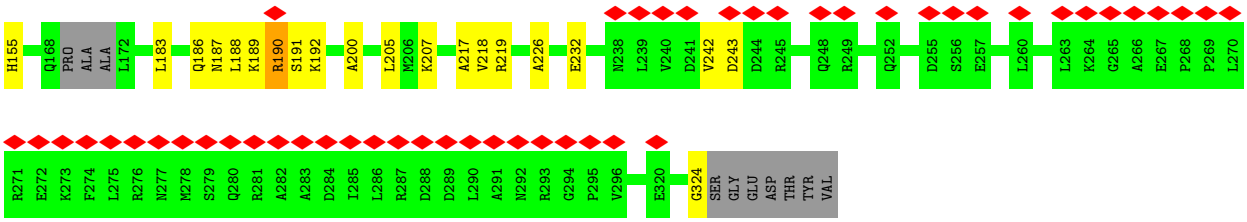
Chain IF:



• Molecule 2: Flagellar motor switch protein FliG

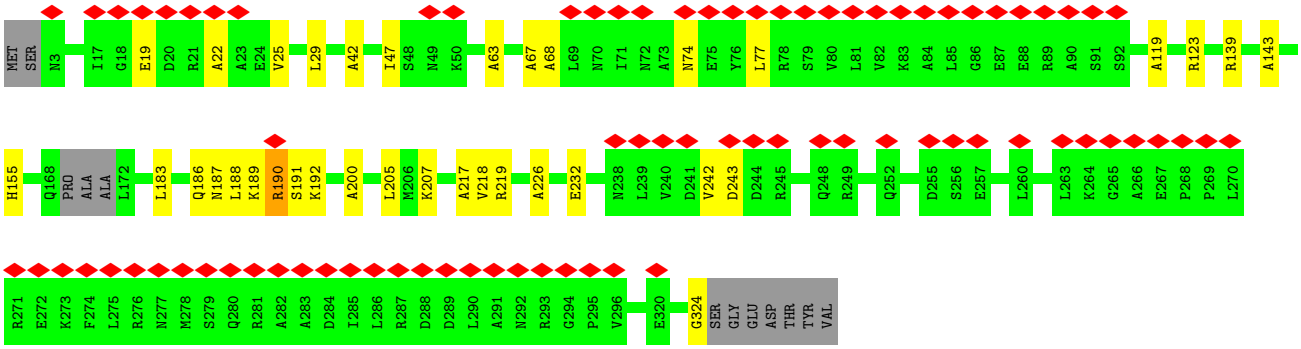
Chain OF:





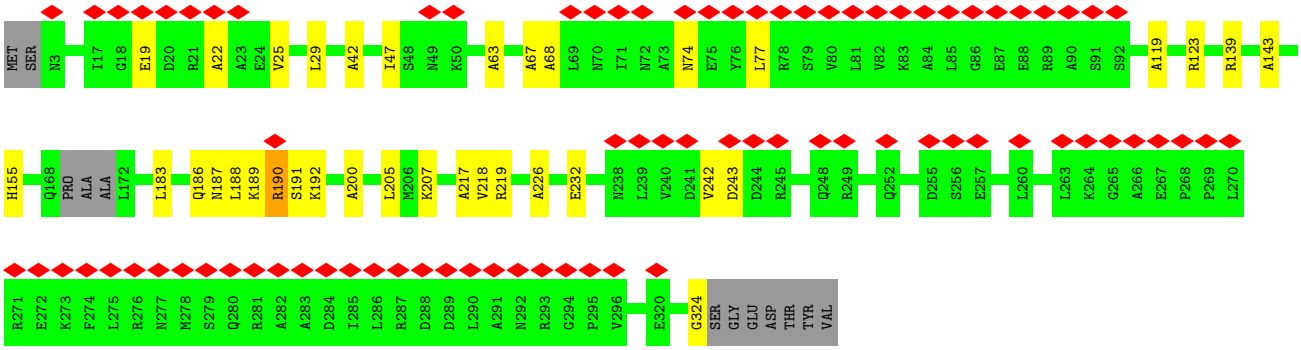
• Molecule 2: Flagellar motor switch protein FliG

Chain UF:



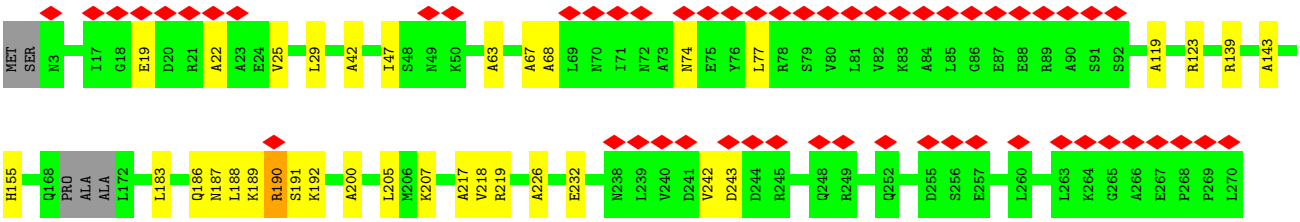
• Molecule 2: Flagellar motor switch protein FliG

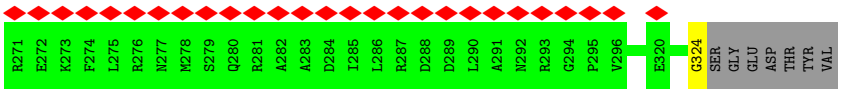
Chain AG:



• Molecule 2: Flagellar motor switch protein FliG

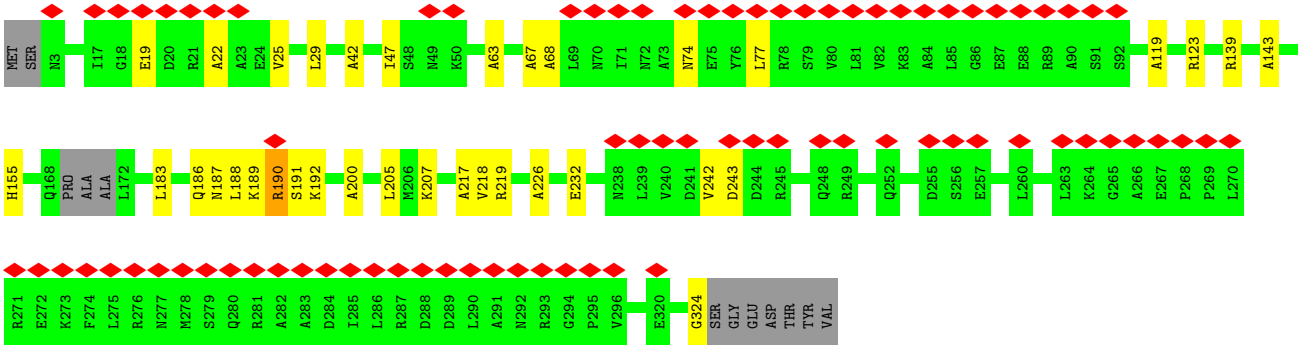
Chain GG:





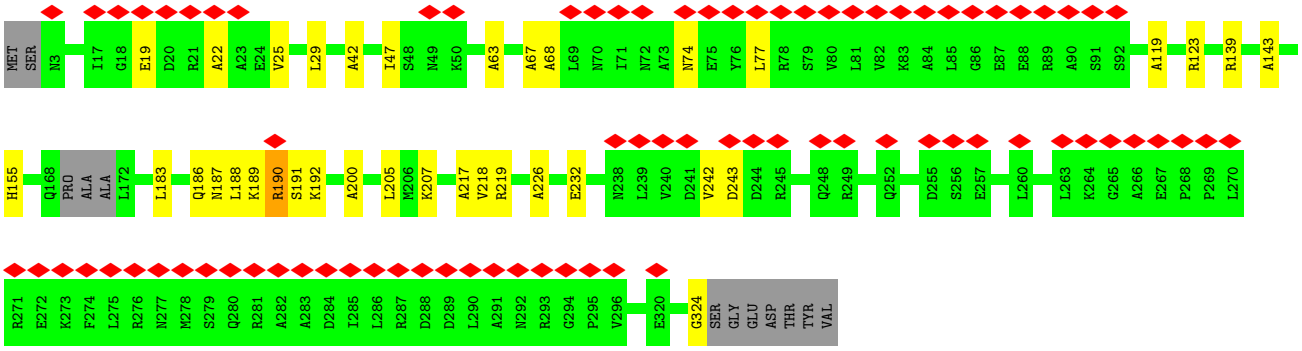
• Molecule 2: Flagellar motor switch protein FliG

Chain MG:



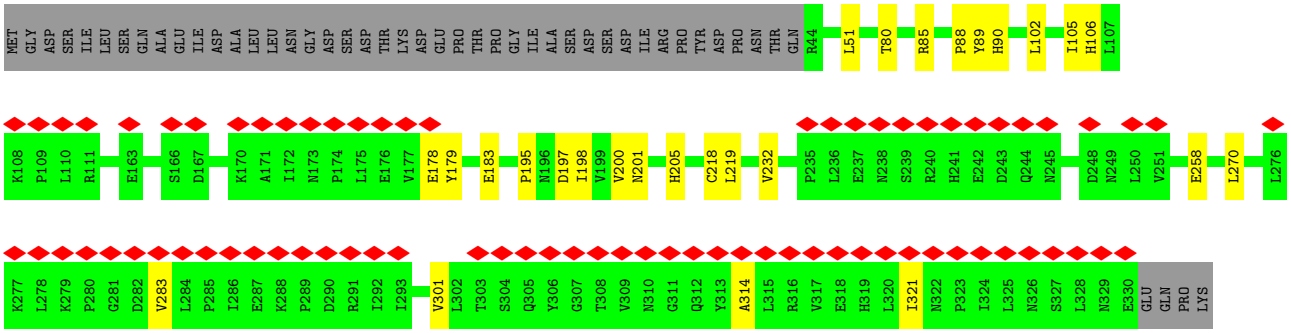
• Molecule 2: Flagellar motor switch protein FliG

Chain SG:



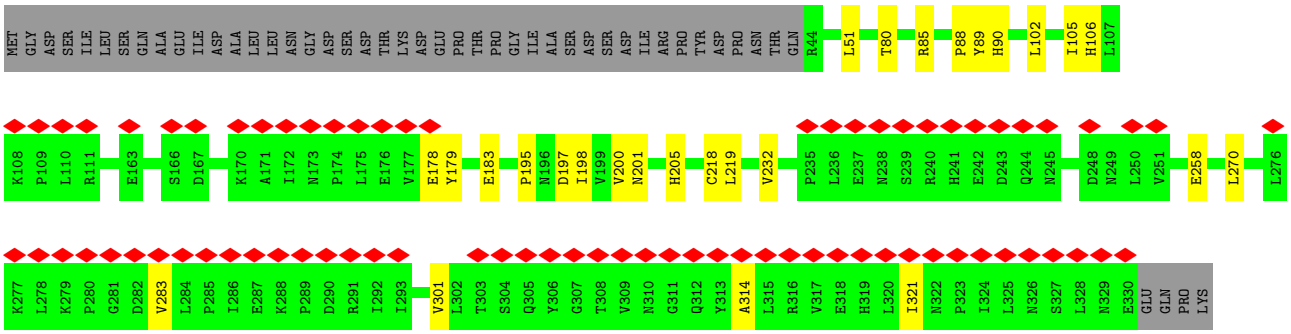
• Molecule 3: Flagellar motor switch protein FliM

Chain M:



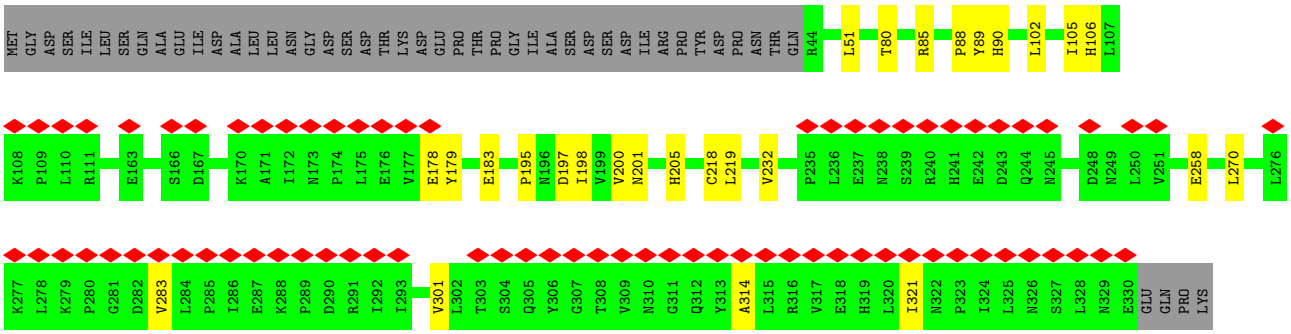
• Molecule 3: Flagellar motor switch protein FliM

Chain C:



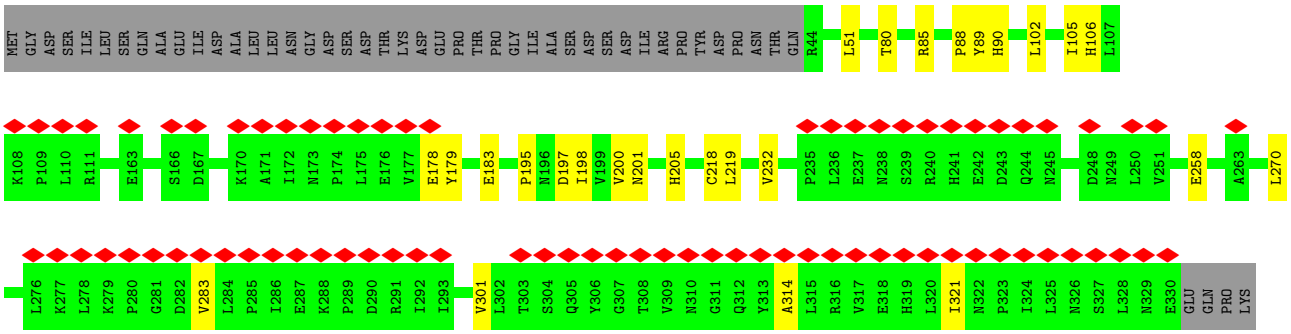
- Molecule 3: Flagellar motor switch protein FliM

Chain K:



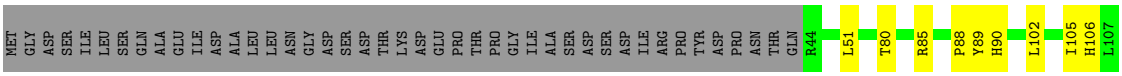
- Molecule 3: Flagellar motor switch protein FliM

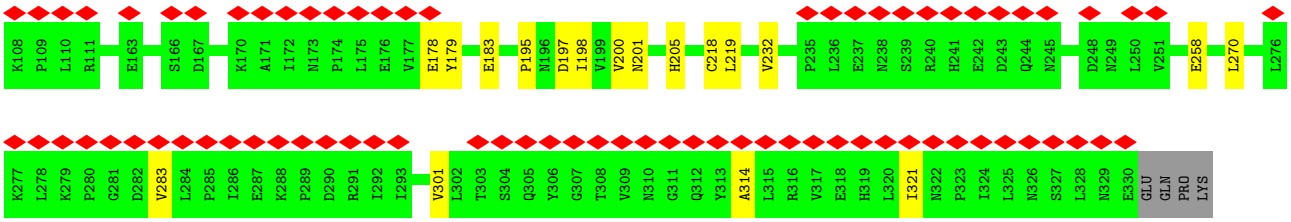
Chain V:



- Molecule 3: Flagellar motor switch protein FliM

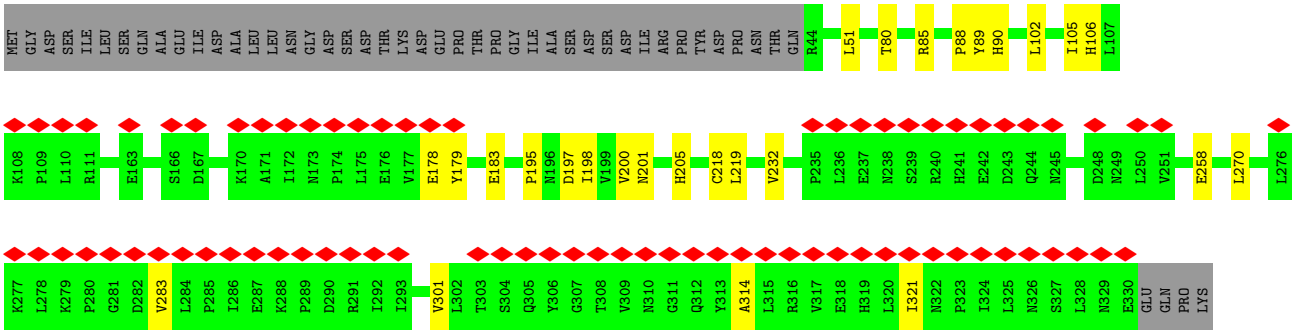
Chain BA:





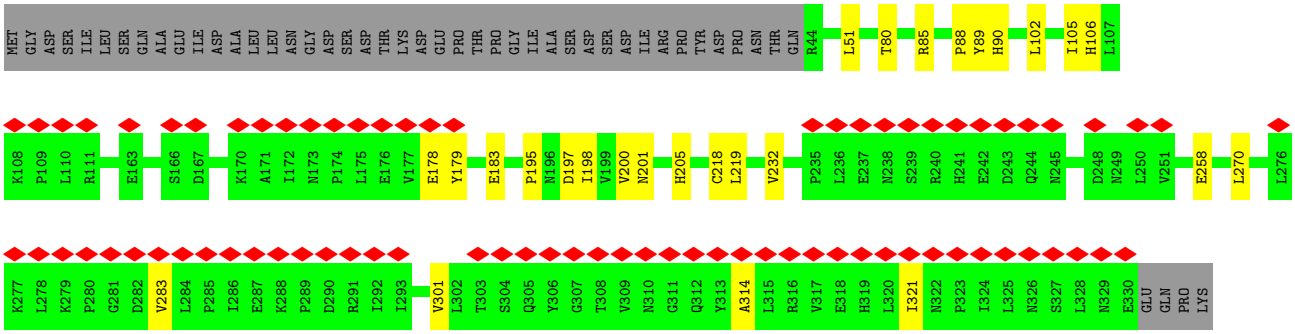
• Molecule 3: Flagellar motor switch protein FliM

Chain HA:



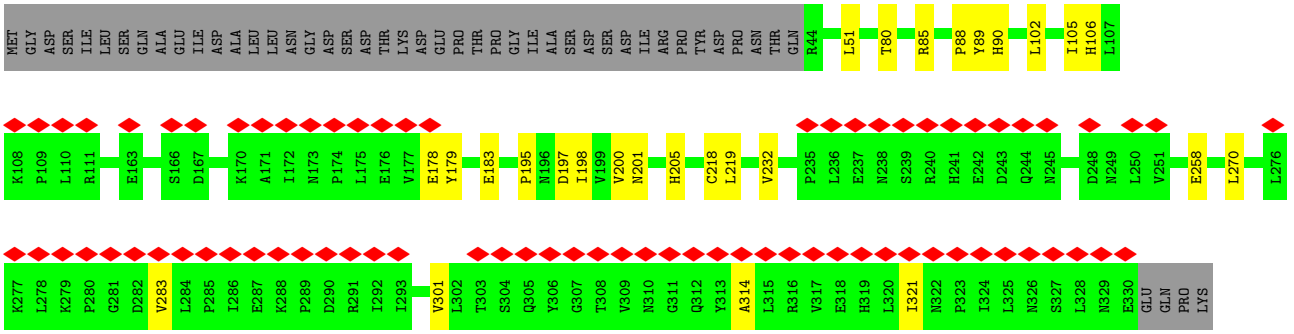
• Molecule 3: Flagellar motor switch protein FliM

Chain NA:



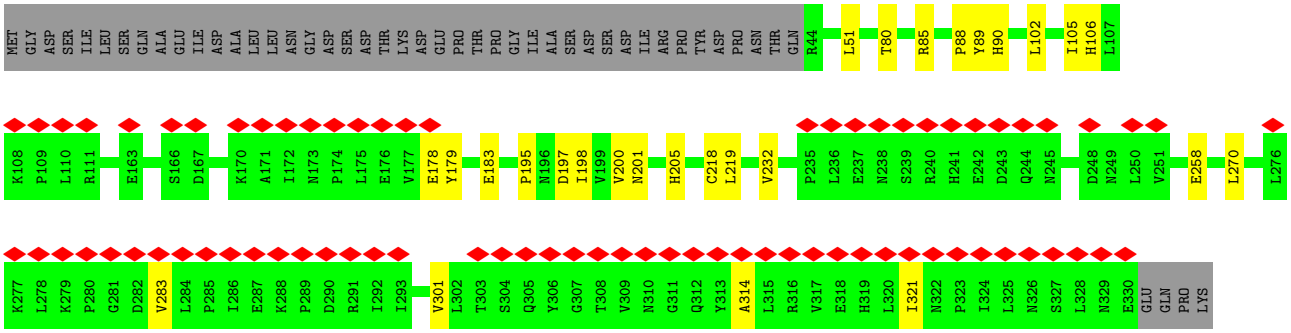
• Molecule 3: Flagellar motor switch protein FliM

Chain TA:



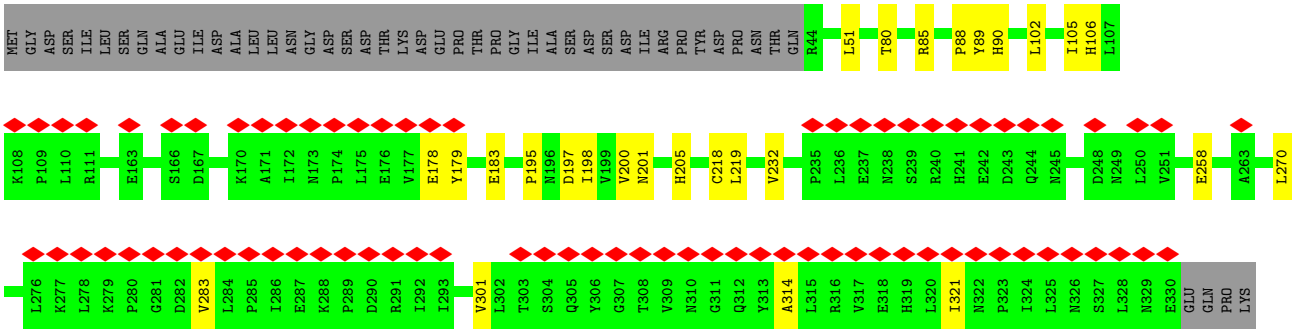
• Molecule 3: Flagellar motor switch protein FliM

Chain ZA:



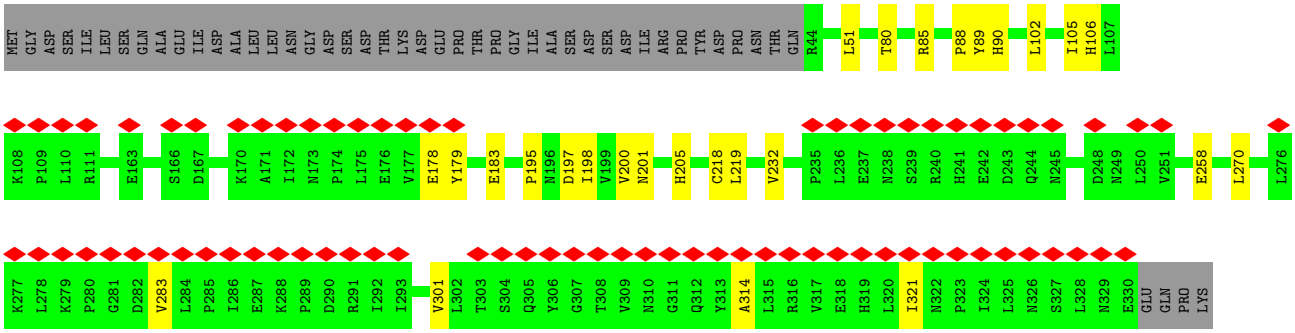
• Molecule 3: Flagellar motor switch protein FliM

Chain FB:



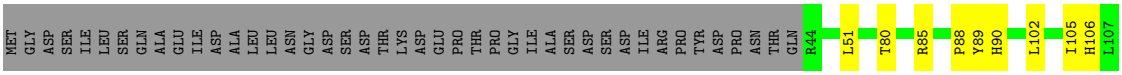
• Molecule 3: Flagellar motor switch protein FliM

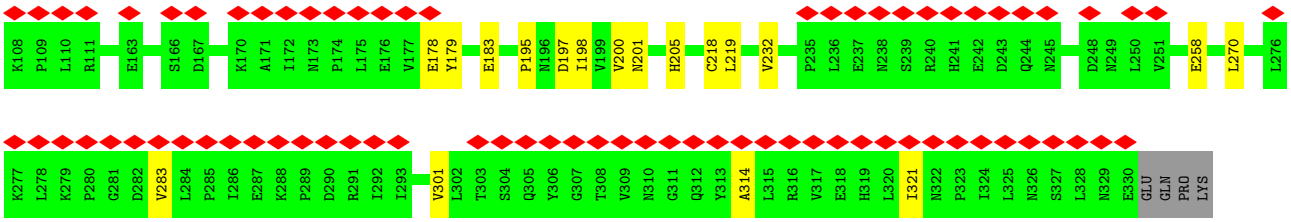
Chain LB:



• Molecule 3: Flagellar motor switch protein FliM

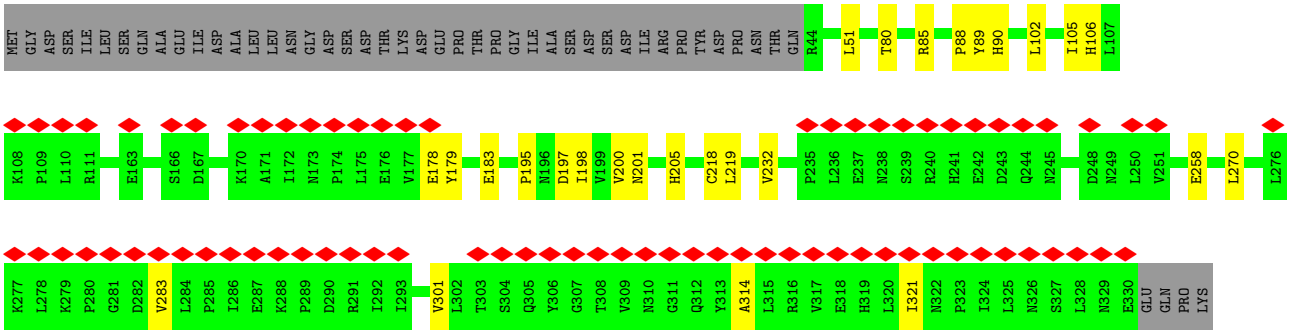
Chain RB:





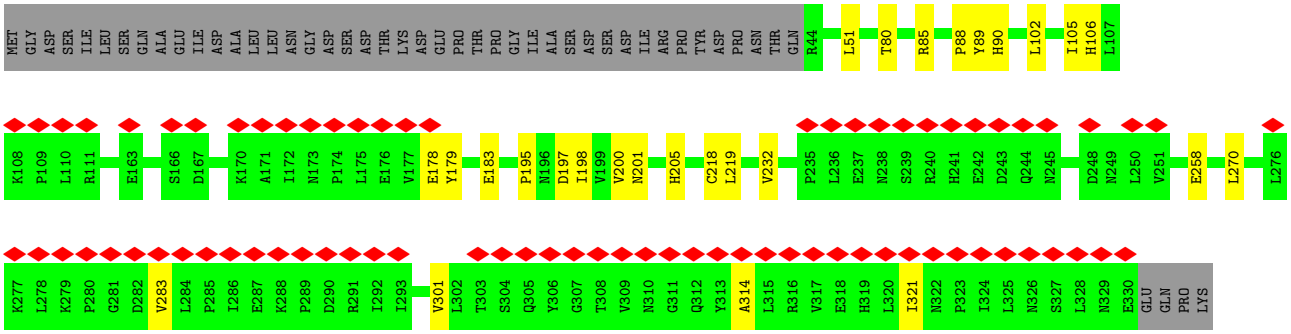
• Molecule 3: Flagellar motor switch protein FliM

Chain XB:



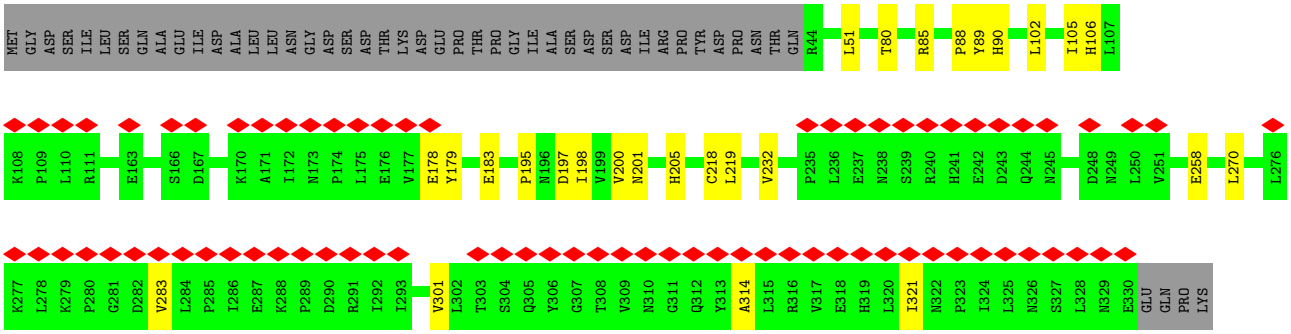
• Molecule 3: Flagellar motor switch protein FliM

Chain DC:



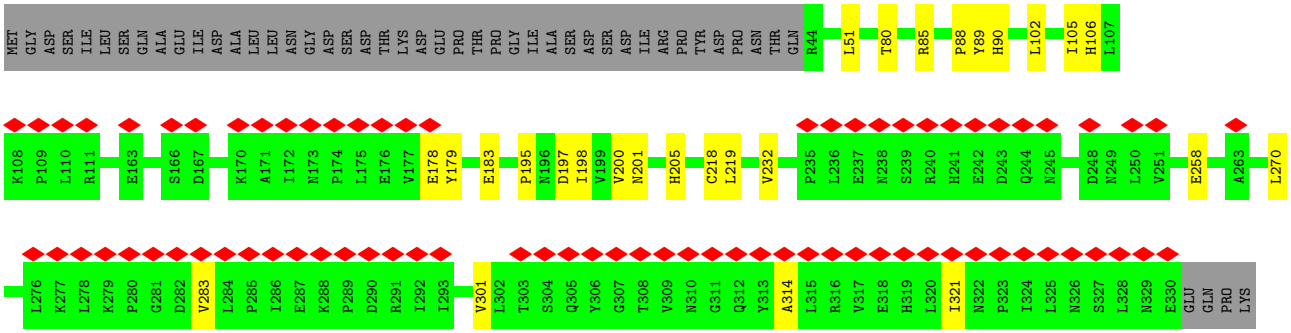
• Molecule 3: Flagellar motor switch protein FliM

Chain JC:



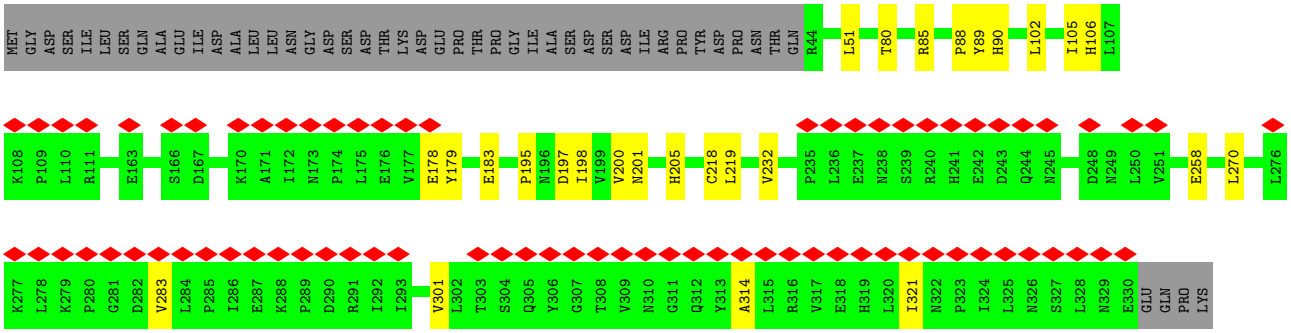
• Molecule 3: Flagellar motor switch protein FliM

Chain PC:



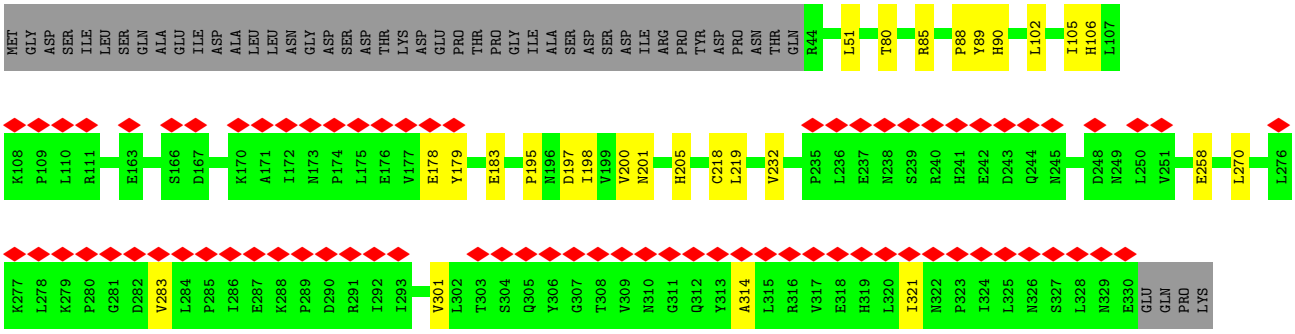
• Molecule 3: Flagellar motor switch protein FliM

Chain VC:



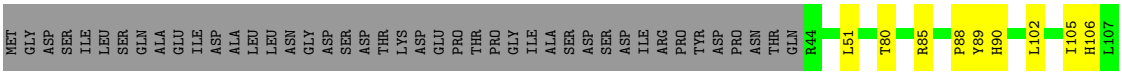
• Molecule 3: Flagellar motor switch protein FliM

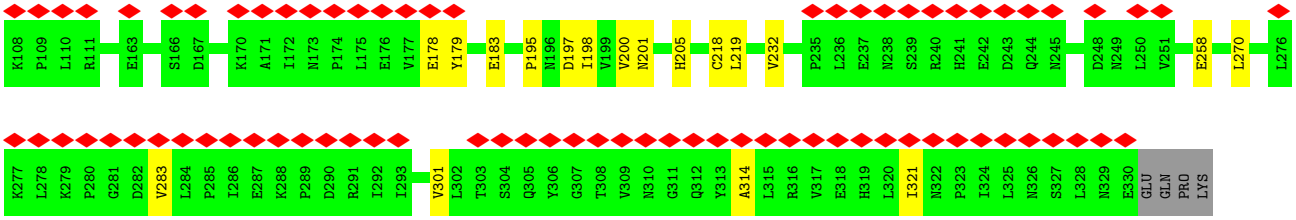
Chain BD:



• Molecule 3: Flagellar motor switch protein FliM

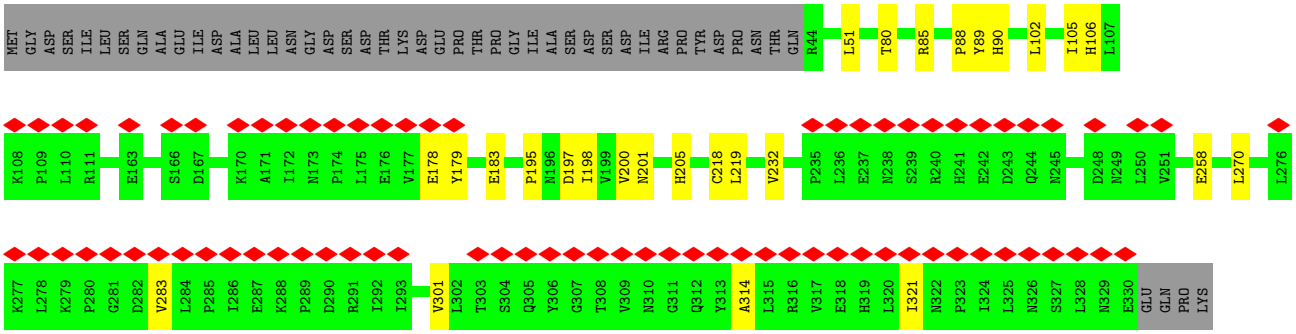
Chain HD:





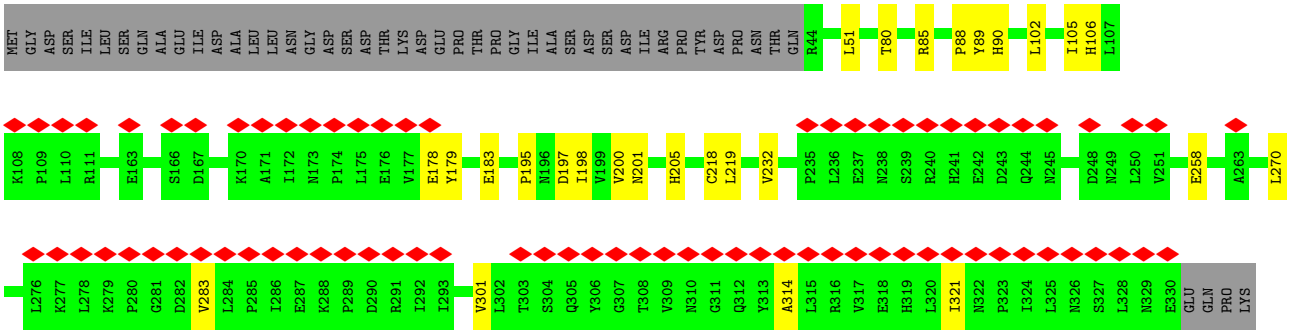
- Molecule 3: Flagellar motor switch protein FliM

Chain ND:



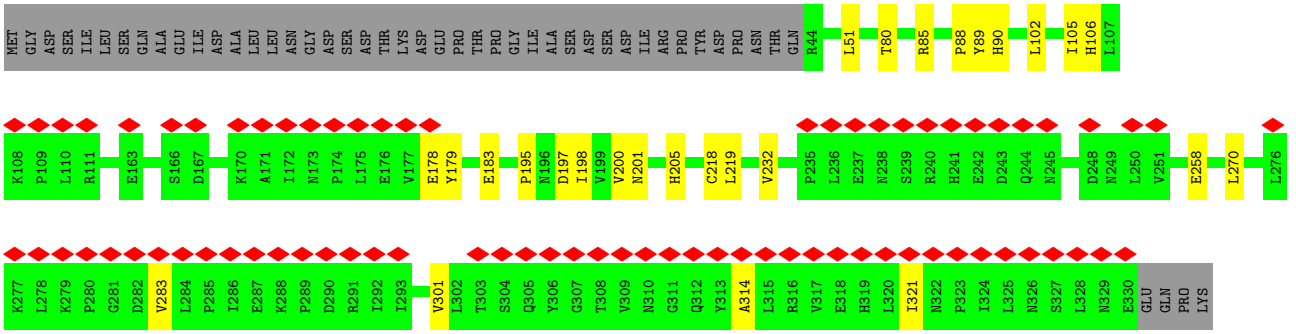
- Molecule 3: Flagellar motor switch protein FliM

Chain TD:



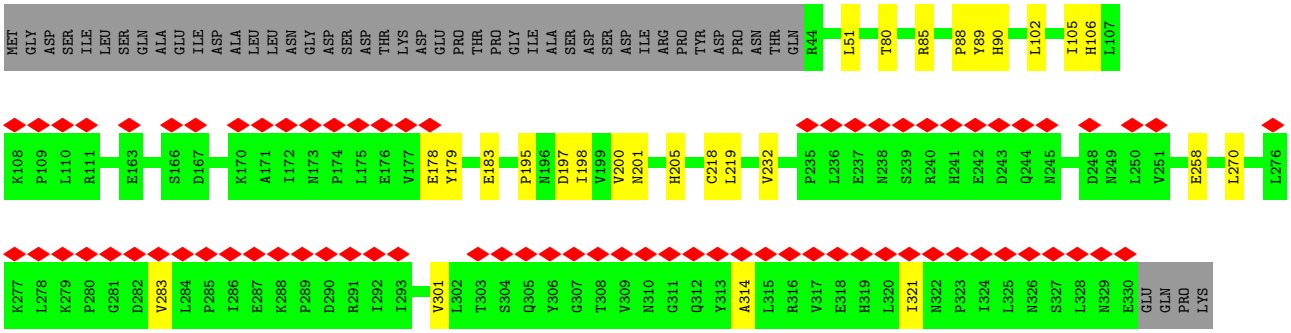
- Molecule 3: Flagellar motor switch protein FliM

Chain ZD:



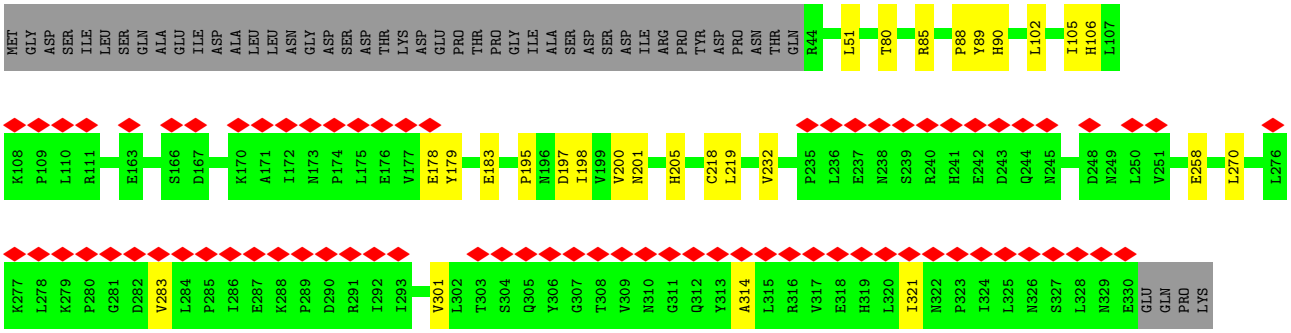
• Molecule 3: Flagellar motor switch protein FliM

Chain FE:



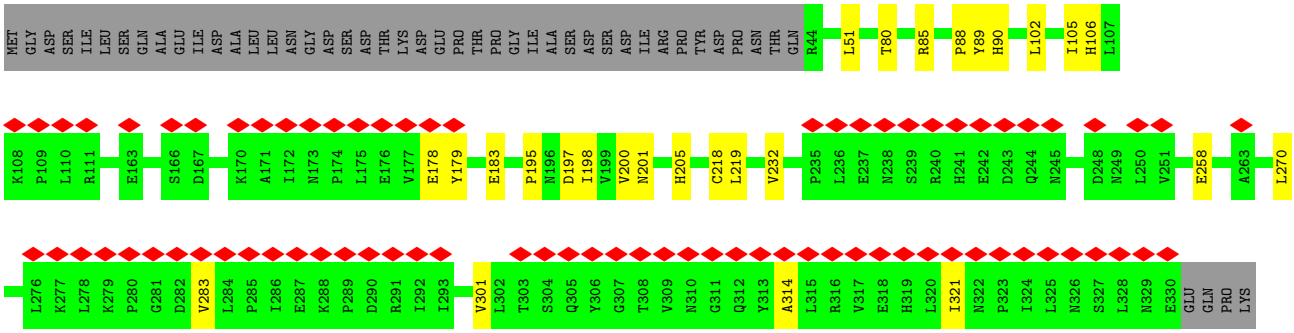
• Molecule 3: Flagellar motor switch protein FliM

Chain LE:



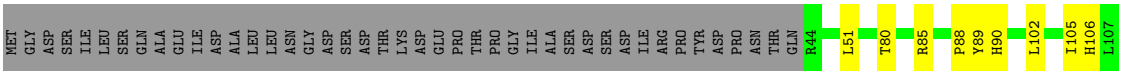
• Molecule 3: Flagellar motor switch protein FliM

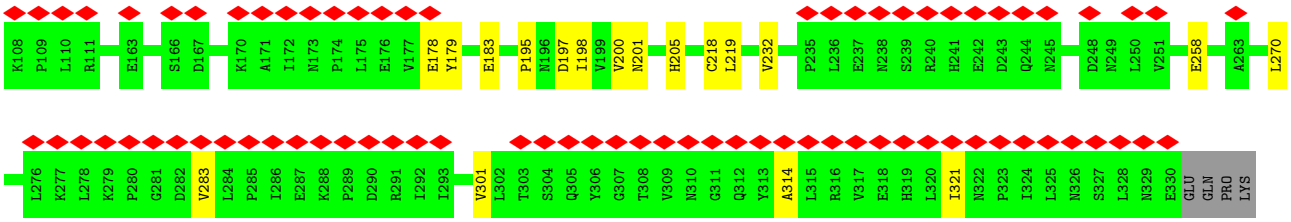
Chain RE:



• Molecule 3: Flagellar motor switch protein FliM

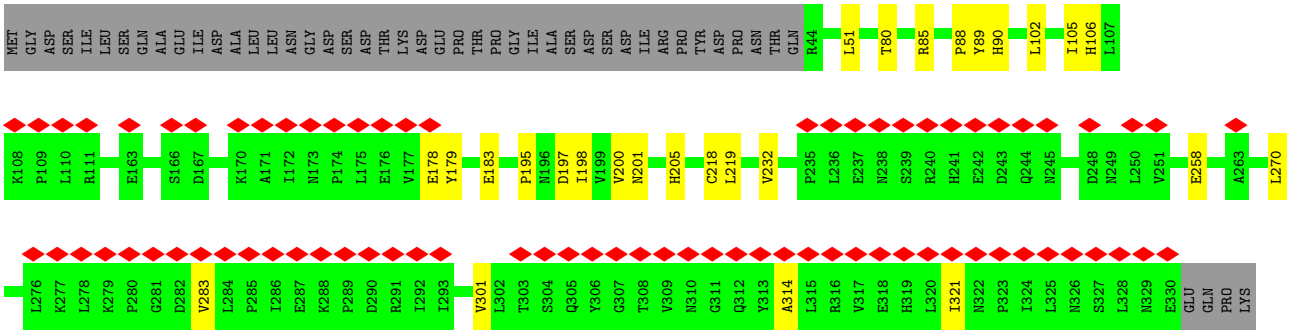
Chain XE:





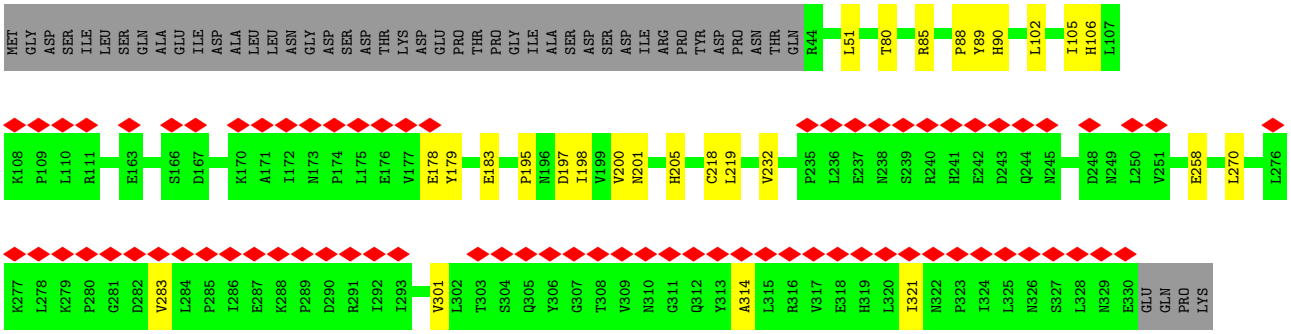
• Molecule 3: Flagellar motor switch protein FliM

Chain DF:



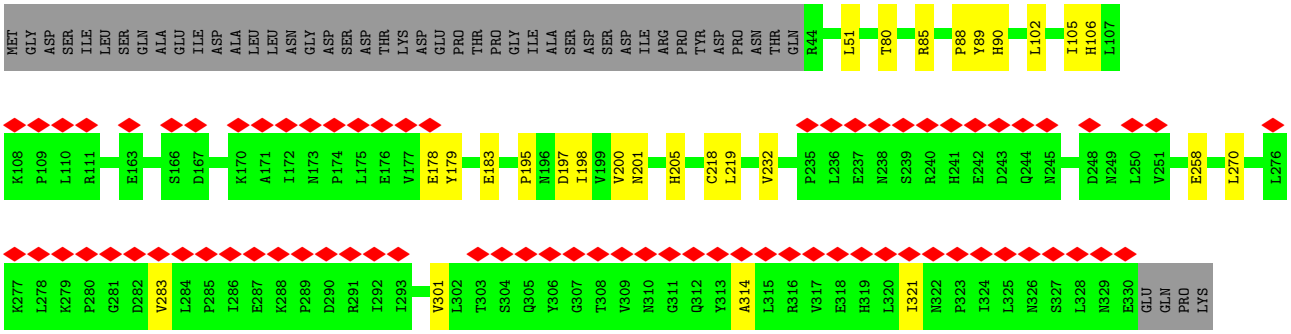
• Molecule 3: Flagellar motor switch protein FliM

Chain JF:



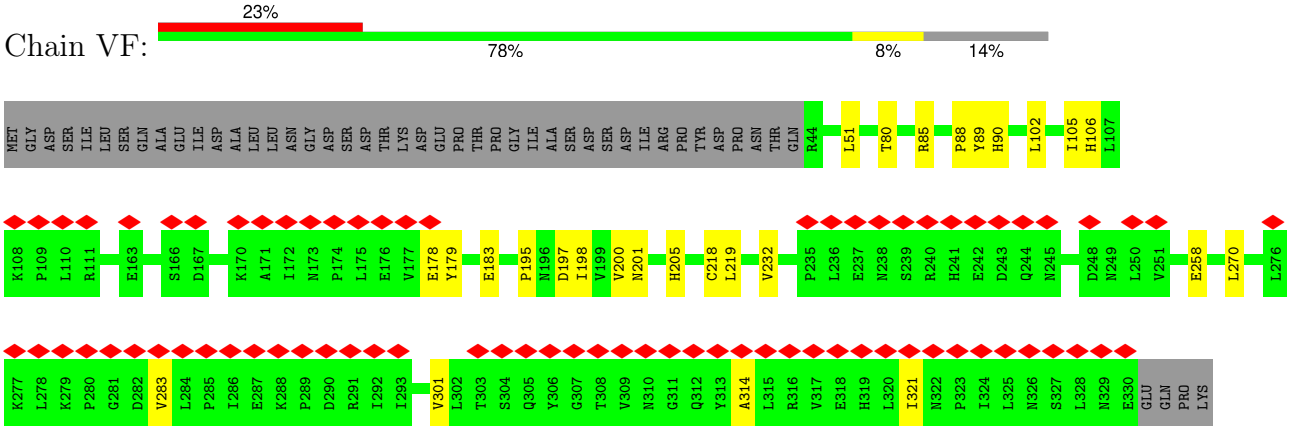
• Molecule 3: Flagellar motor switch protein FliM

Chain PF:



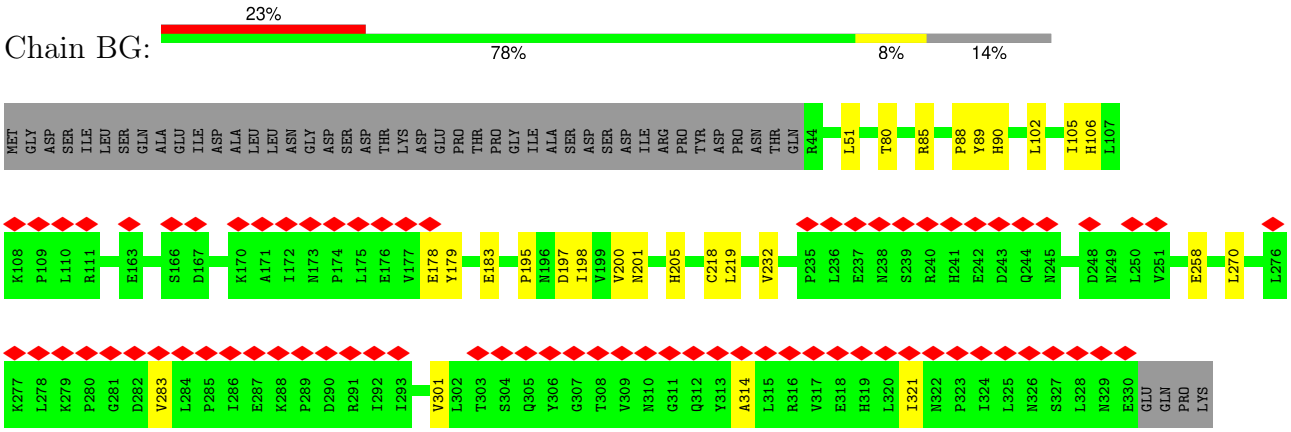
• Molecule 3: Flagellar motor switch protein FliM

Chain VF:



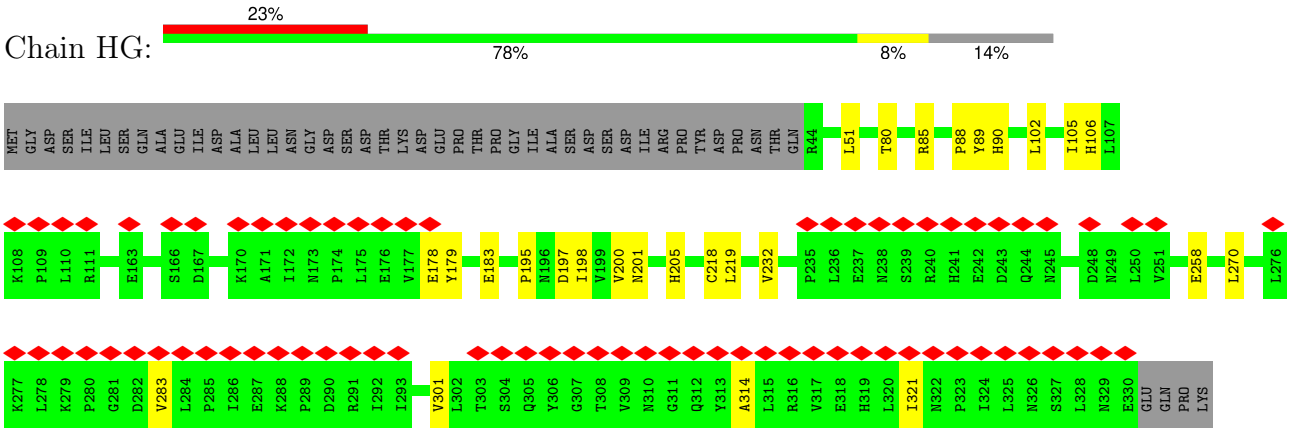
• Molecule 3: Flagellar motor switch protein FliM

Chain BG:



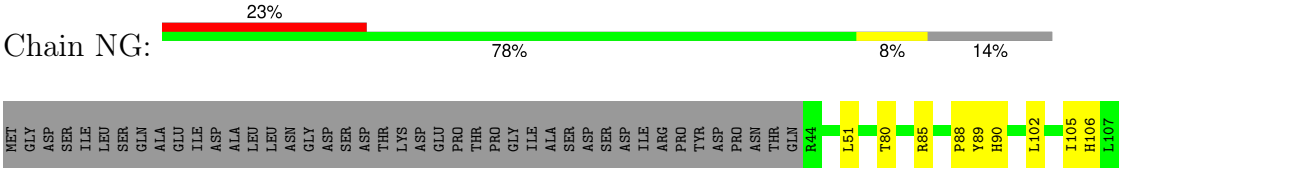
• Molecule 3: Flagellar motor switch protein FliM

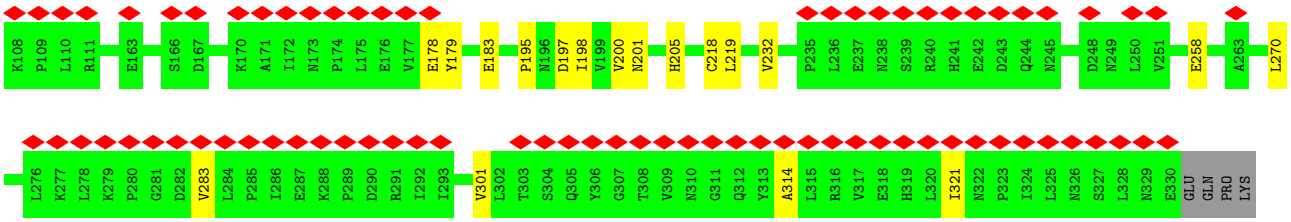
Chain HG:



• Molecule 3: Flagellar motor switch protein FliM

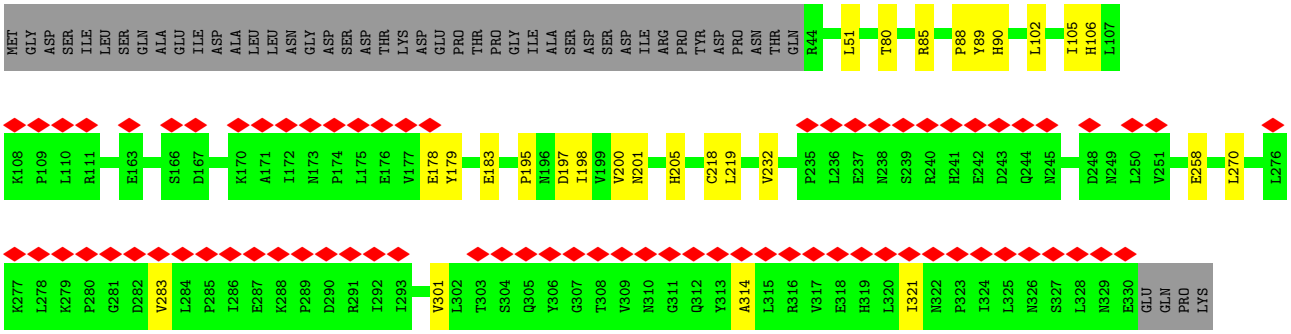
Chain NG:





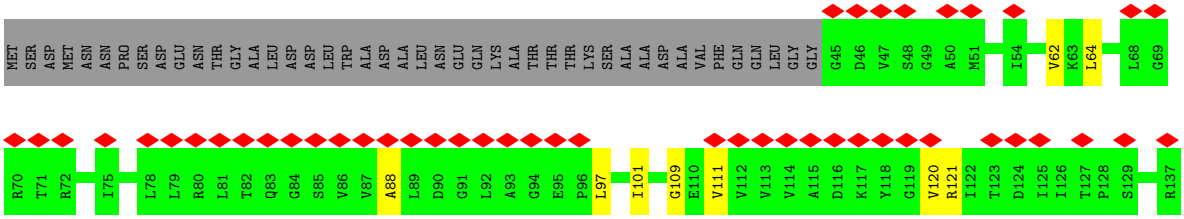
- Molecule 3: Flagellar motor switch protein FliM

Chain TG:



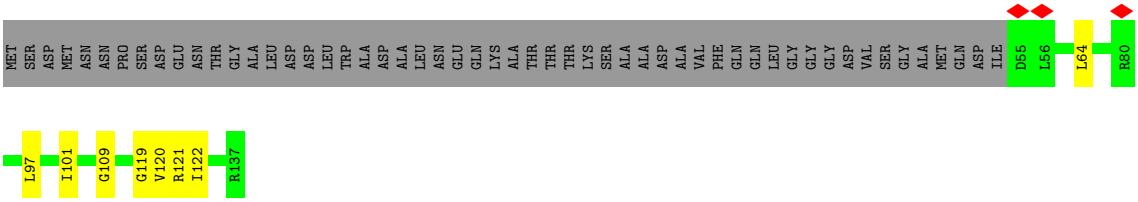
- Molecule 4: Flagellar motor switch protein FliN

Chain N:



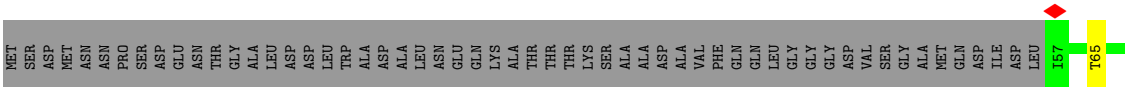
- Molecule 4: Flagellar motor switch protein FliN

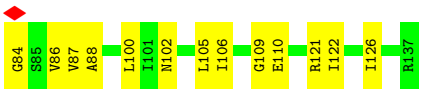
Chain P:



- Molecule 4: Flagellar motor switch protein FliN

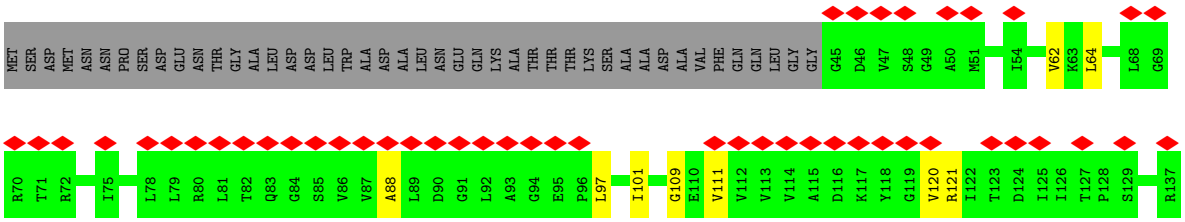
Chain Q:





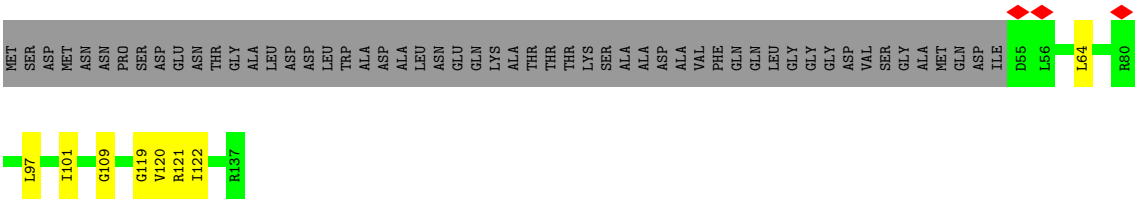
• Molecule 4: Flagellar motor switch protein FliN

Chain D:



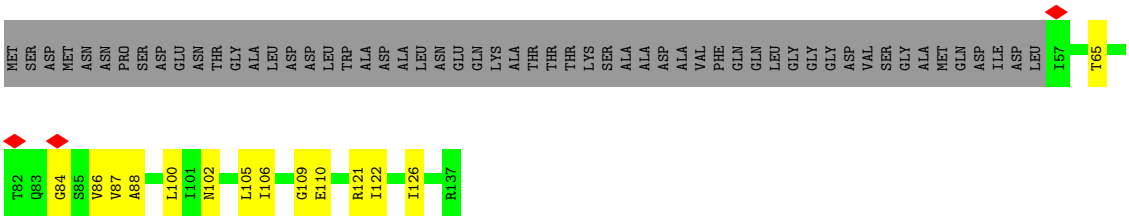
• Molecule 4: Flagellar motor switch protein FliN

Chain E:



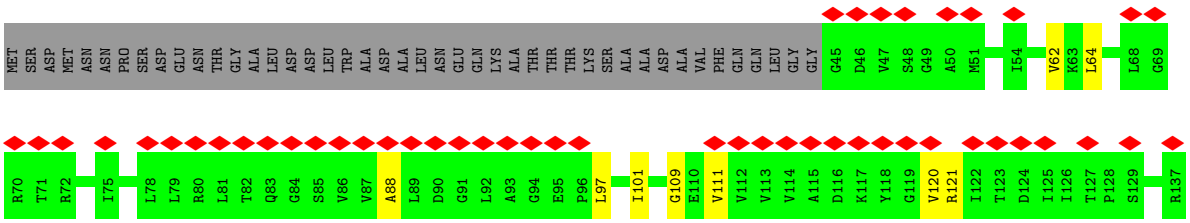
• Molecule 4: Flagellar motor switch protein FliN

Chain H:



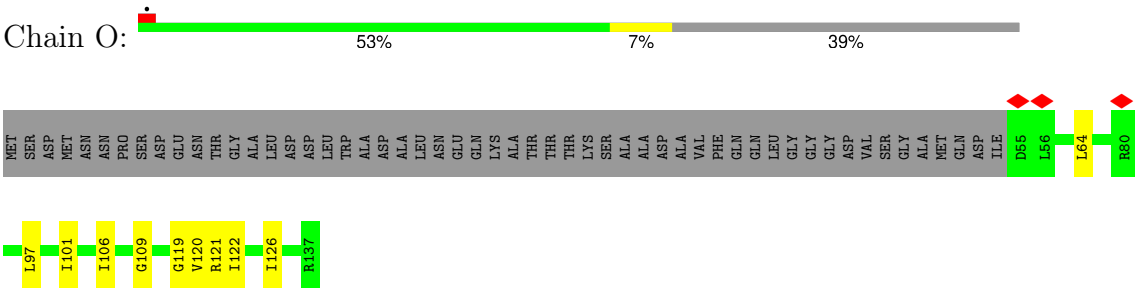
• Molecule 4: Flagellar motor switch protein FliN

Chain L:



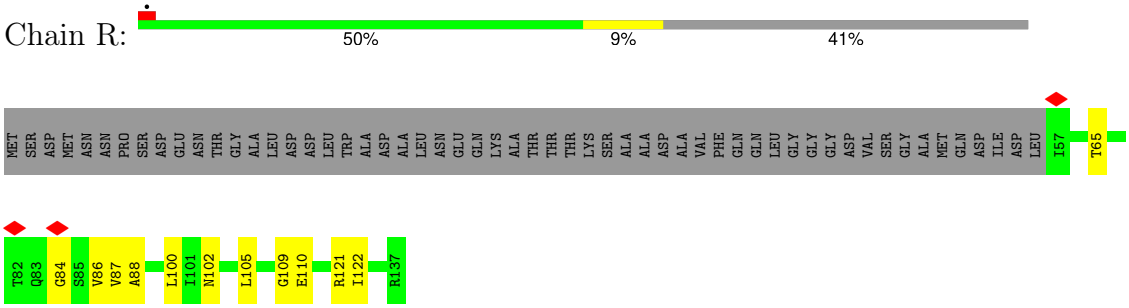
• Molecule 4: Flagellar motor switch protein FliN

Chain O:



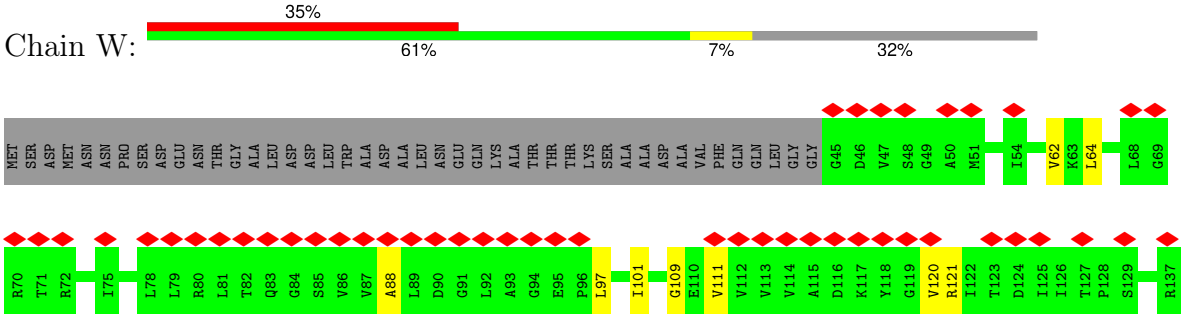
- Molecule 4: Flagellar motor switch protein FliN

Chain R:



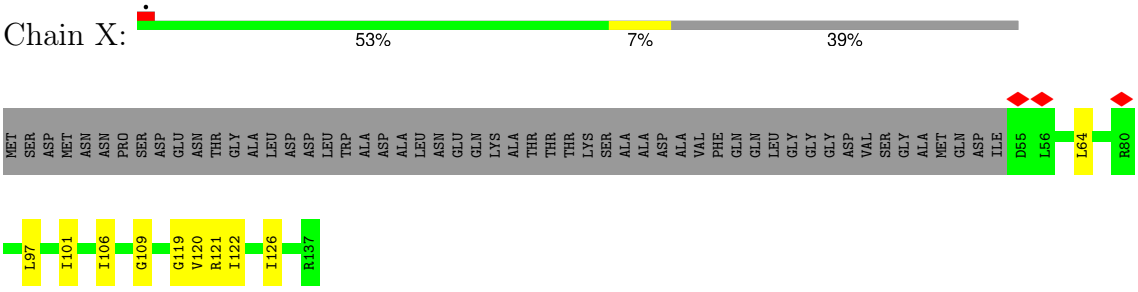
- Molecule 4: Flagellar motor switch protein FliN

Chain W:



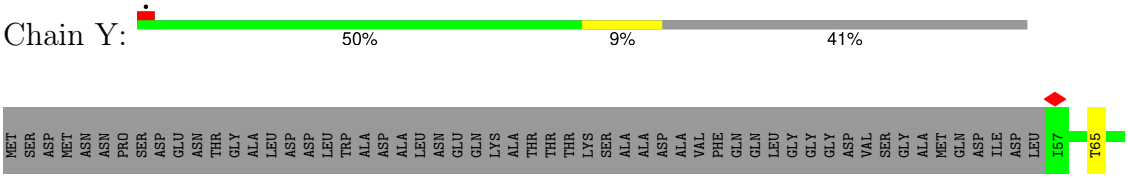
- Molecule 4: Flagellar motor switch protein FliN

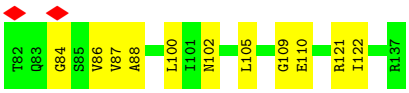
Chain X:



- Molecule 4: Flagellar motor switch protein FliN

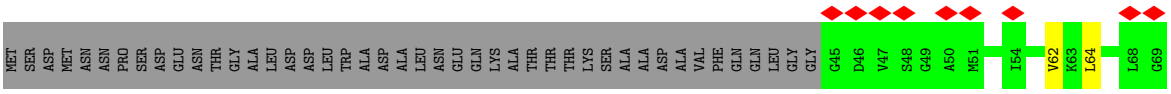
Chain Y:

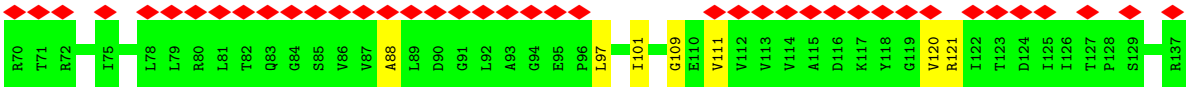




• Molecule 4: Flagellar motor switch protein FliN

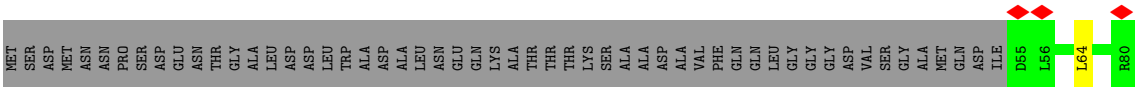
Chain CA:

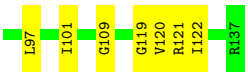




• Molecule 4: Flagellar motor switch protein FliN

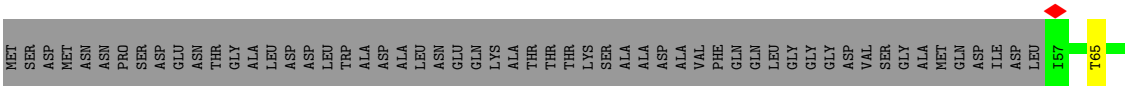
Chain DA:





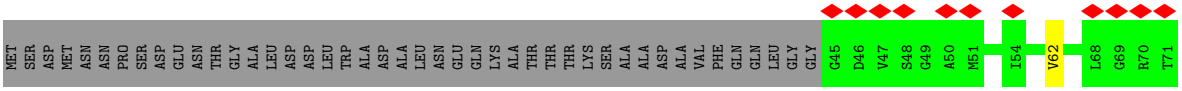
• Molecule 4: Flagellar motor switch protein FliN

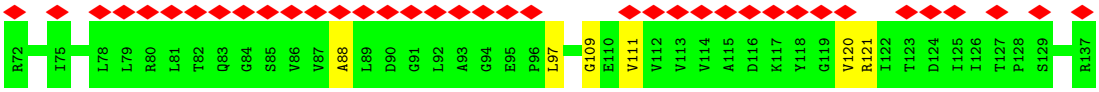
Chain EA:



• Molecule 4: Flagellar motor switch protein FliN

Chain IA:





• Molecule 4: Flagellar motor switch protein FliN

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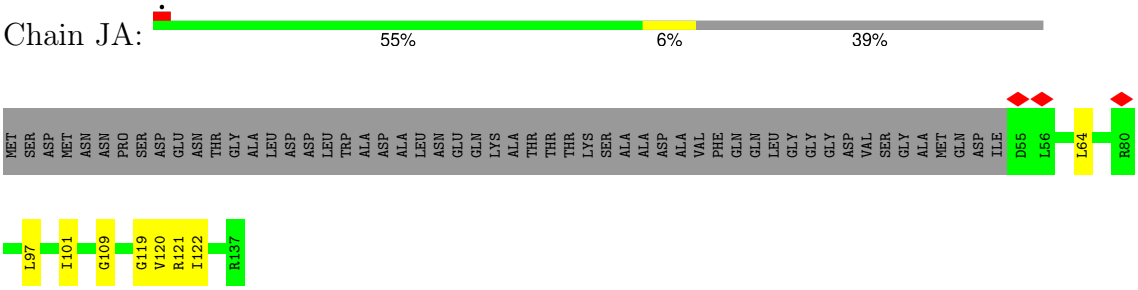
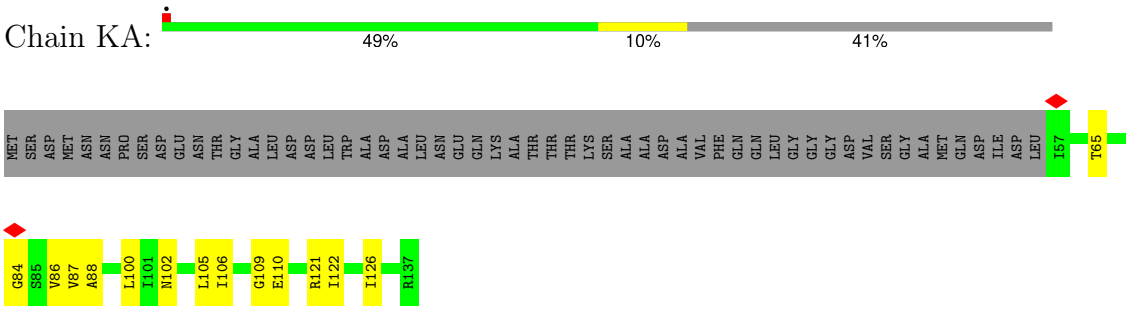


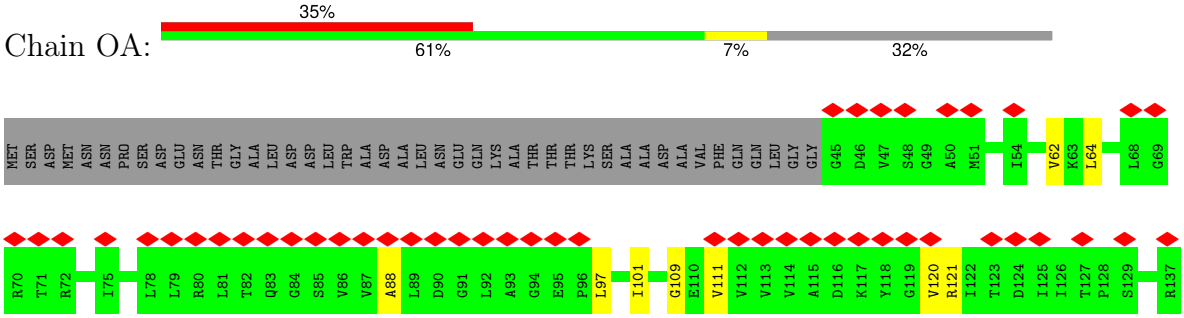
• Molecule 4: Flagellar motor switch protein FliN

Chain KA:



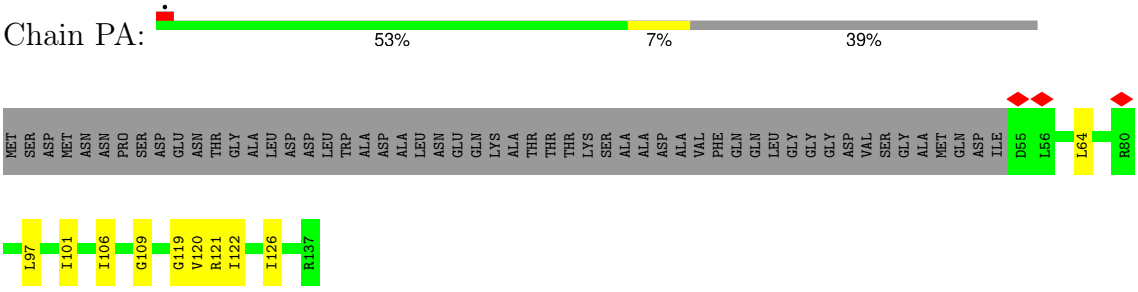
• Molecule 4: Flagellar motor switch protein FliN

Chain OA:



• Molecule 4: Flagellar motor switch protein FliN

Chain PA:



• Molecule 4: Flagellar motor switch protein FliN

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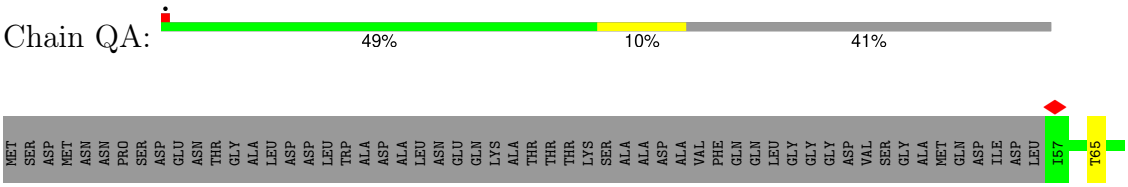

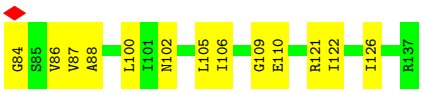

• Molecule 4: Flagellar motor switch protein FliN

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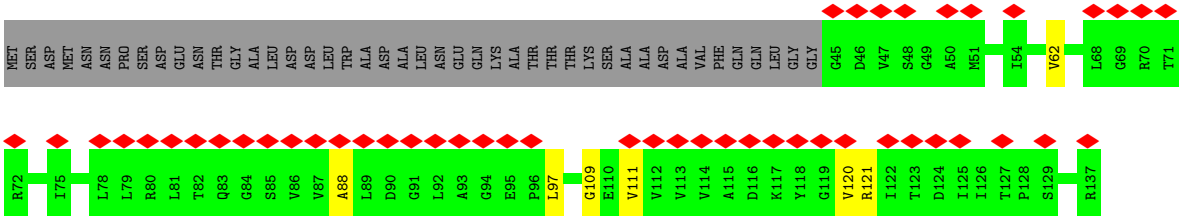
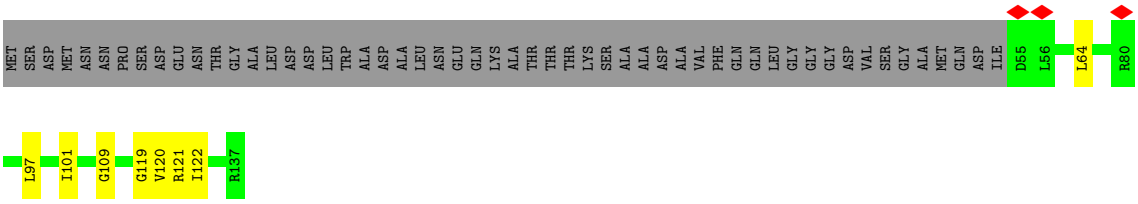


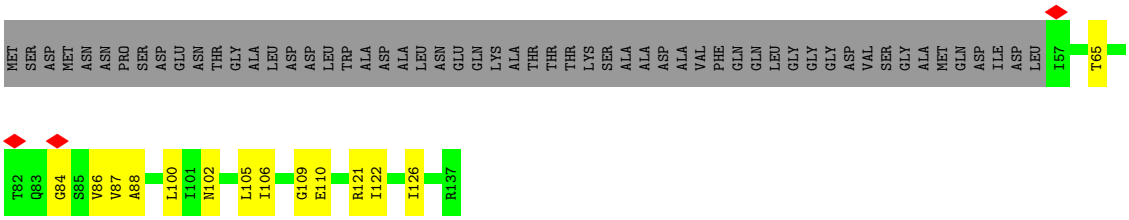
• Molecule 4: Flagellar motor switch protein FliN

Chain VA:



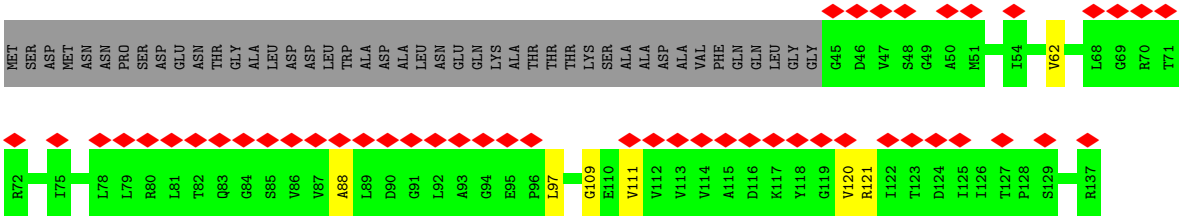
• Molecule 4: Flagellar motor switch protein FliN

Chain WA:



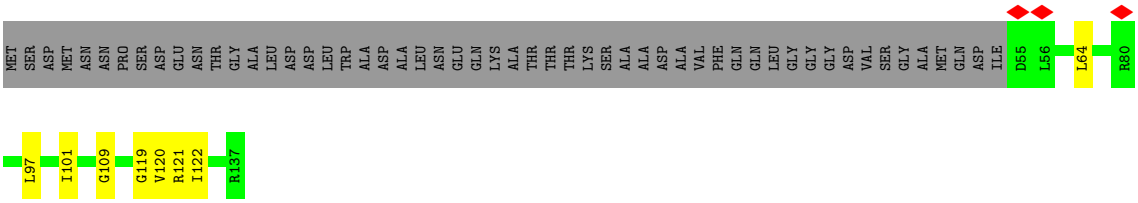
• Molecule 4: Flagellar motor switch protein FliN

Chain AB:



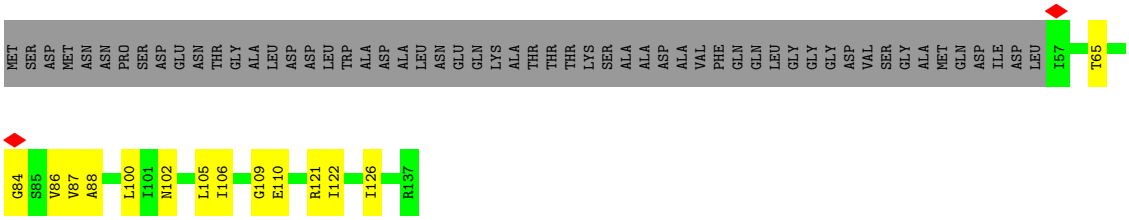
• Molecule 4: Flagellar motor switch protein FliN

Chain BB:



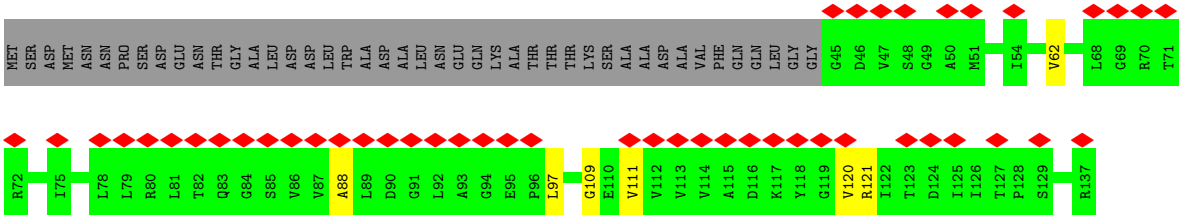
• Molecule 4: Flagellar motor switch protein FliN

Chain CB:



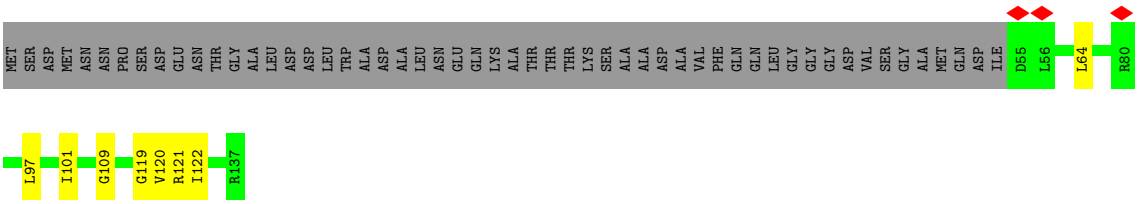
• Molecule 4: Flagellar motor switch protein FliN

Chain GB:



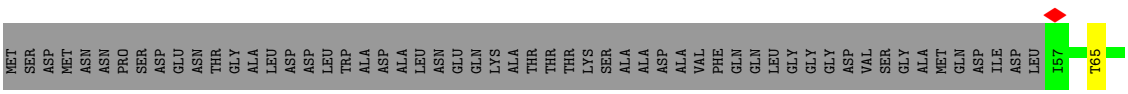
• Molecule 4: Flagellar motor switch protein FliN

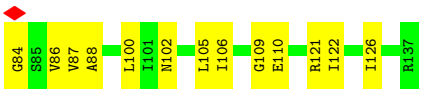
Chain HB:



• Molecule 4: Flagellar motor switch protein FliN

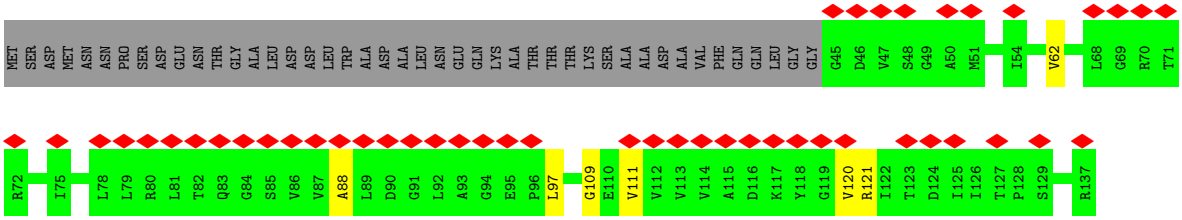
Chain IB:





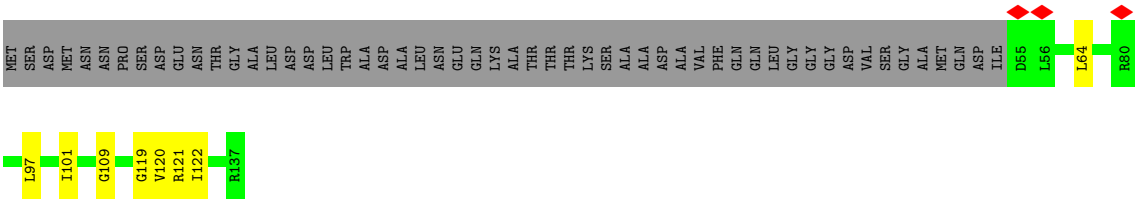
• Molecule 4: Flagellar motor switch protein FliN

Chain MB:



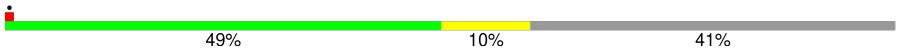
• Molecule 4: Flagellar motor switch protein FliN

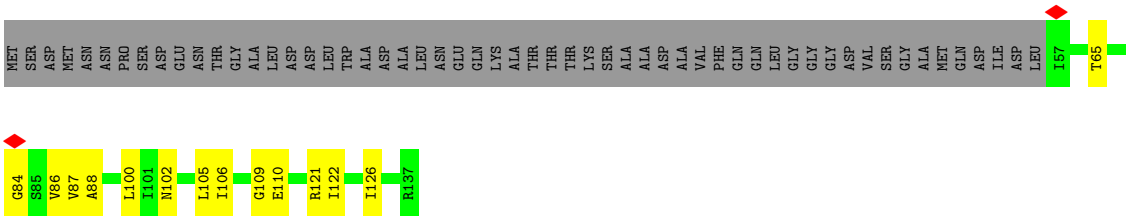
Chain NB:



• Molecule 4: Flagellar motor switch protein FliN

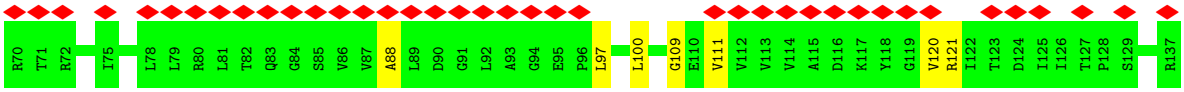
Chain OB:





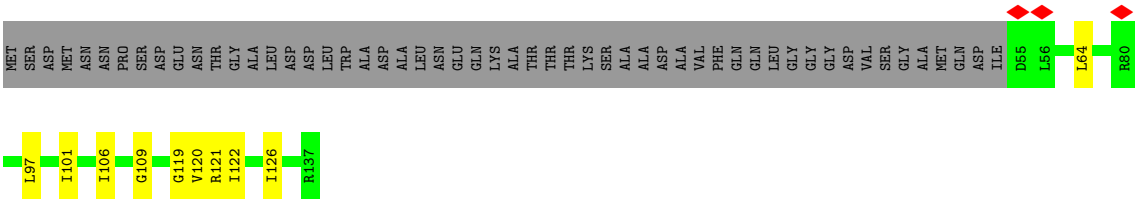
• Molecule 4: Flagellar motor switch protein FliN

Chain SB:



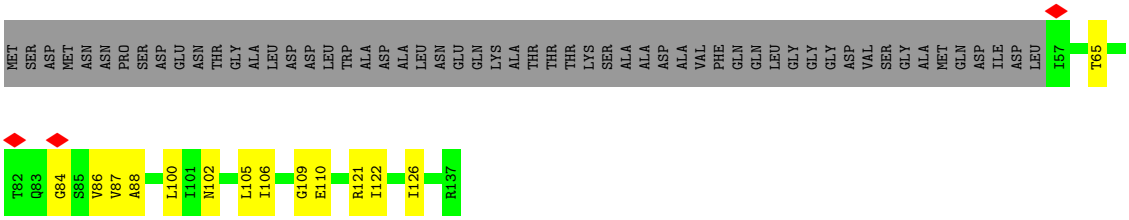
• Molecule 4: Flagellar motor switch protein FliN

Chain TB:



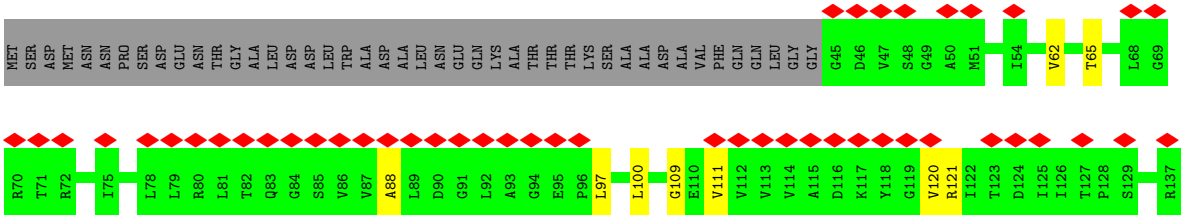
• Molecule 4: Flagellar motor switch protein FliN

Chain UB:



• Molecule 4: Flagellar motor switch protein FliN

Chain YB:



• Molecule 4: Flagellar motor switch protein FliN

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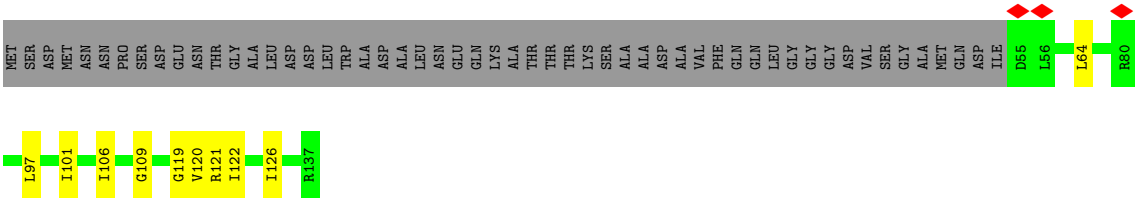
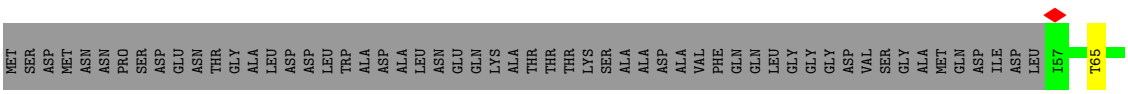
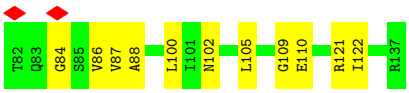


• Molecule 4: Flagellar motor switch protein FliN

Chain AC:





• Molecule 4: Flagellar motor switch protein FliN

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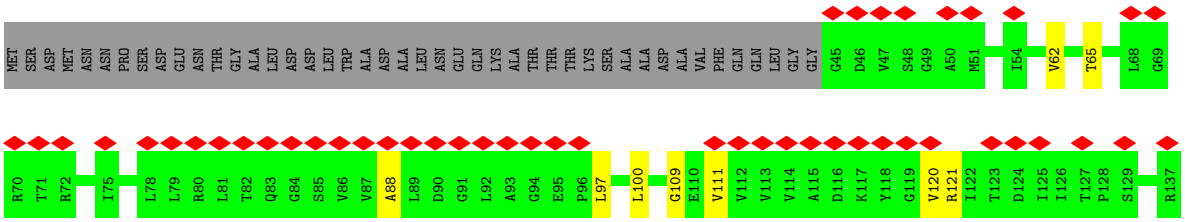
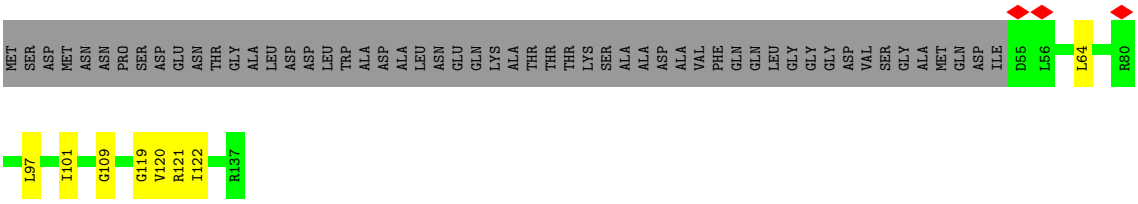


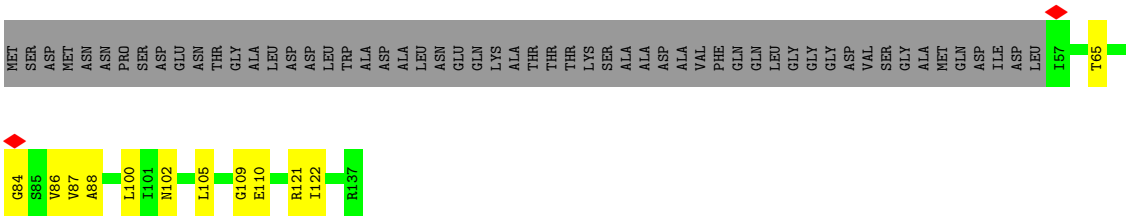
• Molecule 4: Flagellar motor switch protein FliN

Chain FC:



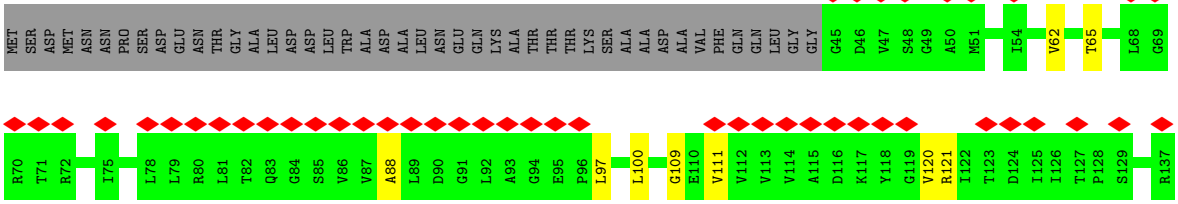
• Molecule 4: Flagellar motor switch protein FliN

Chain GC:



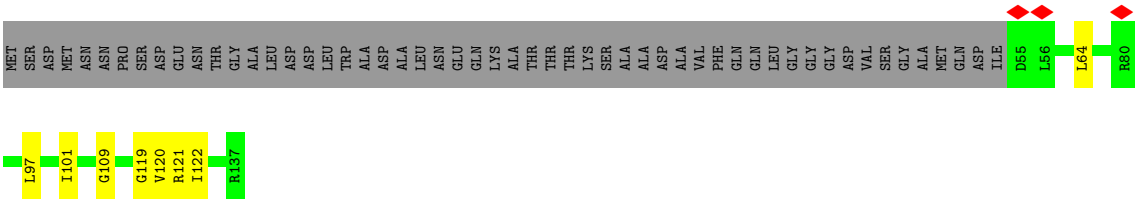
• Molecule 4: Flagellar motor switch protein FliN

Chain KC:



• Molecule 4: Flagellar motor switch protein FliN

Chain LC:



• Molecule 4: Flagellar motor switch protein FliN

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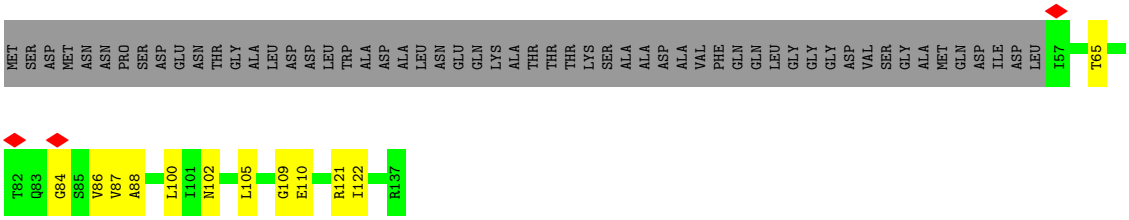
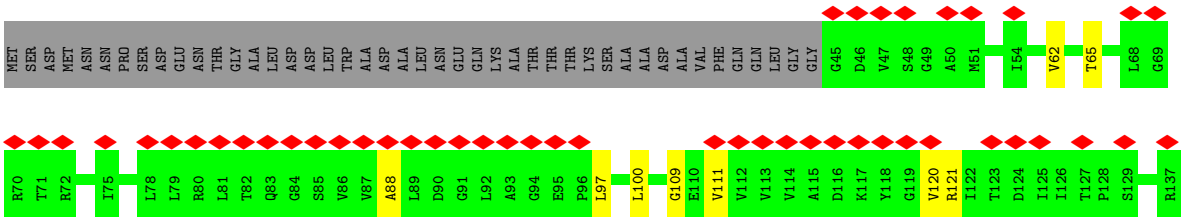


• Molecule 4: Flagellar motor switch protein FliN

Chain QC:



• Molecule 4: Flagellar motor switch protein FliN

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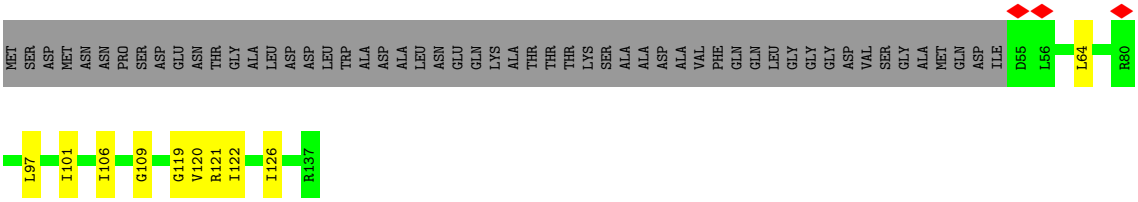

• Molecule 4: Flagellar motor switch protein FliN

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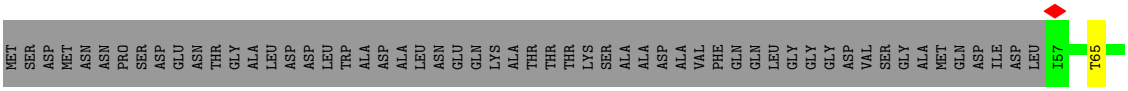
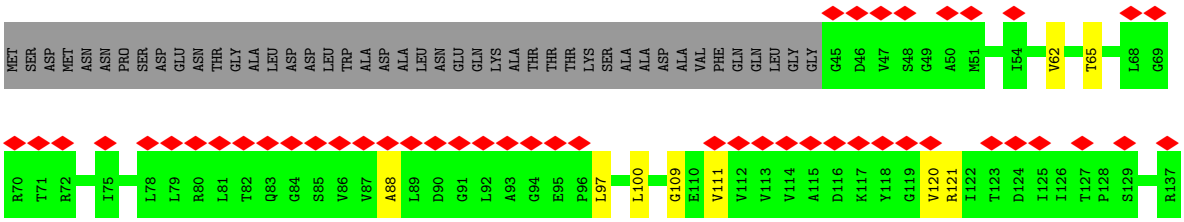


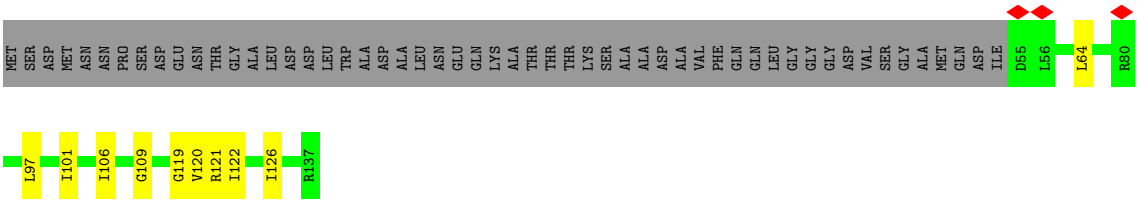
• Molecule 4: Flagellar motor switch protein FliN

Chain WC:



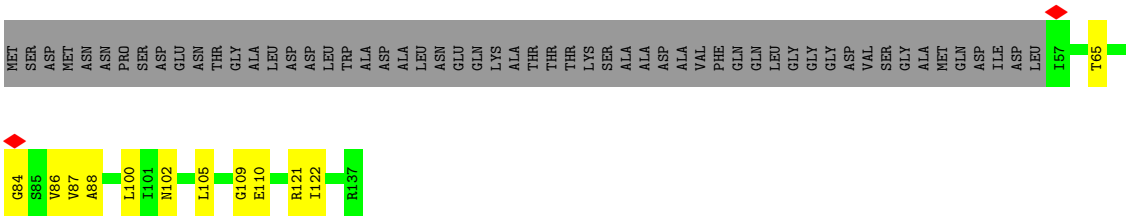
• Molecule 4: Flagellar motor switch protein FliN

Chain XC:



• Molecule 4: Flagellar motor switch protein FliN

Chain YC:



• Molecule 4: Flagellar motor switch protein FliN

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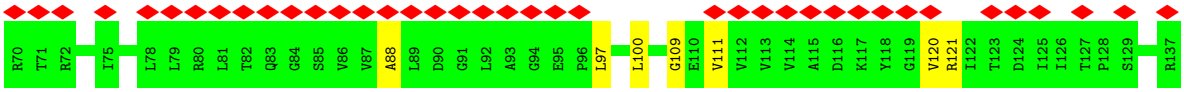
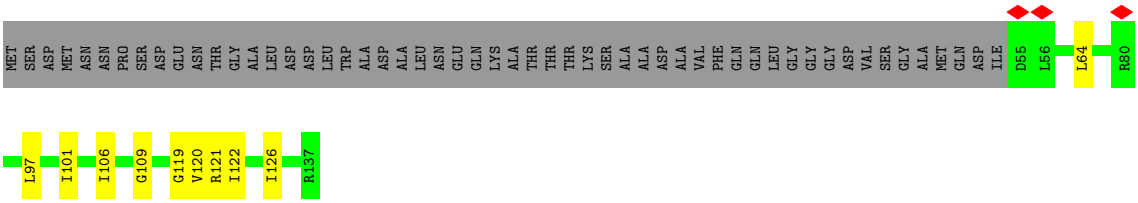


• Molecule 4: Flagellar motor switch protein FliN

Chain DD:



• Molecule 4: Flagellar motor switch protein FliN

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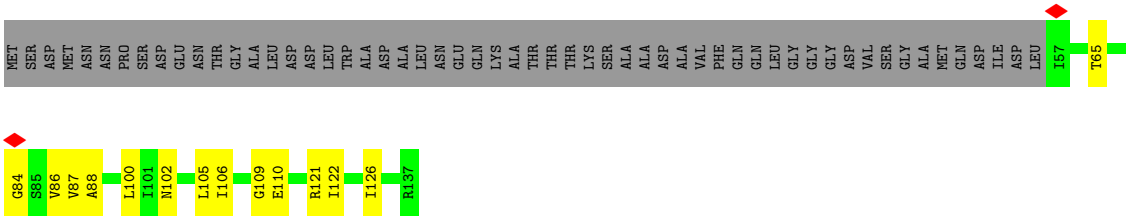

• Molecule 4: Flagellar motor switch protein FliN

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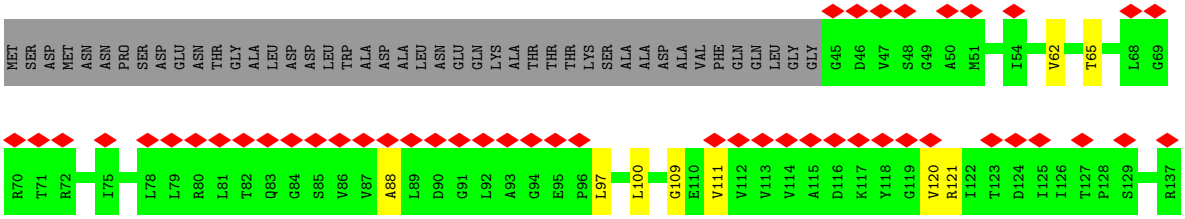

• Molecule 4: Flagellar motor switch protein FliN

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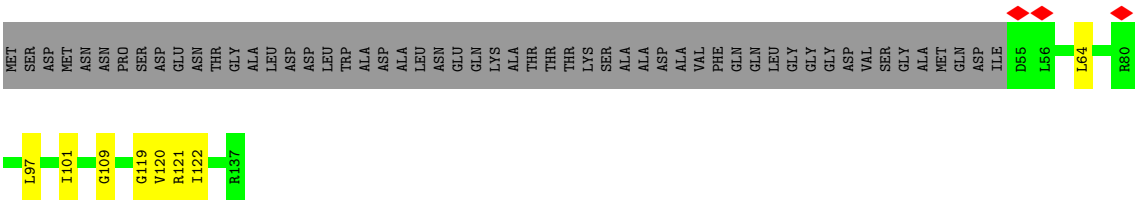

• Molecule 4: Flagellar motor switch protein FliN

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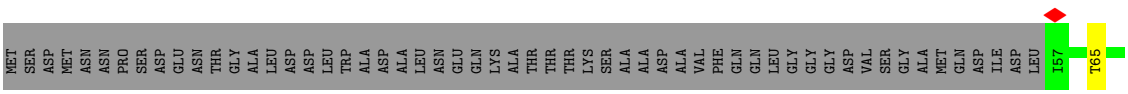

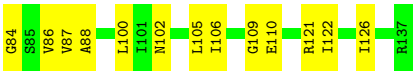

• Molecule 4: Flagellar motor switch protein FliN

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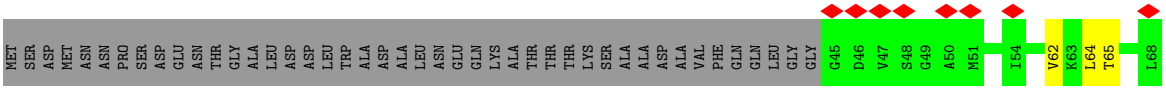
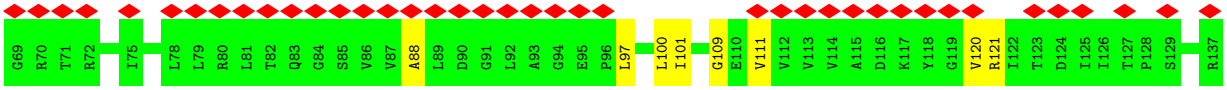
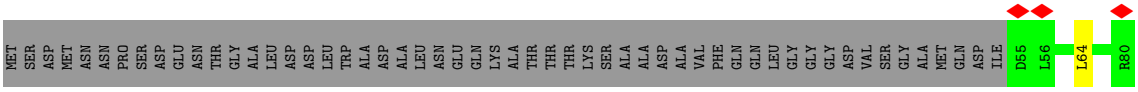
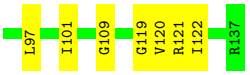




• Molecule 4: Flagellar motor switch protein FliN

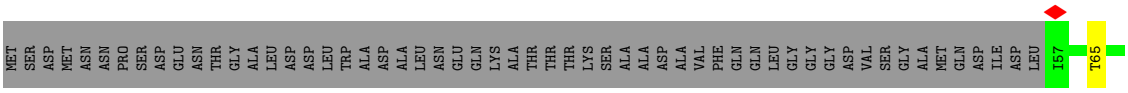
Chain PD:

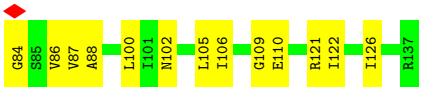




• Molecule 4: Flagellar motor switch protein FliN

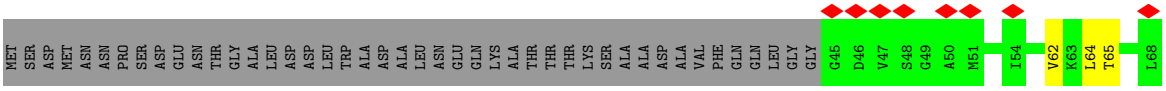
Chain QD:

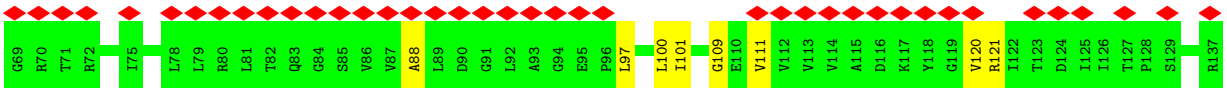




• Molecule 4: Flagellar motor switch protein FliN

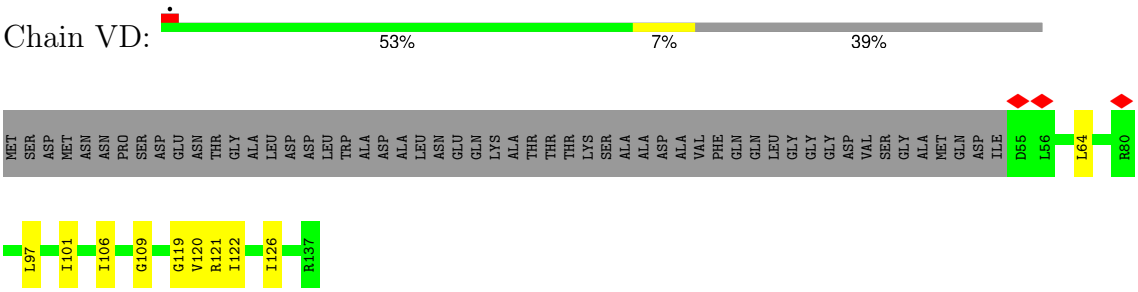
Chain UD:





• Molecule 4: Flagellar motor switch protein FliN

Chain VD:



• Molecule 4: Flagellar motor switch protein FliN

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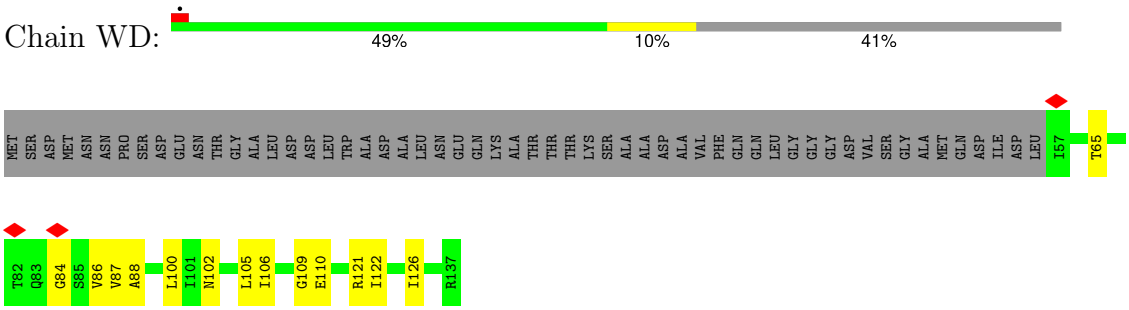
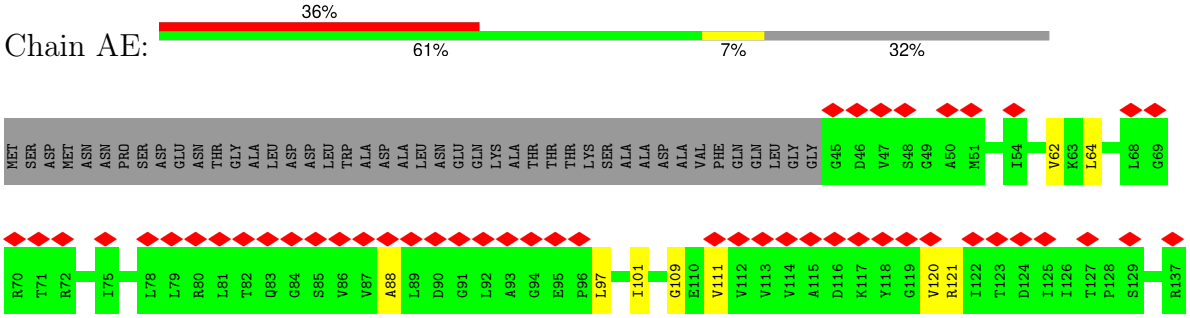


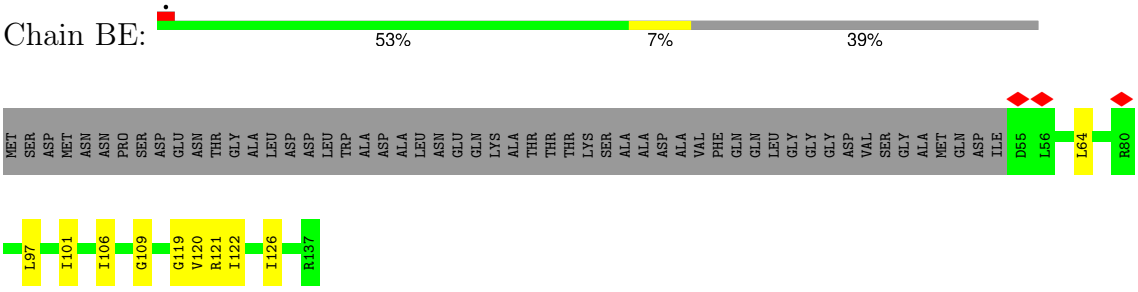
• Molecule 4: Flagellar motor switch protein FliN

Chain AE:



• Molecule 4: Flagellar motor switch protein FliN

Chain BE:



• Molecule 4: Flagellar motor switch protein FliN

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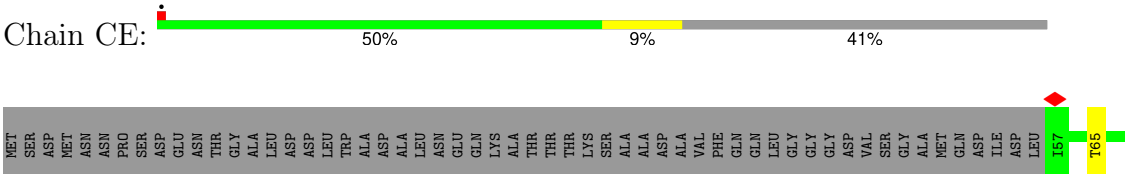
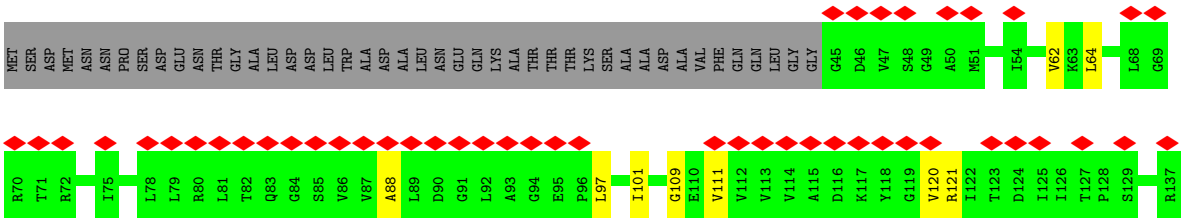


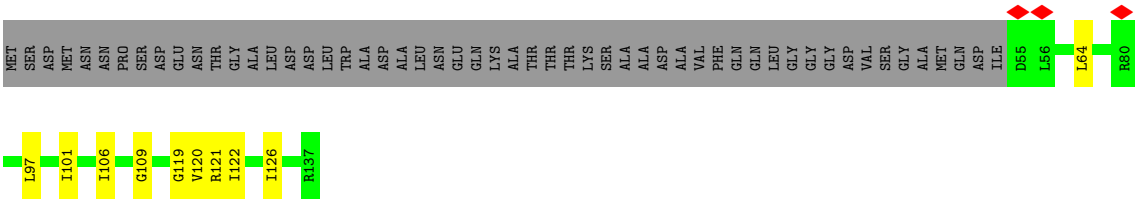
• Molecule 4: Flagellar motor switch protein FliN

Chain GE:



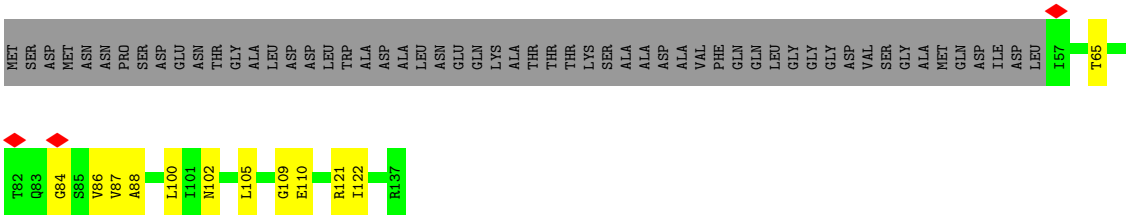
• Molecule 4: Flagellar motor switch protein FliN

Chain HE:



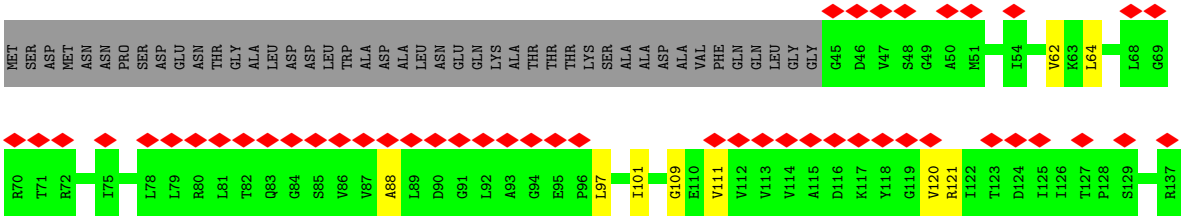
• Molecule 4: Flagellar motor switch protein FliN

Chain IE:



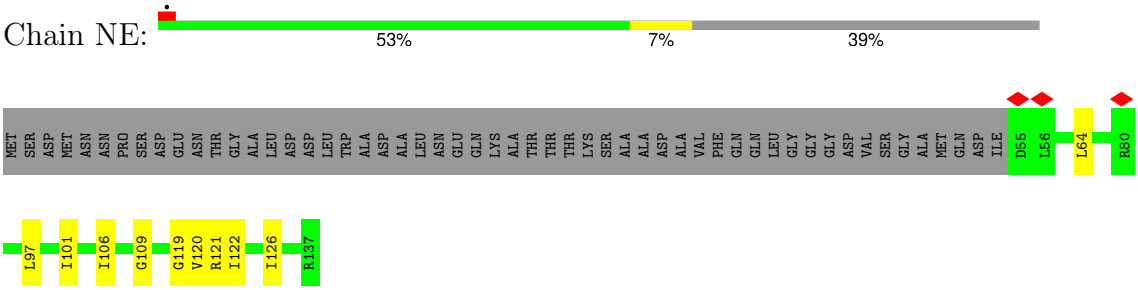
• Molecule 4: Flagellar motor switch protein FliN

Chain ME:



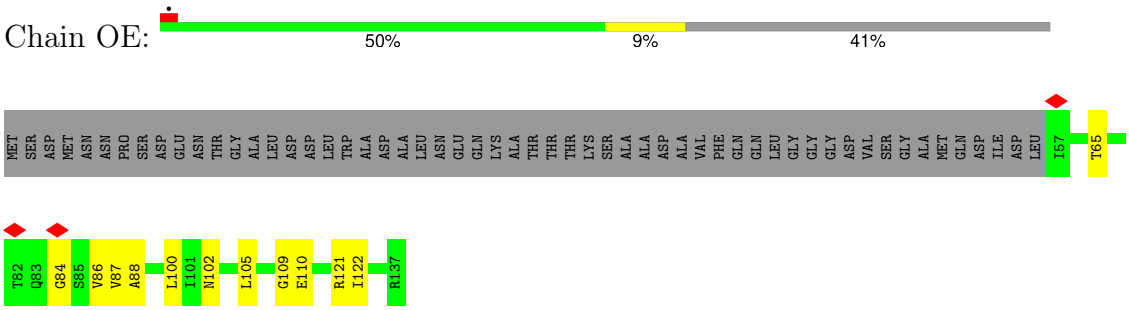
• Molecule 4: Flagellar motor switch protein FliN

Chain NE:



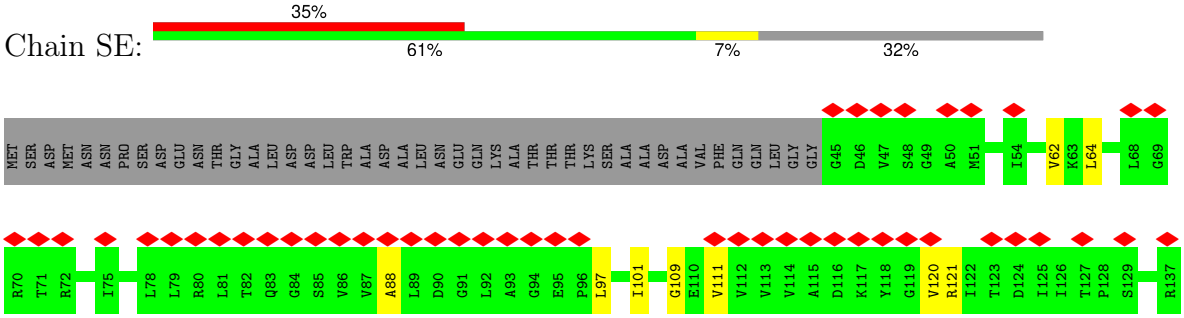
• Molecule 4: Flagellar motor switch protein FliN

Chain OE:



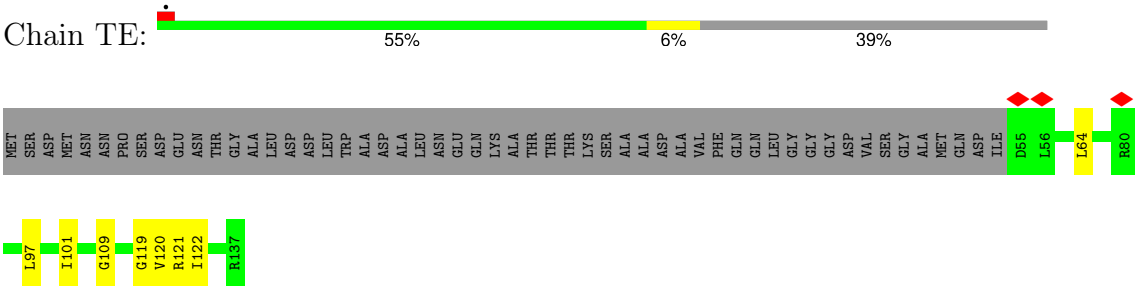
• Molecule 4: Flagellar motor switch protein FliN

Chain SE:



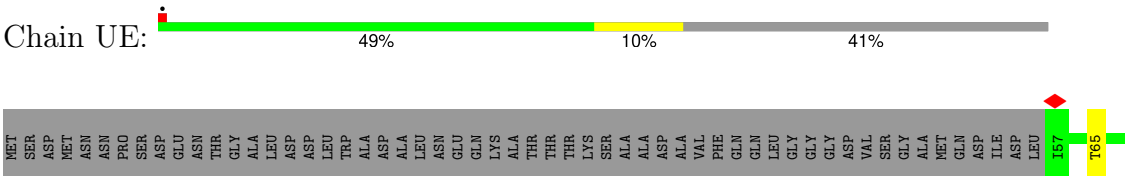
• Molecule 4: Flagellar motor switch protein FliN

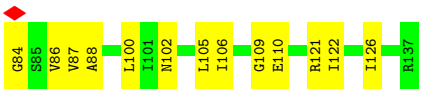
Chain TE:



• Molecule 4: Flagellar motor switch protein FliN

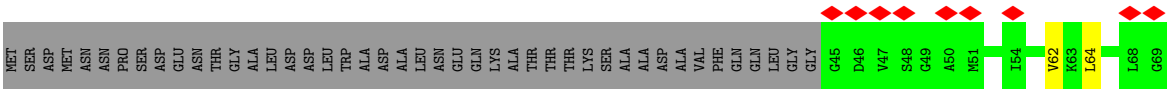
Chain UE:

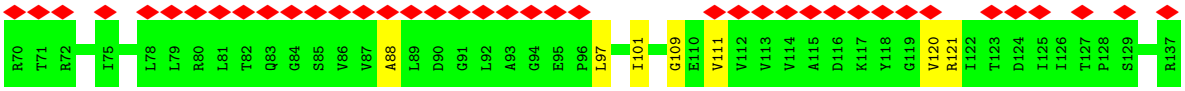




• Molecule 4: Flagellar motor switch protein FliN

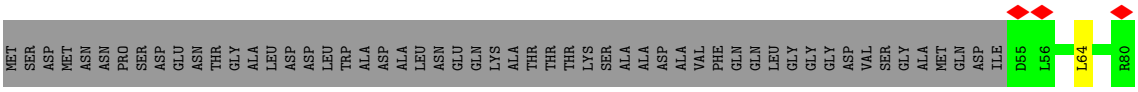
Chain YE:

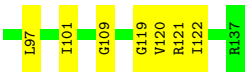




• Molecule 4: Flagellar motor switch protein FliN

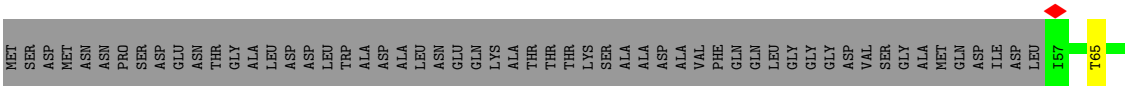
Chain ZE:





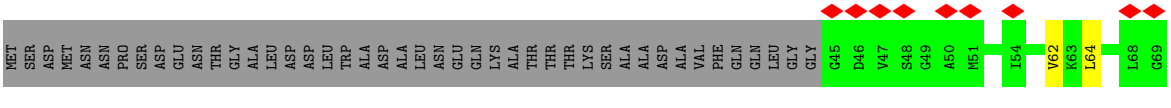
• Molecule 4: Flagellar motor switch protein FliN

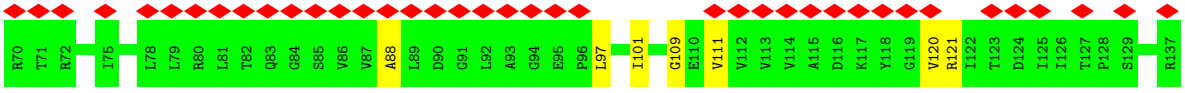
Chain AF:



• Molecule 4: Flagellar motor switch protein FliN

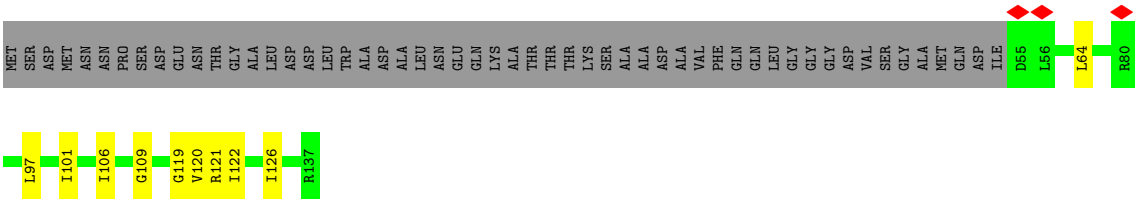
Chain EF:





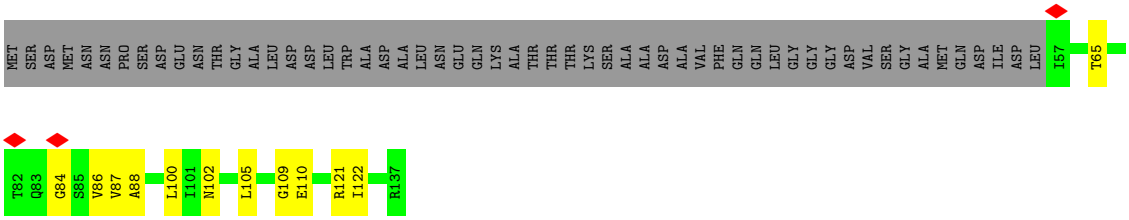
• Molecule 4: Flagellar motor switch protein FliN

Chain FF:



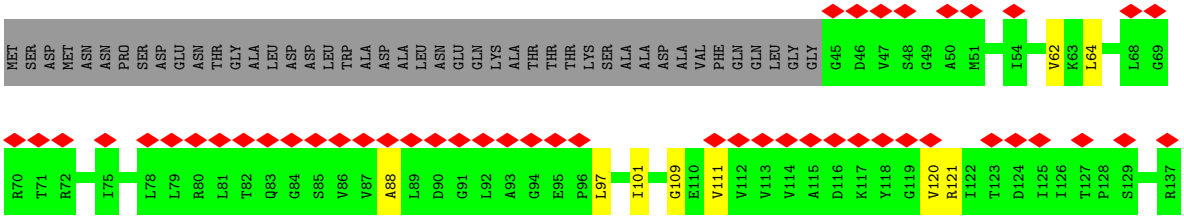
• Molecule 4: Flagellar motor switch protein FliN

Chain GF:



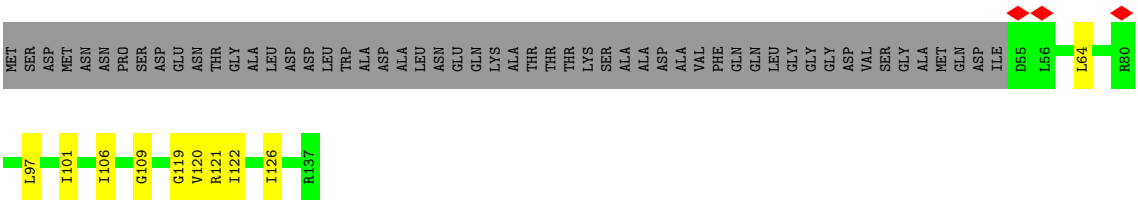
• Molecule 4: Flagellar motor switch protein FliN

Chain KF:



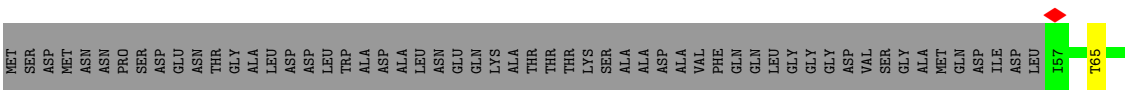
• Molecule 4: Flagellar motor switch protein FliN

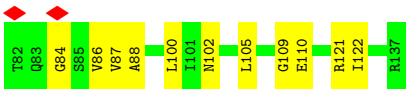
Chain LF:



• Molecule 4: Flagellar motor switch protein FliN

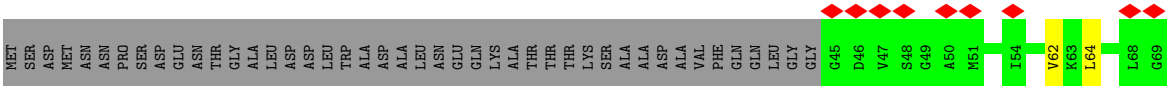
Chain MF:

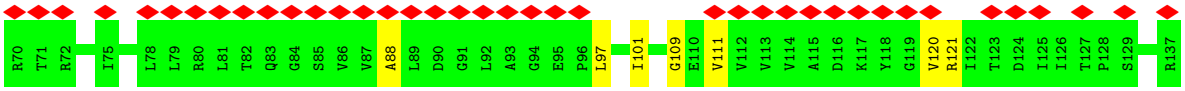




• Molecule 4: Flagellar motor switch protein FliN

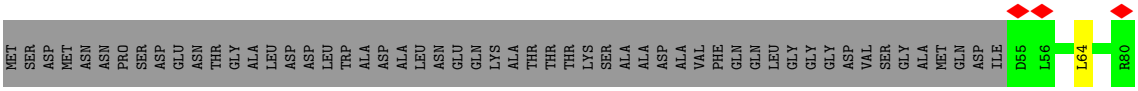
Chain QF:





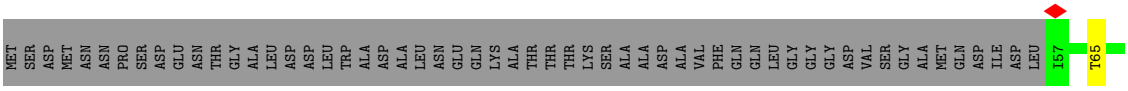
• Molecule 4: Flagellar motor switch protein FliN

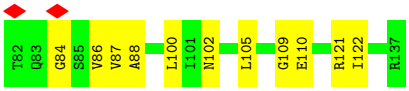
Chain RF:



• Molecule 4: Flagellar motor switch protein FliN

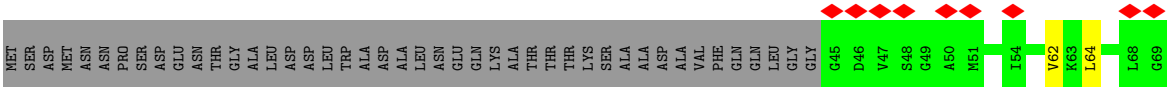
Chain SF:

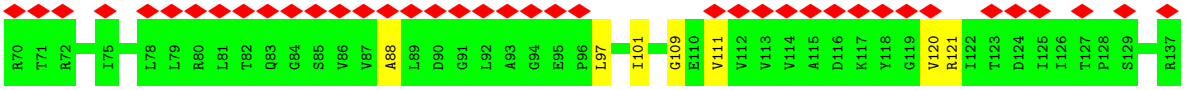




• Molecule 4: Flagellar motor switch protein FliN

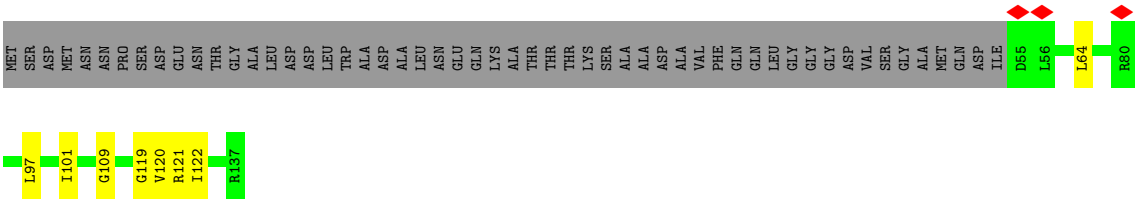
Chain WF:





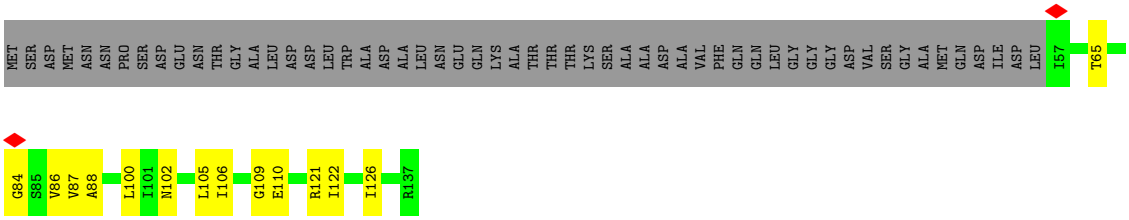
• Molecule 4: Flagellar motor switch protein FliN

Chain XF:



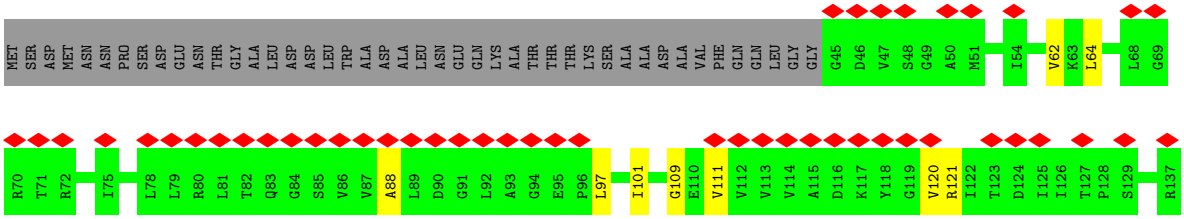
• Molecule 4: Flagellar motor switch protein FliN

Chain YF:



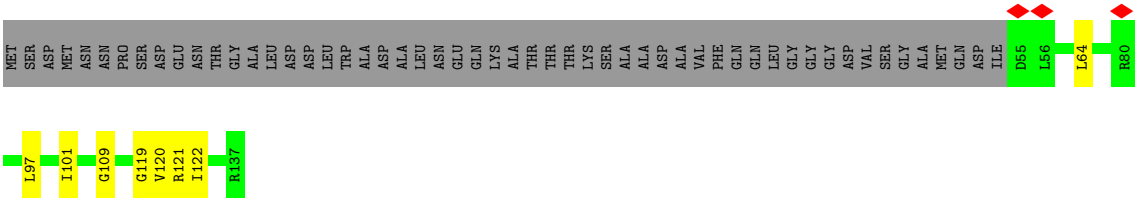
• Molecule 4: Flagellar motor switch protein FliN

Chain CG:



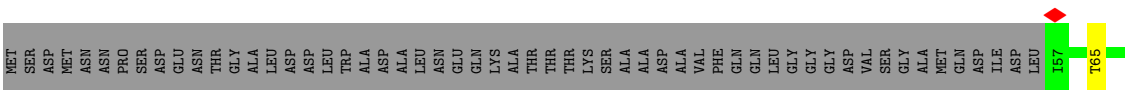
• Molecule 4: Flagellar motor switch protein FliN

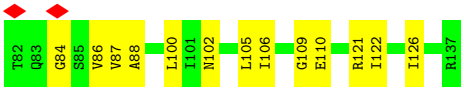
Chain DG:



• Molecule 4: Flagellar motor switch protein FliN

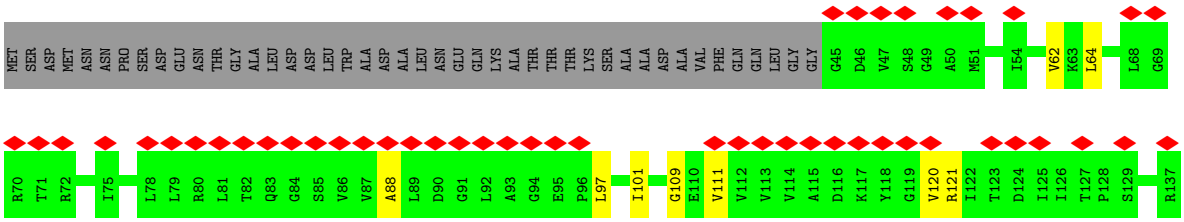
Chain EG:





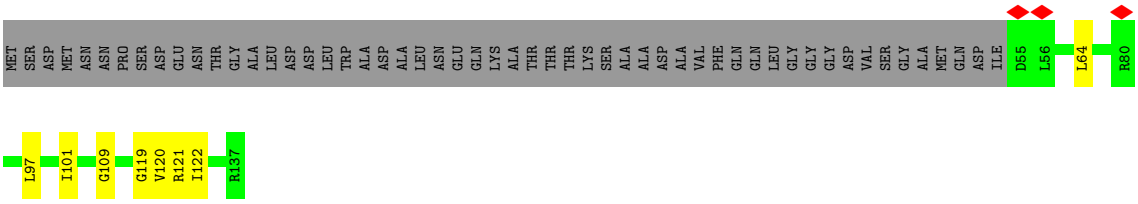
• Molecule 4: Flagellar motor switch protein FliN

Chain IG:



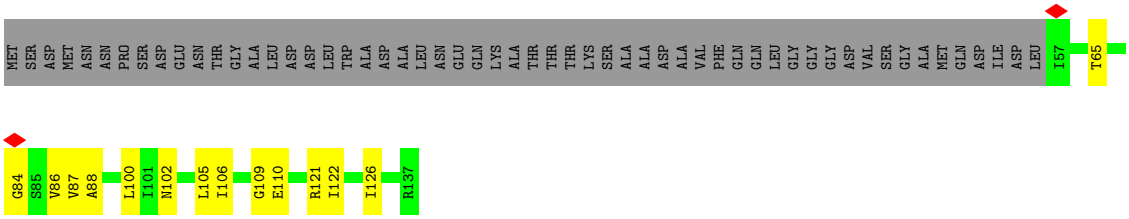
• Molecule 4: Flagellar motor switch protein FliN

Chain JG:



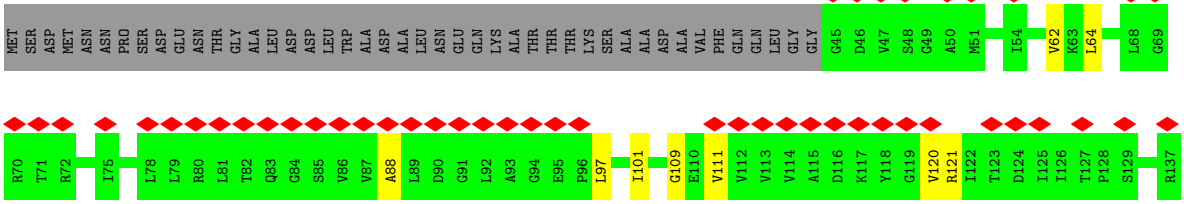
• Molecule 4: Flagellar motor switch protein FliN

Chain KG:



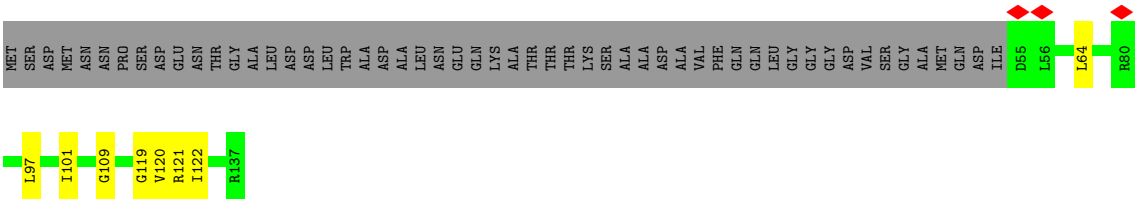
• Molecule 4: Flagellar motor switch protein FliN

Chain OG:



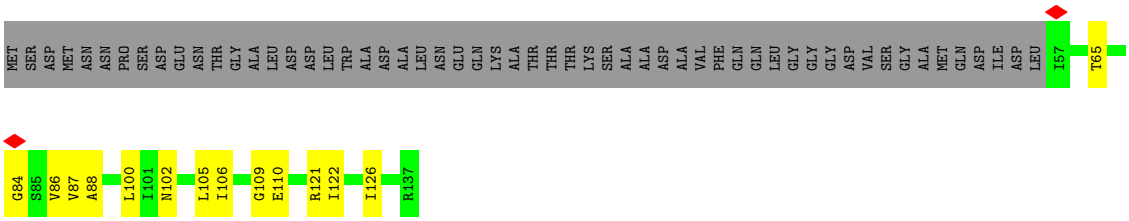
• Molecule 4: Flagellar motor switch protein FliN

Chain PG:



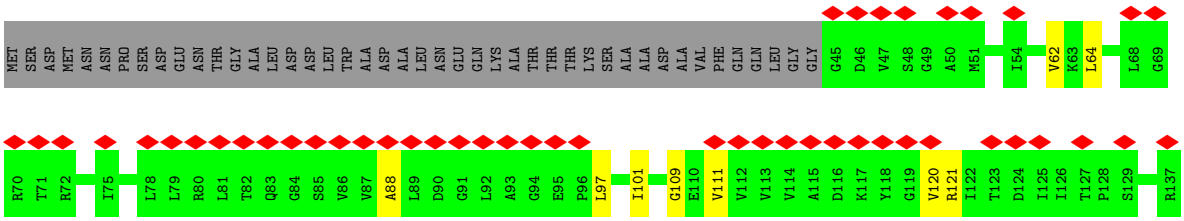
• Molecule 4: Flagellar motor switch protein FliN

Chain QG:



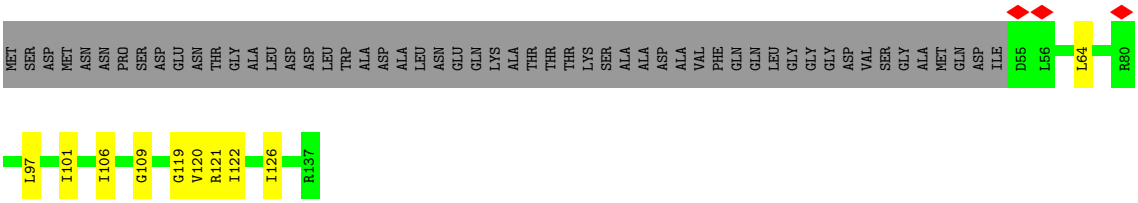
• Molecule 4: Flagellar motor switch protein FliN

Chain UG:



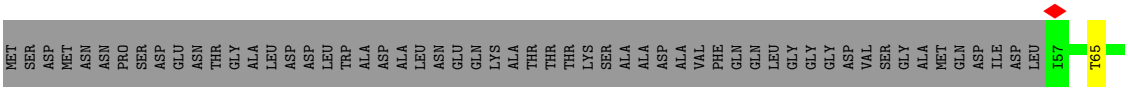
• Molecule 4: Flagellar motor switch protein FliN

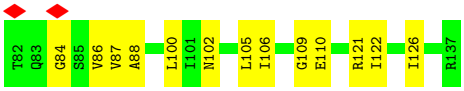
Chain VG:



• Molecule 4: Flagellar motor switch protein FliN

Chain WG:




T82
Q83
G84
S85
V86
V87
A88
L100
I101
N102
L105
I106
G109
E110
R121
I122
I126
R137

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11106	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	59.242	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.283	Depositor
Minimum map value	-0.060	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.175	Depositor
Map size (Å)	1047.04, 1047.04, 1047.04	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.045, 2.045, 2.045	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	A	1.02	0/233	1.25	0/324
1	BC	1.02	0/233	1.25	0/324
1	BF	1.03	0/233	1.26	0/324
1	DB	1.02	0/233	1.26	0/324
1	DE	1.03	0/233	1.25	0/324
1	F	1.02	0/233	1.25	0/324
1	FA	1.02	0/233	1.26	0/324
1	FD	1.02	0/233	1.25	0/324
1	FG	1.02	0/233	1.26	0/324
1	HC	1.03	0/233	1.26	0/324
1	HF	1.02	0/233	1.25	0/324
1	I	1.02	0/233	1.26	0/324
1	JB	1.02	0/233	1.25	0/324
1	JE	1.03	0/233	1.26	0/324
1	LA	1.03	0/233	1.26	0/324
1	LD	1.02	0/233	1.26	0/324
1	LG	1.02	0/233	1.25	0/324
1	NC	1.02	0/233	1.25	0/324
1	NF	1.02	0/233	1.25	0/324
1	PB	1.02	0/233	1.25	0/324
1	PE	1.02	0/233	1.25	0/324
1	RA	1.03	0/233	1.26	0/324
1	RD	1.03	0/233	1.25	0/324
1	RG	1.02	0/233	1.25	0/324
1	S	1.02	0/233	1.25	0/324
1	TC	1.03	0/233	1.25	0/324
1	TF	1.03	0/233	1.25	0/324
1	VB	1.03	0/233	1.25	0/324
1	VE	1.02	0/233	1.25	0/324
1	XA	1.03	0/233	1.25	0/324
1	XD	1.02	0/233	1.25	0/324
1	Z	1.02	0/233	1.25	0/324
1	ZC	1.03	0/233	1.25	0/324
1	ZF	1.03	0/233	1.26	0/324

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	AA	0.72	1/1577 (0.1%)	0.92	5/2195 (0.2%)
2	AD	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	AG	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	B	0.71	1/1577 (0.1%)	0.92	5/2195 (0.2%)
2	CC	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	CF	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	EB	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	EE	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	G	0.71	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	GA	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	GD	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	GG	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	IC	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	IF	0.71	1/1577 (0.1%)	0.92	5/2195 (0.2%)
2	J	0.71	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	KB	0.72	1/1577 (0.1%)	0.92	5/2195 (0.2%)
2	KE	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	MA	0.72	1/1577 (0.1%)	0.92	5/2195 (0.2%)
2	MD	0.71	1/1577 (0.1%)	0.92	5/2195 (0.2%)
2	MG	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	OC	0.71	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	OF	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	QB	0.71	1/1577 (0.1%)	0.92	5/2195 (0.2%)
2	QE	0.71	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	SA	0.71	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	SD	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	SG	0.71	1/1577 (0.1%)	0.92	5/2195 (0.2%)
2	T	0.72	1/1577 (0.1%)	0.92	5/2195 (0.2%)
2	UC	0.71	1/1577 (0.1%)	0.92	5/2195 (0.2%)
2	UF	0.71	1/1577 (0.1%)	0.92	5/2195 (0.2%)
2	WB	0.71	1/1577 (0.1%)	0.92	5/2195 (0.2%)
2	WE	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	YA	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
2	YD	0.72	1/1577 (0.1%)	0.93	5/2195 (0.2%)
3	BA	0.40	0/1419	0.54	0/1976
3	BD	0.40	0/1419	0.54	0/1976
3	BG	0.40	0/1419	0.54	0/1976
3	C	0.40	0/1419	0.54	0/1976
3	DC	0.40	0/1419	0.54	0/1976
3	DF	0.40	0/1419	0.54	0/1976
3	FB	0.40	0/1419	0.54	0/1976
3	FE	0.40	0/1419	0.54	0/1976
3	HA	0.40	0/1419	0.54	0/1976

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	HD	0.40	0/1419	0.54	0/1976
3	HG	0.40	0/1419	0.54	0/1976
3	JC	0.40	0/1419	0.54	0/1976
3	JF	0.40	0/1419	0.54	0/1976
3	K	0.40	0/1419	0.54	0/1976
3	LB	0.40	0/1419	0.54	0/1976
3	LE	0.40	0/1419	0.54	0/1976
3	M	0.40	0/1419	0.54	0/1976
3	NA	0.40	0/1419	0.54	0/1976
3	ND	0.40	0/1419	0.54	0/1976
3	NG	0.40	0/1419	0.55	0/1976
3	PC	0.40	0/1419	0.54	0/1976
3	PF	0.40	0/1419	0.54	0/1976
3	RB	0.40	0/1419	0.54	0/1976
3	RE	0.40	0/1419	0.54	0/1976
3	TA	0.40	0/1419	0.54	0/1976
3	TD	0.40	0/1419	0.54	0/1976
3	TG	0.40	0/1419	0.54	0/1976
3	V	0.40	0/1419	0.54	0/1976
3	VC	0.40	0/1419	0.54	0/1976
3	VF	0.40	0/1419	0.54	0/1976
3	XB	0.40	0/1419	0.54	0/1976
3	XE	0.40	0/1419	0.54	0/1976
3	ZA	0.40	0/1419	0.54	0/1976
3	ZD	0.40	0/1419	0.54	0/1976
4	AB	0.56	0/455	0.65	0/630
4	AC	0.31	0/398	0.42	0/550
4	AE	0.56	0/455	0.65	0/630
4	AF	0.31	0/398	0.42	0/550
4	BB	0.40	0/408	0.49	0/564
4	BE	0.40	0/408	0.49	0/564
4	CA	0.56	0/455	0.65	0/630
4	CB	0.31	0/398	0.42	0/550
4	CD	0.55	0/455	0.65	0/630
4	CE	0.31	0/398	0.42	0/550
4	CG	0.56	0/455	0.66	0/630
4	D	0.55	0/455	0.65	0/630
4	DA	0.40	0/408	0.48	0/564
4	DD	0.40	0/408	0.49	0/564
4	DG	0.40	0/408	0.49	0/564
4	E	0.40	0/408	0.49	0/564
4	EA	0.31	0/398	0.42	0/550
4	EC	0.56	0/455	0.66	0/630

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	ED	0.31	0/398	0.42	0/550
4	EF	0.55	0/455	0.65	0/630
4	EG	0.31	0/398	0.42	0/550
4	FC	0.40	0/408	0.48	0/564
4	FF	0.40	0/408	0.49	0/564
4	GB	0.55	0/455	0.65	0/630
4	GC	0.31	0/398	0.42	0/550
4	GE	0.56	0/455	0.65	0/630
4	GF	0.31	0/398	0.42	0/550
4	H	0.31	0/398	0.42	0/550
4	HB	0.40	0/408	0.48	0/564
4	HE	0.40	0/408	0.49	0/564
4	IA	0.55	0/455	0.65	0/630
4	IB	0.31	0/398	0.42	0/550
4	ID	0.55	0/455	0.66	0/630
4	IE	0.31	0/398	0.42	0/550
4	IG	0.55	0/455	0.65	0/630
4	JA	0.40	0/408	0.49	0/564
4	JD	0.40	0/408	0.49	0/564
4	JG	0.40	0/408	0.49	0/564
4	KA	0.31	0/398	0.42	0/550
4	KC	0.55	0/455	0.66	0/630
4	KD	0.31	0/398	0.42	0/550
4	KF	0.55	0/455	0.66	0/630
4	KG	0.31	0/398	0.42	0/550
4	L	0.56	0/455	0.66	0/630
4	LC	0.40	0/408	0.49	0/564
4	LF	0.40	0/408	0.49	0/564
4	MB	0.56	0/455	0.65	0/630
4	MC	0.31	0/398	0.42	0/550
4	ME	0.56	0/455	0.65	0/630
4	MF	0.31	0/398	0.42	0/550
4	N	0.55	0/455	0.65	0/630
4	NB	0.40	0/408	0.49	0/564
4	NE	0.40	0/408	0.49	0/564
4	O	0.40	0/408	0.48	0/564
4	OA	0.55	0/455	0.65	0/630
4	OB	0.31	0/398	0.42	0/550
4	OD	0.55	0/455	0.65	0/630
4	OE	0.31	0/398	0.42	0/550
4	OG	0.55	0/455	0.66	0/630
4	P	0.40	0/408	0.49	0/564
4	PA	0.40	0/408	0.49	0/564

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	PD	0.40	0/408	0.48	0/564
4	PG	0.40	0/408	0.49	0/564
4	Q	0.31	0/398	0.42	0/550
4	QA	0.31	0/398	0.42	0/550
4	QC	0.56	0/455	0.65	0/630
4	QD	0.31	0/398	0.42	0/550
4	QF	0.56	0/455	0.65	0/630
4	QG	0.31	0/398	0.42	0/550
4	R	0.31	0/398	0.42	0/550
4	RC	0.40	0/408	0.49	0/564
4	RF	0.40	0/408	0.49	0/564
4	SB	0.56	0/455	0.65	0/630
4	SC	0.31	0/398	0.42	0/550
4	SE	0.56	0/455	0.65	0/630
4	SF	0.31	0/398	0.42	0/550
4	TB	0.40	0/408	0.49	0/564
4	TE	0.40	0/408	0.49	0/564
4	UA	0.55	0/455	0.65	0/630
4	UB	0.31	0/398	0.42	0/550
4	UD	0.56	0/455	0.65	0/630
4	UE	0.30	0/398	0.42	0/550
4	UG	0.55	0/455	0.65	0/630
4	VA	0.40	0/408	0.48	0/564
4	VD	0.40	0/408	0.49	0/564
4	VG	0.40	0/408	0.48	0/564
4	W	0.56	0/455	0.65	0/630
4	WA	0.31	0/398	0.42	0/550
4	WC	0.55	0/455	0.65	0/630
4	WD	0.31	0/398	0.42	0/550
4	WF	0.55	0/455	0.65	0/630
4	WG	0.31	0/398	0.42	0/550
4	X	0.40	0/408	0.49	0/564
4	XC	0.40	0/408	0.49	0/564
4	XF	0.40	0/408	0.49	0/564
4	Y	0.31	0/398	0.42	0/550
4	YB	0.56	0/455	0.66	0/630
4	YC	0.31	0/398	0.42	0/550
4	YE	0.56	0/455	0.66	0/630
4	YF	0.31	0/398	0.42	0/550
4	ZB	0.40	0/408	0.49	0/564
4	ZE	0.40	0/408	0.49	0/564
All	All	0.58	34/152660 (0.0%)	0.75	170/212126 (0.1%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	SG	207	LYS	C-N	-6.61	1.25	1.33
2	CC	207	LYS	C-N	-6.59	1.25	1.33
2	AG	207	LYS	C-N	-6.59	1.25	1.33
2	GD	207	LYS	C-N	-6.59	1.25	1.33
2	YA	207	LYS	C-N	-6.58	1.25	1.33
2	WE	207	LYS	C-N	-6.58	1.25	1.33
2	AA	207	LYS	C-N	-6.58	1.25	1.33
2	UC	207	LYS	C-N	-6.58	1.25	1.33
2	EE	207	LYS	C-N	-6.58	1.25	1.33
2	T	207	LYS	C-N	-6.57	1.25	1.33
2	QB	207	LYS	C-N	-6.57	1.25	1.33
2	IC	207	LYS	C-N	-6.57	1.25	1.33
2	GG	207	LYS	C-N	-6.57	1.25	1.33
2	KB	207	LYS	C-N	-6.56	1.25	1.33
2	QE	207	LYS	C-N	-6.55	1.25	1.33
2	B	207	LYS	C-N	-6.55	1.25	1.33
2	OC	207	LYS	C-N	-6.55	1.25	1.33
2	MD	207	LYS	C-N	-6.55	1.25	1.33
2	MG	207	LYS	C-N	-6.55	1.25	1.33
2	EB	207	LYS	C-N	-6.54	1.25	1.33
2	G	207	LYS	C-N	-6.53	1.25	1.33
2	MA	207	LYS	C-N	-6.53	1.25	1.33
2	AD	207	LYS	C-N	-6.53	1.25	1.33
2	SD	207	LYS	C-N	-6.53	1.25	1.33
2	YD	207	LYS	C-N	-6.53	1.25	1.33
2	KE	207	LYS	C-N	-6.53	1.25	1.33
2	GA	207	LYS	C-N	-6.53	1.25	1.33
2	OF	207	LYS	C-N	-6.52	1.25	1.33
2	SA	207	LYS	C-N	-6.52	1.25	1.33
2	IF	207	LYS	C-N	-6.51	1.25	1.33
2	WB	207	LYS	C-N	-6.51	1.25	1.33
2	CF	207	LYS	C-N	-6.51	1.25	1.33
2	UF	207	LYS	C-N	-6.51	1.25	1.33
2	J	207	LYS	C-N	-6.49	1.25	1.33

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	IC	186	GLN	N-CA-C	-7.41	103.38	114.64
2	SG	186	GLN	N-CA-C	-7.40	103.39	114.64
2	UC	186	GLN	N-CA-C	-7.38	103.42	114.64
2	SD	186	GLN	N-CA-C	-7.38	103.43	114.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	YA	186	GLN	N-CA-C	-7.37	103.43	114.64
2	WE	186	GLN	N-CA-C	-7.37	103.44	114.64
2	B	186	GLN	N-CA-C	-7.37	103.44	114.64
2	GA	186	GLN	N-CA-C	-7.37	103.45	114.64
2	OC	186	GLN	N-CA-C	-7.37	103.44	114.64
2	EE	186	GLN	N-CA-C	-7.37	103.45	114.64
2	IF	186	GLN	N-CA-C	-7.37	103.44	114.64
2	MG	186	GLN	N-CA-C	-7.37	103.44	114.64
2	AA	186	GLN	N-CA-C	-7.36	103.45	114.64
2	QB	186	GLN	N-CA-C	-7.36	103.45	114.64
2	AD	186	GLN	N-CA-C	-7.36	103.45	114.64
2	UF	186	GLN	N-CA-C	-7.36	103.45	114.64
2	MA	186	GLN	N-CA-C	-7.36	103.45	114.64
2	KE	186	GLN	N-CA-C	-7.36	103.45	114.64
2	CF	186	GLN	N-CA-C	-7.36	103.46	114.64
2	QE	186	GLN	N-CA-C	-7.35	103.46	114.64
2	T	186	GLN	N-CA-C	-7.35	103.46	114.64
2	GD	186	GLN	N-CA-C	-7.35	103.47	114.64
2	AG	186	GLN	N-CA-C	-7.35	103.47	114.64
2	GG	186	GLN	N-CA-C	-7.35	103.47	114.64
2	CC	186	GLN	N-CA-C	-7.35	103.47	114.64
2	WB	186	GLN	N-CA-C	-7.34	103.48	114.64
2	J	186	GLN	N-CA-C	-7.34	103.49	114.64
2	EB	186	GLN	N-CA-C	-7.34	103.49	114.64
2	G	186	GLN	N-CA-C	-7.33	103.49	114.64
2	YD	186	GLN	N-CA-C	-7.33	103.49	114.64
2	OF	186	GLN	N-CA-C	-7.33	103.50	114.64
2	MD	186	GLN	N-CA-C	-7.33	103.50	114.64
2	SA	186	GLN	N-CA-C	-7.32	103.51	114.64
2	KB	186	GLN	N-CA-C	-7.32	103.51	114.64
2	KE	192	LYS	N-CA-C	-6.83	104.90	113.23
2	G	192	LYS	N-CA-C	-6.82	104.91	113.23
2	AD	192	LYS	N-CA-C	-6.82	104.91	113.23
2	UC	192	LYS	N-CA-C	-6.82	104.92	113.23
2	CF	192	LYS	N-CA-C	-6.81	104.92	113.23
2	MD	192	LYS	N-CA-C	-6.81	104.92	113.23
2	IC	192	LYS	N-CA-C	-6.80	104.93	113.23
2	SG	192	LYS	N-CA-C	-6.80	104.93	113.23
2	KB	192	LYS	N-CA-C	-6.80	104.93	113.23
2	QB	192	LYS	N-CA-C	-6.80	104.93	113.23
2	QE	192	LYS	N-CA-C	-6.80	104.93	113.23
2	IF	192	LYS	N-CA-C	-6.80	104.93	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	YD	192	LYS	N-CA-C	-6.80	104.93	113.23
2	J	192	LYS	N-CA-C	-6.80	104.94	113.23
2	YA	192	LYS	N-CA-C	-6.80	104.94	113.23
2	OC	192	LYS	N-CA-C	-6.80	104.94	113.23
2	T	192	LYS	N-CA-C	-6.79	104.94	113.23
2	SD	192	LYS	N-CA-C	-6.79	104.94	113.23
2	AA	192	LYS	N-CA-C	-6.79	104.95	113.23
2	B	192	LYS	N-CA-C	-6.78	104.96	113.23
2	GD	192	LYS	N-CA-C	-6.78	104.96	113.23
2	WE	192	LYS	N-CA-C	-6.78	104.96	113.23
2	GG	192	LYS	N-CA-C	-6.78	104.96	113.23
2	CC	192	LYS	N-CA-C	-6.77	104.97	113.23
2	OF	192	LYS	N-CA-C	-6.77	104.97	113.23
2	SA	192	LYS	N-CA-C	-6.77	104.97	113.23
2	GA	192	LYS	N-CA-C	-6.76	104.98	113.23
2	MA	192	LYS	N-CA-C	-6.76	104.98	113.23
2	MG	192	LYS	N-CA-C	-6.76	104.98	113.23
2	EB	192	LYS	N-CA-C	-6.76	104.98	113.23
2	WB	192	LYS	N-CA-C	-6.75	104.99	113.23
2	UF	192	LYS	N-CA-C	-6.75	104.99	113.23
2	AG	192	LYS	N-CA-C	-6.75	105.00	113.23
2	EE	192	LYS	N-CA-C	-6.74	105.00	113.23
2	SA	207	LYS	O-C-N	-5.87	116.10	122.79
2	UF	207	LYS	O-C-N	-5.84	116.13	122.79
2	IF	207	LYS	O-C-N	-5.84	116.13	122.79
2	OC	207	LYS	O-C-N	-5.83	116.14	122.79
2	QE	207	LYS	O-C-N	-5.83	116.14	122.79
2	CF	207	LYS	O-C-N	-5.83	116.14	122.79
2	GA	207	LYS	O-C-N	-5.83	116.15	122.79
2	WB	207	LYS	O-C-N	-5.83	116.15	122.79
2	CC	207	LYS	O-C-N	-5.82	116.16	122.79
2	AG	207	LYS	O-C-N	-5.82	116.16	122.79
2	YD	207	LYS	O-C-N	-5.81	116.16	122.79
2	OF	207	LYS	O-C-N	-5.81	116.16	122.79
2	B	207	LYS	O-C-N	-5.81	116.17	122.79
2	AA	207	LYS	O-C-N	-5.81	116.17	122.79
2	J	207	LYS	O-C-N	-5.80	116.18	122.79
2	MA	207	LYS	O-C-N	-5.80	116.18	122.79
2	KE	207	LYS	O-C-N	-5.80	116.18	122.79
2	QB	207	LYS	O-C-N	-5.79	116.19	122.79
2	T	207	LYS	O-C-N	-5.79	116.19	122.79
2	YA	207	LYS	O-C-N	-5.79	116.19	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	WE	207	LYS	O-C-N	-5.79	116.19	122.79
2	EB	207	LYS	O-C-N	-5.78	116.20	122.79
2	KB	207	LYS	O-C-N	-5.78	116.21	122.79
2	MD	207	LYS	O-C-N	-5.77	116.21	122.79
2	EE	207	LYS	O-C-N	-5.77	116.21	122.79
2	SG	207	LYS	O-C-N	-5.77	116.21	122.79
2	G	207	LYS	O-C-N	-5.77	116.21	122.79
2	IC	207	LYS	O-C-N	-5.77	116.21	122.79
2	AD	207	LYS	O-C-N	-5.77	116.21	122.79
2	GG	207	LYS	O-C-N	-5.77	116.21	122.79
2	SD	207	LYS	O-C-N	-5.77	116.21	122.79
2	UC	207	LYS	O-C-N	-5.77	116.21	122.79
2	MG	207	LYS	O-C-N	-5.76	116.23	122.79
2	SA	190	ARG	CA-C-N	-5.74	114.66	123.04
2	SA	190	ARG	C-N-CA	-5.74	114.66	123.04
2	YA	190	ARG	CA-C-N	-5.74	114.67	123.04
2	YA	190	ARG	C-N-CA	-5.74	114.67	123.04
2	QB	190	ARG	CA-C-N	-5.73	114.67	123.04
2	QB	190	ARG	C-N-CA	-5.73	114.67	123.04
2	WB	190	ARG	CA-C-N	-5.73	114.67	123.04
2	WB	190	ARG	C-N-CA	-5.73	114.67	123.04
2	GD	190	ARG	CA-C-N	-5.73	114.67	123.04
2	GD	190	ARG	C-N-CA	-5.73	114.67	123.04
2	IF	190	ARG	CA-C-N	-5.73	114.68	123.04
2	IF	190	ARG	C-N-CA	-5.73	114.68	123.04
2	J	190	ARG	CA-C-N	-5.72	114.69	123.04
2	J	190	ARG	C-N-CA	-5.72	114.69	123.04
2	AD	190	ARG	CA-C-N	-5.72	114.69	123.04
2	AD	190	ARG	C-N-CA	-5.72	114.69	123.04
2	MG	190	ARG	CA-C-N	-5.72	114.69	123.04
2	MG	190	ARG	C-N-CA	-5.72	114.69	123.04
2	QE	190	ARG	CA-C-N	-5.72	114.69	123.04
2	QE	190	ARG	C-N-CA	-5.72	114.69	123.04
2	AA	190	ARG	CA-C-N	-5.72	114.69	123.04
2	AA	190	ARG	C-N-CA	-5.72	114.69	123.04
2	GD	207	LYS	O-C-N	-5.72	116.27	122.79
2	YD	190	ARG	CA-C-N	-5.72	114.69	123.04
2	YD	190	ARG	C-N-CA	-5.72	114.69	123.04
2	SG	190	ARG	CA-C-N	-5.72	114.69	123.04
2	SG	190	ARG	C-N-CA	-5.72	114.69	123.04
2	SD	190	ARG	CA-C-N	-5.71	114.70	123.04
2	SD	190	ARG	C-N-CA	-5.71	114.70	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	WE	190	ARG	CA-C-N	-5.71	114.70	123.04
2	WE	190	ARG	C-N-CA	-5.71	114.70	123.04
2	B	190	ARG	CA-C-N	-5.71	114.70	123.04
2	B	190	ARG	C-N-CA	-5.71	114.70	123.04
2	CF	190	ARG	CA-C-N	-5.71	114.71	123.04
2	CF	190	ARG	C-N-CA	-5.71	114.71	123.04
2	UF	190	ARG	CA-C-N	-5.71	114.71	123.04
2	UF	190	ARG	C-N-CA	-5.71	114.71	123.04
2	EE	190	ARG	CA-C-N	-5.71	114.71	123.04
2	EE	190	ARG	C-N-CA	-5.71	114.71	123.04
2	KE	190	ARG	CA-C-N	-5.70	114.71	123.04
2	KE	190	ARG	C-N-CA	-5.70	114.71	123.04
2	OF	190	ARG	CA-C-N	-5.70	114.71	123.04
2	OF	190	ARG	C-N-CA	-5.70	114.71	123.04
2	KB	190	ARG	CA-C-N	-5.70	114.72	123.04
2	KB	190	ARG	C-N-CA	-5.70	114.72	123.04
2	AG	190	ARG	CA-C-N	-5.70	114.72	123.04
2	AG	190	ARG	C-N-CA	-5.70	114.72	123.04
2	UC	190	ARG	CA-C-N	-5.70	114.72	123.04
2	UC	190	ARG	C-N-CA	-5.70	114.72	123.04
2	MD	190	ARG	CA-C-N	-5.70	114.72	123.04
2	MD	190	ARG	C-N-CA	-5.70	114.72	123.04
2	T	190	ARG	CA-C-N	-5.69	114.74	123.04
2	T	190	ARG	C-N-CA	-5.69	114.74	123.04
2	EB	190	ARG	CA-C-N	-5.69	114.74	123.04
2	EB	190	ARG	C-N-CA	-5.69	114.74	123.04
2	MA	190	ARG	CA-C-N	-5.68	114.74	123.04
2	MA	190	ARG	C-N-CA	-5.68	114.74	123.04
2	OC	190	ARG	CA-C-N	-5.68	114.75	123.04
2	OC	190	ARG	C-N-CA	-5.68	114.75	123.04
2	GA	190	ARG	CA-C-N	-5.68	114.75	123.04
2	GA	190	ARG	C-N-CA	-5.68	114.75	123.04
2	G	190	ARG	CA-C-N	-5.68	114.75	123.04
2	G	190	ARG	C-N-CA	-5.68	114.75	123.04
2	CC	190	ARG	CA-C-N	-5.67	114.76	123.04
2	CC	190	ARG	C-N-CA	-5.67	114.76	123.04
2	IC	190	ARG	CA-C-N	-5.67	114.76	123.04
2	IC	190	ARG	C-N-CA	-5.67	114.76	123.04
2	GG	190	ARG	CA-C-N	-5.67	114.76	123.04
2	GG	190	ARG	C-N-CA	-5.67	114.76	123.04

There are no chirality outliers.

There are no planarity outliers.

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	A	234	0	102	1	0
1	BC	234	0	102	1	0
1	BF	234	0	102	1	0
1	DB	234	0	102	1	0
1	DE	234	0	102	1	0
1	F	234	0	102	1	0
1	FA	234	0	102	1	0
1	FD	234	0	102	1	0
1	FG	234	0	102	1	0
1	HC	234	0	102	1	0
1	HF	234	0	102	1	0
1	I	234	0	102	1	0
1	JB	234	0	102	1	0
1	JE	234	0	102	1	0
1	LA	234	0	102	1	0
1	LD	234	0	102	1	0
1	LG	234	0	102	1	0
1	NC	234	0	102	1	0
1	NF	234	0	102	1	0
1	PB	234	0	102	1	0
1	PE	234	0	102	1	0
1	RA	234	0	102	1	0
1	RD	234	0	102	1	0
1	RG	234	0	102	1	0
1	S	234	0	102	1	0
1	TC	234	0	102	1	0
1	TF	234	0	102	1	0
1	VB	234	0	102	1	0
1	VE	234	0	102	1	0
1	XA	234	0	102	1	0
1	XD	234	0	102	1	0
1	Z	234	0	102	1	0
1	ZC	234	0	102	1	0
1	ZF	234	0	102	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AA	1579	0	738	50	0
2	AD	1579	0	738	49	0
2	AG	1579	0	738	49	0
2	B	1579	0	738	49	0
2	CC	1579	0	738	49	0
2	CF	1579	0	738	48	0
2	EB	1579	0	738	50	0
2	EE	1579	0	738	48	0
2	G	1579	0	738	49	0
2	GA	1579	0	738	51	0
2	GD	1579	0	738	51	0
2	GG	1579	0	738	48	0
2	IC	1579	0	738	50	0
2	IF	1579	0	738	49	0
2	J	1579	0	738	49	0
2	KB	1579	0	738	50	0
2	KE	1579	0	738	51	0
2	MA	1579	0	738	48	0
2	MD	1579	0	738	49	0
2	MG	1579	0	738	47	0
2	OC	1579	0	738	52	0
2	OF	1579	0	738	49	0
2	QB	1579	0	738	49	0
2	QE	1579	0	738	51	0
2	SA	1579	0	738	47	0
2	SD	1579	0	738	48	0
2	SG	1579	0	738	49	0
2	T	1579	0	738	49	0
2	UC	1579	0	738	50	0
2	UF	1579	0	738	49	0
2	WB	1579	0	738	48	0
2	WE	1579	0	738	49	0
2	YA	1579	0	738	49	0
2	YD	1579	0	738	48	0
3	BA	1420	0	604	16	0
3	BD	1420	0	604	17	0
3	BG	1420	0	604	16	0
3	C	1420	0	604	16	0
3	DC	1420	0	604	17	0
3	DF	1420	0	604	16	0
3	FB	1420	0	604	17	0
3	FE	1420	0	604	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	HA	1420	0	604	16	0
3	HD	1420	0	604	16	0
3	HG	1420	0	604	16	0
3	JC	1420	0	604	16	0
3	JF	1420	0	604	16	0
3	K	1420	0	604	16	0
3	LB	1420	0	604	17	0
3	LE	1420	0	604	17	0
3	M	1420	0	604	16	0
3	NA	1420	0	604	16	0
3	ND	1420	0	604	16	0
3	NG	1420	0	604	16	0
3	PC	1420	0	604	16	0
3	PF	1420	0	604	16	0
3	RB	1420	0	604	16	0
3	RE	1420	0	604	16	0
3	TA	1420	0	604	16	0
3	TD	1420	0	604	16	0
3	TG	1420	0	604	16	0
3	V	1420	0	604	16	0
3	VC	1420	0	604	17	0
3	VF	1420	0	604	16	0
3	XB	1420	0	604	16	0
3	XE	1420	0	604	16	0
3	ZA	1420	0	604	17	0
3	ZD	1420	0	604	16	0
4	AB	456	0	206	5	0
4	AC	399	0	177	9	0
4	AE	456	0	206	6	0
4	AF	399	0	177	9	0
4	BB	409	0	181	6	0
4	BE	409	0	181	7	0
4	CA	456	0	206	6	0
4	CB	399	0	177	10	0
4	CD	456	0	206	6	0
4	CE	399	0	177	9	0
4	CG	456	0	206	6	0
4	D	456	0	206	6	0
4	DA	409	0	181	6	0
4	DD	409	0	181	7	0
4	DG	409	0	181	6	0
4	E	409	0	181	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	EA	399	0	177	9	0
4	EC	456	0	206	6	0
4	ED	399	0	177	10	0
4	EF	456	0	206	6	0
4	EG	399	0	177	10	0
4	FC	409	0	181	6	0
4	FF	409	0	181	7	0
4	GB	456	0	206	5	0
4	GC	399	0	177	9	0
4	GE	456	0	206	6	0
4	GF	399	0	177	9	0
4	H	399	0	177	10	0
4	HB	409	0	181	6	0
4	HE	409	0	181	7	0
4	IA	456	0	206	5	0
4	IB	399	0	177	10	0
4	ID	456	0	206	6	0
4	IE	399	0	177	9	0
4	IG	456	0	206	6	0
4	JA	409	0	181	6	0
4	JD	409	0	181	6	0
4	JG	409	0	181	6	0
4	KA	399	0	177	10	0
4	KC	456	0	206	6	0
4	KD	399	0	177	10	0
4	KF	456	0	206	6	0
4	KG	399	0	177	10	0
4	L	456	0	206	6	0
4	LC	409	0	181	6	0
4	LF	409	0	181	7	0
4	MB	456	0	206	5	0
4	MC	399	0	177	9	0
4	ME	456	0	206	6	0
4	MF	399	0	177	9	0
4	N	456	0	206	6	0
4	NB	409	0	181	6	0
4	NE	409	0	181	7	0
4	O	409	0	181	7	0
4	OA	456	0	206	6	0
4	OB	399	0	177	10	0
4	OD	456	0	206	7	0
4	OE	399	0	177	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	OG	456	0	206	6	0
4	P	409	0	181	6	0
4	PA	409	0	181	7	0
4	PD	409	0	181	6	0
4	PG	409	0	181	6	0
4	Q	399	0	177	10	0
4	QA	399	0	177	10	0
4	QC	456	0	206	6	0
4	QD	399	0	177	10	0
4	QF	456	0	206	6	0
4	QG	399	0	177	10	0
4	R	399	0	177	9	0
4	RC	409	0	181	7	0
4	RF	409	0	181	7	0
4	SB	456	0	206	6	0
4	SC	399	0	177	9	0
4	SE	456	0	206	6	0
4	SF	399	0	177	9	0
4	TB	409	0	181	7	0
4	TE	409	0	181	6	0
4	UA	456	0	206	5	0
4	UB	399	0	177	10	0
4	UD	456	0	206	7	0
4	UE	399	0	177	10	0
4	UG	456	0	206	6	0
4	VA	409	0	181	6	0
4	VD	409	0	181	7	0
4	VG	409	0	181	7	0
4	W	456	0	206	6	0
4	WA	399	0	177	10	0
4	WC	456	0	206	6	0
4	WD	399	0	177	10	0
4	WF	456	0	206	6	0
4	WG	399	0	177	10	0
4	X	409	0	181	7	0
4	XC	409	0	181	7	0
4	XF	409	0	181	6	0
4	Y	399	0	177	9	0
4	YB	456	0	206	6	0
4	YC	399	0	177	9	0
4	YE	456	0	206	6	0
4	YF	399	0	177	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	ZB	409	0	181	7	0
4	ZE	409	0	181	6	0
All	All	152898	0	68272	2191	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 (2191) 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)
2:KE:77:LEU:CB	2:QE:42:ALA:HA	1.55	1.35
2:MA:200:ALA:CB	2:MA:232:GLU:CB	2.05	1.35
2:QB:200:ALA:CB	2:QB:232:GLU:CB	2.05	1.35
2:WB:200:ALA:CB	2:WB:232:GLU:CB	2.05	1.35
2:GD:200:ALA:CB	2:GD:232:GLU:CB	2.05	1.35
2:QE:200:ALA:CB	2:QE:232:GLU:CB	2.05	1.35
2:SA:200:ALA:CB	2:SA:232:GLU:CB	2.05	1.35
2:AD:200:ALA:CB	2:AD:232:GLU:CB	2.05	1.35
2:MD:200:ALA:CB	2:MD:232:GLU:CB	2.05	1.35
2:KE:200:ALA:CB	2:KE:232:GLU:CB	2.05	1.35
2:GA:200:ALA:CB	2:GA:232:GLU:CB	2.05	1.34
2:CC:200:ALA:CB	2:CC:232:GLU:CB	2.05	1.34
2:KB:200:ALA:CB	2:KB:232:GLU:CB	2.05	1.34
2:UC:200:ALA:CB	2:UC:232:GLU:CB	2.05	1.34
2:EE:200:ALA:CB	2:EE:232:GLU:CB	2.05	1.34
2:WE:200:ALA:CB	2:WE:232:GLU:CB	2.05	1.34
2:GA:77:LEU:CB	2:MA:42:ALA:HA	1.58	1.34
2:SD:200:ALA:CB	2:SD:232:GLU:CB	2.05	1.34
2:YA:200:ALA:CB	2:YA:232:GLU:CB	2.05	1.34
2:OC:77:LEU:CB	2:UC:42:ALA:HA	1.55	1.34
2:G:200:ALA:CB	2:G:232:GLU:CB	2.05	1.33
2:B:200:ALA:CB	2:B:232:GLU:CB	2.05	1.33
2:AA:200:ALA:CB	2:AA:232:GLU:CB	2.05	1.33
2:IC:200:ALA:CB	2:IC:232:GLU:CB	2.05	1.33
2:UF:200:ALA:CB	2:UF:232:GLU:CB	2.05	1.33
2:OF:200:ALA:CB	2:OF:232:GLU:CB	2.05	1.33
2:J:200:ALA:CB	2:J:232:GLU:CB	2.05	1.33
2:AG:200:ALA:CB	2:AG:232:GLU:CB	2.05	1.33
2:EB:200:ALA:CB	2:EB:232:GLU:CB	2.05	1.33
2:YD:200:ALA:CB	2:YD:232:GLU:CB	2.05	1.33
2:OC:200:ALA:CB	2:OC:232:GLU:CB	2.05	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AD:77:LEU:CB	2:GD:42:ALA:HA	1.58	1.32
2:CF:200:ALA:CB	2:CF:232:GLU:CB	2.05	1.32
2:SG:200:ALA:CB	2:SG:232:GLU:CB	2.05	1.32
2:G:42:ALA:HA	2:SG:77:LEU:CB	1.60	1.32
2:IF:200:ALA:CB	2:IF:232:GLU:CB	2.05	1.32
2:GG:200:ALA:CB	2:GG:232:GLU:CB	2.05	1.32
2:T:200:ALA:CB	2:T:232:GLU:CB	2.05	1.32
2:T:77:LEU:CB	2:AA:42:ALA:HA	1.60	1.31
2:MG:200:ALA:CB	2:MG:232:GLU:CB	2.05	1.31
2:AG:77:LEU:CB	2:GG:42:ALA:HA	1.60	1.31
2:KB:77:LEU:CB	2:QB:42:ALA:HA	1.60	1.31
2:WB:77:LEU:CB	2:CC:42:ALA:HA	1.60	1.31
2:IF:77:LEU:CB	2:OF:42:ALA:HA	1.62	1.30
2:YA:77:LEU:CB	2:EB:42:ALA:HA	1.61	1.29
2:OF:77:LEU:CB	2:UF:42:ALA:HA	1.60	1.29
2:IC:77:LEU:CB	2:OC:42:ALA:HA	1.60	1.29
2:QE:77:LEU:CB	2:WE:42:ALA:HA	1.62	1.29
2:J:77:LEU:CB	2:T:42:ALA:HA	1.61	1.29
2:AA:77:LEU:CB	2:GA:42:ALA:HA	1.63	1.29
2:EB:77:LEU:CB	2:KB:42:ALA:HA	1.61	1.29
2:GG:77:LEU:CB	2:MG:42:ALA:HA	1.64	1.28
2:CF:77:LEU:CB	2:IF:42:ALA:HA	1.64	1.28
2:KB:74:ASN:N	2:QB:42:ALA:O	1.64	1.28
2:B:77:LEU:CB	2:J:42:ALA:HA	1.62	1.28
2:SA:77:LEU:CB	2:YA:42:ALA:HA	1.63	1.27
2:OC:74:ASN:N	2:UC:42:ALA:O	1.65	1.27
2:GD:77:LEU:CB	2:MD:42:ALA:HA	1.63	1.27
2:UF:77:LEU:CB	2:AG:42:ALA:HA	1.64	1.26
2:SD:77:LEU:CB	2:YD:42:ALA:HA	1.65	1.26
2:WE:77:LEU:CB	2:CF:42:ALA:HA	1.66	1.26
2:YD:77:LEU:CB	2:EE:42:ALA:HA	1.63	1.25
2:G:77:LEU:CB	2:B:42:ALA:HA	1.66	1.25
2:MG:77:LEU:CB	2:SG:42:ALA:HA	1.67	1.25
2:CC:77:LEU:CB	2:IC:42:ALA:HA	1.66	1.24
2:MD:77:LEU:CB	2:SD:42:ALA:HA	1.66	1.24
2:OF:74:ASN:N	2:UF:42:ALA:O	1.69	1.24
2:GA:74:ASN:N	2:MA:42:ALA:O	1.69	1.23
2:QB:77:LEU:CB	2:WB:42:ALA:HA	1.67	1.23
2:EE:77:LEU:CB	2:KE:42:ALA:HA	1.66	1.23
2:KE:74:ASN:N	2:QE:42:ALA:O	1.70	1.23
2:AD:74:ASN:N	2:GD:42:ALA:O	1.69	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:MA:77:LEU:CB	2:SA:42:ALA:HA	1.69	1.22
2:T:74:ASN:N	2:AA:42:ALA:O	1.70	1.22
2:AG:74:ASN:N	2:GG:42:ALA:O	1.70	1.22
2:UC:77:LEU:CB	2:AD:42:ALA:HA	1.68	1.22
2:QE:74:ASN:N	2:WE:42:ALA:O	1.71	1.21
2:MA:74:ASN:N	2:SA:42:ALA:O	1.71	1.21
2:YD:74:ASN:N	2:EE:42:ALA:O	1.70	1.21
2:EB:74:ASN:N	2:KB:42:ALA:O	1.72	1.21
2:GG:74:ASN:N	2:MG:42:ALA:O	1.70	1.21
2:WB:74:ASN:N	2:CC:42:ALA:O	1.73	1.21
2:WE:74:ASN:N	2:CF:42:ALA:O	1.70	1.21
2:G:42:ALA:O	2:SG:74:ASN:N	1.72	1.20
2:CC:200:ALA:HB2	2:CC:232:GLU:CB	1.71	1.20
2:CF:74:ASN:N	2:IF:42:ALA:O	1.73	1.19
2:UF:74:ASN:N	2:AG:42:ALA:O	1.72	1.19
2:IC:200:ALA:HB2	2:IC:232:GLU:CB	1.71	1.19
2:SA:74:ASN:N	2:YA:42:ALA:O	1.74	1.19
2:MD:74:ASN:N	2:SD:42:ALA:O	1.71	1.19
2:B:74:ASN:N	2:J:42:ALA:O	1.72	1.19
2:GD:74:ASN:N	2:MD:42:ALA:O	1.72	1.18
2:WB:200:ALA:HB2	2:WB:232:GLU:CB	1.71	1.18
2:J:74:ASN:N	2:T:42:ALA:O	1.74	1.18
2:AA:74:ASN:N	2:GA:42:ALA:O	1.75	1.18
2:OC:200:ALA:HB2	2:OC:232:GLU:CB	1.71	1.17
2:IC:74:ASN:N	2:OC:42:ALA:O	1.76	1.17
2:YA:74:ASN:N	2:EB:42:ALA:O	1.77	1.17
2:CC:74:ASN:N	2:IC:42:ALA:O	1.75	1.17
2:G:74:ASN:N	2:B:42:ALA:O	1.73	1.16
2:SD:74:ASN:N	2:YD:42:ALA:O	1.75	1.16
2:UC:74:ASN:N	2:AD:42:ALA:O	1.74	1.16
2:QB:200:ALA:HB2	2:QB:232:GLU:CB	1.71	1.16
2:GD:200:ALA:HB2	2:GD:232:GLU:CB	1.71	1.16
2:IF:74:ASN:N	2:OF:42:ALA:O	1.78	1.16
2:EE:74:ASN:N	2:KE:42:ALA:O	1.77	1.15
2:QB:74:ASN:N	2:WB:42:ALA:O	1.77	1.15
2:UC:200:ALA:HB2	2:UC:232:GLU:CB	1.70	1.15
2:AD:200:ALA:HB2	2:AD:232:GLU:CB	1.71	1.15
2:MD:200:ALA:HB2	2:MD:232:GLU:CB	1.71	1.15
2:YA:200:ALA:HB2	2:YA:232:GLU:CB	1.71	1.15
2:KB:200:ALA:HB2	2:KB:232:GLU:CB	1.71	1.15
2:MG:74:ASN:N	2:SG:42:ALA:O	1.77	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:200:ALA:HB2	2:EB:232:GLU:CB	1.71	1.14
2:YD:200:ALA:HB2	2:YD:232:GLU:CB	1.70	1.14
2:SA:200:ALA:HB2	2:SA:232:GLU:CB	1.71	1.14
2:EE:200:ALA:HB2	2:EE:232:GLU:CB	1.71	1.14
2:SD:200:ALA:HB2	2:SD:232:GLU:CB	1.71	1.13
2:AG:200:ALA:HB2	2:AG:232:GLU:CB	1.71	1.13
2:GG:200:ALA:HB2	2:GG:232:GLU:CB	1.71	1.13
2:AA:200:ALA:HB2	2:AA:232:GLU:CB	1.70	1.12
2:GA:200:ALA:HB2	2:GA:232:GLU:CB	1.70	1.12
2:KE:200:ALA:HB2	2:KE:232:GLU:CB	1.71	1.12
2:MA:200:ALA:HB2	2:MA:232:GLU:CB	1.71	1.12
2:WE:200:ALA:HB2	2:WE:232:GLU:CB	1.71	1.12
2:UF:200:ALA:HB2	2:UF:232:GLU:CB	1.71	1.11
2:T:200:ALA:HB2	2:T:232:GLU:CB	1.71	1.11
2:QE:200:ALA:HB2	2:QE:232:GLU:CB	1.71	1.11
2:CF:200:ALA:HB2	2:CF:232:GLU:CB	1.71	1.11
2:MG:200:ALA:HB2	2:MG:232:GLU:CB	1.71	1.11
2:OC:155:HIS:CB	2:UC:217:ALA:CB	2.29	1.10
2:G:200:ALA:HB2	2:G:232:GLU:CB	1.71	1.10
2:B:200:ALA:HB2	2:B:232:GLU:CB	1.71	1.10
2:IF:200:ALA:HB2	2:IF:232:GLU:CB	1.71	1.10
2:SG:200:ALA:HB2	2:SG:232:GLU:CB	1.71	1.10
2:J:200:ALA:HB2	2:J:232:GLU:CB	1.71	1.09
2:OC:155:HIS:CB	2:UC:217:ALA:HB1	1.81	1.09
2:OF:200:ALA:HB2	2:OF:232:GLU:CB	1.71	1.09
2:KE:155:HIS:CB	2:QE:217:ALA:HB1	1.84	1.08
2:KE:155:HIS:CB	2:QE:217:ALA:CB	2.30	1.08
2:AD:155:HIS:CB	2:GD:217:ALA:CB	2.32	1.07
2:KB:155:HIS:CB	2:QB:217:ALA:CB	2.33	1.06
2:AD:155:HIS:CB	2:GD:217:ALA:HB1	1.85	1.06
2:G:217:ALA:CB	2:SG:155:HIS:CB	2.34	1.05
2:GA:155:HIS:CB	2:MA:217:ALA:HB1	1.86	1.05
2:KB:155:HIS:CB	2:QB:217:ALA:HB1	1.85	1.05
2:GA:155:HIS:CB	2:MA:217:ALA:CB	2.33	1.05
2:WB:155:HIS:CB	2:CC:217:ALA:CB	2.35	1.05
2:IC:200:ALA:HB1	2:IC:232:GLU:CB	1.87	1.05
2:CC:200:ALA:HB1	2:CC:232:GLU:CB	1.87	1.05
2:T:155:HIS:CB	2:AA:217:ALA:CB	2.34	1.04
2:YA:200:ALA:HB1	2:YA:232:GLU:CB	1.87	1.04
2:OF:155:HIS:CB	2:UF:217:ALA:HB1	1.87	1.04
2:AG:155:HIS:CB	2:GG:217:ALA:CB	2.35	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:200:ALA:HB1	2:EB:232:GLU:CB	1.87	1.04
2:MD:200:ALA:HB1	2:MD:232:GLU:CB	1.87	1.04
2:OF:155:HIS:CB	2:UF:217:ALA:CB	2.34	1.04
2:T:155:HIS:CB	2:AA:217:ALA:HB1	1.88	1.04
2:EB:155:HIS:CB	2:KB:217:ALA:CB	2.35	1.04
2:GD:200:ALA:HB1	2:GD:232:GLU:CB	1.87	1.04
2:IC:155:HIS:CB	2:OC:217:ALA:CB	2.36	1.03
2:OC:200:ALA:HB1	2:OC:232:GLU:CB	1.87	1.03
2:AG:155:HIS:CB	2:GG:217:ALA:HB1	1.88	1.03
2:SA:200:ALA:HB1	2:SA:232:GLU:CB	1.87	1.03
2:WB:200:ALA:HB1	2:WB:232:GLU:CB	1.87	1.03
2:SD:200:ALA:HB1	2:SD:232:GLU:CB	1.87	1.03
2:G:217:ALA:HB1	2:SG:155:HIS:CB	1.88	1.03
2:B:155:HIS:CB	2:J:217:ALA:CB	2.36	1.03
2:YA:155:HIS:CB	2:EB:217:ALA:CB	2.36	1.03
2:J:155:HIS:CB	2:T:217:ALA:CB	2.36	1.03
2:KB:200:ALA:HB1	2:KB:232:GLU:CB	1.87	1.03
2:UF:200:ALA:HB1	2:UF:232:GLU:CB	1.87	1.03
2:GD:155:HIS:CB	2:MD:217:ALA:CB	2.37	1.02
2:AG:200:ALA:HB1	2:AG:232:GLU:CB	1.87	1.02
2:AD:200:ALA:HB1	2:AD:232:GLU:CB	1.87	1.02
2:YD:155:HIS:CB	2:EE:217:ALA:CB	2.37	1.02
2:GG:155:HIS:CB	2:MG:217:ALA:CB	2.37	1.02
2:EB:155:HIS:CB	2:KB:217:ALA:HB1	1.89	1.02
2:QE:155:HIS:CB	2:WE:217:ALA:HB1	1.90	1.02
2:QE:155:HIS:CB	2:WE:217:ALA:CB	2.36	1.02
2:G:200:ALA:HB1	2:G:232:GLU:CB	1.87	1.02
2:IF:155:HIS:CB	2:OF:217:ALA:CB	2.37	1.02
2:B:155:HIS:CB	2:J:217:ALA:HB1	1.90	1.01
2:J:155:HIS:CB	2:T:217:ALA:HB1	1.90	1.01
2:T:200:ALA:HB1	2:T:232:GLU:CB	1.87	1.01
2:WB:155:HIS:CB	2:CC:217:ALA:HB1	1.89	1.01
2:YD:155:HIS:CB	2:EE:217:ALA:HB1	1.90	1.01
2:B:200:ALA:HB1	2:B:232:GLU:CB	1.87	1.01
2:AA:200:ALA:HB1	2:AA:232:GLU:CB	1.87	1.01
2:SA:155:HIS:CB	2:YA:217:ALA:CB	2.38	1.01
2:UC:200:ALA:HB1	2:UC:232:GLU:CB	1.87	1.01
2:OF:200:ALA:HB1	2:OF:232:GLU:CB	1.87	1.01
2:GG:200:ALA:HB1	2:GG:232:GLU:CB	1.87	1.01
2:MA:200:ALA:HB1	2:MA:232:GLU:CB	1.87	1.01
2:YD:200:ALA:HB1	2:YD:232:GLU:CB	1.87	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:WE:200:ALA:HB1	2:WE:232:GLU:CB	1.87	1.01
2:UF:155:HIS:CB	2:AG:217:ALA:CB	2.38	1.01
2:SG:200:ALA:HB1	2:SG:232:GLU:CB	1.87	1.01
2:J:200:ALA:HB1	2:J:232:GLU:CB	1.87	1.01
2:QB:200:ALA:HB1	2:QB:232:GLU:CB	1.87	1.01
2:QE:200:ALA:HB1	2:QE:232:GLU:CB	1.87	1.01
2:GG:155:HIS:CB	2:MG:217:ALA:HB1	1.91	1.01
2:YA:155:HIS:CB	2:EB:217:ALA:HB1	1.91	1.00
2:SD:155:HIS:CB	2:YD:217:ALA:CB	2.39	1.00
2:CF:155:HIS:CB	2:IF:217:ALA:CB	2.38	1.00
2:G:155:HIS:CB	2:B:217:ALA:CB	2.39	1.00
2:AA:155:HIS:CB	2:GA:217:ALA:CB	2.38	1.00
2:AA:155:HIS:CB	2:GA:217:ALA:HB1	1.92	1.00
2:MD:155:HIS:CB	2:SD:217:ALA:CB	2.39	1.00
2:KE:200:ALA:HB1	2:KE:232:GLU:CB	1.87	1.00
2:UF:155:HIS:CB	2:AG:217:ALA:HB1	1.92	1.00
2:CC:155:HIS:CB	2:IC:217:ALA:CB	2.40	1.00
2:CF:200:ALA:HB1	2:CF:232:GLU:CB	1.87	1.00
2:GA:200:ALA:HB1	2:GA:232:GLU:CB	1.87	0.99
2:IC:155:HIS:CB	2:OC:217:ALA:HB1	1.90	0.99
2:GD:155:HIS:CB	2:MD:217:ALA:HB1	1.91	0.99
2:IF:155:HIS:CB	2:OF:217:ALA:HB1	1.92	0.99
2:WE:155:HIS:CB	2:CF:217:ALA:CB	2.39	0.99
2:SA:155:HIS:CB	2:YA:217:ALA:HB1	1.92	0.99
2:WE:155:HIS:CB	2:CF:217:ALA:HB1	1.93	0.99
2:OC:77:LEU:CB	2:UC:42:ALA:CA	2.41	0.99
2:EE:200:ALA:HB1	2:EE:232:GLU:CB	1.87	0.99
2:MG:200:ALA:HB1	2:MG:232:GLU:CB	1.87	0.99
2:EE:155:HIS:CB	2:KE:217:ALA:CB	2.40	0.98
2:CF:155:HIS:CB	2:IF:217:ALA:HB1	1.92	0.98
2:IF:200:ALA:HB1	2:IF:232:GLU:CB	1.87	0.98
2:MG:155:HIS:CB	2:SG:217:ALA:CB	2.41	0.98
2:UC:155:HIS:CB	2:AD:217:ALA:CB	2.41	0.98
2:G:155:HIS:CB	2:B:217:ALA:HB1	1.93	0.98
2:MD:155:HIS:CB	2:SD:217:ALA:HB1	1.93	0.98
2:QB:155:HIS:CB	2:WB:217:ALA:CB	2.42	0.98
2:MA:155:HIS:CB	2:SA:217:ALA:CB	2.41	0.97
2:SD:155:HIS:CB	2:YD:217:ALA:HB1	1.93	0.97
2:KE:77:LEU:CB	2:QE:42:ALA:CA	2.41	0.97
2:EE:155:HIS:CB	2:KE:217:ALA:HB1	1.95	0.97
2:MA:155:HIS:CB	2:SA:217:ALA:HB1	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:MG:155:HIS:CB	2:SG:217:ALA:HB1	1.96	0.95
2:UC:155:HIS:CB	2:AD:217:ALA:HB1	1.96	0.95
2:CC:155:HIS:CB	2:IC:217:ALA:HB1	1.94	0.95
2:AD:77:LEU:CB	2:GD:42:ALA:CA	2.43	0.95
2:QB:155:HIS:CB	2:WB:217:ALA:HB1	1.96	0.94
2:WB:77:LEU:CB	2:CC:42:ALA:CA	2.45	0.94
2:IC:77:LEU:CB	2:OC:42:ALA:CA	2.46	0.94
2:G:42:ALA:CA	2:SG:77:LEU:CB	2.45	0.94
2:GA:77:LEU:CB	2:MA:42:ALA:CA	2.44	0.94
2:YA:77:LEU:CB	2:EB:42:ALA:CA	2.45	0.94
2:T:77:LEU:CB	2:AA:42:ALA:CA	2.45	0.93
2:AG:77:LEU:CB	2:GG:42:ALA:CA	2.46	0.93
2:J:77:LEU:CB	2:T:42:ALA:CA	2.46	0.93
2:KB:77:LEU:CB	2:QB:42:ALA:CA	2.46	0.93
2:OF:77:LEU:CB	2:UF:42:ALA:CA	2.45	0.93
2:EB:77:LEU:CB	2:KB:42:ALA:CA	2.46	0.93
2:B:77:LEU:CB	2:J:42:ALA:CA	2.47	0.92
2:IF:77:LEU:CB	2:OF:42:ALA:CA	2.47	0.92
2:YD:77:LEU:CB	2:EE:42:ALA:CA	2.48	0.91
2:GD:77:LEU:CB	2:MD:42:ALA:CA	2.48	0.91
2:SD:77:LEU:CB	2:YD:42:ALA:CA	2.50	0.90
2:GG:77:LEU:CB	2:MG:42:ALA:CA	2.49	0.90
2:QE:77:LEU:CB	2:WE:42:ALA:CA	2.48	0.90
2:UF:77:LEU:CB	2:AG:42:ALA:CA	2.49	0.90
2:AA:77:LEU:CB	2:GA:42:ALA:CA	2.48	0.90
2:SA:77:LEU:CB	2:YA:42:ALA:CA	2.48	0.89
2:CC:77:LEU:CB	2:IC:42:ALA:CA	2.51	0.89
2:MD:77:LEU:CB	2:SD:42:ALA:CA	2.51	0.88
2:G:77:LEU:CB	2:B:42:ALA:CA	2.51	0.88
2:CF:77:LEU:CB	2:IF:42:ALA:CA	2.49	0.88
2:EE:77:LEU:CB	2:KE:42:ALA:CA	2.51	0.88
2:AA:218:VAL:C	2:AA:226:ALA:HB2	2.00	0.87
2:OC:218:VAL:C	2:OC:226:ALA:HB2	2.00	0.87
2:G:218:VAL:C	2:G:226:ALA:HB2	2.00	0.87
2:SA:218:VAL:C	2:SA:226:ALA:HB2	2.00	0.87
2:WB:218:VAL:C	2:WB:226:ALA:HB2	2.00	0.87
2:SD:218:VAL:C	2:SD:226:ALA:HB2	2.00	0.87
2:IF:218:VAL:C	2:IF:226:ALA:HB2	2.00	0.87
2:B:218:VAL:C	2:B:226:ALA:HB2	2.00	0.87
2:AD:218:VAL:C	2:AD:226:ALA:HB2	2.00	0.87
2:GD:218:VAL:C	2:GD:226:ALA:HB2	2.00	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:YD:218:VAL:C	2:YD:226:ALA:HB2	2.00	0.87
2:OF:218:VAL:C	2:OF:226:ALA:HB2	2.00	0.87
2:EB:218:VAL:C	2:EB:226:ALA:HB2	2.00	0.87
2:KB:218:VAL:C	2:KB:226:ALA:HB2	2.00	0.87
2:SG:218:VAL:C	2:SG:226:ALA:HB2	2.00	0.87
2:KE:218:VAL:C	2:KE:226:ALA:HB2	2.00	0.87
2:CF:218:VAL:C	2:CF:226:ALA:HB2	2.00	0.87
2:MG:218:VAL:C	2:MG:226:ALA:HB2	2.00	0.86
2:J:218:VAL:C	2:J:226:ALA:HB2	2.00	0.86
2:MA:218:VAL:C	2:MA:226:ALA:HB2	2.00	0.86
2:IC:218:VAL:C	2:IC:226:ALA:HB2	2.00	0.86
2:UC:77:LEU:CB	2:AD:42:ALA:CA	2.53	0.86
2:WE:77:LEU:CB	2:CF:42:ALA:CA	2.51	0.86
2:UF:218:VAL:C	2:UF:226:ALA:HB2	2.00	0.86
2:EE:218:VAL:C	2:EE:226:ALA:HB2	2.00	0.86
2:GA:218:VAL:C	2:GA:226:ALA:HB2	2.00	0.86
2:CC:218:VAL:C	2:CC:226:ALA:HB2	2.00	0.86
2:QE:218:VAL:C	2:QE:226:ALA:HB2	2.00	0.86
2:AG:218:VAL:C	2:AG:226:ALA:HB2	2.00	0.86
2:T:218:VAL:C	2:T:226:ALA:HB2	2.00	0.86
2:WE:218:VAL:C	2:WE:226:ALA:HB2	2.00	0.86
2:QB:218:VAL:C	2:QB:226:ALA:HB2	2.00	0.86
2:MG:77:LEU:CB	2:SG:42:ALA:CA	2.52	0.86
2:MD:218:VAL:C	2:MD:226:ALA:HB2	2.00	0.86
2:UC:218:VAL:C	2:UC:226:ALA:HB2	2.00	0.86
2:YA:218:VAL:C	2:YA:226:ALA:HB2	2.00	0.85
2:QB:77:LEU:CB	2:WB:42:ALA:CA	2.52	0.85
2:GG:218:VAL:C	2:GG:226:ALA:HB2	2.00	0.85
2:MA:77:LEU:CB	2:SA:42:ALA:CA	2.54	0.83
3:LE:258:GLU:CB	4:UE:102:ASN:CB	2.65	0.75
2:MA:143:ALA:CB	2:SA:205:LEU:O	2.32	0.75
2:GA:143:ALA:CB	2:MA:205:LEU:O	2.32	0.75
2:YA:143:ALA:CB	2:EB:205:LEU:O	2.34	0.75
2:EB:143:ALA:CB	2:KB:205:LEU:O	2.33	0.75
2:QB:143:ALA:CB	2:WB:205:LEU:O	2.34	0.75
2:WB:143:ALA:CB	2:CC:205:LEU:O	2.33	0.75
2:AA:143:ALA:CB	2:GA:205:LEU:O	2.33	0.74
3:ZA:258:GLU:CB	4:IB:102:ASN:CB	2.65	0.74
3:JC:258:GLU:CB	4:SC:102:ASN:CB	2.66	0.74
2:J:143:ALA:CB	2:T:205:LEU:O	2.33	0.74
2:KB:143:ALA:CB	2:QB:205:LEU:O	2.31	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IC:143:ALA:CB	2:OC:205:LEU:O	2.34	0.74
2:B:143:ALA:CB	2:J:205:LEU:O	2.33	0.74
2:CC:143:ALA:CB	2:IC:205:LEU:O	2.33	0.74
2:UC:143:ALA:CB	2:AD:205:LEU:O	2.33	0.74
2:T:143:ALA:CB	2:AA:205:LEU:O	2.32	0.74
2:OC:143:ALA:CB	2:UC:205:LEU:O	2.31	0.74
2:G:205:LEU:O	2:SG:143:ALA:CB	2.33	0.73
2:SA:143:ALA:CB	2:YA:205:LEU:O	2.33	0.73
2:AD:143:ALA:CB	2:GD:205:LEU:O	2.32	0.73
2:OC:143:ALA:HB3	2:UC:205:LEU:O	1.88	0.73
2:G:143:ALA:CB	2:B:205:LEU:O	2.33	0.73
3:K:258:GLU:CB	4:Y:102:ASN:CB	2.66	0.73
2:GD:143:ALA:CB	2:MD:205:LEU:O	2.33	0.73
3:JF:258:GLU:CB	4:SF:102:ASN:CB	2.66	0.73
3:XB:258:GLU:CB	4:GC:102:ASN:CB	2.67	0.72
3:BD:258:GLU:CB	4:KD:102:ASN:CB	2.67	0.72
2:MD:143:ALA:CB	2:SD:205:LEU:O	2.32	0.72
3:FB:258:GLU:CB	4:OB:102:ASN:CB	2.68	0.72
4:Q:102:ASN:CB	3:TG:258:GLU:CB	2.67	0.72
2:KB:143:ALA:HB3	2:QB:205:LEU:O	1.90	0.72
2:MG:143:ALA:CB	2:SG:205:LEU:O	2.34	0.72
2:SD:143:ALA:CB	2:YD:205:LEU:O	2.33	0.72
2:AG:143:ALA:CB	2:GG:205:LEU:O	2.32	0.72
2:GG:143:ALA:CB	2:MG:205:LEU:O	2.32	0.72
3:HA:258:GLU:CB	4:QA:102:ASN:CB	2.67	0.72
3:PC:258:GLU:CB	4:YC:102:ASN:CB	2.67	0.72
3:BG:258:GLU:CB	4:KG:102:ASN:CB	2.68	0.72
3:V:258:GLU:CB	4:EA:102:ASN:CB	2.68	0.72
2:YD:143:ALA:CB	2:EE:205:LEU:O	2.32	0.72
2:KE:143:ALA:HB3	2:QE:205:LEU:O	1.90	0.72
3:PF:258:GLU:CB	4:YF:102:ASN:CB	2.68	0.72
3:BA:258:GLU:CB	4:KA:102:ASN:CB	2.68	0.71
2:AD:143:ALA:HB3	2:GD:205:LEU:O	1.90	0.71
3:C:258:GLU:CB	4:R:102:ASN:CB	2.68	0.71
2:IF:143:ALA:CB	2:OF:205:LEU:O	2.34	0.71
2:UF:143:ALA:CB	2:AG:205:LEU:O	2.33	0.71
2:GA:143:ALA:HB3	2:MA:205:LEU:O	1.91	0.71
2:EE:143:ALA:CB	2:KE:205:LEU:O	2.34	0.71
2:B:242:VAL:HA	2:B:324:GLY:HA2	1.73	0.71
3:TA:258:GLU:CB	4:CB:102:ASN:CB	2.68	0.71
2:OF:143:ALA:CB	2:UF:205:LEU:O	2.32	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:UF:242:VAL:HA	2:UF:324:GLY:HA2	1.73	0.71
2:AG:242:VAL:HA	2:AG:324:GLY:HA2	1.73	0.71
2:GG:242:VAL:HA	2:GG:324:GLY:HA2	1.73	0.71
2:SG:242:VAL:HA	2:SG:324:GLY:HA2	1.73	0.71
2:G:242:VAL:HA	2:G:324:GLY:HA2	1.73	0.71
2:J:242:VAL:HA	2:J:324:GLY:HA2	1.73	0.71
2:T:242:VAL:HA	2:T:324:GLY:HA2	1.73	0.71
2:AA:242:VAL:HA	2:AA:324:GLY:HA2	1.73	0.71
2:YA:242:VAL:HA	2:YA:324:GLY:HA2	1.73	0.71
2:KB:242:VAL:HA	2:KB:324:GLY:HA2	1.73	0.71
2:WB:242:VAL:HA	2:WB:324:GLY:HA2	1.73	0.71
2:IF:242:VAL:HA	2:IF:324:GLY:HA2	1.73	0.71
2:OF:242:VAL:HA	2:OF:324:GLY:HA2	1.73	0.71
2:MG:242:VAL:HA	2:MG:324:GLY:HA2	1.73	0.71
2:GA:242:VAL:HA	2:GA:324:GLY:HA2	1.73	0.71
2:MA:242:VAL:HA	2:MA:324:GLY:HA2	1.73	0.71
2:QB:242:VAL:HA	2:QB:324:GLY:HA2	1.73	0.71
2:IC:242:VAL:HA	2:IC:324:GLY:HA2	1.73	0.71
2:UC:242:VAL:HA	2:UC:324:GLY:HA2	1.73	0.71
3:TD:258:GLU:CB	4:CE:102:ASN:CB	2.69	0.71
2:QE:242:VAL:HA	2:QE:324:GLY:HA2	1.73	0.71
2:WE:242:VAL:HA	2:WE:324:GLY:HA2	1.73	0.71
2:CF:242:VAL:HA	2:CF:324:GLY:HA2	1.73	0.71
2:SA:242:VAL:HA	2:SA:324:GLY:HA2	1.73	0.71
2:EB:242:VAL:HA	2:EB:324:GLY:HA2	1.73	0.71
2:CC:242:VAL:HA	2:CC:324:GLY:HA2	1.73	0.71
2:GD:242:VAL:HA	2:GD:324:GLY:HA2	1.73	0.71
2:YD:242:VAL:HA	2:YD:324:GLY:HA2	1.73	0.71
2:KE:242:VAL:HA	2:KE:324:GLY:HA2	1.73	0.71
2:WE:143:ALA:CB	2:CF:205:LEU:O	2.32	0.71
2:CF:143:ALA:CB	2:IF:205:LEU:O	2.33	0.71
2:OC:242:VAL:HA	2:OC:324:GLY:HA2	1.73	0.71
2:AD:242:VAL:HA	2:AD:324:GLY:HA2	1.73	0.71
2:MD:242:VAL:HA	2:MD:324:GLY:HA2	1.73	0.71
2:SD:242:VAL:HA	2:SD:324:GLY:HA2	1.73	0.71
3:RE:258:GLU:CB	4:AF:102:ASN:CB	2.69	0.71
2:EE:242:VAL:HA	2:EE:324:GLY:HA2	1.73	0.70
2:KE:143:ALA:CB	2:QE:205:LEU:O	2.33	0.70
2:QE:143:ALA:CB	2:WE:205:LEU:O	2.33	0.70
3:VF:258:GLU:CB	4:EG:102:ASN:CB	2.70	0.70
3:HD:258:GLU:CB	4:QD:102:ASN:CB	2.69	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:143:ALA:HB3	2:AA:205:LEU:O	1.91	0.70
3:DF:258:GLU:CB	4:MF:102:ASN:CB	2.69	0.70
3:RB:258:GLU:CB	4:AC:102:ASN:CB	2.70	0.69
3:DC:258:GLU:CB	4:MC:102:ASN:CB	2.70	0.69
3:FE:258:GLU:CB	4:OE:102:ASN:CB	2.69	0.69
3:NG:258:GLU:CB	4:WG:102:ASN:CB	2.70	0.69
2:EB:143:ALA:HB3	2:KB:205:LEU:O	1.92	0.69
2:OC:155:HIS:CB	2:UC:217:ALA:HB2	2.22	0.69
2:AG:143:ALA:HB3	2:GG:205:LEU:O	1.92	0.69
2:YD:143:ALA:HB3	2:EE:205:LEU:O	1.92	0.69
3:HG:258:GLU:CB	4:QG:102:ASN:CB	2.70	0.69
3:M:258:GLU:CB	4:H:102:ASN:CB	2.70	0.69
2:OF:143:ALA:HB3	2:UF:205:LEU:O	1.91	0.69
2:WB:143:ALA:HB3	2:CC:205:LEU:O	1.92	0.69
2:J:143:ALA:HB3	2:T:205:LEU:O	1.93	0.68
2:GD:143:ALA:HB3	2:MD:205:LEU:O	1.93	0.68
2:G:205:LEU:O	2:SG:143:ALA:HB3	1.92	0.68
3:ZD:258:GLU:CB	4:IE:102:ASN:CB	2.70	0.68
2:WE:143:ALA:HB3	2:CF:205:LEU:O	1.94	0.68
2:GG:143:ALA:HB3	2:MG:205:LEU:O	1.93	0.68
2:B:143:ALA:HB3	2:J:205:LEU:O	1.93	0.68
2:QE:143:ALA:HB3	2:WE:205:LEU:O	1.92	0.68
2:SA:143:ALA:HB3	2:YA:205:LEU:O	1.94	0.68
3:LB:258:GLU:CB	4:UB:102:ASN:CB	2.71	0.68
2:UF:143:ALA:HB3	2:AG:205:LEU:O	1.93	0.68
2:G:143:ALA:HB3	2:B:205:LEU:O	1.94	0.68
2:AA:143:ALA:HB3	2:GA:205:LEU:O	1.94	0.68
3:VC:258:GLU:CB	4:ED:102:ASN:CB	2.71	0.68
3:XE:258:GLU:CB	4:GF:102:ASN:CB	2.72	0.68
2:AD:155:HIS:CB	2:GD:217:ALA:HB2	2.24	0.68
3:ND:258:GLU:CB	4:WD:102:ASN:CB	2.72	0.67
2:MA:143:ALA:HB3	2:SA:205:LEU:O	1.95	0.67
2:MD:143:ALA:HB3	2:SD:205:LEU:O	1.94	0.67
2:KE:155:HIS:CB	2:QE:217:ALA:HB2	2.22	0.67
2:KB:68:ALA:HB1	2:QB:47:ILE:O	1.95	0.67
2:IC:143:ALA:HB3	2:OC:205:LEU:O	1.93	0.67
2:IF:143:ALA:HB3	2:OF:205:LEU:O	1.94	0.67
2:CF:143:ALA:HB3	2:IF:205:LEU:O	1.93	0.67
2:YA:143:ALA:HB3	2:EB:205:LEU:O	1.94	0.66
2:SD:143:ALA:HB3	2:YD:205:LEU:O	1.94	0.66
2:WB:155:HIS:CB	2:CC:217:ALA:HB2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:MG:143:ALA:HB3	2:SG:205:LEU:O	1.96	0.66
2:GA:155:HIS:CB	2:MA:217:ALA:HB2	2.24	0.66
2:CC:143:ALA:HB3	2:IC:205:LEU:O	1.95	0.66
2:YA:155:HIS:CB	2:EB:217:ALA:HB2	2.25	0.66
4:BB:64:LEU:HA	4:BB:101:ILE:HA	1.78	0.66
2:KB:74:ASN:CA	2:QB:42:ALA:O	2.44	0.66
2:UC:143:ALA:HB3	2:AD:205:LEU:O	1.95	0.66
2:MD:219:ARG:N	2:MD:226:ALA:HB2	2.11	0.66
4:TB:64:LEU:HA	4:TB:101:ILE:HA	1.78	0.66
4:ZB:64:LEU:HA	4:ZB:101:ILE:HA	1.78	0.66
2:GD:219:ARG:N	2:GD:226:ALA:HB2	2.11	0.66
2:AG:219:ARG:N	2:AG:226:ALA:HB2	2.11	0.66
2:GG:219:ARG:N	2:GG:226:ALA:HB2	2.11	0.66
4:NB:64:LEU:HA	4:NB:101:ILE:HA	1.78	0.66
4:FC:64:LEU:HA	4:FC:101:ILE:HA	1.78	0.66
2:IC:155:HIS:CB	2:OC:217:ALA:HB2	2.25	0.66
4:RC:64:LEU:HA	4:RC:101:ILE:HA	1.78	0.66
2:QE:219:ARG:N	2:QE:226:ALA:HB2	2.11	0.66
2:WE:219:ARG:N	2:WE:226:ALA:HB2	2.11	0.66
2:J:219:ARG:N	2:J:226:ALA:HB2	2.11	0.65
2:CC:219:ARG:N	2:CC:226:ALA:HB2	2.11	0.65
2:EE:143:ALA:HB3	2:KE:205:LEU:O	1.95	0.65
2:T:219:ARG:N	2:T:226:ALA:HB2	2.11	0.65
4:PA:64:LEU:HA	4:PA:101:ILE:HA	1.78	0.65
4:VA:64:LEU:HA	4:VA:101:ILE:HA	1.78	0.65
4:LC:64:LEU:HA	4:LC:101:ILE:HA	1.78	0.65
2:SD:219:ARG:N	2:SD:226:ALA:HB2	2.11	0.65
4:RF:64:LEU:HA	4:RF:101:ILE:HA	1.78	0.65
2:MG:219:ARG:N	2:MG:226:ALA:HB2	2.11	0.65
2:B:219:ARG:N	2:B:226:ALA:HB2	2.11	0.65
2:SA:219:ARG:N	2:SA:226:ALA:HB2	2.11	0.65
2:EB:155:HIS:CB	2:KB:217:ALA:HB2	2.26	0.65
2:IC:219:ARG:N	2:IC:226:ALA:HB2	2.11	0.65
4:ZE:64:LEU:HA	4:ZE:101:ILE:HA	1.78	0.65
2:UF:219:ARG:N	2:UF:226:ALA:HB2	2.11	0.65
3:NA:258:GLU:CB	4:WA:102:ASN:CB	2.74	0.65
2:YA:219:ARG:N	2:YA:226:ALA:HB2	2.11	0.65
4:HB:64:LEU:HA	4:HB:101:ILE:HA	1.78	0.65
2:AD:219:ARG:N	2:AD:226:ALA:HB2	2.11	0.65
4:DD:64:LEU:HA	4:DD:101:ILE:HA	1.78	0.65
2:KE:219:ARG:N	2:KE:226:ALA:HB2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CF:219:ARG:N	2:CF:226:ALA:HB2	2.11	0.65
4:DA:64:LEU:HA	4:DA:101:ILE:HA	1.78	0.65
2:WB:219:ARG:N	2:WB:226:ALA:HB2	2.11	0.65
2:G:217:ALA:HB2	2:SG:155:HIS:CB	2.25	0.65
4:LF:64:LEU:HA	4:LF:101:ILE:HA	1.78	0.65
2:T:155:HIS:CB	2:AA:217:ALA:HB2	2.26	0.65
4:X:64:LEU:HA	4:X:101:ILE:HA	1.78	0.65
4:JA:64:LEU:HA	4:JA:101:ILE:HA	1.78	0.65
2:QB:143:ALA:HB3	2:WB:205:LEU:O	1.96	0.65
4:JG:64:LEU:HA	4:JG:101:ILE:HA	1.78	0.65
2:G:25:VAL:O	2:G:29:LEU:CB	2.45	0.65
2:GA:25:VAL:O	2:GA:29:LEU:CB	2.45	0.65
2:OC:219:ARG:N	2:OC:226:ALA:HB2	2.11	0.65
4:XC:64:LEU:HA	4:XC:101:ILE:HA	1.78	0.65
2:IF:155:HIS:CB	2:OF:217:ALA:HB2	2.26	0.65
4:DG:64:LEU:HA	4:DG:101:ILE:HA	1.78	0.65
2:AA:219:ARG:N	2:AA:226:ALA:HB2	2.11	0.65
2:EB:219:ARG:N	2:EB:226:ALA:HB2	2.11	0.65
2:YD:219:ARG:N	2:YD:226:ALA:HB2	2.11	0.65
4:TE:64:LEU:HA	4:TE:101:ILE:HA	1.78	0.65
2:IF:219:ARG:N	2:IF:226:ALA:HB2	2.11	0.65
2:G:219:ARG:N	2:G:226:ALA:HB2	2.11	0.65
2:MA:219:ARG:N	2:MA:226:ALA:HB2	2.11	0.65
4:JD:64:LEU:HA	4:JD:101:ILE:HA	1.78	0.65
4:PD:64:LEU:HA	4:PD:101:ILE:HA	1.78	0.65
2:EE:219:ARG:N	2:EE:226:ALA:HB2	2.11	0.65
4:HE:64:LEU:HA	4:HE:101:ILE:HA	1.78	0.65
2:SG:25:VAL:O	2:SG:29:LEU:CB	2.45	0.65
4:VG:64:LEU:HA	4:VG:101:ILE:HA	1.78	0.65
2:AA:25:VAL:O	2:AA:29:LEU:CB	2.45	0.64
2:MA:25:VAL:O	2:MA:29:LEU:CB	2.45	0.64
2:QB:219:ARG:N	2:QB:226:ALA:HB2	2.11	0.64
2:SG:219:ARG:N	2:SG:226:ALA:HB2	2.11	0.64
2:B:25:VAL:O	2:B:29:LEU:CB	2.45	0.64
2:KB:25:VAL:O	2:KB:29:LEU:CB	2.45	0.64
2:QB:25:VAL:O	2:QB:29:LEU:CB	2.45	0.64
2:UC:219:ARG:N	2:UC:226:ALA:HB2	2.11	0.64
2:OF:219:ARG:N	2:OF:226:ALA:HB2	2.11	0.64
4:P:64:LEU:HA	4:P:101:ILE:HA	1.78	0.64
4:E:64:LEU:HA	4:E:101:ILE:HA	1.78	0.64
2:J:155:HIS:CB	2:T:217:ALA:HB2	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:64:LEU:HA	4:O:101:ILE:HA	1.78	0.64
2:MD:25:VAL:O	2:MD:29:LEU:CB	2.45	0.64
2:SD:25:VAL:O	2:SD:29:LEU:CB	2.45	0.64
2:EE:25:VAL:O	2:EE:29:LEU:CB	2.45	0.64
2:UF:25:VAL:O	2:UF:29:LEU:CB	2.45	0.64
2:EB:25:VAL:O	2:EB:29:LEU:CB	2.45	0.64
2:OC:68:ALA:HB1	2:UC:47:ILE:O	1.98	0.64
2:GD:25:VAL:O	2:GD:29:LEU:CB	2.45	0.64
2:YD:25:VAL:O	2:YD:29:LEU:CB	2.45	0.64
4:BE:64:LEU:HA	4:BE:101:ILE:HA	1.78	0.64
2:KE:25:VAL:O	2:KE:29:LEU:CB	2.45	0.64
2:QE:25:VAL:O	2:QE:29:LEU:CB	2.45	0.64
2:KB:219:ARG:N	2:KB:226:ALA:HB2	2.11	0.64
2:UC:25:VAL:O	2:UC:29:LEU:CB	2.45	0.64
2:AD:25:VAL:O	2:AD:29:LEU:CB	2.45	0.64
2:OF:25:VAL:O	2:OF:29:LEU:CB	2.45	0.64
2:SA:25:VAL:O	2:SA:29:LEU:CB	2.45	0.64
2:WB:25:VAL:O	2:WB:29:LEU:CB	2.45	0.64
2:WE:25:VAL:O	2:WE:29:LEU:CB	2.45	0.64
2:OC:25:VAL:O	2:OC:29:LEU:CB	2.45	0.64
4:VD:64:LEU:HA	4:VD:101:ILE:HA	1.78	0.64
2:CF:25:VAL:O	2:CF:29:LEU:CB	2.45	0.64
2:MG:25:VAL:O	2:MG:29:LEU:CB	2.45	0.64
2:GA:219:ARG:N	2:GA:226:ALA:HB2	2.11	0.64
3:NA:105:ILE:HA	3:NA:179:TYR:HA	1.80	0.64
2:IF:25:VAL:O	2:IF:29:LEU:CB	2.45	0.64
2:AG:25:VAL:O	2:AG:29:LEU:CB	2.45	0.64
2:T:25:VAL:O	2:T:29:LEU:CB	2.45	0.64
3:TA:105:ILE:HA	3:TA:179:TYR:HA	1.80	0.64
2:IC:25:VAL:O	2:IC:29:LEU:CB	2.45	0.64
4:FF:64:LEU:HA	4:FF:101:ILE:HA	1.78	0.64
3:HG:105:ILE:HA	3:HG:179:TYR:HA	1.80	0.64
3:TG:105:ILE:HA	3:TG:179:TYR:HA	1.80	0.64
3:C:105:ILE:HA	3:C:179:TYR:HA	1.80	0.64
2:J:25:VAL:O	2:J:29:LEU:CB	2.45	0.64
3:V:105:ILE:HA	3:V:179:TYR:HA	1.80	0.64
3:BA:105:ILE:HA	3:BA:179:TYR:HA	1.80	0.64
3:HA:105:ILE:HA	3:HA:179:TYR:HA	1.80	0.64
4:XF:64:LEU:HA	4:XF:101:ILE:HA	1.78	0.64
3:NG:105:ILE:HA	3:NG:179:TYR:HA	1.80	0.64
3:M:105:ILE:HA	3:M:179:TYR:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:ZA:105:ILE:HA	3:ZA:179:TYR:HA	1.80	0.63
2:CC:25:VAL:O	2:CC:29:LEU:CB	2.45	0.63
3:BG:105:ILE:HA	3:BG:179:TYR:HA	1.80	0.63
3:K:105:ILE:HA	3:K:179:TYR:HA	1.80	0.63
2:YA:77:LEU:CB	2:EB:42:ALA:O	2.46	0.63
3:FB:105:ILE:HA	3:FB:179:TYR:HA	1.80	0.63
2:B:155:HIS:CB	2:J:217:ALA:HB2	2.27	0.63
2:YA:25:VAL:O	2:YA:29:LEU:CB	2.45	0.63
3:JF:90:HIS:N	3:JF:195:PRO:O	2.31	0.63
3:VF:105:ILE:HA	3:VF:179:TYR:HA	1.80	0.63
3:NG:90:HIS:N	3:NG:195:PRO:O	2.31	0.63
3:LB:105:ILE:HA	3:LB:179:TYR:HA	1.80	0.63
4:NE:64:LEU:HA	4:NE:101:ILE:HA	1.78	0.63
3:PF:105:ILE:HA	3:PF:179:TYR:HA	1.80	0.63
3:M:90:HIS:N	3:M:195:PRO:O	2.31	0.63
3:RB:105:ILE:HA	3:RB:179:TYR:HA	1.80	0.63
3:XE:90:HIS:N	3:XE:195:PRO:O	2.31	0.63
2:GG:25:VAL:O	2:GG:29:LEU:CB	2.45	0.63
4:PG:64:LEU:HA	4:PG:101:ILE:HA	1.78	0.63
2:CF:219:ARG:HA	2:CF:226:ALA:CB	2.29	0.63
3:JF:105:ILE:HA	3:JF:179:TYR:HA	1.80	0.63
2:AG:155:HIS:CB	2:GG:217:ALA:HB2	2.26	0.63
3:BG:90:HIS:N	3:BG:195:PRO:O	2.31	0.63
3:K:90:HIS:N	3:K:195:PRO:O	2.31	0.63
3:XB:105:ILE:HA	3:XB:179:TYR:HA	1.80	0.63
2:OC:74:ASN:CA	2:UC:42:ALA:O	2.47	0.63
2:QE:219:ARG:HA	2:QE:226:ALA:CB	2.29	0.63
2:WE:219:ARG:HA	2:WE:226:ALA:CB	2.29	0.63
2:IF:219:ARG:HA	2:IF:226:ALA:CB	2.29	0.63
2:GD:155:HIS:CB	2:MD:217:ALA:HB2	2.28	0.63
3:ND:105:ILE:HA	3:ND:179:TYR:HA	1.80	0.63
2:KE:219:ARG:HA	2:KE:226:ALA:CB	2.29	0.63
3:DF:105:ILE:HA	3:DF:179:TYR:HA	1.80	0.63
2:OF:219:ARG:HA	2:OF:226:ALA:CB	2.29	0.63
2:EE:219:ARG:HA	2:EE:226:ALA:CB	2.29	0.62
3:XE:105:ILE:HA	3:XE:179:TYR:HA	1.80	0.62
2:MD:219:ARG:HA	2:MD:226:ALA:CB	2.29	0.62
2:SD:219:ARG:HA	2:SD:226:ALA:CB	2.29	0.62
3:TD:106:HIS:N	3:TD:178:GLU:O	2.32	0.62
3:LE:90:HIS:N	3:LE:195:PRO:O	2.31	0.62
2:MA:68:ALA:HB1	2:SA:47:ILE:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DC:105:ILE:HA	3:DC:179:TYR:HA	1.80	0.62
2:UC:219:ARG:HA	2:UC:226:ALA:CB	2.29	0.62
2:AD:219:ARG:HA	2:AD:226:ALA:CB	2.29	0.62
2:GD:219:ARG:HA	2:GD:226:ALA:CB	2.29	0.62
2:YD:219:ARG:HA	2:YD:226:ALA:CB	2.29	0.62
3:LE:106:HIS:N	3:LE:178:GLU:O	2.32	0.62
2:IF:77:LEU:CB	2:OF:42:ALA:O	2.47	0.62
2:OF:155:HIS:CB	2:UF:217:ALA:HB2	2.26	0.62
3:PF:90:HIS:N	3:PF:195:PRO:O	2.31	0.62
2:UF:219:ARG:HA	2:UF:226:ALA:CB	2.29	0.62
2:AA:155:HIS:CB	2:GA:217:ALA:HB2	2.28	0.62
3:VC:106:HIS:N	3:VC:178:GLU:O	2.32	0.62
3:ND:106:HIS:N	3:ND:178:GLU:O	2.32	0.62
3:FE:105:ILE:HA	3:FE:179:TYR:HA	1.80	0.62
3:DC:106:HIS:N	3:DC:178:GLU:O	2.32	0.62
2:OC:219:ARG:HA	2:OC:226:ALA:CB	2.29	0.62
3:VC:105:ILE:HA	3:VC:179:TYR:HA	1.80	0.62
3:BD:106:HIS:N	3:BD:178:GLU:O	2.32	0.62
3:BA:90:HIS:N	3:BA:195:PRO:O	2.31	0.62
2:IC:219:ARG:HA	2:IC:226:ALA:CB	2.29	0.62
3:JC:105:ILE:HA	3:JC:179:TYR:HA	1.80	0.62
3:BD:105:ILE:HA	3:BD:179:TYR:HA	1.80	0.62
3:RE:105:ILE:HA	3:RE:179:TYR:HA	1.80	0.62
2:WE:19:GLU:HA	2:WE:22:ALA:HB3	1.82	0.62
3:DF:106:HIS:N	3:DF:178:GLU:O	2.32	0.62
2:T:19:GLU:HA	2:T:22:ALA:HB3	1.82	0.62
2:AA:19:GLU:HA	2:AA:22:ALA:HB3	1.82	0.62
2:GA:219:ARG:HA	2:GA:226:ALA:CB	2.29	0.62
2:YA:19:GLU:HA	2:YA:22:ALA:HB3	1.82	0.62
3:ZD:105:ILE:HA	3:ZD:179:TYR:HA	1.80	0.62
3:FE:106:HIS:N	3:FE:178:GLU:O	2.32	0.62
3:LE:105:ILE:HA	3:LE:179:TYR:HA	1.80	0.62
2:CF:19:GLU:HA	2:CF:22:ALA:HB3	1.82	0.62
2:GG:19:GLU:HA	2:GG:22:ALA:HB3	1.82	0.62
3:PC:105:ILE:HA	3:PC:179:TYR:HA	1.80	0.62
2:YD:155:HIS:CB	2:EE:217:ALA:HB2	2.29	0.62
3:ZD:90:HIS:N	3:ZD:195:PRO:O	2.31	0.62
3:RE:106:HIS:N	3:RE:178:GLU:O	2.32	0.62
2:AG:219:ARG:HA	2:AG:226:ALA:CB	2.29	0.62
3:FE:90:HIS:N	3:FE:195:PRO:O	2.31	0.62
3:RE:90:HIS:N	3:RE:195:PRO:O	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AG:19:GLU:HA	2:AG:22:ALA:HB3	1.82	0.62
2:MG:19:GLU:HA	2:MG:22:ALA:HB3	1.82	0.62
3:C:106:HIS:N	3:C:178:GLU:O	2.32	0.62
2:J:219:ARG:HA	2:J:226:ALA:CB	2.29	0.62
3:BA:106:HIS:N	3:BA:178:GLU:O	2.32	0.62
3:HA:106:HIS:N	3:HA:178:GLU:O	2.32	0.62
2:EB:19:GLU:HA	2:EB:22:ALA:HB3	1.82	0.62
2:KB:19:GLU:HA	2:KB:22:ALA:HB3	1.82	0.62
2:QB:219:ARG:HA	2:QB:226:ALA:CB	2.29	0.62
3:JC:106:HIS:N	3:JC:178:GLU:O	2.32	0.62
2:QE:19:GLU:HA	2:QE:22:ALA:HB3	1.82	0.62
3:JF:106:HIS:N	3:JF:178:GLU:O	2.32	0.62
3:M:106:HIS:N	3:M:178:GLU:O	2.32	0.61
2:J:19:GLU:HA	2:J:22:ALA:HB3	1.82	0.61
2:J:77:LEU:CB	2:T:42:ALA:O	2.48	0.61
3:LB:106:HIS:N	3:LB:178:GLU:O	2.32	0.61
2:CC:219:ARG:HA	2:CC:226:ALA:CB	2.29	0.61
2:SD:19:GLU:HA	2:SD:22:ALA:HB3	1.82	0.61
3:ZD:106:HIS:N	3:ZD:178:GLU:O	2.32	0.61
3:DF:90:HIS:N	3:DF:195:PRO:O	2.31	0.61
2:GG:219:ARG:HA	2:GG:226:ALA:CB	2.29	0.61
2:B:219:ARG:HA	2:B:226:ALA:CB	2.29	0.61
2:MA:219:ARG:HA	2:MA:226:ALA:CB	2.29	0.61
2:SA:219:ARG:HA	2:SA:226:ALA:CB	2.29	0.61
2:YA:219:ARG:HA	2:YA:226:ALA:CB	2.29	0.61
2:OC:19:GLU:HA	2:OC:22:ALA:HB3	1.82	0.61
3:VF:106:HIS:N	3:VF:178:GLU:O	2.32	0.61
3:C:90:HIS:N	3:C:195:PRO:O	2.31	0.61
2:T:219:ARG:HA	2:T:226:ALA:CB	2.29	0.61
2:AA:219:ARG:HA	2:AA:226:ALA:CB	2.29	0.61
2:GA:19:GLU:HA	2:GA:22:ALA:HB3	1.82	0.61
3:NA:90:HIS:N	3:NA:195:PRO:O	2.31	0.61
2:IC:19:GLU:HA	2:IC:22:ALA:HB3	1.82	0.61
2:IC:77:LEU:CB	2:OC:42:ALA:O	2.47	0.61
3:PC:106:HIS:N	3:PC:178:GLU:O	2.32	0.61
2:MD:19:GLU:HA	2:MD:22:ALA:HB3	1.82	0.61
2:YD:19:GLU:HA	2:YD:22:ALA:HB3	1.82	0.61
3:XE:106:HIS:N	3:XE:178:GLU:O	2.32	0.61
2:IF:19:GLU:HA	2:IF:22:ALA:HB3	1.82	0.61
2:MG:219:ARG:HA	2:MG:226:ALA:CB	2.29	0.61
2:SG:19:GLU:HA	2:SG:22:ALA:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:90:HIS:N	3:V:195:PRO:O	2.31	0.61
2:SA:155:HIS:CB	2:YA:217:ALA:HB2	2.28	0.61
2:EB:219:ARG:HA	2:EB:226:ALA:CB	2.29	0.61
3:HD:105:ILE:HA	3:HD:179:TYR:HA	1.80	0.61
3:TD:90:HIS:N	3:TD:195:PRO:O	2.31	0.61
3:TD:105:ILE:HA	3:TD:179:TYR:HA	1.80	0.61
2:KE:77:LEU:CB	2:QE:42:ALA:O	2.48	0.61
3:BG:106:HIS:N	3:BG:178:GLU:O	2.32	0.61
2:MA:74:ASN:CA	2:SA:42:ALA:O	2.48	0.61
3:FB:106:HIS:N	3:FB:178:GLU:O	2.32	0.61
3:XB:106:HIS:N	3:XB:178:GLU:O	2.32	0.61
2:YD:68:ALA:HB1	2:EE:47:ILE:O	2.00	0.61
2:QE:155:HIS:CB	2:WE:217:ALA:HB2	2.28	0.61
2:OF:68:ALA:HB1	2:UF:47:ILE:O	2.00	0.61
2:SG:219:ARG:HA	2:SG:226:ALA:CB	2.29	0.61
2:G:219:ARG:HA	2:G:226:ALA:CB	2.29	0.61
3:HA:90:HIS:N	3:HA:195:PRO:O	2.31	0.61
3:ZA:106:HIS:N	3:ZA:178:GLU:O	2.32	0.61
2:KB:219:ARG:HA	2:KB:226:ALA:CB	2.29	0.61
2:CC:155:HIS:CB	2:IC:217:ALA:HB2	2.30	0.61
3:HD:106:HIS:N	3:HD:178:GLU:O	2.32	0.61
3:ND:90:HIS:N	3:ND:195:PRO:O	2.31	0.61
3:K:106:HIS:N	3:K:178:GLU:O	2.32	0.61
3:V:106:HIS:N	3:V:178:GLU:O	2.32	0.61
3:NA:106:HIS:N	3:NA:178:GLU:O	2.32	0.61
2:CC:19:GLU:HA	2:CC:22:ALA:HB3	1.82	0.61
2:SD:155:HIS:CB	2:YD:217:ALA:HB2	2.29	0.61
2:UF:19:GLU:HA	2:UF:22:ALA:HB3	1.82	0.61
3:NG:106:HIS:N	3:NG:178:GLU:O	2.32	0.61
3:TG:90:HIS:N	3:TG:195:PRO:O	2.31	0.61
3:TG:106:HIS:N	3:TG:178:GLU:O	2.32	0.61
2:B:19:GLU:HA	2:B:22:ALA:HB3	1.82	0.61
2:SA:19:GLU:HA	2:SA:22:ALA:HB3	1.82	0.61
3:TA:106:HIS:N	3:TA:178:GLU:O	2.32	0.61
3:RB:106:HIS:N	3:RB:178:GLU:O	2.32	0.61
2:WB:219:ARG:HA	2:WB:226:ALA:CB	2.29	0.61
2:UC:19:GLU:HA	2:UC:22:ALA:HB3	1.82	0.61
3:HG:106:HIS:N	3:HG:178:GLU:O	2.32	0.61
3:ZA:90:HIS:N	3:ZA:195:PRO:O	2.31	0.61
2:QB:19:GLU:HA	2:QB:22:ALA:HB3	1.82	0.61
3:HD:90:HIS:N	3:HD:195:PRO:O	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:WE:68:ALA:HB1	2:CF:47:ILE:O	2.00	0.61
4:OA:97:LEU:N	4:OA:109:GLY:O	2.34	0.61
4:AB:97:LEU:N	4:AB:109:GLY:O	2.34	0.61
4:GB:97:LEU:N	4:GB:109:GLY:O	2.34	0.61
2:GD:19:GLU:HA	2:GD:22:ALA:HB3	1.82	0.61
2:MD:68:ALA:HB1	2:SD:47:ILE:O	2.00	0.61
2:WE:74:ASN:CA	2:CF:42:ALA:O	2.48	0.61
2:GG:68:ALA:HB1	2:MG:47:ILE:O	2.00	0.61
4:CA:97:LEU:N	4:CA:109:GLY:O	2.34	0.60
4:IA:97:LEU:N	4:IA:109:GLY:O	2.34	0.60
4:UA:97:LEU:N	4:UA:109:GLY:O	2.34	0.60
2:EE:19:GLU:HA	2:EE:22:ALA:HB3	1.82	0.60
3:PF:106:HIS:N	3:PF:178:GLU:O	2.32	0.60
2:GG:155:HIS:CB	2:MG:217:ALA:HB2	2.29	0.60
2:G:19:GLU:HA	2:G:22:ALA:HB3	1.82	0.60
3:TA:90:HIS:N	3:TA:195:PRO:O	2.31	0.60
4:MB:97:LEU:N	4:MB:109:GLY:O	2.34	0.60
3:VC:90:HIS:N	3:VC:195:PRO:O	2.31	0.60
2:OF:19:GLU:HA	2:OF:22:ALA:HB3	1.82	0.60
4:L:97:LEU:N	4:L:109:GLY:O	2.34	0.60
2:MA:19:GLU:HA	2:MA:22:ALA:HB3	1.82	0.60
3:LB:90:HIS:N	3:LB:195:PRO:O	2.31	0.60
4:SB:97:LEU:N	4:SB:109:GLY:O	2.34	0.60
3:BD:90:HIS:N	3:BD:195:PRO:O	2.31	0.60
2:KE:19:GLU:HA	2:KE:22:ALA:HB3	1.82	0.60
4:W:97:LEU:N	4:W:109:GLY:O	2.34	0.60
2:QB:155:HIS:CB	2:WB:217:ALA:HB2	2.31	0.60
2:WB:77:LEU:CB	2:CC:42:ALA:O	2.49	0.60
2:AD:68:ALA:HB1	2:GD:47:ILE:O	2.01	0.60
4:SE:97:LEU:N	4:SE:109:GLY:O	2.34	0.60
2:G:42:ALA:O	2:SG:77:LEU:CB	2.49	0.60
2:T:68:ALA:HB1	2:AA:47:ILE:O	2.02	0.60
3:FB:90:HIS:N	3:FB:195:PRO:O	2.31	0.60
4:YB:97:LEU:N	4:YB:109:GLY:O	2.34	0.60
3:JC:90:HIS:N	3:JC:195:PRO:O	2.31	0.60
4:GE:97:LEU:N	4:GE:109:GLY:O	2.34	0.60
4:ME:97:LEU:N	4:ME:109:GLY:O	2.34	0.60
3:HG:90:HIS:N	3:HG:195:PRO:O	2.31	0.60
3:XB:90:HIS:N	3:XB:195:PRO:O	2.31	0.60
4:YE:97:LEU:N	4:YE:109:GLY:O	2.34	0.60
2:OF:74:ASN:CA	2:UF:42:ALA:O	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:97:LEU:N	4:D:109:GLY:O	2.34	0.60
3:PC:90:HIS:N	3:PC:195:PRO:O	2.31	0.60
3:V:314:ALA:HA	4:W:88:ALA:HA	1.84	0.60
2:AA:77:LEU:CB	2:GA:42:ALA:O	2.49	0.60
3:ZA:314:ALA:HA	4:AB:88:ALA:HA	1.84	0.60
3:FB:314:ALA:HA	4:GB:88:ALA:HA	1.84	0.60
2:WB:19:GLU:HA	2:WB:22:ALA:HB3	1.82	0.60
3:DC:314:ALA:HA	4:EC:88:ALA:HA	1.84	0.60
4:EC:97:LEU:N	4:EC:109:GLY:O	2.34	0.60
2:MD:155:HIS:CB	2:SD:217:ALA:HB2	2.31	0.60
2:SD:77:LEU:CB	2:YD:42:ALA:O	2.50	0.60
4:AE:97:LEU:N	4:AE:109:GLY:O	2.34	0.60
4:EF:97:LEU:N	4:EF:109:GLY:O	2.34	0.60
4:N:97:LEU:N	4:N:109:GLY:O	2.34	0.60
2:T:74:ASN:CA	2:AA:42:ALA:O	2.50	0.60
3:RB:90:HIS:N	3:RB:195:PRO:O	2.31	0.60
3:JC:314:ALA:HA	4:KC:88:ALA:HA	1.84	0.60
4:KF:97:LEU:N	4:KF:109:GLY:O	2.34	0.60
2:AG:68:ALA:HB1	2:GG:47:ILE:O	2.02	0.60
2:G:155:HIS:CB	2:B:217:ALA:HB2	2.30	0.60
3:K:314:ALA:HA	4:L:88:ALA:HA	1.84	0.60
3:BA:314:ALA:HA	4:CA:88:ALA:HA	1.84	0.60
3:DC:90:HIS:N	3:DC:195:PRO:O	2.31	0.60
2:AD:19:GLU:HA	2:AD:22:ALA:HB3	1.82	0.60
3:ND:314:ALA:HA	4:OD:88:ALA:HA	1.84	0.60
4:UD:97:LEU:N	4:UD:109:GLY:O	2.34	0.60
2:EE:77:LEU:CB	2:KE:42:ALA:O	2.50	0.60
2:GA:74:ASN:CA	2:MA:42:ALA:O	2.50	0.59
2:GA:77:LEU:CB	2:MA:42:ALA:O	2.50	0.59
2:EB:77:LEU:CB	2:KB:42:ALA:O	2.50	0.59
4:KC:97:LEU:N	4:KC:109:GLY:O	2.34	0.59
3:HD:314:ALA:HA	4:ID:88:ALA:HA	1.84	0.59
3:ND:102:LEU:O	3:ND:183:GLU:N	2.31	0.59
3:TD:314:ALA:HA	4:UD:88:ALA:HA	1.84	0.59
3:PC:314:ALA:HA	4:QC:88:ALA:HA	1.84	0.59
4:DD:122:ILE:O	4:ED:84:GLY:N	2.34	0.59
4:PD:122:ILE:O	4:QD:84:GLY:N	2.34	0.59
4:HE:122:ILE:O	4:IE:84:GLY:N	2.34	0.59
4:UG:97:LEU:N	4:UG:109:GLY:O	2.34	0.59
3:TA:314:ALA:HA	4:UA:88:ALA:HA	1.84	0.59
4:NB:122:ILE:O	4:OB:84:GLY:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:XB:314:ALA:HA	4:YB:88:ALA:HA	1.84	0.59
2:AD:77:LEU:CB	2:GD:42:ALA:O	2.50	0.59
4:JD:122:ILE:O	4:KD:84:GLY:N	2.34	0.59
4:VD:122:ILE:O	4:WD:84:GLY:N	2.34	0.59
4:BE:122:ILE:O	4:CE:84:GLY:N	2.34	0.59
4:QF:97:LEU:N	4:QF:109:GLY:O	2.34	0.59
2:UF:155:HIS:CB	2:AG:217:ALA:HB2	2.29	0.59
2:GG:74:ASN:CA	2:MG:42:ALA:O	2.49	0.59
2:B:77:LEU:CB	2:J:42:ALA:O	2.50	0.59
4:HB:122:ILE:O	4:IB:84:GLY:N	2.34	0.59
4:OD:97:LEU:N	4:OD:109:GLY:O	2.34	0.59
4:NE:122:ILE:O	4:OE:84:GLY:N	2.34	0.59
4:TE:122:ILE:O	4:UE:84:GLY:N	2.34	0.59
2:GA:68:ALA:HB1	2:MA:47:ILE:O	2.01	0.59
2:SA:77:LEU:CB	2:YA:42:ALA:O	2.50	0.59
3:LB:314:ALA:HA	4:MB:88:ALA:HA	1.84	0.59
3:HD:102:LEU:O	3:HD:183:GLU:N	2.31	0.59
3:RE:314:ALA:HA	4:SE:88:ALA:HA	1.84	0.59
4:ZE:122:ILE:O	4:AF:84:GLY:N	2.34	0.59
4:FF:122:ILE:O	4:GF:84:GLY:N	2.34	0.59
2:UF:68:ALA:HB1	2:AG:47:ILE:O	2.02	0.59
3:HG:314:ALA:HA	4:IG:88:ALA:HA	1.84	0.59
4:VA:122:ILE:O	4:WA:84:GLY:N	2.34	0.59
4:BB:122:ILE:O	4:CB:84:GLY:N	2.34	0.59
2:UC:155:HIS:CB	2:AD:217:ALA:HB2	2.32	0.59
2:QE:68:ALA:HB1	2:WE:47:ILE:O	2.02	0.59
3:XE:314:ALA:HA	4:YE:88:ALA:HA	1.84	0.59
3:NG:314:ALA:HA	4:OG:88:ALA:HA	1.84	0.59
4:OG:97:LEU:N	4:OG:109:GLY:O	2.34	0.59
2:KB:155:HIS:CB	2:QB:217:ALA:HB2	2.27	0.59
2:EE:155:HIS:CB	2:KE:217:ALA:HB2	2.30	0.59
4:LF:122:ILE:O	4:MF:84:GLY:N	2.34	0.59
3:VF:90:HIS:N	3:VF:195:PRO:O	2.31	0.59
3:BG:314:ALA:HA	4:CG:88:ALA:HA	1.84	0.59
2:G:68:ALA:HB1	2:B:47:ILE:O	2.03	0.59
3:C:102:LEU:O	3:C:183:GLU:N	2.31	0.59
3:C:314:ALA:HA	4:D:88:ALA:HA	1.84	0.59
3:HA:314:ALA:HA	4:IA:88:ALA:HA	1.84	0.59
3:BD:314:ALA:HA	4:CD:88:ALA:HA	1.84	0.59
3:DF:314:ALA:HA	4:EF:88:ALA:HA	1.84	0.59
4:IG:97:LEU:N	4:IG:109:GLY:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:TG:102:LEU:O	3:TG:183:GLU:N	2.31	0.59
3:M:102:LEU:O	3:M:183:GLU:N	2.31	0.59
2:B:68:ALA:HB1	2:J:47:ILE:O	2.03	0.59
3:K:102:LEU:O	3:K:183:GLU:N	2.31	0.59
4:O:97:LEU:N	4:O:109:GLY:O	2.36	0.59
4:JA:122:ILE:O	4:KA:84:GLY:N	2.34	0.59
4:PA:122:ILE:O	4:QA:84:GLY:N	2.34	0.59
2:AD:74:ASN:CA	2:GD:42:ALA:O	2.50	0.59
4:ID:97:LEU:N	4:ID:109:GLY:O	2.34	0.59
4:RF:122:ILE:O	4:SF:84:GLY:N	2.34	0.59
4:WF:97:LEU:N	4:WF:109:GLY:O	2.34	0.59
2:G:74:ASN:CA	2:B:42:ALA:O	2.51	0.59
4:E:97:LEU:N	4:E:109:GLY:O	2.36	0.59
3:V:102:LEU:O	3:V:183:GLU:N	2.31	0.59
4:X:97:LEU:N	4:X:109:GLY:O	2.36	0.59
2:EB:68:ALA:HB1	2:KB:47:ILE:O	2.03	0.59
3:BD:102:LEU:O	3:BD:183:GLU:N	2.31	0.59
2:GD:77:LEU:CB	2:MD:42:ALA:O	2.51	0.59
3:ZD:314:ALA:HA	4:AE:88:ALA:HA	1.84	0.59
4:NE:97:LEU:N	4:NE:109:GLY:O	2.36	0.59
4:TE:97:LEU:N	4:TE:109:GLY:O	2.36	0.59
4:ZE:97:LEU:N	4:ZE:109:GLY:O	2.36	0.59
4:FF:97:LEU:N	4:FF:109:GLY:O	2.36	0.59
4:RF:97:LEU:N	4:RF:109:GLY:O	2.36	0.59
4:XF:97:LEU:N	4:XF:109:GLY:O	2.36	0.59
4:XF:122:ILE:O	4:YF:84:GLY:N	2.34	0.59
3:TG:314:ALA:HA	4:UG:88:ALA:HA	1.84	0.59
4:VG:97:LEU:N	4:VG:109:GLY:O	2.36	0.59
4:P:97:LEU:N	4:P:109:GLY:O	2.36	0.58
2:T:77:LEU:CB	2:AA:42:ALA:O	2.51	0.58
4:DA:97:LEU:N	4:DA:109:GLY:O	2.36	0.58
4:DA:122:ILE:O	4:EA:84:GLY:N	2.34	0.58
4:JA:97:LEU:N	4:JA:109:GLY:O	2.36	0.58
4:PA:97:LEU:N	4:PA:109:GLY:O	2.36	0.58
2:MD:74:ASN:CA	2:SD:42:ALA:O	2.49	0.58
4:HE:97:LEU:N	4:HE:109:GLY:O	2.36	0.58
2:CF:77:LEU:CB	2:IF:42:ALA:O	2.51	0.58
4:LF:97:LEU:N	4:LF:109:GLY:O	2.36	0.58
2:AG:74:ASN:CA	2:GG:42:ALA:O	2.50	0.58
4:DG:122:ILE:O	4:EG:84:GLY:N	2.34	0.58
4:JG:97:LEU:N	4:JG:109:GLY:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:PG:97:LEU:N	4:PG:109:GLY:O	2.36	0.58
4:X:122:ILE:O	4:Y:84:GLY:N	2.34	0.58
3:VC:314:ALA:HA	4:WC:88:ALA:HA	1.84	0.58
4:BE:97:LEU:N	4:BE:109:GLY:O	2.36	0.58
3:LE:314:ALA:HA	4:ME:88:ALA:HA	1.84	0.58
4:DG:97:LEU:N	4:DG:109:GLY:O	2.36	0.58
4:JG:122:ILE:O	4:KG:84:GLY:N	2.34	0.58
2:MG:155:HIS:CB	2:SG:217:ALA:HB2	2.31	0.58
4:PG:122:ILE:O	4:QG:84:GLY:N	2.34	0.58
4:E:122:ILE:O	4:H:84:GLY:N	2.34	0.58
4:O:122:ILE:O	4:R:84:GLY:N	2.34	0.58
3:BA:102:LEU:O	3:BA:183:GLU:N	2.31	0.58
3:NA:314:ALA:HA	4:OA:88:ALA:HA	1.84	0.58
4:VA:97:LEU:N	4:VA:109:GLY:O	2.36	0.58
4:PD:97:LEU:N	4:PD:109:GLY:O	2.36	0.58
4:VD:97:LEU:N	4:VD:109:GLY:O	2.36	0.58
2:CF:155:HIS:CB	2:IF:217:ALA:HB2	2.28	0.58
4:CG:97:LEU:N	4:CG:109:GLY:O	2.34	0.58
4:P:122:ILE:O	4:Q:84:GLY:N	2.34	0.58
2:B:74:ASN:CA	2:J:42:ALA:O	2.52	0.58
3:VC:102:LEU:O	3:VC:183:GLU:N	2.31	0.58
4:JD:97:LEU:N	4:JD:109:GLY:O	2.36	0.58
3:JF:314:ALA:HA	4:KF:88:ALA:HA	1.84	0.58
3:VF:314:ALA:HA	4:WF:88:ALA:HA	1.84	0.58
4:VG:122:ILE:O	4:WG:84:GLY:N	2.34	0.58
4:BB:97:LEU:N	4:BB:109:GLY:O	2.37	0.58
4:HB:97:LEU:N	4:HB:109:GLY:O	2.36	0.58
2:KE:68:ALA:HB1	2:QE:47:ILE:O	2.03	0.58
3:HA:102:LEU:O	3:HA:183:GLU:N	2.31	0.58
4:NB:97:LEU:N	4:NB:109:GLY:O	2.36	0.58
4:AC:65:THR:N	4:AC:100:LEU:O	2.37	0.58
4:LC:97:LEU:N	4:LC:109:GLY:O	2.36	0.58
4:QC:97:LEU:N	4:QC:109:GLY:O	2.34	0.58
4:RC:97:LEU:N	4:RC:109:GLY:O	2.36	0.58
2:UC:68:ALA:HB1	2:AD:47:ILE:O	2.03	0.58
4:WC:97:LEU:N	4:WC:109:GLY:O	2.34	0.58
4:XC:97:LEU:N	4:XC:109:GLY:O	2.36	0.58
4:DD:97:LEU:N	4:DD:109:GLY:O	2.36	0.58
2:MG:77:LEU:CB	2:SG:42:ALA:O	2.50	0.58
3:RB:314:ALA:HA	4:SB:88:ALA:HA	1.84	0.58
4:TB:97:LEU:N	4:TB:109:GLY:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CD:97:LEU:N	4:CD:109:GLY:O	2.34	0.58
2:GD:68:ALA:HB1	2:MD:47:ILE:O	2.03	0.58
2:QE:77:LEU:CB	2:WE:42:ALA:O	2.51	0.58
2:UF:74:ASN:CA	2:AG:42:ALA:O	2.51	0.58
2:AG:77:LEU:CB	2:GG:42:ALA:O	2.51	0.58
3:M:314:ALA:HA	4:N:88:ALA:HA	1.84	0.58
2:QB:77:LEU:CB	2:WB:42:ALA:O	2.51	0.58
4:ZB:97:LEU:N	4:ZB:109:GLY:O	2.36	0.58
4:FC:97:LEU:N	4:FC:109:GLY:O	2.36	0.58
3:PC:102:LEU:O	3:PC:183:GLU:N	2.31	0.58
2:QE:74:ASN:CA	2:WE:42:ALA:O	2.50	0.58
3:NA:102:LEU:O	3:NA:183:GLU:N	2.31	0.58
2:OF:77:LEU:CB	2:UF:42:ALA:O	2.52	0.58
2:CC:77:LEU:CB	2:IC:42:ALA:O	2.51	0.58
4:GC:65:THR:N	4:GC:100:LEU:O	2.37	0.58
3:FE:314:ALA:HA	4:GE:88:ALA:HA	1.84	0.58
2:WE:155:HIS:CB	2:CF:217:ALA:HB2	2.31	0.58
3:VF:102:LEU:O	3:VF:183:GLU:N	2.31	0.58
4:R:65:THR:N	4:R:100:LEU:O	2.37	0.57
4:Y:65:THR:N	4:Y:100:LEU:O	2.37	0.57
4:EA:65:THR:N	4:EA:100:LEU:O	2.37	0.57
4:QA:65:THR:N	4:QA:100:LEU:O	2.37	0.57
2:SA:68:ALA:HB1	2:YA:47:ILE:O	2.04	0.57
3:TA:102:LEU:O	3:TA:183:GLU:N	2.31	0.57
4:WA:65:THR:N	4:WA:100:LEU:O	2.37	0.57
4:CB:65:THR:N	4:CB:100:LEU:O	2.37	0.57
4:IB:65:THR:N	4:IB:100:LEU:O	2.37	0.57
3:TD:88:PRO:HA	3:TD:198:ILE:HA	1.86	0.57
2:UF:77:LEU:CB	2:AG:42:ALA:O	2.52	0.57
4:EG:65:THR:N	4:EG:100:LEU:O	2.37	0.57
2:G:47:ILE:O	2:SG:68:ALA:HB1	2.03	0.57
4:Q:65:THR:N	4:Q:100:LEU:O	2.37	0.57
4:H:65:THR:N	4:H:100:LEU:O	2.37	0.57
4:KA:65:THR:N	4:KA:100:LEU:O	2.37	0.57
4:OB:65:THR:N	4:OB:100:LEU:O	2.37	0.57
4:UB:65:THR:N	4:UB:100:LEU:O	2.37	0.57
3:JC:102:LEU:O	3:JC:183:GLU:N	2.31	0.57
2:OC:77:LEU:CB	2:UC:42:ALA:O	2.52	0.57
2:YD:74:ASN:CA	2:EE:42:ALA:O	2.49	0.57
3:FE:88:PRO:HA	3:FE:198:ILE:HA	1.86	0.57
2:CF:68:ALA:HB1	2:IF:47:ILE:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:WG:65:THR:N	4:WG:100:LEU:O	2.37	0.57
3:ZA:102:LEU:O	3:ZA:183:GLU:N	2.31	0.57
2:WB:74:ASN:CA	2:CC:42:ALA:O	2.53	0.57
3:XB:85:ARG:N	3:XB:201:ASN:O	2.36	0.57
2:UC:77:LEU:CB	2:AD:42:ALA:O	2.52	0.57
3:HD:88:PRO:HA	3:HD:198:ILE:HA	1.86	0.57
3:LE:88:PRO:HA	3:LE:198:ILE:HA	1.86	0.57
3:PF:314:ALA:HA	4:QF:88:ALA:HA	1.84	0.57
4:QG:65:THR:N	4:QG:100:LEU:O	2.37	0.57
2:G:77:LEU:CB	2:B:42:ALA:O	2.52	0.57
2:CC:68:ALA:HB1	2:IC:47:ILE:O	2.04	0.57
2:CC:74:ASN:CA	2:IC:42:ALA:O	2.53	0.57
3:DC:102:LEU:O	3:DC:183:GLU:N	2.31	0.57
4:KG:65:THR:N	4:KG:100:LEU:O	2.37	0.57
3:K:88:PRO:HA	3:K:198:ILE:HA	1.86	0.57
3:HA:88:PRO:HA	3:HA:198:ILE:HA	1.86	0.57
3:FB:102:LEU:O	3:FB:183:GLU:N	2.31	0.57
3:LB:102:LEU:O	3:LB:183:GLU:N	2.31	0.57
3:XB:102:LEU:O	3:XB:183:GLU:N	2.31	0.57
4:MC:65:THR:N	4:MC:100:LEU:O	2.37	0.57
3:VC:88:PRO:HA	3:VC:198:ILE:HA	1.86	0.57
3:ND:88:PRO:HA	3:ND:198:ILE:HA	1.86	0.57
2:YD:77:LEU:CB	2:EE:42:ALA:O	2.52	0.57
3:FE:85:ARG:N	3:FE:201:ASN:O	2.36	0.57
3:XE:88:PRO:HA	3:XE:198:ILE:HA	1.86	0.57
3:PF:102:LEU:O	3:PF:183:GLU:N	2.31	0.57
4:YF:65:THR:N	4:YF:100:LEU:O	2.37	0.57
3:NA:88:PRO:HA	3:NA:198:ILE:HA	1.86	0.57
3:ZA:88:PRO:HA	3:ZA:198:ILE:HA	1.86	0.57
3:RB:102:LEU:O	3:RB:183:GLU:N	2.31	0.57
3:ZD:88:PRO:HA	3:ZD:198:ILE:HA	1.86	0.57
4:IE:65:THR:N	4:IE:100:LEU:O	2.37	0.57
3:V:88:PRO:HA	3:V:198:ILE:HA	1.86	0.57
3:RB:85:ARG:N	3:RB:201:ASN:O	2.36	0.57
3:BD:88:PRO:HA	3:BD:198:ILE:HA	1.86	0.57
3:ZD:85:ARG:N	3:ZD:201:ASN:O	2.36	0.57
3:LE:85:ARG:N	3:LE:201:ASN:O	2.36	0.57
4:OE:65:THR:N	4:OE:100:LEU:O	2.37	0.57
3:RE:88:PRO:HA	3:RE:198:ILE:HA	1.86	0.57
4:AF:65:THR:N	4:AF:100:LEU:O	2.37	0.57
3:JF:88:PRO:HA	3:JF:198:ILE:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:MF:65:THR:N	4:MF:100:LEU:O	2.37	0.57
4:SF:65:THR:N	4:SF:100:LEU:O	2.37	0.57
3:TG:88:PRO:HA	3:TG:198:ILE:HA	1.86	0.57
3:PC:88:PRO:HA	3:PC:198:ILE:HA	1.86	0.57
2:UC:74:ASN:CA	2:AD:42:ALA:O	2.52	0.57
2:GD:74:ASN:CA	2:MD:42:ALA:O	2.51	0.57
4:CE:65:THR:N	4:CE:100:LEU:O	2.37	0.57
4:UE:65:THR:N	4:UE:100:LEU:O	2.37	0.57
3:PC:85:ARG:N	3:PC:201:ASN:O	2.36	0.57
4:SC:65:THR:N	4:SC:100:LEU:O	2.37	0.57
4:WD:65:THR:N	4:WD:100:LEU:O	2.37	0.57
3:DF:88:PRO:HA	3:DF:198:ILE:HA	1.86	0.57
3:M:88:PRO:HA	3:M:198:ILE:HA	1.86	0.57
3:RB:201:ASN:HA	3:RB:218:CYS:HA	1.87	0.57
4:YC:65:THR:N	4:YC:100:LEU:O	2.37	0.57
3:BD:201:ASN:HA	3:BD:218:CYS:HA	1.87	0.57
3:ND:201:ASN:HA	3:ND:218:CYS:HA	1.87	0.57
4:GF:65:THR:N	4:GF:100:LEU:O	2.37	0.57
3:JF:102:LEU:O	3:JF:183:GLU:N	2.31	0.57
3:VF:88:PRO:HA	3:VF:198:ILE:HA	1.86	0.57
3:NA:201:ASN:HA	3:NA:218:CYS:HA	1.87	0.56
3:DC:201:ASN:HA	3:DC:218:CYS:HA	1.87	0.56
3:JC:201:ASN:HA	3:JC:218:CYS:HA	1.87	0.56
4:ED:65:THR:N	4:ED:100:LEU:O	2.37	0.56
3:HD:201:ASN:HA	3:HD:218:CYS:HA	1.87	0.56
4:QD:65:THR:N	4:QD:100:LEU:O	2.37	0.56
2:AA:74:ASN:CA	2:GA:42:ALA:O	2.53	0.56
3:TA:201:ASN:HA	3:TA:218:CYS:HA	1.87	0.56
3:FB:88:PRO:HA	3:FB:198:ILE:HA	1.86	0.56
3:FB:201:ASN:HA	3:FB:218:CYS:HA	1.88	0.56
3:RB:88:PRO:HA	3:RB:198:ILE:HA	1.86	0.56
3:XB:201:ASN:HA	3:XB:218:CYS:HA	1.87	0.56
3:JC:88:PRO:HA	3:JC:198:ILE:HA	1.86	0.56
3:PC:201:ASN:HA	3:PC:218:CYS:HA	1.87	0.56
3:VC:201:ASN:HA	3:VC:218:CYS:HA	1.87	0.56
4:KD:65:THR:N	4:KD:100:LEU:O	2.37	0.56
3:TD:201:ASN:HA	3:TD:218:CYS:HA	1.87	0.56
3:LE:201:ASN:HA	3:LE:218:CYS:HA	1.87	0.56
2:J:68:ALA:HB1	2:T:47:ILE:O	2.06	0.56
3:K:201:ASN:HA	3:K:218:CYS:HA	1.87	0.56
3:BA:201:ASN:HA	3:BA:218:CYS:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:HA:201:ASN:HA	3:HA:218:CYS:HA	1.87	0.56
3:ZA:201:ASN:HA	3:ZA:218:CYS:HA	1.88	0.56
3:LB:201:ASN:HA	3:LB:218:CYS:HA	1.88	0.56
2:QB:74:ASN:CA	2:WB:42:ALA:O	2.54	0.56
3:DC:88:PRO:HA	3:DC:198:ILE:HA	1.86	0.56
3:ZD:201:ASN:HA	3:ZD:218:CYS:HA	1.88	0.56
3:FE:201:ASN:HA	3:FE:218:CYS:HA	1.87	0.56
3:XE:201:ASN:HA	3:XE:218:CYS:HA	1.87	0.56
3:PF:88:PRO:HA	3:PF:198:ILE:HA	1.86	0.56
2:WB:68:ALA:HB1	2:CC:47:ILE:O	2.04	0.56
2:MD:77:LEU:CB	2:SD:42:ALA:O	2.54	0.56
3:TD:85:ARG:N	3:TD:201:ASN:O	2.36	0.56
2:J:74:ASN:CA	2:T:42:ALA:O	2.54	0.56
3:V:201:ASN:HA	3:V:218:CYS:HA	1.87	0.56
2:SA:74:ASN:CA	2:YA:42:ALA:O	2.52	0.56
3:RE:85:ARG:N	3:RE:201:ASN:O	2.36	0.56
3:DF:102:LEU:O	3:DF:183:GLU:N	2.31	0.56
3:HG:88:PRO:HA	3:HG:198:ILE:HA	1.86	0.56
2:G:42:ALA:O	2:SG:74:ASN:CA	2.52	0.56
3:M:201:ASN:HA	3:M:218:CYS:HA	1.87	0.56
3:ZA:85:ARG:N	3:ZA:201:ASN:O	2.36	0.56
3:RE:201:ASN:HA	3:RE:218:CYS:HA	1.87	0.56
3:BG:88:PRO:HA	3:BG:198:ILE:HA	1.86	0.56
3:BA:88:PRO:HA	3:BA:198:ILE:HA	1.86	0.56
2:EB:74:ASN:CA	2:KB:42:ALA:O	2.52	0.56
3:XB:88:PRO:HA	3:XB:198:ILE:HA	1.86	0.56
3:JF:201:ASN:HA	3:JF:218:CYS:HA	1.87	0.56
3:C:88:PRO:HA	3:C:198:ILE:HA	1.86	0.56
3:TA:85:ARG:N	3:TA:201:ASN:O	2.36	0.56
3:LB:85:ARG:N	3:LB:201:ASN:O	2.36	0.56
2:SD:68:ALA:HB1	2:YD:47:ILE:O	2.06	0.56
2:WE:77:LEU:CB	2:CF:42:ALA:O	2.54	0.56
3:DF:201:ASN:HA	3:DF:218:CYS:HA	1.87	0.56
3:VF:201:ASN:HA	3:VF:218:CYS:HA	1.87	0.56
2:GG:77:LEU:CB	2:MG:42:ALA:O	2.53	0.56
3:NG:201:ASN:HA	3:NG:218:CYS:HA	1.87	0.56
2:AA:68:ALA:HB1	2:GA:47:ILE:O	2.05	0.56
3:BG:201:ASN:HA	3:BG:218:CYS:HA	1.87	0.56
2:MG:68:ALA:HB1	2:SG:47:ILE:O	2.06	0.56
3:C:201:ASN:HA	3:C:218:CYS:HA	1.87	0.56
3:TA:88:PRO:HA	3:TA:198:ILE:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:FB:85:ARG:N	3:FB:201:ASN:O	2.36	0.56
2:QB:68:ALA:HB1	2:WB:47:ILE:O	2.06	0.56
2:KE:74:ASN:CA	2:QE:42:ALA:O	2.52	0.56
3:JF:85:ARG:N	3:JF:201:ASN:O	2.36	0.56
3:HG:201:ASN:HA	3:HG:218:CYS:HA	1.87	0.56
3:TG:201:ASN:HA	3:TG:218:CYS:HA	1.87	0.56
3:JC:85:ARG:N	3:JC:201:ASN:O	2.36	0.55
3:XE:102:LEU:O	3:XE:183:GLU:N	2.31	0.55
3:PF:201:ASN:HA	3:PF:218:CYS:HA	1.87	0.55
3:NG:88:PRO:HA	3:NG:198:ILE:HA	1.86	0.55
2:MA:155:HIS:CB	2:SA:217:ALA:HB2	2.34	0.55
4:SC:109:GLY:HA3	4:SC:122:ILE:HA	1.88	0.55
3:LB:88:PRO:HA	3:LB:198:ILE:HA	1.86	0.55
3:DF:85:ARG:N	3:DF:201:ASN:O	2.36	0.55
3:NA:85:ARG:N	3:NA:201:ASN:O	2.36	0.55
4:YC:109:GLY:HA3	4:YC:122:ILE:HA	1.88	0.55
2:KE:77:LEU:CB	2:QE:42:ALA:C	2.79	0.55
2:CF:74:ASN:CA	2:IF:42:ALA:O	2.51	0.55
4:JA:121:ARG:HA	4:KA:86:VAL:HA	1.89	0.55
2:EE:68:ALA:HB1	2:KE:47:ILE:O	2.06	0.55
3:PF:85:ARG:N	3:PF:201:ASN:O	2.36	0.55
4:KG:109:GLY:HA3	4:KG:122:ILE:HA	1.88	0.55
4:NB:121:ARG:HA	4:OB:86:VAL:HA	1.89	0.55
4:TB:121:ARG:HA	4:UB:86:VAL:HA	1.89	0.55
4:XC:121:ARG:HA	4:YC:86:VAL:HA	1.89	0.55
4:EG:109:GLY:HA3	4:EG:122:ILE:HA	1.88	0.55
4:Q:109:GLY:HA3	4:Q:122:ILE:HA	1.88	0.55
4:IB:109:GLY:HA3	4:IB:122:ILE:HA	1.88	0.55
4:OB:109:GLY:HA3	4:OB:122:ILE:HA	1.88	0.55
4:MC:109:GLY:HA3	4:MC:122:ILE:HA	1.88	0.55
3:ND:85:ARG:N	3:ND:201:ASN:O	2.36	0.55
4:MF:109:GLY:HA3	4:MF:122:ILE:HA	1.88	0.55
4:SF:109:GLY:HA3	4:SF:122:ILE:HA	1.88	0.55
4:H:109:GLY:HA3	4:H:122:ILE:HA	1.88	0.55
4:PA:121:ARG:HA	4:QA:86:VAL:HA	1.89	0.55
4:ZB:122:ILE:O	4:AC:84:GLY:N	2.34	0.55
4:RC:121:ARG:HA	4:SC:86:VAL:HA	1.89	0.55
3:RE:102:LEU:O	3:RE:183:GLU:N	2.31	0.55
3:XE:85:ARG:N	3:XE:201:ASN:O	2.36	0.55
4:WG:109:GLY:HA3	4:WG:122:ILE:HA	1.88	0.55
3:ZA:283:VAL:HA	4:AB:121:ARG:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DC:89:TYR:N	3:DC:197:ASP:O	2.40	0.55
2:IC:68:ALA:HB1	2:OC:47:ILE:O	2.07	0.55
4:DD:121:ARG:HA	4:ED:86:VAL:HA	1.89	0.55
4:QG:109:GLY:HA3	4:QG:122:ILE:HA	1.88	0.55
4:DA:121:ARG:HA	4:EA:86:VAL:HA	1.89	0.55
3:TA:270:LEU:O	4:UA:62:VAL:N	2.27	0.55
3:TA:283:VAL:HA	4:UA:121:ARG:HA	1.89	0.55
4:UB:109:GLY:HA3	4:UB:122:ILE:HA	1.88	0.55
4:ZB:121:ARG:HA	4:AC:86:VAL:HA	1.89	0.55
2:IC:74:ASN:CA	2:OC:42:ALA:O	2.55	0.55
3:VC:89:TYR:N	3:VC:197:ASP:O	2.40	0.55
4:BE:121:ARG:HA	4:CE:86:VAL:HA	1.89	0.55
4:YF:109:GLY:HA3	4:YF:122:ILE:HA	1.88	0.55
4:P:121:ARG:HA	4:Q:86:VAL:HA	1.89	0.54
3:V:85:ARG:N	3:V:201:ASN:O	2.35	0.54
4:HB:121:ARG:HA	4:IB:86:VAL:HA	1.89	0.54
3:LB:89:TYR:N	3:LB:197:ASP:O	2.40	0.54
3:RB:283:VAL:HA	4:SB:121:ARG:HA	1.89	0.54
3:XB:283:VAL:HA	4:YB:121:ARG:HA	1.89	0.54
3:JC:283:VAL:HA	4:KC:121:ARG:HA	1.89	0.54
3:PC:283:VAL:HA	4:QC:121:ARG:HA	1.89	0.54
4:ED:109:GLY:HA3	4:ED:122:ILE:HA	1.88	0.54
2:GG:183:LEU:O	2:GG:187:ASN:N	2.41	0.54
2:MG:183:LEU:O	2:MG:187:ASN:N	2.41	0.54
2:SG:183:LEU:O	2:SG:187:ASN:N	2.41	0.54
4:Y:109:GLY:HA3	4:Y:122:ILE:HA	1.88	0.54
3:BA:283:VAL:HA	4:CA:121:ARG:HA	1.89	0.54
3:HA:283:VAL:HA	4:IA:121:ARG:HA	1.89	0.54
3:FB:283:VAL:HA	4:GB:121:ARG:HA	1.89	0.54
3:LB:283:VAL:HA	4:MB:121:ARG:HA	1.89	0.54
3:ND:89:TYR:N	3:ND:197:ASP:O	2.40	0.54
2:YD:183:LEU:O	2:YD:187:ASN:N	2.41	0.54
4:CE:109:GLY:HA3	4:CE:122:ILE:HA	1.88	0.54
4:HE:121:ARG:HA	4:IE:86:VAL:HA	1.89	0.54
4:UE:109:GLY:HA3	4:UE:122:ILE:HA	1.88	0.54
4:AF:109:GLY:HA3	4:AF:122:ILE:HA	1.88	0.54
2:G:183:LEU:O	2:G:187:ASN:N	2.41	0.54
4:R:109:GLY:HA3	4:R:122:ILE:HA	1.88	0.54
4:CB:109:GLY:HA3	4:CB:122:ILE:HA	1.88	0.54
3:DC:283:VAL:HA	4:EC:121:ARG:HA	1.89	0.54
4:FC:122:ILE:O	4:GC:84:GLY:N	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:LC:121:ARG:HA	4:MC:86:VAL:HA	1.89	0.54
2:OC:139:ARG:C	2:UC:205:LEU:CB	2.81	0.54
3:HD:270:LEU:O	4:ID:62:VAL:N	2.27	0.54
2:SD:183:LEU:O	2:SD:187:ASN:N	2.41	0.54
4:VD:121:ARG:HA	4:WD:86:VAL:HA	1.89	0.54
4:WD:109:GLY:HA3	4:WD:122:ILE:HA	1.88	0.54
2:EE:183:LEU:O	2:EE:187:ASN:N	2.41	0.54
2:AG:183:LEU:O	2:AG:187:ASN:N	2.41	0.54
4:E:121:ARG:HA	4:H:86:VAL:HA	1.89	0.54
3:K:85:ARG:N	3:K:201:ASN:O	2.36	0.54
3:NA:283:VAL:HA	4:OA:121:ARG:HA	1.89	0.54
4:VA:121:ARG:HA	4:WA:86:VAL:HA	1.89	0.54
4:GC:109:GLY:HA3	4:GC:122:ILE:HA	1.88	0.54
3:LE:102:LEU:O	3:LE:183:GLU:N	2.31	0.54
3:VF:85:ARG:N	3:VF:201:ASN:O	2.36	0.54
3:BA:85:ARG:N	3:BA:201:ASN:O	2.36	0.54
4:EA:109:GLY:HA3	4:EA:122:ILE:HA	1.88	0.54
3:TA:89:TYR:N	3:TA:197:ASP:O	2.40	0.54
3:VC:270:LEU:O	4:WC:62:VAL:N	2.27	0.54
4:XC:122:ILE:O	4:YC:84:GLY:N	2.34	0.54
2:MD:183:LEU:O	2:MD:187:ASN:N	2.41	0.54
3:FE:89:TYR:N	3:FE:197:ASP:O	2.40	0.54
4:GF:109:GLY:HA3	4:GF:122:ILE:HA	1.88	0.54
3:NG:85:ARG:N	3:NG:201:ASN:O	2.36	0.54
4:VG:121:ARG:HA	4:WG:86:VAL:HA	1.89	0.54
2:B:183:LEU:O	2:B:187:ASN:N	2.41	0.54
3:K:283:VAL:HA	4:L:121:ARG:HA	1.89	0.54
2:MA:77:LEU:CB	2:SA:42:ALA:O	2.55	0.54
4:RC:122:ILE:O	4:SC:84:GLY:N	2.34	0.54
2:OF:183:LEU:O	2:OF:187:ASN:N	2.41	0.54
2:UF:183:LEU:O	2:UF:187:ASN:N	2.41	0.54
3:HG:85:ARG:N	3:HG:201:ASN:O	2.36	0.54
3:HA:85:ARG:N	3:HA:201:ASN:O	2.36	0.54
3:VC:283:VAL:HA	4:WC:121:ARG:HA	1.89	0.54
4:JD:121:ARG:HA	4:KD:86:VAL:HA	1.89	0.54
3:TD:270:LEU:O	4:UD:62:VAL:N	2.27	0.54
4:IE:109:GLY:HA3	4:IE:122:ILE:HA	1.88	0.54
2:KE:139:ARG:C	2:QE:205:LEU:CB	2.80	0.54
2:KE:183:LEU:O	2:KE:187:ASN:N	2.41	0.54
4:NE:121:ARG:HA	4:OE:86:VAL:HA	1.89	0.54
2:QE:183:LEU:O	2:QE:187:ASN:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:XE:270:LEU:O	4:YE:62:VAL:N	2.27	0.54
2:CF:183:LEU:O	2:CF:187:ASN:N	2.41	0.54
2:IF:183:LEU:O	2:IF:187:ASN:N	2.41	0.54
3:C:283:VAL:HA	4:D:121:ARG:HA	1.89	0.54
2:J:183:LEU:O	2:J:187:ASN:N	2.41	0.54
3:V:283:VAL:HA	4:W:121:ARG:HA	1.89	0.54
4:KA:109:GLY:HA3	4:KA:122:ILE:HA	1.88	0.54
3:BD:283:VAL:HA	4:CD:121:ARG:HA	1.89	0.54
2:GD:183:LEU:O	2:GD:187:ASN:N	2.41	0.54
3:HD:283:VAL:HA	4:ID:121:ARG:HA	1.89	0.54
4:QD:109:GLY:HA3	4:QD:122:ILE:HA	1.88	0.54
4:OE:109:GLY:HA3	4:OE:122:ILE:HA	1.88	0.54
2:WE:183:LEU:O	2:WE:187:ASN:N	2.41	0.54
3:XE:89:TYR:N	3:XE:197:ASP:O	2.40	0.54
3:JF:51:LEU:HA	3:JF:232:VAL:HA	1.90	0.54
4:LF:121:ARG:HA	4:MF:86:VAL:HA	1.89	0.54
3:PF:283:VAL:HA	4:QF:121:ARG:HA	1.89	0.54
4:RF:121:ARG:HA	4:SF:86:VAL:HA	1.89	0.54
2:T:183:LEU:O	2:T:187:ASN:N	2.41	0.54
3:HA:51:LEU:HA	3:HA:232:VAL:HA	1.90	0.54
3:HA:270:LEU:O	4:IA:62:VAL:N	2.27	0.54
3:TA:51:LEU:HA	3:TA:232:VAL:HA	1.90	0.54
2:YA:68:ALA:HB1	2:EB:47:ILE:O	2.08	0.54
3:ZA:51:LEU:HA	3:ZA:232:VAL:HA	1.90	0.54
3:LB:51:LEU:HA	3:LB:232:VAL:HA	1.90	0.54
4:AC:109:GLY:HA3	4:AC:122:ILE:HA	1.88	0.54
4:LC:122:ILE:O	4:MC:84:GLY:N	2.34	0.54
3:RE:51:LEU:HA	3:RE:232:VAL:HA	1.90	0.54
3:XE:283:VAL:HA	4:YE:121:ARG:HA	1.89	0.54
3:VF:51:LEU:HA	3:VF:232:VAL:HA	1.90	0.54
3:BG:51:LEU:HA	3:BG:232:VAL:HA	1.90	0.54
2:MG:74:ASN:CA	2:SG:42:ALA:O	2.54	0.54
4:PG:121:ARG:HA	4:QG:86:VAL:HA	1.89	0.54
3:TG:51:LEU:HA	3:TG:232:VAL:HA	1.90	0.54
3:TG:85:ARG:N	3:TG:201:ASN:O	2.36	0.54
3:K:51:LEU:HA	3:K:232:VAL:HA	1.90	0.54
4:O:121:ARG:HA	4:R:86:VAL:HA	1.89	0.54
4:X:121:ARG:HA	4:Y:86:VAL:HA	1.89	0.54
2:AA:183:LEU:O	2:AA:187:ASN:N	2.41	0.54
3:BA:51:LEU:HA	3:BA:232:VAL:HA	1.90	0.54
2:GA:183:LEU:O	2:GA:187:ASN:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DC:51:LEU:HA	3:DC:232:VAL:HA	1.90	0.54
3:DC:85:ARG:N	3:DC:201:ASN:O	2.36	0.54
3:JC:270:LEU:O	4:KC:62:VAL:N	2.27	0.54
2:AD:183:LEU:O	2:AD:187:ASN:N	2.41	0.54
4:PD:121:ARG:HA	4:QD:86:VAL:HA	1.89	0.54
3:RE:283:VAL:HA	4:SE:121:ARG:HA	1.89	0.54
3:DF:51:LEU:HA	3:DF:232:VAL:HA	1.90	0.54
3:PF:89:TYR:N	3:PF:197:ASP:O	2.40	0.54
3:NG:51:LEU:HA	3:NG:232:VAL:HA	1.90	0.54
3:M:283:VAL:HA	4:N:121:ARG:HA	1.89	0.53
3:C:51:LEU:HA	3:C:232:VAL:HA	1.90	0.53
3:C:85:ARG:N	3:C:201:ASN:O	2.35	0.53
4:FC:121:ARG:HA	4:GC:86:VAL:HA	1.89	0.53
2:OC:77:LEU:CB	2:UC:42:ALA:C	2.82	0.53
2:UC:183:LEU:O	2:UC:187:ASN:N	2.41	0.53
3:ZD:51:LEU:HA	3:ZD:232:VAL:HA	1.90	0.53
3:FE:102:LEU:O	3:FE:183:GLU:N	2.31	0.53
3:DF:283:VAL:HA	4:EF:121:ARG:HA	1.89	0.53
3:VF:283:VAL:HA	4:WF:121:ARG:HA	1.89	0.53
4:XF:121:ARG:HA	4:YF:86:VAL:HA	1.89	0.53
3:BA:89:TYR:N	3:BA:197:ASP:O	2.40	0.53
2:MA:183:LEU:O	2:MA:187:ASN:N	2.41	0.53
4:QA:109:GLY:HA3	4:QA:122:ILE:HA	1.88	0.53
2:YA:77:LEU:CB	2:EB:42:ALA:C	2.81	0.53
4:BB:121:ARG:HA	4:CB:86:VAL:HA	1.89	0.53
2:IC:77:LEU:CB	2:OC:42:ALA:C	2.81	0.53
2:OC:183:LEU:O	2:OC:187:ASN:N	2.40	0.53
2:AD:77:LEU:CB	2:GD:42:ALA:C	2.82	0.53
4:KD:109:GLY:HA3	4:KD:122:ILE:HA	1.88	0.53
3:ND:283:VAL:HA	4:OD:121:ARG:HA	1.89	0.53
2:EE:218:VAL:O	2:EE:226:ALA:HB2	2.09	0.53
3:JF:283:VAL:HA	4:KF:121:ARG:HA	1.89	0.53
3:HG:89:TYR:N	3:HG:197:ASP:O	2.40	0.53
2:T:218:VAL:O	2:T:226:ALA:HB2	2.09	0.53
3:V:89:TYR:N	3:V:197:ASP:O	2.40	0.53
2:SA:183:LEU:O	2:SA:187:ASN:N	2.41	0.53
4:WA:109:GLY:HA3	4:WA:122:ILE:HA	1.88	0.53
3:RB:51:LEU:HA	3:RB:232:VAL:HA	1.90	0.53
3:RB:89:TYR:N	3:RB:197:ASP:O	2.40	0.53
3:VC:51:LEU:HA	3:VC:232:VAL:HA	1.90	0.53
3:HD:85:ARG:N	3:HD:201:ASN:O	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:FE:283:VAL:HA	4:GE:121:ARG:HA	1.89	0.53
4:FF:121:ARG:HA	4:GF:86:VAL:HA	1.89	0.53
3:NG:283:VAL:HA	4:OG:121:ARG:HA	1.89	0.53
3:TG:283:VAL:HA	4:UG:121:ARG:HA	1.89	0.53
2:J:218:VAL:O	2:J:226:ALA:HB2	2.09	0.53
2:WB:183:LEU:O	2:WB:187:ASN:N	2.40	0.53
2:IC:183:LEU:O	2:IC:187:ASN:N	2.41	0.53
3:JC:89:TYR:N	3:JC:197:ASP:O	2.40	0.53
2:UC:218:VAL:O	2:UC:226:ALA:HB2	2.09	0.53
2:SD:74:ASN:CA	2:YD:42:ALA:O	2.54	0.53
2:EE:74:ASN:CA	2:KE:42:ALA:O	2.54	0.53
2:KE:218:VAL:O	2:KE:226:ALA:HB2	2.09	0.53
2:IF:218:VAL:O	2:IF:226:ALA:HB2	2.09	0.53
3:BG:85:ARG:N	3:BG:201:ASN:O	2.36	0.53
3:HG:283:VAL:HA	4:IG:121:ARG:HA	1.89	0.53
3:C:89:TYR:N	3:C:197:ASP:O	2.40	0.53
3:V:270:LEU:O	4:W:62:VAL:N	2.27	0.53
2:AA:218:VAL:O	2:AA:226:ALA:HB2	2.09	0.53
2:YA:183:LEU:O	2:YA:187:ASN:N	2.41	0.53
2:EB:183:LEU:O	2:EB:187:ASN:N	2.41	0.53
2:EB:218:VAL:O	2:EB:226:ALA:HB2	2.09	0.53
2:KB:183:LEU:O	2:KB:187:ASN:N	2.41	0.53
2:KB:218:VAL:O	2:KB:226:ALA:HB2	2.09	0.53
2:QB:183:LEU:O	2:QB:187:ASN:N	2.41	0.53
2:CC:183:LEU:O	2:CC:187:ASN:N	2.41	0.53
2:OC:218:VAL:O	2:OC:226:ALA:HB2	2.09	0.53
2:AD:218:VAL:O	2:AD:226:ALA:HB2	2.09	0.53
3:HD:51:LEU:HA	3:HD:232:VAL:HA	1.90	0.53
3:ND:51:LEU:HA	3:ND:232:VAL:HA	1.90	0.53
3:TD:283:VAL:HA	4:UD:121:ARG:HA	1.89	0.53
2:YD:218:VAL:O	2:YD:226:ALA:HB2	2.09	0.53
3:ZD:283:VAL:HA	4:AE:121:ARG:HA	1.89	0.53
3:LE:51:LEU:HA	3:LE:232:VAL:HA	1.90	0.53
3:LE:283:VAL:HA	4:ME:121:ARG:HA	1.89	0.53
3:BG:283:VAL:HA	4:CG:121:ARG:HA	1.89	0.53
2:MG:218:VAL:O	2:MG:226:ALA:HB2	2.09	0.53
3:HA:89:TYR:N	3:HA:197:ASP:O	2.40	0.53
3:FE:270:LEU:O	4:GE:62:VAL:N	2.27	0.53
2:OF:218:VAL:O	2:OF:226:ALA:HB2	2.09	0.53
3:BG:89:TYR:N	3:BG:197:ASP:O	2.40	0.53
2:GG:218:VAL:O	2:GG:226:ALA:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:YA:218:VAL:O	2:YA:226:ALA:HB2	2.09	0.53
3:ZA:89:TYR:N	3:ZA:197:ASP:O	2.40	0.53
4:ZE:121:ARG:HA	4:AF:86:VAL:HA	1.89	0.53
2:CF:218:VAL:O	2:CF:226:ALA:HB2	2.09	0.53
2:IF:77:LEU:CB	2:OF:42:ALA:C	2.82	0.53
2:SG:218:VAL:O	2:SG:226:ALA:HB2	2.09	0.53
3:M:85:ARG:N	3:M:201:ASN:O	2.36	0.53
3:XB:270:LEU:O	4:YB:62:VAL:N	2.27	0.53
3:PC:51:LEU:HA	3:PC:232:VAL:HA	1.90	0.53
3:BD:89:TYR:N	3:BD:197:ASP:O	2.40	0.53
4:JG:121:ARG:HA	4:KG:86:VAL:HA	1.89	0.53
3:C:270:LEU:O	4:D:62:VAL:N	2.27	0.53
2:KB:77:LEU:CB	2:QB:42:ALA:O	2.56	0.53
3:ZD:102:LEU:O	3:ZD:183:GLU:N	2.31	0.53
3:FE:51:LEU:HA	3:FE:232:VAL:HA	1.90	0.53
4:TE:121:ARG:HA	4:UE:86:VAL:HA	1.89	0.53
4:DG:121:ARG:HA	4:EG:86:VAL:HA	1.89	0.53
2:B:218:VAL:O	2:B:226:ALA:HB2	2.09	0.53
2:QB:218:VAL:O	2:QB:226:ALA:HB2	2.09	0.53
3:JC:51:LEU:HA	3:JC:232:VAL:HA	1.90	0.53
2:QE:218:VAL:O	2:QE:226:ALA:HB2	2.09	0.53
3:XE:51:LEU:HA	3:XE:232:VAL:HA	1.90	0.53
3:TG:89:TYR:N	3:TG:197:ASP:O	2.40	0.53
2:GA:218:VAL:O	2:GA:226:ALA:HB2	2.09	0.52
2:SA:218:VAL:O	2:SA:226:ALA:HB2	2.09	0.52
3:XB:51:LEU:HA	3:XB:232:VAL:HA	1.90	0.52
2:IC:218:VAL:O	2:IC:226:ALA:HB2	2.09	0.52
2:GD:218:VAL:O	2:GD:226:ALA:HB2	2.09	0.52
2:SD:218:VAL:O	2:SD:226:ALA:HB2	2.09	0.52
4:TB:122:ILE:O	4:UB:84:GLY:N	2.34	0.52
3:PF:51:LEU:HA	3:PF:232:VAL:HA	1.90	0.52
2:AG:218:VAL:O	2:AG:226:ALA:HB2	2.09	0.52
3:M:51:LEU:HA	3:M:232:VAL:HA	1.90	0.52
3:V:51:LEU:HA	3:V:232:VAL:HA	1.90	0.52
3:NA:51:LEU:HA	3:NA:232:VAL:HA	1.90	0.52
2:WB:77:LEU:CB	2:CC:42:ALA:C	2.82	0.52
3:TD:51:LEU:HA	3:TD:232:VAL:HA	1.90	0.52
3:TD:89:TYR:N	3:TD:197:ASP:O	2.40	0.52
2:IF:68:ALA:HB1	2:OF:47:ILE:O	2.09	0.52
2:UF:218:VAL:O	2:UF:226:ALA:HB2	2.09	0.52
3:FB:51:LEU:HA	3:FB:232:VAL:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:HG:51:LEU:HA	3:HG:232:VAL:HA	1.90	0.52
2:T:219:ARG:CA	2:T:226:ALA:CB	2.88	0.52
2:YA:74:ASN:CA	2:EB:42:ALA:O	2.56	0.52
2:WE:218:VAL:O	2:WE:226:ALA:HB2	2.09	0.52
3:JF:270:LEU:O	4:KF:62:VAL:N	2.27	0.52
3:NG:89:TYR:N	3:NG:197:ASP:O	2.40	0.52
2:G:42:ALA:C	2:SG:77:LEU:CB	2.82	0.52
2:J:219:ARG:CA	2:J:226:ALA:CB	2.88	0.52
2:AA:219:ARG:CA	2:AA:226:ALA:CB	2.88	0.52
2:GA:219:ARG:CA	2:GA:226:ALA:CB	2.88	0.52
3:LE:89:TYR:N	3:LE:197:ASP:O	2.40	0.52
3:BG:270:LEU:O	4:CG:62:VAL:N	2.27	0.52
2:G:218:VAL:O	2:G:226:ALA:HB2	2.09	0.52
2:G:219:ARG:CA	2:G:226:ALA:CB	2.88	0.52
2:B:219:ARG:CA	2:B:226:ALA:CB	2.88	0.52
2:J:77:LEU:CB	2:T:42:ALA:C	2.82	0.52
2:GA:77:LEU:CB	2:MA:42:ALA:C	2.82	0.52
2:MA:219:ARG:CA	2:MA:226:ALA:CB	2.88	0.52
3:LB:270:LEU:O	4:MB:62:VAL:N	2.27	0.52
3:TD:102:LEU:O	3:TD:183:GLU:N	2.31	0.52
3:K:270:LEU:O	4:L:62:VAL:N	2.27	0.52
2:SA:219:ARG:CA	2:SA:226:ALA:CB	2.88	0.52
2:YA:219:ARG:CA	2:YA:226:ALA:CB	2.88	0.52
3:DF:89:TYR:N	3:DF:197:ASP:O	2.40	0.52
2:SG:219:ARG:CA	2:SG:226:ALA:CB	2.88	0.52
2:WB:218:VAL:O	2:WB:226:ALA:HB2	2.09	0.52
3:BD:51:LEU:HA	3:BD:232:VAL:HA	1.90	0.52
2:MD:218:VAL:O	2:MD:226:ALA:HB2	2.09	0.52
3:RE:270:LEU:O	4:SE:62:VAL:N	2.27	0.52
3:VF:89:TYR:N	3:VF:197:ASP:O	2.40	0.52
2:MG:219:ARG:CA	2:MG:226:ALA:CB	2.88	0.52
2:MA:218:VAL:O	2:MA:226:ALA:HB2	2.09	0.52
2:EB:219:ARG:CA	2:EB:226:ALA:CB	2.88	0.52
2:KB:219:ARG:CA	2:KB:226:ALA:CB	2.88	0.52
2:CC:218:VAL:O	2:CC:226:ALA:HB2	2.09	0.52
2:AD:139:ARG:C	2:GD:205:LEU:CB	2.83	0.52
2:IF:219:ARG:N	2:IF:226:ALA:CB	2.74	0.51
3:NA:89:TYR:N	3:NA:197:ASP:O	2.40	0.51
2:QB:219:ARG:CA	2:QB:226:ALA:CB	2.88	0.51
2:KE:219:ARG:HA	2:KE:226:ALA:HB3	1.93	0.51
2:CF:219:ARG:HA	2:CF:226:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:UF:219:ARG:N	2:UF:226:ALA:CB	2.74	0.51
2:GG:219:ARG:CA	2:GG:226:ALA:CB	2.88	0.51
2:SD:219:ARG:HA	2:SD:226:ALA:HB3	1.93	0.51
2:QE:219:ARG:N	2:QE:226:ALA:CB	2.74	0.51
2:WE:219:ARG:N	2:WE:226:ALA:CB	2.74	0.51
2:CF:219:ARG:N	2:CF:226:ALA:CB	2.74	0.51
2:OF:219:ARG:N	2:OF:226:ALA:CB	2.74	0.51
2:AG:219:ARG:N	2:AG:226:ALA:CB	2.74	0.51
2:GA:139:ARG:C	2:MA:205:LEU:CB	2.83	0.51
2:WB:219:ARG:CA	2:WB:226:ALA:CB	2.88	0.51
2:OF:77:LEU:CB	2:UF:42:ALA:C	2.84	0.51
2:UF:219:ARG:HA	2:UF:226:ALA:HB3	1.93	0.51
2:GG:219:ARG:N	2:GG:226:ALA:CB	2.74	0.51
3:ZA:270:LEU:O	4:AB:62:VAL:N	2.27	0.51
2:OC:219:ARG:N	2:OC:226:ALA:CB	2.74	0.51
2:UC:219:ARG:N	2:UC:226:ALA:CB	2.74	0.51
3:BD:85:ARG:N	3:BD:201:ASN:O	2.36	0.51
2:KE:219:ARG:N	2:KE:226:ALA:CB	2.74	0.51
2:KE:219:ARG:CA	2:KE:226:ALA:CB	2.88	0.51
2:QE:219:ARG:CA	2:QE:226:ALA:CB	2.88	0.51
2:CF:219:ARG:CA	2:CF:226:ALA:CB	2.88	0.51
2:AG:77:LEU:CB	2:GG:42:ALA:C	2.83	0.51
2:AG:219:ARG:CA	2:AG:226:ALA:CB	2.88	0.51
3:K:89:TYR:N	3:K:197:ASP:O	2.40	0.51
2:EE:219:ARG:N	2:EE:226:ALA:CB	2.74	0.51
2:EE:219:ARG:HA	2:EE:226:ALA:HB3	1.93	0.51
2:EE:219:ARG:CA	2:EE:226:ALA:CB	2.88	0.51
2:WE:219:ARG:HA	2:WE:226:ALA:HB3	1.93	0.51
2:WE:219:ARG:CA	2:WE:226:ALA:CB	2.88	0.51
2:T:219:ARG:N	2:T:226:ALA:CB	2.74	0.51
2:AA:219:ARG:N	2:AA:226:ALA:CB	2.74	0.51
2:EB:77:LEU:CB	2:KB:42:ALA:C	2.83	0.51
3:XB:89:TYR:N	3:XB:197:ASP:O	2.40	0.51
2:CC:219:ARG:CA	2:CC:226:ALA:CB	2.88	0.51
2:IC:219:ARG:N	2:IC:226:ALA:CB	2.74	0.51
2:AD:219:ARG:N	2:AD:226:ALA:CB	2.74	0.51
2:AD:219:ARG:HA	2:AD:226:ALA:HB3	1.93	0.51
2:MD:219:ARG:HA	2:MD:226:ALA:HB3	1.93	0.51
2:IF:219:ARG:CA	2:IF:226:ALA:CB	2.88	0.51
2:OF:219:ARG:HA	2:OF:226:ALA:HB3	1.93	0.51
2:UF:219:ARG:CA	2:UF:226:ALA:CB	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:MG:219:ARG:N	2:MG:226:ALA:CB	2.74	0.51
3:NG:270:LEU:O	4:OG:62:VAL:N	2.27	0.51
2:GA:219:ARG:N	2:GA:226:ALA:CB	2.74	0.51
3:FB:89:TYR:N	3:FB:197:ASP:O	2.40	0.51
2:CC:219:ARG:N	2:CC:226:ALA:CB	2.74	0.51
2:OC:219:ARG:CA	2:OC:226:ALA:CB	2.88	0.51
2:UC:219:ARG:CA	2:UC:226:ALA:CB	2.88	0.51
2:GD:219:ARG:N	2:GD:226:ALA:CB	2.74	0.51
2:YD:219:ARG:CA	2:YD:226:ALA:CB	2.88	0.51
3:RE:89:TYR:N	3:RE:197:ASP:O	2.40	0.51
2:MG:219:ARG:HA	2:MG:226:ALA:HB3	1.93	0.51
2:T:77:LEU:CB	2:AA:42:ALA:C	2.83	0.51
2:MA:219:ARG:N	2:MA:226:ALA:CB	2.74	0.51
2:WB:139:ARG:C	2:CC:205:LEU:CB	2.84	0.51
2:AD:219:ARG:CA	2:AD:226:ALA:CB	2.88	0.51
2:GD:219:ARG:CA	2:GD:226:ALA:CB	2.88	0.51
2:MD:219:ARG:CA	2:MD:226:ALA:CB	2.88	0.51
2:SD:219:ARG:CA	2:SD:226:ALA:CB	2.88	0.51
2:YD:219:ARG:N	2:YD:226:ALA:CB	2.74	0.51
2:OF:219:ARG:CA	2:OF:226:ALA:CB	2.88	0.51
3:BG:102:LEU:O	3:BG:183:GLU:N	2.31	0.51
2:GG:219:ARG:HA	2:GG:226:ALA:HB3	1.93	0.51
2:J:219:ARG:N	2:J:226:ALA:CB	2.74	0.51
2:IC:219:ARG:HA	2:IC:226:ALA:HB3	1.93	0.51
2:IC:219:ARG:CA	2:IC:226:ALA:CB	2.88	0.51
2:UC:219:ARG:HA	2:UC:226:ALA:HB3	1.92	0.51
2:G:205:LEU:CB	2:SG:139:ARG:C	2.84	0.50
2:J:119:ALA:O	2:J:123:ARG:N	2.44	0.50
2:AA:119:ALA:O	2:AA:123:ARG:N	2.44	0.50
2:SA:119:ALA:O	2:SA:123:ARG:N	2.44	0.50
2:SA:219:ARG:N	2:SA:226:ALA:CB	2.74	0.50
2:WB:119:ALA:O	2:WB:123:ARG:N	2.44	0.50
2:OC:119:ALA:O	2:OC:123:ARG:N	2.44	0.50
3:PC:89:TYR:N	3:PC:197:ASP:O	2.40	0.50
2:AD:119:ALA:O	2:AD:123:ARG:N	2.44	0.50
2:GD:119:ALA:O	2:GD:123:ARG:N	2.44	0.50
2:SG:119:ALA:O	2:SG:123:ARG:N	2.44	0.50
2:SG:219:ARG:N	2:SG:226:ALA:CB	2.74	0.50
2:B:219:ARG:N	2:B:226:ALA:CB	2.74	0.50
2:AA:77:LEU:CB	2:GA:42:ALA:C	2.84	0.50
3:NA:270:LEU:O	4:OA:62:VAL:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:WB:219:ARG:N	2:WB:226:ALA:CB	2.74	0.50
2:MD:219:ARG:N	2:MD:226:ALA:CB	2.74	0.50
3:VF:270:LEU:O	4:WF:62:VAL:N	2.27	0.50
2:G:219:ARG:HA	2:G:226:ALA:HB3	1.93	0.50
2:B:119:ALA:O	2:B:123:ARG:N	2.44	0.50
3:K:200:VAL:N	3:K:219:LEU:O	2.44	0.50
3:BA:200:VAL:N	3:BA:219:LEU:O	2.44	0.50
2:GA:119:ALA:O	2:GA:123:ARG:N	2.44	0.50
2:KB:119:ALA:O	2:KB:123:ARG:N	2.44	0.50
2:SD:219:ARG:N	2:SD:226:ALA:CB	2.74	0.50
3:HG:102:LEU:O	3:HG:183:GLU:N	2.31	0.50
3:M:270:LEU:O	4:N:62:VAL:N	2.27	0.50
2:B:77:LEU:CB	2:J:42:ALA:C	2.84	0.50
3:V:200:VAL:N	3:V:219:LEU:O	2.44	0.50
3:HA:200:VAL:N	3:HA:219:LEU:O	2.44	0.50
2:EB:119:ALA:O	2:EB:123:ARG:N	2.44	0.50
2:IC:119:ALA:O	2:IC:123:ARG:N	2.44	0.50
2:OC:139:ARG:O	2:UC:205:LEU:CB	2.60	0.50
2:YD:119:ALA:O	2:YD:123:ARG:N	2.44	0.50
2:QE:219:ARG:HA	2:QE:226:ALA:HB3	1.93	0.50
2:IF:219:ARG:HA	2:IF:226:ALA:HB3	1.93	0.50
2:G:219:ARG:N	2:G:226:ALA:CB	2.74	0.50
3:C:200:VAL:N	3:C:219:LEU:O	2.44	0.50
2:T:219:ARG:HA	2:T:226:ALA:HB3	1.92	0.50
2:QB:219:ARG:HA	2:QB:226:ALA:HB3	1.93	0.50
2:YD:219:ARG:HA	2:YD:226:ALA:HB3	1.93	0.50
3:M:200:VAL:N	3:M:219:LEU:O	2.44	0.50
2:B:219:ARG:HA	2:B:226:ALA:HB3	1.93	0.50
3:NA:200:VAL:N	3:NA:219:LEU:O	2.44	0.50
2:SA:77:LEU:CB	2:YA:42:ALA:C	2.84	0.50
3:TA:200:VAL:N	3:TA:219:LEU:O	2.44	0.50
2:YA:219:ARG:N	2:YA:226:ALA:CB	2.74	0.50
2:QB:219:ARG:N	2:QB:226:ALA:CB	2.74	0.50
2:GD:77:LEU:CB	2:MD:42:ALA:C	2.85	0.50
2:GD:219:ARG:HA	2:GD:226:ALA:HB3	1.93	0.50
2:SD:77:LEU:CB	2:YD:42:ALA:C	2.85	0.50
2:QE:77:LEU:CB	2:WE:42:ALA:C	2.85	0.50
3:DF:270:LEU:O	4:EF:62:VAL:N	2.27	0.50
3:NG:102:LEU:O	3:NG:183:GLU:N	2.31	0.50
4:O:119:GLY:HA2	4:R:88:ALA:HA	1.94	0.50
3:BA:270:LEU:O	4:CA:62:VAL:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:TB:119:GLY:HA2	4:UB:88:ALA:HA	1.94	0.50
2:CC:119:ALA:O	2:CC:123:ARG:N	2.44	0.50
4:LC:119:GLY:HA2	4:MC:88:ALA:HA	1.94	0.50
2:OC:219:ARG:HA	2:OC:226:ALA:HB3	1.92	0.50
2:IF:74:ASN:CA	2:OF:42:ALA:O	2.57	0.50
1:NF:552:ARG:HA	2:OF:67:ALA:HB2	1.94	0.50
4:JA:119:GLY:HA2	4:KA:88:ALA:HA	1.94	0.50
2:YA:219:ARG:HA	2:YA:226:ALA:HB3	1.93	0.50
3:ZA:200:VAL:N	3:ZA:219:LEU:O	2.44	0.50
4:BB:119:GLY:HA2	4:CB:88:ALA:HA	1.94	0.50
2:IC:139:ARG:C	2:OC:205:LEU:CB	2.85	0.50
3:HD:89:TYR:N	3:HD:197:ASP:O	2.40	0.50
1:JE:552:ARG:HA	2:KE:67:ALA:HB2	1.94	0.50
1:VE:552:ARG:HA	2:WE:67:ALA:HB2	1.94	0.50
1:HF:552:ARG:HA	2:IF:67:ALA:HB2	1.94	0.50
1:ZF:552:ARG:HA	2:AG:67:ALA:HB2	1.94	0.50
2:AG:219:ARG:HA	2:AG:226:ALA:HB3	1.93	0.50
3:TG:200:VAL:N	3:TG:219:LEU:O	2.44	0.50
4:VG:119:GLY:HA2	4:WG:88:ALA:HA	1.94	0.50
2:GA:219:ARG:HA	2:GA:226:ALA:HB3	1.92	0.50
2:MA:119:ALA:O	2:MA:123:ARG:N	2.44	0.50
2:YA:119:ALA:O	2:YA:123:ARG:N	2.44	0.50
2:YA:139:ARG:C	2:EB:205:LEU:CB	2.85	0.50
1:XD:552:ARG:HA	2:YD:67:ALA:HB2	1.94	0.50
1:DE:552:ARG:HA	2:EE:67:ALA:HB2	1.94	0.50
2:CF:77:LEU:CB	2:IF:42:ALA:C	2.85	0.50
2:OF:139:ARG:C	2:UF:205:LEU:CB	2.85	0.50
2:AG:139:ARG:C	2:GG:205:LEU:CB	2.85	0.50
2:MA:219:ARG:HA	2:MA:226:ALA:HB3	1.93	0.49
2:EB:219:ARG:N	2:EB:226:ALA:CB	2.74	0.49
2:WB:219:ARG:HA	2:WB:226:ALA:HB3	1.93	0.49
4:DD:119:GLY:HA2	4:ED:88:ALA:HA	1.94	0.49
3:ZD:89:TYR:N	3:ZD:197:ASP:O	2.40	0.49
1:PE:552:ARG:HA	2:QE:67:ALA:HB2	1.94	0.49
1:BF:552:ARG:HA	2:CF:67:ALA:HB2	1.94	0.49
3:JF:200:VAL:N	3:JF:219:LEU:O	2.44	0.49
3:PF:200:VAL:N	3:PF:219:LEU:O	2.44	0.49
1:TF:552:ARG:HA	2:UF:67:ALA:HB2	1.94	0.49
3:NG:200:VAL:N	3:NG:219:LEU:O	2.44	0.49
2:G:119:ALA:O	2:G:123:ARG:N	2.44	0.49
3:M:89:TYR:N	3:M:197:ASP:O	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:PA:119:GLY:HA2	4:QA:88:ALA:HA	1.94	0.49
2:EB:219:ARG:HA	2:EB:226:ALA:HB3	1.93	0.49
3:FB:200:VAL:N	3:FB:219:LEU:O	2.44	0.49
2:KB:219:ARG:N	2:KB:226:ALA:CB	2.74	0.49
2:CC:219:ARG:HA	2:CC:226:ALA:HB3	1.93	0.49
3:ND:270:LEU:O	4:OD:62:VAL:N	2.27	0.49
3:DF:200:VAL:N	3:DF:219:LEU:O	2.44	0.49
3:JF:89:TYR:N	3:JF:197:ASP:O	2.40	0.49
1:LG:552:ARG:HA	2:MG:67:ALA:HB2	1.94	0.49
2:QB:119:ALA:O	2:QB:123:ARG:N	2.44	0.49
4:ZB:119:GLY:HA2	4:AC:88:ALA:HA	1.94	0.49
2:UC:119:ALA:O	2:UC:123:ARG:N	2.44	0.49
3:BD:270:LEU:O	4:CD:62:VAL:N	2.27	0.49
1:LD:552:ARG:HA	2:MD:67:ALA:HB2	1.94	0.49
3:VF:200:VAL:N	3:VF:219:LEU:O	2.44	0.49
3:BG:200:VAL:N	3:BG:219:LEU:O	2.44	0.49
1:FG:552:ARG:HA	2:GG:67:ALA:HB2	1.94	0.49
4:P:119:GLY:HA2	4:Q:88:ALA:HA	1.94	0.49
2:T:119:ALA:O	2:T:123:ARG:N	2.44	0.49
4:X:119:GLY:HA2	4:Y:88:ALA:HA	1.94	0.49
2:AA:219:ARG:HA	2:AA:226:ALA:HB3	1.93	0.49
4:HB:119:GLY:HA2	4:IB:88:ALA:HA	1.94	0.49
1:FD:552:ARG:HA	2:GD:67:ALA:HB2	1.94	0.49
1:RD:552:ARG:HA	2:SD:67:ALA:HB2	1.94	0.49
3:RE:200:VAL:N	3:RE:219:LEU:O	2.44	0.49
3:XE:200:VAL:N	3:XE:219:LEU:O	2.44	0.49
2:GG:119:ALA:O	2:GG:123:ARG:N	2.44	0.49
3:HG:200:VAL:N	3:HG:219:LEU:O	2.44	0.49
1:F:552:ARG:HA	2:G:67:ALA:HB2	1.94	0.49
3:LB:200:VAL:N	3:LB:219:LEU:O	2.44	0.49
2:WB:63:ALA:HA	2:WB:67:ALA:HB3	1.94	0.49
4:RC:119:GLY:HA2	4:SC:88:ALA:HA	1.94	0.49
2:UC:63:ALA:HA	2:UC:67:ALA:HB3	1.94	0.49
4:VD:119:GLY:HA2	4:WD:88:ALA:HA	1.94	0.49
4:DG:119:GLY:HA2	4:EG:88:ALA:HA	1.94	0.49
4:JG:119:GLY:HA2	4:KG:88:ALA:HA	1.94	0.49
1:RG:552:ARG:HA	2:SG:67:ALA:HB2	1.94	0.49
2:YA:63:ALA:HA	2:YA:67:ALA:HB3	1.94	0.49
3:XB:301:VAL:O	3:XB:321:ILE:N	2.45	0.49
3:DC:301:VAL:O	3:DC:321:ILE:N	2.45	0.49
2:IC:63:ALA:HA	2:IC:67:ALA:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PC:301:VAL:O	3:PC:321:ILE:N	2.45	0.49
3:VC:301:VAL:O	3:VC:321:ILE:N	2.45	0.49
1:ZC:552:ARG:HA	2:AD:67:ALA:HB2	1.94	0.49
3:ZD:270:LEU:O	4:AE:62:VAL:N	2.27	0.49
3:LE:200:VAL:N	3:LE:219:LEU:O	2.44	0.49
4:RF:119:GLY:HA2	4:SF:88:ALA:HA	1.94	0.49
2:UF:77:LEU:CB	2:AG:42:ALA:C	2.86	0.49
2:SG:219:ARG:HA	2:SG:226:ALA:HB3	1.93	0.49
1:A:552:ARG:HA	2:B:67:ALA:HB2	1.94	0.49
2:T:139:ARG:C	2:AA:205:LEU:CB	2.85	0.49
4:W:111:VAL:HA	4:W:120:VAL:HA	1.95	0.49
2:SA:219:ARG:HA	2:SA:226:ALA:HB3	1.93	0.49
2:KB:63:ALA:HA	2:KB:67:ALA:HB3	1.95	0.49
3:RB:200:VAL:N	3:RB:219:LEU:O	2.44	0.49
3:JC:301:VAL:O	3:JC:321:ILE:N	2.45	0.49
3:BD:301:VAL:O	3:BD:321:ILE:N	2.45	0.49
3:HD:301:VAL:O	3:HD:321:ILE:N	2.45	0.49
4:ZE:119:GLY:HA2	4:AF:88:ALA:HA	1.94	0.49
2:IF:139:ARG:C	2:OF:205:LEU:CB	2.86	0.49
2:J:219:ARG:HA	2:J:226:ALA:HB3	1.93	0.49
4:DA:119:GLY:HA2	4:EA:88:ALA:HA	1.94	0.49
4:VA:119:GLY:HA2	4:WA:88:ALA:HA	1.94	0.49
2:EB:63:ALA:HA	2:EB:67:ALA:HB3	1.94	0.49
3:RB:301:VAL:O	3:RB:321:ILE:N	2.45	0.49
2:CC:63:ALA:HA	2:CC:67:ALA:HB3	1.94	0.49
1:NC:552:ARG:HA	2:OC:67:ALA:HB2	1.94	0.49
1:TC:552:ARG:HA	2:UC:67:ALA:HB2	1.94	0.49
2:MD:119:ALA:O	2:MD:123:ARG:N	2.44	0.49
3:ND:301:VAL:O	3:ND:321:ILE:N	2.45	0.49
3:TD:301:VAL:O	3:TD:321:ILE:N	2.45	0.49
3:FE:200:VAL:N	3:FE:219:LEU:O	2.44	0.49
4:D:111:VAL:HA	4:D:120:VAL:HA	1.95	0.49
1:I:552:ARG:HA	2:J:67:ALA:HB2	1.94	0.49
4:L:111:VAL:HA	4:L:120:VAL:HA	1.95	0.49
4:CA:111:VAL:HA	4:CA:120:VAL:HA	1.95	0.49
4:IA:111:VAL:HA	4:IA:120:VAL:HA	1.95	0.49
4:OA:111:VAL:HA	4:OA:120:VAL:HA	1.95	0.49
4:UA:111:VAL:HA	4:UA:120:VAL:HA	1.95	0.49
3:FB:80:THR:O	3:FB:205:HIS:N	2.35	0.49
3:LB:301:VAL:O	3:LB:321:ILE:N	2.45	0.49
4:NB:119:GLY:HA2	4:OB:88:ALA:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:MC:110:GLU:O	4:MC:121:ARG:N	2.42	0.49
3:PC:270:LEU:O	4:QC:62:VAL:N	2.27	0.49
2:GD:63:ALA:HA	2:GD:67:ALA:HB3	1.94	0.49
4:PD:119:GLY:HA2	4:QD:88:ALA:HA	1.94	0.49
2:EE:77:LEU:CB	2:KE:42:ALA:C	2.85	0.49
4:HE:119:GLY:HA2	4:IE:88:ALA:HA	1.94	0.49
4:NE:119:GLY:HA2	4:OE:88:ALA:HA	1.94	0.49
2:AG:63:ALA:HA	2:AG:67:ALA:HB3	1.95	0.49
4:N:111:VAL:HA	4:N:120:VAL:HA	1.95	0.49
2:QB:63:ALA:HA	2:QB:67:ALA:HB3	1.95	0.49
3:RB:270:LEU:O	4:SB:62:VAL:N	2.27	0.49
3:XB:200:VAL:N	3:XB:219:LEU:O	2.44	0.49
4:FC:119:GLY:HA2	4:GC:88:ALA:HA	1.94	0.49
3:VC:85:ARG:N	3:VC:201:ASN:O	2.36	0.49
4:XC:119:GLY:HA2	4:YC:88:ALA:HA	1.94	0.49
3:ZD:200:VAL:N	3:ZD:219:LEU:O	2.44	0.49
3:ZD:301:VAL:O	3:ZD:321:ILE:N	2.45	0.49
2:UF:63:ALA:HA	2:UF:67:ALA:HB3	1.94	0.49
3:HG:270:LEU:O	4:IG:62:VAL:N	2.27	0.49
4:UG:111:VAL:HA	4:UG:120:VAL:HA	1.95	0.49
4:E:119:GLY:HA2	4:H:88:ALA:HA	1.94	0.48
1:Z:552:ARG:HA	2:AA:67:ALA:HB2	1.94	0.48
2:EB:139:ARG:C	2:KB:205:LEU:CB	2.86	0.48
3:FB:301:VAL:O	3:FB:321:ILE:N	2.45	0.48
1:BC:552:ARG:HA	2:CC:67:ALA:HB2	1.94	0.48
3:DC:200:VAL:N	3:DC:219:LEU:O	2.44	0.48
4:GC:110:GLU:O	4:GC:121:ARG:N	2.42	0.48
1:HC:552:ARG:HA	2:IC:67:ALA:HB2	1.94	0.48
2:OC:63:ALA:HA	2:OC:67:ALA:HB3	1.95	0.48
2:AD:63:ALA:HA	2:AD:67:ALA:HB3	1.95	0.48
4:JD:119:GLY:HA2	4:KD:88:ALA:HA	1.94	0.48
2:EE:119:ALA:O	2:EE:123:ARG:N	2.44	0.48
2:WE:119:ALA:O	2:WE:123:ARG:N	2.44	0.48
4:LF:119:GLY:HA2	4:MF:88:ALA:HA	1.94	0.48
2:J:139:ARG:C	2:T:205:LEU:CB	2.85	0.48
1:S:552:ARG:HA	2:T:67:ALA:HB2	1.94	0.48
4:GB:111:VAL:HA	4:GB:120:VAL:HA	1.95	0.48
2:KB:219:ARG:HA	2:KB:226:ALA:HB3	1.93	0.48
4:OB:110:GLU:O	4:OB:121:ARG:N	2.42	0.48
4:UB:110:GLU:O	4:UB:121:ARG:N	2.42	0.48
4:AC:110:GLU:O	4:AC:121:ARG:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GG:77:LEU:CB	2:MG:42:ALA:C	2.86	0.48
4:IG:111:VAL:HA	4:IG:120:VAL:HA	1.95	0.48
4:OG:111:VAL:HA	4:OG:120:VAL:HA	1.95	0.48
2:B:63:ALA:HA	2:B:67:ALA:HB3	1.95	0.48
1:FA:552:ARG:HA	2:GA:67:ALA:HB2	1.94	0.48
2:MA:63:ALA:HA	2:MA:67:ALA:HB3	1.95	0.48
3:ZA:301:VAL:O	3:ZA:321:ILE:N	2.45	0.48
4:AB:111:VAL:HA	4:AB:120:VAL:HA	1.95	0.48
2:KB:77:LEU:CB	2:QB:42:ALA:C	2.86	0.48
1:PB:552:ARG:HA	2:QB:67:ALA:HB2	1.94	0.48
1:VB:552:ARG:HA	2:WB:67:ALA:HB2	1.94	0.48
2:CC:77:LEU:CB	2:IC:42:ALA:C	2.86	0.48
3:JC:200:VAL:N	3:JC:219:LEU:O	2.44	0.48
2:MD:63:ALA:HA	2:MD:67:ALA:HB3	1.94	0.48
3:ND:200:VAL:N	3:ND:219:LEU:O	2.44	0.48
2:SD:63:ALA:HA	2:SD:67:ALA:HB3	1.95	0.48
3:TD:200:VAL:N	3:TD:219:LEU:O	2.44	0.48
3:FE:301:VAL:O	3:FE:321:ILE:N	2.45	0.48
4:CG:111:VAL:HA	4:CG:120:VAL:HA	1.95	0.48
2:GG:63:ALA:HA	2:GG:67:ALA:HB3	1.94	0.48
2:G:63:ALA:HA	2:G:67:ALA:HB3	1.95	0.48
3:BA:80:THR:O	3:BA:205:HIS:N	2.35	0.48
3:TA:301:VAL:O	3:TA:321:ILE:N	2.45	0.48
4:CB:110:GLU:O	4:CB:121:ARG:N	2.42	0.48
1:DB:552:ARG:HA	2:EB:67:ALA:HB2	1.94	0.48
4:IB:110:GLU:O	4:IB:121:ARG:N	2.42	0.48
2:KB:139:ARG:C	2:QB:205:LEU:CB	2.86	0.48
4:MB:111:VAL:HA	4:MB:120:VAL:HA	1.95	0.48
4:SB:111:VAL:HA	4:SB:120:VAL:HA	1.95	0.48
3:PC:200:VAL:N	3:PC:219:LEU:O	2.44	0.48
3:HD:200:VAL:N	3:HD:219:LEU:O	2.44	0.48
2:YD:77:LEU:CB	2:EE:42:ALA:C	2.86	0.48
3:LE:301:VAL:O	3:LE:321:ILE:N	2.45	0.48
2:WE:63:ALA:HA	2:WE:67:ALA:HB3	1.95	0.48
4:WF:111:VAL:HA	4:WF:120:VAL:HA	1.95	0.48
1:LA:552:ARG:HA	2:MA:67:ALA:HB2	1.94	0.48
1:JB:552:ARG:HA	2:KB:67:ALA:HB2	1.94	0.48
3:VC:200:VAL:N	3:VC:219:LEU:O	2.44	0.48
3:BD:200:VAL:N	3:BD:219:LEU:O	2.44	0.48
3:LE:270:LEU:O	4:ME:62:VAL:N	2.27	0.48
4:FF:119:GLY:HA2	4:GF:88:ALA:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:OF:63:ALA:HA	2:OF:67:ALA:HB3	1.94	0.48
4:PG:119:GLY:HA2	4:QG:88:ALA:HA	1.94	0.48
3:NA:301:VAL:O	3:NA:321:ILE:N	2.45	0.48
2:SA:63:ALA:HA	2:SA:67:ALA:HB3	1.95	0.48
4:WA:110:GLU:O	4:WA:121:ARG:N	2.42	0.48
1:XA:552:ARG:HA	2:YA:67:ALA:HB2	1.94	0.48
2:QE:63:ALA:HA	2:QE:67:ALA:HB3	1.95	0.48
3:RE:301:VAL:O	3:RE:321:ILE:N	2.45	0.48
2:MG:77:LEU:CB	2:SG:42:ALA:C	2.86	0.48
4:KA:100:LEU:HA	4:KA:105:LEU:HA	1.96	0.48
1:RA:552:ARG:HA	2:SA:67:ALA:HB2	1.94	0.48
4:WA:100:LEU:HA	4:WA:105:LEU:HA	1.96	0.48
3:DC:270:LEU:O	4:EC:62:VAL:N	2.27	0.48
2:YD:63:ALA:HA	2:YD:67:ALA:HB3	1.95	0.48
2:KE:139:ARG:O	2:QE:205:LEU:CB	2.61	0.48
3:PF:270:LEU:O	4:QF:62:VAL:N	2.27	0.48
2:J:63:ALA:HA	2:J:67:ALA:HB3	1.95	0.48
4:QA:110:GLU:O	4:QA:121:ARG:N	2.42	0.48
4:IB:100:LEU:HA	4:IB:105:LEU:HA	1.96	0.48
4:UB:100:LEU:HA	4:UB:105:LEU:HA	1.96	0.48
4:YB:111:VAL:HA	4:YB:120:VAL:HA	1.95	0.48
4:AE:111:VAL:HA	4:AE:120:VAL:HA	1.95	0.48
4:TE:119:GLY:HA2	4:UE:88:ALA:HA	1.94	0.48
4:KF:111:VAL:HA	4:KF:120:VAL:HA	1.95	0.48
2:G:77:LEU:CB	2:B:42:ALA:C	2.87	0.48
2:B:139:ARG:C	2:J:205:LEU:CB	2.87	0.48
2:AA:63:ALA:HA	2:AA:67:ALA:HB3	1.95	0.48
4:EA:100:LEU:HA	4:EA:105:LEU:HA	1.96	0.48
2:GA:63:ALA:HA	2:GA:67:ALA:HB3	1.95	0.48
3:HA:301:VAL:O	3:HA:321:ILE:N	2.45	0.48
4:KA:110:GLU:O	4:KA:121:ARG:N	2.42	0.48
4:CB:100:LEU:HA	4:CB:105:LEU:HA	1.96	0.48
4:OB:100:LEU:HA	4:OB:105:LEU:HA	1.96	0.48
2:EE:63:ALA:HA	2:EE:67:ALA:HB3	1.95	0.48
3:RE:80:THR:O	3:RE:205:HIS:N	2.35	0.48
3:XE:301:VAL:O	3:XE:321:ILE:N	2.45	0.48
2:CF:63:ALA:HA	2:CF:67:ALA:HB3	1.95	0.48
2:SG:63:ALA:HA	2:SG:67:ALA:HB3	1.94	0.48
4:H:100:LEU:HA	4:H:105:LEU:HA	1.96	0.48
4:R:100:LEU:HA	4:R:105:LEU:HA	1.96	0.48
4:BE:119:GLY:HA2	4:CE:88:ALA:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:QF:111:VAL:HA	4:QF:120:VAL:HA	1.95	0.48
4:XF:119:GLY:HA2	4:YF:88:ALA:HA	1.94	0.48
4:Q:100:LEU:HA	4:Q:105:LEU:HA	1.96	0.47
3:BA:301:VAL:O	3:BA:321:ILE:N	2.45	0.47
4:EA:110:GLU:O	4:EA:121:ARG:N	2.42	0.47
4:AC:100:LEU:HA	4:AC:105:LEU:HA	1.96	0.47
2:AD:139:ARG:O	2:GD:205:LEU:CB	2.62	0.47
4:UD:111:VAL:HA	4:UD:120:VAL:HA	1.95	0.47
2:KE:63:ALA:HA	2:KE:67:ALA:HB3	1.94	0.47
4:YE:111:VAL:HA	4:YE:120:VAL:HA	1.95	0.47
3:DF:301:VAL:O	3:DF:321:ILE:N	2.45	0.47
4:Y:100:LEU:HA	4:Y:105:LEU:HA	1.96	0.47
2:QB:77:LEU:CB	2:WB:42:ALA:C	2.87	0.47
4:EC:111:VAL:HA	4:EC:120:VAL:HA	1.95	0.47
4:KC:111:VAL:HA	4:KC:120:VAL:HA	1.95	0.47
4:MC:100:LEU:HA	4:MC:105:LEU:HA	1.96	0.47
4:SC:100:LEU:HA	4:SC:105:LEU:HA	1.96	0.47
4:WC:111:VAL:HA	4:WC:120:VAL:HA	1.95	0.47
4:GE:111:VAL:HA	4:GE:120:VAL:HA	1.95	0.47
2:CF:119:ALA:O	2:CF:123:ARG:N	2.44	0.47
2:OF:119:ALA:O	2:OF:123:ARG:N	2.44	0.47
2:MG:63:ALA:HA	2:MG:67:ALA:HB3	1.94	0.47
4:QA:100:LEU:HA	4:QA:105:LEU:HA	1.96	0.47
2:EB:200:ALA:HB3	2:EB:232:GLU:CB	2.32	0.47
2:YD:139:ARG:C	2:EE:205:LEU:CB	2.88	0.47
3:XE:80:THR:O	3:XE:205:HIS:N	2.35	0.47
4:EF:111:VAL:HA	4:EF:120:VAL:HA	1.95	0.47
3:V:301:VAL:O	3:V:321:ILE:N	2.45	0.47
4:Y:110:GLU:O	4:Y:121:ARG:N	2.42	0.47
4:GC:100:LEU:HA	4:GC:105:LEU:HA	1.96	0.47
4:CD:111:VAL:HA	4:CD:120:VAL:HA	1.95	0.47
4:ME:111:VAL:HA	4:ME:120:VAL:HA	1.95	0.47
2:QE:119:ALA:O	2:QE:123:ARG:N	2.44	0.47
2:IF:119:ALA:O	2:IF:123:ARG:N	2.44	0.47
3:JF:301:VAL:O	3:JF:321:ILE:N	2.45	0.47
2:AG:119:ALA:O	2:AG:123:ARG:N	2.44	0.47
2:SG:200:ALA:HB3	2:SG:232:GLU:CB	2.32	0.47
4:QC:111:VAL:HA	4:QC:120:VAL:HA	1.95	0.47
2:UC:77:LEU:CB	2:AD:42:ALA:C	2.88	0.47
4:QG:100:LEU:HA	4:QG:105:LEU:HA	1.96	0.47
3:TG:270:LEU:O	4:UG:62:VAL:N	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:301:VAL:O	3:K:321:ILE:N	2.45	0.47
2:T:63:ALA:HA	2:T:67:ALA:HB3	1.95	0.47
2:YA:139:ARG:CB	2:EB:205:LEU:CB	2.92	0.47
2:GD:139:ARG:C	2:MD:205:LEU:CB	2.88	0.47
4:KD:100:LEU:HA	4:KD:105:LEU:HA	1.96	0.47
2:KE:119:ALA:O	2:KE:123:ARG:N	2.44	0.47
2:IF:63:ALA:HA	2:IF:67:ALA:HB3	1.95	0.47
4:WG:100:LEU:HA	4:WG:105:LEU:HA	1.96	0.47
3:M:301:VAL:O	3:M:321:ILE:N	2.45	0.47
3:C:301:VAL:O	3:C:321:ILE:N	2.45	0.47
2:AA:139:ARG:C	2:GA:205:LEU:CB	2.87	0.47
2:AA:200:ALA:HB3	2:AA:232:GLU:CB	2.32	0.47
2:KB:139:ARG:O	2:QB:205:LEU:CB	2.63	0.47
4:YC:100:LEU:HA	4:YC:105:LEU:HA	1.96	0.47
4:ED:100:LEU:HA	4:ED:105:LEU:HA	1.96	0.47
4:ID:111:VAL:HA	4:ID:120:VAL:HA	1.95	0.47
4:OD:111:VAL:HA	4:OD:120:VAL:HA	1.95	0.47
4:QD:100:LEU:HA	4:QD:105:LEU:HA	1.96	0.47
4:SE:111:VAL:HA	4:SE:120:VAL:HA	1.95	0.47
2:WE:77:LEU:CB	2:CF:42:ALA:C	2.88	0.47
2:IF:139:ARG:CB	2:OF:205:LEU:CB	2.93	0.47
3:PF:301:VAL:O	3:PF:321:ILE:N	2.45	0.47
2:UF:119:ALA:O	2:UF:123:ARG:N	2.44	0.47
3:VF:301:VAL:O	3:VF:321:ILE:N	2.45	0.47
2:GG:139:ARG:C	2:MG:205:LEU:CB	2.88	0.47
4:KG:100:LEU:HA	4:KG:105:LEU:HA	1.96	0.47
2:MG:119:ALA:O	2:MG:123:ARG:N	2.44	0.47
4:R:110:GLU:O	4:R:121:ARG:N	2.42	0.47
2:GA:139:ARG:O	2:MA:205:LEU:CB	2.63	0.47
3:LB:80:THR:O	3:LB:205:HIS:N	2.35	0.47
2:IC:139:ARG:CB	2:OC:205:LEU:CB	2.93	0.47
2:MD:77:LEU:CB	2:SD:42:ALA:C	2.88	0.47
3:DF:80:THR:O	3:DF:205:HIS:N	2.35	0.47
3:NG:80:THR:O	3:NG:205:HIS:N	2.35	0.47
3:TG:301:VAL:O	3:TG:321:ILE:N	2.45	0.47
2:SA:139:ARG:C	2:YA:205:LEU:CB	2.88	0.47
4:SF:100:LEU:HA	4:SF:105:LEU:HA	1.96	0.47
4:YF:110:GLU:O	4:YF:121:ARG:N	2.42	0.47
3:BG:301:VAL:O	3:BG:321:ILE:N	2.45	0.47
3:NG:301:VAL:O	3:NG:321:ILE:N	2.45	0.47
3:M:80:THR:O	3:M:205:HIS:N	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:VC:80:THR:O	3:VC:205:HIS:N	2.35	0.47
2:SD:139:ARG:C	2:YD:205:LEU:CB	2.89	0.47
2:QE:139:ARG:C	2:WE:205:LEU:CB	2.87	0.47
4:YF:100:LEU:HA	4:YF:105:LEU:HA	1.96	0.47
3:HG:301:VAL:O	3:HG:321:ILE:N	2.45	0.47
4:H:110:GLU:O	4:H:121:ARG:N	2.42	0.46
4:CE:100:LEU:HA	4:CE:105:LEU:HA	1.96	0.46
2:CF:139:ARG:C	2:IF:205:LEU:CB	2.88	0.46
4:SF:110:GLU:O	4:SF:121:ARG:N	2.42	0.46
2:UF:139:ARG:C	2:AG:205:LEU:CB	2.88	0.46
4:EG:100:LEU:HA	4:EG:105:LEU:HA	1.96	0.46
4:Q:110:GLU:O	4:Q:121:ARG:N	2.42	0.46
3:FB:270:LEU:O	4:GB:62:VAL:N	2.27	0.46
4:WD:100:LEU:HA	4:WD:105:LEU:HA	1.96	0.46
4:IE:100:LEU:HA	4:IE:105:LEU:HA	1.96	0.46
4:MF:100:LEU:HA	4:MF:105:LEU:HA	1.96	0.46
2:SD:119:ALA:O	2:SD:123:ARG:N	2.44	0.46
4:AF:100:LEU:HA	4:AF:105:LEU:HA	1.96	0.46
4:MF:110:GLU:O	4:MF:121:ARG:N	2.42	0.46
4:GF:100:LEU:HA	4:GF:105:LEU:HA	1.96	0.46
4:OE:100:LEU:HA	4:OE:105:LEU:HA	1.96	0.46
4:UE:100:LEU:HA	4:UE:105:LEU:HA	1.96	0.46
4:GF:110:GLU:O	4:GF:121:ARG:N	2.42	0.46
3:JF:80:THR:O	3:JF:205:HIS:N	2.35	0.46
3:HA:80:THR:O	3:HA:205:HIS:N	2.35	0.46
3:TG:80:THR:O	3:TG:205:HIS:N	2.35	0.46
4:AF:110:GLU:O	4:AF:121:ARG:N	2.42	0.46
2:UF:200:ALA:HB3	2:UF:232:GLU:CB	2.32	0.46
2:OC:147:ALA:HA	2:UC:210:GLN:CB	2.46	0.45
3:BG:80:THR:O	3:BG:205:HIS:N	2.35	0.45
4:WG:110:GLU:O	4:WG:121:ARG:N	2.42	0.45
2:KE:139:ARG:CB	2:QE:205:LEU:CB	2.94	0.45
4:YF:106:ILE:O	4:YF:126:ILE:N	2.40	0.45
2:T:139:ARG:O	2:AA:205:LEU:CB	2.64	0.45
2:CC:139:ARG:C	2:IC:205:LEU:CB	2.90	0.45
4:UE:110:GLU:O	4:UE:121:ARG:N	2.42	0.45
4:QG:110:GLU:O	4:QG:121:ARG:N	2.42	0.45
4:CB:106:ILE:O	4:CB:126:ILE:N	2.40	0.45
2:EE:139:ARG:C	2:KE:205:LEU:CB	2.90	0.45
3:PF:80:THR:O	3:PF:205:HIS:N	2.35	0.45
2:G:139:ARG:C	2:B:205:LEU:CB	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:139:ARG:O	2:KB:205:LEU:CB	2.65	0.45
3:RB:80:THR:O	3:RB:205:HIS:N	2.35	0.45
2:OF:139:ARG:O	2:UF:205:LEU:CB	2.64	0.45
4:EG:106:ILE:O	4:EG:126:ILE:N	2.40	0.45
2:G:205:LEU:CB	2:SG:139:ARG:O	2.64	0.44
4:OE:110:GLU:O	4:OE:121:ARG:N	2.42	0.44
4:KG:110:GLU:O	4:KG:121:ARG:N	2.42	0.44
4:ED:106:ILE:O	4:ED:126:ILE:N	2.40	0.44
2:J:139:ARG:CB	2:T:205:LEU:CB	2.95	0.44
2:MA:77:LEU:CB	2:SA:42:ALA:C	2.90	0.44
2:WB:139:ARG:O	2:CC:205:LEU:CB	2.65	0.44
2:MD:139:ARG:C	2:SD:205:LEU:CB	2.91	0.44
4:KG:106:ILE:O	4:KG:126:ILE:N	2.40	0.44
2:OC:200:ALA:HB3	2:OC:232:GLU:CB	2.32	0.44
4:SC:110:GLU:O	4:SC:121:ARG:N	2.42	0.44
3:BD:80:THR:O	3:BD:205:HIS:N	2.35	0.44
4:PD:120:VAL:N	4:QD:87:VAL:O	2.51	0.44
2:SD:200:ALA:HB3	2:SD:232:GLU:CB	2.32	0.44
4:NE:120:VAL:N	4:OE:87:VAL:O	2.51	0.44
2:MG:139:ARG:C	2:SG:205:LEU:CB	2.91	0.44
4:O:120:VAL:N	4:R:87:VAL:O	2.51	0.44
2:KB:200:ALA:HB3	2:KB:232:GLU:CB	2.32	0.44
2:WB:139:ARG:CB	2:CC:205:LEU:CB	2.95	0.44
4:JD:120:VAL:N	4:KD:87:VAL:O	2.51	0.44
4:IE:110:GLU:O	4:IE:121:ARG:N	2.42	0.44
4:PG:120:VAL:N	4:QG:87:VAL:O	2.51	0.44
2:G:200:ALA:HB3	2:G:232:GLU:CB	2.32	0.44
4:X:120:VAL:N	4:Y:87:VAL:O	2.51	0.44
2:IC:139:ARG:O	2:OC:205:LEU:CB	2.66	0.44
2:AG:139:ARG:O	2:GG:205:LEU:CB	2.65	0.44
4:EG:110:GLU:O	4:EG:121:ARG:N	2.42	0.44
2:YA:139:ARG:O	2:EB:205:LEU:CB	2.66	0.44
4:RF:120:VAL:N	4:SF:87:VAL:O	2.51	0.44
2:GA:200:ALA:HB3	2:GA:232:GLU:CB	2.32	0.44
4:BB:120:VAL:N	4:CB:87:VAL:O	2.51	0.44
2:QB:139:ARG:C	2:WB:205:LEU:CB	2.91	0.44
4:HE:120:VAL:N	4:IE:87:VAL:O	2.51	0.44
4:TE:120:VAL:N	4:UE:87:VAL:O	2.51	0.44
2:WE:139:ARG:C	2:CF:205:LEU:CB	2.90	0.44
4:LF:120:VAL:N	4:MF:87:VAL:O	2.51	0.44
4:JG:120:VAL:N	4:KG:87:VAL:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:VG:120:VAL:N	4:WG:87:VAL:O	2.51	0.44
4:VA:120:VAL:N	4:WA:87:VAL:O	2.51	0.43
4:FC:120:VAL:N	4:GC:87:VAL:O	2.51	0.43
4:LC:120:VAL:N	4:MC:87:VAL:O	2.51	0.43
4:CE:110:GLU:O	4:CE:121:ARG:N	2.42	0.43
3:FE:80:THR:O	3:FE:205:HIS:N	2.35	0.43
4:DG:120:VAL:N	4:EG:87:VAL:O	2.51	0.43
4:DA:120:VAL:N	4:EA:87:VAL:O	2.51	0.43
4:VD:120:VAL:N	4:WD:87:VAL:O	2.51	0.43
2:KE:190:ARG:O	2:KE:191:SER:C	2.61	0.43
3:VF:80:THR:O	3:VF:205:HIS:N	2.35	0.43
2:G:205:LEU:CB	2:SG:139:ARG:CB	2.96	0.43
3:C:80:THR:O	3:C:205:HIS:N	2.35	0.43
4:E:120:VAL:N	4:H:87:VAL:O	2.51	0.43
4:HB:120:VAL:N	4:IB:87:VAL:O	2.51	0.43
4:DD:120:VAL:N	4:ED:87:VAL:O	2.51	0.43
2:EE:190:ARG:O	2:EE:191:SER:C	2.62	0.43
2:KE:147:ALA:HA	2:QE:210:GLN:CB	2.48	0.43
2:QE:190:ARG:O	2:QE:191:SER:C	2.61	0.43
2:WE:200:ALA:HB3	2:WE:232:GLU:CB	2.32	0.43
4:QG:106:ILE:O	4:QG:126:ILE:N	2.40	0.43
4:PA:120:VAL:N	4:QA:87:VAL:O	2.51	0.43
4:IB:106:ILE:O	4:IB:126:ILE:N	2.40	0.43
4:ZB:120:VAL:N	4:AC:87:VAL:O	2.51	0.43
2:GD:139:ARG:O	2:MD:205:LEU:CB	2.67	0.43
2:YD:139:ARG:O	2:EE:205:LEU:CB	2.66	0.43
2:WE:190:ARG:O	2:WE:191:SER:C	2.61	0.43
4:RC:120:VAL:N	4:SC:87:VAL:O	2.51	0.43
2:SD:139:ARG:CB	2:YD:205:LEU:CB	2.97	0.43
2:QE:139:ARG:O	2:WE:205:LEU:CB	2.66	0.43
2:CF:190:ARG:O	2:CF:191:SER:C	2.61	0.43
4:FF:120:VAL:N	4:GF:87:VAL:O	2.51	0.43
4:XF:120:VAL:N	4:YF:87:VAL:O	2.51	0.43
4:KD:106:ILE:O	4:KD:126:ILE:N	2.40	0.43
4:WD:110:GLU:O	4:WD:121:ARG:N	2.42	0.43
2:IF:190:ARG:O	2:IF:191:SER:C	2.61	0.43
2:OF:188:LEU:O	2:OF:189:LYS:C	2.62	0.43
2:J:139:ARG:O	2:T:205:LEU:CB	2.66	0.43
4:ZE:120:VAL:N	4:AF:87:VAL:O	2.51	0.43
2:IF:188:LEU:O	2:IF:189:LYS:C	2.62	0.43
2:UF:188:LEU:O	2:UF:189:LYS:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AG:188:LEU:O	2:AG:189:LYS:C	2.62	0.43
2:GG:188:LEU:O	2:GG:189:LYS:C	2.62	0.43
4:P:120:VAL:N	4:Q:87:VAL:O	2.51	0.43
3:NA:80:THR:O	3:NA:205:HIS:N	2.35	0.43
4:BE:120:VAL:N	4:CE:87:VAL:O	2.51	0.43
2:CF:188:LEU:O	2:CF:189:LYS:C	2.62	0.43
2:MG:188:LEU:O	2:MG:189:LYS:C	2.62	0.43
2:SG:188:LEU:O	2:SG:189:LYS:C	2.62	0.43
2:B:139:ARG:O	2:J:205:LEU:CB	2.66	0.43
2:OF:190:ARG:O	2:OF:191:SER:C	2.61	0.43
2:SA:139:ARG:O	2:YA:205:LEU:CB	2.67	0.43
2:EB:139:ARG:CB	2:KB:205:LEU:CB	2.97	0.43
4:NB:120:VAL:N	4:OB:87:VAL:O	2.51	0.43
2:UF:190:ARG:O	2:UF:191:SER:C	2.61	0.43
4:WG:106:ILE:O	4:WG:126:ILE:N	2.40	0.43
2:G:188:LEU:O	2:G:189:LYS:C	2.62	0.42
4:JA:120:VAL:N	4:KA:87:VAL:O	2.51	0.42
2:OC:73:ALA:HA	2:UC:43:ASN:HA	2.00	0.42
3:HD:80:THR:O	3:HD:205:HIS:N	2.35	0.42
3:ND:80:THR:O	3:ND:205:HIS:N	2.35	0.42
4:QD:110:GLU:O	4:QD:121:ARG:N	2.42	0.42
2:B:188:LEU:O	2:B:189:LYS:C	2.62	0.42
2:MA:190:ARG:O	2:MA:191:SER:C	2.61	0.42
2:UC:139:ARG:C	2:AD:205:LEU:CB	2.92	0.42
4:XC:120:VAL:N	4:YC:87:VAL:O	2.51	0.42
2:AD:139:ARG:CB	2:GD:205:LEU:CB	2.97	0.42
2:AG:190:ARG:O	2:AG:191:SER:C	2.61	0.42
2:AA:139:ARG:CB	2:GA:205:LEU:CB	2.97	0.42
2:GA:190:ARG:O	2:GA:191:SER:C	2.61	0.42
2:SA:190:ARG:O	2:SA:191:SER:C	2.61	0.42
3:BD:80:THR:N	3:BD:205:HIS:O	2.33	0.42
3:TD:80:THR:O	3:TD:205:HIS:N	2.35	0.42
2:J:188:LEU:O	2:J:189:LYS:C	2.62	0.42
2:AA:139:ARG:O	2:GA:205:LEU:CB	2.67	0.42
2:AA:190:ARG:O	2:AA:191:SER:C	2.61	0.42
3:XB:80:THR:O	3:XB:205:HIS:N	2.35	0.42
2:GA:139:ARG:CB	2:MA:205:LEU:CB	2.97	0.42
2:YA:190:ARG:O	2:YA:191:SER:C	2.61	0.42
4:QC:65:THR:N	4:QC:100:LEU:O	2.40	0.42
2:EE:139:ARG:CB	2:KE:205:LEU:CB	2.97	0.42
2:GG:190:ARG:O	2:GG:191:SER:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:80:THR:O	3:K:205:HIS:N	2.35	0.42
2:T:188:LEU:O	2:T:189:LYS:C	2.62	0.42
2:T:190:ARG:O	2:T:191:SER:C	2.61	0.42
4:WC:65:THR:N	4:WC:100:LEU:O	2.40	0.42
4:KD:110:GLU:O	4:KD:121:ARG:N	2.42	0.42
2:KB:188:LEU:O	2:KB:189:LYS:C	2.62	0.42
4:KC:65:THR:N	4:KC:100:LEU:O	2.40	0.42
3:PC:80:THR:O	3:PC:205:HIS:N	2.35	0.42
3:ZD:80:THR:O	3:ZD:205:HIS:N	2.35	0.42
2:MG:190:ARG:O	2:MG:191:SER:C	2.61	0.42
2:AA:188:LEU:O	2:AA:189:LYS:C	2.62	0.42
3:TA:80:THR:O	3:TA:205:HIS:N	2.35	0.42
2:EB:188:LEU:O	2:EB:189:LYS:C	2.62	0.42
2:EB:190:ARG:O	2:EB:191:SER:C	2.61	0.42
2:KB:147:ALA:HA	2:QB:210:GLN:CB	2.49	0.42
2:QB:188:LEU:O	2:QB:189:LYS:C	2.62	0.42
4:CD:65:THR:N	4:CD:100:LEU:O	2.40	0.42
2:KE:73:ALA:HA	2:QE:43:ASN:HA	2.00	0.42
2:GG:139:ARG:O	2:MG:205:LEU:CB	2.67	0.42
4:Q:106:ILE:O	4:Q:126:ILE:N	2.40	0.42
2:SA:139:ARG:CB	2:YA:205:LEU:CB	2.97	0.42
2:KB:190:ARG:O	2:KB:191:SER:C	2.61	0.42
4:TB:120:VAL:N	4:UB:87:VAL:O	2.51	0.42
2:WB:188:LEU:O	2:WB:189:LYS:C	2.62	0.42
2:IC:190:ARG:O	2:IC:191:SER:C	2.61	0.42
2:MD:200:ALA:HB3	2:MD:232:GLU:CB	2.32	0.42
4:QD:106:ILE:O	4:QD:126:ILE:N	2.40	0.42
3:HG:80:THR:O	3:HG:205:HIS:N	2.35	0.42
2:J:190:ARG:O	2:J:191:SER:C	2.61	0.42
2:GA:188:LEU:O	2:GA:189:LYS:C	2.62	0.42
2:YA:188:LEU:O	2:YA:189:LYS:C	2.62	0.42
4:OB:106:ILE:O	4:OB:126:ILE:N	2.40	0.42
2:CC:188:LEU:O	2:CC:189:LYS:C	2.62	0.42
2:CC:190:ARG:O	2:CC:191:SER:C	2.61	0.42
2:IC:200:ALA:HB3	2:IC:232:GLU:CB	2.32	0.42
3:JC:80:THR:O	3:JC:205:HIS:N	2.35	0.42
2:OC:190:ARG:O	2:OC:191:SER:C	2.61	0.42
4:ED:110:GLU:O	4:ED:121:ARG:N	2.42	0.42
2:SG:190:ARG:O	2:SG:191:SER:C	2.61	0.42
2:OC:188:LEU:O	2:OC:189:LYS:C	2.62	0.41
2:AD:188:LEU:O	2:AD:189:LYS:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GD:188:LEU:O	2:GD:189:LYS:C	2.62	0.41
2:SD:139:ARG:O	2:YD:205:LEU:CB	2.68	0.41
2:CF:139:ARG:CB	2:IF:205:LEU:CB	2.98	0.41
2:AG:139:ARG:CB	2:GG:205:LEU:CB	2.98	0.41
2:AG:200:ALA:HB3	2:AG:232:GLU:CB	2.32	0.41
2:T:139:ARG:CB	2:AA:205:LEU:CB	2.98	0.41
2:MA:139:ARG:C	2:SA:205:LEU:CB	2.93	0.41
2:MA:188:LEU:O	2:MA:189:LYS:C	2.62	0.41
2:SA:188:LEU:O	2:SA:189:LYS:C	2.62	0.41
3:ZA:80:THR:O	3:ZA:205:HIS:N	2.35	0.41
2:WB:190:ARG:O	2:WB:191:SER:C	2.61	0.41
4:EC:65:THR:N	4:EC:100:LEU:O	2.40	0.41
2:IC:188:LEU:O	2:IC:189:LYS:C	2.62	0.41
2:UC:188:LEU:O	2:UC:189:LYS:C	2.62	0.41
2:UC:190:ARG:O	2:UC:191:SER:C	2.61	0.41
4:ID:65:THR:N	4:ID:100:LEU:O	2.40	0.41
2:MD:188:LEU:O	2:MD:189:LYS:C	2.62	0.41
2:G:190:ARG:O	2:G:191:SER:C	2.61	0.41
3:LB:80:THR:N	3:LB:205:HIS:O	2.33	0.41
2:QB:190:ARG:O	2:QB:191:SER:C	2.61	0.41
2:CC:139:ARG:CB	2:IC:205:LEU:CB	2.99	0.41
3:DC:80:THR:O	3:DC:205:HIS:N	2.35	0.41
4:YC:110:GLU:O	4:YC:121:ARG:N	2.42	0.41
2:MD:139:ARG:O	2:SD:205:LEU:CB	2.68	0.41
3:LE:80:THR:N	3:LE:205:HIS:O	2.33	0.41
2:UF:139:ARG:O	2:AG:205:LEU:CB	2.67	0.41
2:OC:139:ARG:CB	2:UC:205:LEU:CB	2.99	0.41
2:AD:190:ARG:O	2:AD:191:SER:C	2.61	0.41
2:SD:188:LEU:O	2:SD:189:LYS:C	2.62	0.41
2:YD:188:LEU:O	2:YD:189:LYS:C	2.62	0.41
2:IF:139:ARG:O	2:OF:205:LEU:CB	2.67	0.41
2:MG:139:ARG:CB	2:SG:205:LEU:CB	2.98	0.41
2:B:139:ARG:CB	2:J:205:LEU:CB	2.98	0.41
2:B:190:ARG:O	2:B:191:SER:C	2.61	0.41
4:KA:106:ILE:O	4:KA:126:ILE:N	2.40	0.41
3:DC:85:ARG:O	3:DC:201:ASN:N	2.34	0.41
2:GD:139:ARG:CB	2:MD:205:LEU:CB	2.99	0.41
2:CF:139:ARG:O	2:IF:205:LEU:CB	2.67	0.41
4:QA:106:ILE:O	4:QA:126:ILE:N	2.40	0.41
2:AD:147:ALA:HA	2:GD:210:GLN:CB	2.50	0.41
4:WA:106:ILE:O	4:WA:126:ILE:N	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:YB:65:THR:N	4:YB:100:LEU:O	2.40	0.41
2:GD:190:ARG:O	2:GD:191:SER:C	2.61	0.41
2:EE:188:LEU:O	2:EE:189:LYS:C	2.62	0.41
3:VC:80:THR:N	3:VC:205:HIS:O	2.33	0.41
4:OD:65:THR:N	4:OD:100:LEU:O	2.40	0.41
2:KE:188:LEU:O	2:KE:189:LYS:C	2.62	0.41
2:OF:139:ARG:CB	2:UF:205:LEU:CB	2.99	0.41
4:QF:64:LEU:HA	4:QF:101:ILE:HA	2.03	0.41
4:CG:64:LEU:HA	4:CG:101:ILE:HA	2.03	0.41
4:N:64:LEU:HA	4:N:101:ILE:HA	2.03	0.41
4:H:106:ILE:O	4:H:126:ILE:N	2.40	0.41
4:L:64:LEU:HA	4:L:101:ILE:HA	2.03	0.41
3:V:80:THR:O	3:V:205:HIS:N	2.35	0.41
3:FB:80:THR:N	3:FB:205:HIS:O	2.33	0.41
2:QB:139:ARG:CB	2:WB:205:LEU:CB	2.99	0.41
4:XC:106:ILE:O	4:XC:126:ILE:HA	2.21	0.41
4:BE:106:ILE:O	4:BE:126:ILE:HA	2.21	0.41
4:HE:106:ILE:O	4:HE:126:ILE:HA	2.21	0.41
2:QE:188:LEU:O	2:QE:189:LYS:C	2.62	0.41
4:SE:64:LEU:HA	4:SE:101:ILE:HA	2.03	0.41
4:UE:106:ILE:O	4:UE:126:ILE:N	2.40	0.41
4:EF:64:LEU:HA	4:EF:101:ILE:HA	2.03	0.41
4:KF:64:LEU:HA	4:KF:101:ILE:HA	2.03	0.41
4:LF:106:ILE:O	4:LF:126:ILE:HA	2.21	0.41
4:WF:64:LEU:HA	4:WF:101:ILE:HA	2.03	0.41
4:OG:64:LEU:HA	4:OG:101:ILE:HA	2.03	0.41
4:D:64:LEU:HA	4:D:101:ILE:HA	2.03	0.41
2:MD:190:ARG:O	2:MD:191:SER:C	2.61	0.41
4:GE:64:LEU:HA	4:GE:101:ILE:HA	2.03	0.41
3:LE:80:THR:O	3:LE:205:HIS:N	2.35	0.41
4:FF:106:ILE:O	4:FF:126:ILE:HA	2.21	0.41
4:CA:64:LEU:HA	4:CA:101:ILE:HA	2.03	0.40
2:GA:147:ALA:HA	2:MA:210:GLN:CB	2.51	0.40
2:AD:73:ALA:HA	2:GD:43:ASN:HA	2.03	0.40
4:DD:106:ILE:O	4:DD:126:ILE:HA	2.21	0.40
4:WD:106:ILE:O	4:WD:126:ILE:N	2.40	0.40
4:ME:64:LEU:HA	4:ME:101:ILE:HA	2.03	0.40
4:YE:64:LEU:HA	4:YE:101:ILE:HA	2.03	0.40
4:IG:64:LEU:HA	4:IG:101:ILE:HA	2.03	0.40
4:UG:64:LEU:HA	4:UG:101:ILE:HA	2.03	0.40
2:G:139:ARG:O	2:B:205:LEU:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:106:ILE:O	4:O:126:ILE:HA	2.21	0.40
4:PA:106:ILE:O	4:PA:126:ILE:HA	2.21	0.40
2:QB:200:ALA:HB3	2:QB:232:GLU:CB	2.32	0.40
2:CC:139:ARG:O	2:IC:205:LEU:CB	2.69	0.40
4:RC:106:ILE:O	4:RC:126:ILE:HA	2.21	0.40
2:UC:200:ALA:HB3	2:UC:232:GLU:CB	2.32	0.40
2:QE:139:ARG:CB	2:WE:205:LEU:CB	2.99	0.40
2:WE:139:ARG:O	2:CF:205:LEU:CB	2.68	0.40
4:VG:106:ILE:O	4:VG:126:ILE:HA	2.21	0.40
4:X:106:ILE:O	4:X:126:ILE:HA	2.21	0.40
4:SB:65:THR:N	4:SB:100:LEU:O	2.40	0.40
4:TB:106:ILE:O	4:TB:126:ILE:HA	2.21	0.40
4:VD:106:ILE:O	4:VD:126:ILE:HA	2.21	0.40
2:YD:200:ALA:HB3	2:YD:232:GLU:CB	2.32	0.40
4:NE:106:ILE:O	4:NE:126:ILE:HA	2.21	0.40
2:WE:188:LEU:O	2:WE:189:LYS:C	2.62	0.40
4:RF:106:ILE:O	4:RF:126:ILE:HA	2.21	0.40
4:OA:64:LEU:HA	4:OA:101:ILE:HA	2.03	0.40
3:ZA:80:THR:N	3:ZA:205:HIS:O	2.33	0.40
4:ZB:106:ILE:O	4:ZB:126:ILE:HA	2.21	0.40
4:AE:64:LEU:HA	4:AE:101:ILE:HA	2.03	0.40
2:EE:139:ARG:O	2:KE:205:LEU:CB	2.70	0.40
2:B:200:ALA:HB3	2:B:232:GLU:CB	2.32	0.40
4:W:64:LEU:HA	4:W:101:ILE:HA	2.03	0.40
4:UB:106:ILE:O	4:UB:126:ILE:N	2.40	0.40
4:OD:64:LEU:HA	4:OD:101:ILE:HA	2.03	0.40
4:UD:64:LEU:HA	4:UD:101:ILE:HA	2.03	0.40
4:UD:65:THR:N	4:UD:100:LEU:O	2.40	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	A	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	BC	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	BF	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	DB	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	DE	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	F	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	FA	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	FD	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	FG	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	HC	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	HF	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	I	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	JB	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	JE	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	LA	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	LD	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	LG	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	NC	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	NF	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	PB	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	PE	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	RA	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	RD	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	RG	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	S	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	TC	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	TF	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	VB	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	VE	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	XA	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	XD	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	Z	45/560 (8%)	44 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	ZC	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	ZF	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
2	AA	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	AD	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	AG	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	B	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	CC	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	CF	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	EB	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	EE	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	G	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	GA	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	GD	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	GG	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	IC	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	IF	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	J	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	KB	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	KE	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	MA	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	MD	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	MG	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	OC	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	OF	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	QB	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	QE	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	SA	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	SD	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	SG	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	T	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	UC	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	UF	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	WB	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	WE	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	YA	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
2	YD	315/331 (95%)	299 (95%)	15 (5%)	1 (0%)	37	73
3	BA	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	BD	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	BG	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	C	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	DC	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	DF	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	FB	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	FE	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	HA	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	HD	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	HG	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	JC	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	JF	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	K	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	LB	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	LE	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	M	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	NA	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	ND	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	NG	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	PC	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	PF	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	RB	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	RE	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	TA	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	TD	285/334 (85%)	274 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	TG	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	V	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	VC	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	VF	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	XB	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	XE	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	ZA	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	ZD	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
4	AB	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	AC	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	AE	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	AF	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	BB	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	BE	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	CA	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	CB	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	CD	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	CE	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	CG	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	D	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	DA	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	DD	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	DG	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	E	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	EA	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	EC	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	ED	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	EF	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	EG	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	FC	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	FF	81/137 (59%)	73 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	GB	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	GC	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	GE	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	GF	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	H	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	HB	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	HE	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	IA	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	IB	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	ID	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	IE	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	IG	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	JA	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	JD	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	JG	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	KA	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	KC	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	KD	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	KF	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	KG	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	L	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	LC	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	LF	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	MB	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	MC	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	ME	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	MF	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	N	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	NB	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	NE	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	O	81/137 (59%)	73 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	OA	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	OB	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	OD	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	OE	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	OG	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	P	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	PA	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	PD	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	PG	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	Q	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	QA	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	QC	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	QD	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	QF	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	QG	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	R	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	RC	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	RF	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	SB	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	SC	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	SE	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	SF	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	TB	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	TE	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	UA	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	UB	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	UD	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	UE	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	UG	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	VA	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	VD	81/137 (59%)	73 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	VG	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	W	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	WA	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	WC	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	WD	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	WF	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	WG	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	X	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	XC	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	XF	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	Y	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	YB	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	YC	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	YE	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	YF	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	ZB	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
4	ZE	81/137 (59%)	73 (90%)	8 (10%)	0	100	100
All	All	30464/55624 (55%)	28968 (95%)	1462 (5%)	34 (0%)	50	83

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	243	ASP
2	B	243	ASP
2	J	243	ASP
2	T	243	ASP
2	AA	243	ASP
2	GA	243	ASP
2	MA	243	ASP
2	SA	243	ASP
2	YA	243	ASP
2	EB	243	ASP
2	KB	243	ASP
2	QB	243	ASP
2	WB	243	ASP
2	CC	243	ASP

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Mol	Chain	Res	Type
2	IC	243	ASP
2	OC	243	ASP
2	UC	243	ASP
2	AD	243	ASP
2	GD	243	ASP
2	MD	243	ASP
2	SD	243	ASP
2	YD	243	ASP
2	EE	243	ASP
2	KE	243	ASP
2	QE	243	ASP
2	WE	243	ASP
2	CF	243	ASP
2	IF	243	ASP
2	OF	243	ASP
2	UF	243	ASP
2	AG	243	ASP
2	GG	243	ASP
2	MG	243	ASP
2	SG	243	ASP

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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)

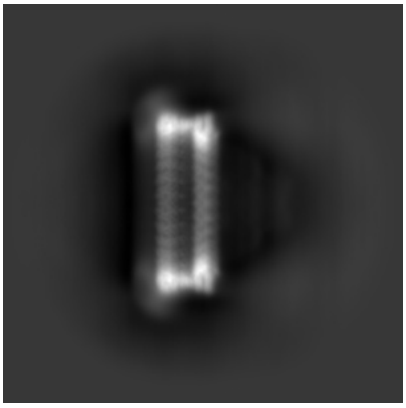
This section contains visualisations of the EMDB entry EMD-43328. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

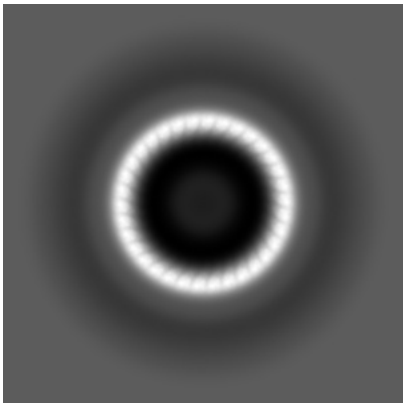
6.1 Orthogonal projections (i)

6.1.1 Primary map

X



Y

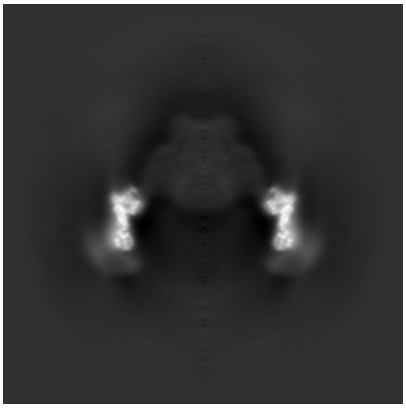


Z

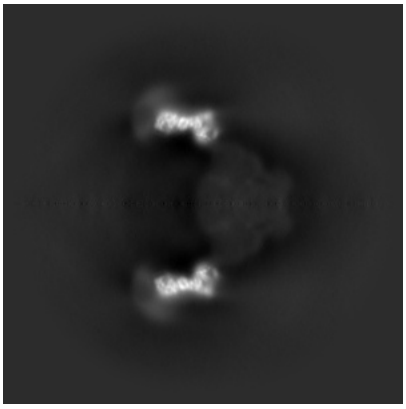
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

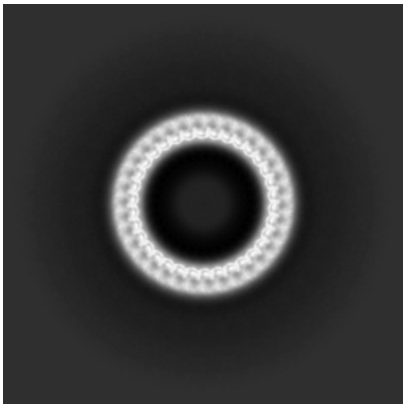
6.2.1 Primary map



X Index: 256



Y Index: 256

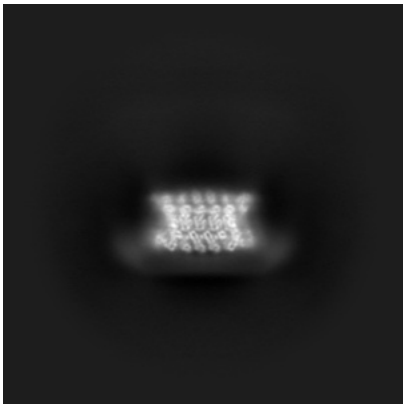


Z Index: 256

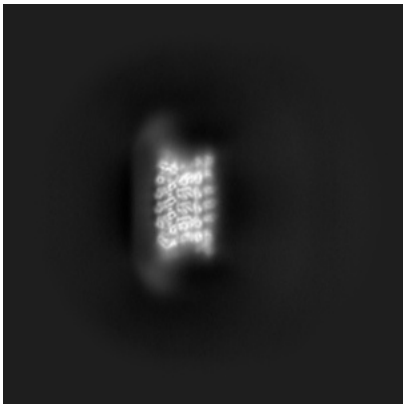
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 157



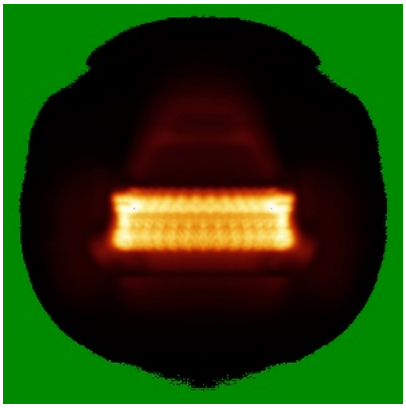
Y Index: 157

Z Index: 252

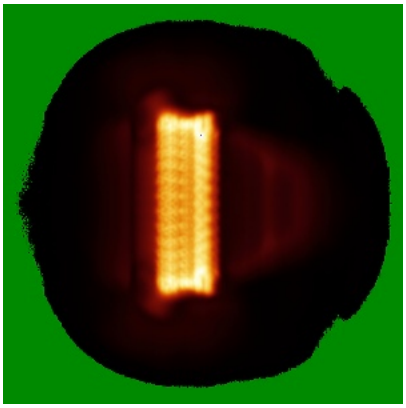
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

The images above show the 3D surface view of the map at the recommended contour level 0.175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

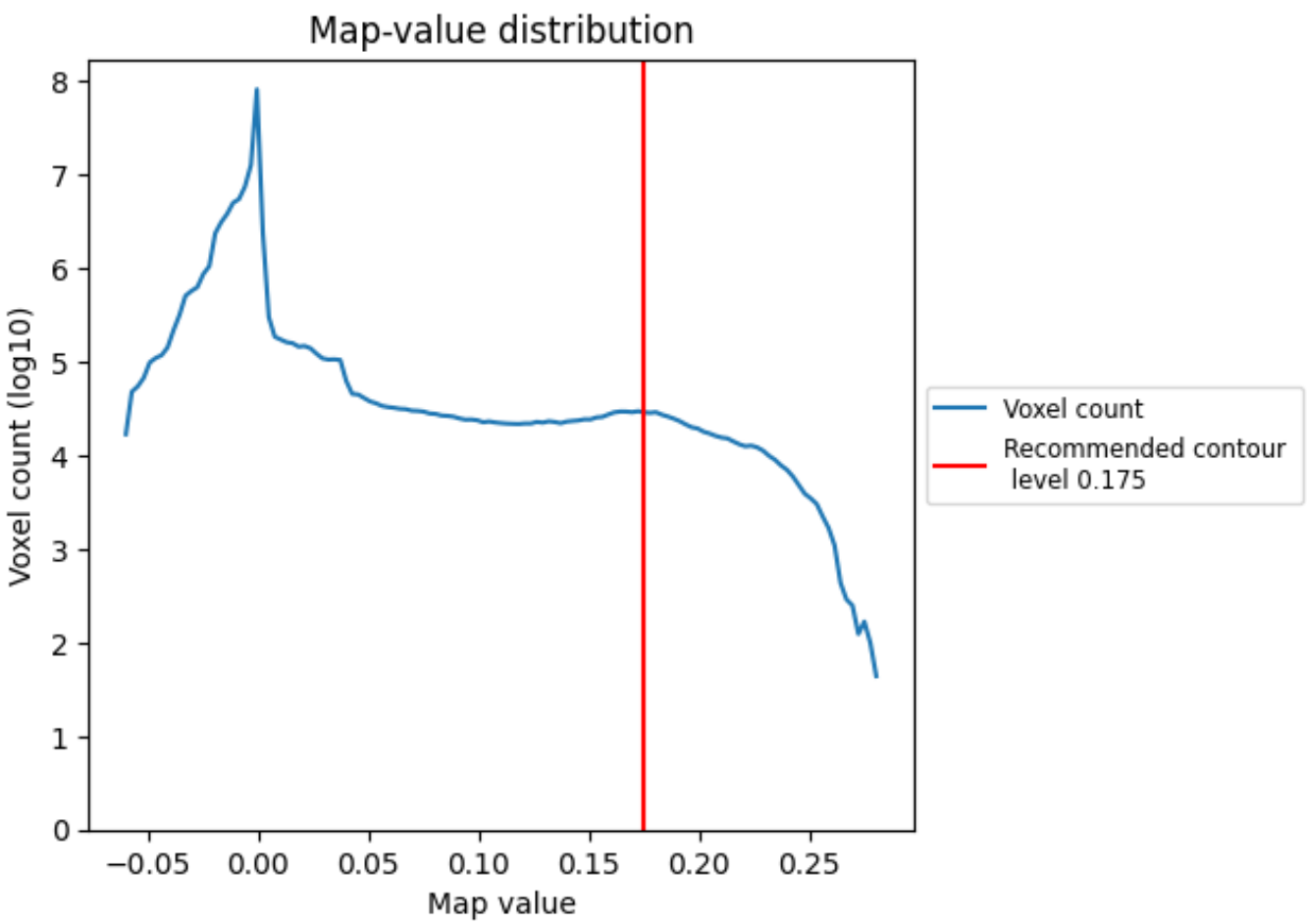
6.6 Mask visualisation (i)

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

7 Map analysis (i)

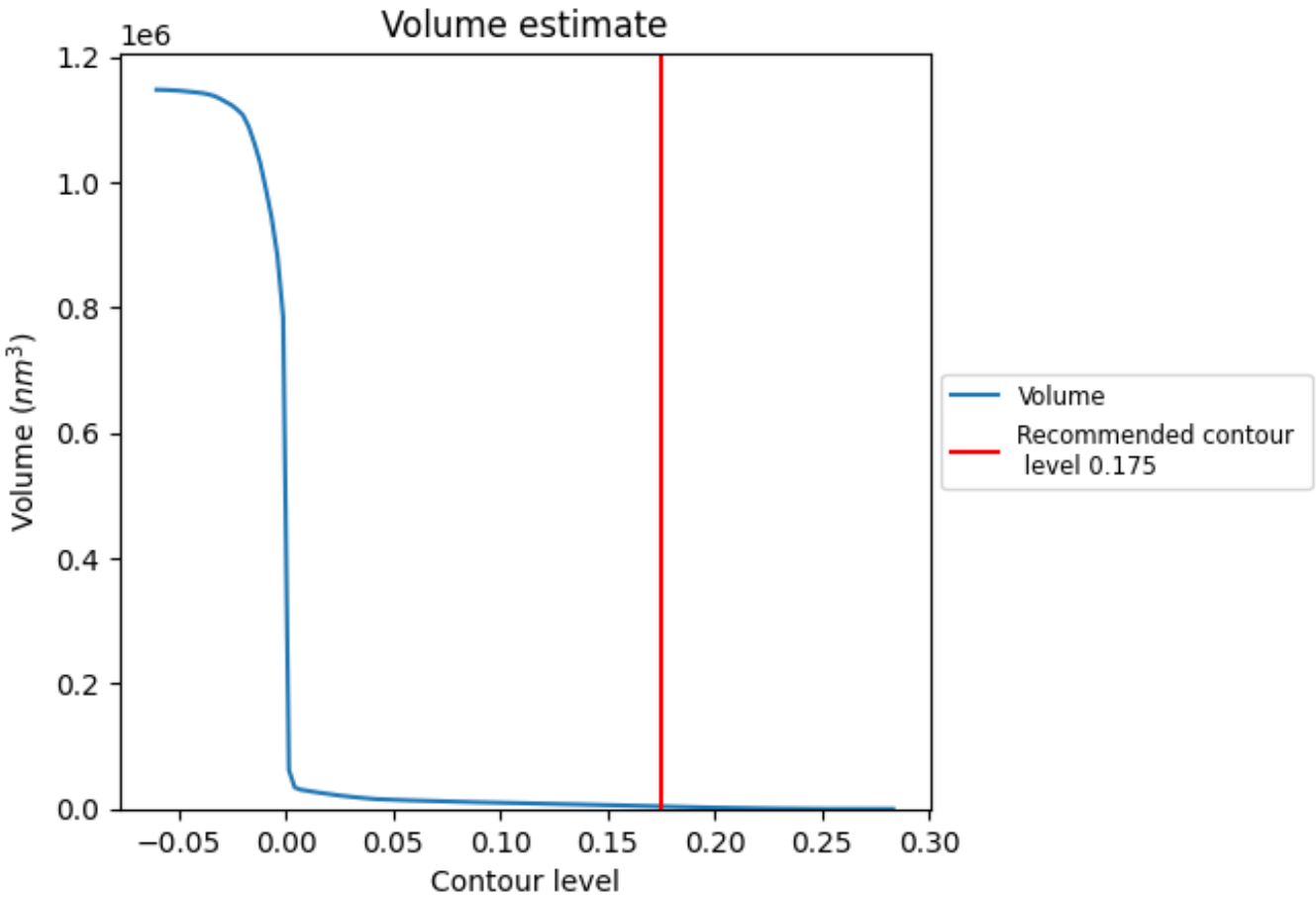
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

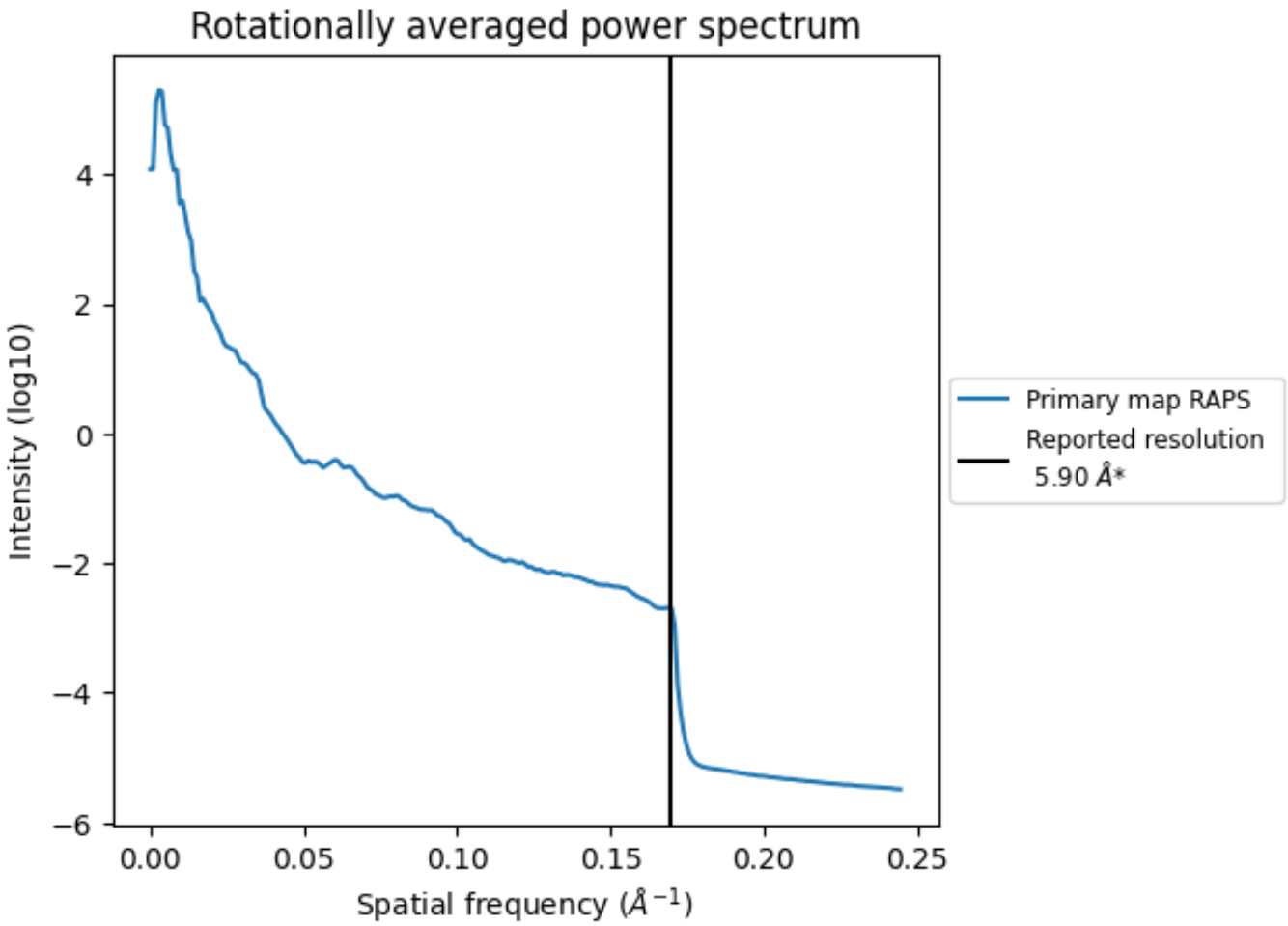
7.2 Volume estimate (i)



The volume at the recommended contour level is 4028 nm^3; this corresponds to an approximate mass of 3639 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 0.169 Å^{-1}

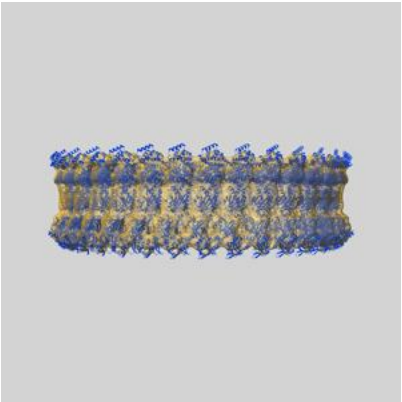
8 Fourier-Shell correlation (i)

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

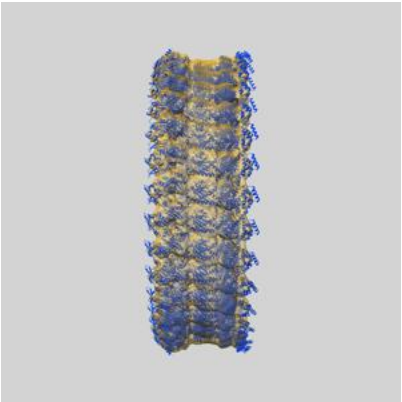
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-43328 and PDB model 8VKR. Per-residue inclusion information can be found in section 3 on page 22.

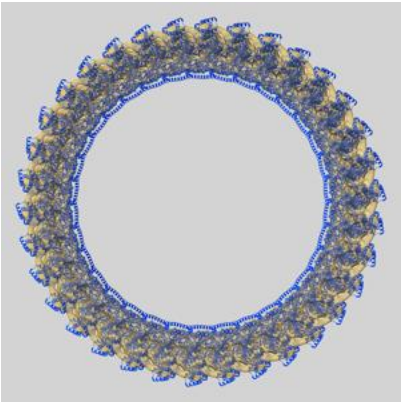
9.1 Map-model overlay (i)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.175 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

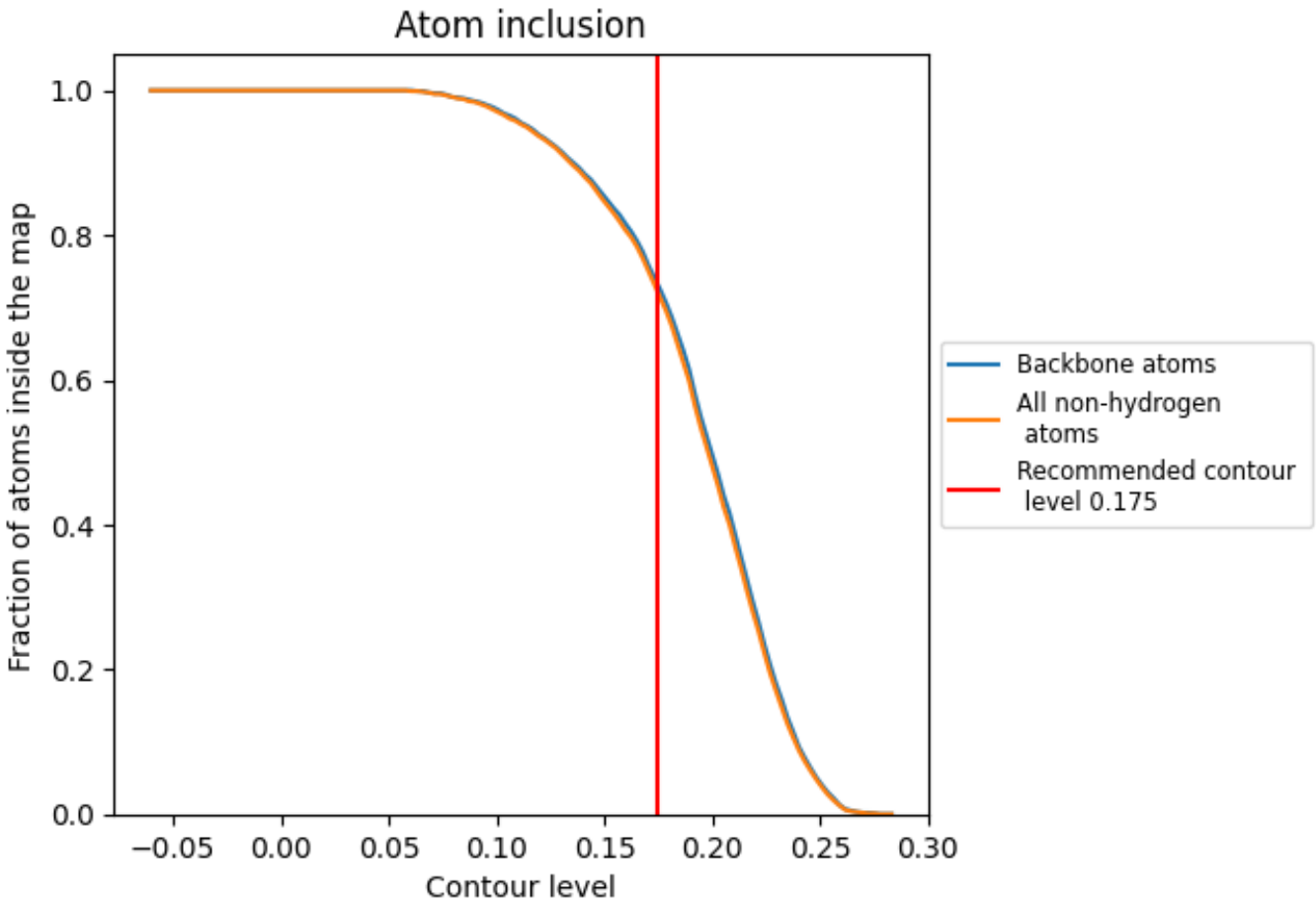
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.175).

9.4 Atom inclusion (i)



At the recommended contour level, 73% 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 (0.175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7200	0.1760
A	0.2270	0.0810
AA	0.7330	0.1670
AB	0.4850	0.1760
AC	0.9470	0.2060
AD	0.7320	0.1650
AE	0.4820	0.1750
AF	0.9520	0.2090
AG	0.7320	0.1680
B	0.7330	0.1680
BA	0.7280	0.1930
BB	0.9660	0.1860
BC	0.2270	0.0900
BD	0.7270	0.1930
BE	0.9660	0.1860
BF	0.2270	0.0780
BG	0.7280	0.1900
C	0.7270	0.1920
CA	0.4820	0.1730
CB	0.9500	0.2020
CC	0.7320	0.1650
CD	0.4870	0.1790
CE	0.9500	0.2090
CF	0.7310	0.1680
CG	0.4850	0.1770
D	0.4820	0.1740
DA	0.9660	0.1880
DB	0.2270	0.0840
DC	0.7280	0.1910
DD	0.9660	0.1810
DE	0.2270	0.0880
DF	0.7250	0.1920
DG	0.9660	0.1890
E	0.9660	0.1900
EA	0.9500	0.2040

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Chain	Atom inclusion	Q-score
EB	0.7310	0.1640
EC	0.4850	0.1740
ED	0.9500	0.2100
EE	0.7330	0.1650
EF	0.4820	0.1830
EG	0.9470	0.2030
F	0.2270	0.0820
FA	0.2270	0.0820
FB	0.7250	0.1940
FC	0.9660	0.1850
FD	0.2270	0.0930
FE	0.7260	0.1900
FF	0.9630	0.1860
FG	0.2270	0.0770
G	0.7330	0.1690
GA	0.7330	0.1660
GB	0.4820	0.1790
GC	0.9500	0.1990
GD	0.7320	0.1640
GE	0.4850	0.1810
GF	0.9450	0.2060
GG	0.7320	0.1670
H	0.9470	0.2040
HA	0.7260	0.1930
HB	0.9660	0.1850
HC	0.2270	0.0920
HD	0.7260	0.1910
HE	0.9660	0.1850
HF	0.2270	0.0760
HG	0.7300	0.1930
I	0.2270	0.0790
IA	0.4820	0.1800
IB	0.9500	0.1970
IC	0.7330	0.1640
ID	0.4850	0.1770
IE	0.9470	0.2090
IF	0.7330	0.1680
IG	0.4850	0.1780
J	0.7330	0.1670
JA	0.9660	0.1890
JB	0.2270	0.0830
JC	0.7300	0.1950

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Chain	Atom inclusion	Q-score
JD	0.9630	0.1860
JE	0.2270	0.0880
JF	0.7300	0.1910
JG	0.9630	0.1850
K	0.7260	0.1920
KA	0.9500	0.2050
KB	0.7330	0.1630
KC	0.4870	0.1750
KD	0.9550	0.2060
KE	0.7320	0.1650
KF	0.4850	0.1780
KG	0.9520	0.2100
L	0.4870	0.1820
LA	0.2220	0.0850
LB	0.7280	0.1940
LC	0.9660	0.1810
LD	0.2270	0.0870
LE	0.7260	0.1910
LF	0.9660	0.1870
LG	0.2270	0.0760
M	0.7280	0.1930
MA	0.7330	0.1650
MB	0.4850	0.1730
MC	0.9470	0.2080
MD	0.7330	0.1650
ME	0.4820	0.1830
MF	0.9470	0.2100
MG	0.7330	0.1680
N	0.4870	0.1790
NA	0.7250	0.1940
NB	0.9660	0.1840
NC	0.2270	0.0870
ND	0.7260	0.1920
NE	0.9660	0.1880
NF	0.2270	0.0790
NG	0.7280	0.1900
O	0.9660	0.1930
OA	0.4850	0.1770
OB	0.9520	0.2000
OC	0.7330	0.1640
OD	0.4870	0.1820
OE	0.9470	0.2080

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Chain	Atom inclusion	Q-score
OF	0.7330	0.1670
OG	0.4890	0.1800
P	0.9660	0.1860
PA	0.9630	0.1900
PB	0.2270	0.0900
PC	0.7280	0.1940
PD	0.9630	0.1870
PE	0.2270	0.0860
PF	0.7270	0.1890
PG	0.9660	0.1890
Q	0.9500	0.2070
QA	0.9520	0.2020
QB	0.7320	0.1620
QC	0.4850	0.1820
QD	0.9520	0.2090
QE	0.7310	0.1660
QF	0.4850	0.1790
QG	0.9500	0.2050
R	0.9470	0.2030
RA	0.2270	0.0830
RB	0.7280	0.1900
RC	0.9660	0.1840
RD	0.2270	0.0850
RE	0.7250	0.1900
RF	0.9660	0.1890
RG	0.2270	0.0760
S	0.2270	0.0770
SA	0.7320	0.1650
SB	0.4870	0.1760
SC	0.9500	0.2080
SD	0.7330	0.1650
SE	0.4870	0.1810
SF	0.9470	0.2060
SG	0.7320	0.1680
T	0.7330	0.1670
TA	0.7290	0.1920
TB	0.9630	0.1850
TC	0.2270	0.0880
TD	0.7260	0.1900
TE	0.9630	0.1860
TF	0.2270	0.0810
TG	0.7260	0.1910

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Chain	Atom inclusion	Q-score
UA	0.4850	0.1760
UB	0.9470	0.2020
UC	0.7310	0.1630
UD	0.4870	0.1790
UE	0.9520	0.2100
UF	0.7330	0.1680
UG	0.4850	0.1780
V	0.7260	0.1910
VA	0.9630	0.1870
VB	0.2270	0.0900
VC	0.7250	0.1930
VD	0.9630	0.1820
VE	0.2270	0.0810
VF	0.7280	0.1930
VG	0.9660	0.1870
W	0.4850	0.1780
WA	0.9470	0.2030
WB	0.7330	0.1650
WC	0.4870	0.1820
WD	0.9470	0.2060
WE	0.7330	0.1660
WF	0.4850	0.1770
WG	0.9470	0.2070
X	0.9660	0.1890
XA	0.2270	0.0840
XB	0.7300	0.1940
XC	0.9660	0.1850
XD	0.2270	0.0860
XE	0.7250	0.1910
XF	0.9630	0.1890
Y	0.9470	0.2000
YA	0.7330	0.1630
YB	0.4850	0.1750
YC	0.9520	0.2120
YD	0.7330	0.1650
YE	0.4850	0.1770
YF	0.9520	0.2100
Z	0.2270	0.0800
ZA	0.7280	0.1930
ZB	0.9660	0.1830
ZC	0.2270	0.0890
ZD	0.7280	0.1920

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Chain	Atom inclusion	Q-score
ZE	0.9630	0.1880
ZF	0.2270	0.0790