



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:23 PM UTC

PDB ID : 8VKQ / pdb_00008vkq
EMDB ID : EMD-43327
Title : CW Flagellar Switch Complex - FliF, FliG, FliM, and FliN forming the C-ring from Salmonella
Authors : Singh, P.K.; Iverson, T.M.
Deposited on : 2024-01-09
Resolution : 4.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

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

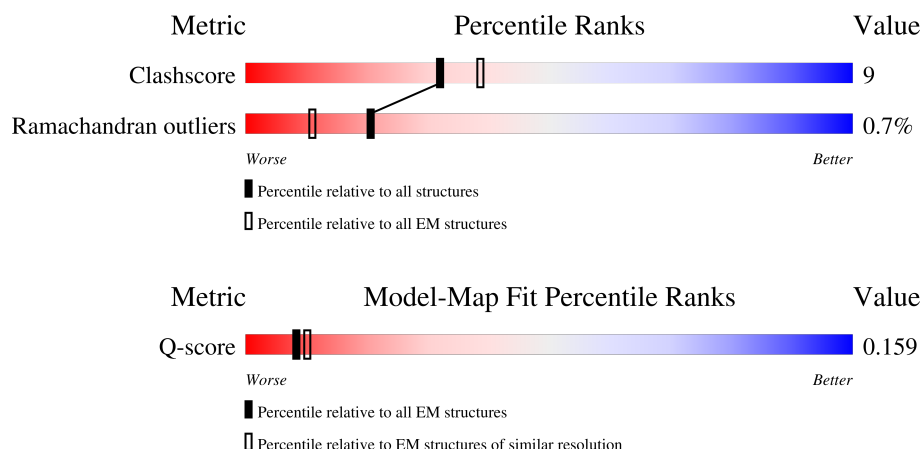
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	2407 (4.10 - 5.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	560	6% 8% 92%
1	BC	560	6% 8% 92%
1	BF	560	6% 8% 92%
1	DB	560	6% 8% 92%
1	DE	560	6% 8% 92%

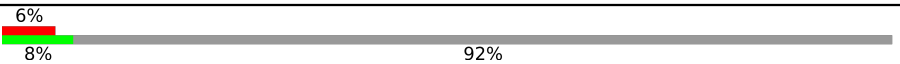
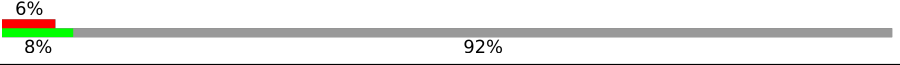
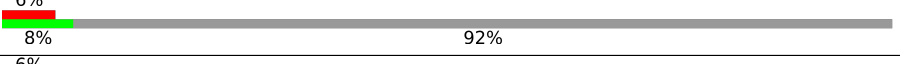
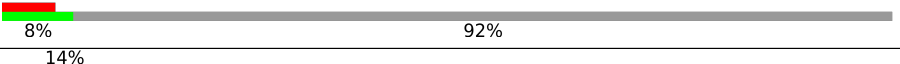
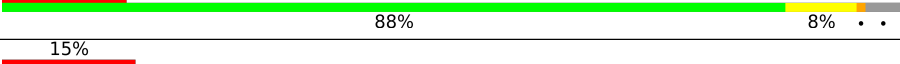
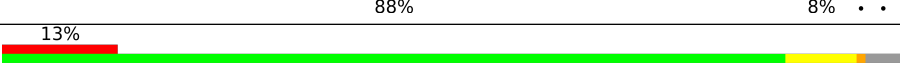
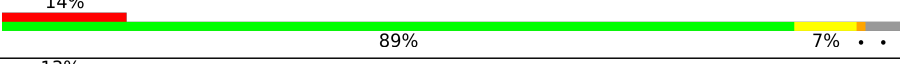
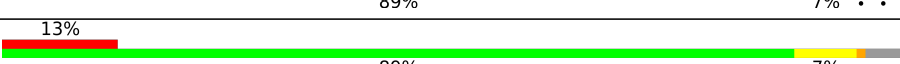
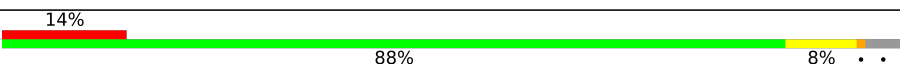
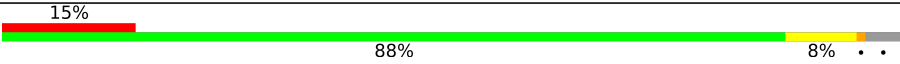
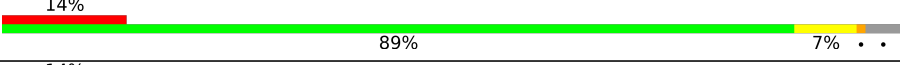
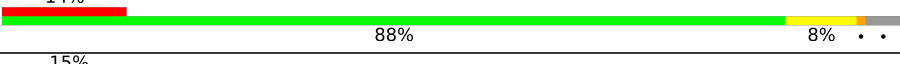
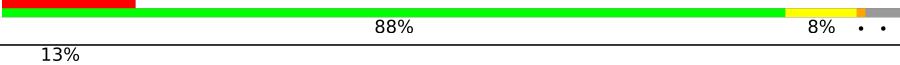
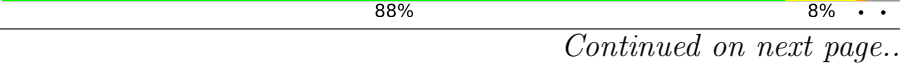
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Mol	Chain	Length	Quality of chain	
1	F	560		92%
1	FA	560		92%
1	FD	560		92%
1	FG	560		92%
1	HC	560		92%
1	HF	560		92%
1	I	560		92%
1	JB	560		92%
1	JE	560		92%
1	LA	560		92%
1	LD	560		92%
1	LG	560		92%
1	NC	560		92%
1	NF	560		92%
1	PB	560		92%
1	PE	560		92%
1	RA	560		92%
1	RD	560		92%
1	RG	560		92%
1	S	560		92%
1	TC	560		92%
1	TF	560		92%
1	VB	560		92%
1	VE	560		92%
1	XA	560		92%

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Mol	Chain	Length	Quality of chain
1	XD	560	
1	Z	560	
1	ZC	560	
1	ZF	560	
2	AA	331	
2	AD	331	
2	AG	331	
2	B	331	
2	CC	331	
2	CF	331	
2	EB	331	
2	EE	331	
2	G	331	
2	GA	331	
2	GD	331	
2	GG	331	
2	IC	331	
2	IF	331	
2	J	331	
2	KB	331	
2	KE	331	
2	MA	331	
2	MD	331	
2	MG	331	
2	OC	331	

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Mol	Chain	Length	Quality of chain
2	OF	331	
2	QB	331	
2	QE	331	
2	SA	331	
2	SD	331	
2	SG	331	
2	T	331	
2	UC	331	
2	UF	331	
2	WB	331	
2	WE	331	
2	YA	331	
2	YD	331	
3	BA	334	
3	BD	334	
3	BG	334	
3	C	334	
3	DC	334	
3	DF	334	
3	FB	334	
3	FE	334	
3	HA	334	
3	HD	334	
3	HG	334	
3	JC	334	

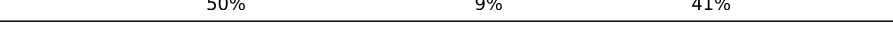
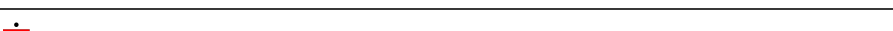
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Mol	Chain	Length	Quality of chain
3	JF	334	
3	K	334	
3	LB	334	
3	LE	334	
3	M	334	
3	NA	334	
3	ND	334	
3	NG	334	
3	PC	334	
3	PF	334	
3	RB	334	
3	RE	334	
3	TA	334	
3	TD	334	
3	TG	334	
3	V	334	
3	VC	334	
3	VF	334	
3	XB	334	
3	XE	334	
3	ZA	334	
3	ZD	334	
4	AB	137	
4	AC	137	
4	AE	137	

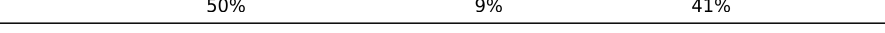
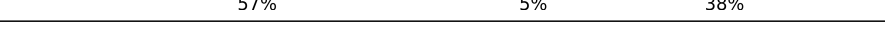
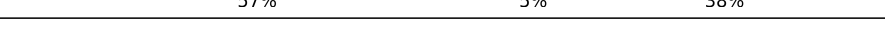
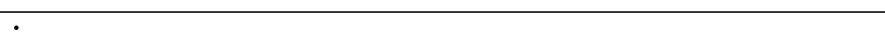
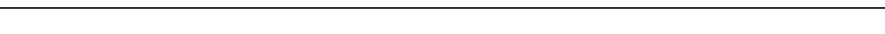
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Mol	Chain	Length	Quality of chain
4	AF	137	
4	BB	137	
4	BE	137	
4	CA	137	
4	CB	137	
4	CD	137	
4	CE	137	
4	CG	137	
4	D	137	
4	DA	137	
4	DD	137	
4	DG	137	
4	E	137	
4	EA	137	
4	EC	137	
4	ED	137	
4	EF	137	
4	EG	137	
4	FC	137	
4	FF	137	
4	GB	137	
4	GC	137	
4	GE	137	
4	GF	137	
4	H	137	

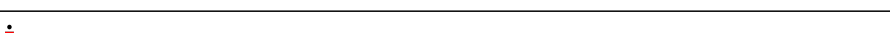
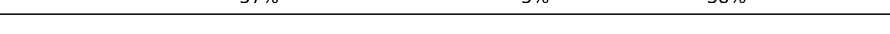
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Mol	Chain	Length	Quality of chain
4	HB	137	
4	HE	137	
4	IA	137	
4	IB	137	
4	ID	137	
4	IE	137	
4	IG	137	
4	JA	137	
4	JD	137	
4	JG	137	
4	KA	137	
4	KC	137	
4	KD	137	
4	KF	137	
4	KG	137	
4	L	137	
4	LC	137	
4	LF	137	
4	MB	137	
4	MC	137	
4	ME	137	
4	MF	137	
4	N	137	
4	NB	137	
4	NE	137	

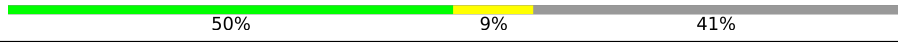
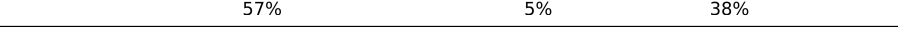
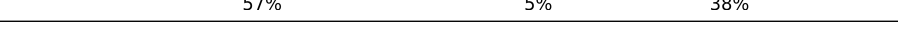
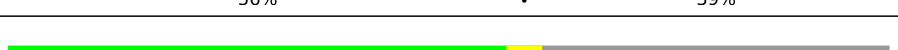
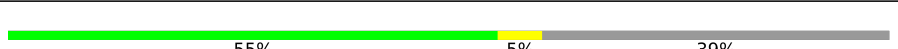
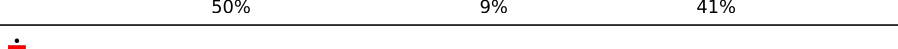
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Mol	Chain	Length	Quality of chain
4	O	137	
4	OA	137	
4	OB	137	
4	OD	137	
4	OE	137	
4	OG	137	
4	P	137	
4	PA	137	
4	PD	137	
4	PG	137	
4	Q	137	
4	QA	137	
4	QC	137	
4	QD	137	
4	QF	137	
4	QG	137	
4	R	137	
4	RC	137	
4	RF	137	
4	SB	137	
4	SC	137	
4	SE	137	
4	SF	137	
4	TB	137	
4	TE	137	

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Mol	Chain	Length	Quality of chain
4	UA	137	
4	UB	137	
4	UD	137	
4	UE	137	
4	UG	137	
4	VA	137	
4	VD	137	
4	VG	137	
4	W	137	
4	WA	137	
4	WC	137	
4	WD	137	
4	WF	137	
4	WG	137	
4	X	137	
4	XC	137	
4	XF	137	
4	Y	137	
4	YB	137	
4	YC	137	
4	YE	137	
4	YF	137	
4	ZB	137	
4	ZE	137	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 150620 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
1	F	47	Total	C	N	O	0	0
			235	140	47	48		
1	A	47	Total	C	N	O	0	0
			235	140	47	48		
1	I	47	Total	C	N	O	0	0
			235	140	47	48		
1	S	47	Total	C	N	O	0	0
			235	140	47	48		
1	Z	47	Total	C	N	O	0	0
			235	140	47	48		
1	FA	47	Total	C	N	O	0	0
			235	140	47	48		
1	LA	47	Total	C	N	O	0	0
			235	140	47	48		
1	RA	47	Total	C	N	O	0	0
			235	140	47	48		
1	XA	47	Total	C	N	O	0	0
			235	140	47	48		
1	DB	47	Total	C	N	O	0	0
			235	140	47	48		
1	JB	47	Total	C	N	O	0	0
			235	140	47	48		
1	PB	47	Total	C	N	O	0	0
			235	140	47	48		
1	VB	47	Total	C	N	O	0	0
			235	140	47	48		
1	BC	47	Total	C	N	O	0	0
			235	140	47	48		
1	HC	47	Total	C	N	O	0	0
			235	140	47	48		
1	NC	47	Total	C	N	O	0	0
			235	140	47	48		
1	TC	47	Total	C	N	O	0	0
			235	140	47	48		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	ZC	47	Total	C	N	O	0	0
			235	140	47	48		
1	FD	47	Total	C	N	O	0	0
			235	140	47	48		
1	LD	47	Total	C	N	O	0	0
			235	140	47	48		
1	RD	47	Total	C	N	O	0	0
			235	140	47	48		
1	XD	47	Total	C	N	O	0	0
			235	140	47	48		
1	DE	47	Total	C	N	O	0	0
			235	140	47	48		
1	JE	47	Total	C	N	O	0	0
			235	140	47	48		
1	PE	47	Total	C	N	O	0	0
			235	140	47	48		
1	VE	47	Total	C	N	O	0	0
			235	140	47	48		
1	BF	47	Total	C	N	O	0	0
			235	140	47	48		
1	HF	47	Total	C	N	O	0	0
			235	140	47	48		
1	NF	47	Total	C	N	O	0	0
			235	140	47	48		
1	TF	47	Total	C	N	O	0	0
			235	140	47	48		
1	ZF	47	Total	C	N	O	0	0
			235	140	47	48		
1	FG	47	Total	C	N	O	0	0
			235	140	47	48		
1	LG	47	Total	C	N	O	0	0
			235	140	47	48		
1	RG	47	Total	C	N	O	0	0
			235	140	47	48		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	319	Total	C	N	O	0	0
			1580	942	319	319		
2	B	319	Total	C	N	O	0	0
			1580	942	319	319		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	J	319	Total	C	N	O	0	0
			1580	942	319	319		
2	T	319	Total	C	N	O	0	0
			1580	942	319	319		
2	AA	319	Total	C	N	O	0	0
			1580	942	319	319		
2	GA	319	Total	C	N	O	0	0
			1580	942	319	319		
2	MA	319	Total	C	N	O	0	0
			1580	942	319	319		
2	SA	319	Total	C	N	O	0	0
			1580	942	319	319		
2	YA	319	Total	C	N	O	0	0
			1580	942	319	319		
2	EB	319	Total	C	N	O	0	0
			1580	942	319	319		
2	KB	319	Total	C	N	O	0	0
			1580	942	319	319		
2	QB	319	Total	C	N	O	0	0
			1580	942	319	319		
2	WB	319	Total	C	N	O	0	0
			1580	942	319	319		
2	CC	319	Total	C	N	O	0	0
			1580	942	319	319		
2	IC	319	Total	C	N	O	0	0
			1580	942	319	319		
2	OC	319	Total	C	N	O	0	0
			1580	942	319	319		
2	UC	319	Total	C	N	O	0	0
			1580	942	319	319		
2	AD	319	Total	C	N	O	0	0
			1580	942	319	319		
2	GD	319	Total	C	N	O	0	0
			1580	942	319	319		
2	MD	319	Total	C	N	O	0	0
			1580	942	319	319		
2	SD	319	Total	C	N	O	0	0
			1580	942	319	319		
2	YD	319	Total	C	N	O	0	0
			1580	942	319	319		
2	EE	319	Total	C	N	O	0	0
			1580	942	319	319		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	KE	319	Total	C	N	O	0	0
			1580	942	319	319		
2	QE	319	Total	C	N	O	0	0
			1580	942	319	319		
2	WE	319	Total	C	N	O	0	0
			1580	942	319	319		
2	CF	319	Total	C	N	O	0	0
			1580	942	319	319		
2	IF	319	Total	C	N	O	0	0
			1580	942	319	319		
2	OF	319	Total	C	N	O	0	0
			1580	942	319	319		
2	UF	319	Total	C	N	O	0	0
			1580	942	319	319		
2	AG	319	Total	C	N	O	0	0
			1580	942	319	319		
2	GG	319	Total	C	N	O	0	0
			1580	942	319	319		
2	MG	319	Total	C	N	O	0	0
			1580	942	319	319		
2	SG	319	Total	C	N	O	0	0
			1580	942	319	319		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	M	281	Total	C	N	O	0	0
			1390	828	281	281		
3	C	281	Total	C	N	O	0	0
			1390	828	281	281		
3	K	281	Total	C	N	O	0	0
			1390	828	281	281		
3	V	281	Total	C	N	O	0	0
			1390	828	281	281		
3	BA	281	Total	C	N	O	0	0
			1390	828	281	281		
3	HA	281	Total	C	N	O	0	0
			1390	828	281	281		
3	NA	281	Total	C	N	O	0	0
			1390	828	281	281		
3	TA	281	Total	C	N	O	0	0
			1390	828	281	281		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	ZA	281	Total 1390	C 828	N 281	O 281	0	0
3	FB	281	Total 1390	C 828	N 281	O 281	0	0
3	LB	281	Total 1390	C 828	N 281	O 281	0	0
3	RB	281	Total 1390	C 828	N 281	O 281	0	0
3	XB	281	Total 1390	C 828	N 281	O 281	0	0
3	DC	281	Total 1390	C 828	N 281	O 281	0	0
3	JC	281	Total 1390	C 828	N 281	O 281	0	0
3	PC	281	Total 1390	C 828	N 281	O 281	0	0
3	VC	281	Total 1390	C 828	N 281	O 281	0	0
3	BD	281	Total 1390	C 828	N 281	O 281	0	0
3	HD	281	Total 1390	C 828	N 281	O 281	0	0
3	ND	281	Total 1390	C 828	N 281	O 281	0	0
3	TD	281	Total 1390	C 828	N 281	O 281	0	0
3	ZD	281	Total 1390	C 828	N 281	O 281	0	0
3	FE	281	Total 1390	C 828	N 281	O 281	0	0
3	LE	281	Total 1390	C 828	N 281	O 281	0	0
3	RE	281	Total 1390	C 828	N 281	O 281	0	0
3	XE	281	Total 1390	C 828	N 281	O 281	0	0
3	DF	281	Total 1390	C 828	N 281	O 281	0	0
3	JF	281	Total 1390	C 828	N 281	O 281	0	0
3	PF	281	Total 1390	C 828	N 281	O 281	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	VF	281	Total	C	N	O	0	0
			1390	828	281	281		
3	BG	281	Total	C	N	O	0	0
			1390	828	281	281		
3	HG	281	Total	C	N	O	0	0
			1390	828	281	281		
3	NG	281	Total	C	N	O	0	0
			1390	828	281	281		
3	TG	281	Total	C	N	O	0	0
			1390	828	281	281		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	N	85	Total	C	N	O	0	0
			418	248	85	85		
4	P	83	Total	C	N	O	0	0
			409	242	83	84		
4	Q	81	Total	C	N	O	0	0
			398	236	81	81		
4	D	85	Total	C	N	O	0	0
			418	248	85	85		
4	E	83	Total	C	N	O	0	0
			409	242	83	84		
4	H	81	Total	C	N	O	0	0
			398	236	81	81		
4	L	85	Total	C	N	O	0	0
			418	248	85	85		
4	O	83	Total	C	N	O	0	0
			409	242	83	84		
4	R	81	Total	C	N	O	0	0
			398	236	81	81		
4	W	85	Total	C	N	O	0	0
			418	248	85	85		
4	X	83	Total	C	N	O	0	0
			409	242	83	84		
4	Y	81	Total	C	N	O	0	0
			398	236	81	81		
4	CA	85	Total	C	N	O	0	0
			418	248	85	85		
4	DA	83	Total	C	N	O	0	0
			409	242	83	84		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	EA	81	Total	C	N	O	0	0
			398	236	81	81		
4	IA	85	Total	C	N	O	0	0
			418	248	85	85		
4	JA	83	Total	C	N	O	0	0
			409	242	83	84		
4	KA	81	Total	C	N	O	0	0
			398	236	81	81		
4	OA	85	Total	C	N	O	0	0
			418	248	85	85		
4	PA	83	Total	C	N	O	0	0
			409	242	83	84		
4	QA	81	Total	C	N	O	0	0
			398	236	81	81		
4	UA	85	Total	C	N	O	0	0
			418	248	85	85		
4	VA	83	Total	C	N	O	0	0
			409	242	83	84		
4	WA	81	Total	C	N	O	0	0
			398	236	81	81		
4	AB	85	Total	C	N	O	0	0
			418	248	85	85		
4	BB	83	Total	C	N	O	0	0
			409	242	83	84		
4	CB	81	Total	C	N	O	0	0
			398	236	81	81		
4	GB	85	Total	C	N	O	0	0
			418	248	85	85		
4	HB	83	Total	C	N	O	0	0
			409	242	83	84		
4	IB	81	Total	C	N	O	0	0
			398	236	81	81		
4	MB	85	Total	C	N	O	0	0
			418	248	85	85		
4	NB	83	Total	C	N	O	0	0
			409	242	83	84		
4	OB	81	Total	C	N	O	0	0
			398	236	81	81		
4	SB	85	Total	C	N	O	0	0
			418	248	85	85		
4	TB	83	Total	C	N	O	0	0
			409	242	83	84		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	UB	81	Total	C	N	O	0	0
			398	236	81	81		
4	YB	85	Total	C	N	O	0	0
			418	248	85	85		
4	ZB	83	Total	C	N	O	0	0
			409	242	83	84		
4	AC	81	Total	C	N	O	0	0
			398	236	81	81		
4	EC	85	Total	C	N	O	0	0
			418	248	85	85		
4	FC	83	Total	C	N	O	0	0
			409	242	83	84		
4	GC	81	Total	C	N	O	0	0
			398	236	81	81		
4	KC	85	Total	C	N	O	0	0
			418	248	85	85		
4	LC	83	Total	C	N	O	0	0
			409	242	83	84		
4	MC	81	Total	C	N	O	0	0
			398	236	81	81		
4	QC	85	Total	C	N	O	0	0
			418	248	85	85		
4	RC	83	Total	C	N	O	0	0
			409	242	83	84		
4	SC	81	Total	C	N	O	0	0
			398	236	81	81		
4	WC	85	Total	C	N	O	0	0
			418	248	85	85		
4	XC	83	Total	C	N	O	0	0
			409	242	83	84		
4	YC	81	Total	C	N	O	0	0
			398	236	81	81		
4	CD	85	Total	C	N	O	0	0
			418	248	85	85		
4	DD	83	Total	C	N	O	0	0
			409	242	83	84		
4	ED	81	Total	C	N	O	0	0
			398	236	81	81		
4	ID	85	Total	C	N	O	0	0
			418	248	85	85		
4	JD	83	Total	C	N	O	0	0
			409	242	83	84		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	KD	81	Total	C	N	O	0	0
			398	236	81	81		
4	OD	85	Total	C	N	O	0	0
			418	248	85	85		
4	PD	83	Total	C	N	O	0	0
			409	242	83	84		
4	QD	81	Total	C	N	O	0	0
			398	236	81	81		
4	UD	85	Total	C	N	O	0	0
			418	248	85	85		
4	VD	83	Total	C	N	O	0	0
			409	242	83	84		
4	WD	81	Total	C	N	O	0	0
			398	236	81	81		
4	AE	85	Total	C	N	O	0	0
			418	248	85	85		
4	BE	83	Total	C	N	O	0	0
			409	242	83	84		
4	CE	81	Total	C	N	O	0	0
			398	236	81	81		
4	GE	85	Total	C	N	O	0	0
			418	248	85	85		
4	HE	83	Total	C	N	O	0	0
			409	242	83	84		
4	IE	81	Total	C	N	O	0	0
			398	236	81	81		
4	ME	85	Total	C	N	O	0	0
			418	248	85	85		
4	NE	83	Total	C	N	O	0	0
			409	242	83	84		
4	OE	81	Total	C	N	O	0	0
			398	236	81	81		
4	SE	85	Total	C	N	O	0	0
			418	248	85	85		
4	TE	83	Total	C	N	O	0	0
			409	242	83	84		
4	UE	81	Total	C	N	O	0	0
			398	236	81	81		
4	YE	85	Total	C	N	O	0	0
			418	248	85	85		
4	ZE	83	Total	C	N	O	0	0
			409	242	83	84		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	AF	81	Total	C	N	O	0	0
			398	236	81	81		
4	EF	85	Total	C	N	O	0	0
			418	248	85	85		
4	FF	83	Total	C	N	O	0	0
			409	242	83	84		
4	GF	81	Total	C	N	O	0	0
			398	236	81	81		
4	KF	85	Total	C	N	O	0	0
			418	248	85	85		
4	LF	83	Total	C	N	O	0	0
			409	242	83	84		
4	MF	81	Total	C	N	O	0	0
			398	236	81	81		
4	QF	85	Total	C	N	O	0	0
			418	248	85	85		
4	RF	83	Total	C	N	O	0	0
			409	242	83	84		
4	SF	81	Total	C	N	O	0	0
			398	236	81	81		
4	WF	85	Total	C	N	O	0	0
			418	248	85	85		
4	XF	83	Total	C	N	O	0	0
			409	242	83	84		
4	YF	81	Total	C	N	O	0	0
			398	236	81	81		
4	CG	85	Total	C	N	O	0	0
			418	248	85	85		
4	DG	83	Total	C	N	O	0	0
			409	242	83	84		
4	EG	81	Total	C	N	O	0	0
			398	236	81	81		
4	IG	85	Total	C	N	O	0	0
			418	248	85	85		
4	JG	83	Total	C	N	O	0	0
			409	242	83	84		
4	KG	81	Total	C	N	O	0	0
			398	236	81	81		
4	OG	85	Total	C	N	O	0	0
			418	248	85	85		
4	PG	83	Total	C	N	O	0	0
			409	242	83	84		

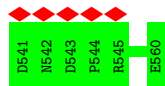
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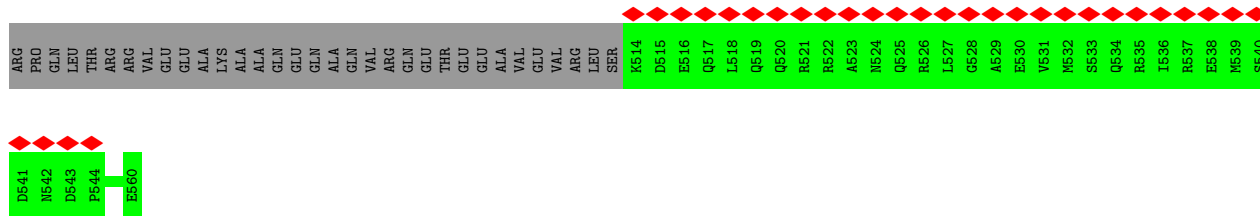
Mol	Chain	Residues	Atoms				AltConf	Trace
4	QG	81	Total	C	N	O	0	0
			398	236	81	81		
4	UG	85	Total	C	N	O	0	0
			418	248	85	85		
4	VG	83	Total	C	N	O	0	0
			409	242	83	84		
4	WG	81	Total	C	N	O	0	0
			398	236	81	81		

- Molecule 1: Flagellar M-ring protein

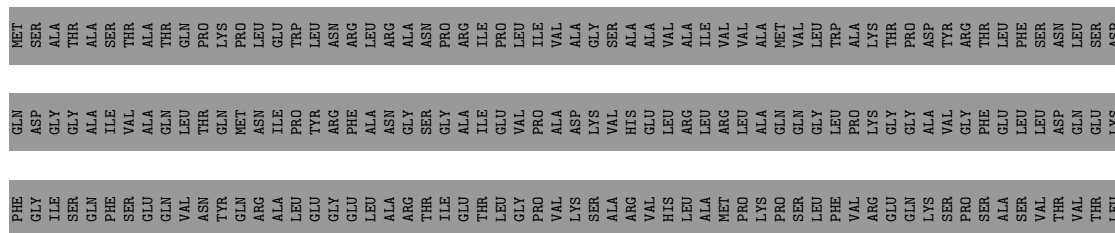
[illegible]



Chain S: 6% 8% 92%



Chain Z: 6% 8% 92%

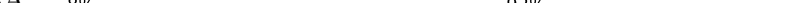


D541
N542
D543
P544

E560

Chain FA:

Diagram illustrating a group of nodes (D541, N542, D543, P544) connected to a single node (E560).

Chain LA: 

Chain RA:

D641	ARG	K5 14
N542	PRO	D5 15
D643	GLN	E5 16
P544	LEU	Q5 17
R545	THR	L5 18
V546	ARG	Q5 19
	VAL	Q5 20
	GLU	R5 21
	ALA	R5 22
	GLU	A5 23
	VAL	N5 24
	ARG	Q5 25
	LEU	R5 26
	SER	L5 27
		G5 28
		A5 29
		E5 30
		V5 31
		M5 32
		S5 33
		Q5 34
		R5 35
		T5 36
		R5 37
		E5 38
		M5 39
		S5 40

Chain XA:

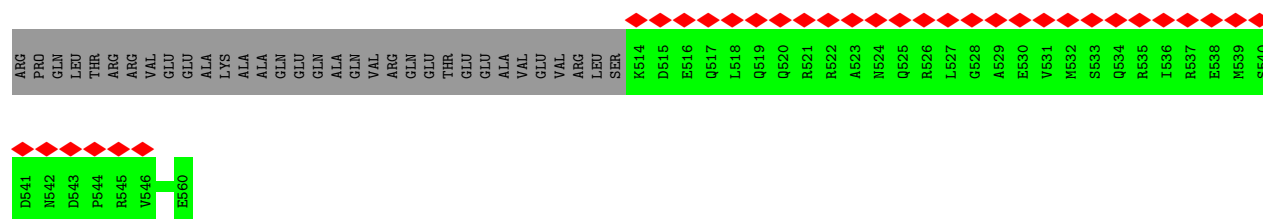
D641	ARG	GLY	ASN	SER	VAL	GLU	PHE	GLU	GLY	GLN	GLN	MET
N542	GLN	SER	GLU	GLU	GLU	GLU	GLY	GLU	ILE	ASP	ASP	SER
D643	LEU	ASP	THR	THR	VAL	GLN	GLY	ARG	GLN	GLY	GLY	THR
P644	THR	LYS	ASN	ASN	ILE	GLN	PHE	ALA	GLN	ALA	ALA	SER
R645	ARG	ARG	GLY	VAL	GLY	GLY	GLY	ALA	SER	VAL	VAL	THR
V646	VAL	ASP	THR	THR	ARG	THR	TYR	ARG	GLU	ALA	ALA	GLN
	GLU	LEU	GLU	ARG	ILE	GLY	VAL	GLN	VAL	GLN	THR	GLN
	ALA	ASN	THR	THR	ALA	GLY	GLY	ILE	ASN	ILE	PRO	LYS
	LYS	VAL	ILE	ARG	PRO	PRO	PRO	LEU	SER	GLN	GLN	PRO
	ALA	VAL	ARG	GLY	LEU	GLY	GLY	ALA	GLN	MET	LEU	LEU
	ALA	ASN	HIS	GLY	SER	VAL	ARG	VAL	ASN	ASN	GLY	GLY
	GLN	SER	THR	THR	ALA	ALA	ALA	VAL	ILE	ILE	GLY	GLY
	GLN	THR	THR	THR	ILE	VAL	THR	VAL	GLY	GLY	GLY	THR
	ARG	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	GLU	GLU	GLU	GLU	VAL	VAL	GLU	GLU	GLY	GLY	GLY	GLY
	VAL	PRO	PRO	ALA	ILE	ILE	ILE	GLY	GLY	GLY	GLY	GLY
	GLU	PHE	VAL	VAL	VAL	ALA	PRO	GLY	GLY	GLY	GLY	GLY
	VAL	TRP	VAL	VAL	LEU	LEU	VAL	VAL	VAL	ALA	ALA	VAL
	ARG	GLN	GLN	VAL	PRO	PRO	THR	ASP	LYS	ASP	ASP	VAL
	LEU	GLN	ASN	ASN	THR	THR	THR	PHE	THR	LYS	LYS	GLY
	SER	GLN	THR	THR	ALA	ALA	ALA	ALA	ALA	VAL	VAL	GLY
	K514	PHE	THR	LYS	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
	D615	ILE	LEU	GLN	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY
	E516	ASP	ALA	ALA	ASN	ASN	GLU	SER	HIS	ARG	ARG	ALA
	Q617	GLN	GLN	GLY	GLN	GLN	THR	HIS	THR	VAL	LEU	ALA
	L518	LEU	LEU	ASP	GLY	GLU	GLU	GLU	MET	ARG	ARG	ILE
	Q619	ALA	LEU	LYS	ASN	ASN	GLU	LEU	PRO	LEU	VAL	VAL
	Q620	ALA	ALA	PRO	THR	THR	HIS	THR	LYS	ALA	ALA	VAL
	R621	GLY	LEU	LEU	PRO	TYR	TYR	GLN	PRO	GLN	MET	MET
	R522	ARG	GLY	PRO	GLN	SER	SER	SER	SER	GLN	VAL	VAL
	A623	TRP	THR	THR	THR	THR	PHE	THR	PHE	LEU	LEU	TRP
	N524	LEU	ALA	ALA	THR	THR	ARG	GLY	ARG	LYS	LYS	LYS
	Q625	LEU	GLN	THR	THR	THR	ALA	GLU	GLU	GLY	GLY	THR
	R526	VAL	MET	ASN	ASN	SER	SER	ASP	GLU	GLY	GLY	PRO
	L527	VAL	LYS	SER	ASN	SER	LYS	LEU	VAL	ASP	ASP	ALA
	G528	ALA	ILE	SER	ASN	ALA	THR	THR	GLY	VAL	VAL	ALA
	A529	TRP	GLU	ALA	ALA	LEU	SER	ALA	GLY	GLY	PHE	THR
	E530	ILE	ASP	GLY	ARG	ARG	ALA	ALA	ALA	GLU	GLU	LEU
	V531	LEU	LEU	PRO	PRO	SER	SER	SER	SER	LEU	LEU	PHE
	M532	TRP	THR	THR	ARG	ARG	VAL	VAL	VAL	ASP	LEU	ASN
	S533	ARG	GLU	GLU	SER	GLN	THR	VAL	VAL	GLN	GLN	LEU
	G534	LYS	VAL	THR	THR	LEU	ALA	VAL	VAL	ASP	GLY	ASN
		ALA	MET	ARG	GLN	THR	THR	ILE	THR	LYS	THR	SER

Chain DB: 6% 8% 92%

MET	SER	ALA	ALA	THR	THR	SER	THR	ALA	GLN	PRO	LYS	LEU	GLY	TRP	ASN	ARG	LEU	ARG	ALA	ASN	PRO	ARG	ILE	LEU	ILE	VAL	ALA	GLY	SER	ALA	ALA	VAL	ALA	ALA	ILE	VAL	VAL	VAL	MET	VAL	VAL	LEU	TRP	TYR	ARG	THR	LEU	PHE	SER	ASN	LEU	SER	SER
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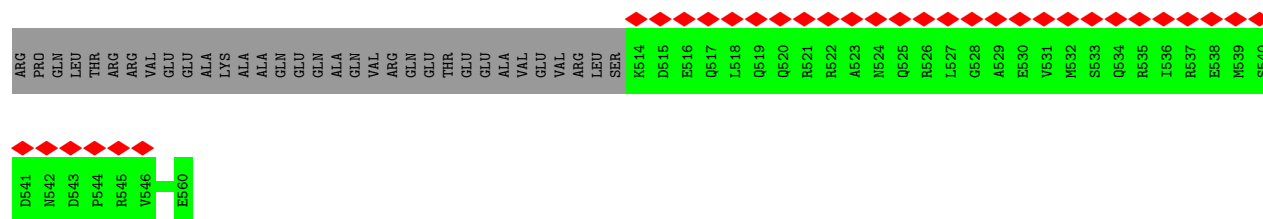
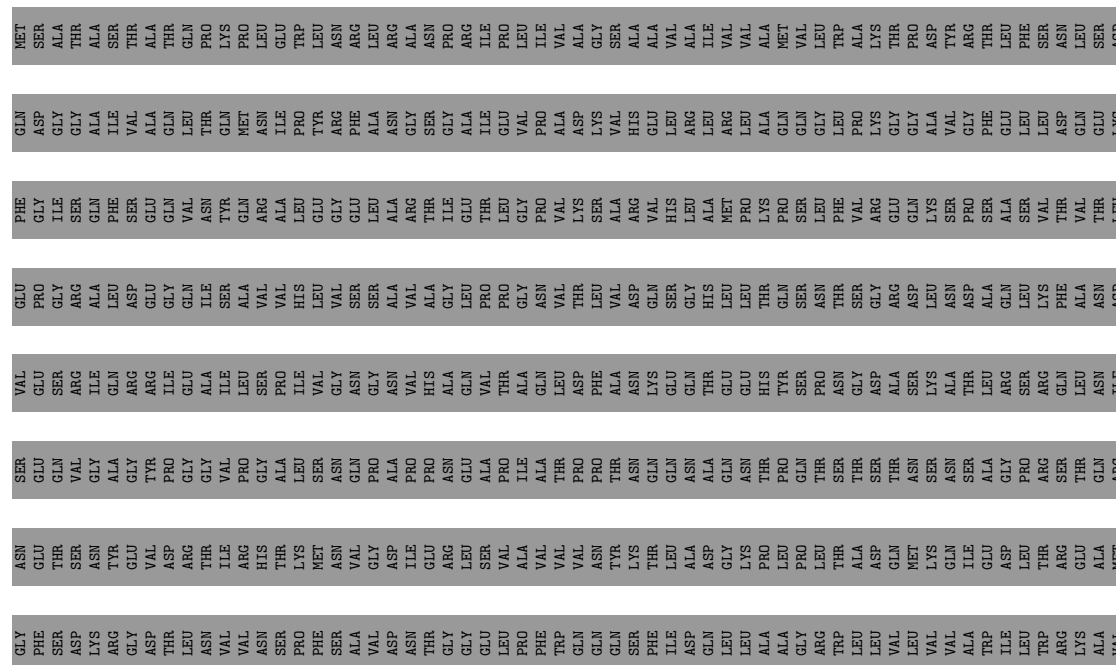
- Molecule 1: Flagellar M-ring protein

[illegible]



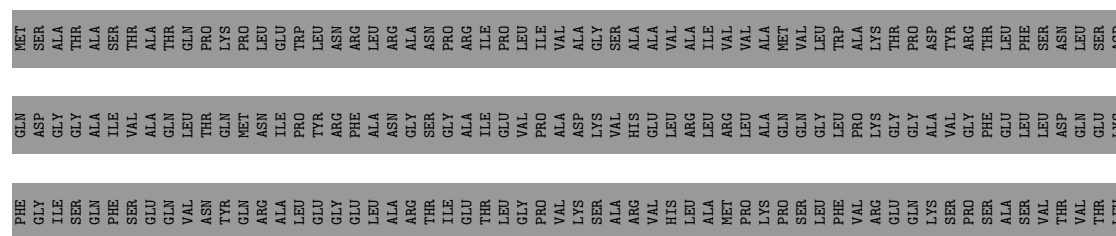
• Molecule 1: Flagellar M-ring protein

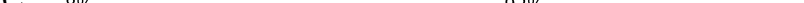
Chain PB: 6% 8% 92%

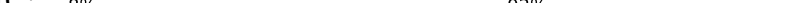


• Molecule 1: Flagellar M-ring protein

Chain VB: 6% 8% 92%



Chain HC: 

Chain NC: 



D641	D642	D643	P644	R645	V646	E660	ARG	PRO	GLN	LEU	THR	ARG	ARG	VAL	GLU	GLU	ALA	LYS	ALA	ALA	GLN	GLN	GLN	ALA	GLN	VAL	ARG	GLN	GLU	THR	GLU	GLU	ALA	VAL	GLU	VAL	ARG	ARG	LEU	SER	K514	D615	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
------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

Chain TC:

D641	ARG	GLY	ASN	SER	VAL	GLU	PRO	PHE	GLU	PHE	GLN	MET
N542	PRO	SER	GLU	GLU	GLY	GLU	GLY	GLY	GLU	GLY	ASP	SER
D643	GLN	THR	THR	THR	VAL	GLN	GLN	ILE	GLN	ILE	GLY	ALA
P544	THR	LYS	ASN	ASN	GLY	TYR	ALA	ALA	GLN	GLN	ALA	SER
R645	ARG	ARG	GLY	GLU	GLY	VAL	TYR	GLY	ASP	SER	VAL	THR
V546	VAL	ASP	THR	THR	ASP	TYR	ALA	GLY	GLU	GLU	ALA	ALA
E560	GLU	LEU	ARG	GLY	GLY	GLY	GLY	GLY	GLN	VAL	LEU	GLN
	ALA	ALA	ASN	THR	VAL	GLY	VAL	ILE	ILE	SER	THR	LYS
	LYS	VAL	ARG	ARG	PRO	PRO	PRO	GLY	LEU	GLN	MET	PRO
	ALA	VAL	ASN	HIS	GLY	GLY	SER	GLY	VAL	ARG	ASN	LEU
	GLN	SER	THR	THR	ALA	ALA	ALA	ILE	PRO	ILE	PRO	TRP
	GLU	LEU	LYS	MET	ILE	VAL	VAL	GLY	HIS	GLY	PRO	GLY
	ALA	PRO	ASN	ASN	GLY	VAL	ASN	GLY	GLY	ARG	ASN	ASN
	GLN	VAL	VAL	GLN	ASN	SER	GLN	GLY	GLY	PHE	LEU	ARG
	VAL	ALA	GLY	PRO	GLY	SER	SER	GLY	LEU	ALA	ALA	ARG
	ARG	ASP	ASN	ILE	ALA	PRO	PRO	ARG	ALA	ARG	GLY	ALA
	GLN	ASN	ILE	GLU	THR	PRO	PRO	THR	ALA	THR	SER	ASN
	GLU	THR	GLY	GLY	THR	ASN	ALA	ILE	HIS	ILE	PRO	ASN
	THR	GLY	ARG	ASN	ALA	GLU	ALA	GLY	GLY	ILE	PRO	PRO
	GLU	GLY	LEU	LEU	GLN	THR	THR	LEU	VAL	VAL	ALA	VAL
	GLU	GLU	SER	VAL	VAL	ALA	ALA	PRO	ASN	PRO	PRO	ILE
	ALA	LEU	VAL	VAL	GLN	THR	LEU	GLY	VAL	ALA	ALA	VAL
	VAL	THR	VAL	VAL	LEU	THR	THR	SER	GLY	GLY	ALA	VAL
	ARG	GLN	VAL	VAL	ASP	PRO	ASP	LYS	THR	LYS	ASP	ALA
	LEU	GLN	ASN	ASN	THR	PRO	THR	THR	VAL	GLN	GLN	MET
	SER	GLN	THR	THR	GLY	GLN	GLN	GLY	GLY	PRO	GLN	VAL
		R514	PHE	THR	GLN	ASN	ASN	GLY	GLY	SER	GLN	MET
		D515	ILE	LEU	GLN	ASN	ASN	GLY	GLY	THR	GLN	VAL
		E516	ASP	ALA	ASN	GLY	GLY	THR	GLY	LEU	GLY	VAL
		Q517	GLN	ASP	ALA	GLN	ALA	THR	HIS	ALA	LEU	ALA
		L518	LEU	GLY	GLN	GLN	GLY	GLY	LEU	MET	ARG	ILE
		O519	LEU	LYS	ASN	ASN	ASN	GLY	LEU	PRO	LEU	ALA
		Q520	ALA	PRO	THR	THR	THR	HIS	THR	LYS	ALA	VAL
		R521	GLY	LEU	PRO	PRO	TYR	TYR	GLN	PRO	ALA	MET
		R522	ARG	PRO	GLN	GLN	SER	SER	SER	SER	GLN	VAL
		A523	TRP	THR	LEU	THR	ASN	THR	THR	PHE	LEU	LEU
		N524	LEU	ALA	GLN	THR	SER	ASP	GLY	ARG	LYS	THR
		Q525	VAL	MET	ASN	THR	ASN	ALA	ALA	GLY	GLY	PRO
		R526	VAL	LYS	SER	SER	SER	SER	ASP	GLY	GLY	THR
		L527	VAL	GLN	ASN	ASN	ASN	LYS	LEU	VAL	ALA	TYR
		Q528	ALA	ILE	GLY	SER	SER	THR	THR	GLY	PHE	THR
		A529	TRP	ASP	ALA	ALA	ALA	ARG	ALA	ALA	GLY	LEU
		E530	ILE	THR	GLY	GLY	PRO	SER	GLN	GLY	LEU	PHE
		V531	LEU	LEU	THR	PRO	ARG	THR	SER	VAL	LEU	ASN
		H532	TRP	THR	THR	THR	ARG	THR	THR	THR	ASP	ASN
		H533	ARG	GLU	GLU	GLY	SER	GLN	PHE	VAL	GLN	LEU
		S534	LYS	THR	THR	THR	THR	VAL	ALA	VAL	GLY	ASN
		S535	VAL	MET	ALA	GLN	ARG	THR	ASN	THR	LYS	SER

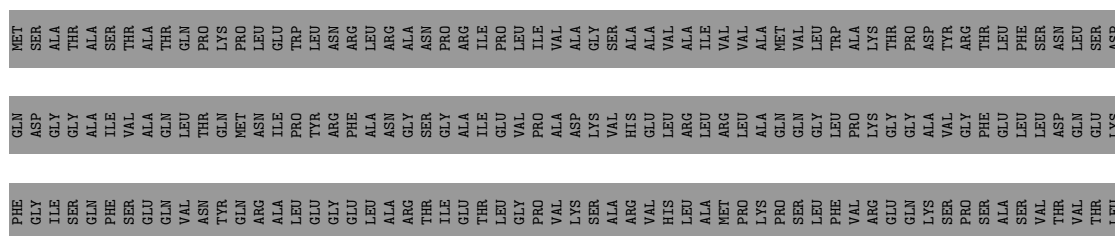
Chain ZC: 6% 8% 92%

[illegible]

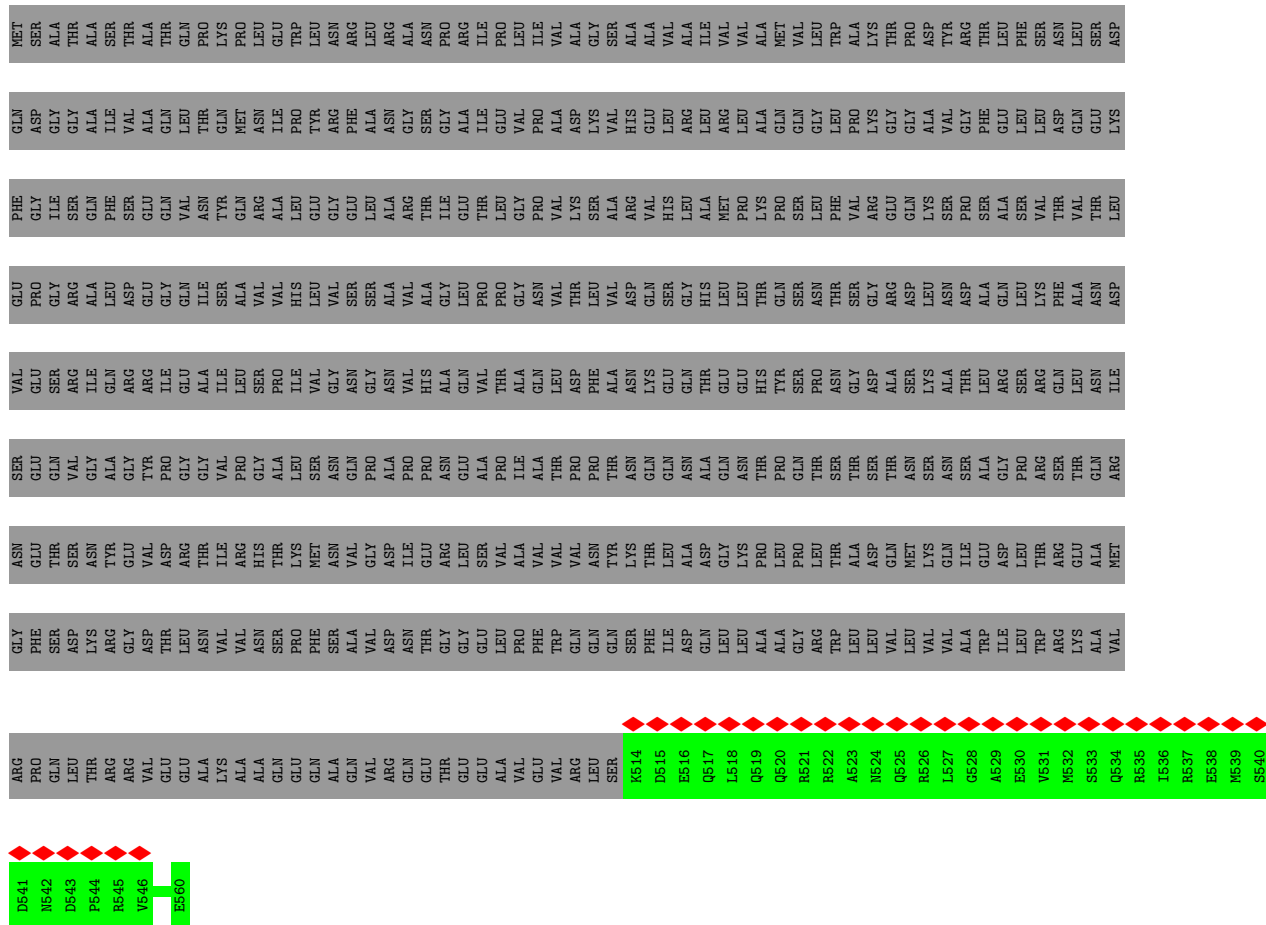
Diagram illustrating a sequence of nodes: D541, N542, D543, P544, R545, V546, and E560. The nodes D541 through V546 are grouped together in a green box, and E560 is shown separately in another green box. Red diamonds are positioned above the first five nodes (D541, N542, D543, P544, R545).

Chain FD:

[illegible]



Chain DE:



Chain JE:



D641	N642	D643	P644	R645	V646	E660	ARG	PRO	GLN	LEU	THR	ARG	ARG	VAL	GLU	GLU	ALA	LYS	ALA	ALA	GLN	GLN	GLN	ALA	GLN	VAL	ARG	GLN	GLU	THR	GLU	GLU	ALA	VAL	GLU	VAL	ARG	LEU	SER	R614	D615	E616	Q617	L618	Q619	Q620	R621	R622	A623	N624	Q625	R626	L627	Q628	A629	E630	V631	N632	S633	Q634	R635	L636	R637	E638	N639	S640
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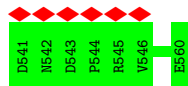
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N542	PRO	PHE	GLU	ASN	GLN	GLU	THR	GLN	GLY	GLY	GLY	ASP	SER	GLN
D643	LEU	ASP	SER	THR	VAL	THR	ASN	ARG	ILE	GLY	ARG	GLY	THR	ALA
F644	THR	LYS	ASN	ASN	GLY	ASN	TYR	GLY	ALA	LEU	ALA	ILE	SER	SER
R645	ARG	ARG	GLY	GLU	ALA	GLY	THR	PRO	PHE	ASP	SER	VAL	THR	ALA
V546	VAL	THR	VAL	VAL	TYR	ASP	GLY	ILE	GLY	GLU	GLU	ALA	ALA	ALA
E560	GLU	GLU	ARG	THR	GLY	GLY	THR	GLN	VAL	GLN	GLN	LEU	THR	THR
	ALA	ASN	THR	THR	GLY	THR	ILE	ALA	ASN	ILE	ILE	LEU	PRO	PRO
	LYS	VAL	ILE	ILE	VAL	PRO	VAL	TYR	SER	SER	SER	GLN	LYS	LYS
	ALA	VAL	VAL	ARG	PRO	PRO	LEU	GLN	ALA	ALA	ALA	MET	LEU	PRO
	ALA	ASN	HIS	HIS	GLY	ALA	SER	VAL	ARG	ASN	ILE	ASN	LEU	LEU
	GLN	SER	THR	THR	ALA	ASP	VAL	PRO	ALA	ASN	ALA	ASN	ARG	ARG
	GLU	PRO	LYS	LYS	ILE	ASP	ILE	HIS	THR	VAL	VAL	GLY	LEU	ASN
	THR	PHE	MET	MET	SER	SER	GLY	VAL	GLY	LEU	GLY	THR	TYR	LEU
	ALA	SER	ASN	ASN	ASN	ASN	ASN	ASN	THR	VAL	ASN	ARG	ASN	ASN
	GLN	VAL	VAL	VAL	GLN	GLN	GLN	GLN	GLU	GLU	SER	PHE	LEU	ARG
D643	VAL	ALA	VAL	GLY	GLY	GLU	THR	PRO	GLY	GLY	LEU	ALA	LEU	LEU
R645	ARG	ASP	ASP	ASP	ALA	ASP	ALA	ALA	ASN	ALA	ALA	ASN	ARG	ARG
D643	GLN	ASN	ILE	ILE	PRO	THR	PRO	VAL	VAL	VAL	VAL	GLY	ALA	ALA
V546	GLU	THR	GLU	GLU	THR	GLY	GLY	ALA	THR	VAL	VAL	GLY	GLY	GLN
E560	THR	GLY	ARG	ARG	GLU	THR	ILE	HIS	ILE	VAL	VAL	LYS	THR	THR
	GLU	GLY	LEU	LEU	VAL	VAL	ALA	GLN	GLY	VAL	THR	GLY	GLY	GLY
	ALA	PRO	ALA	ALA	ILE	ALA	ALA	GLN	GLY	ASN	PRO	ALA	ALA	ALA
	VAL	TRP	VAL	VAL	VAL	THR	THR	LEU	PRO	VAL	VAL	ALA	VAL	VAL
	ARG	GLN	GLN	VAL	ASN	ASN	PRO	ASN	THR	THR	VAL	ARG	ALA	ALA
	LEU	GLN	GLN	ASN	TYR	ASN	THR	ALA	ASP	VAL	VAL	ALA	ALA	ALA
	SER	SER	SER	LYS	LYS	THR	PHE	GLN	VAL	GLN	HIS	GLY	VAL	VAL
	D615	PHE	ILE	LEU	LEU	THR	THR	GLN	VAL	SER	SER	LEU	VAL	VAL
	E516	ASP	GLN	ASP	ALA	ALA	ASP	ALA	THR	VAL	GLY	ARG	ALA	ALA
	Q517	LEU	LEU	GLY	GLY	GLN	GLU	THR	MET	ARG	LEU	LEU	ILE	ILE
L518	LEU	LEU	LYS	ASN	ASN	GLU	PRO	PRO	LYS	LEU	VAL	ALA	ALA	
Q519	ALA	ALA	PRO	PRO	THR	THR	THR	THR	THR	THR	LYS	ALA	ALA	
Q520	ALA	ALA	LEU	LEU	PRO	PRO	TYR	GLN	PRO	GLN	GLN	MET	MET	
R521	GLY	GLY	PRO	PRO	GLN	GLN	SER	SER	SER	SER	GLN	VAL	VAL	
A522	ARG	ARG	LEU	LEU	THR	THR	THR	ASN	LEU	GLY	GLY	LEU	TRP	
A523	TRP	LEU	THR	ALA	SER	THR	THR	GLY	PHE	PRO	PRO	ALA	ALA	
N524	LEU	LEU	ASP	ASN	THR	THR	THR	ASP	ARG	GLY	LYS	LYS	THR	
Q525	VAL	VAL	GLN	GLN	THR	THR	THR	ALA	ARG	GLN	GLY	GLY	THR	
R526	LEU	LEU	MET	MET	ASN	SER	SER	SER	GLN	ASN	GLY	GLY	PRO	
L527	VAL	VAL	GLN	GLN	LYS	SER	LYS	LYS	VAL	LEU	ALA	ASP	TYR	
G528	ALA	ALA	ILE	ILE	ASN	SER	SER	THR	GLY	ASP	GLY	ARG	ARG	
A529	TRP	TRP	GLU	GLU	ALA	ALA	ALA	LEU	SER	ALA	PHE	THR	THR	
E530	ILE	ILE	ASP	ASP	GLY	GLY	GLY	ARG	ALA	GLN	GLU	GLU	LEU	
V531	LEU	LEU	THR	THR	LEU	LEU	THR	SER	SER	LEU	LEU	LEU	PHE	
M532	TRP	TRP	THR	THR	ARG	ARG	ARG	GLN	VAL	VAL	VAL	ASP	SER	
M532	ARG	ARG	GLU	GLU	THR	THR	THR	GLN	VAL	VAL	VAL	ASP	ASN	
S533	LYS	LYS	GLU	GLU	THR	THR	THR	ALA	VAL	VAL	VAL	GLN	LEU	
G534	ALA	ALA	MET	MET	ALA	ALA	THR	GLN	THR	ASN	THR	GLN	SER	
G534	VAL	VAL	THR	THR	ARG	ARG	THR	ASN	ILE	ASN	THR	LYS	ARG	ARG



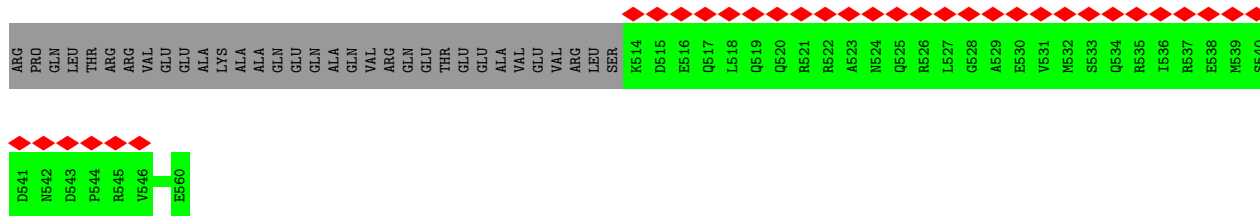
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- Molecule 1: Flagellar M-ring protein

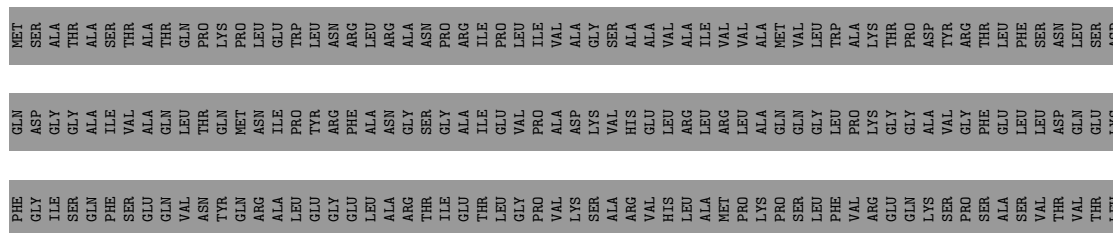
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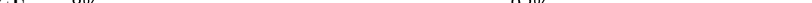


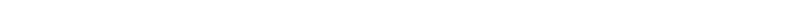
Chain HF:



Chain NF: 6% 8% 92%



Chain ZF: 

Chain FG: 

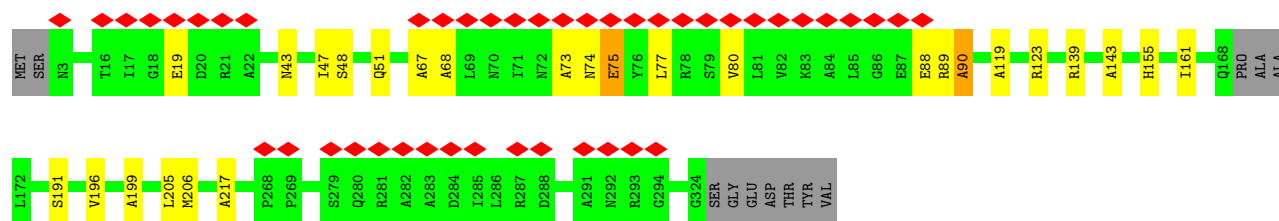
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D643	GLN	E5 16
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R545	THR	L5 18
V546	ARG	Q5 19
	VAL	Q5 20
	GLU	R5 21
	ALA	R5 22
	GLU	A5 23
	VAL	N5 24
	ARG	Q5 25
	LEU	R5 26
	SER	L5 27
		G5 28
		A5 29
		E5 30
		V5 31
		M5 32
		S5 33
		Q5 34
		R5 35
		T5 36
		R5 37
		E5 38
		M5 39
		S5 40

Chain LG:

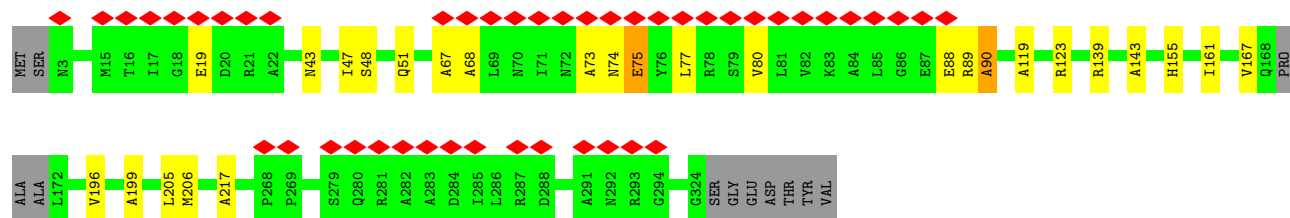
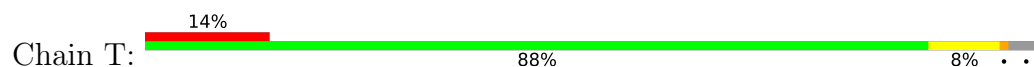
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D643	LEU	ASP	ASN	VAL	GLY	ARG	GLN	ALA	ALA	ALA	THR
P644	THR	LYS	ASN	THR	ALA	GLY	PHE	LEU	ILE	ILE	SER
R645	ARG	ARG	GLY	GLU	GLY	ARG	SER	ASP	VAL	VAL	THR
V646	VAL	ASP	THR	TYR	THR	ARG	GLU	GLU	GLN	ALA	ALA
E560	GLU	THR	THR	GLY	GLY	VAL	ASN	VAL	THR	GLN	LYS
	GLU	ALA	THR	VAL	GLY	ILE	SER	SER	GLN	GLN	PRO
D642	GLN	VAL	ASN	PRO	GLY	LEU	GLN	LEU	MET	LEU	LEU
D643	ARG	ASP	THR	GLY	PRO	SER	ARG	LEU	ASN	GLY	GLY
P644	GLN	ASN	ILE	PRO	VAL	ALA	ALA	ALA	ILE	PRO	TRP
R645	GLU	THR	GLU	PRO	VAL	HIS	THR	GLY	SER	TYR	ASN
V646	THR	GLY	ARG	ASN	GLY	GLN	ILE	GLY	GLY	PRO	ASN
E560	GLU	GLY	LEU	GLU	VAL	VAL	GLU	VAL	ALA	ALA	VAL
	GLU	GLU	SER	ALA	SER	THR	THR	PRO	GLY	GLU	LEU
D642	VAL	PHE	VAL	ALA	GLN	LEU	VAL	VAL	ALA	ALA	VAL
D643	ARG	GLN	VAL	PRO	ASP	PHE	LYS	THR	VAL	VAL	ALA
P644	LEU	THR	THR	THR	GLN	GLY	VAL	ARG	HIS	HIS	ALA
R645	GLU	PHE	THR	GLN	LYS	SER	VAL	ASN	GLY	GLY	ALA
V646	VAL	ILE	LEU	LEU	GLN	SER	HIS	SER	LEU	LEU	VAL
E560	ARG	GLN	GLN	PRO	THR	THR	GLY	ASP	GLY	GLN	MET
	LEU	GLN	ASN	THR	ALA	VAL	LYS	THR	GLY	GLN	VAL
K514	SER	GLN	THR	THR	GLN	GLY	VAL	ASN	ARG	ALA	ALA
	D615	PHE	THR	THR	GLN	GLY	VAL	ASN	VAL	GLY	GLY
E516	ASP	ILE	ASP	ALA	GLN	SER	HIS	GLY	LEU	ALA	ALA
Q617	GLN	GLN	GLY	GLY	GLN	HIS	THR	ALA	MET	ARG	ILE
L518	LEU	LEU	ASP	GLY	GLU	GLU	VAL	PRO	ARG	VAL	VAL
Q619	ALA	ALA	PRO	PRO	ASN	LYS	THR	LYS	PRO	LEU	ALA
Q620	ALA	ALA	LEU	PRO	THR	HIS	THR	THR	ALA	ALA	VAL
R621	GLY	GLY	PRO	GLN	TYR	TYR	PRO	PRO	GLN	GLN	MET
R522	ARG	ARG	LEU	THR	THR	SER	SER	SER	GLN	GLY	VAL
A623	TRP	TRP	THR	SER	ASN	THR	PHE	THR	LEU	LEU	TRP
N524	LEU	LEU	ALA	THR	GLY	GLY	ARG	GLY	PRO	PRO	LYS
Q625	LEU	VAL	GLN	THR	ALA	THR	GLU	GLU	GLY	GLY	LYS
Q626	VAL	VAL	MET	ASN	ASN	SER	ASN	ASN	GLN	PRO	THR
L527	VAL	VAL	GLN	SER	LYS	LYS	VAL	VAL	ASP	ASP	ALA
G528	ALA	ALA	ILE	SER	ALA	THR	SER	GLY	VAL	GLY	ALA
A529	TRP	TRP	GLU	ALA	LEU	ALA	SER	ALA	PHE	PHE	THR
E530	ILE	ILE	ASP	GLY	ARG	ARG	ALA	ALA	GLU	GLU	LEU
V531	LEU	LEU	LEU	PRO	THR	SER	SER	VAL	LEU	LEU	PHE
M532	TRP	TRP	THR	ARG	ARG	GLN	VAL	THR	ASP	ASP	ASN
S633	ARG	LYS	GLU	THR	THR	GLN	VAL	ALA	GLN	GLN	LEU
G534	ALA	VAL	MET	GLN	ARG	ASN	THR	ASN	ASN	LYS	SER

Chain RG:

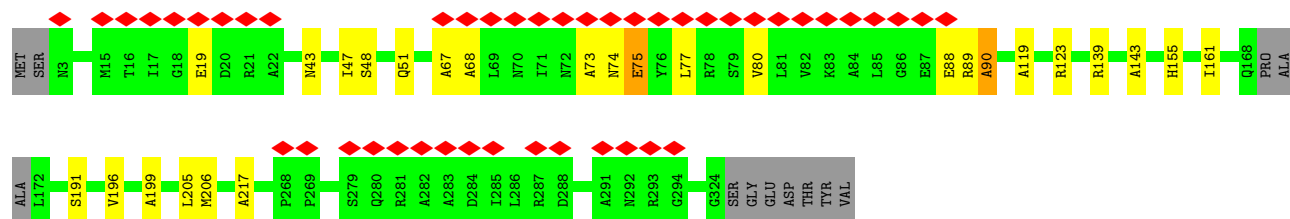
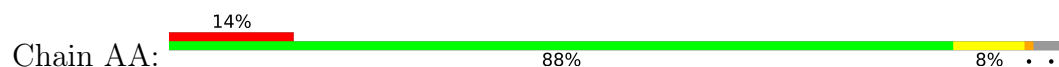
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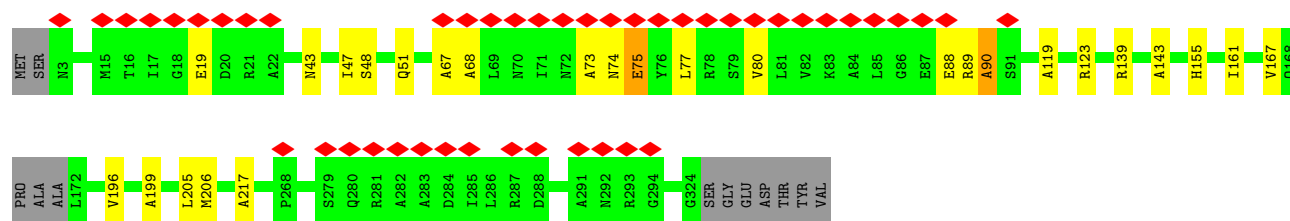
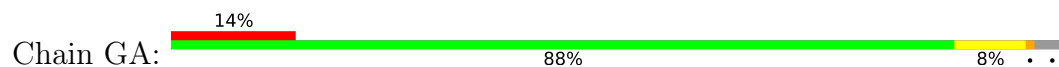
• Molecule 2: Flagellar motor switch protein FliG



• Molecule 2: Flagellar motor switch protein FliG



• Molecule 2: Flagellar motor switch protein FliG

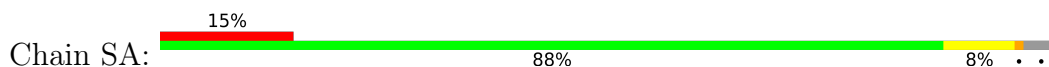


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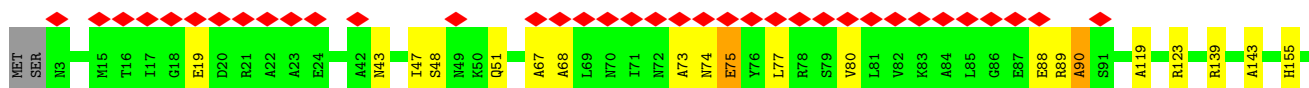
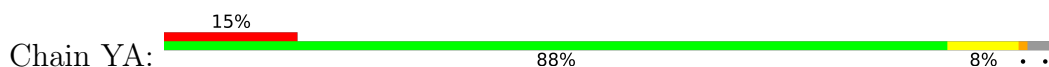




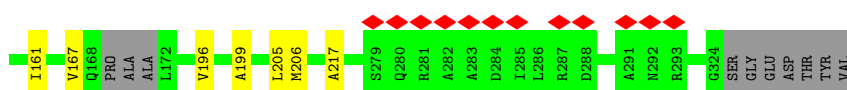
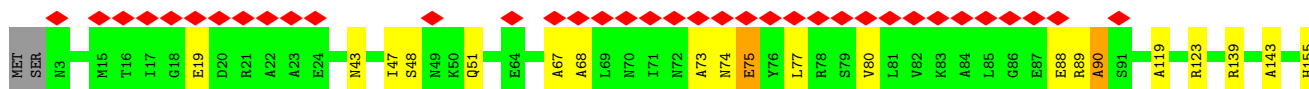
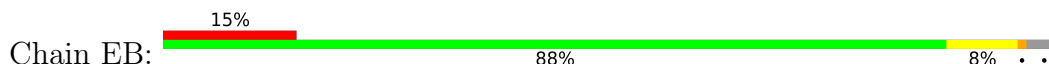
• Molecule 2: Flagellar motor switch protein Flig



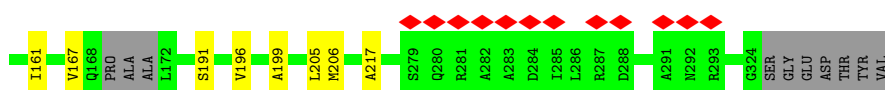
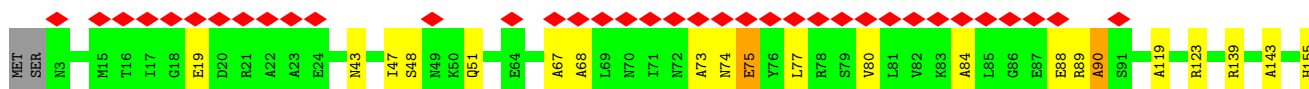
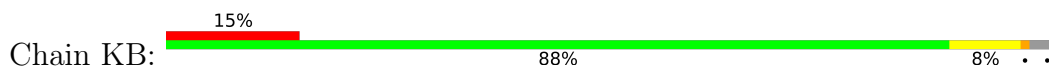
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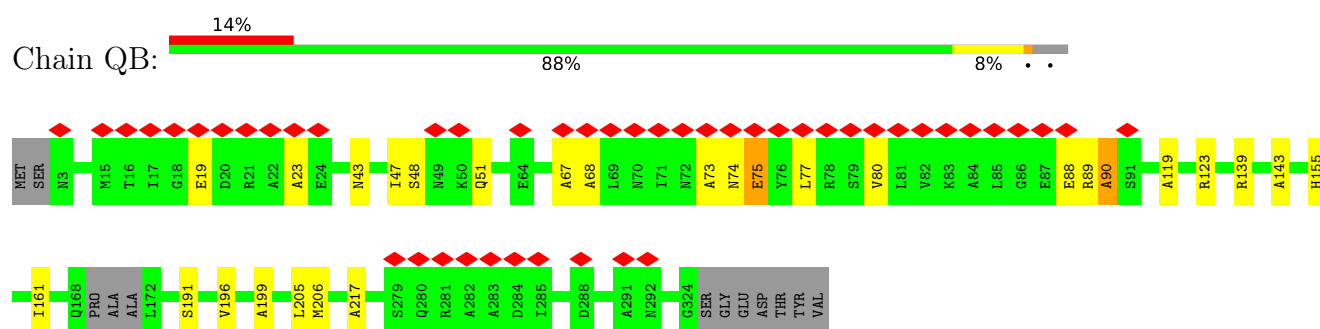
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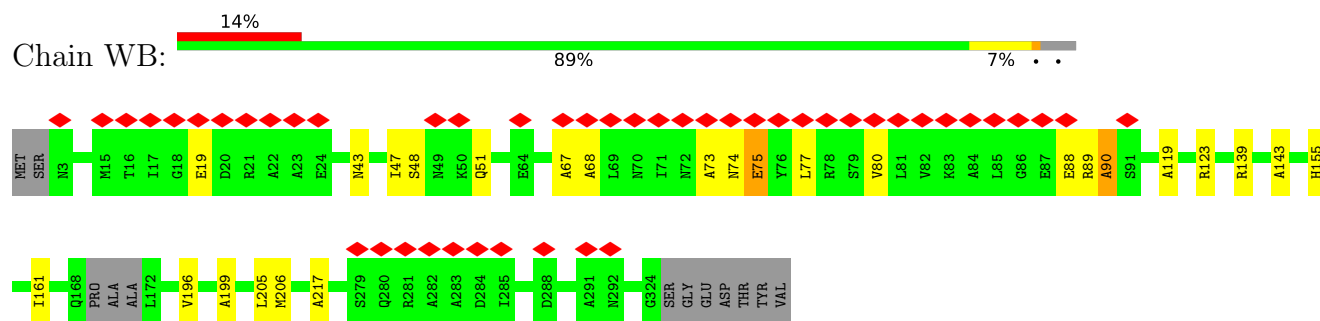
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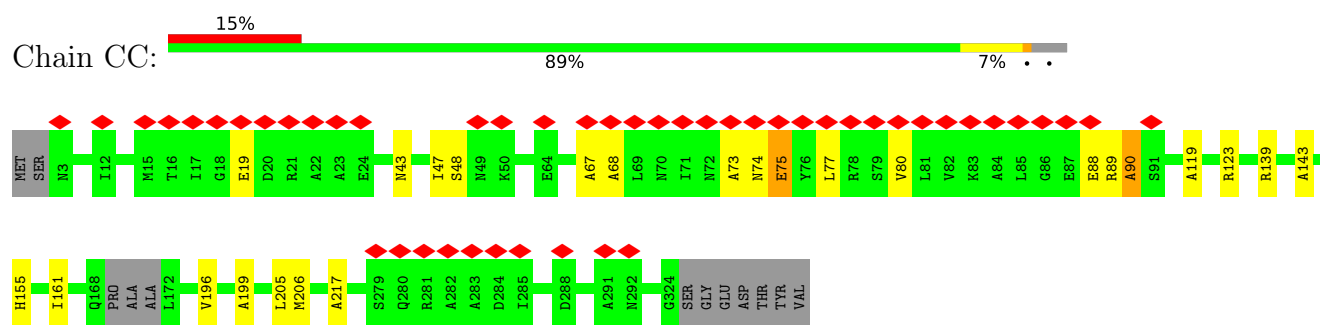
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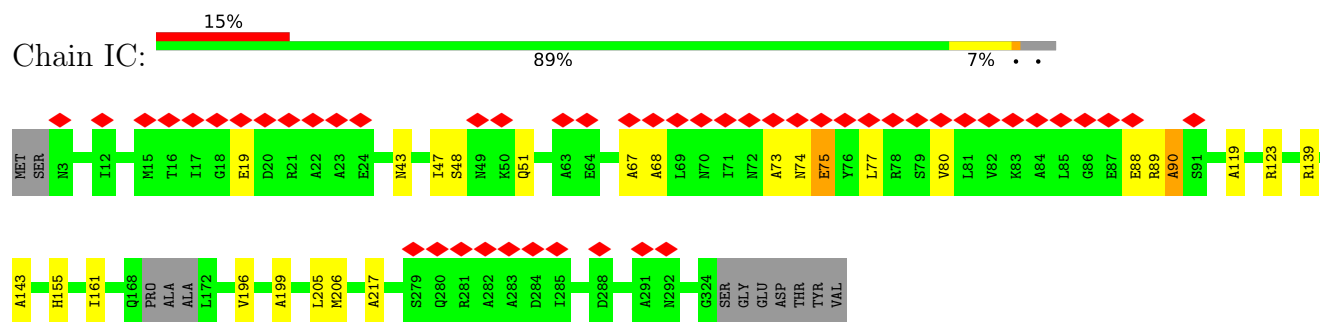
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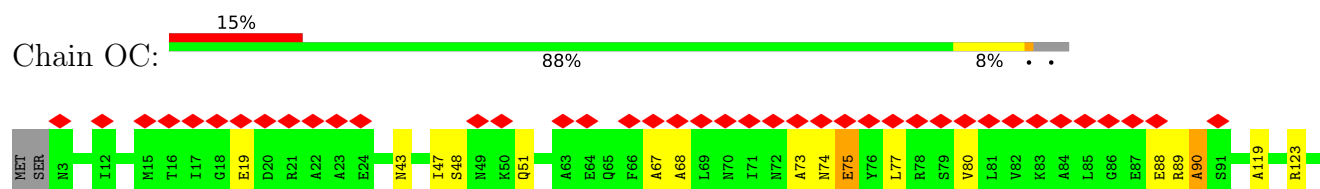
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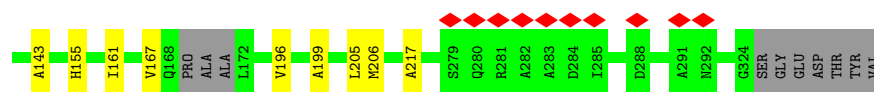


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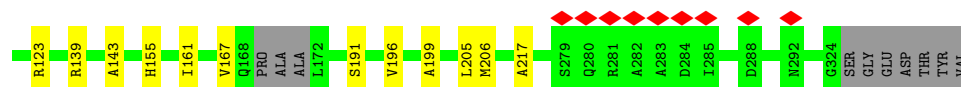
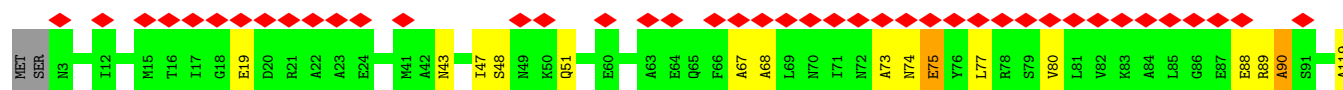
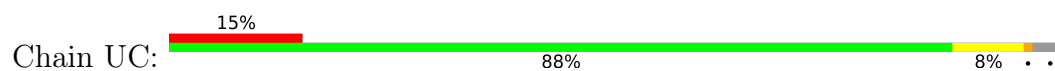


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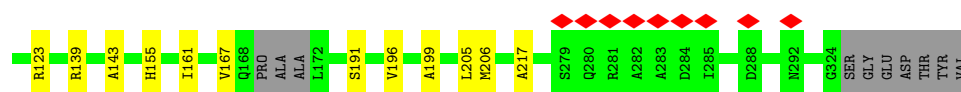
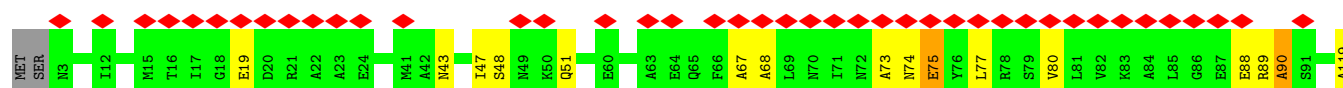
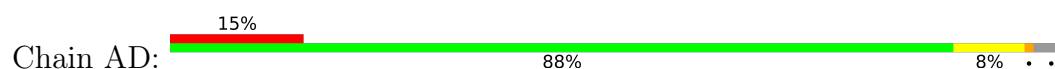




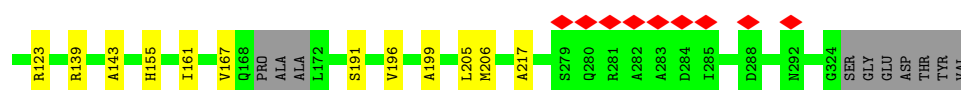
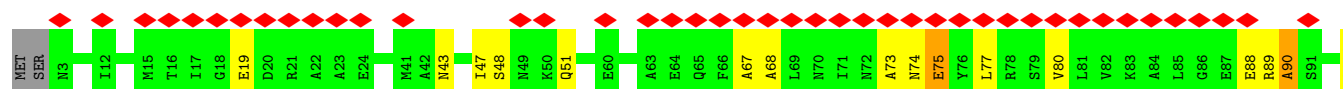
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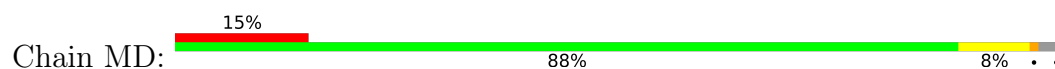
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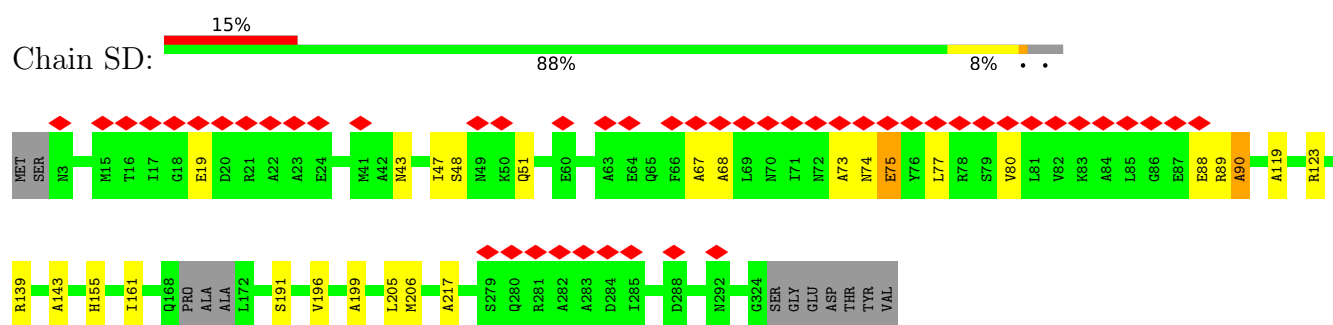
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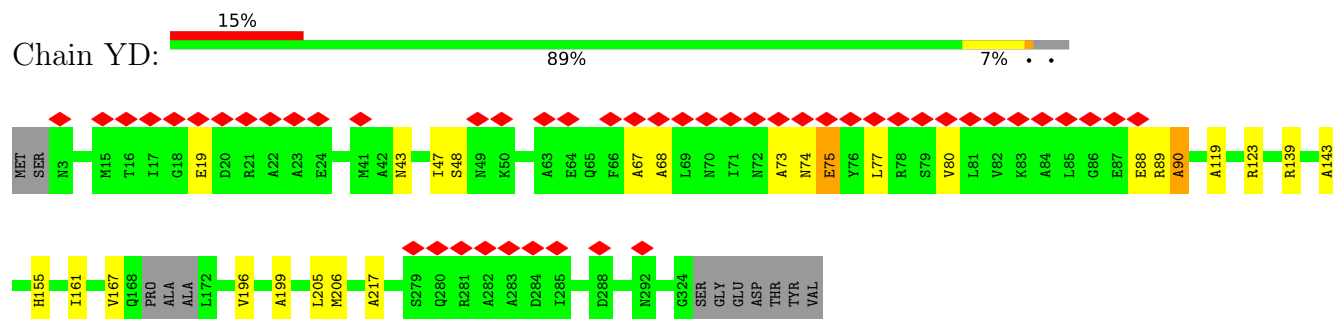
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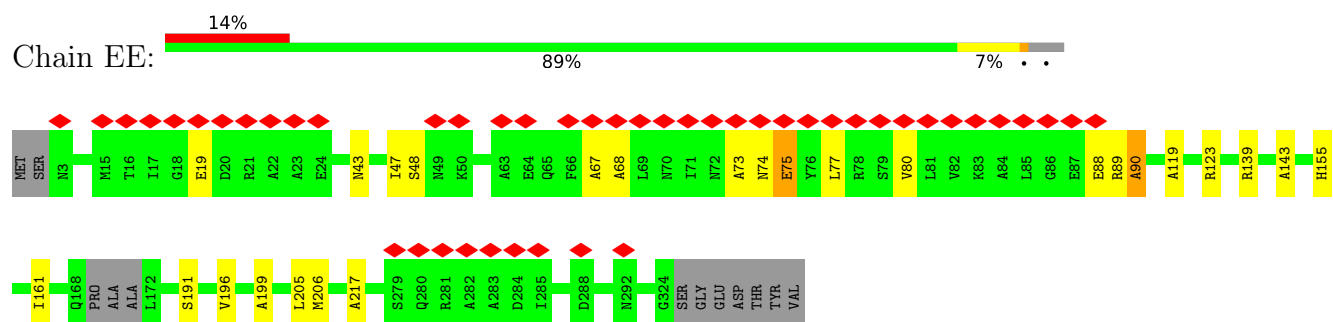
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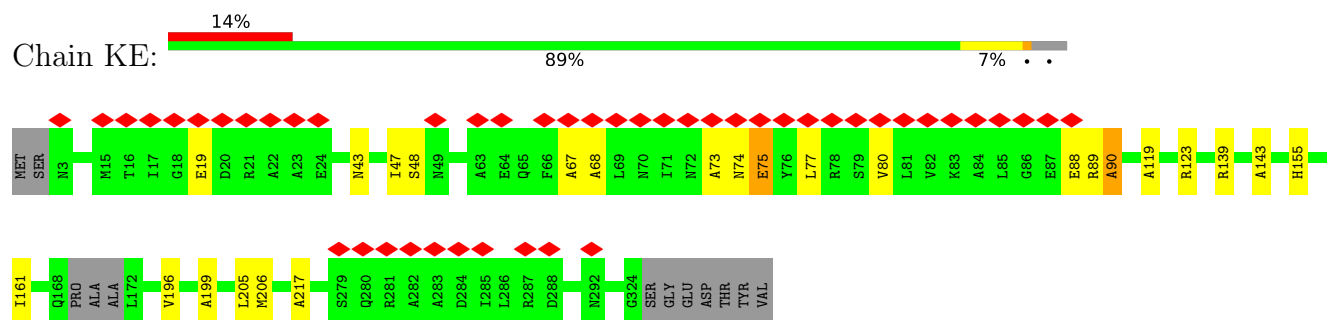
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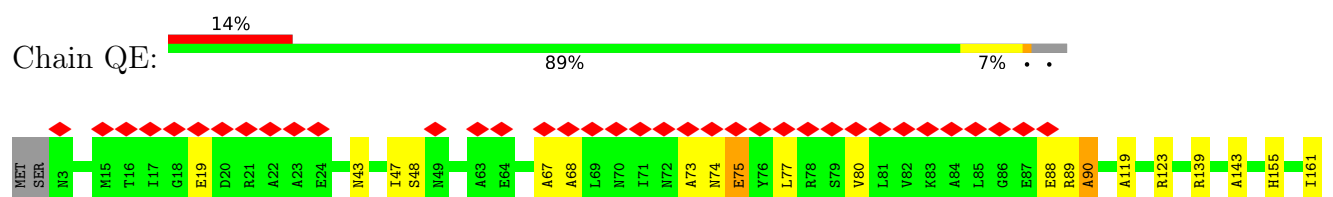
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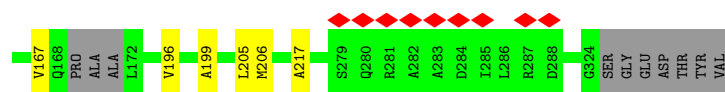


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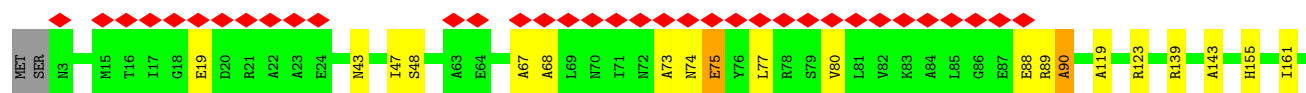
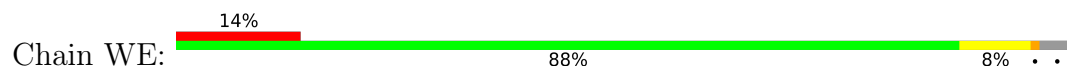


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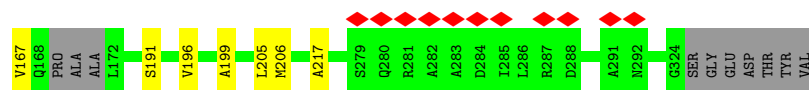
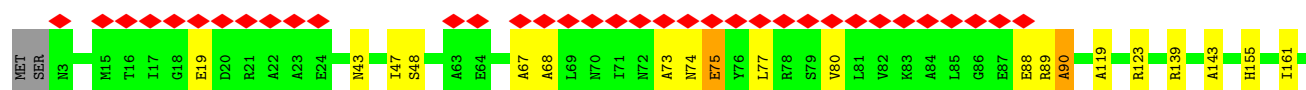
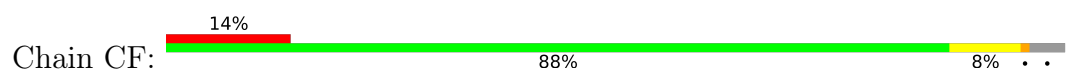




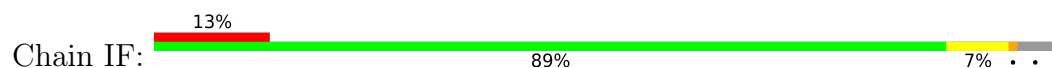
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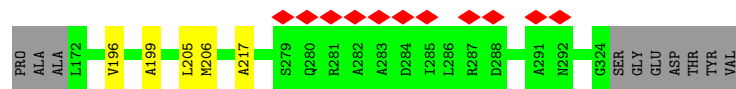
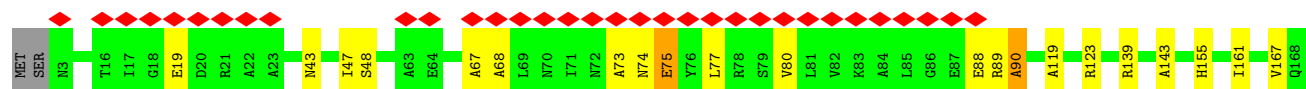
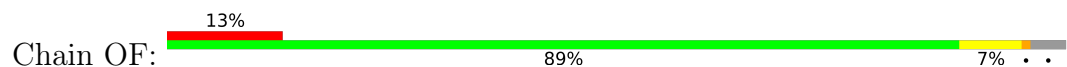
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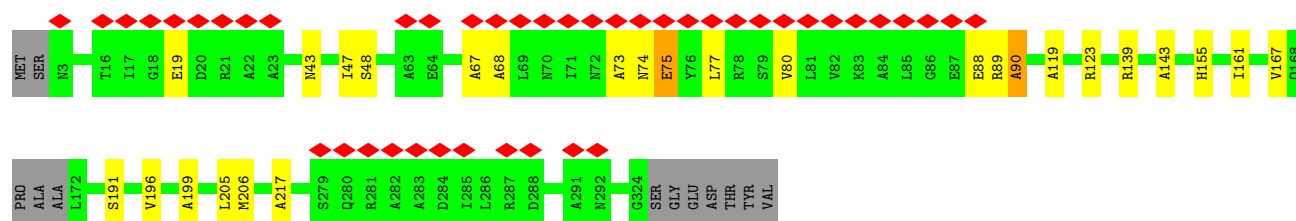


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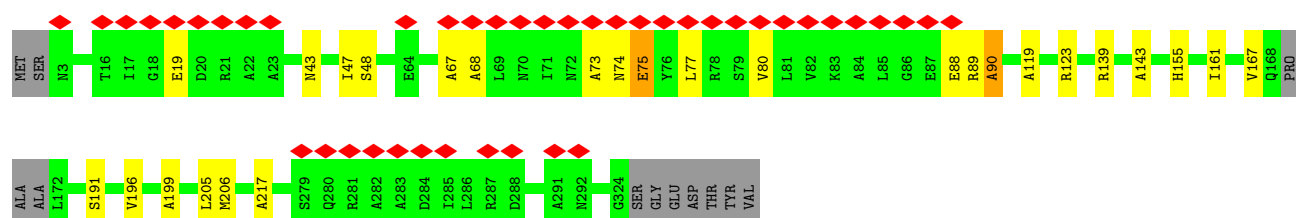
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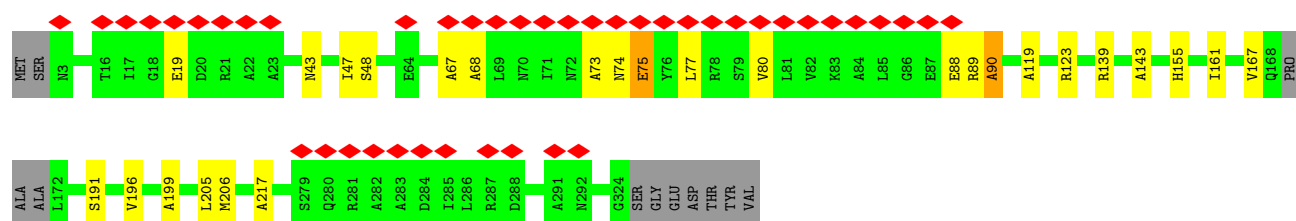
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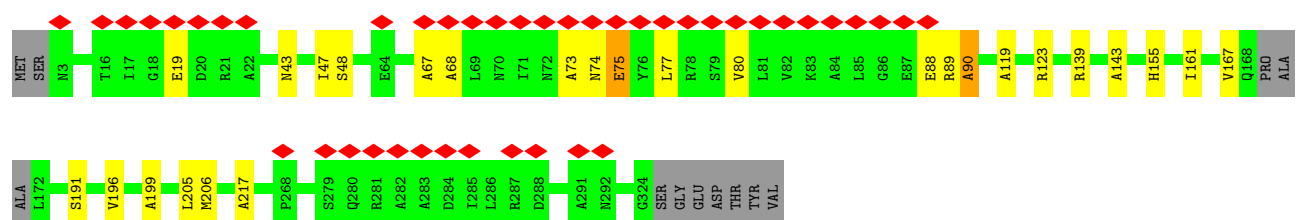
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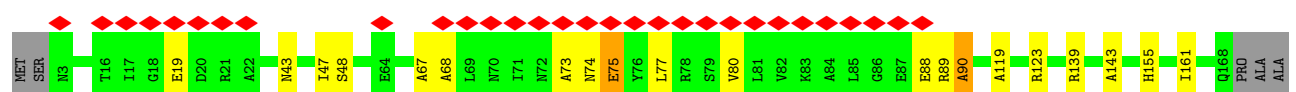
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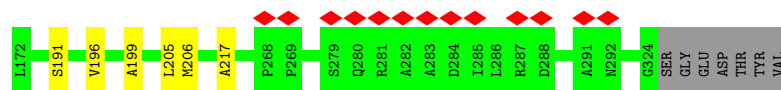
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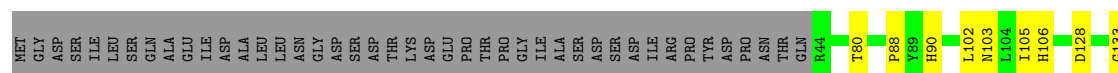
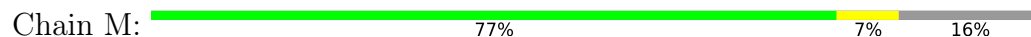
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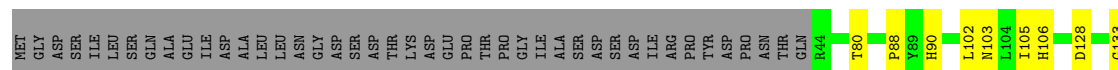
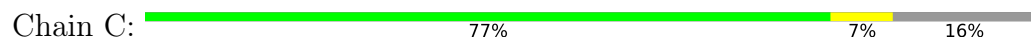




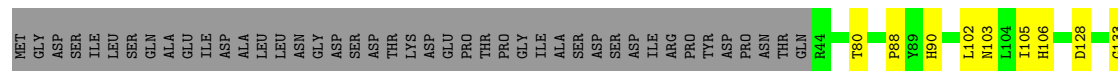
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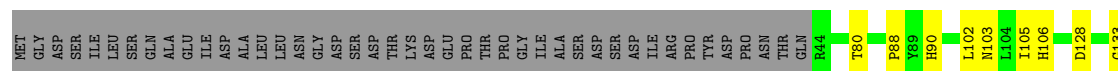
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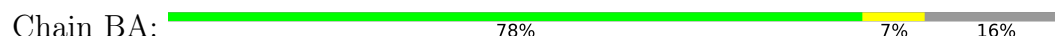
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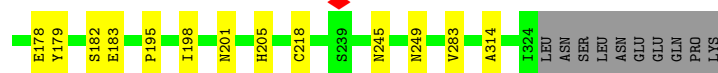
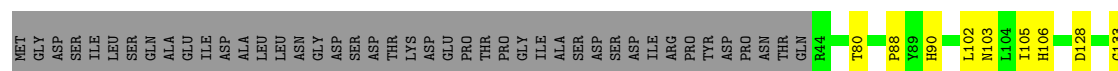


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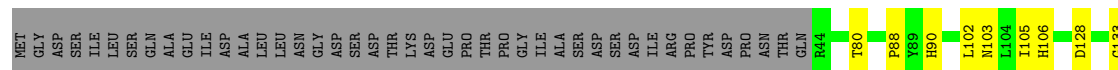
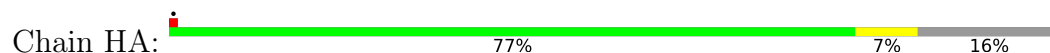


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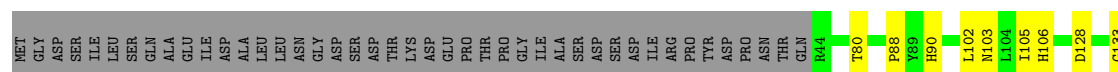
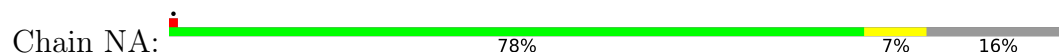




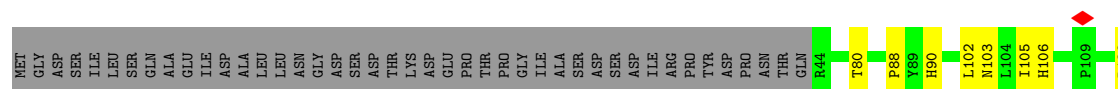
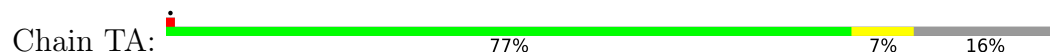
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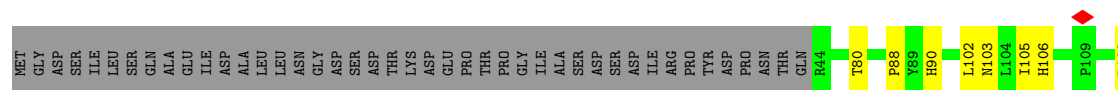
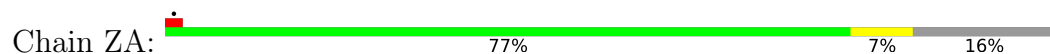
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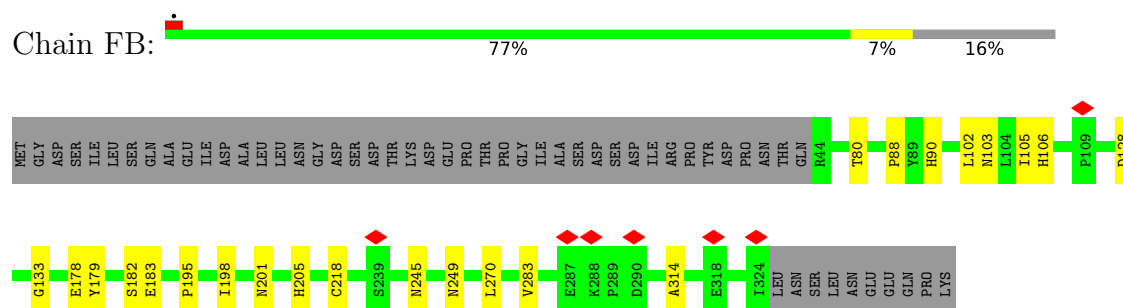
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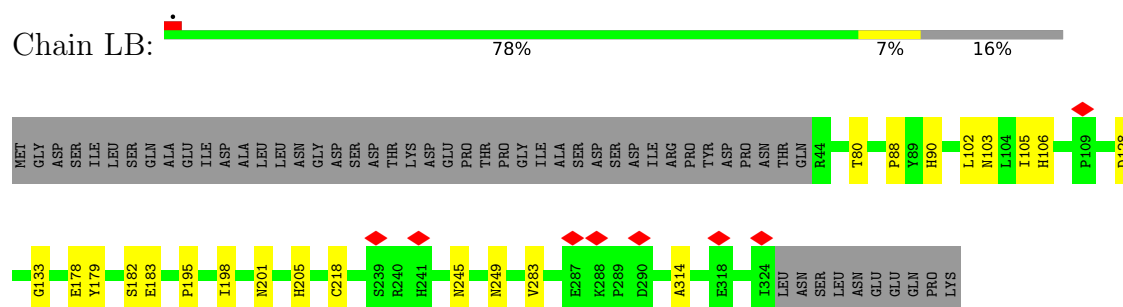
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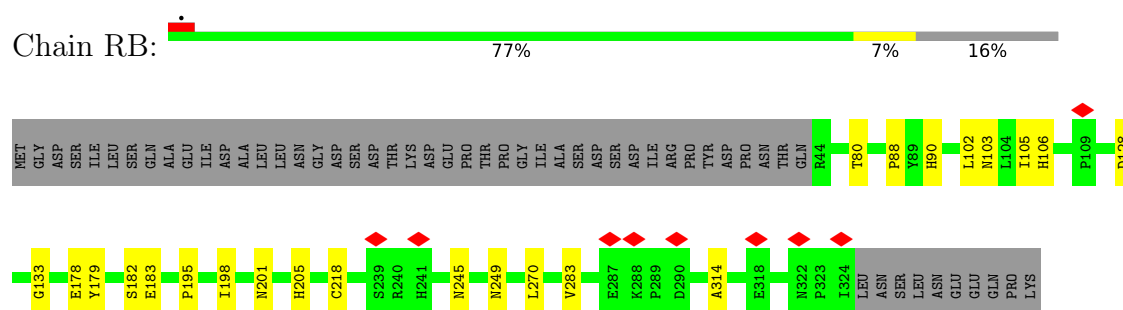
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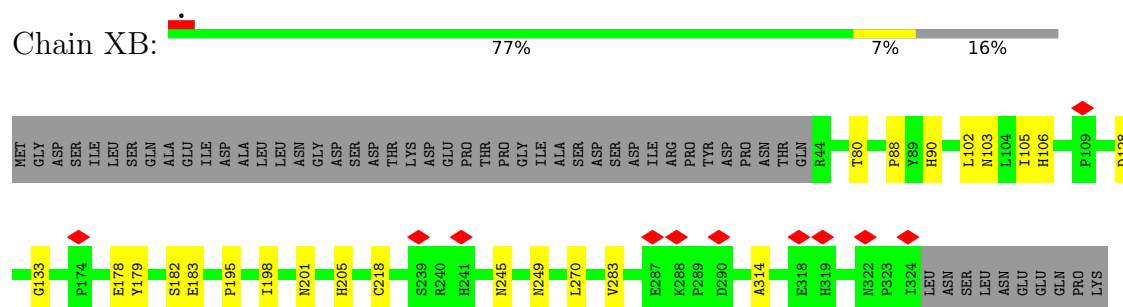
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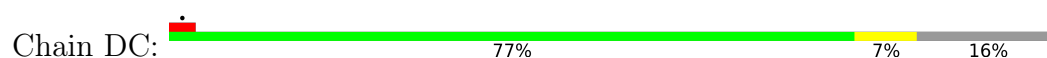
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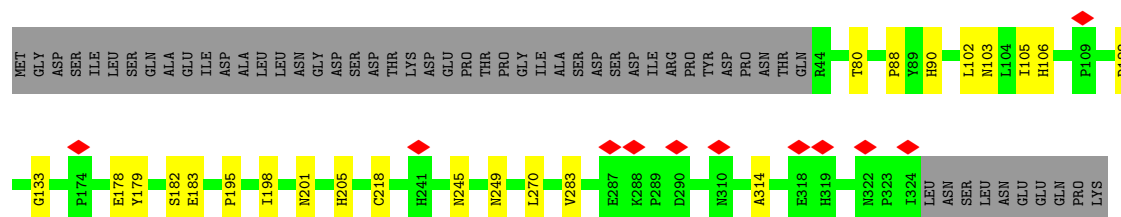


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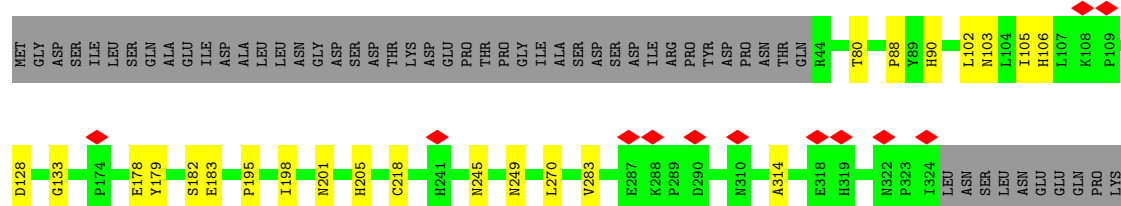
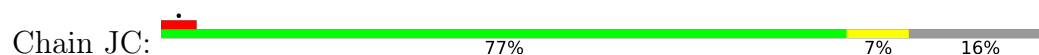


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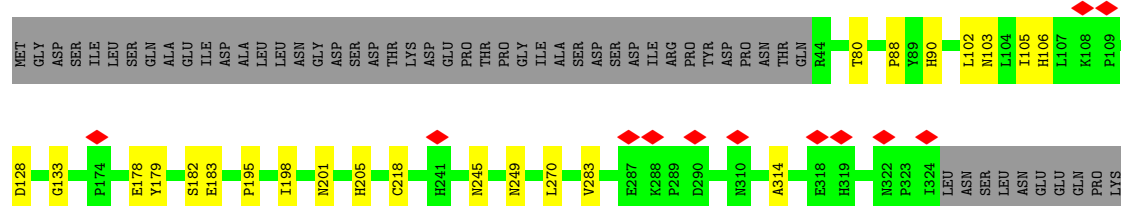
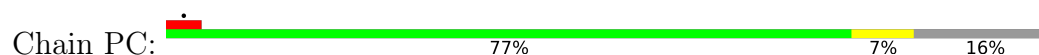




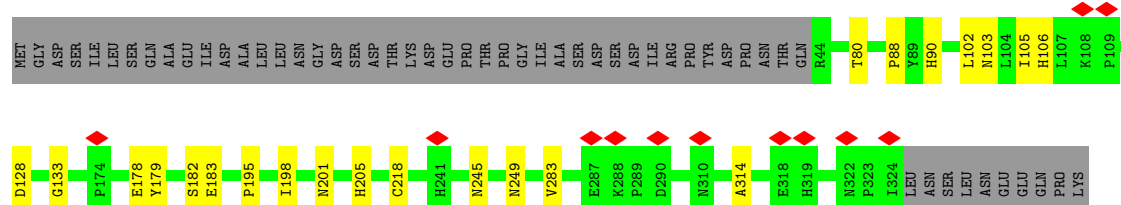
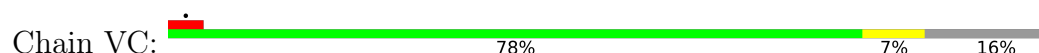
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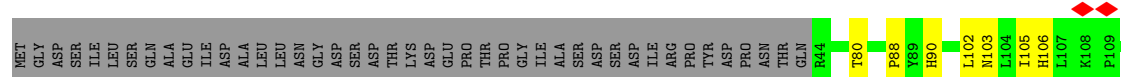
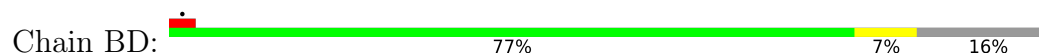
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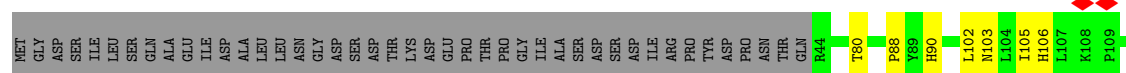
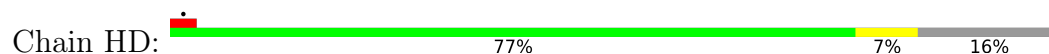


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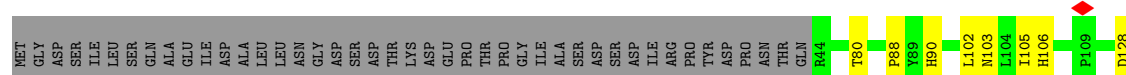
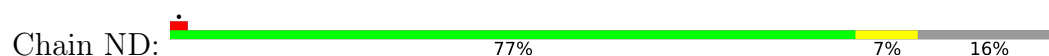




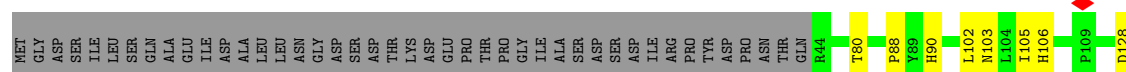
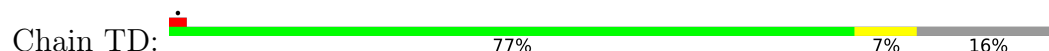
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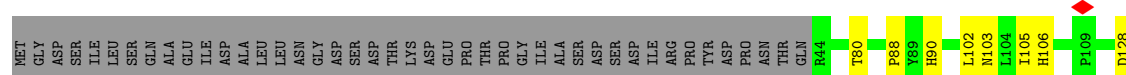
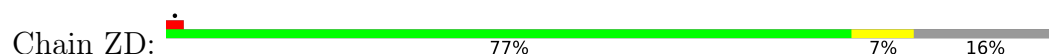
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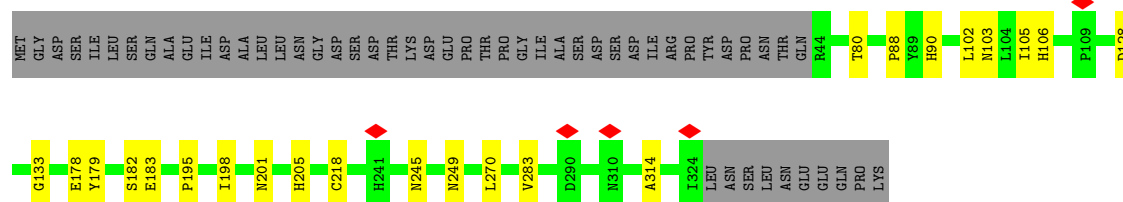


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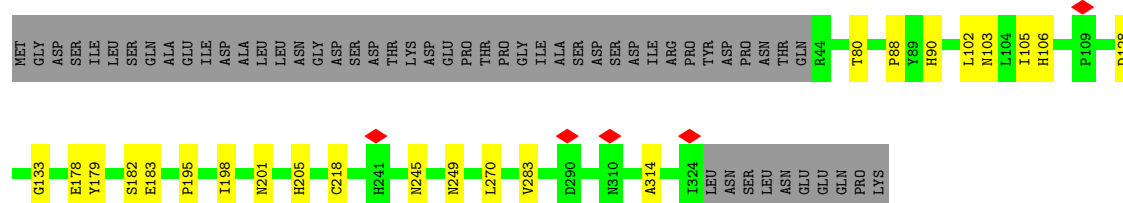
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Chain FE:  77% 7% 16%



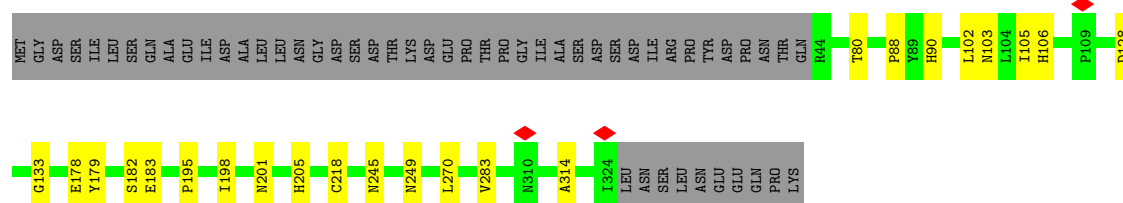
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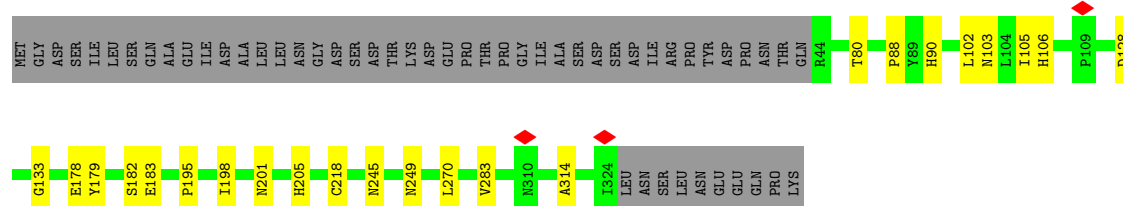
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Chain RE:  77% 7% 16%



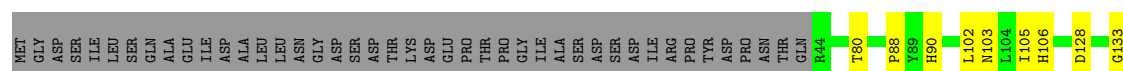
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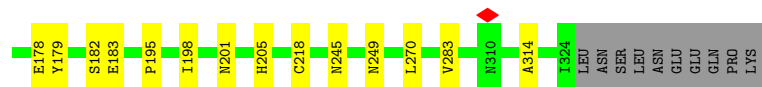
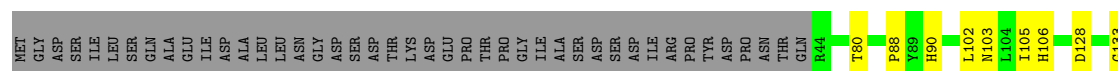
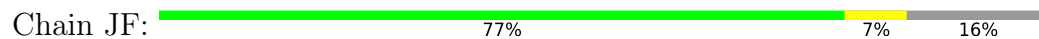
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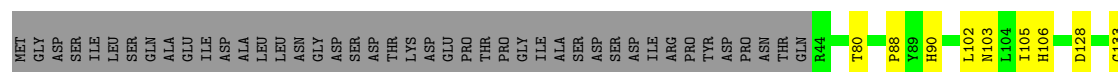
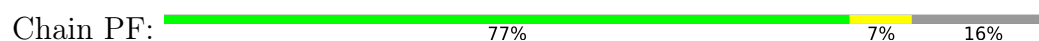




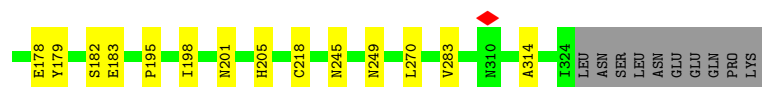
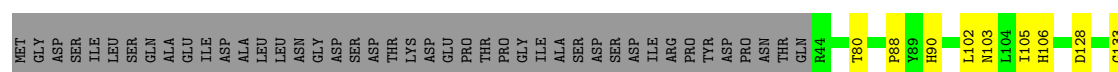
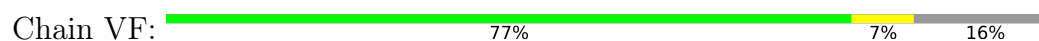
• Molecule 3: Flagellar motor switch protein FliM



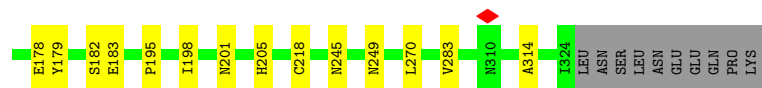
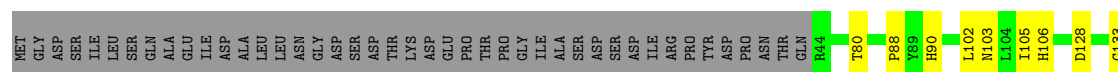
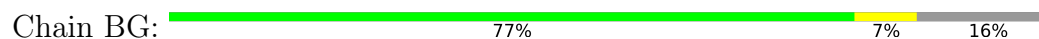
• Molecule 3: Flagellar motor switch protein FliM



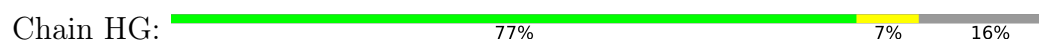
• Molecule 3: Flagellar motor switch protein FliM

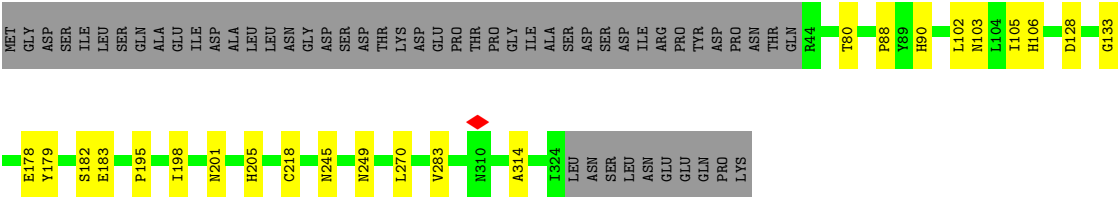


• Molecule 3: Flagellar motor switch protein FliM

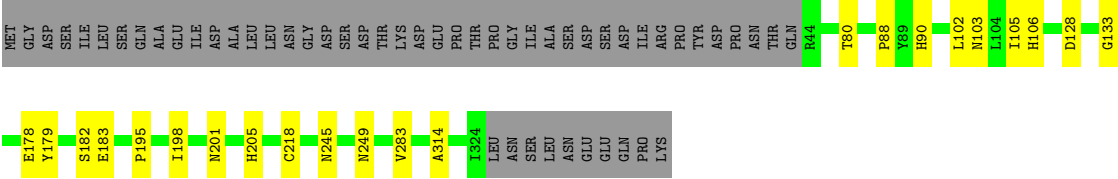
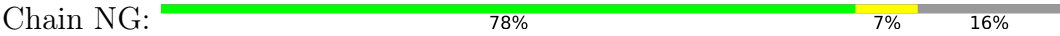


• Molecule 3: Flagellar motor switch protein FliM

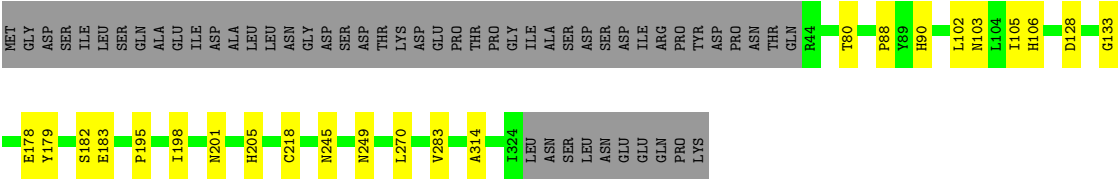
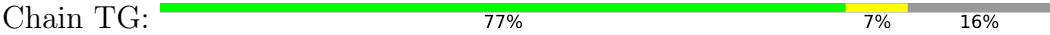




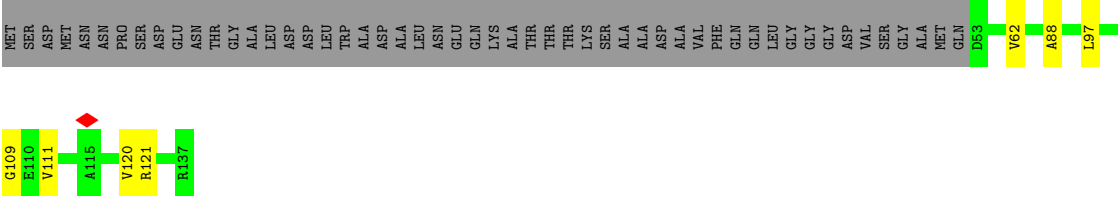
• Molecule 3: Flagellar motor switch protein FliM



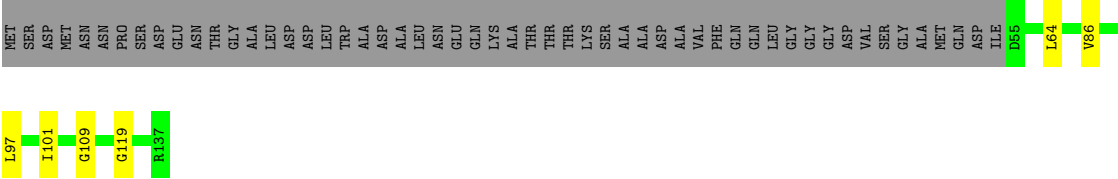
• Molecule 3: Flagellar motor switch protein FliM



• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

Chain Q:  50% 9% 41%

MET SER ASP MET MET ASN ASN PRO SER ASP GLU THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU LEU ASN ASN GLN LYS ALA ALA THR THR THR LYS SER ALA ALA ASP ASP ALA VAL PHE GLN GLN LEU LEU GLY GLY GLY ASP VAL SER GLY ALA MET GLN ASP ASP LEU I57 T65

I75 L79 A88 L100 L105 G109 E110 V111 V120 R121 I122 R137

- Molecule 4: Flagellar motor switch protein FliN

Chain D:  57% 5% 38%

MET SER ASP MET MET ASN ASN PRO SER ASP GLU THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU LEU ASN ASN GLN LYS ALA ALA THR THR THR LYS SER ALA ALA ASP ASP ALA VAL PHE GLN GLN LEU LEU GLY GLY GLY ASP VAL SER GLY ALA MET GLN D53 V62 A88 L97

G109 E110 V111 V114 A115 V120 R121 R137

- Molecule 4: Flagellar motor switch protein FliN

Chain E:  56% 0% 39%

MET SER ASP MET MET ASN ASN PRO SER ASP GLU THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU LEU ASN ASN GLN LYS ALA ALA THR THR THR LYS SER ALA ALA ASP ASP ALA VAL PHE GLN GLN LEU LEU GLY GLY GLY ASP VAL SER GLY ALA MET GLN ASP ASP LEU ILE D55 L64 V66

L97 I101 G109 G119 R137

- Molecule 4: Flagellar motor switch protein FliN

Chain H:  50% 9% 41%

MET SER ASP MET MET ASN ASN PRO SER ASP GLU THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU LEU ASN ASN GLN LYS ALA ALA THR THR THR LYS SER ALA ALA ASP ASP ALA VAL PHE GLN GLN LEU LEU GLY GLY GLY ASP VAL SER GLY ALA MET GLN ASP ASP LEU I57 T65

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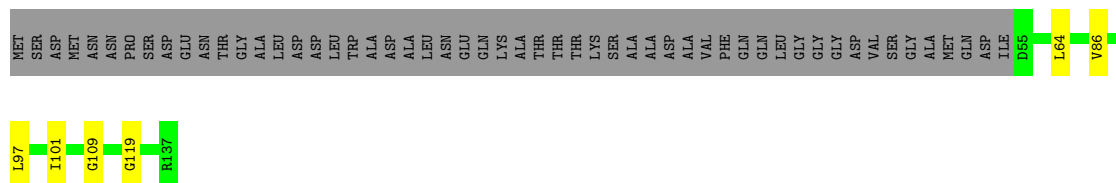
- Molecule 4: Flagellar motor switch protein FliN

Chain L:  57% 5% 38%

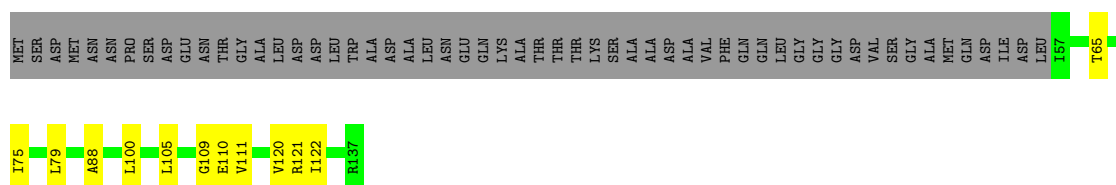
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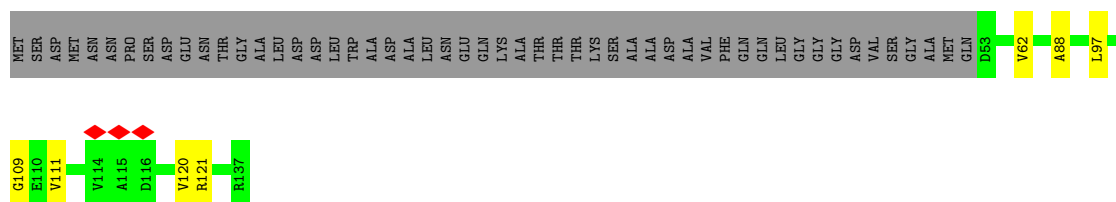
● Molecule 4: Flagellar motor switch protein FliN

Chain O:  56% 39%

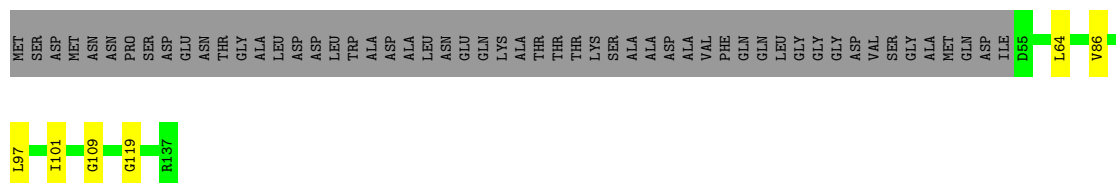
● Molecule 4: Flagellar motor switch protein FliN

Chain R:  50% 9% 41%

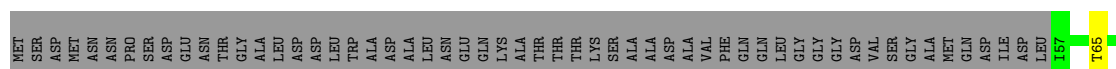
● Molecule 4: Flagellar motor switch protein FliN

Chain W:  57% 5% 38%

● Molecule 4: Flagellar motor switch protein FliN

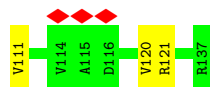
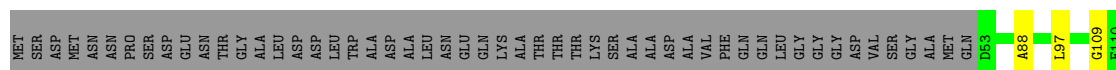
Chain X:  56% 39%

● Molecule 4: Flagellar motor switch protein FliN

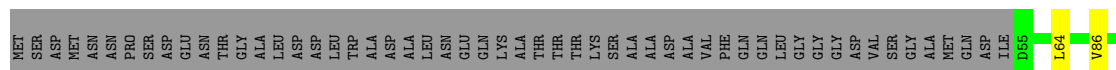
Chain Y:  50% 9% 41%



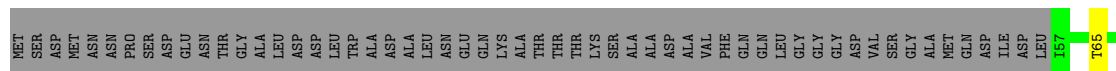
- Molecule 4: Flagellar motor switch protein FliN



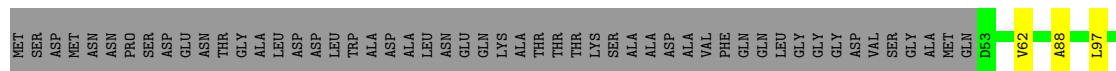
- Molecule 4: Flagellar motor switch protein FliN



- Molecule 4: Flagellar motor switch protein FliN

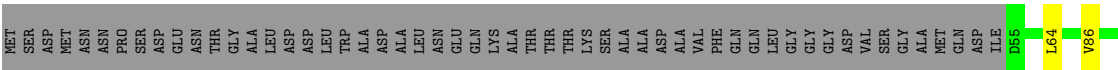


- Molecule 4: Flagellar motor switch protein FliN



- Molecule 4: Flagellar motor switch protein FliN

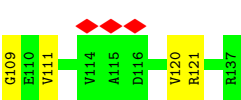




• Molecule 4: Flagellar motor switch protein FliN



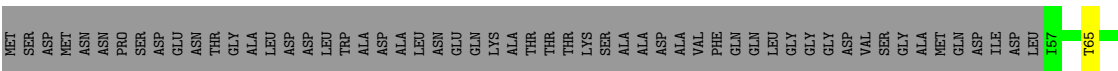
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• Molecule 4: Flagellar motor switch protein FliN

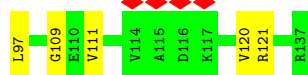
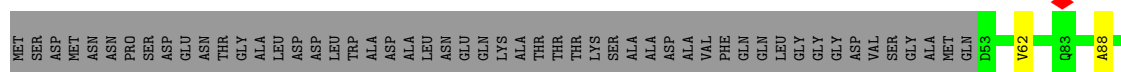


• Molecule 4: Flagellar motor switch protein FliN



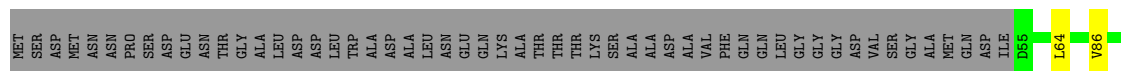
• Molecule 4: Flagellar motor switch protein FliN

Chain UA:  57% 5% 38%



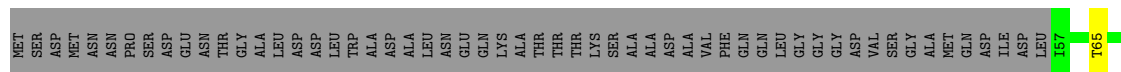
- Molecule 4: Flagellar motor switch protein FliN

Chain VA:  56% 39%



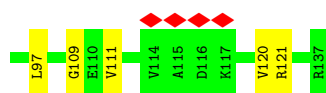
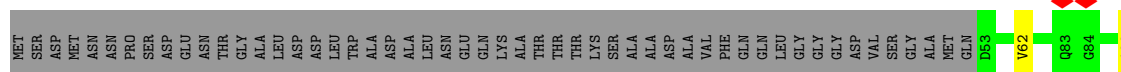
- Molecule 4: Flagellar motor switch protein FliN

Chain WA:  50% 9% 41%



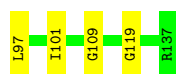
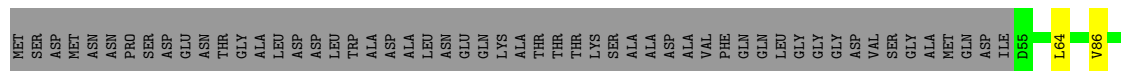
- Molecule 4: Flagellar motor switch protein FliN

Chain AB:  57% 5% 38%



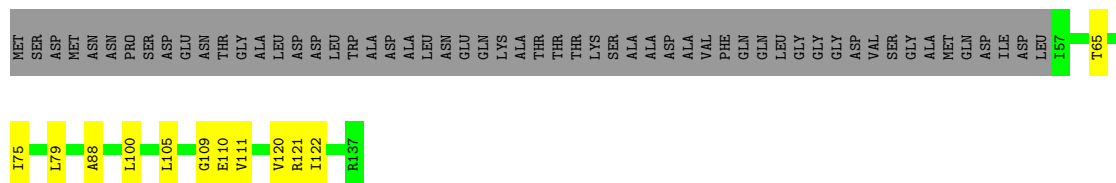
- Molecule 4: Flagellar motor switch protein FliN

Chain BB:  56% 39%



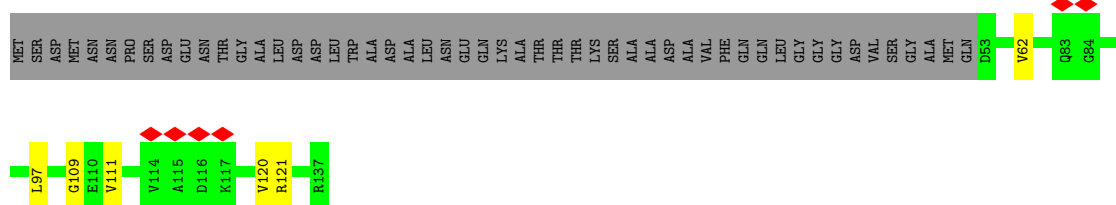
- Molecule 4: Flagellar motor switch protein FliN

Chain CB:  50% 9% 41%



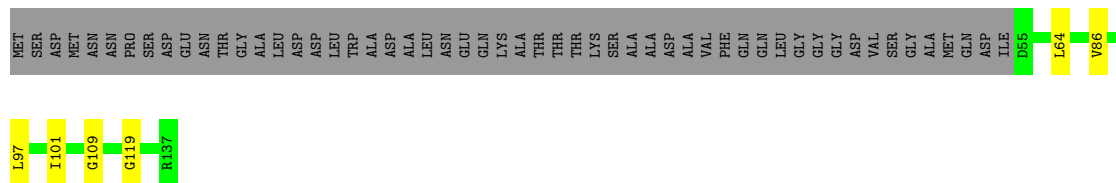
- Molecule 4: Flagellar motor switch protein FliN

Chain GB:  57% 5% 38%



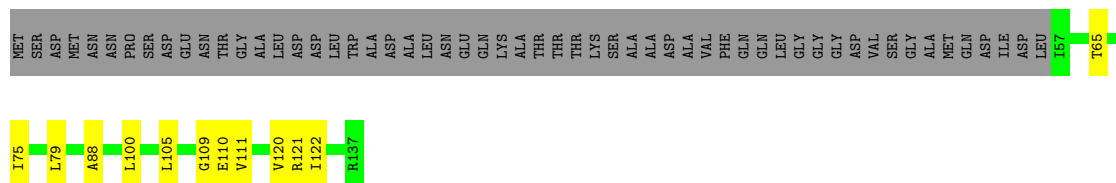
- Molecule 4: Flagellar motor switch protein FliN

Chain HB:  56% 39%



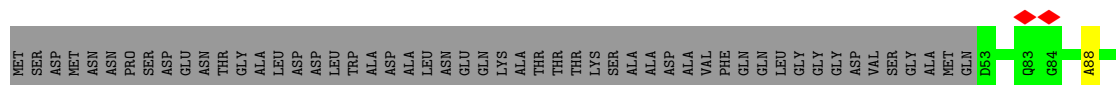
- Molecule 4: Flagellar motor switch protein FliN

Chain IB:  50% 9% 41%



- Molecule 4: Flagellar motor switch protein FliN

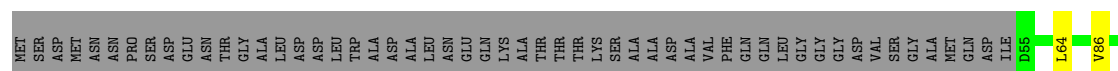
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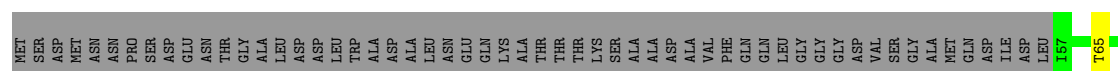
- Molecule 4: Flagellar motor switch protein FliN

Chain NB: 56% 39%



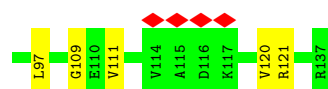
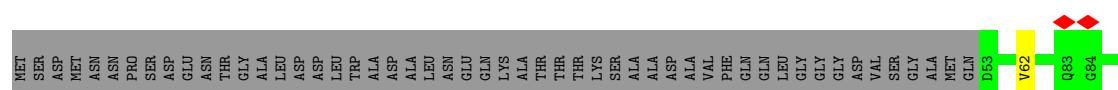
- Molecule 4: Flagellar motor switch protein FliN

Chain OB: 50% 9% 41%



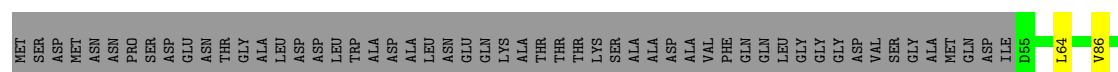
- Molecule 4: Flagellar motor switch protein FliN

Chain SB: 57% 5% 38%



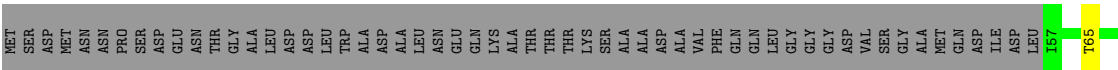
- Molecule 4: Flagellar motor switch protein FliN

Chain TB: 56% 39%

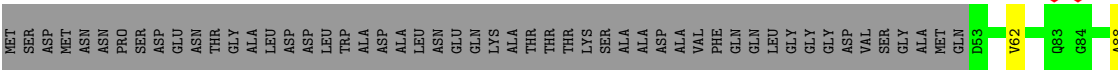


- Molecule 4: Flagellar motor switch protein FliN

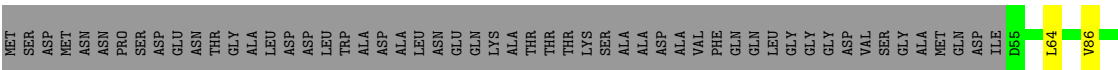
Chain UB: 50% 9% 41%



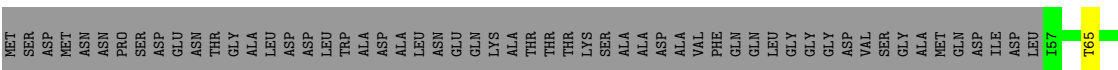
• Molecule 4: Flagellar motor switch protein FliN



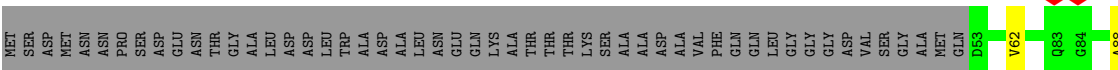
• Molecule 4: Flagellar motor switch protein FliN



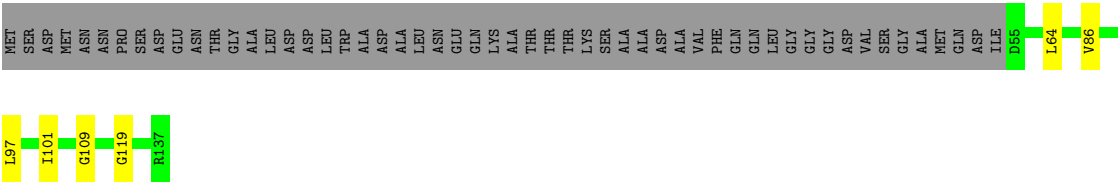
• Molecule 4: Flagellar motor switch protein FliN



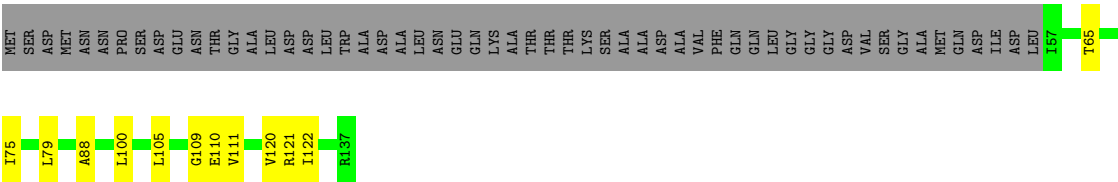
• Molecule 4: Flagellar motor switch protein FliN



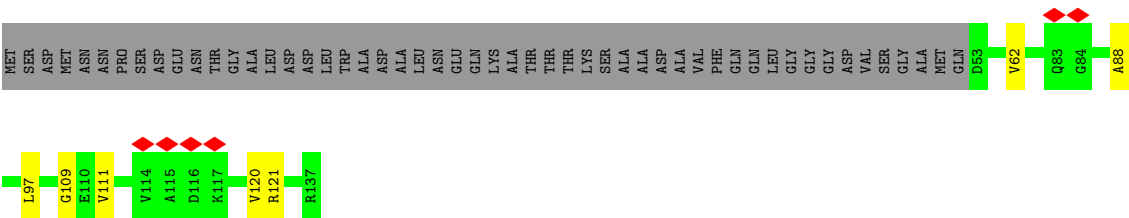
• Molecule 4: Flagellar motor switch protein FliN



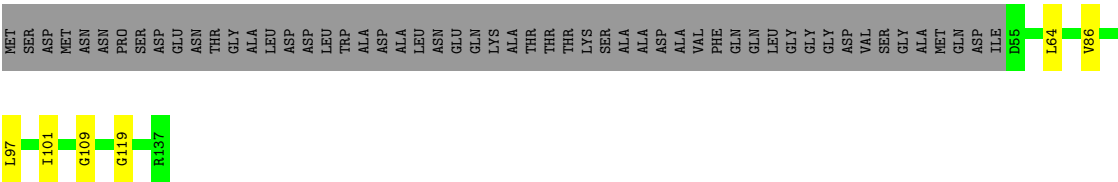
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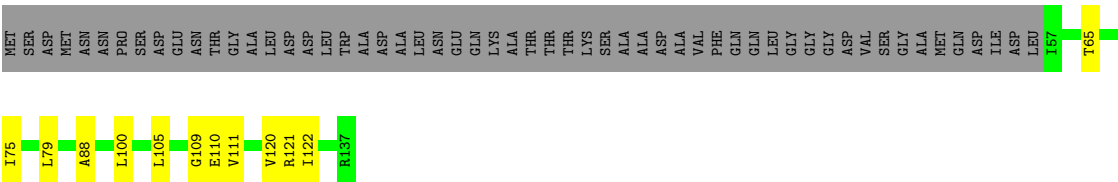
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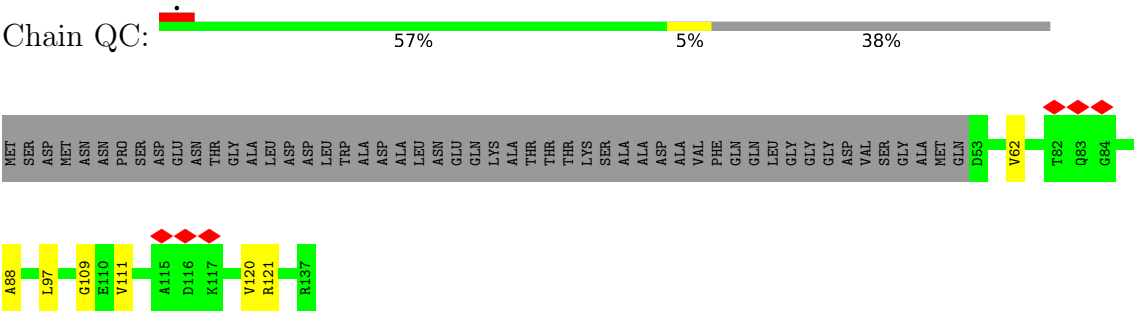
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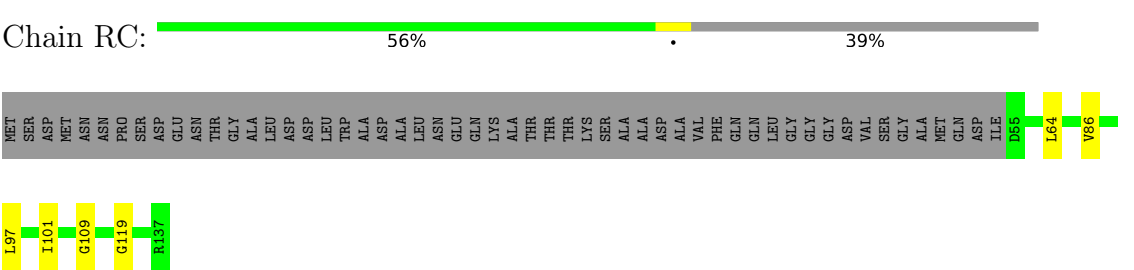
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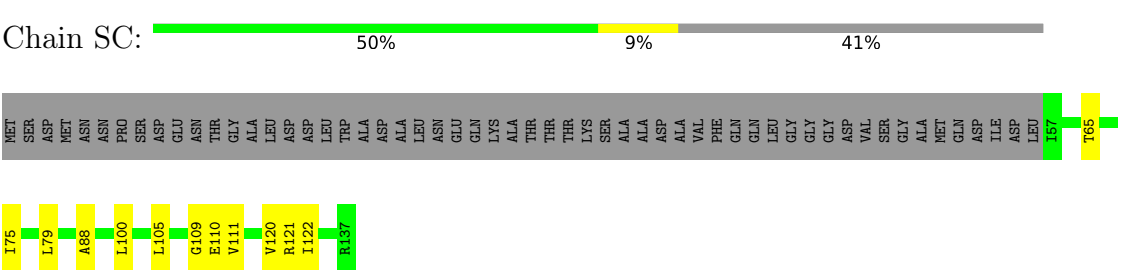
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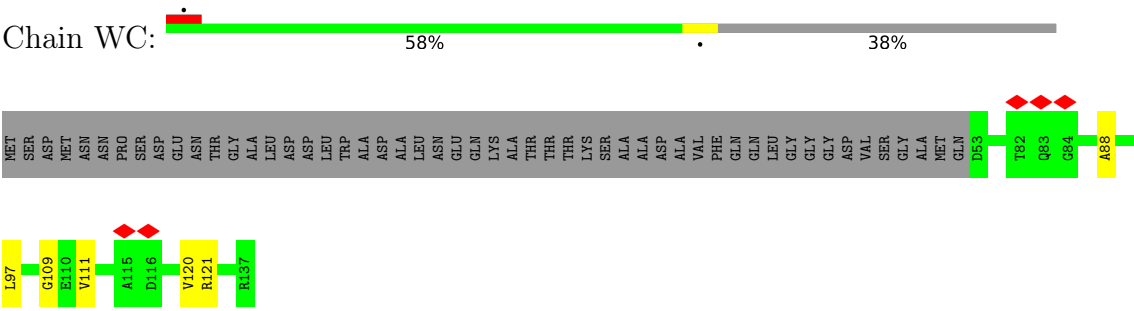
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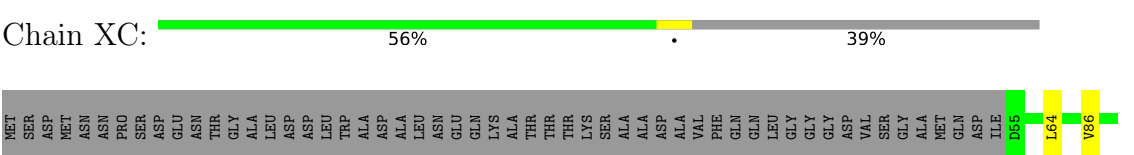
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN



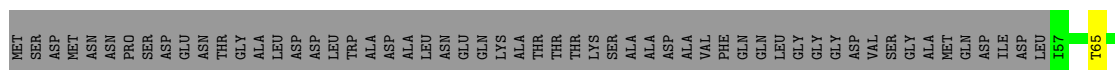
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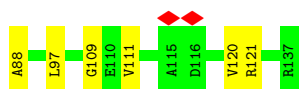
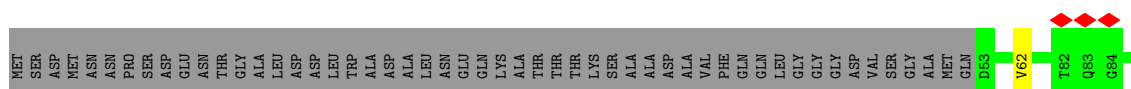
- Molecule 4: Flagellar motor switch protein FliN

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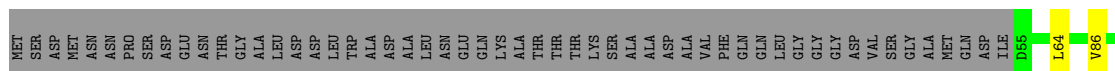
- Molecule 4: Flagellar motor switch protein FliN

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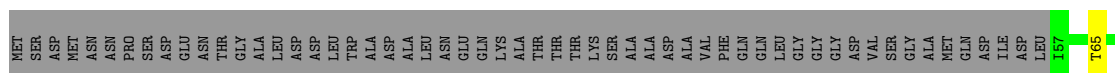
- Molecule 4: Flagellar motor switch protein FliN

Chain DD:



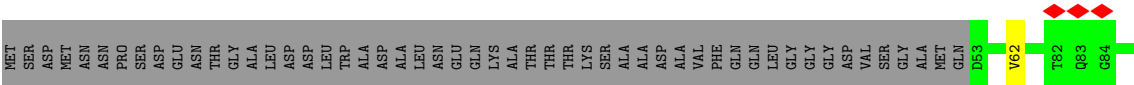
- Molecule 4: Flagellar motor switch protein FliN

Chain ED:

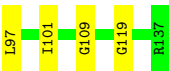
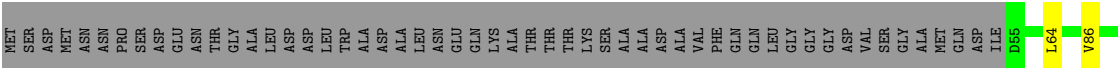


- Molecule 4: Flagellar motor switch protein FliN

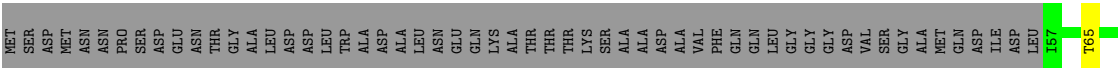
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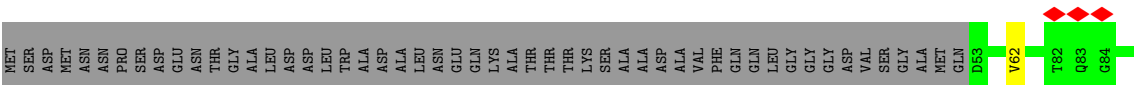
• Molecule 4: Flagellar motor switch protein FliN



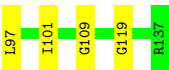
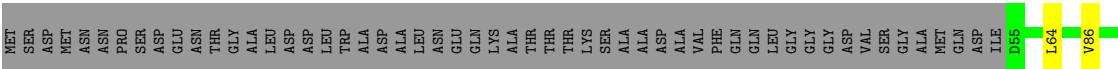
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

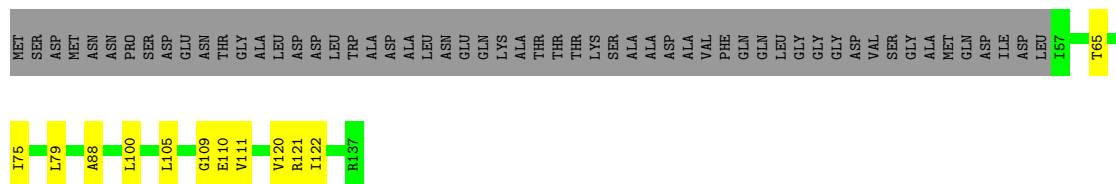


• Molecule 4: Flagellar motor switch protein FliN



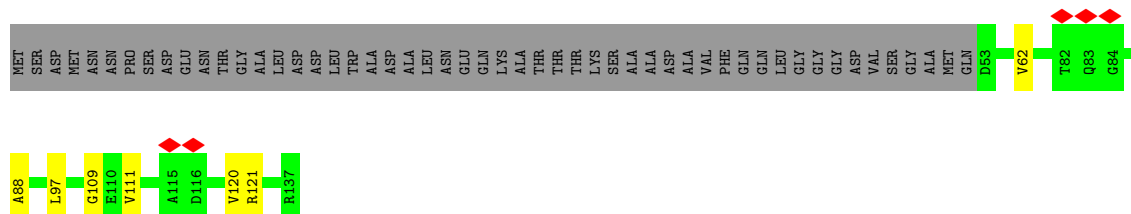
• Molecule 4: Flagellar motor switch protein FliN

Chain QD:  50% 9% 41%



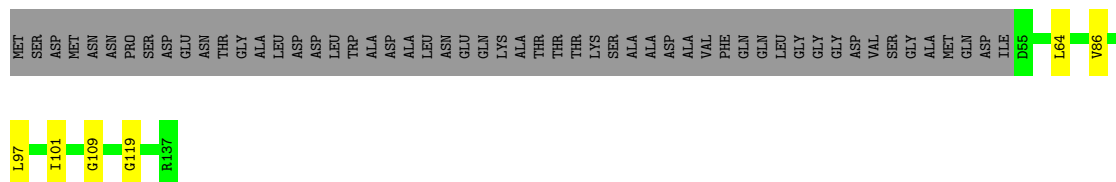
- Molecule 4: Flagellar motor switch protein FliN

Chain UD:  57% 5% 38%



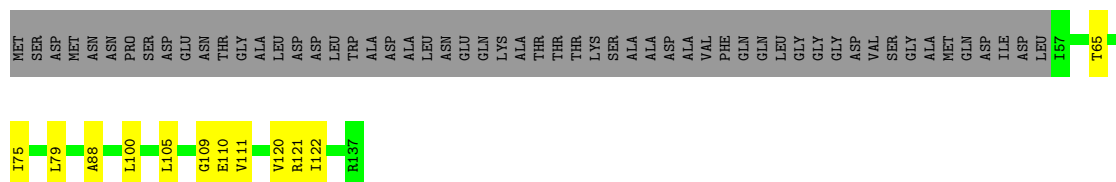
- Molecule 4: Flagellar motor switch protein FliN

Chain VD:  56% 39%



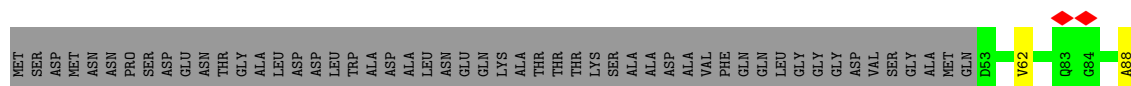
- Molecule 4: Flagellar motor switch protein FliN

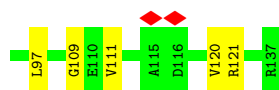
Chain WD:  50% 9% 41%



- Molecule 4: Flagellar motor switch protein FliN

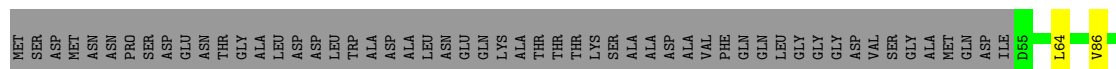
Chain AE:  57% 5% 38%





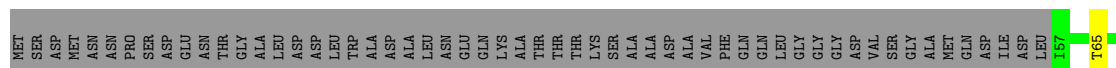
• Molecule 4: Flagellar motor switch protein FliN

Chain BE: 55% 5% 39%



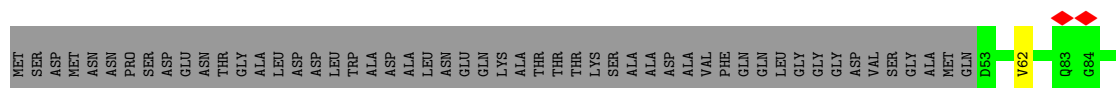
• Molecule 4: Flagellar motor switch protein FliN

Chain CE: 50% 9% 41%



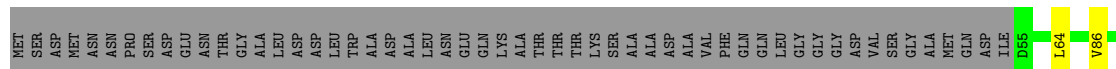
• Molecule 4: Flagellar motor switch protein FliN

Chain GE: 57% 5% 38%



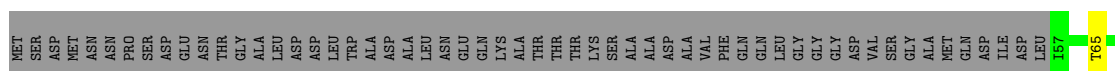
• Molecule 4: Flagellar motor switch protein FliN

Chain HE: 55% 5% 39%

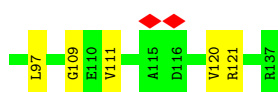
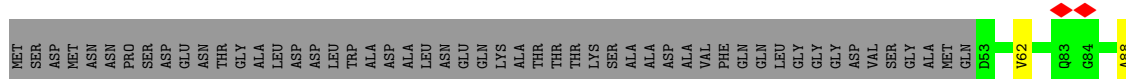


• Molecule 4: Flagellar motor switch protein FliN

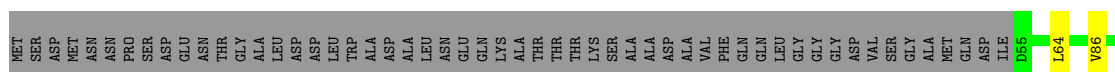
Chain IE: 50% 9% 41%



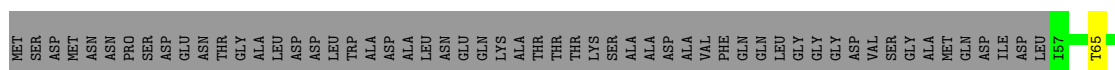
- Molecule 4: Flagellar motor switch protein FliN



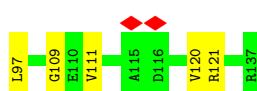
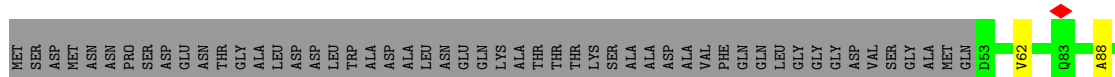
- Molecule 4: Flagellar motor switch protein FliN



- Molecule 4: Flagellar motor switch protein FliN

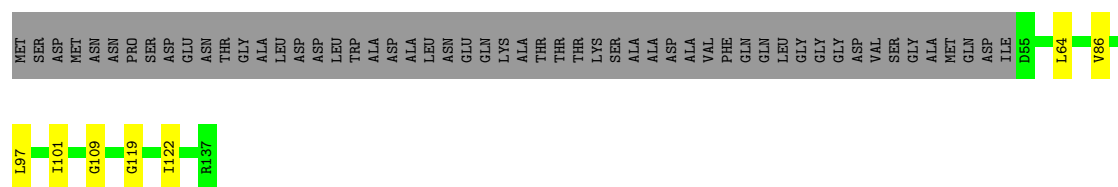


- Molecule 4: Flagellar motor switch protein FliN



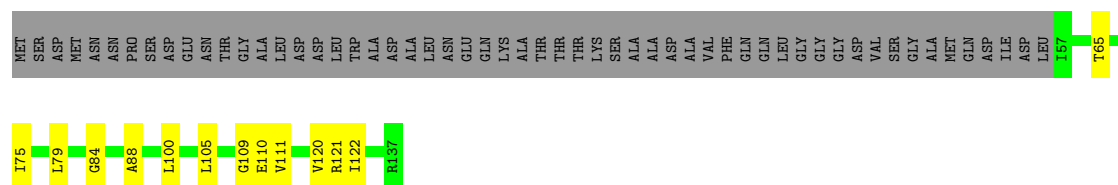
- Molecule 4: Flagellar motor switch protein FliN

Chain TE:  55% 5% 39%



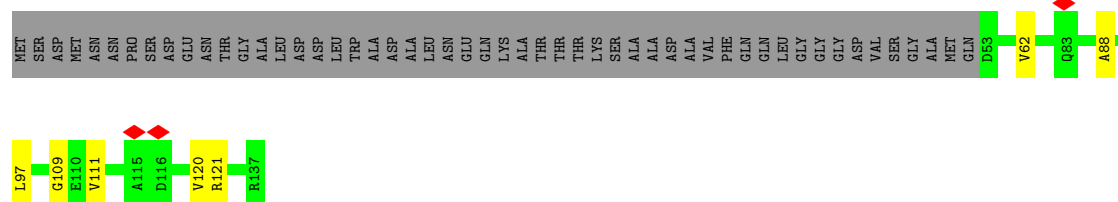
- Molecule 4: Flagellar motor switch protein FliN

Chain UE:  50% 9% 41%



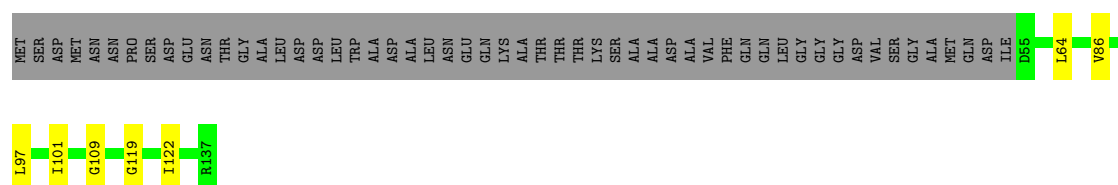
- Molecule 4: Flagellar motor switch protein FliN

Chain YE:  57% 5% 38%



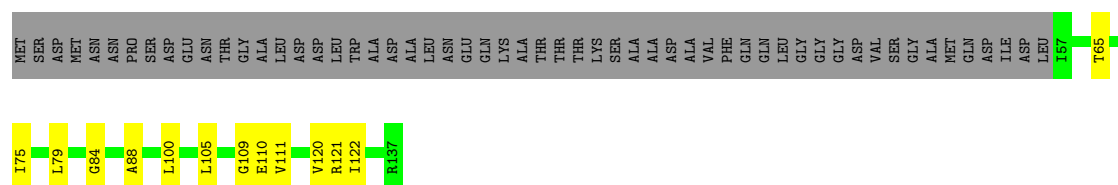
- Molecule 4: Flagellar motor switch protein FliN

Chain ZE:  55% 5% 39%



- Molecule 4: Flagellar motor switch protein FliN

Chain AF:  50% 9% 41%



• Molecule 4: Flagellar motor switch protein FliN

Chain EF:  57% 5% 38%

MET	SER	ASP	MET	ASN	PRO	SER	ASP	GLU	THR	GLY	ALA	LEU	ASP	LEU	TRP	ALA	ASP	LEU	ALA	ASN	GLU	GLN	LYS	ALA	ALA	ALA	ASP	ASP	VAL	PHE	GLN	GLN	LEU	GLY	GLY	ASP	VAL	SER	GLY	ALA	MET	GLN	D53	V62	A88	L97
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G109	E110	V111	A115	D116	V120	R121	R137
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• Molecule 4: Flagellar motor switch protein FliN

Chain FF:  55% 5% 39%

MET	SER	ASP	MET	ASN	PRO	SER	ASP	GLU	THR	GLY	ALA	LEU	ASP	LEU	TRP	ALA	ASP	LEU	ALA	ASN	GLU	GLN	LYS	ALA	ALA	ALA	ASP	ASP	VAL	PHE	GLN	GLN	LEU	GLY	GLY	ASP	VAL	SER	GLY	ALA	MET	GLN	ASP	ILE	D55	L64	V86
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L97	I101	G109	G119	I122	R137
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• Molecule 4: Flagellar motor switch protein FliN

Chain GF:  50% 9% 41%

MET	SER	ASP	MET	ASN	PRO	SER	ASP	GLU	ASN	THR	GLY	ALA	LEU	ASP	LEU	TRP	ALA	ASP	LEU	LEU	GLU	GLN	LYS	THR	THR	THR	LYS	ALA	ALA	ALA	ASP	ASP	VAL	PHE	GLN	GLN	LEU	GLY	GLY	ASP	VAL	SER	GLY	ALA	MET	GLN	ASP	ASP	LEU	I57	T65
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I75	L79	G84	A83	L100	L105	G109	E110	V111	V120	I122	R137
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• Molecule 4: Flagellar motor switch protein FliN

Chain KF:  57% 5% 38%

MET	SER	ASP	MET	ASN	PRO	SER	ASP	GLU	THR	GLY	ALA	LEU	ASP	LEU	TRP	ALA	ASP	LEU	ALA	ASN	GLU	GLN	LYS	ALA	ALA	ALA	ASP	ASP	VAL	PHE	GLN	GLN	LEU	GLY	GLY	ASP	VAL	SER	GLY	ALA	MET	GLN	D53	V62	A88	L97
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G109	E110	V111	A115	D116	V120	R121	R137
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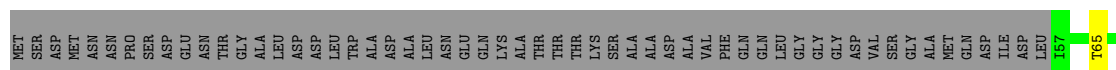
• Molecule 4: Flagellar motor switch protein FliN

Chain LF:  55% 5% 39%

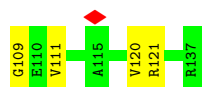
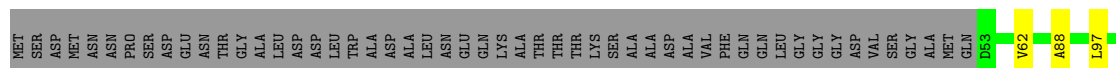
MET	SER	ASP	MET	ASN	PRO	SER	ASP	GLU	THR	GLY	ALA	LEU	ASP	LEU	TRP	ALA	ASP	LEU	ALA	ASN	GLU	GLN	LYS	ALA	ALA	ALA	ASP	ASP	VAL	PHE	GLN	GLN	LEU	GLY	GLY	ASP	VAL	SER	GLY	ALA	MET	GLN	ASP	ASP	ILE	D55	L64	V86
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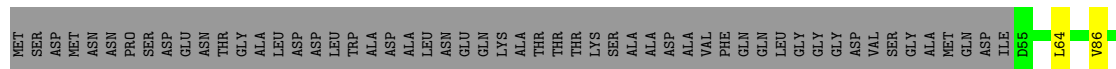
- Molecule 4: Flagellar motor switch protein FliN



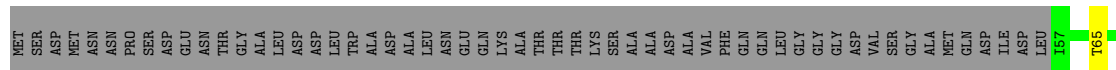
- Molecule 4: Flagellar motor switch protein FliN



- Molecule 4: Flagellar motor switch protein FliN

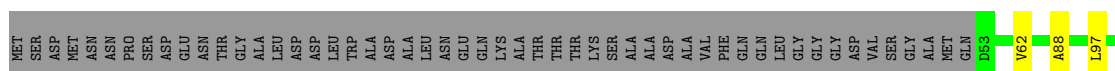


- Molecule 4: Flagellar motor switch protein FliN

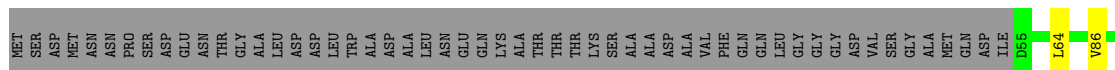


- Molecule 4: Flagellar motor switch protein FliN

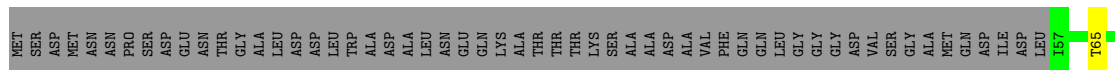




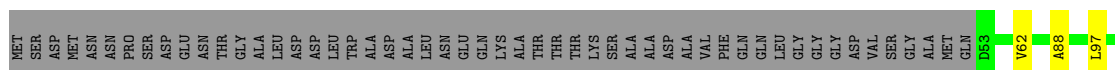
- Molecule 4: Flagellar motor switch protein FliN



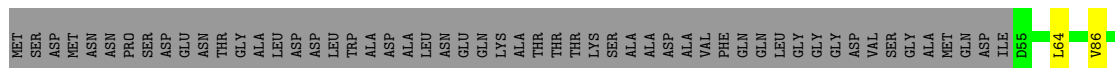
- Molecule 4: Flagellar motor switch protein FliN



- Molecule 4: Flagellar motor switch protein FliN

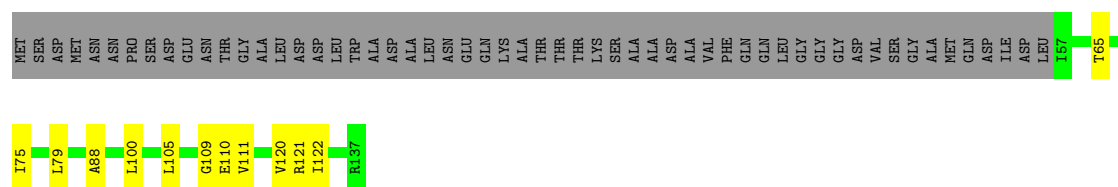


- Molecule 4: Flagellar motor switch protein FliN



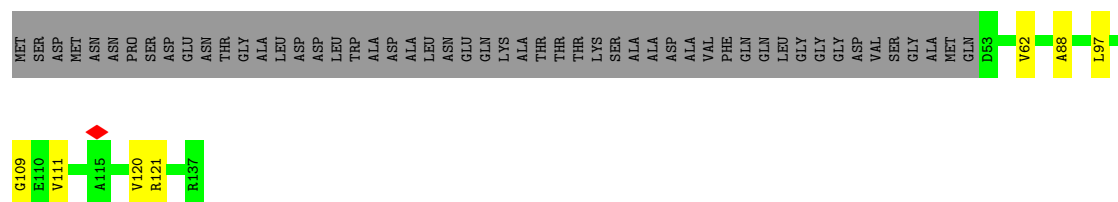
- Molecule 4: Flagellar motor switch protein FliN

Chain EG:  50% 9% 41%



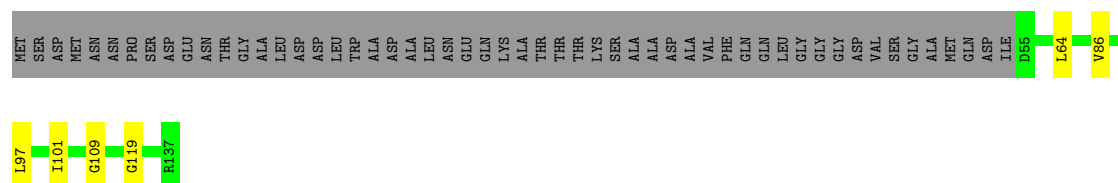
- Molecule 4: Flagellar motor switch protein FliN

Chain IG:  57% 5% 38%



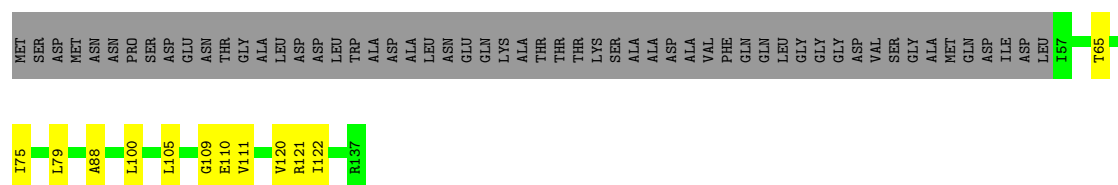
- Molecule 4: Flagellar motor switch protein FliN

Chain JG:  56% 39%



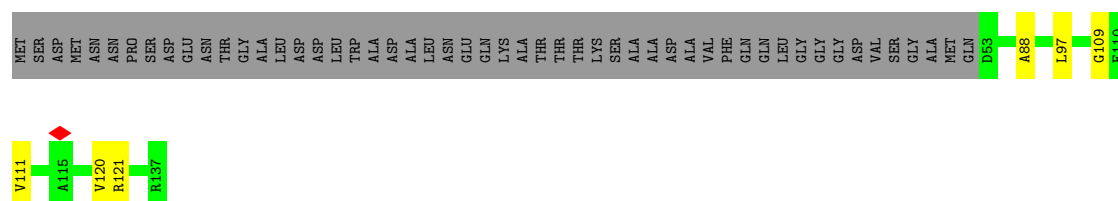
- Molecule 4: Flagellar motor switch protein FliN

Chain KG:  50% 9% 41%

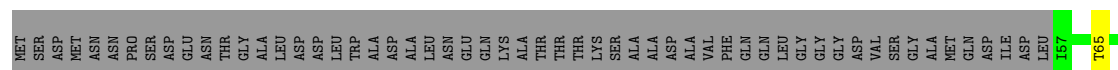
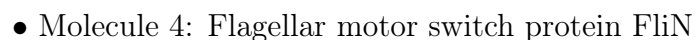
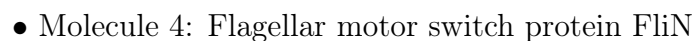
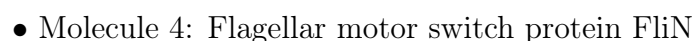
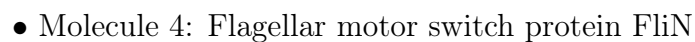


- Molecule 4: Flagellar motor switch protein FliN

Chain OG:  58% 38%



Chain PG: 56% 1% 39%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7201	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 ($e^-/\text{\AA}^2$)	56.323	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	0.376	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.151	Depositor
Map size (Å)	1049.6, 1049.6, 1049.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.05, 2.05, 2.05	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/234	0.48	0/324
1	BC	0.19	0/234	0.48	0/324
1	BF	0.19	0/234	0.48	0/324
1	DB	0.19	0/234	0.48	0/324
1	DE	0.19	0/234	0.48	0/324
1	F	0.19	0/234	0.48	0/324
1	FA	0.19	0/234	0.48	0/324
1	FD	0.19	0/234	0.48	0/324
1	FG	0.19	0/234	0.48	0/324
1	HC	0.19	0/234	0.48	0/324
1	HF	0.19	0/234	0.48	0/324
1	I	0.19	0/234	0.48	0/324
1	JB	0.19	0/234	0.48	0/324
1	JE	0.19	0/234	0.49	0/324
1	LA	0.19	0/234	0.49	0/324
1	LD	0.19	0/234	0.48	0/324
1	LG	0.19	0/234	0.48	0/324
1	NC	0.19	0/234	0.48	0/324
1	NF	0.19	0/234	0.48	0/324
1	PB	0.19	0/234	0.48	0/324
1	PE	0.19	0/234	0.48	0/324
1	RA	0.19	0/234	0.48	0/324
1	RD	0.19	0/234	0.48	0/324
1	RG	0.19	0/234	0.48	0/324
1	S	0.19	0/234	0.48	0/324
1	TC	0.19	0/234	0.48	0/324
1	TF	0.19	0/234	0.48	0/324
1	VB	0.19	0/234	0.48	0/324
1	VE	0.19	0/234	0.48	0/324
1	XA	0.19	0/234	0.48	0/324
1	XD	0.19	0/234	0.48	0/324
1	Z	0.19	0/234	0.48	0/324
1	ZC	0.19	0/234	0.48	0/324
1	ZF	0.19	0/234	0.48	0/324

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	AA	0.55	0/1578	0.73	0/2197
2	AD	0.55	0/1578	0.73	0/2197
2	AG	0.55	0/1578	0.73	0/2197
2	B	0.55	0/1578	0.73	0/2197
2	CC	0.55	0/1578	0.73	0/2197
2	CF	0.56	0/1578	0.73	0/2197
2	EB	0.55	0/1578	0.73	0/2197
2	EE	0.55	0/1578	0.73	0/2197
2	G	0.55	0/1578	0.73	0/2197
2	GA	0.56	0/1578	0.73	0/2197
2	GD	0.55	0/1578	0.73	0/2197
2	GG	0.55	0/1578	0.73	0/2197
2	IC	0.55	0/1578	0.73	0/2197
2	IF	0.55	0/1578	0.73	0/2197
2	J	0.55	0/1578	0.73	0/2197
2	KB	0.55	0/1578	0.73	0/2197
2	KE	0.55	0/1578	0.73	0/2197
2	MA	0.55	0/1578	0.73	0/2197
2	MD	0.55	0/1578	0.73	0/2197
2	MG	0.55	0/1578	0.73	0/2197
2	OC	0.56	0/1578	0.73	0/2197
2	OF	0.55	0/1578	0.73	0/2197
2	QB	0.55	0/1578	0.73	0/2197
2	QE	0.55	0/1578	0.73	0/2197
2	SA	0.55	0/1578	0.73	0/2197
2	SD	0.56	0/1578	0.73	0/2197
2	SG	0.55	0/1578	0.73	0/2197
2	T	0.55	0/1578	0.73	0/2197
2	UC	0.55	0/1578	0.73	0/2197
2	UF	0.56	0/1578	0.73	0/2197
2	WB	0.55	0/1578	0.73	0/2197
2	WE	0.55	0/1578	0.73	0/2197
2	YA	0.55	0/1578	0.73	0/2197
2	YD	0.55	0/1578	0.73	0/2197
3	BA	0.24	0/1389	0.43	0/1934
3	BD	0.23	0/1389	0.43	0/1934
3	BG	0.24	0/1389	0.43	0/1934
3	C	0.24	0/1389	0.43	0/1934
3	DC	0.24	0/1389	0.43	0/1934
3	DF	0.24	0/1389	0.43	0/1934
3	FB	0.23	0/1389	0.43	0/1934
3	FE	0.24	0/1389	0.43	0/1934
3	HA	0.24	0/1389	0.43	0/1934

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	HD	0.24	0/1389	0.43	0/1934
3	HG	0.24	0/1389	0.43	0/1934
3	JC	0.24	0/1389	0.43	0/1934
3	JF	0.23	0/1389	0.43	0/1934
3	K	0.23	0/1389	0.43	0/1934
3	LB	0.24	0/1389	0.43	0/1934
3	LE	0.24	0/1389	0.43	0/1934
3	M	0.23	0/1389	0.43	0/1934
3	NA	0.24	0/1389	0.43	0/1934
3	ND	0.23	0/1389	0.43	0/1934
3	NG	0.24	0/1389	0.43	0/1934
3	PC	0.24	0/1389	0.43	0/1934
3	PF	0.24	0/1389	0.43	0/1934
3	RB	0.24	0/1389	0.43	0/1934
3	RE	0.24	0/1389	0.43	0/1934
3	TA	0.23	0/1389	0.43	0/1934
3	TD	0.23	0/1389	0.43	0/1934
3	TG	0.24	0/1389	0.43	0/1934
3	V	0.24	0/1389	0.43	0/1934
3	VC	0.23	0/1389	0.43	0/1934
3	VF	0.24	0/1389	0.43	0/1934
3	XB	0.23	0/1389	0.43	0/1934
3	XE	0.24	0/1389	0.43	0/1934
3	ZA	0.24	0/1389	0.43	0/1934
3	ZD	0.23	0/1389	0.43	0/1934
4	AB	0.13	0/417	0.37	0/578
4	AC	0.12	0/397	0.33	0/550
4	AE	0.13	0/417	0.37	0/578
4	AF	0.12	0/397	0.33	0/550
4	BB	0.13	0/408	0.32	0/564
4	BE	0.13	0/408	0.32	0/564
4	CA	0.13	0/417	0.37	0/578
4	CB	0.12	0/397	0.33	0/550
4	CD	0.13	0/417	0.37	0/578
4	CE	0.12	0/397	0.33	0/550
4	CG	0.13	0/417	0.37	0/578
4	D	0.13	0/417	0.37	0/578
4	DA	0.13	0/408	0.32	0/564
4	DD	0.13	0/408	0.32	0/564
4	DG	0.13	0/408	0.32	0/564
4	E	0.13	0/408	0.32	0/564
4	EA	0.12	0/397	0.33	0/550
4	EC	0.13	0/417	0.37	0/578

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	ED	0.12	0/397	0.33	0/550
4	EF	0.13	0/417	0.37	0/578
4	EG	0.12	0/397	0.33	0/550
4	FC	0.13	0/408	0.32	0/564
4	FF	0.13	0/408	0.32	0/564
4	GB	0.13	0/417	0.37	0/578
4	GC	0.12	0/397	0.33	0/550
4	GE	0.13	0/417	0.37	0/578
4	GF	0.12	0/397	0.33	0/550
4	H	0.12	0/397	0.33	0/550
4	HB	0.13	0/408	0.32	0/564
4	HE	0.13	0/408	0.32	0/564
4	IA	0.13	0/417	0.37	0/578
4	IB	0.12	0/397	0.33	0/550
4	ID	0.13	0/417	0.37	0/578
4	IE	0.12	0/397	0.33	0/550
4	IG	0.13	0/417	0.37	0/578
4	JA	0.13	0/408	0.32	0/564
4	JD	0.13	0/408	0.32	0/564
4	JG	0.13	0/408	0.32	0/564
4	KA	0.12	0/397	0.33	0/550
4	KC	0.13	0/417	0.37	0/578
4	KD	0.12	0/397	0.33	0/550
4	KF	0.13	0/417	0.37	0/578
4	KG	0.12	0/397	0.33	0/550
4	L	0.13	0/417	0.37	0/578
4	LC	0.13	0/408	0.32	0/564
4	LF	0.13	0/408	0.32	0/564
4	MB	0.13	0/417	0.37	0/578
4	MC	0.12	0/397	0.33	0/550
4	ME	0.13	0/417	0.37	0/578
4	MF	0.12	0/397	0.33	0/550
4	N	0.13	0/417	0.37	0/578
4	NB	0.13	0/408	0.32	0/564
4	NE	0.13	0/408	0.32	0/564
4	O	0.13	0/408	0.32	0/564
4	OA	0.13	0/417	0.37	0/578
4	OB	0.12	0/397	0.33	0/550
4	OD	0.13	0/417	0.37	0/578
4	OE	0.12	0/397	0.33	0/550
4	OG	0.13	0/417	0.37	0/578
4	P	0.13	0/408	0.32	0/564
4	PA	0.13	0/408	0.32	0/564

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	PD	0.13	0/408	0.32	0/564
4	PG	0.13	0/408	0.32	0/564
4	Q	0.12	0/397	0.33	0/550
4	QA	0.12	0/397	0.33	0/550
4	QC	0.13	0/417	0.37	0/578
4	QD	0.12	0/397	0.33	0/550
4	QF	0.13	0/417	0.37	0/578
4	QG	0.12	0/397	0.33	0/550
4	R	0.12	0/397	0.33	0/550
4	RC	0.13	0/408	0.32	0/564
4	RF	0.13	0/408	0.32	0/564
4	SB	0.13	0/417	0.37	0/578
4	SC	0.12	0/397	0.33	0/550
4	SE	0.13	0/417	0.37	0/578
4	SF	0.12	0/397	0.33	0/550
4	TB	0.13	0/408	0.32	0/564
4	TE	0.13	0/408	0.32	0/564
4	UA	0.13	0/417	0.37	0/578
4	UB	0.12	0/397	0.33	0/550
4	UD	0.13	0/417	0.37	0/578
4	UE	0.12	0/397	0.33	0/550
4	UG	0.13	0/417	0.37	0/578
4	VA	0.13	0/408	0.32	0/564
4	VD	0.13	0/408	0.32	0/564
4	VG	0.13	0/408	0.32	0/564
4	W	0.13	0/417	0.37	0/578
4	WA	0.12	0/397	0.33	0/550
4	WC	0.13	0/417	0.37	0/578
4	WD	0.12	0/397	0.33	0/550
4	WF	0.13	0/417	0.37	0/578
4	WG	0.12	0/397	0.33	0/550
4	X	0.13	0/408	0.32	0/564
4	XC	0.13	0/408	0.32	0/564
4	XF	0.13	0/408	0.32	0/564
4	Y	0.12	0/397	0.33	0/550
4	YB	0.13	0/417	0.37	0/578
4	YC	0.12	0/397	0.33	0/550
4	YE	0.13	0/417	0.37	0/578
4	YF	0.12	0/397	0.33	0/550
4	ZB	0.13	0/408	0.32	0/564
4	ZE	0.13	0/408	0.32	0/564
All	All	0.37	0/150382	0.54	0/208998

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	235	0	102	0	0
1	BC	235	0	102	0	0
1	BF	235	0	102	0	0
1	DB	235	0	102	0	0
1	DE	235	0	102	0	0
1	F	235	0	102	0	0
1	FA	235	0	102	0	0
1	FD	235	0	102	0	0
1	FG	235	0	102	0	0
1	HC	235	0	102	0	0
1	HF	235	0	102	0	0
1	I	235	0	102	0	0
1	JB	235	0	102	0	0
1	JE	235	0	102	0	0
1	LA	235	0	102	0	0
1	LD	235	0	102	0	0
1	LG	235	0	102	0	0
1	NC	235	0	102	0	0
1	NF	235	0	102	0	0
1	PB	235	0	102	0	0
1	PE	235	0	102	0	0
1	RA	235	0	102	0	0
1	RD	235	0	102	0	0
1	RG	235	0	102	0	0
1	S	235	0	102	0	0
1	TC	235	0	102	0	0
1	TF	235	0	102	0	0
1	VB	235	0	102	0	0
1	VE	235	0	102	0	0
1	XA	235	0	102	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	XD	235	0	102	0	0
1	Z	235	0	102	0	0
1	ZC	235	0	102	0	0
1	ZF	235	0	102	0	0
2	AA	1580	0	739	49	0
2	AD	1580	0	739	51	0
2	AG	1580	0	739	49	0
2	B	1580	0	739	48	0
2	CC	1580	0	739	47	0
2	CF	1580	0	739	49	0
2	EB	1580	0	739	51	0
2	EE	1580	0	739	48	0
2	G	1580	0	739	48	0
2	GA	1580	0	739	50	0
2	GD	1580	0	739	52	0
2	GG	1580	0	739	51	0
2	IC	1580	0	739	49	0
2	IF	1580	0	739	47	0
2	J	1580	0	739	49	0
2	KB	1580	0	739	61	0
2	KE	1580	0	739	48	0
2	MA	1580	0	739	61	0
2	MD	1580	0	739	51	0
2	MG	1580	0	739	48	0
2	OC	1580	0	739	55	0
2	OF	1580	0	739	50	0
2	QB	1580	0	739	60	0
2	QE	1580	0	739	51	0
2	SA	1580	0	739	57	0
2	SD	1580	0	739	50	0
2	SG	1580	0	739	47	0
2	T	1580	0	739	51	0
2	UC	1580	0	739	54	0
2	UF	1580	0	739	50	0
2	WB	1580	0	739	47	0
2	WE	1580	0	739	51	0
2	YA	1580	0	739	50	0
2	YD	1580	0	739	48	0
3	BA	1390	0	592	13	0
3	BD	1390	0	592	14	0
3	BG	1390	0	592	13	0
3	C	1390	0	592	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	DC	1390	0	592	14	0
3	DF	1390	0	592	14	0
3	FB	1390	0	592	14	0
3	FE	1390	0	592	13	0
3	HA	1390	0	592	13	0
3	HD	1390	0	592	14	0
3	HG	1390	0	592	14	0
3	JC	1390	0	592	14	0
3	JF	1390	0	592	14	0
3	K	1390	0	592	14	0
3	LB	1390	0	592	13	0
3	LE	1390	0	592	14	0
3	M	1390	0	592	13	0
3	NA	1390	0	592	12	0
3	ND	1390	0	592	14	0
3	NG	1390	0	592	13	0
3	PC	1390	0	592	14	0
3	PF	1390	0	592	14	0
3	RB	1390	0	592	13	0
3	RE	1390	0	592	14	0
3	TA	1390	0	592	14	0
3	TD	1390	0	592	14	0
3	TG	1390	0	592	14	0
3	V	1390	0	592	14	0
3	VC	1390	0	592	13	0
3	VF	1390	0	592	13	0
3	XB	1390	0	592	14	0
3	XE	1390	0	592	14	0
3	ZA	1390	0	592	14	0
3	ZD	1390	0	592	13	0
4	AB	418	0	185	5	0
4	AC	398	0	177	8	0
4	AE	418	0	185	5	0
4	AF	398	0	177	9	0
4	BB	409	0	181	4	0
4	BE	409	0	181	5	0
4	CA	418	0	185	4	0
4	CB	398	0	177	8	0
4	CD	418	0	185	5	0
4	CE	398	0	177	9	0
4	CG	418	0	185	5	0
4	D	418	0	185	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	DA	409	0	181	4	0
4	DD	409	0	181	4	0
4	DG	409	0	181	4	0
4	E	409	0	181	4	0
4	EA	398	0	177	8	0
4	EC	418	0	185	5	0
4	ED	398	0	177	8	0
4	EF	418	0	185	5	0
4	EG	398	0	177	8	0
4	FC	409	0	181	4	0
4	FF	409	0	181	5	0
4	GB	418	0	185	5	0
4	GC	398	0	177	8	0
4	GE	418	0	185	5	0
4	GF	398	0	177	9	0
4	H	398	0	177	8	0
4	HB	409	0	181	4	0
4	HE	409	0	181	5	0
4	IA	418	0	185	5	0
4	IB	398	0	177	8	0
4	ID	418	0	185	5	0
4	IE	398	0	177	9	0
4	IG	418	0	185	5	0
4	JA	409	0	181	4	0
4	JD	409	0	181	4	0
4	JG	409	0	181	4	0
4	KA	398	0	177	8	0
4	KC	418	0	185	5	0
4	KD	398	0	177	8	0
4	KF	418	0	185	5	0
4	KG	398	0	177	8	0
4	L	418	0	185	5	0
4	LC	409	0	181	4	0
4	LF	409	0	181	5	0
4	MB	418	0	185	4	0
4	MC	398	0	177	8	0
4	ME	418	0	185	5	0
4	MF	398	0	177	9	0
4	N	418	0	185	5	0
4	NB	409	0	181	4	0
4	NE	409	0	181	5	0
4	O	409	0	181	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	OA	418	0	185	4	0
4	OB	398	0	177	8	0
4	OD	418	0	185	5	0
4	OE	398	0	177	9	0
4	OG	418	0	185	4	0
4	P	409	0	181	4	0
4	PA	409	0	181	4	0
4	PD	409	0	181	4	0
4	PG	409	0	181	4	0
4	Q	398	0	177	8	0
4	QA	398	0	177	8	0
4	QC	418	0	185	5	0
4	QD	398	0	177	8	0
4	QF	418	0	185	5	0
4	QG	398	0	177	8	0
4	R	398	0	177	8	0
4	RC	409	0	181	4	0
4	RF	409	0	181	5	0
4	SB	418	0	185	5	0
4	SC	398	0	177	8	0
4	SE	418	0	185	5	0
4	SF	398	0	177	9	0
4	TB	409	0	181	4	0
4	TE	409	0	181	5	0
4	UA	418	0	185	5	0
4	UB	398	0	177	8	0
4	UD	418	0	185	5	0
4	UE	398	0	177	9	0
4	UG	418	0	185	5	0
4	VA	409	0	181	4	0
4	VD	409	0	181	4	0
4	VG	409	0	181	4	0
4	W	418	0	185	5	0
4	WA	398	0	177	8	0
4	WC	418	0	185	4	0
4	WD	398	0	177	8	0
4	WF	418	0	185	5	0
4	WG	398	0	177	8	0
4	X	409	0	181	4	0
4	XC	409	0	181	4	0
4	XF	409	0	181	5	0
4	Y	398	0	177	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	YB	418	0	185	5	0
4	YC	398	0	177	8	0
4	YE	418	0	185	5	0
4	YF	398	0	177	9	0
4	ZB	409	0	181	4	0
4	ZE	409	0	181	5	0
All	All	150620	0	67184	1862	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 9.

All (1862) 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:KB:84:ALA:HB3	2:QB:23:ALA:CB	1.27	1.65
2:KB:84:ALA:CB	2:QB:23:ALA:HB1	1.27	1.64
2:MA:84:ALA:HB3	2:SA:23:ALA:CB	1.22	1.63
2:MA:84:ALA:CB	2:SA:23:ALA:CB	1.76	1.60
2:KB:84:ALA:CB	2:QB:23:ALA:CB	1.77	1.56
2:MA:84:ALA:CB	2:SA:23:ALA:HB1	1.30	1.45
2:MA:143:ALA:HB2	2:SA:205:LEU:CB	1.48	1.41
2:SA:143:ALA:HB2	2:YA:205:LEU:CB	1.52	1.40
2:KB:143:ALA:HB2	2:QB:205:LEU:CB	1.48	1.40
2:B:143:ALA:HB2	2:J:205:LEU:CB	1.52	1.40
2:GG:143:ALA:HB2	2:MG:205:LEU:CB	1.50	1.40
2:T:143:ALA:HB2	2:AA:205:LEU:CB	1.52	1.39
2:EB:143:ALA:HB2	2:KB:205:LEU:CB	1.52	1.39
2:G:143:ALA:HB2	2:B:205:LEU:CB	1.50	1.39
2:UF:143:ALA:HB2	2:AG:205:LEU:CB	1.51	1.39
2:GA:143:ALA:HB2	2:MA:205:LEU:CB	1.53	1.39
2:OF:143:ALA:HB2	2:UF:205:LEU:CB	1.52	1.39
2:AG:143:ALA:HB2	2:GG:205:LEU:CB	1.52	1.39
2:QB:143:ALA:HB2	2:WB:205:LEU:CB	1.52	1.39
2:CC:143:ALA:HB2	2:IC:205:LEU:CB	1.51	1.39
2:WE:143:ALA:HB2	2:CF:205:LEU:CB	1.50	1.38
2:MD:143:ALA:HB2	2:SD:205:LEU:CB	1.50	1.38
2:MG:143:ALA:HB2	2:SG:205:LEU:CB	1.51	1.38
2:G:205:LEU:CB	2:SG:143:ALA:HB2	1.53	1.38
2:OC:143:ALA:HB2	2:UC:205:LEU:CB	1.51	1.38
2:UC:143:ALA:HB2	2:AD:205:LEU:CB	1.51	1.38
2:YD:143:ALA:HB2	2:EE:205:LEU:CB	1.51	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CF:143:ALA:HB2	2:IF:205:LEU:CB	1.51	1.38
2:AD:143:ALA:HB2	2:GD:205:LEU:CB	1.52	1.37
2:QE:143:ALA:HB2	2:WE:205:LEU:CB	1.51	1.37
2:GD:143:ALA:HB2	2:MD:205:LEU:CB	1.51	1.37
2:IF:143:ALA:HB2	2:OF:205:LEU:CB	1.54	1.37
2:J:143:ALA:HB2	2:T:205:LEU:CB	1.54	1.36
2:AA:143:ALA:HB2	2:GA:205:LEU:CB	1.53	1.36
2:WB:143:ALA:HB2	2:CC:205:LEU:CB	1.53	1.36
2:KE:143:ALA:HB2	2:QE:205:LEU:CB	1.54	1.35
2:SD:143:ALA:HB2	2:YD:205:LEU:CB	1.52	1.35
2:IC:143:ALA:HB2	2:OC:205:LEU:CB	1.54	1.35
2:EE:143:ALA:HB2	2:KE:205:LEU:CB	1.52	1.35
2:YA:143:ALA:HB2	2:EB:205:LEU:CB	1.55	1.34
2:MA:80:VAL:CB	2:SA:19:GLU:CB	2.12	1.27
2:KB:143:ALA:CB	2:QB:205:LEU:CB	2.16	1.24
2:UC:80:VAL:CB	2:AD:19:GLU:CB	2.15	1.23
2:WE:80:VAL:CB	2:CF:19:GLU:CB	2.16	1.23
2:EE:80:VAL:CB	2:KE:19:GLU:CB	2.17	1.23
2:MA:143:ALA:CB	2:SA:205:LEU:CB	2.17	1.23
2:MD:80:VAL:CB	2:SD:19:GLU:CB	2.16	1.23
2:QB:80:VAL:CB	2:WB:19:GLU:CB	2.16	1.22
2:KB:80:VAL:CB	2:QB:19:GLU:CB	2.18	1.22
2:MG:80:VAL:CB	2:SG:19:GLU:CB	2.15	1.22
2:SD:80:VAL:CB	2:YD:19:GLU:CB	2.18	1.22
2:G:80:VAL:CB	2:B:19:GLU:CB	2.16	1.21
2:CC:80:VAL:CB	2:IC:19:GLU:CB	2.17	1.21
2:CF:80:VAL:CB	2:IF:19:GLU:CB	2.18	1.21
2:UF:80:VAL:CB	2:AG:19:GLU:CB	2.17	1.21
2:YD:80:VAL:CB	2:EE:19:GLU:CB	2.18	1.21
2:QE:80:VAL:CB	2:WE:19:GLU:CB	2.19	1.21
2:SA:80:VAL:CB	2:YA:19:GLU:CB	2.19	1.20
2:GD:80:VAL:CB	2:MD:19:GLU:CB	2.18	1.20
2:GG:80:VAL:CB	2:MG:19:GLU:CB	2.18	1.20
2:GG:143:ALA:CB	2:MG:205:LEU:CB	2.20	1.20
2:AA:80:VAL:CB	2:GA:19:GLU:CB	2.19	1.19
2:WE:143:ALA:CB	2:CF:205:LEU:CB	2.20	1.19
2:IF:80:VAL:CB	2:OF:19:GLU:CB	2.19	1.19
2:EB:80:VAL:CB	2:KB:19:GLU:CB	2.20	1.19
2:OC:143:ALA:CB	2:UC:205:LEU:CB	2.20	1.19
2:MD:143:ALA:CB	2:SD:205:LEU:CB	2.20	1.19
2:UF:143:ALA:CB	2:AG:205:LEU:CB	2.21	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:VAL:CB	2:J:19:GLU:CB	2.19	1.18
2:YD:143:ALA:CB	2:EE:205:LEU:CB	2.21	1.18
2:OF:143:ALA:CB	2:UF:205:LEU:CB	2.22	1.18
2:UC:143:ALA:CB	2:AD:205:LEU:CB	2.22	1.18
2:OF:80:VAL:CB	2:UF:19:GLU:CB	2.21	1.18
2:AG:143:ALA:CB	2:GG:205:LEU:CB	2.22	1.18
2:WB:80:VAL:CB	2:CC:19:GLU:CB	2.21	1.17
2:IC:80:VAL:CB	2:OC:19:GLU:CB	2.21	1.17
2:CF:143:ALA:CB	2:IF:205:LEU:CB	2.22	1.17
2:QE:143:ALA:CB	2:WE:205:LEU:CB	2.22	1.17
2:G:143:ALA:CB	2:B:205:LEU:CB	2.21	1.17
2:T:80:VAL:CB	2:AA:19:GLU:CB	2.21	1.17
2:KB:68:ALA:HB2	2:QB:47:ILE:O	1.44	1.17
2:AG:80:VAL:CB	2:GG:19:GLU:CB	2.21	1.17
2:EB:143:ALA:CB	2:KB:205:LEU:CB	2.23	1.17
2:GD:143:ALA:CB	2:MD:205:LEU:CB	2.22	1.17
2:OC:80:VAL:CB	2:UC:19:GLU:CB	2.23	1.17
2:J:80:VAL:CB	2:T:19:GLU:CB	2.21	1.16
2:SA:143:ALA:CB	2:YA:205:LEU:CB	2.23	1.16
2:AD:80:VAL:CB	2:GD:19:GLU:CB	2.22	1.16
2:MG:143:ALA:CB	2:SG:205:LEU:CB	2.22	1.16
2:GA:143:ALA:CB	2:MA:205:LEU:CB	2.23	1.16
2:OC:68:ALA:HB2	2:UC:47:ILE:O	1.45	1.16
2:GA:80:VAL:CB	2:MA:19:GLU:CB	2.22	1.16
2:YA:80:VAL:CB	2:EB:19:GLU:CB	2.22	1.16
2:T:143:ALA:CB	2:AA:205:LEU:CB	2.22	1.16
2:CC:143:ALA:CB	2:IC:205:LEU:CB	2.23	1.16
2:G:19:GLU:CB	2:SG:80:VAL:CB	2.22	1.16
2:EE:143:ALA:CB	2:KE:205:LEU:CB	2.24	1.16
2:AD:143:ALA:CB	2:GD:205:LEU:CB	2.22	1.15
2:SD:143:ALA:CB	2:YD:205:LEU:CB	2.24	1.15
2:KE:80:VAL:CB	2:QE:19:GLU:CB	2.24	1.15
2:G:205:LEU:CB	2:SG:143:ALA:CB	2.24	1.15
2:B:143:ALA:CB	2:J:205:LEU:CB	2.23	1.15
2:WB:143:ALA:CB	2:CC:205:LEU:CB	2.24	1.15
2:AA:143:ALA:CB	2:GA:205:LEU:CB	2.24	1.15
2:QB:143:ALA:CB	2:WB:205:LEU:CB	2.23	1.15
2:GA:68:ALA:HB2	2:MA:47:ILE:O	1.47	1.14
2:OC:143:ALA:HB1	2:UC:205:LEU:C	1.72	1.14
2:YD:68:ALA:HB2	2:EE:47:ILE:O	1.48	1.14
2:KE:143:ALA:CB	2:QE:205:LEU:CB	2.24	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:OF:68:ALA:HB2	2:UF:47:ILE:O	1.48	1.14
2:IF:143:ALA:CB	2:OF:205:LEU:CB	2.26	1.14
2:T:68:ALA:HB2	2:AA:47:ILE:O	1.48	1.14
2:OC:67:ALA:O	2:UC:48:SER:HA	1.48	1.14
2:MA:68:ALA:HB2	2:SA:47:ILE:O	1.48	1.13
2:AD:68:ALA:HB2	2:GD:47:ILE:O	1.48	1.13
2:KB:143:ALA:HB1	2:QB:205:LEU:C	1.72	1.13
2:WE:68:ALA:HB2	2:CF:47:ILE:O	1.48	1.13
2:WB:68:ALA:HB2	2:CC:47:ILE:O	1.49	1.13
2:G:47:ILE:O	2:SG:68:ALA:HB2	1.49	1.12
2:J:143:ALA:CB	2:T:205:LEU:CB	2.25	1.12
2:GD:68:ALA:HB2	2:MD:47:ILE:O	1.49	1.12
2:GA:67:ALA:O	2:MA:48:SER:HA	1.50	1.12
2:IC:143:ALA:CB	2:OC:205:LEU:CB	2.26	1.12
2:AG:68:ALA:HB2	2:GG:47:ILE:O	1.48	1.12
2:G:68:ALA:HB2	2:B:47:ILE:O	1.50	1.12
2:B:68:ALA:HB2	2:J:47:ILE:O	1.49	1.12
2:YA:143:ALA:CB	2:EB:205:LEU:CB	2.27	1.12
2:MD:68:ALA:HB2	2:SD:47:ILE:O	1.48	1.12
2:OF:143:ALA:HB1	2:UF:205:LEU:C	1.75	1.12
2:CF:68:ALA:HB2	2:IF:47:ILE:O	1.49	1.12
2:GG:68:ALA:HB2	2:MG:47:ILE:O	1.48	1.12
2:AD:143:ALA:HB1	2:GD:205:LEU:C	1.74	1.11
2:QE:68:ALA:HB2	2:WE:47:ILE:O	1.48	1.11
2:KE:143:ALA:HB1	2:QE:205:LEU:C	1.75	1.11
2:AG:143:ALA:HB1	2:GG:205:LEU:C	1.76	1.11
2:UC:68:ALA:HB2	2:AD:47:ILE:O	1.50	1.11
2:EB:68:ALA:HB2	2:KB:47:ILE:O	1.49	1.11
2:IC:68:ALA:HB2	2:OC:47:ILE:O	1.51	1.11
2:SD:68:ALA:HB2	2:YD:47:ILE:O	1.51	1.11
2:KE:67:ALA:O	2:QE:48:SER:HA	1.49	1.11
2:G:48:SER:HA	2:SG:67:ALA:O	1.51	1.10
2:AA:68:ALA:HB2	2:GA:47:ILE:O	1.51	1.10
2:YD:143:ALA:HB1	2:EE:205:LEU:C	1.76	1.10
2:KE:68:ALA:HB2	2:QE:47:ILE:O	1.49	1.10
2:KB:67:ALA:O	2:QB:48:SER:HA	1.51	1.10
2:EE:68:ALA:HB2	2:KE:47:ILE:O	1.51	1.10
2:MG:68:ALA:HB2	2:SG:47:ILE:O	1.51	1.10
2:GA:143:ALA:HB1	2:MA:205:LEU:C	1.74	1.10
2:WE:143:ALA:HB1	2:CF:205:LEU:C	1.77	1.10
2:UF:68:ALA:HB2	2:AG:47:ILE:O	1.49	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GG:143:ALA:HB1	2:MG:205:LEU:C	1.76	1.10
2:G:205:LEU:C	2:SG:143:ALA:HB1	1.76	1.10
2:MA:84:ALA:CB	2:SA:23:ALA:HB3	1.59	1.10
2:SA:68:ALA:HB2	2:YA:47:ILE:O	1.50	1.10
2:QE:143:ALA:HB1	2:WE:205:LEU:C	1.76	1.10
2:AG:67:ALA:O	2:GG:48:SER:HA	1.52	1.10
2:J:68:ALA:HB2	2:T:47:ILE:O	1.51	1.09
2:T:143:ALA:HB1	2:AA:205:LEU:C	1.75	1.09
2:CF:143:ALA:HB1	2:IF:205:LEU:C	1.77	1.09
2:J:67:ALA:O	2:T:48:SER:HA	1.53	1.09
2:YA:67:ALA:O	2:EB:48:SER:HA	1.53	1.09
2:YA:68:ALA:HB2	2:EB:47:ILE:O	1.52	1.09
2:WB:143:ALA:HB1	2:CC:205:LEU:C	1.76	1.09
2:CC:68:ALA:HB2	2:IC:47:ILE:O	1.51	1.09
2:MD:143:ALA:HB1	2:SD:205:LEU:C	1.77	1.09
2:QE:67:ALA:O	2:WE:48:SER:HA	1.53	1.09
2:UF:143:ALA:HB1	2:AG:205:LEU:C	1.77	1.09
2:AD:67:ALA:O	2:GD:48:SER:HA	1.50	1.09
2:J:143:ALA:HB1	2:T:205:LEU:C	1.78	1.08
2:T:67:ALA:O	2:AA:48:SER:HA	1.51	1.08
2:IC:67:ALA:O	2:OC:48:SER:HA	1.53	1.08
2:G:143:ALA:HB1	2:B:205:LEU:C	1.78	1.08
2:GD:143:ALA:HB1	2:MD:205:LEU:C	1.77	1.08
2:YD:67:ALA:O	2:EE:48:SER:HA	1.53	1.08
2:OF:67:ALA:O	2:UF:48:SER:HA	1.51	1.08
2:IF:68:ALA:HB2	2:OF:47:ILE:O	1.52	1.08
2:EB:67:ALA:O	2:KB:48:SER:HA	1.52	1.08
2:B:67:ALA:O	2:J:48:SER:HA	1.53	1.07
2:EB:143:ALA:HB1	2:KB:205:LEU:C	1.76	1.07
2:WB:67:ALA:O	2:CC:48:SER:HA	1.52	1.07
2:B:143:ALA:HB1	2:J:205:LEU:C	1.77	1.07
2:AA:143:ALA:HB1	2:GA:205:LEU:C	1.78	1.07
2:QB:68:ALA:HB2	2:WB:47:ILE:O	1.52	1.07
2:IC:143:ALA:HB1	2:OC:205:LEU:C	1.78	1.07
2:GD:67:ALA:O	2:MD:48:SER:HA	1.54	1.07
2:CF:67:ALA:O	2:IF:48:SER:HA	1.54	1.07
2:SD:143:ALA:HB1	2:YD:205:LEU:C	1.79	1.07
2:UF:67:ALA:O	2:AG:48:SER:HA	1.54	1.07
2:SA:67:ALA:O	2:YA:48:SER:HA	1.54	1.07
2:YA:143:ALA:HB1	2:EB:205:LEU:C	1.78	1.07
2:IF:67:ALA:O	2:OF:48:SER:HA	1.55	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SA:143:ALA:HB1	2:YA:205:LEU:C	1.78	1.06
2:AA:67:ALA:O	2:GA:48:SER:HA	1.54	1.06
2:MA:143:ALA:HB1	2:SA:205:LEU:C	1.79	1.06
2:EE:143:ALA:HB1	2:KE:205:LEU:C	1.79	1.06
2:MG:143:ALA:HB1	2:SG:205:LEU:C	1.80	1.06
2:IF:143:ALA:HB1	2:OF:205:LEU:C	1.80	1.06
2:CC:143:ALA:HB1	2:IC:205:LEU:C	1.79	1.06
2:CC:67:ALA:O	2:IC:48:SER:HA	1.56	1.05
2:GG:67:ALA:O	2:MG:48:SER:HA	1.53	1.05
2:QB:143:ALA:HB1	2:WB:205:LEU:C	1.80	1.05
2:KB:84:ALA:HB2	2:QB:23:ALA:HB3	1.05	1.05
2:UC:143:ALA:HB1	2:AD:205:LEU:C	1.79	1.05
2:MA:84:ALA:HB2	2:SA:23:ALA:HB3	1.05	1.04
2:WE:67:ALA:O	2:CF:48:SER:HA	1.55	1.04
2:MD:67:ALA:O	2:SD:48:SER:HA	1.55	1.04
2:EE:67:ALA:O	2:KE:48:SER:HA	1.56	1.04
2:SD:67:ALA:O	2:YD:48:SER:HA	1.55	1.04
2:G:67:ALA:O	2:B:48:SER:HA	1.56	1.04
2:UC:67:ALA:O	2:AD:48:SER:HA	1.57	1.03
2:MG:67:ALA:O	2:SG:48:SER:HA	1.58	1.03
2:QB:67:ALA:O	2:WB:48:SER:HA	1.57	1.02
2:MA:67:ALA:O	2:SA:48:SER:HA	1.58	1.01
2:OC:143:ALA:CB	2:UC:205:LEU:C	2.35	0.99
2:KE:143:ALA:CB	2:QE:205:LEU:C	2.37	0.98
2:GA:143:ALA:CB	2:MA:205:LEU:C	2.37	0.98
2:AD:143:ALA:CB	2:GD:205:LEU:C	2.37	0.97
2:KB:143:ALA:CB	2:QB:205:LEU:C	2.38	0.96
2:OF:143:ALA:CB	2:UF:205:LEU:C	2.38	0.96
2:G:205:LEU:C	2:SG:143:ALA:CB	2.39	0.96
2:T:143:ALA:CB	2:AA:205:LEU:C	2.38	0.95
2:AG:143:ALA:CB	2:GG:205:LEU:C	2.39	0.95
2:WB:143:ALA:CB	2:CC:205:LEU:C	2.39	0.95
2:B:143:ALA:CB	2:J:205:LEU:C	2.41	0.94
2:J:143:ALA:CB	2:T:205:LEU:C	2.40	0.94
2:YD:143:ALA:CB	2:EE:205:LEU:C	2.41	0.94
2:YA:143:ALA:CB	2:EB:205:LEU:C	2.40	0.94
2:GG:143:ALA:CB	2:MG:205:LEU:C	2.40	0.94
2:CF:143:ALA:CB	2:IF:205:LEU:C	2.41	0.93
2:EB:143:ALA:CB	2:KB:205:LEU:C	2.40	0.93
2:QE:143:ALA:CB	2:WE:205:LEU:C	2.40	0.93
2:UF:143:ALA:CB	2:AG:205:LEU:C	2.42	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:KB:84:ALA:CB	2:QB:23:ALA:HB3	1.64	0.93
2:WE:143:ALA:CB	2:CF:205:LEU:C	2.42	0.93
2:SA:143:ALA:CB	2:YA:205:LEU:C	2.42	0.93
2:IF:143:ALA:CB	2:OF:205:LEU:C	2.42	0.93
2:IC:143:ALA:CB	2:OC:205:LEU:C	2.40	0.92
2:GD:143:ALA:CB	2:MD:205:LEU:C	2.41	0.92
2:G:143:ALA:CB	2:B:205:LEU:C	2.43	0.92
2:AA:143:ALA:CB	2:GA:205:LEU:C	2.42	0.92
2:SD:143:ALA:CB	2:YD:205:LEU:C	2.42	0.92
2:EE:143:ALA:CB	2:KE:205:LEU:C	2.43	0.91
2:MD:143:ALA:CB	2:SD:205:LEU:C	2.43	0.91
2:CC:143:ALA:CB	2:IC:205:LEU:C	2.43	0.90
2:UC:143:ALA:CB	2:AD:205:LEU:C	2.44	0.89
2:MG:143:ALA:CB	2:SG:205:LEU:C	2.45	0.89
2:MA:143:ALA:CB	2:SA:205:LEU:C	2.45	0.89
2:OC:68:ALA:CB	2:UC:47:ILE:O	2.20	0.89
2:QB:143:ALA:CB	2:WB:205:LEU:C	2.45	0.88
2:AD:68:ALA:CB	2:GD:47:ILE:O	2.22	0.87
2:GA:68:ALA:CB	2:MA:47:ILE:O	2.22	0.87
2:KB:68:ALA:CB	2:QB:47:ILE:O	2.21	0.87
2:KE:68:ALA:CB	2:QE:47:ILE:O	2.22	0.86
2:OC:155:HIS:CB	2:UC:217:ALA:CB	2.53	0.86
2:OF:68:ALA:CB	2:UF:47:ILE:O	2.23	0.86
2:T:68:ALA:CB	2:AA:47:ILE:O	2.23	0.86
2:EB:68:ALA:CB	2:KB:47:ILE:O	2.24	0.86
2:WB:68:ALA:CB	2:CC:47:ILE:O	2.23	0.86
2:OC:67:ALA:O	2:UC:48:SER:CA	2.25	0.85
2:YD:68:ALA:CB	2:EE:47:ILE:O	2.24	0.85
2:GG:68:ALA:CB	2:MG:47:ILE:O	2.24	0.85
2:YA:68:ALA:CB	2:EB:47:ILE:O	2.25	0.85
2:G:47:ILE:O	2:SG:68:ALA:CB	2.23	0.85
2:SA:68:ALA:CB	2:YA:47:ILE:O	2.25	0.85
2:IC:68:ALA:CB	2:OC:47:ILE:O	2.25	0.85
2:MD:68:ALA:CB	2:SD:47:ILE:O	2.25	0.85
2:KB:155:HIS:CB	2:QB:217:ALA:CB	2.55	0.85
2:B:68:ALA:CB	2:J:47:ILE:O	2.24	0.85
2:QE:68:ALA:CB	2:WE:47:ILE:O	2.24	0.84
2:GD:68:ALA:CB	2:MD:47:ILE:O	2.24	0.84
2:UF:68:ALA:CB	2:AG:47:ILE:O	2.24	0.84
2:AG:68:ALA:CB	2:GG:47:ILE:O	2.23	0.84
2:J:68:ALA:CB	2:T:47:ILE:O	2.24	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CC:68:ALA:CB	2:IC:47:ILE:O	2.26	0.84
2:CF:68:ALA:CB	2:IF:47:ILE:O	2.25	0.84
2:AA:68:ALA:CB	2:GA:47:ILE:O	2.25	0.84
2:WE:68:ALA:CB	2:CF:47:ILE:O	2.24	0.84
2:SD:68:ALA:CB	2:YD:47:ILE:O	2.25	0.83
2:QB:68:ALA:CB	2:WB:47:ILE:O	2.27	0.83
2:EE:68:ALA:CB	2:KE:47:ILE:O	2.26	0.83
2:MA:68:ALA:CB	2:SA:47:ILE:O	2.26	0.83
2:KB:67:ALA:O	2:QB:48:SER:CA	2.26	0.83
2:G:68:ALA:CB	2:B:47:ILE:O	2.26	0.82
2:GA:155:HIS:CB	2:MA:217:ALA:CB	2.57	0.82
2:UC:68:ALA:CB	2:AD:47:ILE:O	2.26	0.82
2:AD:67:ALA:O	2:GD:48:SER:CA	2.27	0.82
2:T:67:ALA:O	2:AA:48:SER:CA	2.28	0.82
2:OF:67:ALA:O	2:UF:48:SER:CA	2.28	0.82
2:AD:155:HIS:CB	2:GD:217:ALA:CB	2.58	0.82
2:IF:68:ALA:CB	2:OF:47:ILE:O	2.26	0.82
2:GA:67:ALA:O	2:MA:48:SER:CA	2.27	0.81
2:MG:68:ALA:CB	2:SG:47:ILE:O	2.27	0.81
2:KE:155:HIS:CB	2:QE:217:ALA:CB	2.58	0.81
2:OF:155:HIS:CB	2:UF:217:ALA:CB	2.59	0.81
2:KE:67:ALA:O	2:QE:48:SER:CA	2.27	0.81
2:GG:67:ALA:O	2:MG:48:SER:CA	2.29	0.81
2:YD:67:ALA:O	2:EE:48:SER:CA	2.30	0.80
2:QE:67:ALA:O	2:WE:48:SER:CA	2.30	0.80
2:WB:67:ALA:O	2:CC:48:SER:CA	2.29	0.80
2:T:155:HIS:CB	2:AA:217:ALA:CB	2.59	0.80
2:EB:67:ALA:O	2:KB:48:SER:CA	2.29	0.80
2:B:67:ALA:O	2:J:48:SER:CA	2.30	0.79
2:GD:67:ALA:O	2:MD:48:SER:CA	2.30	0.79
2:G:48:SER:CA	2:SG:67:ALA:O	2.29	0.79
2:WB:155:HIS:CB	2:CC:217:ALA:CB	2.61	0.79
2:AG:155:HIS:CB	2:GG:217:ALA:CB	2.60	0.79
2:WE:67:ALA:O	2:CF:48:SER:CA	2.30	0.79
2:EB:155:HIS:CB	2:KB:217:ALA:CB	2.61	0.79
2:GG:155:HIS:CB	2:MG:217:ALA:CB	2.60	0.79
2:G:217:ALA:CB	2:SG:155:HIS:CB	2.61	0.78
2:OC:143:ALA:HB1	2:UC:206:MET:N	1.97	0.78
2:QE:155:HIS:CB	2:WE:217:ALA:CB	2.61	0.78
2:SA:67:ALA:O	2:YA:48:SER:CA	2.31	0.78
2:AG:67:ALA:O	2:GG:48:SER:CA	2.29	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:67:ALA:O	2:B:48:SER:CA	2.32	0.78
2:AA:67:ALA:O	2:GA:48:SER:CA	2.32	0.78
2:J:67:ALA:O	2:T:48:SER:CA	2.31	0.78
2:UF:67:ALA:O	2:AG:48:SER:CA	2.31	0.78
2:YD:155:HIS:CB	2:EE:217:ALA:CB	2.61	0.78
2:MD:67:ALA:O	2:SD:48:SER:CA	2.31	0.77
2:WE:155:HIS:CB	2:CF:217:ALA:CB	2.62	0.77
2:UF:155:HIS:CB	2:AG:217:ALA:CB	2.62	0.77
2:GD:155:HIS:CB	2:MD:217:ALA:CB	2.62	0.77
2:CF:67:ALA:O	2:IF:48:SER:CA	2.31	0.77
2:YA:67:ALA:O	2:EB:48:SER:CA	2.31	0.77
2:KE:139:ARG:O	2:QE:205:LEU:CB	2.33	0.77
2:MA:67:ALA:O	2:SA:48:SER:CA	2.33	0.77
2:OC:139:ARG:O	2:UC:205:LEU:CB	2.33	0.77
2:IC:155:HIS:CB	2:OC:217:ALA:CB	2.63	0.77
2:B:155:HIS:CB	2:J:217:ALA:CB	2.62	0.77
2:MA:161:ILE:CB	2:SA:199:ALA:HB2	2.13	0.76
2:IC:67:ALA:O	2:OC:48:SER:CA	2.31	0.76
2:MD:155:HIS:CB	2:SD:217:ALA:CB	2.63	0.76
2:EE:67:ALA:O	2:KE:48:SER:CA	2.33	0.76
2:SA:155:HIS:CB	2:YA:217:ALA:CB	2.64	0.76
2:MD:161:ILE:CB	2:SD:199:ALA:HB2	2.16	0.76
2:YA:155:HIS:CB	2:EB:217:ALA:CB	2.64	0.76
2:CC:67:ALA:O	2:IC:48:SER:CA	2.33	0.76
2:KB:143:ALA:HB1	2:QB:206:MET:N	1.99	0.76
2:CF:155:HIS:CB	2:IF:217:ALA:CB	2.63	0.76
2:J:155:HIS:CB	2:T:217:ALA:CB	2.63	0.75
2:WE:161:ILE:CB	2:CF:199:ALA:HB2	2.16	0.75
2:KB:161:ILE:CB	2:QB:199:ALA:HB2	2.16	0.75
2:UC:161:ILE:CB	2:AD:199:ALA:HB2	2.16	0.75
2:KE:143:ALA:HB1	2:QE:206:MET:N	2.01	0.75
2:G:161:ILE:CB	2:B:199:ALA:HB2	2.16	0.75
2:GA:139:ARG:O	2:MA:205:LEU:CB	2.34	0.75
2:UC:67:ALA:O	2:AD:48:SER:CA	2.33	0.75
2:AD:139:ARG:O	2:GD:205:LEU:CB	2.35	0.75
2:MA:155:HIS:CB	2:SA:217:ALA:CB	2.65	0.75
2:AA:155:HIS:CB	2:GA:217:ALA:CB	2.64	0.75
2:MG:67:ALA:O	2:SG:48:SER:CA	2.34	0.75
2:MG:161:ILE:CB	2:SG:199:ALA:HB2	2.16	0.75
2:G:155:HIS:CB	2:B:217:ALA:CB	2.64	0.75
2:SD:67:ALA:O	2:YD:48:SER:CA	2.32	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:YD:161:ILE:CB	2:EE:199:ALA:HB2	2.17	0.75
2:GA:143:ALA:HB1	2:MA:206:MET:N	2.00	0.74
2:GD:161:ILE:CB	2:MD:199:ALA:HB2	2.17	0.74
2:CC:155:HIS:CB	2:IC:217:ALA:CB	2.66	0.74
2:SD:155:HIS:CB	2:YD:217:ALA:CB	2.65	0.74
2:OF:143:ALA:HB1	2:UF:206:MET:N	2.02	0.74
2:G:205:LEU:CB	2:SG:139:ARG:O	2.36	0.74
2:AD:143:ALA:HB1	2:GD:206:MET:N	2.01	0.74
2:QB:161:ILE:CB	2:WB:199:ALA:HB2	2.17	0.74
2:CC:161:ILE:CB	2:IC:199:ALA:HB2	2.17	0.74
2:SD:161:ILE:CB	2:YD:199:ALA:HB2	2.18	0.74
2:EE:161:ILE:CB	2:KE:199:ALA:HB2	2.17	0.74
2:QE:161:ILE:CB	2:WE:199:ALA:HB2	2.17	0.74
2:UC:155:HIS:CB	2:AD:217:ALA:CB	2.66	0.74
2:GG:161:ILE:CB	2:MG:199:ALA:HB2	2.17	0.74
2:OF:139:ARG:O	2:UF:205:LEU:CB	2.36	0.73
2:AA:161:ILE:CB	2:GA:199:ALA:HB2	2.18	0.73
2:YA:139:ARG:O	2:EB:205:LEU:CB	2.36	0.73
2:IF:155:HIS:CB	2:OF:217:ALA:CB	2.66	0.73
2:B:161:ILE:CB	2:J:199:ALA:HB2	2.18	0.73
2:SA:161:ILE:CB	2:YA:199:ALA:HB2	2.18	0.73
2:IF:67:ALA:O	2:OF:48:SER:CA	2.33	0.73
2:KB:84:ALA:HB2	2:QB:23:ALA:CB	1.68	0.73
2:T:139:ARG:O	2:AA:205:LEU:CB	2.36	0.73
2:WB:139:ARG:O	2:CC:205:LEU:CB	2.36	0.73
2:IC:139:ARG:O	2:OC:205:LEU:CB	2.36	0.73
2:AG:143:ALA:HB1	2:GG:206:MET:N	2.03	0.73
2:UF:161:ILE:CB	2:AG:199:ALA:HB2	2.17	0.73
2:EE:155:HIS:CB	2:KE:217:ALA:CB	2.66	0.73
2:AG:139:ARG:O	2:GG:205:LEU:CB	2.37	0.73
2:AG:161:ILE:CB	2:GG:199:ALA:HB2	2.18	0.73
4:VD:64:LEU:HA	4:VD:101:ILE:HA	1.71	0.73
4:NE:64:LEU:HA	4:NE:101:ILE:HA	1.71	0.73
2:CF:161:ILE:CB	2:IF:199:ALA:HB2	2.17	0.73
4:FF:64:LEU:HA	4:FF:101:ILE:HA	1.71	0.73
2:OF:161:ILE:CB	2:UF:199:ALA:HB2	2.18	0.72
4:XF:64:LEU:HA	4:XF:101:ILE:HA	1.71	0.72
2:T:143:ALA:HB1	2:AA:206:MET:N	2.02	0.72
2:T:161:ILE:CB	2:AA:199:ALA:HB2	2.18	0.72
2:GA:161:ILE:CB	2:MA:199:ALA:HB2	2.19	0.72
2:EB:139:ARG:O	2:KB:205:LEU:CB	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:161:ILE:CB	2:KB:199:ALA:HB2	2.18	0.72
4:DD:64:LEU:HA	4:DD:101:ILE:HA	1.71	0.72
4:BE:64:LEU:HA	4:BE:101:ILE:HA	1.71	0.72
4:TE:64:LEU:HA	4:TE:101:ILE:HA	1.71	0.72
2:G:199:ALA:HB2	2:SG:161:ILE:CB	2.19	0.72
4:LF:64:LEU:HA	4:LF:101:ILE:HA	1.71	0.72
2:J:139:ARG:O	2:T:205:LEU:CB	2.37	0.72
2:QB:67:ALA:O	2:WB:48:SER:CA	2.34	0.72
2:QB:155:HIS:CB	2:WB:217:ALA:CB	2.68	0.72
4:JD:64:LEU:HA	4:JD:101:ILE:HA	1.71	0.72
2:KB:139:ARG:O	2:QB:205:LEU:CB	2.37	0.72
2:OC:161:ILE:CB	2:UC:199:ALA:HB2	2.19	0.72
4:PG:64:LEU:HA	4:PG:101:ILE:HA	1.71	0.72
2:G:206:MET:N	2:SG:143:ALA:HB1	2.03	0.72
2:J:161:ILE:CB	2:T:199:ALA:HB2	2.20	0.72
4:DG:64:LEU:HA	4:DG:101:ILE:HA	1.71	0.72
2:WB:143:ALA:HB1	2:CC:206:MET:N	2.04	0.72
4:RC:64:LEU:HA	4:RC:101:ILE:HA	1.71	0.72
4:LC:64:LEU:HA	4:LC:101:ILE:HA	1.71	0.72
2:EB:143:ALA:HB1	2:KB:206:MET:N	2.04	0.71
2:B:139:ARG:O	2:J:205:LEU:CB	2.38	0.71
2:AD:161:ILE:CB	2:GD:199:ALA:HB2	2.19	0.71
4:E:64:LEU:HA	4:E:101:ILE:HA	1.71	0.71
2:IF:161:ILE:CB	2:OF:199:ALA:HB2	2.19	0.71
4:ZB:64:LEU:HA	4:ZB:101:ILE:HA	1.71	0.71
4:HE:64:LEU:HA	4:HE:101:ILE:HA	1.71	0.71
2:QE:139:ARG:O	2:WE:205:LEU:CB	2.38	0.71
2:QE:143:ALA:HB1	2:WE:206:MET:N	2.05	0.71
4:ZE:64:LEU:HA	4:ZE:101:ILE:HA	1.71	0.71
4:VG:64:LEU:HA	4:VG:101:ILE:HA	1.71	0.71
4:PD:64:LEU:HA	4:PD:101:ILE:HA	1.71	0.71
4:RF:64:LEU:HA	4:RF:101:ILE:HA	1.71	0.71
2:GG:143:ALA:HB1	2:MG:206:MET:N	2.04	0.71
2:MG:155:HIS:CB	2:SG:217:ALA:CB	2.67	0.71
4:HB:64:LEU:HA	4:HB:101:ILE:HA	1.71	0.71
4:JG:64:LEU:HA	4:JG:101:ILE:HA	1.71	0.71
4:P:64:LEU:HA	4:P:101:ILE:HA	1.71	0.71
2:B:143:ALA:HB1	2:J:206:MET:N	2.05	0.71
4:DA:64:LEU:HA	4:DA:101:ILE:HA	1.71	0.71
4:TB:64:LEU:HA	4:TB:101:ILE:HA	1.71	0.71
2:WB:161:ILE:CB	2:CC:199:ALA:HB2	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IC:161:ILE:CB	2:OC:199:ALA:HB2	2.20	0.71
4:X:64:LEU:HA	4:X:101:ILE:HA	1.71	0.70
4:PA:64:LEU:HA	4:PA:101:ILE:HA	1.71	0.70
2:SA:139:ARG:O	2:YA:205:LEU:CB	2.39	0.70
2:IC:143:ALA:HB1	2:OC:206:MET:N	2.06	0.70
2:YD:143:ALA:HB1	2:EE:206:MET:N	2.05	0.70
2:IF:139:ARG:O	2:OF:205:LEU:CB	2.39	0.70
4:VA:64:LEU:HA	4:VA:101:ILE:HA	1.71	0.70
4:XC:64:LEU:HA	4:XC:101:ILE:HA	1.71	0.70
2:GD:139:ARG:O	2:MD:205:LEU:CB	2.39	0.70
2:UF:143:ALA:HB1	2:AG:206:MET:N	2.06	0.70
2:GG:139:ARG:O	2:MG:205:LEU:CB	2.39	0.70
4:JA:64:LEU:HA	4:JA:101:ILE:HA	1.71	0.70
2:YD:139:ARG:O	2:EE:205:LEU:CB	2.39	0.70
2:KE:161:ILE:CB	2:QE:199:ALA:HB2	2.20	0.70
4:O:64:LEU:HA	4:O:101:ILE:HA	1.71	0.70
4:NB:64:LEU:HA	4:NB:101:ILE:HA	1.71	0.70
2:YA:143:ALA:HB1	2:EB:206:MET:N	2.06	0.70
2:YA:161:ILE:CB	2:EB:199:ALA:HB2	2.21	0.70
4:BB:64:LEU:HA	4:BB:101:ILE:HA	1.71	0.70
2:UF:139:ARG:O	2:AG:205:LEU:CB	2.40	0.70
2:J:143:ALA:HB1	2:T:206:MET:N	2.06	0.70
2:AA:139:ARG:O	2:GA:205:LEU:CB	2.39	0.70
4:FC:64:LEU:HA	4:FC:101:ILE:HA	1.71	0.70
2:GD:143:ALA:HB1	2:MD:206:MET:N	2.06	0.69
2:CF:139:ARG:O	2:IF:205:LEU:CB	2.39	0.69
2:SD:139:ARG:O	2:YD:205:LEU:CB	2.40	0.69
2:SA:143:ALA:HB1	2:YA:206:MET:N	2.07	0.69
2:WE:143:ALA:HB1	2:CF:206:MET:N	2.06	0.69
2:CF:143:ALA:HB1	2:IF:206:MET:N	2.06	0.69
2:MD:143:ALA:HB1	2:SD:206:MET:N	2.07	0.69
2:EE:139:ARG:O	2:KE:205:LEU:CB	2.41	0.69
2:WE:139:ARG:O	2:CF:205:LEU:CB	2.41	0.68
2:G:143:ALA:HB1	2:B:206:MET:N	2.08	0.68
2:CC:139:ARG:O	2:IC:205:LEU:CB	2.42	0.68
2:KB:143:ALA:HB3	2:QB:205:LEU:CB	2.19	0.68
2:MD:139:ARG:O	2:SD:205:LEU:CB	2.42	0.68
2:G:139:ARG:O	2:B:205:LEU:CB	2.42	0.67
2:CC:143:ALA:HB1	2:IC:206:MET:N	2.09	0.67
2:SD:143:ALA:HB1	2:YD:206:MET:N	2.08	0.67
2:GG:143:ALA:HB3	2:MG:205:LEU:CB	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:KB:155:HIS:CB	2:QB:217:ALA:HB3	2.25	0.67
2:IF:143:ALA:HB1	2:OF:206:MET:N	2.09	0.67
2:AA:143:ALA:HB1	2:GA:206:MET:N	2.07	0.67
2:OC:143:ALA:HB3	2:UC:205:LEU:CB	2.22	0.67
2:UC:139:ARG:O	2:AD:205:LEU:CB	2.43	0.67
2:EE:143:ALA:HB1	2:KE:206:MET:N	2.09	0.66
2:MA:143:ALA:HB1	2:SA:206:MET:N	2.10	0.66
2:OC:155:HIS:CB	2:UC:217:ALA:HB3	2.26	0.66
3:RB:88:PRO:HA	3:RB:198:ILE:HA	1.78	0.66
2:WE:143:ALA:HB3	2:CF:205:LEU:CB	2.24	0.66
2:QB:139:ARG:O	2:WB:205:LEU:CB	2.43	0.66
3:ND:88:PRO:HA	3:ND:198:ILE:HA	1.78	0.66
4:QD:110:GLU:O	4:QD:121:ARG:N	2.29	0.66
3:FE:88:PRO:HA	3:FE:198:ILE:HA	1.78	0.66
3:JF:88:PRO:HA	3:JF:198:ILE:HA	1.78	0.66
4:KA:110:GLU:O	4:KA:121:ARG:N	2.29	0.66
4:QA:110:GLU:O	4:QA:121:ARG:N	2.29	0.66
4:WA:110:GLU:O	4:WA:121:ARG:N	2.29	0.66
3:ZA:88:PRO:HA	3:ZA:198:ILE:HA	1.78	0.66
4:CB:110:GLU:O	4:CB:121:ARG:N	2.29	0.66
3:JC:88:PRO:HA	3:JC:198:ILE:HA	1.78	0.66
3:RE:88:PRO:HA	3:RE:198:ILE:HA	1.78	0.66
4:IB:110:GLU:O	4:IB:121:ARG:N	2.29	0.66
3:VC:88:PRO:HA	3:VC:198:ILE:HA	1.78	0.66
4:KD:110:GLU:O	4:KD:121:ARG:N	2.29	0.66
3:XE:88:PRO:HA	3:XE:198:ILE:HA	1.78	0.66
4:EA:110:GLU:O	4:EA:121:ARG:N	2.29	0.66
3:BG:88:PRO:HA	3:BG:198:ILE:HA	1.78	0.66
3:HA:88:PRO:HA	3:HA:198:ILE:HA	1.78	0.66
3:BD:88:PRO:HA	3:BD:198:ILE:HA	1.78	0.66
4:ED:110:GLU:O	4:ED:121:ARG:N	2.29	0.66
3:DC:88:PRO:HA	3:DC:198:ILE:HA	1.78	0.66
3:K:88:PRO:HA	3:K:198:ILE:HA	1.78	0.65
3:PF:88:PRO:HA	3:PF:198:ILE:HA	1.78	0.65
2:MG:139:ARG:O	2:SG:205:LEU:CB	2.44	0.65
3:TG:88:PRO:HA	3:TG:198:ILE:HA	1.78	0.65
4:Y:110:GLU:O	4:Y:121:ARG:N	2.29	0.65
3:FB:88:PRO:HA	3:FB:198:ILE:HA	1.78	0.65
3:ZD:88:PRO:HA	3:ZD:198:ILE:HA	1.78	0.65
3:NA:88:PRO:HA	3:NA:198:ILE:HA	1.78	0.65
2:UC:143:ALA:HB1	2:AD:206:MET:N	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:YC:110:GLU:O	4:YC:121:ARG:N	2.29	0.65
3:XB:88:PRO:HA	3:XB:198:ILE:HA	1.78	0.65
4:MF:110:GLU:O	4:MF:121:ARG:N	2.29	0.65
4:R:110:GLU:O	4:R:121:ARG:N	2.29	0.65
3:V:88:PRO:HA	3:V:198:ILE:HA	1.78	0.65
3:LB:88:PRO:HA	3:LB:198:ILE:HA	1.78	0.65
3:HG:88:PRO:HA	3:HG:198:ILE:HA	1.78	0.65
3:M:88:PRO:HA	3:M:198:ILE:HA	1.78	0.65
3:TD:88:PRO:HA	3:TD:198:ILE:HA	1.78	0.65
3:VF:88:PRO:HA	3:VF:198:ILE:HA	1.78	0.65
4:SC:110:GLU:O	4:SC:121:ARG:N	2.29	0.65
3:HD:88:PRO:HA	3:HD:198:ILE:HA	1.78	0.65
4:GF:110:GLU:O	4:GF:121:ARG:N	2.29	0.65
4:H:110:GLU:O	4:H:121:ARG:N	2.29	0.65
2:IC:143:ALA:HB1	2:OC:205:LEU:O	1.97	0.65
3:DF:88:PRO:HA	3:DF:198:ILE:HA	1.78	0.65
3:TA:88:PRO:HA	3:TA:198:ILE:HA	1.78	0.65
2:YA:143:ALA:HB1	2:EB:205:LEU:O	1.97	0.65
2:KB:161:ILE:CB	2:QB:199:ALA:CB	2.75	0.65
2:YD:143:ALA:HB3	2:EE:205:LEU:CB	2.25	0.65
3:NG:88:PRO:HA	3:NG:198:ILE:HA	1.78	0.65
2:MA:161:ILE:CB	2:SA:199:ALA:CB	2.75	0.64
2:QB:143:ALA:HB1	2:WB:206:MET:N	2.11	0.64
3:C:88:PRO:HA	3:C:198:ILE:HA	1.78	0.64
3:BA:88:PRO:HA	3:BA:198:ILE:HA	1.78	0.64
2:WB:143:ALA:HB1	2:CC:205:LEU:O	1.98	0.64
4:MC:110:GLU:O	4:MC:121:ARG:N	2.29	0.64
2:OC:143:ALA:HB1	2:UC:205:LEU:O	1.98	0.64
2:KE:143:ALA:HB1	2:QE:205:LEU:O	1.97	0.64
4:EA:109:GLY:HA3	4:EA:122:ILE:HA	1.80	0.64
3:PC:88:PRO:HA	3:PC:198:ILE:HA	1.78	0.64
4:YC:109:GLY:HA3	4:YC:122:ILE:HA	1.80	0.64
3:LE:88:PRO:HA	3:LE:198:ILE:HA	1.78	0.64
2:MG:143:ALA:HB1	2:SG:206:MET:N	2.11	0.64
4:Y:109:GLY:HA3	4:Y:122:ILE:HA	1.80	0.64
4:IB:109:GLY:HA3	4:IB:122:ILE:HA	1.80	0.64
4:SC:109:GLY:HA3	4:SC:122:ILE:HA	1.80	0.64
4:CE:109:GLY:HA3	4:CE:122:ILE:HA	1.80	0.64
4:AF:110:GLU:O	4:AF:121:ARG:N	2.29	0.64
4:Q:110:GLU:O	4:Q:121:ARG:N	2.29	0.64
4:OB:109:GLY:HA3	4:OB:122:ILE:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:MC:109:GLY:HA3	4:MC:122:ILE:HA	1.80	0.64
4:WD:109:GLY:HA3	4:WD:122:ILE:HA	1.80	0.64
4:QG:109:GLY:HA3	4:QG:122:ILE:HA	1.80	0.64
4:R:109:GLY:HA3	4:R:122:ILE:HA	1.80	0.64
2:MA:139:ARG:O	2:SA:205:LEU:CB	2.46	0.64
2:EB:143:ALA:HB1	2:KB:205:LEU:O	1.98	0.64
4:IE:109:GLY:HA3	4:IE:122:ILE:HA	1.80	0.64
4:KG:109:GLY:HA3	4:KG:122:ILE:HA	1.80	0.64
4:KA:109:GLY:HA3	4:KA:122:ILE:HA	1.80	0.64
4:CB:109:GLY:HA3	4:CB:122:ILE:HA	1.80	0.64
2:KB:143:ALA:CB	2:QB:205:LEU:CA	2.76	0.64
4:GC:110:GLU:O	4:GC:121:ARG:N	2.29	0.64
4:GF:109:GLY:HA3	4:GF:122:ILE:HA	1.80	0.64
4:WG:109:GLY:HA3	4:WG:122:ILE:HA	1.80	0.64
4:ED:109:GLY:HA3	4:ED:122:ILE:HA	1.80	0.64
2:CF:143:ALA:HB3	2:IF:205:LEU:CB	2.27	0.64
4:MF:109:GLY:HA3	4:MF:122:ILE:HA	1.80	0.64
4:UB:109:GLY:HA3	4:UB:122:ILE:HA	1.80	0.63
4:UE:110:GLU:O	4:UE:121:ARG:N	2.29	0.63
2:IF:143:ALA:HB1	2:OF:205:LEU:O	1.98	0.63
4:QD:109:GLY:HA3	4:QD:122:ILE:HA	1.80	0.63
2:QE:143:ALA:HB1	2:WE:205:LEU:O	1.99	0.63
2:AG:143:ALA:HB1	2:GG:205:LEU:O	1.98	0.63
4:WG:110:GLU:O	4:WG:121:ARG:N	2.29	0.63
4:AC:110:GLU:O	4:AC:121:ARG:N	2.29	0.63
4:AF:109:GLY:HA3	4:AF:122:ILE:HA	1.80	0.63
4:WA:109:GLY:HA3	4:WA:122:ILE:HA	1.80	0.63
4:GC:109:GLY:HA3	4:GC:122:ILE:HA	1.80	0.63
2:GD:143:ALA:HB1	2:MD:205:LEU:O	1.99	0.63
4:SF:109:GLY:HA3	4:SF:122:ILE:HA	1.80	0.63
2:UF:161:ILE:CB	2:AG:199:ALA:CB	2.77	0.63
2:G:205:LEU:O	2:SG:143:ALA:HB1	1.97	0.63
4:YC:65:THR:N	4:YC:100:LEU:O	2.32	0.63
2:OF:143:ALA:HB1	2:UF:205:LEU:O	1.98	0.63
4:EG:109:GLY:HA3	4:EG:122:ILE:HA	1.80	0.63
2:T:143:ALA:HB1	2:AA:205:LEU:O	1.98	0.63
4:AC:65:THR:N	4:AC:100:LEU:O	2.32	0.63
4:GC:65:THR:N	4:GC:100:LEU:O	2.32	0.63
4:MC:65:THR:N	4:MC:100:LEU:O	2.32	0.63
2:OC:143:ALA:HB2	2:UC:205:LEU:CA	2.27	0.63
4:SC:65:THR:N	4:SC:100:LEU:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:ED:65:THR:N	4:ED:100:LEU:O	2.32	0.63
4:KD:65:THR:N	4:KD:100:LEU:O	2.32	0.63
2:SD:143:ALA:HB1	2:YD:205:LEU:O	1.99	0.63
2:YD:143:ALA:HB1	2:EE:205:LEU:O	1.99	0.63
4:OE:65:THR:N	4:OE:100:LEU:O	2.32	0.63
2:GG:161:ILE:CB	2:MG:199:ALA:CB	2.76	0.63
4:Q:109:GLY:HA3	4:Q:122:ILE:HA	1.80	0.63
4:H:109:GLY:HA3	4:H:122:ILE:HA	1.80	0.63
4:OB:65:THR:N	4:OB:100:LEU:O	2.32	0.63
4:UB:65:THR:N	4:UB:100:LEU:O	2.32	0.63
2:OC:143:ALA:CB	2:UC:205:LEU:CA	2.77	0.63
4:QD:65:THR:N	4:QD:100:LEU:O	2.32	0.63
4:WD:65:THR:N	4:WD:100:LEU:O	2.32	0.63
4:CE:65:THR:N	4:CE:100:LEU:O	2.32	0.63
4:IE:65:THR:N	4:IE:100:LEU:O	2.32	0.63
4:UE:65:THR:N	4:UE:100:LEU:O	2.32	0.63
4:SF:110:GLU:O	4:SF:121:ARG:N	2.29	0.63
2:B:161:ILE:CB	2:J:199:ALA:CB	2.77	0.63
4:IB:65:THR:N	4:IB:100:LEU:O	2.32	0.63
2:MD:161:ILE:CB	2:SD:199:ALA:CB	2.76	0.63
4:OE:109:GLY:HA3	4:OE:122:ILE:HA	1.80	0.63
4:OE:110:GLU:O	4:OE:121:ARG:N	2.29	0.63
4:AF:65:THR:N	4:AF:100:LEU:O	2.32	0.63
2:MG:161:ILE:CB	2:SG:199:ALA:CB	2.77	0.63
2:G:161:ILE:CB	2:B:199:ALA:CB	2.77	0.62
2:B:143:ALA:HB1	2:J:205:LEU:O	1.98	0.62
2:GA:161:ILE:CB	2:MA:199:ALA:CB	2.77	0.62
4:QA:109:GLY:HA3	4:QA:122:ILE:HA	1.80	0.62
4:CB:65:THR:N	4:CB:100:LEU:O	2.32	0.62
4:UB:110:GLU:O	4:UB:121:ARG:N	2.29	0.62
4:AC:109:GLY:HA3	4:AC:122:ILE:HA	1.80	0.62
4:KD:109:GLY:HA3	4:KD:122:ILE:HA	1.80	0.62
2:WE:161:ILE:CB	2:CF:199:ALA:CB	2.76	0.62
4:GF:65:THR:N	4:GF:100:LEU:O	2.32	0.62
4:MF:65:THR:N	4:MF:100:LEU:O	2.32	0.62
2:AG:161:ILE:CB	2:GG:199:ALA:CB	2.77	0.62
4:WA:65:THR:N	4:WA:100:LEU:O	2.32	0.62
2:CC:73:ALA:HB1	2:CC:77:LEU:H	1.65	0.62
2:UC:73:ALA:HB1	2:UC:77:LEU:H	1.64	0.62
2:CF:143:ALA:HB1	2:IF:205:LEU:O	1.99	0.62
4:SF:65:THR:N	4:SF:100:LEU:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:YF:110:GLU:O	4:YF:121:ARG:N	2.29	0.62
2:G:73:ALA:HB1	2:G:77:LEU:H	1.65	0.62
2:G:205:LEU:CB	2:SG:143:ALA:HB3	2.28	0.62
2:GA:73:ALA:HB1	2:GA:77:LEU:H	1.65	0.62
2:MA:143:ALA:HB3	2:SA:205:LEU:CB	2.23	0.62
4:QA:65:THR:N	4:QA:100:LEU:O	2.32	0.62
2:YA:73:ALA:HB1	2:YA:77:LEU:H	1.65	0.62
2:QB:161:ILE:CB	2:WB:199:ALA:CB	2.77	0.62
2:OC:161:ILE:CB	2:UC:199:ALA:CB	2.76	0.62
2:QE:161:ILE:CB	2:WE:199:ALA:CB	2.77	0.62
2:OF:143:ALA:HB3	2:UF:205:LEU:CB	2.26	0.62
4:QG:110:GLU:O	4:QG:121:ARG:N	2.29	0.62
2:J:73:ALA:HB1	2:J:77:LEU:H	1.64	0.62
2:UC:143:ALA:HB3	2:AD:205:LEU:CB	2.28	0.62
2:AD:161:ILE:CB	2:GD:199:ALA:CB	2.77	0.62
4:IE:110:GLU:O	4:IE:121:ARG:N	2.29	0.62
4:YF:65:THR:N	4:YF:100:LEU:O	2.32	0.62
2:T:73:ALA:HB1	2:T:77:LEU:H	1.65	0.62
2:AA:143:ALA:HB1	2:GA:205:LEU:O	1.98	0.62
4:KA:65:THR:N	4:KA:100:LEU:O	2.32	0.62
2:EB:161:ILE:CB	2:KB:199:ALA:CB	2.77	0.62
2:KB:73:ALA:HB1	2:KB:77:LEU:H	1.65	0.62
2:QB:143:ALA:HB1	2:WB:205:LEU:O	2.00	0.62
2:MD:73:ALA:HB1	2:MD:77:LEU:H	1.65	0.62
4:UE:109:GLY:HA3	4:UE:122:ILE:HA	1.80	0.62
2:CF:161:ILE:CB	2:IF:199:ALA:CB	2.77	0.62
2:UF:143:ALA:HB1	2:AG:205:LEU:O	1.99	0.62
4:EG:110:GLU:O	4:EG:121:ARG:N	2.29	0.62
2:GG:73:ALA:HB1	2:GG:77:LEU:H	1.65	0.62
4:EA:65:THR:N	4:EA:100:LEU:O	2.32	0.62
2:GA:143:ALA:HB1	2:MA:205:LEU:O	1.97	0.62
2:SA:161:ILE:CB	2:YA:199:ALA:CB	2.77	0.62
2:QB:73:ALA:HB1	2:QB:77:LEU:H	1.65	0.62
2:UC:161:ILE:CB	2:AD:199:ALA:CB	2.77	0.62
2:YD:161:ILE:CB	2:EE:199:ALA:CB	2.76	0.62
2:OF:161:ILE:CB	2:UF:199:ALA:CB	2.77	0.62
4:EG:65:THR:N	4:EG:100:LEU:O	2.32	0.62
4:KG:65:THR:N	4:KG:100:LEU:O	2.32	0.62
2:G:199:ALA:CB	2:SG:161:ILE:CB	2.78	0.62
4:Y:65:THR:N	4:Y:100:LEU:O	2.32	0.62
4:OB:110:GLU:O	4:OB:121:ARG:N	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:OF:73:ALA:HB1	2:OF:77:LEU:H	1.65	0.62
4:QG:65:THR:N	4:QG:100:LEU:O	2.32	0.62
4:Q:65:THR:N	4:Q:100:LEU:O	2.32	0.62
2:J:143:ALA:HB1	2:T:205:LEU:O	1.97	0.62
2:T:161:ILE:CB	2:AA:199:ALA:CB	2.77	0.62
2:SA:143:ALA:HB1	2:YA:205:LEU:O	1.99	0.62
2:WB:161:ILE:CB	2:CC:199:ALA:CB	2.78	0.62
2:CC:161:ILE:CB	2:IC:199:ALA:CB	2.77	0.62
4:CE:110:GLU:O	4:CE:121:ARG:N	2.29	0.62
2:EE:73:ALA:HB1	2:EE:77:LEU:H	1.65	0.62
4:H:65:THR:N	4:H:100:LEU:O	2.32	0.62
4:R:65:THR:N	4:R:100:LEU:O	2.32	0.62
2:AA:161:ILE:CB	2:GA:199:ALA:CB	2.78	0.62
2:KB:143:ALA:HB2	2:QB:205:LEU:CA	2.28	0.62
2:KB:143:ALA:HB1	2:QB:205:LEU:O	2.00	0.62
2:AD:155:HIS:CB	2:GD:217:ALA:HB3	2.30	0.62
2:EE:161:ILE:CB	2:KE:199:ALA:CB	2.78	0.62
2:WE:73:ALA:HB1	2:WE:77:LEU:H	1.65	0.62
4:KG:110:GLU:O	4:KG:121:ARG:N	2.29	0.62
2:SG:73:ALA:HB1	2:SG:77:LEU:H	1.65	0.62
4:WG:65:THR:N	4:WG:100:LEU:O	2.32	0.62
2:GA:155:HIS:CB	2:MA:217:ALA:HB3	2.30	0.62
2:MA:73:ALA:HB1	2:MA:77:LEU:H	1.65	0.62
2:IC:73:ALA:HB1	2:IC:77:LEU:H	1.65	0.62
2:IC:161:ILE:CB	2:OC:199:ALA:CB	2.78	0.62
2:GD:161:ILE:CB	2:MD:199:ALA:CB	2.77	0.62
2:SD:161:ILE:CB	2:YD:199:ALA:CB	2.77	0.62
4:YF:109:GLY:HA3	4:YF:122:ILE:HA	1.80	0.62
2:B:143:ALA:HB3	2:J:205:LEU:CB	2.27	0.61
2:J:161:ILE:CB	2:T:199:ALA:CB	2.78	0.61
2:SA:73:ALA:HB1	2:SA:77:LEU:H	1.65	0.61
2:OC:73:ALA:HB1	2:OC:77:LEU:H	1.65	0.61
2:GD:73:ALA:HB1	2:GD:77:LEU:H	1.65	0.61
2:EE:143:ALA:HB1	2:KE:205:LEU:O	1.99	0.61
2:IF:161:ILE:CB	2:OF:199:ALA:CB	2.78	0.61
2:UF:143:ALA:HB3	2:AG:205:LEU:CB	2.26	0.61
2:AD:143:ALA:HB1	2:GD:205:LEU:O	1.98	0.61
4:WD:110:GLU:O	4:WD:121:ARG:N	2.29	0.61
2:WE:143:ALA:HB1	2:CF:205:LEU:O	2.00	0.61
2:YD:73:ALA:HB1	2:YD:77:LEU:H	1.65	0.61
2:AG:73:ALA:HB1	2:AG:77:LEU:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:MG:143:ALA:HB1	2:SG:205:LEU:O	2.00	0.61
2:KE:161:ILE:CB	2:QE:199:ALA:CB	2.78	0.61
2:GA:143:ALA:HB3	2:MA:205:LEU:CB	2.26	0.61
2:WB:73:ALA:HB1	2:WB:77:LEU:H	1.65	0.61
2:OC:73:ALA:C	2:OC:75:GLU:H	2.09	0.61
2:AD:73:ALA:HB1	2:AD:77:LEU:H	1.65	0.61
2:QE:73:ALA:HB1	2:QE:77:LEU:H	1.65	0.61
2:IF:73:ALA:HB1	2:IF:77:LEU:H	1.65	0.61
2:GG:143:ALA:HB1	2:MG:205:LEU:O	1.99	0.61
2:G:143:ALA:HB1	2:B:205:LEU:O	2.00	0.61
2:AA:73:ALA:C	2:AA:75:GLU:H	2.09	0.61
2:GA:143:ALA:HB2	2:MA:205:LEU:CA	2.29	0.61
2:GD:73:ALA:C	2:GD:75:GLU:H	2.09	0.61
2:KE:73:ALA:HB1	2:KE:77:LEU:H	1.65	0.61
2:MG:73:ALA:HB1	2:MG:77:LEU:H	1.65	0.61
2:SG:73:ALA:C	2:SG:75:GLU:H	2.09	0.61
2:GA:73:ALA:C	2:GA:75:GLU:H	2.09	0.61
2:YA:161:ILE:CB	2:EB:199:ALA:CB	2.79	0.61
2:EB:73:ALA:C	2:EB:75:GLU:H	2.09	0.61
2:EB:143:ALA:HB3	2:KB:205:LEU:CB	2.27	0.61
2:B:73:ALA:HB1	2:B:77:LEU:H	1.65	0.61
2:J:73:ALA:C	2:J:75:GLU:H	2.09	0.61
2:EB:73:ALA:HB1	2:EB:77:LEU:H	1.65	0.61
2:KB:73:ALA:C	2:KB:75:GLU:H	2.09	0.61
2:WB:73:ALA:C	2:WB:75:GLU:H	2.09	0.61
2:MD:143:ALA:HB1	2:SD:205:LEU:O	2.00	0.61
2:UF:73:ALA:HB1	2:UF:77:LEU:H	1.65	0.61
2:GG:73:ALA:C	2:GG:75:GLU:H	2.09	0.61
2:AA:73:ALA:HB1	2:AA:77:LEU:H	1.65	0.61
2:CC:143:ALA:HB1	2:IC:205:LEU:O	1.99	0.61
2:AG:73:ALA:C	2:AG:75:GLU:H	2.09	0.61
2:G:73:ALA:C	2:G:75:GLU:H	2.09	0.60
2:GA:143:ALA:CB	2:MA:205:LEU:CA	2.79	0.60
2:SD:73:ALA:HB1	2:SD:77:LEU:H	1.65	0.60
2:YD:73:ALA:C	2:YD:75:GLU:H	2.09	0.60
2:QE:73:ALA:C	2:QE:75:GLU:H	2.09	0.60
2:CF:73:ALA:HB1	2:CF:77:LEU:H	1.65	0.60
2:IF:73:ALA:C	2:IF:75:GLU:H	2.09	0.60
2:MA:73:ALA:C	2:MA:75:GLU:H	2.09	0.60
2:EB:143:ALA:HB2	2:KB:205:LEU:CA	2.30	0.60
2:IC:73:ALA:C	2:IC:75:GLU:H	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:YA:73:ALA:C	2:YA:75:GLU:H	2.09	0.60
2:OF:73:ALA:C	2:OF:75:GLU:H	2.09	0.60
2:AD:143:ALA:HB3	2:GD:205:LEU:CB	2.25	0.60
2:T:73:ALA:C	2:T:75:GLU:H	2.09	0.60
2:T:155:HIS:CB	2:AA:217:ALA:HB3	2.31	0.60
2:QB:73:ALA:C	2:QB:75:GLU:H	2.09	0.60
2:UC:73:ALA:C	2:UC:75:GLU:H	2.09	0.60
2:AD:73:ALA:C	2:AD:75:GLU:H	2.09	0.60
2:MG:73:ALA:C	2:MG:75:GLU:H	2.09	0.60
2:SA:73:ALA:C	2:SA:75:GLU:H	2.09	0.60
2:B:73:ALA:C	2:B:75:GLU:H	2.09	0.60
2:MA:143:ALA:HB1	2:SA:205:LEU:O	2.02	0.60
2:CC:73:ALA:C	2:CC:75:GLU:H	2.09	0.60
2:UC:143:ALA:HB1	2:AD:205:LEU:O	2.00	0.60
2:T:143:ALA:HB2	2:AA:205:LEU:CA	2.30	0.60
2:SD:73:ALA:C	2:SD:75:GLU:H	2.09	0.60
2:AG:143:ALA:HB2	2:GG:205:LEU:CA	2.30	0.60
2:WE:73:ALA:C	2:WE:75:GLU:H	2.09	0.60
2:OF:155:HIS:CB	2:UF:217:ALA:HB3	2.31	0.60
2:EE:143:ALA:HB3	2:KE:205:LEU:CB	2.30	0.59
2:KE:143:ALA:HB2	2:QE:205:LEU:CA	2.29	0.59
3:FB:201:ASN:HA	3:FB:218:CYS:HA	1.84	0.59
3:RB:201:ASN:HA	3:RB:218:CYS:HA	1.84	0.59
2:EE:73:ALA:C	2:EE:75:GLU:H	2.09	0.59
2:CF:73:ALA:C	2:CF:75:GLU:H	2.09	0.59
2:UF:73:ALA:C	2:UF:75:GLU:H	2.09	0.59
3:TA:201:ASN:HA	3:TA:218:CYS:HA	1.84	0.59
3:DC:201:ASN:HA	3:DC:218:CYS:HA	1.84	0.59
2:EB:155:HIS:CB	2:KB:217:ALA:HB3	2.33	0.59
3:LB:201:ASN:HA	3:LB:218:CYS:HA	1.84	0.59
3:XB:201:ASN:HA	3:XB:218:CYS:HA	1.84	0.59
2:MD:73:ALA:C	2:MD:75:GLU:H	2.09	0.59
2:T:143:ALA:CB	2:AA:205:LEU:CA	2.80	0.59
3:ZA:201:ASN:HA	3:ZA:218:CYS:HA	1.84	0.59
3:PC:201:ASN:HA	3:PC:218:CYS:HA	1.84	0.59
2:MD:143:ALA:HB3	2:SD:205:LEU:CB	2.25	0.59
2:T:143:ALA:HB3	2:AA:205:LEU:CB	2.26	0.59
2:WB:143:ALA:HB2	2:CC:205:LEU:CA	2.30	0.59
2:KE:73:ALA:C	2:KE:75:GLU:H	2.09	0.59
3:HA:201:ASN:HA	3:HA:218:CYS:HA	1.84	0.59
3:JC:201:ASN:HA	3:JC:218:CYS:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AD:143:ALA:CB	2:GD:205:LEU:CA	2.80	0.59
2:GD:143:ALA:HB2	2:MD:205:LEU:CA	2.31	0.59
2:OF:143:ALA:CB	2:UF:205:LEU:CA	2.80	0.59
3:BG:201:ASN:HA	3:BG:218:CYS:HA	1.84	0.59
3:NA:201:ASN:HA	3:NA:218:CYS:HA	1.84	0.59
2:SA:143:ALA:HB3	2:YA:205:LEU:CB	2.29	0.59
3:VC:201:ASN:HA	3:VC:218:CYS:HA	1.84	0.59
3:BD:201:ASN:HA	3:BD:218:CYS:HA	1.84	0.59
2:GD:143:ALA:HB3	2:MD:205:LEU:CB	2.27	0.59
3:VF:201:ASN:HA	3:VF:218:CYS:HA	1.84	0.59
2:EB:143:ALA:CB	2:KB:205:LEU:CA	2.81	0.59
2:YD:155:HIS:CB	2:EE:217:ALA:HB3	2.32	0.59
3:BA:201:ASN:HA	3:BA:218:CYS:HA	1.84	0.59
2:QE:143:ALA:HB3	2:WE:205:LEU:CB	2.26	0.59
3:RE:201:ASN:HA	3:RE:218:CYS:HA	1.84	0.59
3:XE:201:ASN:HA	3:XE:218:CYS:HA	1.84	0.59
2:OF:143:ALA:HB2	2:UF:205:LEU:CA	2.29	0.59
2:GG:143:ALA:CB	2:MG:205:LEU:CA	2.80	0.59
3:V:201:ASN:HA	3:V:218:CYS:HA	1.84	0.58
2:KB:84:ALA:HB1	2:QB:23:ALA:C	2.28	0.58
2:G:217:ALA:HB3	2:SG:155:HIS:CB	2.33	0.58
3:ND:201:ASN:HA	3:ND:218:CYS:HA	1.84	0.58
2:KE:143:ALA:CB	2:QE:205:LEU:CA	2.80	0.58
3:DF:201:ASN:HA	3:DF:218:CYS:HA	1.84	0.58
2:B:143:ALA:HB2	2:J:205:LEU:CA	2.31	0.58
2:B:155:HIS:CB	2:J:217:ALA:HB3	2.33	0.58
2:AG:143:ALA:HB3	2:GG:205:LEU:CB	2.27	0.58
3:HG:201:ASN:HA	3:HG:218:CYS:HA	1.84	0.58
2:G:205:LEU:CA	2:SG:143:ALA:HB2	2.30	0.58
3:K:201:ASN:HA	3:K:218:CYS:HA	1.84	0.58
2:IC:143:ALA:HB2	2:OC:205:LEU:CA	2.31	0.58
3:HD:201:ASN:HA	3:HD:218:CYS:HA	1.84	0.58
2:IF:143:ALA:HB3	2:OF:205:LEU:CB	2.32	0.58
2:AG:143:ALA:CB	2:GG:205:LEU:CA	2.81	0.58
2:KE:155:HIS:CB	2:QE:217:ALA:HB3	2.31	0.58
2:QE:143:ALA:CB	2:WE:205:LEU:CA	2.81	0.58
3:PF:201:ASN:HA	3:PF:218:CYS:HA	1.84	0.58
2:GD:155:HIS:CB	2:MD:217:ALA:HB3	2.33	0.58
2:MD:143:ALA:CB	2:SD:205:LEU:CA	2.81	0.58
3:C:201:ASN:HA	3:C:218:CYS:HA	1.84	0.58
2:MD:155:HIS:CB	2:SD:217:ALA:HB3	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GG:143:ALA:HB2	2:MG:205:LEU:CA	2.30	0.58
2:GG:155:HIS:CB	2:MG:217:ALA:HB3	2.31	0.58
2:WB:155:HIS:CB	2:CC:217:ALA:HB3	2.33	0.58
2:YD:143:ALA:CB	2:EE:205:LEU:CA	2.81	0.58
3:ZD:201:ASN:HA	3:ZD:218:CYS:HA	1.84	0.58
3:LE:201:ASN:HA	3:LE:218:CYS:HA	1.84	0.58
2:QE:143:ALA:HB2	2:WE:205:LEU:CA	2.31	0.58
2:G:205:LEU:CA	2:SG:143:ALA:CB	2.82	0.58
3:M:201:ASN:HA	3:M:218:CYS:HA	1.84	0.58
2:WB:143:ALA:HB3	2:CC:205:LEU:CB	2.28	0.58
2:GD:143:ALA:CB	2:MD:205:LEU:CA	2.82	0.58
2:G:143:ALA:HB3	2:B:205:LEU:CB	2.27	0.58
2:MA:143:ALA:CB	2:SA:205:LEU:CA	2.81	0.58
2:AD:143:ALA:HB2	2:GD:205:LEU:CA	2.29	0.58
3:TD:201:ASN:HA	3:TD:218:CYS:HA	1.84	0.58
2:WE:143:ALA:CB	2:CF:205:LEU:CA	2.81	0.58
2:WE:155:HIS:CB	2:CF:217:ALA:HB3	2.32	0.58
2:UF:155:HIS:CB	2:AG:217:ALA:HB3	2.33	0.58
3:BD:102:LEU:O	3:BD:183:GLU:N	2.30	0.57
3:ZD:314:ALA:HA	4:AE:88:ALA:HA	1.86	0.57
3:FE:314:ALA:HA	4:GE:88:ALA:HA	1.86	0.57
3:LE:314:ALA:HA	4:ME:88:ALA:HA	1.86	0.57
3:RE:314:ALA:HA	4:SE:88:ALA:HA	1.86	0.57
3:JF:314:ALA:HA	4:KF:88:ALA:HA	1.86	0.57
4:DG:97:LEU:N	4:DG:109:GLY:O	2.37	0.57
4:JG:97:LEU:N	4:JG:109:GLY:O	2.37	0.57
4:PG:97:LEU:N	4:PG:109:GLY:O	2.37	0.57
2:B:143:ALA:CB	2:J:205:LEU:CA	2.82	0.57
3:ND:314:ALA:HA	4:OD:88:ALA:HA	1.86	0.57
2:SD:143:ALA:HB2	2:YD:205:LEU:CA	2.32	0.57
3:XE:314:ALA:HA	4:YE:88:ALA:HA	1.86	0.57
2:AG:155:HIS:CB	2:GG:217:ALA:HB3	2.32	0.57
2:KB:84:ALA:CB	2:QB:23:ALA:CA	2.78	0.57
2:WB:143:ALA:CB	2:CC:205:LEU:CA	2.82	0.57
3:TD:314:ALA:HA	4:UD:88:ALA:HA	1.86	0.57
4:HE:97:LEU:N	4:HE:109:GLY:O	2.37	0.57
2:KE:143:ALA:HB3	2:QE:205:LEU:CB	2.28	0.57
3:DF:314:ALA:HA	4:EF:88:ALA:HA	1.86	0.57
3:JF:102:LEU:O	3:JF:183:GLU:N	2.30	0.57
3:JF:201:ASN:HA	3:JF:218:CYS:HA	1.84	0.57
3:NG:102:LEU:O	3:NG:183:GLU:N	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:NG:201:ASN:HA	3:NG:218:CYS:HA	1.84	0.57
4:VG:97:LEU:N	4:VG:109:GLY:O	2.37	0.57
4:VD:97:LEU:N	4:VD:109:GLY:O	2.37	0.57
4:BE:97:LEU:N	4:BE:109:GLY:O	2.37	0.57
4:NE:97:LEU:N	4:NE:109:GLY:O	2.37	0.57
2:QE:155:HIS:CB	2:WE:217:ALA:HB3	2.32	0.57
3:XE:102:LEU:O	3:XE:183:GLU:N	2.30	0.57
3:DF:102:LEU:O	3:DF:183:GLU:N	2.30	0.57
4:RF:97:LEU:N	4:RF:109:GLY:O	2.37	0.57
3:VF:314:ALA:HA	4:WF:88:ALA:HA	1.86	0.57
3:TG:201:ASN:HA	3:TG:218:CYS:HA	1.84	0.57
3:HD:314:ALA:HA	4:ID:88:ALA:HA	1.86	0.57
3:RE:102:LEU:O	3:RE:183:GLU:N	2.30	0.57
2:CF:143:ALA:CB	2:IF:205:LEU:CA	2.82	0.57
4:LF:97:LEU:N	4:LF:109:GLY:O	2.37	0.57
3:PF:314:ALA:HA	4:QF:88:ALA:HA	1.86	0.57
4:XF:97:LEU:N	4:XF:109:GLY:O	2.37	0.57
4:P:97:LEU:N	4:P:109:GLY:O	2.37	0.57
2:MA:155:HIS:CB	2:SA:217:ALA:HB3	2.33	0.57
2:SA:155:HIS:CB	2:YA:217:ALA:HB3	2.35	0.57
3:BD:314:ALA:HA	4:CD:88:ALA:HA	1.86	0.57
3:FE:201:ASN:HA	3:FE:218:CYS:HA	1.84	0.57
4:TE:97:LEU:N	4:TE:109:GLY:O	2.37	0.57
4:ZE:97:LEU:N	4:ZE:109:GLY:O	2.37	0.57
4:FF:97:LEU:N	4:FF:109:GLY:O	2.37	0.57
3:PF:102:LEU:O	3:PF:183:GLU:N	2.30	0.57
2:G:143:ALA:CB	2:B:205:LEU:CA	2.82	0.57
4:TB:97:LEU:N	4:TB:109:GLY:O	2.37	0.57
3:VC:102:LEU:O	3:VC:183:GLU:N	2.30	0.57
4:PD:97:LEU:N	4:PD:109:GLY:O	2.37	0.57
3:LE:102:LEU:O	3:LE:183:GLU:N	2.30	0.57
2:UF:143:ALA:CB	2:AG:205:LEU:CA	2.81	0.57
3:BG:314:ALA:HA	4:CG:88:ALA:HA	1.86	0.57
4:E:97:LEU:N	4:E:109:GLY:O	2.37	0.57
2:J:143:ALA:HB3	2:T:205:LEU:CB	2.30	0.57
4:NB:97:LEU:N	4:NB:109:GLY:O	2.37	0.57
4:ZB:97:LEU:N	4:ZB:109:GLY:O	2.37	0.57
4:FC:97:LEU:N	4:FC:109:GLY:O	2.37	0.57
3:VC:314:ALA:HA	4:WC:88:ALA:HA	1.86	0.57
3:VF:102:LEU:O	3:VF:183:GLU:N	2.30	0.57
3:TG:102:LEU:O	3:TG:183:GLU:N	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:155:HIS:CB	2:B:217:ALA:HB3	2.35	0.57
4:O:97:LEU:N	4:O:109:GLY:O	2.37	0.57
3:HA:314:ALA:HA	4:IA:88:ALA:HA	1.86	0.57
2:CC:143:ALA:HB3	2:IC:205:LEU:CB	2.29	0.57
3:PC:314:ALA:HA	4:QC:88:ALA:HA	1.86	0.57
3:FE:102:LEU:O	3:FE:183:GLU:N	2.30	0.57
3:HG:314:ALA:HA	4:IG:88:ALA:HA	1.86	0.57
4:X:97:LEU:N	4:X:109:GLY:O	2.37	0.57
2:AA:143:ALA:CB	2:GA:205:LEU:CA	2.83	0.57
4:HB:97:LEU:N	4:HB:109:GLY:O	2.37	0.57
3:NA:314:ALA:HA	4:OA:88:ALA:HA	1.86	0.56
4:LC:97:LEU:N	4:LC:109:GLY:O	2.37	0.56
4:JD:97:LEU:N	4:JD:109:GLY:O	2.37	0.56
2:EE:143:ALA:HB2	2:KE:205:LEU:CA	2.33	0.56
2:CF:143:ALA:HB2	2:IF:205:LEU:CA	2.31	0.56
3:BG:102:LEU:O	3:BG:183:GLU:N	2.30	0.56
3:LB:314:ALA:HA	4:MB:88:ALA:HA	1.86	0.56
2:CC:143:ALA:CB	2:IC:205:LEU:CA	2.84	0.56
2:IC:143:ALA:CB	2:OC:205:LEU:CA	2.84	0.56
2:IC:155:HIS:CB	2:OC:217:ALA:HB3	2.35	0.56
3:JC:314:ALA:HA	4:KC:88:ALA:HA	1.86	0.56
3:PC:102:LEU:O	3:PC:183:GLU:N	2.30	0.56
2:YD:143:ALA:HB2	2:EE:205:LEU:CA	2.31	0.56
3:M:102:LEU:O	3:M:183:GLU:N	2.30	0.56
3:BA:314:ALA:HA	4:CA:88:ALA:HA	1.86	0.56
4:DA:97:LEU:N	4:DA:109:GLY:O	2.37	0.56
4:JA:97:LEU:N	4:JA:109:GLY:O	2.37	0.56
2:SA:143:ALA:CB	2:YA:205:LEU:CA	2.83	0.56
2:YA:143:ALA:HB2	2:EB:205:LEU:CA	2.32	0.56
4:BB:97:LEU:N	4:BB:109:GLY:O	2.37	0.56
4:QC:97:LEU:N	4:QC:109:GLY:O	2.38	0.56
4:RC:97:LEU:N	4:RC:109:GLY:O	2.37	0.56
4:DD:97:LEU:N	4:DD:109:GLY:O	2.37	0.56
2:MD:143:ALA:HB2	2:SD:205:LEU:CA	2.32	0.56
3:ZD:102:LEU:O	3:ZD:183:GLU:N	2.30	0.56
4:SE:97:LEU:N	4:SE:109:GLY:O	2.38	0.56
4:YE:97:LEU:N	4:YE:109:GLY:O	2.38	0.56
4:EF:97:LEU:N	4:EF:109:GLY:O	2.38	0.56
4:KF:97:LEU:N	4:KF:109:GLY:O	2.38	0.56
3:HG:102:LEU:O	3:HG:183:GLU:N	2.30	0.56
3:NG:314:ALA:HA	4:OG:88:ALA:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:TG:314:ALA:HA	4:UG:88:ALA:HA	1.86	0.56
3:FB:314:ALA:HA	4:GB:88:ALA:HA	1.86	0.56
3:RB:314:ALA:HA	4:SB:88:ALA:HA	1.86	0.56
3:XB:314:ALA:HA	4:YB:88:ALA:HA	1.86	0.56
3:DC:314:ALA:HA	4:EC:88:ALA:HA	1.86	0.56
4:KC:97:LEU:N	4:KC:109:GLY:O	2.38	0.56
4:XC:97:LEU:N	4:XC:109:GLY:O	2.37	0.56
3:M:314:ALA:HA	4:N:88:ALA:HA	1.86	0.56
2:J:155:HIS:CB	2:T:217:ALA:HB3	2.35	0.56
4:PA:97:LEU:N	4:PA:109:GLY:O	2.37	0.56
4:EC:97:LEU:N	4:EC:109:GLY:O	2.38	0.56
4:QF:97:LEU:N	4:QF:109:GLY:O	2.38	0.56
4:VA:97:LEU:N	4:VA:109:GLY:O	2.37	0.56
3:TD:102:LEU:O	3:TD:183:GLU:N	2.30	0.56
4:ME:97:LEU:N	4:ME:109:GLY:O	2.38	0.56
3:C:314:ALA:HA	4:D:88:ALA:HA	1.86	0.56
3:TA:314:ALA:HA	4:UA:88:ALA:HA	1.86	0.56
3:JC:102:LEU:O	3:JC:183:GLU:N	2.30	0.56
2:UC:155:HIS:CB	2:AD:217:ALA:HB3	2.36	0.56
2:SD:143:ALA:CB	2:YD:205:LEU:CA	2.83	0.56
2:AA:143:ALA:HB2	2:GA:205:LEU:CA	2.32	0.56
4:GE:97:LEU:N	4:GE:109:GLY:O	2.38	0.56
4:WF:97:LEU:N	4:WF:109:GLY:O	2.38	0.56
3:C:102:LEU:O	3:C:183:GLU:N	2.30	0.56
4:YB:97:LEU:N	4:YB:109:GLY:O	2.38	0.56
2:CF:155:HIS:CB	2:IF:217:ALA:HB3	2.34	0.56
3:ND:102:LEU:O	3:ND:183:GLU:N	2.30	0.56
4:SF:111:VAL:HA	4:SF:120:VAL:HA	1.88	0.56
2:G:143:ALA:HB2	2:B:205:LEU:CA	2.32	0.55
3:V:314:ALA:HA	4:W:88:ALA:HA	1.86	0.55
2:UC:143:ALA:CB	2:AD:205:LEU:CA	2.83	0.55
4:GF:111:VAL:HA	4:GF:120:VAL:HA	1.88	0.55
2:MG:143:ALA:HB3	2:SG:205:LEU:CB	2.29	0.55
3:K:314:ALA:HA	4:L:88:ALA:HA	1.86	0.55
4:SB:97:LEU:N	4:SB:109:GLY:O	2.38	0.55
3:DC:102:LEU:O	3:DC:183:GLU:N	2.30	0.55
4:AE:97:LEU:N	4:AE:109:GLY:O	2.38	0.55
4:UE:111:VAL:HA	4:UE:120:VAL:HA	1.88	0.55
2:J:143:ALA:HB2	2:T:205:LEU:CA	2.31	0.55
3:K:102:LEU:O	3:K:183:GLU:N	2.30	0.55
2:YA:155:HIS:CB	2:EB:217:ALA:HB3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:ZA:314:ALA:HA	4:AB:88:ALA:HA	1.86	0.55
4:EG:111:VAL:HA	4:EG:120:VAL:HA	1.88	0.55
2:J:143:ALA:CB	2:T:205:LEU:CA	2.83	0.55
2:WE:143:ALA:HB2	2:CF:205:LEU:CA	2.31	0.55
2:MG:143:ALA:CB	2:SG:205:LEU:CA	2.84	0.55
4:QG:111:VAL:HA	4:QG:120:VAL:HA	1.88	0.55
2:AA:143:ALA:HB3	2:GA:205:LEU:CB	2.30	0.55
2:AA:155:HIS:CB	2:GA:217:ALA:HB3	2.36	0.55
2:YA:143:ALA:CB	2:EB:205:LEU:CA	2.84	0.55
4:IE:111:VAL:HA	4:IE:120:VAL:HA	1.88	0.55
4:AF:111:VAL:HA	4:AF:120:VAL:HA	1.88	0.55
4:Q:111:VAL:HA	4:Q:120:VAL:HA	1.88	0.55
4:AB:97:LEU:N	4:AB:109:GLY:O	2.38	0.55
4:GB:97:LEU:N	4:GB:109:GLY:O	2.38	0.55
3:HD:102:LEU:O	3:HD:183:GLU:N	2.30	0.55
4:UD:97:LEU:N	4:UD:109:GLY:O	2.38	0.55
4:MF:111:VAL:HA	4:MF:120:VAL:HA	1.88	0.55
4:YF:111:VAL:HA	4:YF:120:VAL:HA	1.88	0.55
4:OA:97:LEU:N	4:OA:109:GLY:O	2.38	0.55
4:UA:97:LEU:N	4:UA:109:GLY:O	2.38	0.55
4:WG:111:VAL:HA	4:WG:120:VAL:HA	1.88	0.55
4:MB:97:LEU:N	4:MB:109:GLY:O	2.38	0.55
3:XB:102:LEU:O	3:XB:183:GLU:N	2.30	0.55
2:SD:155:HIS:CB	2:YD:217:ALA:HB3	2.36	0.55
4:OE:111:VAL:HA	4:OE:120:VAL:HA	1.88	0.55
4:KG:111:VAL:HA	4:KG:120:VAL:HA	1.88	0.55
3:V:102:LEU:O	3:V:183:GLU:N	2.30	0.55
4:IA:97:LEU:N	4:IA:109:GLY:O	2.38	0.55
2:YA:143:ALA:HB3	2:EB:205:LEU:CB	2.32	0.55
4:AC:111:VAL:HA	4:AC:120:VAL:HA	1.88	0.55
4:R:111:VAL:HA	4:R:120:VAL:HA	1.88	0.55
4:W:97:LEU:N	4:W:109:GLY:O	2.38	0.55
4:CA:97:LEU:N	4:CA:109:GLY:O	2.38	0.55
4:OD:97:LEU:N	4:OD:109:GLY:O	2.38	0.55
4:WD:111:VAL:HA	4:WD:120:VAL:HA	1.88	0.55
4:L:97:LEU:N	4:L:109:GLY:O	2.38	0.54
3:RB:102:LEU:O	3:RB:183:GLU:N	2.30	0.54
2:CC:155:HIS:CB	2:IC:217:ALA:HB3	2.36	0.54
4:CE:111:VAL:HA	4:CE:120:VAL:HA	1.88	0.54
2:EE:155:HIS:CB	2:KE:217:ALA:HB3	2.37	0.54
4:D:97:LEU:N	4:D:109:GLY:O	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:111:VAL:HA	4:H:120:VAL:HA	1.88	0.54
3:BA:102:LEU:O	3:BA:183:GLU:N	2.30	0.54
4:WA:111:VAL:HA	4:WA:120:VAL:HA	1.88	0.54
2:MA:84:ALA:HB1	2:SA:23:ALA:C	2.32	0.54
4:CB:111:VAL:HA	4:CB:120:VAL:HA	1.88	0.54
4:UB:111:VAL:HA	4:UB:120:VAL:HA	1.88	0.54
4:GC:111:VAL:HA	4:GC:120:VAL:HA	1.88	0.54
2:MG:143:ALA:HB2	2:SG:205:LEU:CA	2.34	0.54
4:N:97:LEU:N	4:N:109:GLY:O	2.38	0.54
4:Y:111:VAL:HA	4:Y:120:VAL:HA	1.88	0.54
4:KD:111:VAL:HA	4:KD:120:VAL:HA	1.88	0.54
3:HA:102:LEU:O	3:HA:183:GLU:N	2.30	0.54
3:LB:102:LEU:O	3:LB:183:GLU:N	2.30	0.54
2:IF:143:ALA:CB	2:OF:205:LEU:CA	2.85	0.54
4:EA:111:VAL:HA	4:EA:120:VAL:HA	1.88	0.54
4:QA:111:VAL:HA	4:QA:120:VAL:HA	1.88	0.54
2:QB:143:ALA:HB3	2:WB:205:LEU:CB	2.30	0.54
2:CC:143:ALA:HB2	2:IC:205:LEU:CA	2.33	0.54
4:ID:97:LEU:N	4:ID:109:GLY:O	2.38	0.54
4:QD:111:VAL:HA	4:QD:120:VAL:HA	1.88	0.54
2:QB:143:ALA:CB	2:WB:205:LEU:CA	2.85	0.54
4:ED:111:VAL:HA	4:ED:120:VAL:HA	1.88	0.54
2:EE:143:ALA:CB	2:KE:205:LEU:CA	2.84	0.54
4:UG:97:LEU:N	4:UG:109:GLY:O	2.38	0.54
3:NA:102:LEU:O	3:NA:183:GLU:N	2.30	0.54
3:FB:102:LEU:O	3:FB:183:GLU:N	2.30	0.54
4:KA:111:VAL:HA	4:KA:120:VAL:HA	1.88	0.54
3:TA:102:LEU:O	3:TA:183:GLU:N	2.30	0.54
3:ZA:102:LEU:O	3:ZA:183:GLU:N	2.30	0.54
4:IB:111:VAL:HA	4:IB:120:VAL:HA	1.88	0.54
4:YC:111:VAL:HA	4:YC:120:VAL:HA	1.88	0.54
2:IC:143:ALA:HB3	2:OC:205:LEU:CB	2.31	0.54
4:MC:111:VAL:HA	4:MC:120:VAL:HA	1.88	0.54
4:OG:97:LEU:N	4:OG:109:GLY:O	2.38	0.54
4:OB:111:VAL:HA	4:OB:120:VAL:HA	1.88	0.53
2:QB:155:HIS:CB	2:WB:217:ALA:HB3	2.38	0.53
4:CD:97:LEU:N	4:CD:109:GLY:O	2.38	0.53
4:SC:111:VAL:HA	4:SC:120:VAL:HA	1.88	0.53
2:IF:155:HIS:CB	2:OF:217:ALA:HB3	2.38	0.53
4:IG:97:LEU:N	4:IG:109:GLY:O	2.38	0.53
2:UF:143:ALA:HB2	2:AG:205:LEU:CA	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:WC:97:LEU:N	4:WC:109:GLY:O	2.38	0.53
4:CG:97:LEU:N	4:CG:109:GLY:O	2.38	0.53
2:KB:84:ALA:CB	2:QB:23:ALA:C	2.82	0.52
2:SD:143:ALA:HB3	2:YD:205:LEU:CB	2.29	0.52
3:V:283:VAL:HA	4:W:121:ARG:HA	1.92	0.52
3:NA:283:VAL:HA	4:OA:121:ARG:HA	1.92	0.52
3:PC:106:HIS:N	3:PC:178:GLU:O	2.43	0.52
3:TA:283:VAL:HA	4:UA:121:ARG:HA	1.92	0.52
3:LB:283:VAL:HA	4:MB:121:ARG:HA	1.92	0.52
2:QB:143:ALA:HB2	2:WB:205:LEU:CA	2.34	0.52
3:M:283:VAL:HA	4:N:121:ARG:HA	1.92	0.52
3:K:283:VAL:HA	4:L:121:ARG:HA	1.92	0.52
3:BA:283:VAL:HA	4:CA:121:ARG:HA	1.92	0.52
3:ZA:106:HIS:N	3:ZA:178:GLU:O	2.43	0.52
3:XB:106:HIS:N	3:XB:178:GLU:O	2.43	0.52
3:FE:106:HIS:N	3:FE:178:GLU:O	2.43	0.52
2:MG:155:HIS:CB	2:SG:217:ALA:HB3	2.37	0.52
3:ZA:283:VAL:HA	4:AB:121:ARG:HA	1.92	0.52
3:FB:283:VAL:HA	4:GB:121:ARG:HA	1.92	0.52
3:TG:283:VAL:HA	4:UG:121:ARG:HA	1.92	0.52
3:C:283:VAL:HA	4:D:121:ARG:HA	1.92	0.52
3:HA:283:VAL:HA	4:IA:121:ARG:HA	1.92	0.52
3:RB:283:VAL:HA	4:SB:121:ARG:HA	1.92	0.52
3:DC:283:VAL:HA	4:EC:121:ARG:HA	1.92	0.52
3:ND:106:HIS:N	3:ND:178:GLU:O	2.43	0.52
3:XE:106:HIS:N	3:XE:178:GLU:O	2.43	0.52
3:JC:283:VAL:HA	4:KC:121:ARG:HA	1.92	0.52
3:FB:106:HIS:N	3:FB:178:GLU:O	2.43	0.52
2:KB:84:ALA:HB3	2:QB:23:ALA:CA	2.28	0.52
3:XB:283:VAL:HA	4:YB:121:ARG:HA	1.92	0.52
3:HG:283:VAL:HA	4:IG:121:ARG:HA	1.92	0.52
3:HA:106:HIS:N	3:HA:178:GLU:O	2.43	0.52
3:VC:283:VAL:HA	4:WC:121:ARG:HA	1.92	0.52
3:BG:283:VAL:HA	4:CG:121:ARG:HA	1.92	0.52
3:VC:106:HIS:N	3:VC:178:GLU:O	2.43	0.52
3:NG:283:VAL:HA	4:OG:121:ARG:HA	1.92	0.52
3:PC:283:VAL:HA	4:QC:121:ARG:HA	1.92	0.51
3:BD:283:VAL:HA	4:CD:121:ARG:HA	1.92	0.51
4:KD:75:ILE:O	4:KD:79:LEU:N	2.38	0.51
3:PF:106:HIS:N	3:PF:178:GLU:O	2.43	0.51
2:IF:143:ALA:HB2	2:OF:205:LEU:CA	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:VF:283:VAL:HA	4:WF:121:ARG:HA	1.92	0.51
4:Q:75:ILE:O	4:Q:79:LEU:N	2.38	0.51
3:K:106:HIS:N	3:K:178:GLU:O	2.43	0.51
3:NA:106:HIS:N	3:NA:178:GLU:O	2.43	0.51
2:OC:143:ALA:HB1	2:UC:206:MET:CA	2.41	0.51
3:HD:105:ILE:HA	3:HD:179:TYR:HA	1.92	0.51
3:JF:283:VAL:HA	4:KF:121:ARG:HA	1.92	0.51
3:PF:283:VAL:HA	4:QF:121:ARG:HA	1.92	0.51
3:DC:105:ILE:HA	3:DC:179:TYR:HA	1.92	0.51
3:VC:105:ILE:HA	3:VC:179:TYR:HA	1.92	0.51
3:TD:283:VAL:HA	4:UD:121:ARG:HA	1.92	0.51
3:TG:106:HIS:N	3:TG:178:GLU:O	2.43	0.51
3:M:105:ILE:HA	3:M:179:TYR:HA	1.92	0.51
3:DC:106:HIS:N	3:DC:178:GLU:O	2.43	0.51
3:DF:283:VAL:HA	4:EF:121:ARG:HA	1.92	0.51
3:HG:105:ILE:HA	3:HG:179:TYR:HA	1.92	0.51
3:HG:106:HIS:N	3:HG:178:GLU:O	2.43	0.51
3:NG:105:ILE:HA	3:NG:179:TYR:HA	1.92	0.51
3:TG:105:ILE:HA	3:TG:179:TYR:HA	1.92	0.51
3:M:106:HIS:N	3:M:178:GLU:O	2.43	0.51
3:V:106:HIS:N	3:V:178:GLU:O	2.43	0.51
3:HD:283:VAL:HA	4:ID:121:ARG:HA	1.92	0.51
3:ND:283:VAL:HA	4:OD:121:ARG:HA	1.92	0.51
3:LE:106:HIS:N	3:LE:178:GLU:O	2.43	0.51
3:LE:283:VAL:HA	4:ME:121:ARG:HA	1.92	0.51
3:BG:105:ILE:HA	3:BG:179:TYR:HA	1.92	0.51
3:C:105:ILE:HA	3:C:179:TYR:HA	1.92	0.51
3:K:105:ILE:HA	3:K:179:TYR:HA	1.92	0.51
4:WA:75:ILE:O	4:WA:79:LEU:N	2.38	0.51
3:PC:105:ILE:HA	3:PC:179:TYR:HA	1.92	0.51
3:ZD:283:VAL:HA	4:AE:121:ARG:HA	1.92	0.51
2:KE:143:ALA:HB1	2:QE:206:MET:CA	2.41	0.51
3:VF:105:ILE:HA	3:VF:179:TYR:HA	1.92	0.51
3:LB:105:ILE:HA	3:LB:179:TYR:HA	1.92	0.51
3:TD:103:ASN:HA	3:TD:182:SER:HA	1.93	0.51
3:ZD:105:ILE:HA	3:ZD:179:TYR:HA	1.92	0.51
3:RE:283:VAL:HA	4:SE:121:ARG:HA	1.92	0.51
4:MF:75:ILE:O	4:MF:79:LEU:N	2.38	0.51
4:YF:75:ILE:O	4:YF:79:LEU:N	2.38	0.51
3:TD:106:HIS:N	3:TD:178:GLU:O	2.43	0.51
3:FE:283:VAL:HA	4:GE:121:ARG:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DF:106:HIS:N	3:DF:178:GLU:O	2.43	0.51
3:PF:105:ILE:HA	3:PF:179:TYR:HA	1.92	0.51
3:BG:106:HIS:N	3:BG:178:GLU:O	2.43	0.51
3:HG:103:ASN:HA	3:HG:182:SER:HA	1.93	0.51
3:K:90:HIS:N	3:K:195:PRO:O	2.40	0.50
3:V:105:ILE:HA	3:V:179:TYR:HA	1.92	0.50
3:LE:103:ASN:HA	3:LE:182:SER:HA	1.94	0.50
3:XE:283:VAL:HA	4:YE:121:ARG:HA	1.92	0.50
3:JF:105:ILE:HA	3:JF:179:TYR:HA	1.92	0.50
3:PF:103:ASN:HA	3:PF:182:SER:HA	1.94	0.50
3:M:103:ASN:HA	3:M:182:SER:HA	1.94	0.50
3:BD:103:ASN:HA	3:BD:182:SER:HA	1.94	0.50
4:ED:75:ILE:O	4:ED:79:LEU:N	2.38	0.50
3:ND:105:ILE:HA	3:ND:179:TYR:HA	1.92	0.50
3:TG:103:ASN:HA	3:TG:182:SER:HA	1.93	0.50
3:K:103:ASN:HA	3:K:182:SER:HA	1.93	0.50
3:BA:90:HIS:N	3:BA:195:PRO:O	2.40	0.50
3:BA:105:ILE:HA	3:BA:179:TYR:HA	1.92	0.50
4:KA:75:ILE:O	4:KA:79:LEU:N	2.38	0.50
3:LB:106:HIS:N	3:LB:178:GLU:O	2.43	0.50
3:RB:105:ILE:HA	3:RB:179:TYR:HA	1.92	0.50
3:DF:90:HIS:N	3:DF:195:PRO:O	2.40	0.50
3:NA:90:HIS:N	3:NA:195:PRO:O	2.40	0.50
3:PC:103:ASN:HA	3:PC:182:SER:HA	1.94	0.50
3:HD:103:ASN:HA	3:HD:182:SER:HA	1.94	0.50
3:XE:103:ASN:HA	3:XE:182:SER:HA	1.94	0.50
3:DF:103:ASN:HA	3:DF:182:SER:HA	1.94	0.50
3:DF:105:ILE:HA	3:DF:179:TYR:HA	1.92	0.50
3:V:103:ASN:HA	3:V:182:SER:HA	1.94	0.50
3:ZA:90:HIS:N	3:ZA:195:PRO:O	2.40	0.50
3:XB:90:HIS:N	3:XB:195:PRO:O	2.40	0.50
3:XB:103:ASN:HA	3:XB:182:SER:HA	1.93	0.50
3:JC:103:ASN:HA	3:JC:182:SER:HA	1.94	0.50
3:VF:106:HIS:N	3:VF:178:GLU:O	2.43	0.50
3:C:106:HIS:N	3:C:178:GLU:O	2.43	0.50
3:HA:103:ASN:HA	3:HA:182:SER:HA	1.94	0.50
3:HA:105:ILE:HA	3:HA:179:TYR:HA	1.92	0.50
3:ZA:105:ILE:HA	3:ZA:179:TYR:HA	1.92	0.50
3:LB:90:HIS:N	3:LB:195:PRO:O	2.40	0.50
3:JC:105:ILE:HA	3:JC:179:TYR:HA	1.92	0.50
3:TD:105:ILE:HA	3:TD:179:TYR:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:LE:90:HIS:N	3:LE:195:PRO:O	2.40	0.50
3:RE:105:ILE:HA	3:RE:179:TYR:HA	1.92	0.50
3:XE:105:ILE:HA	3:XE:179:TYR:HA	1.92	0.50
3:PF:90:HIS:N	3:PF:195:PRO:O	2.40	0.50
3:BG:103:ASN:HA	3:BG:182:SER:HA	1.93	0.50
3:NA:103:ASN:HA	3:NA:182:SER:HA	1.93	0.50
3:NA:105:ILE:HA	3:NA:179:TYR:HA	1.92	0.50
4:QA:75:ILE:O	4:QA:79:LEU:N	2.38	0.50
3:ZA:245:ASN:O	3:ZA:249:ASN:N	2.45	0.50
3:XB:105:ILE:HA	3:XB:179:TYR:HA	1.92	0.50
3:ZD:103:ASN:HA	3:ZD:182:SER:HA	1.94	0.50
3:FE:103:ASN:HA	3:FE:182:SER:HA	1.93	0.50
3:LE:105:ILE:HA	3:LE:179:TYR:HA	1.92	0.50
3:RE:245:ASN:O	3:RE:249:ASN:N	2.45	0.50
3:TA:105:ILE:HA	3:TA:179:TYR:HA	1.92	0.50
3:ZA:103:ASN:HA	3:ZA:182:SER:HA	1.94	0.50
3:FB:103:ASN:HA	3:FB:182:SER:HA	1.94	0.50
3:RB:103:ASN:HA	3:RB:182:SER:HA	1.94	0.50
3:BD:106:HIS:N	3:BD:178:GLU:O	2.43	0.50
3:VF:103:ASN:HA	3:VF:182:SER:HA	1.94	0.50
3:NA:245:ASN:O	3:NA:249:ASN:N	2.45	0.50
2:EE:73:ALA:HB1	2:EE:77:LEU:N	2.27	0.50
3:XE:90:HIS:N	3:XE:195:PRO:O	2.40	0.50
3:DF:245:ASN:O	3:DF:249:ASN:N	2.45	0.50
4:GF:75:ILE:O	4:GF:79:LEU:N	2.38	0.50
3:TA:106:HIS:N	3:TA:178:GLU:O	2.43	0.49
4:HE:119:GLY:HA2	4:IE:88:ALA:HA	1.94	0.49
4:WG:75:ILE:O	4:WG:79:LEU:N	2.38	0.49
4:DA:119:GLY:HA2	4:EA:88:ALA:HA	1.94	0.49
4:UB:75:ILE:O	4:UB:79:LEU:N	2.38	0.49
3:BD:105:ILE:HA	3:BD:179:TYR:HA	1.92	0.49
2:MD:73:ALA:HB1	2:MD:77:LEU:N	2.27	0.49
4:VD:119:GLY:HA2	4:WD:88:ALA:HA	1.94	0.49
2:WE:73:ALA:HB1	2:WE:77:LEU:N	2.27	0.49
3:VF:90:HIS:N	3:VF:195:PRO:O	2.40	0.49
3:BA:245:ASN:O	3:BA:249:ASN:N	2.45	0.49
4:DD:119:GLY:HA2	4:ED:88:ALA:HA	1.94	0.49
4:JD:119:GLY:HA2	4:KD:88:ALA:HA	1.94	0.49
3:ND:103:ASN:HA	3:ND:182:SER:HA	1.93	0.49
2:QE:73:ALA:HB1	2:QE:77:LEU:N	2.27	0.49
3:RE:90:HIS:N	3:RE:195:PRO:O	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:TE:119:GLY:HA2	4:UE:88:ALA:HA	1.94	0.49
2:IF:73:ALA:HB1	2:IF:77:LEU:N	2.27	0.49
3:PF:245:ASN:O	3:PF:249:ASN:N	2.45	0.49
3:NG:106:HIS:N	3:NG:178:GLU:O	2.43	0.49
4:E:119:GLY:HA2	4:H:88:ALA:HA	1.94	0.49
2:GA:73:ALA:HB1	2:GA:77:LEU:N	2.27	0.49
2:SA:73:ALA:HB1	2:SA:77:LEU:N	2.27	0.49
4:VA:119:GLY:HA2	4:WA:88:ALA:HA	1.94	0.49
2:EB:73:ALA:HB1	2:EB:77:LEU:N	2.27	0.49
2:AD:73:ALA:HB1	2:AD:77:LEU:N	2.27	0.49
4:PD:119:GLY:HA2	4:QD:88:ALA:HA	1.94	0.49
2:SD:73:ALA:HB1	2:SD:77:LEU:N	2.27	0.49
4:ZE:119:GLY:HA2	4:AF:88:ALA:HA	1.94	0.49
3:JF:103:ASN:HA	3:JF:182:SER:HA	1.93	0.49
3:NG:103:ASN:HA	3:NG:182:SER:HA	1.94	0.49
3:K:245:ASN:O	3:K:249:ASN:N	2.45	0.49
3:BA:106:HIS:N	3:BA:178:GLU:O	2.43	0.49
4:RC:119:GLY:HA2	4:SC:88:ALA:HA	1.94	0.49
4:BE:119:GLY:HA2	4:CE:88:ALA:HA	1.94	0.49
3:FE:105:ILE:HA	3:FE:179:TYR:HA	1.92	0.49
4:NE:119:GLY:HA2	4:OE:88:ALA:HA	1.94	0.49
3:BG:245:ASN:O	3:BG:249:ASN:N	2.45	0.49
3:HG:90:HIS:N	3:HG:195:PRO:O	2.40	0.49
4:XC:119:GLY:HA2	4:YC:88:ALA:HA	1.94	0.49
4:YC:75:ILE:O	4:YC:79:LEU:N	2.38	0.49
2:AD:143:ALA:HB1	2:GD:206:MET:CA	2.43	0.49
3:ZD:90:HIS:N	3:ZD:195:PRO:O	2.40	0.49
3:RE:103:ASN:HA	3:RE:182:SER:HA	1.94	0.49
2:AG:73:ALA:HB1	2:AG:77:LEU:N	2.27	0.49
4:PG:119:GLY:HA2	4:QG:88:ALA:HA	1.94	0.49
3:M:245:ASN:O	3:M:249:ASN:N	2.45	0.49
2:T:73:ALA:HB1	2:T:77:LEU:N	2.27	0.49
3:TA:128:ASP:O	3:TA:133:GLY:N	2.42	0.49
3:ZA:128:ASP:O	3:ZA:133:GLY:N	2.42	0.49
3:RB:128:ASP:O	3:RB:133:GLY:N	2.42	0.49
3:VC:103:ASN:HA	3:VC:182:SER:HA	1.93	0.49
2:OF:73:ALA:HB1	2:OF:77:LEU:N	2.27	0.49
3:NG:245:ASN:O	3:NG:249:ASN:N	2.45	0.49
4:X:119:GLY:HA2	4:Y:88:ALA:HA	1.94	0.49
2:GA:143:ALA:HB1	2:MA:206:MET:CA	2.42	0.49
3:FB:105:ILE:HA	3:FB:179:TYR:HA	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:UC:73:ALA:HB1	2:UC:77:LEU:N	2.27	0.49
3:TD:90:HIS:N	3:TD:195:PRO:O	2.40	0.49
2:KE:73:ALA:HB1	2:KE:77:LEU:N	2.27	0.49
4:FF:119:GLY:HA2	4:GF:88:ALA:HA	1.94	0.49
4:LF:119:GLY:HA2	4:MF:88:ALA:HA	1.94	0.49
3:C:103:ASN:HA	3:C:182:SER:HA	1.94	0.49
4:EA:75:ILE:O	4:EA:79:LEU:N	2.38	0.49
4:PA:119:GLY:HA2	4:QA:88:ALA:HA	1.94	0.49
4:NB:119:GLY:HA2	4:OB:88:ALA:HA	1.94	0.49
3:XB:128:ASP:O	3:XB:133:GLY:N	2.42	0.49
4:FC:119:GLY:HA2	4:GC:88:ALA:HA	1.94	0.49
2:IC:73:ALA:HB1	2:IC:77:LEU:N	2.27	0.49
3:JC:106:HIS:N	3:JC:178:GLU:O	2.43	0.49
2:YD:73:ALA:HB1	2:YD:77:LEU:N	2.27	0.49
4:P:119:GLY:HA2	4:Q:88:ALA:HA	1.94	0.49
2:B:73:ALA:HB1	2:B:77:LEU:N	2.27	0.49
3:BA:103:ASN:HA	3:BA:182:SER:HA	1.94	0.49
3:DC:103:ASN:HA	3:DC:182:SER:HA	1.94	0.49
4:LC:119:GLY:HA2	4:MC:88:ALA:HA	1.94	0.49
2:UC:143:ALA:HB2	2:AD:205:LEU:CA	2.33	0.49
3:XE:245:ASN:O	3:XE:249:ASN:N	2.45	0.49
3:TA:245:ASN:O	3:TA:249:ASN:N	2.45	0.48
3:LB:103:ASN:HA	3:LB:182:SER:HA	1.93	0.48
3:JF:106:HIS:N	3:JF:178:GLU:O	2.43	0.48
4:SF:75:ILE:O	4:SF:79:LEU:N	2.38	0.48
2:UF:73:ALA:HB1	2:UF:77:LEU:N	2.27	0.48
4:O:119:GLY:HA2	4:R:88:ALA:HA	1.94	0.48
3:TA:103:ASN:HA	3:TA:182:SER:HA	1.93	0.48
3:LB:128:ASP:O	3:LB:133:GLY:N	2.42	0.48
4:AF:75:ILE:O	4:AF:79:LEU:N	2.38	0.48
4:RF:119:GLY:HA2	4:SF:88:ALA:HA	1.94	0.48
4:XF:119:GLY:HA2	4:YF:88:ALA:HA	1.94	0.48
2:SG:73:ALA:HB1	2:SG:77:LEU:N	2.27	0.48
4:JA:119:GLY:HA2	4:KA:88:ALA:HA	1.94	0.48
3:FB:128:ASP:O	3:FB:133:GLY:N	2.42	0.48
4:OB:75:ILE:O	4:OB:79:LEU:N	2.38	0.48
3:BD:270:LEU:O	4:CD:62:VAL:N	2.31	0.48
3:FE:80:THR:N	3:FE:205:HIS:O	2.32	0.48
3:FE:90:HIS:N	3:FE:195:PRO:O	2.40	0.48
2:CF:73:ALA:HB1	2:CF:77:LEU:N	2.27	0.48
3:NA:128:ASP:O	3:NA:133:GLY:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:HB:119:GLY:HA2	4:IB:88:ALA:HA	1.94	0.48
4:TB:119:GLY:HA2	4:UB:88:ALA:HA	1.94	0.48
4:UE:75:ILE:O	4:UE:79:LEU:N	2.38	0.48
2:MG:73:ALA:HB1	2:MG:77:LEU:N	2.27	0.48
4:VG:119:GLY:HA2	4:WG:88:ALA:HA	1.94	0.48
2:OC:73:ALA:HB1	2:OC:77:LEU:N	2.27	0.48
3:RE:106:HIS:N	3:RE:178:GLU:O	2.43	0.48
3:JF:245:ASN:O	3:JF:249:ASN:N	2.45	0.48
3:BG:90:HIS:N	3:BG:195:PRO:O	2.40	0.48
2:GG:73:ALA:HB1	2:GG:77:LEU:N	2.27	0.48
3:HA:245:ASN:O	3:HA:249:ASN:N	2.45	0.48
4:BB:119:GLY:HA2	4:CB:88:ALA:HA	1.94	0.48
2:QB:73:ALA:HB1	2:QB:77:LEU:N	2.27	0.48
4:ZB:119:GLY:HA2	4:AC:88:ALA:HA	1.94	0.48
2:CC:73:ALA:HB1	2:CC:77:LEU:N	2.27	0.48
2:GD:73:ALA:HB1	2:GD:77:LEU:N	2.27	0.48
3:XE:270:LEU:O	4:YE:62:VAL:N	2.31	0.48
4:JG:119:GLY:HA2	4:KG:88:ALA:HA	1.94	0.48
3:BA:128:ASP:O	3:BA:133:GLY:N	2.42	0.48
3:FB:245:ASN:O	3:FB:249:ASN:N	2.45	0.48
3:DC:128:ASP:O	3:DC:133:GLY:N	2.42	0.48
3:JC:270:LEU:O	4:KC:62:VAL:N	2.31	0.48
3:ZD:106:HIS:N	3:ZD:178:GLU:O	2.43	0.48
3:JF:90:HIS:N	3:JF:195:PRO:O	2.40	0.48
2:J:73:ALA:HB1	2:J:77:LEU:N	2.27	0.48
3:V:128:ASP:O	3:V:133:GLY:N	2.42	0.48
2:MA:84:ALA:HB2	2:SA:23:ALA:CB	1.72	0.48
4:SC:75:ILE:O	4:SC:79:LEU:N	2.38	0.48
3:HD:90:HIS:N	3:HD:195:PRO:O	2.40	0.48
4:WD:100:LEU:HA	4:WD:105:LEU:HA	1.96	0.48
3:ZD:80:THR:N	3:ZD:205:HIS:O	2.32	0.48
3:NG:90:HIS:N	3:NG:195:PRO:O	2.40	0.48
3:V:245:ASN:O	3:V:249:ASN:N	2.45	0.48
4:Y:100:LEU:HA	4:Y:105:LEU:HA	1.96	0.48
3:PC:128:ASP:O	3:PC:133:GLY:N	2.42	0.48
4:WD:75:ILE:O	4:WD:79:LEU:N	2.38	0.48
3:LE:245:ASN:O	3:LE:249:ASN:N	2.45	0.48
4:OE:100:LEU:HA	4:OE:105:LEU:HA	1.96	0.48
3:VF:245:ASN:O	3:VF:249:ASN:N	2.45	0.48
4:DG:119:GLY:HA2	4:EG:88:ALA:HA	1.94	0.48
3:M:90:HIS:N	3:M:195:PRO:O	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:245:ASN:O	3:C:249:ASN:N	2.45	0.48
4:EA:100:LEU:HA	4:EA:105:LEU:HA	1.96	0.48
4:QA:100:LEU:HA	4:QA:105:LEU:HA	1.96	0.48
3:RB:106:HIS:N	3:RB:178:GLU:O	2.43	0.48
2:WB:73:ALA:HB1	2:WB:77:LEU:N	2.27	0.48
3:TD:270:LEU:O	4:UD:62:VAL:N	2.31	0.48
4:CE:100:LEU:HA	4:CE:105:LEU:HA	1.96	0.48
3:BG:270:LEU:O	4:CG:62:VAL:N	2.31	0.48
4:Q:100:LEU:HA	4:Q:105:LEU:HA	1.96	0.47
4:R:100:LEU:HA	4:R:105:LEU:HA	1.96	0.47
3:HA:128:ASP:O	3:HA:133:GLY:N	2.42	0.47
4:WA:100:LEU:HA	4:WA:105:LEU:HA	1.96	0.47
2:YA:73:ALA:HB1	2:YA:77:LEU:N	2.27	0.47
3:RB:245:ASN:O	3:RB:249:ASN:N	2.45	0.47
3:JC:128:ASP:O	3:JC:133:GLY:N	2.42	0.47
4:ED:100:LEU:HA	4:ED:105:LEU:HA	1.96	0.47
4:QD:100:LEU:HA	4:QD:105:LEU:HA	1.96	0.47
3:HG:245:ASN:O	3:HG:249:ASN:N	2.45	0.47
3:TG:245:ASN:O	3:TG:249:ASN:N	2.45	0.47
2:T:143:ALA:HB1	2:AA:206:MET:CA	2.44	0.47
4:KA:100:LEU:HA	4:KA:105:LEU:HA	1.96	0.47
3:VC:128:ASP:O	3:VC:133:GLY:N	2.42	0.47
4:YC:100:LEU:HA	4:YC:105:LEU:HA	1.96	0.47
4:IE:100:LEU:HA	4:IE:105:LEU:HA	1.96	0.47
4:UE:100:LEU:HA	4:UE:105:LEU:HA	1.96	0.47
2:G:73:ALA:HB1	2:G:77:LEU:N	2.27	0.47
4:H:100:LEU:HA	4:H:105:LEU:HA	1.96	0.47
4:QG:75:ILE:O	4:QG:79:LEU:N	2.38	0.47
3:TG:90:HIS:N	3:TG:195:PRO:O	2.40	0.47
2:T:88:GLU:C	2:T:90:ALA:H	2.23	0.47
2:KB:73:ALA:HB1	2:KB:77:LEU:N	2.27	0.47
4:KD:100:LEU:HA	4:KD:105:LEU:HA	1.96	0.47
3:TD:80:THR:N	3:TD:205:HIS:O	2.32	0.47
3:ZD:245:ASN:O	3:ZD:249:ASN:N	2.45	0.47
4:GF:100:LEU:HA	4:GF:105:LEU:HA	1.96	0.47
4:MF:100:LEU:HA	4:MF:105:LEU:HA	1.96	0.47
4:WG:100:LEU:HA	4:WG:105:LEU:HA	1.96	0.47
2:G:88:GLU:C	2:G:90:ALA:H	2.23	0.47
4:Y:75:ILE:O	4:Y:79:LEU:N	2.38	0.47
2:AA:73:ALA:HB1	2:AA:77:LEU:N	2.27	0.47
2:MA:88:GLU:C	2:MA:90:ALA:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SA:143:ALA:HB2	2:YA:205:LEU:CA	2.32	0.47
2:YA:88:GLU:C	2:YA:90:ALA:H	2.23	0.47
4:IB:100:LEU:HA	4:IB:105:LEU:HA	1.96	0.47
2:MG:88:GLU:C	2:MG:90:ALA:H	2.23	0.47
3:K:128:ASP:O	3:K:133:GLY:N	2.42	0.47
4:CB:100:LEU:HA	4:CB:105:LEU:HA	1.96	0.47
4:OB:100:LEU:HA	4:OB:105:LEU:HA	1.96	0.47
2:QB:88:GLU:C	2:QB:90:ALA:H	2.23	0.47
4:MC:100:LEU:HA	4:MC:105:LEU:HA	1.96	0.47
3:PC:80:THR:N	3:PC:205:HIS:O	2.32	0.47
3:BD:90:HIS:N	3:BD:195:PRO:O	2.40	0.47
3:HD:106:HIS:N	3:HD:178:GLU:O	2.43	0.47
2:UF:88:GLU:C	2:UF:90:ALA:H	2.23	0.47
2:B:88:GLU:C	2:B:90:ALA:H	2.23	0.47
2:GA:88:GLU:C	2:GA:90:ALA:H	2.23	0.47
2:EB:88:GLU:C	2:EB:90:ALA:H	2.23	0.47
4:IB:75:ILE:O	4:IB:79:LEU:N	2.38	0.47
4:UB:100:LEU:HA	4:UB:105:LEU:HA	1.96	0.47
4:SC:100:LEU:HA	4:SC:105:LEU:HA	1.96	0.47
3:ND:90:HIS:N	3:ND:195:PRO:O	2.40	0.47
4:AF:100:LEU:HA	4:AF:105:LEU:HA	1.96	0.47
2:CF:88:GLU:C	2:CF:90:ALA:H	2.23	0.47
2:OF:143:ALA:HB1	2:UF:206:MET:CA	2.44	0.47
4:SF:100:LEU:HA	4:SF:105:LEU:HA	1.96	0.47
4:KG:100:LEU:HA	4:KG:105:LEU:HA	1.96	0.47
4:QG:100:LEU:HA	4:QG:105:LEU:HA	1.96	0.47
2:MA:73:ALA:HB1	2:MA:77:LEU:N	2.27	0.47
2:YA:143:ALA:HB1	2:EB:206:MET:CA	2.45	0.47
3:RB:270:LEU:O	4:SB:62:VAL:N	2.31	0.47
2:WB:143:ALA:HB1	2:CC:206:MET:CA	2.45	0.47
4:GC:100:LEU:HA	4:GC:105:LEU:HA	1.96	0.47
2:IC:88:GLU:C	2:IC:90:ALA:H	2.23	0.47
3:BD:128:ASP:O	3:BD:133:GLY:N	2.42	0.47
4:EG:100:LEU:HA	4:EG:105:LEU:HA	1.96	0.47
2:GG:88:GLU:C	2:GG:90:ALA:H	2.23	0.47
3:TA:80:THR:O	3:TA:205:HIS:N	2.38	0.47
3:TA:80:THR:N	3:TA:205:HIS:O	2.32	0.47
2:AD:88:GLU:C	2:AD:90:ALA:H	2.23	0.47
4:AC:100:LEU:HA	4:AC:105:LEU:HA	1.96	0.47
3:ND:245:ASN:O	3:ND:249:ASN:N	2.45	0.47
2:KE:88:GLU:C	2:KE:90:ALA:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:206:MET:CA	2:SG:143:ALA:HB1	2.44	0.46
2:EB:143:ALA:HB1	2:KB:206:MET:CA	2.46	0.46
2:KB:167:VAL:CB	2:QB:191:SER:HA	2.45	0.46
4:YF:100:LEU:HA	4:YF:105:LEU:HA	1.96	0.46
2:AG:143:ALA:HB1	2:GG:206:MET:CA	2.45	0.46
2:J:88:GLU:C	2:J:90:ALA:H	2.23	0.46
2:MA:84:ALA:CB	2:SA:23:ALA:C	2.87	0.46
4:MC:75:ILE:O	4:MC:79:LEU:N	2.38	0.46
3:PC:90:HIS:N	3:PC:195:PRO:O	2.40	0.46
3:ND:80:THR:N	3:ND:205:HIS:O	2.32	0.46
3:C:80:THR:N	3:C:205:HIS:O	2.32	0.46
2:OF:88:GLU:C	2:OF:90:ALA:H	2.23	0.46
4:R:75:ILE:O	4:R:79:LEU:N	2.38	0.46
2:KB:88:GLU:C	2:KB:90:ALA:H	2.23	0.46
2:CC:88:GLU:C	2:CC:90:ALA:H	2.23	0.46
2:IF:119:ALA:O	2:IF:123:ARG:N	2.49	0.46
3:V:90:HIS:N	3:V:195:PRO:O	2.40	0.46
3:LB:245:ASN:O	3:LB:249:ASN:N	2.45	0.46
3:JC:80:THR:N	3:JC:205:HIS:O	2.32	0.46
2:SD:119:ALA:O	2:SD:123:ARG:N	2.49	0.46
2:QE:119:ALA:O	2:QE:123:ARG:N	2.49	0.46
3:C:128:ASP:O	3:C:133:GLY:N	2.42	0.46
2:KB:73:ALA:C	2:KB:75:GLU:N	2.74	0.46
2:KB:143:ALA:HB1	2:QB:206:MET:CA	2.46	0.46
2:IC:73:ALA:C	2:IC:75:GLU:N	2.74	0.46
2:IC:143:ALA:HB1	2:OC:206:MET:CA	2.45	0.46
2:UC:88:GLU:C	2:UC:90:ALA:H	2.23	0.46
4:QD:75:ILE:O	4:QD:79:LEU:N	2.38	0.46
2:YD:119:ALA:O	2:YD:123:ARG:N	2.49	0.46
2:KE:119:ALA:O	2:KE:123:ARG:N	2.49	0.46
4:OE:75:ILE:O	4:OE:79:LEU:N	2.38	0.46
2:WE:88:GLU:C	2:WE:90:ALA:H	2.23	0.46
2:AG:119:ALA:O	2:AG:123:ARG:N	2.49	0.46
3:M:128:ASP:O	3:M:133:GLY:N	2.42	0.46
3:C:90:HIS:N	3:C:195:PRO:O	2.40	0.46
2:GA:73:ALA:C	2:GA:75:GLU:N	2.74	0.46
2:EB:73:ALA:C	2:EB:75:GLU:N	2.74	0.46
2:AD:119:ALA:O	2:AD:123:ARG:N	2.49	0.46
2:MD:73:ALA:C	2:MD:75:GLU:N	2.74	0.46
3:TG:270:LEU:O	4:UG:62:VAL:N	2.31	0.46
2:J:143:ALA:HB1	2:T:206:MET:CA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:80:THR:O	3:K:205:HIS:N	2.38	0.46
2:AA:73:ALA:C	2:AA:75:GLU:N	2.74	0.46
2:SA:88:GLU:C	2:SA:90:ALA:H	2.23	0.46
2:OC:73:ALA:C	2:OC:75:GLU:N	2.74	0.46
2:MD:88:GLU:C	2:MD:90:ALA:H	2.23	0.46
2:EE:88:GLU:C	2:EE:90:ALA:H	2.23	0.46
3:LE:270:LEU:O	4:ME:62:VAL:N	2.31	0.46
3:TG:128:ASP:O	3:TG:133:GLY:N	2.42	0.46
2:EB:119:ALA:O	2:EB:123:ARG:N	2.49	0.46
2:GD:119:ALA:O	2:GD:123:ARG:N	2.49	0.46
3:HD:128:ASP:O	3:HD:133:GLY:N	2.42	0.46
3:ND:128:ASP:O	3:ND:133:GLY:N	2.42	0.46
2:CF:119:ALA:O	2:CF:123:ARG:N	2.49	0.46
2:SG:88:GLU:C	2:SG:90:ALA:H	2.23	0.46
2:AA:119:ALA:O	2:AA:123:ARG:N	2.49	0.46
2:GA:119:ALA:O	2:GA:123:ARG:N	2.49	0.46
2:MA:73:ALA:C	2:MA:75:GLU:N	2.74	0.46
3:ZA:270:LEU:O	4:AB:62:VAL:N	2.31	0.46
2:SD:73:ALA:C	2:SD:75:GLU:N	2.74	0.46
2:SG:119:ALA:O	2:SG:123:ARG:N	2.49	0.46
2:MA:143:ALA:HB2	2:SA:205:LEU:CA	2.33	0.45
2:MA:167:VAL:CB	2:SA:191:SER:HA	2.47	0.45
2:QB:73:ALA:C	2:QB:75:GLU:N	2.74	0.45
3:DC:270:LEU:O	4:EC:62:VAL:N	2.31	0.45
2:IC:119:ALA:O	2:IC:123:ARG:N	2.49	0.45
2:OC:119:ALA:O	2:OC:123:ARG:N	2.49	0.45
3:BD:245:ASN:O	3:BD:249:ASN:N	2.45	0.45
3:TD:128:ASP:O	3:TD:133:GLY:N	2.42	0.45
2:OF:119:ALA:O	2:OF:123:ARG:N	2.49	0.45
2:UF:119:ALA:O	2:UF:123:ARG:N	2.49	0.45
2:KB:119:ALA:O	2:KB:123:ARG:N	2.49	0.45
3:JC:90:HIS:N	3:JC:195:PRO:O	2.40	0.45
3:VC:90:HIS:N	3:VC:195:PRO:O	2.40	0.45
3:NG:128:ASP:O	3:NG:133:GLY:N	2.42	0.45
2:YA:119:ALA:O	2:YA:123:ARG:N	2.49	0.45
3:HD:80:THR:N	3:HD:205:HIS:O	2.32	0.45
2:GG:119:ALA:O	2:GG:123:ARG:N	2.49	0.45
4:H:75:ILE:O	4:H:79:LEU:N	2.38	0.45
3:PC:270:LEU:O	4:QC:62:VAL:N	2.31	0.45
2:WE:73:ALA:C	2:WE:75:GLU:N	2.74	0.45
2:WE:119:ALA:O	2:WE:123:ARG:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:PF:270:LEU:O	4:QF:62:VAL:N	2.31	0.45
2:MG:73:ALA:C	2:MG:75:GLU:N	2.74	0.45
2:MG:119:ALA:O	2:MG:123:ARG:N	2.49	0.45
2:SG:73:ALA:C	2:SG:75:GLU:N	2.74	0.45
2:T:119:ALA:O	2:T:123:ARG:N	2.49	0.45
4:HB:86:VAL:HA	4:IB:120:VAL:O	2.17	0.45
2:WB:119:ALA:O	2:WB:123:ARG:N	2.49	0.45
3:DC:80:THR:N	3:DC:205:HIS:O	2.32	0.45
3:ZD:128:ASP:O	3:ZD:133:GLY:N	2.42	0.45
2:QE:73:ALA:C	2:QE:75:GLU:N	2.74	0.45
2:AA:88:GLU:C	2:AA:90:ALA:H	2.23	0.45
4:VA:86:VAL:HA	4:WA:120:VAL:O	2.17	0.45
4:BB:86:VAL:HA	4:CB:120:VAL:O	2.17	0.45
4:CB:75:ILE:O	4:CB:79:LEU:N	2.38	0.45
4:GC:75:ILE:O	4:GC:79:LEU:N	2.38	0.45
2:UC:119:ALA:O	2:UC:123:ARG:N	2.49	0.45
2:MD:119:ALA:O	2:MD:123:ARG:N	2.49	0.45
3:LE:80:THR:O	3:LE:205:HIS:N	2.38	0.45
2:CF:73:ALA:C	2:CF:75:GLU:N	2.74	0.45
2:G:73:ALA:C	2:G:75:GLU:N	2.74	0.45
2:G:119:ALA:O	2:G:123:ARG:N	2.49	0.45
2:B:119:ALA:O	2:B:123:ARG:N	2.49	0.45
2:J:119:ALA:O	2:J:123:ARG:N	2.49	0.45
2:MA:119:ALA:O	2:MA:123:ARG:N	2.49	0.45
4:PA:86:VAL:HA	4:QA:120:VAL:O	2.17	0.45
3:ZA:80:THR:O	3:ZA:205:HIS:N	2.38	0.45
4:NB:86:VAL:HA	4:OB:120:VAL:O	2.17	0.45
3:VC:245:ASN:O	3:VC:249:ASN:N	2.45	0.45
2:YD:73:ALA:C	2:YD:75:GLU:N	2.74	0.45
4:FF:86:VAL:HA	4:GF:120:VAL:O	2.17	0.45
3:K:270:LEU:O	4:L:62:VAL:N	2.31	0.45
3:HA:270:LEU:O	4:IA:62:VAL:N	2.31	0.45
4:JA:86:VAL:HA	4:KA:120:VAL:O	2.17	0.45
4:TB:86:VAL:HA	4:UB:120:VAL:O	2.17	0.45
4:ZB:86:VAL:HA	4:AC:120:VAL:O	2.17	0.45
3:JC:80:THR:O	3:JC:205:HIS:N	2.37	0.45
2:YD:88:GLU:C	2:YD:90:ALA:H	2.23	0.45
2:EE:119:ALA:O	2:EE:123:ARG:N	2.49	0.45
2:KE:143:ALA:HB1	2:QE:206:MET:HA	1.98	0.45
2:QE:143:ALA:HB1	2:WE:206:MET:CA	2.47	0.45
2:AG:88:GLU:C	2:AG:90:ALA:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:FB:270:LEU:O	4:GB:62:VAL:N	2.31	0.45
2:QB:119:ALA:O	2:QB:123:ARG:N	2.49	0.45
4:FC:86:VAL:HA	4:GC:120:VAL:O	2.17	0.45
2:GD:88:GLU:C	2:GD:90:ALA:H	2.23	0.45
3:HG:128:ASP:O	3:HG:133:GLY:N	2.42	0.45
4:KG:75:ILE:O	4:KG:79:LEU:N	2.38	0.45
4:DA:86:VAL:HA	4:EA:120:VAL:O	2.17	0.45
3:HA:90:HIS:N	3:HA:195:PRO:O	2.40	0.45
2:CC:119:ALA:O	2:CC:123:ARG:N	2.49	0.45
2:SD:88:GLU:C	2:SD:90:ALA:H	2.23	0.45
4:ZE:86:VAL:HA	4:AF:120:VAL:O	2.17	0.45
2:IF:73:ALA:C	2:IF:75:GLU:N	2.74	0.45
4:LF:86:VAL:HA	4:MF:120:VAL:O	2.17	0.45
3:FB:90:HIS:N	3:FB:195:PRO:O	2.40	0.44
4:LC:86:VAL:HA	4:MC:120:VAL:O	2.17	0.44
2:UF:73:ALA:C	2:UF:75:GLU:N	2.74	0.44
4:PG:86:VAL:HA	4:QG:120:VAL:O	2.17	0.44
2:B:143:ALA:HB1	2:J:206:MET:CA	2.47	0.44
3:DC:245:ASN:O	3:DC:249:ASN:N	2.45	0.44
3:FE:128:ASP:O	3:FE:133:GLY:N	2.42	0.44
3:RE:80:THR:O	3:RE:205:HIS:N	2.38	0.44
4:VG:86:VAL:HA	4:WG:120:VAL:O	2.17	0.44
2:B:73:ALA:C	2:B:75:GLU:N	2.74	0.44
4:X:86:VAL:HA	4:Y:120:VAL:O	2.17	0.44
2:SA:119:ALA:O	2:SA:123:ARG:N	2.49	0.44
3:RB:80:THR:N	3:RB:205:HIS:O	2.32	0.44
3:RB:90:HIS:N	3:RB:195:PRO:O	2.40	0.44
4:RC:86:VAL:HA	4:SC:120:VAL:O	2.17	0.44
4:VD:86:VAL:HA	4:WD:120:VAL:O	2.17	0.44
4:IE:75:ILE:O	4:IE:79:LEU:N	2.38	0.44
4:JG:86:VAL:HA	4:KG:120:VAL:O	2.17	0.44
4:O:86:VAL:HA	4:R:120:VAL:O	2.17	0.44
3:NA:80:THR:N	3:NA:205:HIS:O	2.32	0.44
3:DC:90:HIS:N	3:DC:195:PRO:O	2.40	0.44
4:XC:86:VAL:HA	4:YC:120:VAL:O	2.17	0.44
3:HD:245:ASN:O	3:HD:249:ASN:N	2.45	0.44
4:TE:86:VAL:HA	4:UE:120:VAL:O	2.17	0.44
4:RF:86:VAL:HA	4:SF:120:VAL:O	2.17	0.44
3:JC:245:ASN:O	3:JC:249:ASN:N	2.45	0.44
3:PC:245:ASN:O	3:PC:249:ASN:N	2.45	0.44
4:PD:86:VAL:HA	4:QD:120:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:86:VAL:HA	4:CE:120:VAL:O	2.17	0.44
2:QE:88:GLU:O	2:QE:90:ALA:N	2.46	0.44
2:IF:88:GLU:C	2:IF:90:ALA:H	2.23	0.44
3:M:80:THR:N	3:M:205:HIS:O	2.32	0.44
3:TA:90:HIS:N	3:TA:195:PRO:O	2.40	0.44
3:TA:270:LEU:O	4:UA:62:VAL:N	2.31	0.44
2:WB:88:GLU:C	2:WB:90:ALA:H	2.23	0.44
3:FE:270:LEU:O	4:GE:62:VAL:N	2.31	0.44
3:JF:80:THR:N	3:JF:205:HIS:O	2.32	0.44
3:PF:80:THR:N	3:PF:205:HIS:O	2.32	0.44
3:NG:80:THR:O	3:NG:205:HIS:N	2.38	0.44
4:P:86:VAL:HA	4:Q:120:VAL:O	2.17	0.44
4:E:86:VAL:HA	4:H:120:VAL:O	2.17	0.44
3:XB:80:THR:N	3:XB:205:HIS:O	2.32	0.44
2:OC:88:GLU:C	2:OC:90:ALA:H	2.23	0.44
3:BD:80:THR:N	3:BD:205:HIS:O	2.32	0.44
4:DD:86:VAL:HA	4:ED:120:VAL:O	2.17	0.44
2:GD:143:ALA:HB1	2:MD:206:MET:CA	2.48	0.44
2:YD:143:ALA:HB1	2:EE:206:MET:CA	2.48	0.44
3:DF:80:THR:N	3:DF:205:HIS:O	2.32	0.44
4:DG:86:VAL:HA	4:EG:120:VAL:O	2.17	0.44
2:QE:88:GLU:C	2:QE:90:ALA:H	2.23	0.44
3:JF:128:ASP:O	3:JF:133:GLY:N	2.42	0.44
2:OF:73:ALA:C	2:OF:75:GLU:N	2.74	0.44
3:VF:80:THR:N	3:VF:205:HIS:O	2.32	0.44
3:BG:128:ASP:O	3:BG:133:GLY:N	2.42	0.44
2:AA:143:ALA:HB1	2:GA:206:MET:CA	2.48	0.44
4:AC:75:ILE:O	4:AC:79:LEU:N	2.38	0.44
3:HD:270:LEU:O	4:ID:62:VAL:N	2.31	0.44
4:JD:86:VAL:HA	4:KD:120:VAL:O	2.17	0.44
3:DF:128:ASP:O	3:DF:133:GLY:N	2.42	0.44
3:PF:128:ASP:O	3:PF:133:GLY:N	2.42	0.44
4:HE:86:VAL:HA	4:IE:120:VAL:O	2.17	0.43
3:LE:128:ASP:O	3:LE:133:GLY:N	2.42	0.43
3:XE:80:THR:O	3:XE:205:HIS:N	2.38	0.43
3:XE:128:ASP:O	3:XE:133:GLY:N	2.42	0.43
2:GG:143:ALA:HB1	2:MG:206:MET:CA	2.48	0.43
3:V:80:THR:O	3:V:205:HIS:N	2.37	0.43
2:KE:73:ALA:C	2:KE:75:GLU:N	2.74	0.43
4:NE:86:VAL:HA	4:OE:120:VAL:O	2.17	0.43
3:RE:128:ASP:O	3:RE:133:GLY:N	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:XE:80:THR:N	3:XE:205:HIS:O	2.32	0.43
3:VF:128:ASP:O	3:VF:133:GLY:N	2.42	0.43
3:BG:80:THR:N	3:BG:205:HIS:O	2.32	0.43
2:J:73:ALA:C	2:J:75:GLU:N	2.74	0.43
4:WC:111:VAL:HA	4:WC:120:VAL:HA	2.00	0.43
2:KB:67:ALA:O	2:QB:48:SER:C	2.61	0.43
4:AE:111:VAL:HA	4:AE:120:VAL:HA	2.00	0.43
4:CE:75:ILE:O	4:CE:79:LEU:N	2.38	0.43
4:XF:86:VAL:HA	4:YF:120:VAL:O	2.17	0.43
2:QB:88:GLU:O	2:QB:90:ALA:N	2.46	0.43
2:OC:143:ALA:HB1	2:UC:206:MET:HA	2.00	0.43
2:OC:167:VAL:CB	2:UC:191:SER:HA	2.49	0.43
3:JF:270:LEU:O	4:KF:62:VAL:N	2.31	0.43
4:N:111:VAL:HA	4:N:120:VAL:HA	2.00	0.43
4:QC:111:VAL:HA	4:QC:120:VAL:HA	2.00	0.43
4:CD:111:VAL:HA	4:CD:120:VAL:HA	2.00	0.43
4:UD:111:VAL:HA	4:UD:120:VAL:HA	2.00	0.43
4:L:111:VAL:HA	4:L:120:VAL:HA	2.00	0.43
2:MA:84:ALA:CB	2:SA:23:ALA:CA	2.80	0.43
2:SA:143:ALA:HB1	2:YA:206:MET:CA	2.48	0.43
2:UC:88:GLU:O	2:UC:90:ALA:N	2.46	0.43
4:GE:111:VAL:HA	4:GE:120:VAL:HA	2.00	0.43
3:DF:270:LEU:O	4:EF:62:VAL:N	2.31	0.43
3:HG:80:THR:N	3:HG:205:HIS:O	2.32	0.43
4:OG:111:VAL:HA	4:OG:120:VAL:HA	2.00	0.43
4:CA:111:VAL:HA	4:CA:120:VAL:HA	2.00	0.43
3:FB:80:THR:O	3:FB:205:HIS:N	2.38	0.43
3:FB:80:THR:N	3:FB:205:HIS:O	2.32	0.43
4:SB:111:VAL:HA	4:SB:120:VAL:HA	2.00	0.43
3:FE:245:ASN:O	3:FE:249:ASN:N	2.45	0.43
3:RE:80:THR:N	3:RE:205:HIS:O	2.32	0.43
2:UF:143:ALA:HB1	2:AG:206:MET:CA	2.49	0.43
4:UG:111:VAL:HA	4:UG:120:VAL:HA	2.00	0.43
4:W:111:VAL:HA	4:W:120:VAL:HA	2.00	0.43
2:AD:143:ALA:HB1	2:GD:206:MET:HA	2.01	0.43
3:ND:270:LEU:O	4:OD:62:VAL:N	2.31	0.43
3:ZD:270:LEU:O	4:AE:62:VAL:N	2.31	0.43
3:PF:80:THR:O	3:PF:205:HIS:N	2.38	0.43
4:D:111:VAL:HA	4:D:120:VAL:HA	2.00	0.43
2:GA:143:ALA:HB1	2:MA:206:MET:HA	2.00	0.43
4:MB:111:VAL:HA	4:MB:120:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:YB:111:VAL:HA	4:YB:120:VAL:HA	2.00	0.43
2:SD:143:ALA:HB1	2:YD:206:MET:CA	2.49	0.43
4:CG:111:VAL:HA	4:CG:120:VAL:HA	2.00	0.43
2:G:206:MET:HA	2:SG:143:ALA:HB1	2.01	0.42
2:T:88:GLU:O	2:T:90:ALA:N	2.46	0.42
4:OA:111:VAL:HA	4:OA:120:VAL:HA	2.00	0.42
2:YA:143:ALA:HB1	2:EB:206:MET:HA	2.00	0.42
4:KC:111:VAL:HA	4:KC:120:VAL:HA	2.00	0.42
2:CF:143:ALA:HB1	2:IF:206:MET:CA	2.48	0.42
3:DF:80:THR:O	3:DF:205:HIS:N	2.37	0.42
2:IF:143:ALA:HB1	2:OF:206:MET:CA	2.48	0.42
2:OC:143:ALA:CB	2:UC:206:MET:N	2.72	0.42
3:VC:80:THR:N	3:VC:205:HIS:O	2.32	0.42
4:OD:111:VAL:HA	4:OD:120:VAL:HA	2.00	0.42
4:EF:111:VAL:HA	4:EF:120:VAL:HA	2.00	0.42
3:HG:270:LEU:O	4:IG:62:VAL:N	2.31	0.42
4:IG:111:VAL:HA	4:IG:120:VAL:HA	2.00	0.42
3:NG:80:THR:N	3:NG:205:HIS:O	2.32	0.42
2:T:73:ALA:C	2:T:75:GLU:N	2.74	0.42
2:MA:88:GLU:O	2:MA:90:ALA:N	2.46	0.42
3:ZA:80:THR:N	3:ZA:205:HIS:O	2.32	0.42
4:ID:111:VAL:HA	4:ID:120:VAL:HA	2.00	0.42
4:QF:111:VAL:HA	4:QF:120:VAL:HA	2.00	0.42
2:GA:155:HIS:CB	2:MA:217:ALA:HB2	2.48	0.42
4:IA:111:VAL:HA	4:IA:120:VAL:HA	2.00	0.42
3:XB:245:ASN:O	3:XB:249:ASN:N	2.45	0.42
3:TD:245:ASN:O	3:TD:249:ASN:N	2.45	0.42
4:YE:111:VAL:HA	4:YE:120:VAL:HA	2.00	0.42
4:WF:111:VAL:HA	4:WF:120:VAL:HA	2.00	0.42
3:HG:80:THR:O	3:HG:205:HIS:N	2.38	0.42
2:G:88:GLU:O	2:G:90:ALA:N	2.46	0.42
3:V:270:LEU:O	4:W:62:VAL:N	2.31	0.42
2:OC:67:ALA:O	2:UC:48:SER:C	2.63	0.42
3:PC:80:THR:O	3:PC:205:HIS:N	2.38	0.42
2:YD:167:VAL:CB	2:EE:191:SER:HA	2.49	0.42
2:WE:167:VAL:CB	2:CF:191:SER:HA	2.49	0.42
3:VF:270:LEU:O	4:WF:62:VAL:N	2.31	0.42
4:ME:111:VAL:HA	4:ME:120:VAL:HA	2.00	0.42
4:KF:111:VAL:HA	4:KF:120:VAL:HA	2.00	0.42
3:TG:80:THR:N	3:TG:205:HIS:O	2.32	0.42
4:AB:111:VAL:HA	4:AB:120:VAL:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:GB:111:VAL:HA	4:GB:120:VAL:HA	2.00	0.42
2:WB:73:ALA:C	2:WB:75:GLU:N	2.74	0.42
3:XB:270:LEU:O	4:YB:62:VAL:N	2.31	0.42
3:LE:80:THR:N	3:LE:205:HIS:O	2.32	0.42
2:GG:167:VAL:CB	2:MG:191:SER:HA	2.49	0.42
2:J:143:ALA:HB1	2:T:206:MET:HA	2.01	0.42
2:CC:73:ALA:C	2:CC:75:GLU:N	2.74	0.42
4:EC:111:VAL:HA	4:EC:120:VAL:HA	2.00	0.42
2:MD:167:VAL:CB	2:SD:191:SER:HA	2.49	0.42
3:RE:270:LEU:O	4:SE:62:VAL:N	2.31	0.42
4:UA:111:VAL:HA	4:UA:120:VAL:HA	2.00	0.42
2:WB:143:ALA:HB1	2:CC:206:MET:HA	2.01	0.42
2:OC:88:GLU:O	2:OC:90:ALA:N	2.46	0.42
2:WE:143:ALA:HB1	2:CF:206:MET:CA	2.50	0.42
3:C:270:LEU:O	4:D:62:VAL:N	2.31	0.42
2:KB:155:HIS:CB	2:QB:217:ALA:HB1	2.48	0.42
2:OC:155:HIS:CB	2:UC:217:ALA:HB1	2.47	0.42
2:UF:167:VAL:CB	2:AG:191:SER:HA	2.50	0.42
4:EG:75:ILE:O	4:EG:79:LEU:N	2.38	0.42
2:G:167:VAL:CB	2:B:191:SER:HA	2.50	0.41
3:HA:80:THR:N	3:HA:205:HIS:O	2.32	0.41
3:LB:80:THR:N	3:LB:205:HIS:O	2.32	0.41
2:MD:88:GLU:O	2:MD:90:ALA:N	2.46	0.41
2:EE:143:ALA:HB1	2:KE:206:MET:CA	2.50	0.41
2:KE:155:HIS:CB	2:QE:217:ALA:HB2	2.48	0.41
4:SE:111:VAL:HA	4:SE:120:VAL:HA	2.00	0.41
2:AG:73:ALA:C	2:AG:75:GLU:N	2.74	0.41
3:VC:80:THR:O	3:VC:205:HIS:N	2.37	0.41
2:IC:143:ALA:HB1	2:OC:206:MET:HA	2.01	0.41
3:BD:80:THR:O	3:BD:205:HIS:N	2.38	0.41
4:BE:122:ILE:O	4:CE:84:GLY:N	2.36	0.41
4:HE:122:ILE:O	4:IE:84:GLY:N	2.36	0.41
2:GG:88:GLU:O	2:GG:90:ALA:N	2.46	0.41
2:YA:195:GLY:O	2:YA:197:ARG:N	2.48	0.41
2:AD:73:ALA:C	2:AD:75:GLU:N	2.74	0.41
4:NE:122:ILE:O	4:OE:84:GLY:N	2.36	0.41
4:TE:122:ILE:O	4:UE:84:GLY:N	2.36	0.41
3:JF:80:THR:O	3:JF:205:HIS:N	2.38	0.41
2:T:143:ALA:HB1	2:AA:206:MET:HA	2.02	0.41
2:SA:73:ALA:C	2:SA:75:GLU:N	2.74	0.41
2:YA:73:ALA:C	2:YA:75:GLU:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:88:GLU:O	2:EB:90:ALA:N	2.46	0.41
3:HD:80:THR:O	3:HD:205:HIS:N	2.38	0.41
4:ZE:122:ILE:O	4:AF:84:GLY:N	2.36	0.41
2:MA:67:ALA:O	2:SA:48:SER:C	2.63	0.41
2:IC:88:GLU:O	2:IC:90:ALA:N	2.46	0.41
2:UC:73:ALA:C	2:UC:75:GLU:N	2.74	0.41
2:MD:67:ALA:O	2:SD:48:SER:C	2.64	0.41
2:QE:167:VAL:CB	2:WE:191:SER:HA	2.50	0.41
2:GG:67:ALA:O	2:MG:48:SER:C	2.64	0.41
3:K:80:THR:N	3:K:205:HIS:O	2.32	0.41
2:AD:155:HIS:CB	2:GD:217:ALA:HB2	2.49	0.41
3:TD:80:THR:O	3:TD:205:HIS:N	2.38	0.41
4:FF:122:ILE:O	4:GF:84:GLY:N	2.36	0.41
3:V:80:THR:N	3:V:205:HIS:O	2.32	0.41
3:BA:80:THR:O	3:BA:205:HIS:N	2.38	0.41
3:BA:80:THR:N	3:BA:205:HIS:O	2.32	0.41
2:SA:48:SER:H	2:SA:51:GLN:CB	2.34	0.41
2:GD:167:VAL:CB	2:MD:191:SER:HA	2.51	0.41
3:ND:80:THR:O	3:ND:205:HIS:N	2.37	0.41
2:MG:167:VAL:CB	2:SG:191:SER:HA	2.51	0.41
3:TG:80:THR:O	3:TG:205:HIS:N	2.37	0.41
2:B:195:GLY:O	2:B:197:ARG:N	2.48	0.41
2:GA:48:SER:H	2:GA:51:GLN:CB	2.34	0.41
2:MA:48:SER:H	2:MA:51:GLN:CB	2.34	0.41
2:YA:48:SER:H	2:YA:51:GLN:CB	2.34	0.41
2:YA:143:ALA:CB	2:EB:206:MET:N	2.79	0.41
3:LB:80:THR:O	3:LB:205:HIS:N	2.38	0.41
2:SD:88:GLU:O	2:SD:90:ALA:N	2.46	0.41
2:YD:67:ALA:O	2:EE:48:SER:C	2.64	0.41
2:EE:88:GLU:O	2:EE:90:ALA:N	2.46	0.41
2:CF:167:VAL:CB	2:IF:191:SER:HA	2.51	0.41
4:LF:122:ILE:O	4:MF:84:GLY:N	2.36	0.41
2:OF:88:GLU:O	2:OF:90:ALA:N	2.46	0.41
2:OF:143:ALA:HB1	2:UF:206:MET:HA	2.02	0.41
4:RF:122:ILE:O	4:SF:84:GLY:N	2.36	0.41
2:B:167:VAL:CB	2:J:191:SER:HA	2.52	0.41
2:AD:48:SER:H	2:AD:51:GLN:CB	2.34	0.41
2:GD:48:SER:H	2:GD:51:GLN:CB	2.34	0.41
2:MD:143:ALA:HB1	2:SD:206:MET:CA	2.51	0.41
2:WE:67:ALA:O	2:CF:48:SER:C	2.64	0.41
2:AG:167:VAL:CB	2:GG:191:SER:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:270:LEU:O	4:N:62:VAL:N	2.31	0.40
2:T:167:VAL:CB	2:AA:191:SER:HA	2.51	0.40
2:AA:48:SER:H	2:AA:51:GLN:CB	2.34	0.40
2:GA:167:VAL:CB	2:MA:191:SER:HA	2.51	0.40
2:EB:48:SER:H	2:EB:51:GLN:CB	2.34	0.40
3:DC:80:THR:O	3:DC:205:HIS:N	2.38	0.40
2:UC:167:VAL:CB	2:AD:191:SER:HA	2.51	0.40
2:AD:167:VAL:CB	2:GD:191:SER:HA	2.51	0.40
2:WE:88:GLU:O	2:WE:90:ALA:N	2.46	0.40
2:OF:167:VAL:CB	2:UF:191:SER:HA	2.51	0.40
2:AG:143:ALA:HB1	2:GG:206:MET:HA	2.02	0.40
2:WB:48:SER:H	2:WB:51:GLN:CB	2.34	0.40
2:IC:48:SER:H	2:IC:51:GLN:CB	2.34	0.40
2:OC:48:SER:H	2:OC:51:GLN:CB	2.34	0.40
2:UC:48:SER:H	2:UC:51:GLN:CB	2.34	0.40
4:XF:122:ILE:O	4:YF:84:GLY:N	2.36	0.40
2:EB:167:VAL:CB	2:KB:191:SER:HA	2.52	0.40
2:KB:48:SER:H	2:KB:51:GLN:CB	2.34	0.40
2:CC:143:ALA:HB1	2:IC:206:MET:CA	2.51	0.40
2:MD:48:SER:H	2:MD:51:GLN:CB	2.34	0.40
2:OF:67:ALA:O	2:UF:48:SER:C	2.65	0.40
2:AD:67:ALA:O	2:GD:48:SER:C	2.65	0.40
2:QE:67:ALA:O	2:WE:48:SER:C	2.65	0.40
2:GG:73:ALA:C	2:GG:75:GLU:N	2.74	0.40
2:J:48:SER:H	2:J:51:GLN:CB	2.34	0.40
2:T:48:SER:H	2:T:51:GLN:CB	2.34	0.40
2:QB:48:SER:H	2:QB:51:GLN:CB	2.34	0.40
3:XB:80:THR:O	3:XB:205:HIS:N	2.38	0.40
2:OC:67:ALA:O	2:UC:47:ILE:O	2.40	0.40
2:GD:73:ALA:C	2:GD:75:GLU:N	2.74	0.40
2:SD:48:SER:H	2:SD:51:GLN:CB	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	45/560 (8%)	45 (100%)	0	0	100	100
1	BC	45/560 (8%)	45 (100%)	0	0	100	100
1	BF	45/560 (8%)	45 (100%)	0	0	100	100
1	DB	45/560 (8%)	45 (100%)	0	0	100	100
1	DE	45/560 (8%)	45 (100%)	0	0	100	100
1	F	45/560 (8%)	45 (100%)	0	0	100	100
1	FA	45/560 (8%)	45 (100%)	0	0	100	100
1	FD	45/560 (8%)	45 (100%)	0	0	100	100
1	FG	45/560 (8%)	45 (100%)	0	0	100	100
1	HC	45/560 (8%)	45 (100%)	0	0	100	100
1	HF	45/560 (8%)	45 (100%)	0	0	100	100
1	I	45/560 (8%)	45 (100%)	0	0	100	100
1	JB	45/560 (8%)	45 (100%)	0	0	100	100
1	JE	45/560 (8%)	45 (100%)	0	0	100	100
1	LA	45/560 (8%)	45 (100%)	0	0	100	100
1	LD	45/560 (8%)	45 (100%)	0	0	100	100
1	LG	45/560 (8%)	45 (100%)	0	0	100	100
1	NC	45/560 (8%)	45 (100%)	0	0	100	100
1	NF	45/560 (8%)	45 (100%)	0	0	100	100
1	PB	45/560 (8%)	45 (100%)	0	0	100	100
1	PE	45/560 (8%)	45 (100%)	0	0	100	100
1	RA	45/560 (8%)	45 (100%)	0	0	100	100
1	RD	45/560 (8%)	45 (100%)	0	0	100	100
1	RG	45/560 (8%)	45 (100%)	0	0	100	100
1	S	45/560 (8%)	45 (100%)	0	0	100	100
1	TC	45/560 (8%)	45 (100%)	0	0	100	100
1	TF	45/560 (8%)	45 (100%)	0	0	100	100
1	VB	45/560 (8%)	45 (100%)	0	0	100	100
1	VE	45/560 (8%)	45 (100%)	0	0	100	100
1	XA	45/560 (8%)	45 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	XD	45/560 (8%)	45 (100%)	0	0	100	100
1	Z	45/560 (8%)	45 (100%)	0	0	100	100
1	ZC	45/560 (8%)	45 (100%)	0	0	100	100
1	ZF	45/560 (8%)	45 (100%)	0	0	100	100
2	AA	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	AD	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	AG	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	B	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	CC	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	CF	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	EB	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	EE	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	G	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	GA	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	GD	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	GG	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	IC	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	IF	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	J	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	KB	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	KE	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	MA	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	MD	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	MG	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	OC	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	OF	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	QB	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	QE	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	SA	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	SD	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	SG	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	UC	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	UF	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	WB	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	WE	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	YA	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
2	YD	315/331 (95%)	300 (95%)	9 (3%)	6 (2%)	6	32
3	BA	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	BD	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	BG	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	C	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	DC	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	DF	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	FB	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	FE	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	HA	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	HD	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	HG	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	JC	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	JF	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	K	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	LB	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	LE	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	M	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	NA	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	ND	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	NG	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	PC	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	PF	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	RB	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	RE	279/334 (84%)	268 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	TA	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	TD	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	TG	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	V	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	VC	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	VF	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	XB	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	XE	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	ZA	279/334 (84%)	268 (96%)	11 (4%)	0	100	100
3	ZD	279/334 (84%)	267 (96%)	12 (4%)	0	100	100
4	AB	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	AC	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	AE	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	AF	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	BB	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	BE	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	CA	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	CB	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	CD	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	CE	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	CG	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	D	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	DA	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	DD	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	DG	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	E	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	EA	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	EC	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	ED	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	EF	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	EG	79/137 (58%)	74 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	FC	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	FF	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	GB	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	GC	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	GE	83/137 (61%)	80 (96%)	3 (4%)	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%)	72 (89%)	9 (11%)	0	100	100
4	HE	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	IA	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	IB	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	ID	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	IE	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	IG	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	JA	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	JD	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	JG	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	KA	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	KC	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	KD	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	KF	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	KG	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	L	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	LC	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	LF	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	MB	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	MC	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	ME	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	MF	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	N	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	NB	81/137 (59%)	72 (89%)	9 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	NE	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	O	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	OA	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	OB	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	OD	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	OE	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	OG	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	P	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	PA	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	PD	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	PG	81/137 (59%)	72 (89%)	9 (11%)	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	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	QD	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	QF	83/137 (61%)	80 (96%)	3 (4%)	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%)	72 (89%)	9 (11%)	0	100	100
4	RF	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	SB	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	SC	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	SE	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	SF	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	TB	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	TE	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	UA	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	UB	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	UD	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	UE	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	UG	83/137 (61%)	80 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	VA	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	VD	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	VG	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	W	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	WA	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	WC	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	WD	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	WF	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	WG	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	X	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	XC	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	XF	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	Y	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	YB	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	YC	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	YE	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
4	YF	79/137 (58%)	74 (94%)	5 (6%)	0	100	100
4	ZB	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
4	ZE	81/137 (59%)	72 (89%)	9 (11%)	0	100	100
All	All	29988/55624 (54%)	28525 (95%)	1259 (4%)	204 (1%)	20	55

All (204) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	43	ASN
2	B	43	ASN
2	J	43	ASN
2	T	43	ASN
2	AA	43	ASN
2	GA	43	ASN
2	MA	43	ASN
2	SA	43	ASN
2	YA	43	ASN
2	EB	43	ASN
2	KB	43	ASN

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Mol	Chain	Res	Type
2	QB	43	ASN
2	WB	43	ASN
2	CC	43	ASN
2	IC	43	ASN
2	OC	43	ASN
2	UC	43	ASN
2	AD	43	ASN
2	GD	43	ASN
2	MD	43	ASN
2	SD	43	ASN
2	YD	43	ASN
2	EE	43	ASN
2	KE	43	ASN
2	QE	43	ASN
2	WE	43	ASN
2	CF	43	ASN
2	IF	43	ASN
2	OF	43	ASN
2	UF	43	ASN
2	AG	43	ASN
2	GG	43	ASN
2	MG	43	ASN
2	SG	43	ASN
2	G	75	GLU
2	G	196	VAL
2	B	75	GLU
2	B	196	VAL
2	J	75	GLU
2	J	196	VAL
2	T	75	GLU
2	T	196	VAL
2	AA	75	GLU
2	AA	196	VAL
2	GA	75	GLU
2	GA	196	VAL
2	MA	75	GLU
2	MA	196	VAL
2	SA	75	GLU
2	SA	196	VAL
2	YA	75	GLU
2	YA	196	VAL
2	EB	75	GLU

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Mol	Chain	Res	Type
2	EB	196	VAL
2	KB	75	GLU
2	KB	196	VAL
2	QB	75	GLU
2	QB	196	VAL
2	WB	75	GLU
2	WB	196	VAL
2	CC	75	GLU
2	CC	196	VAL
2	IC	75	GLU
2	IC	196	VAL
2	OC	75	GLU
2	OC	196	VAL
2	UC	75	GLU
2	UC	196	VAL
2	AD	75	GLU
2	AD	196	VAL
2	GD	75	GLU
2	GD	196	VAL
2	MD	75	GLU
2	MD	196	VAL
2	SD	75	GLU
2	SD	196	VAL
2	YD	75	GLU
2	YD	196	VAL
2	EE	75	GLU
2	EE	196	VAL
2	KE	75	GLU
2	KE	196	VAL
2	QE	75	GLU
2	QE	196	VAL
2	WE	75	GLU
2	WE	196	VAL
2	CF	75	GLU
2	CF	196	VAL
2	IF	75	GLU
2	IF	196	VAL
2	OF	75	GLU
2	OF	196	VAL
2	UF	75	GLU
2	UF	196	VAL
2	AG	75	GLU

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Mol	Chain	Res	Type
2	AG	196	VAL
2	GG	75	GLU
2	GG	196	VAL
2	MG	75	GLU
2	MG	196	VAL
2	SG	75	GLU
2	SG	196	VAL
2	G	89	ARG
2	G	90	ALA
2	B	89	ARG
2	B	90	ALA
2	J	89	ARG
2	J	90	ALA
2	T	89	ARG
2	T	90	ALA
2	AA	89	ARG
2	AA	90	ALA
2	GA	89	ARG
2	GA	90	ALA
2	MA	89	ARG
2	MA	90	ALA
2	SA	89	ARG
2	SA	90	ALA
2	YA	89	ARG
2	YA	90	ALA
2	EB	89	ARG
2	EB	90	ALA
2	KB	89	ARG
2	KB	90	ALA
2	QB	89	ARG
2	QB	90	ALA
2	WB	89	ARG
2	WB	90	ALA
2	CC	89	ARG
2	CC	90	ALA
2	IC	89	ARG
2	IC	90	ALA
2	OC	89	ARG
2	OC	90	ALA
2	UC	89	ARG
2	UC	90	ALA
2	AD	89	ARG

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Mol	Chain	Res	Type
2	AD	90	ALA
2	GD	89	ARG
2	GD	90	ALA
2	MD	89	ARG
2	MD	90	ALA
2	SD	89	ARG
2	SD	90	ALA
2	YD	89	ARG
2	YD	90	ALA
2	EE	89	ARG
2	EE	90	ALA
2	KE	89	ARG
2	KE	90	ALA
2	QE	89	ARG
2	QE	90	ALA
2	WE	89	ARG
2	WE	90	ALA
2	CF	89	ARG
2	CF	90	ALA
2	IF	89	ARG
2	IF	90	ALA
2	OF	89	ARG
2	OF	90	ALA
2	UF	89	ARG
2	UF	90	ALA
2	AG	89	ARG
2	AG	90	ALA
2	GG	89	ARG
2	GG	90	ALA
2	MG	89	ARG
2	MG	90	ALA
2	SG	89	ARG
2	SG	90	ALA
2	G	74	ASN
2	B	74	ASN
2	J	74	ASN
2	T	74	ASN
2	AA	74	ASN
2	GA	74	ASN
2	MA	74	ASN
2	SA	74	ASN
2	YA	74	ASN

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Mol	Chain	Res	Type
2	EB	74	ASN
2	KB	74	ASN
2	QB	74	ASN
2	WB	74	ASN
2	CC	74	ASN
2	IC	74	ASN
2	OC	74	ASN
2	UC	74	ASN
2	AD	74	ASN
2	GD	74	ASN
2	MD	74	ASN
2	SD	74	ASN
2	YD	74	ASN
2	EE	74	ASN
2	KE	74	ASN
2	QE	74	ASN
2	WE	74	ASN
2	CF	74	ASN
2	IF	74	ASN
2	OF	74	ASN
2	UF	74	ASN
2	AG	74	ASN
2	GG	74	ASN
2	MG	74	ASN
2	SG	74	ASN

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.

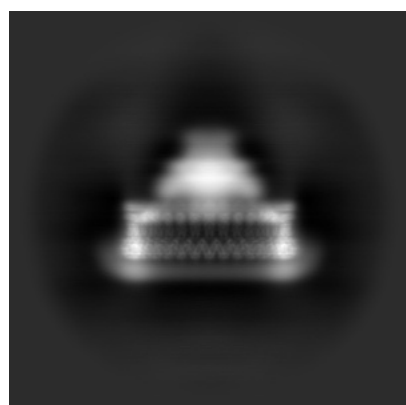
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43327. These allow visual inspection of the internal detail of the map and identification of artifacts.

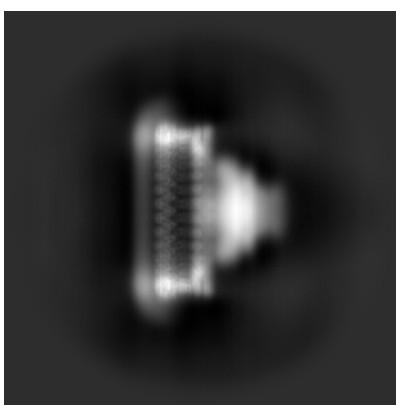
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

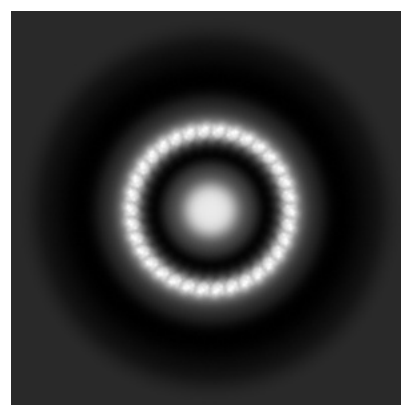
6.1.1 Primary map



X



Y

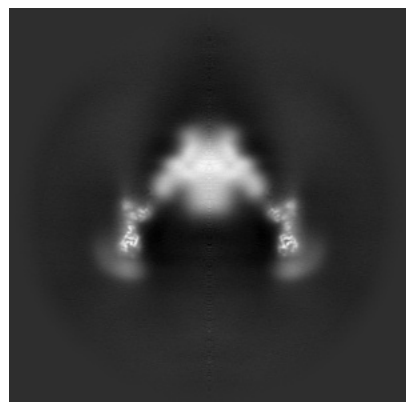


Z

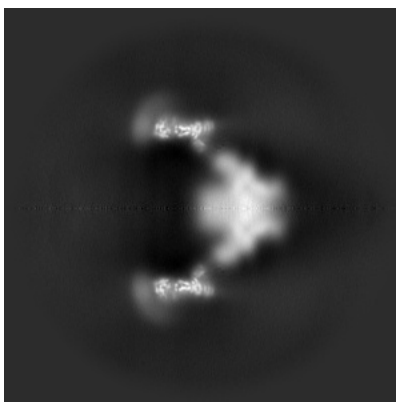
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

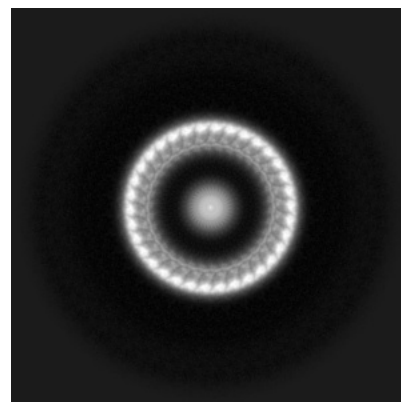
6.2.1 Primary map



X Index: 256



Y Index: 256

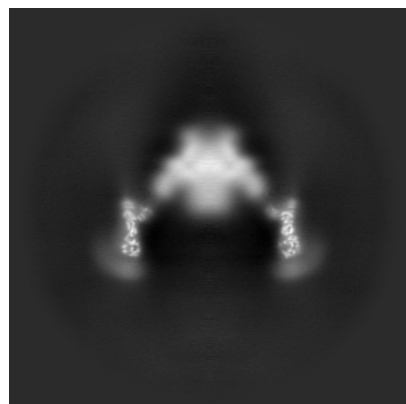


Z Index: 256

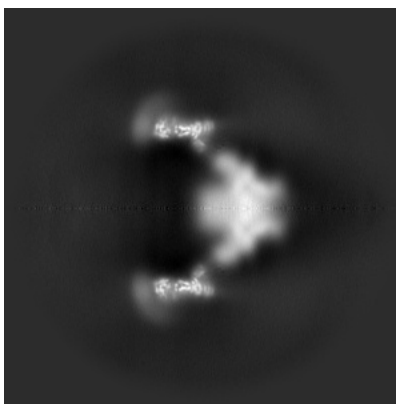
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

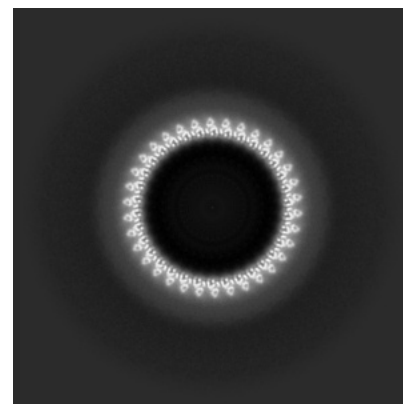
6.3.1 Primary map



X Index: 250



Y Index: 256

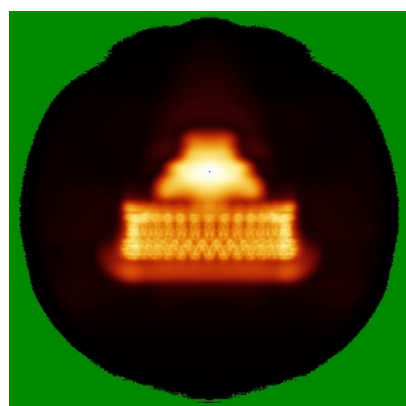


Z Index: 211

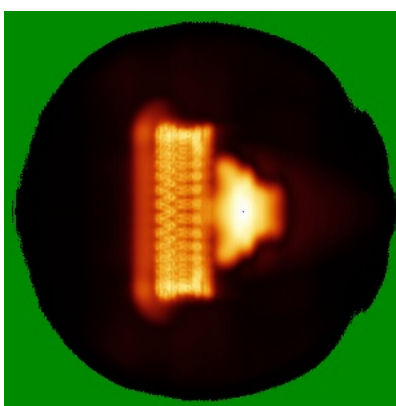
The images above show the largest variance slices of the map in three orthogonal directions.

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

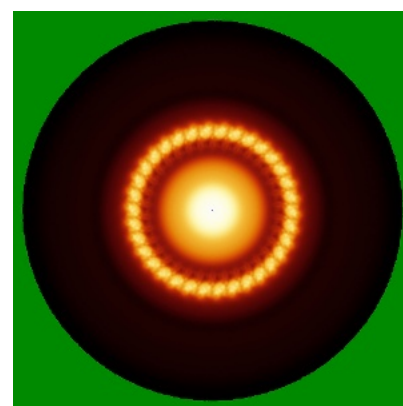
6.4.1 Primary map



X



Y

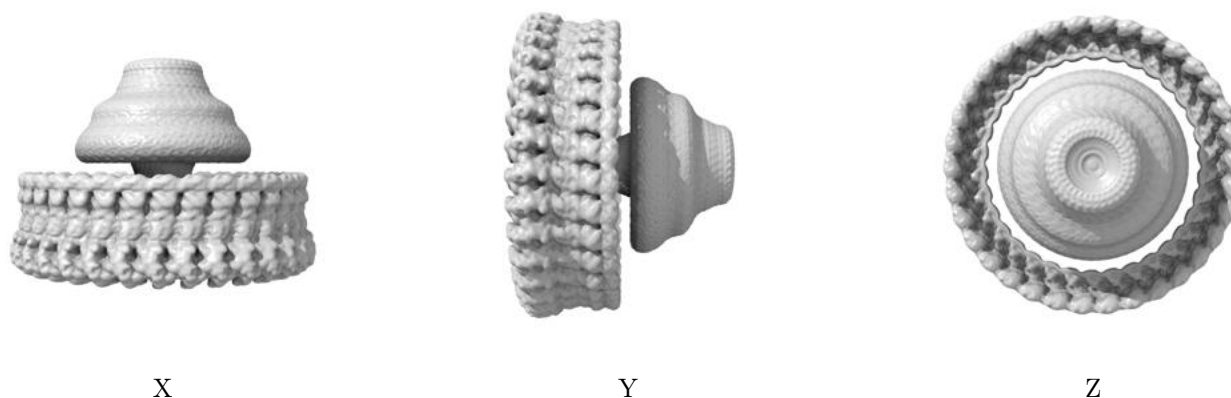


Z

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

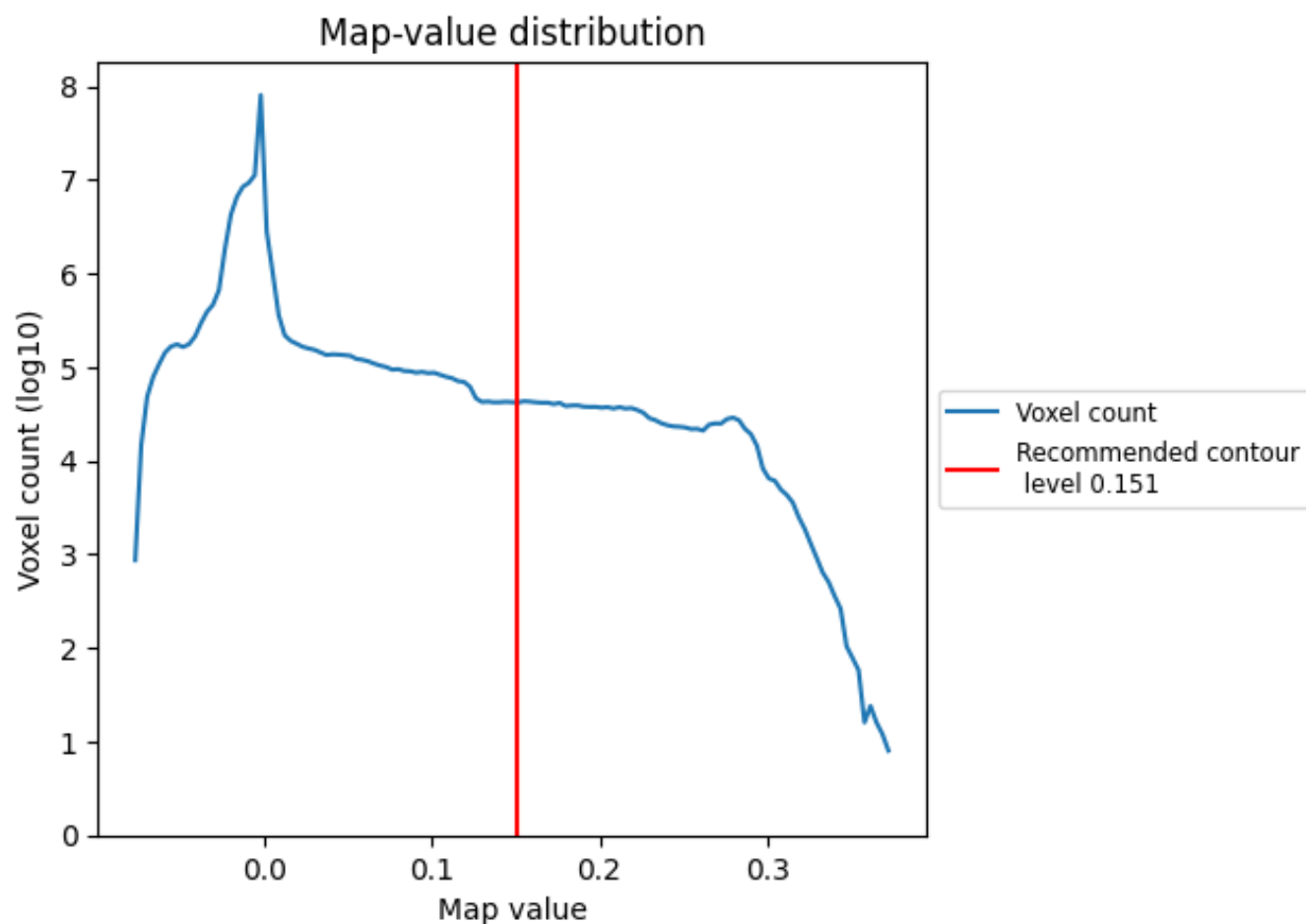
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

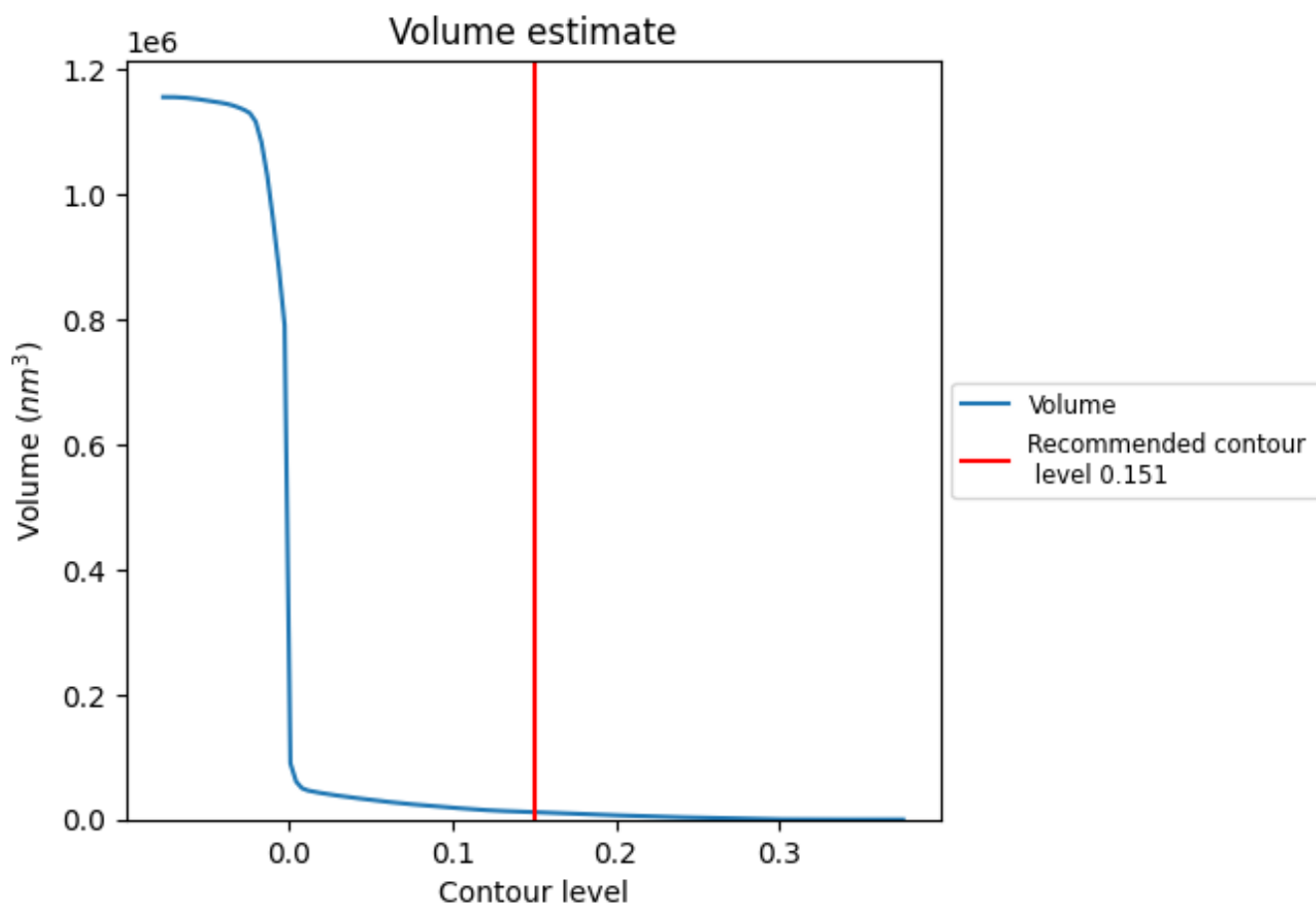
This section contains the results of statistical analysis of the map.

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.

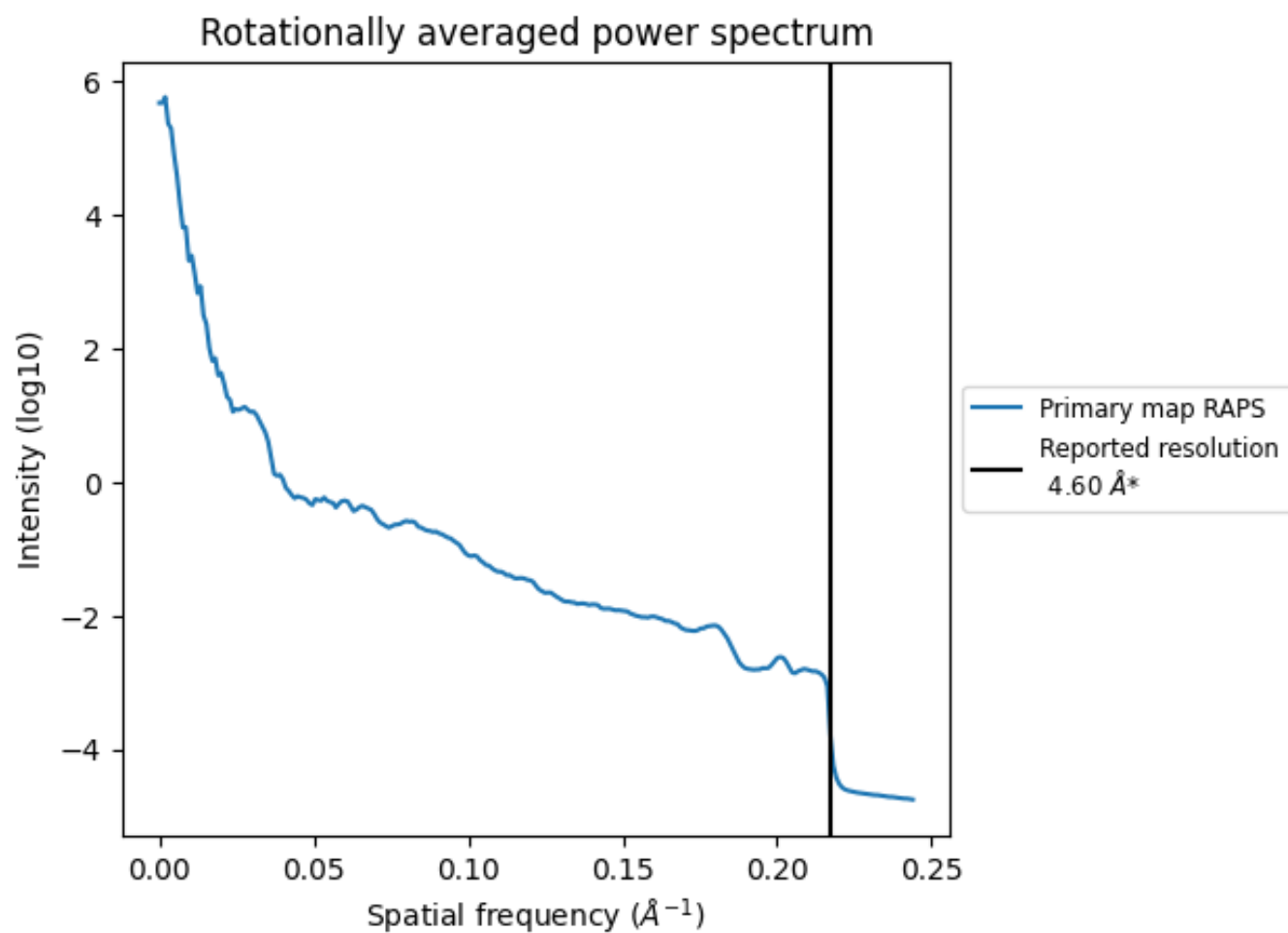
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11612 nm³; this corresponds to an approximate mass of 10489 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

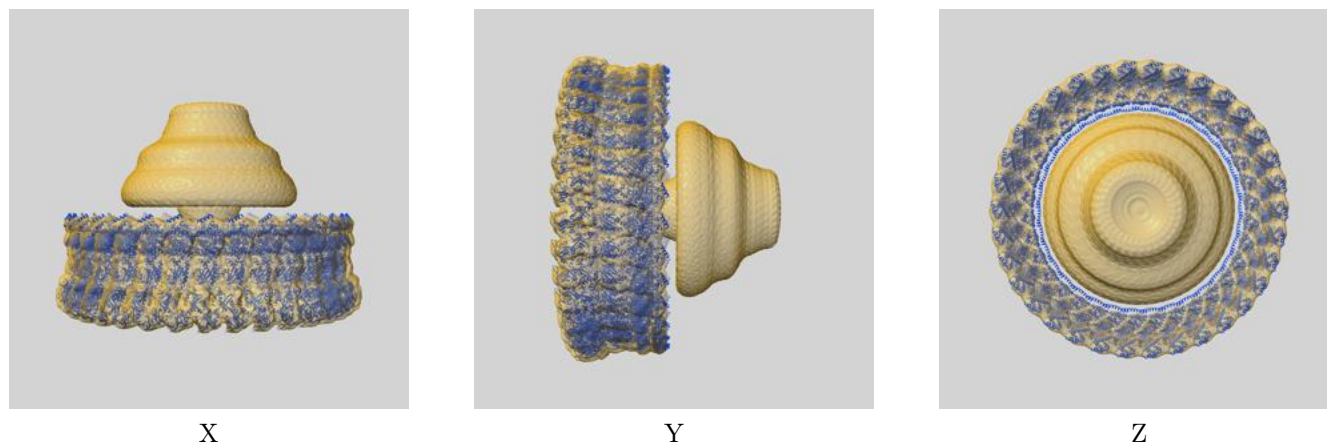
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

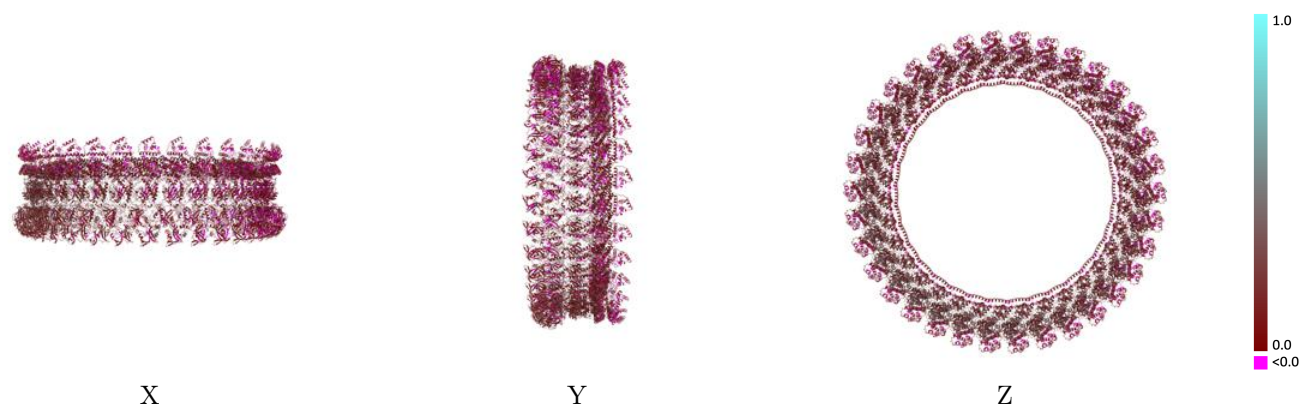
This section contains information regarding the fit between EMDB map EMD-43327 and PDB model 8VKQ. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



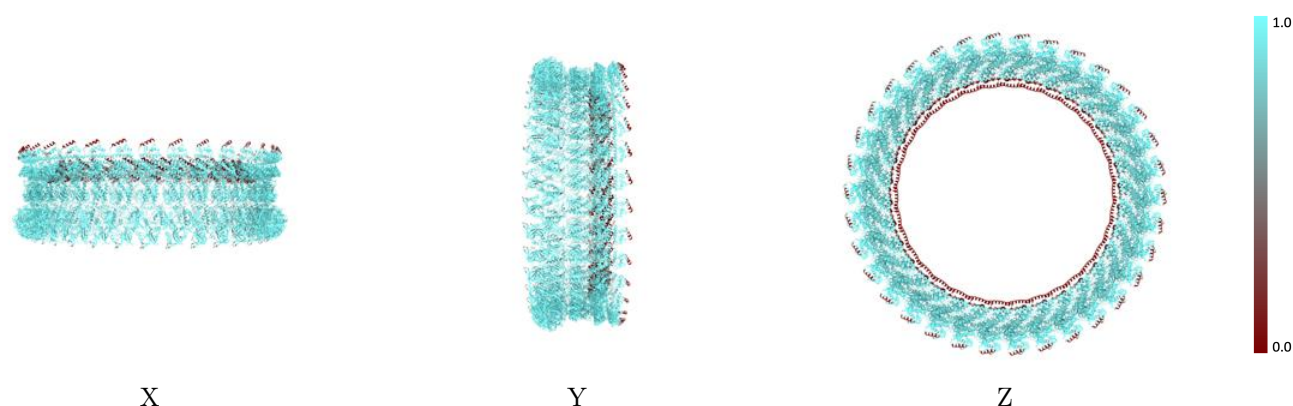
The images above show the 3D surface view of the map at the recommended contour level 0.151 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



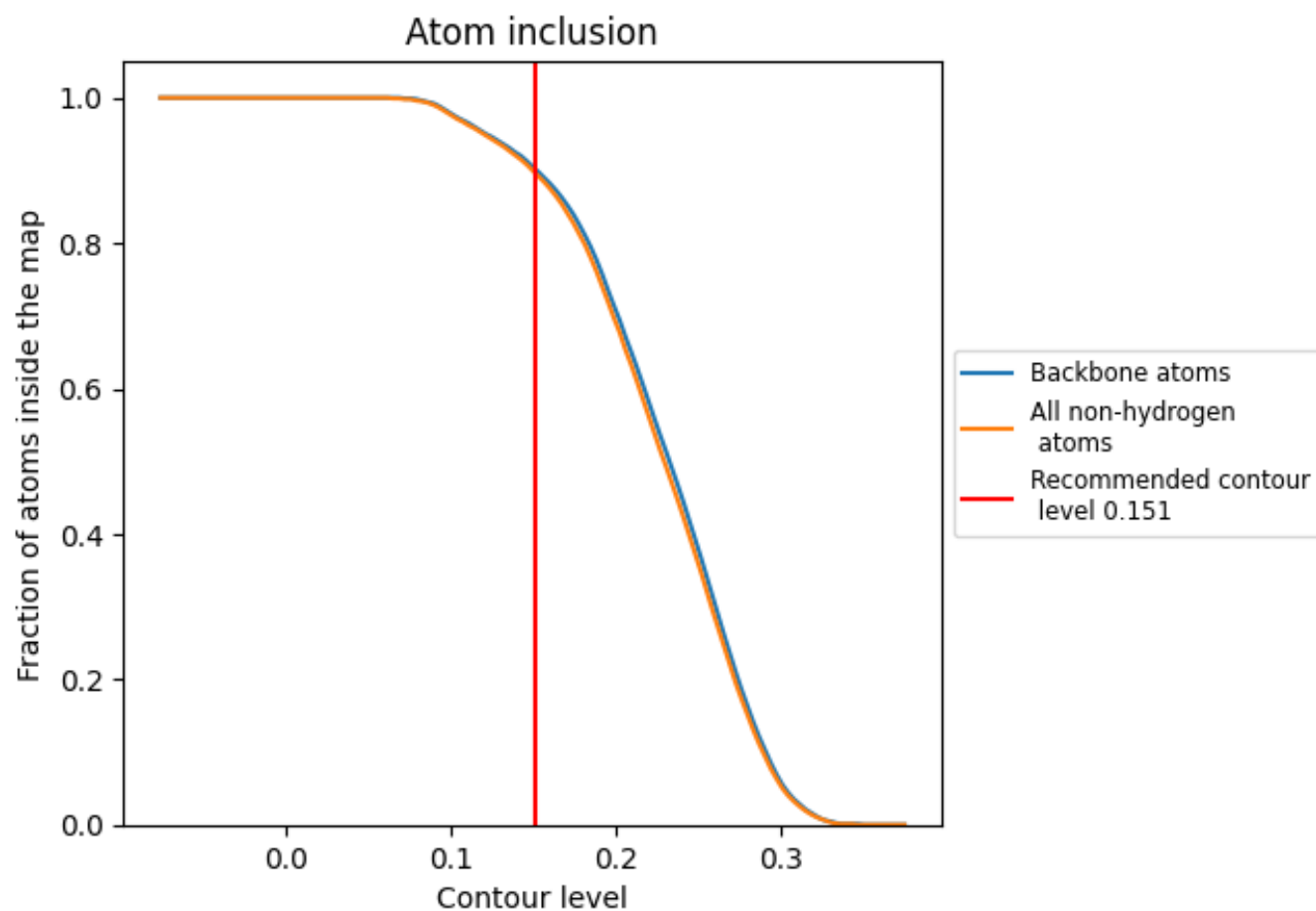
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.151).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.151) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8970	 0.1590
A	 0.3320	 0.1460
AA	 0.8560	 0.1270
AB	 0.9330	 0.1210
AC	 1.0000	 0.1000
AD	 0.8340	 0.1160
AE	 0.9400	 0.2040
AF	 1.0000	 0.2340
AG	 0.8650	 0.1680
B	 0.8610	 0.1470
BA	 0.9890	 0.1600
BB	 1.0000	 0.1060
BC	 0.3020	 0.1390
BD	 0.9500	 0.1340
BE	 1.0000	 0.1720
BF	 0.3020	 0.1310
BG	 0.9950	 0.2570
C	 0.9940	 0.2060
CA	 0.9550	 0.1550
CB	 0.9980	 0.1210
CC	 0.8350	 0.1040
CD	 0.9310	 0.1590
CE	 1.0000	 0.1820
CF	 0.8580	 0.1630
CG	 0.9790	 0.2320
D	 0.9710	 0.1900
DA	 1.0000	 0.1550
DB	 0.3190	 0.1490
DC	 0.9460	 0.1120
DD	 0.9950	 0.1150
DE	 0.2940	 0.1250
DF	 0.9890	 0.2430
DG	 1.0000	 0.2550
E	 1.0000	 0.2000
EA	 1.0000	 0.1800



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Chain	Atom inclusion	Q-score
EB	 0.8420	 0.1070
EC	 0.9310	 0.1210
ED	 0.9980	 0.1230
EE	 0.8480	 0.1440
EF	 0.9690	 0.2320
EG	 1.0000	 0.2660
F	 0.3320	 0.1400
FA	 0.3360	 0.1470
FB	 0.9590	 0.1150
FC	 0.9950	 0.0870
FD	 0.2940	 0.1300
FE	 0.9740	 0.1920
FF	 1.0000	 0.2430
FG	 0.3190	 0.1430
G	 0.8640	 0.1520
GA	 0.8510	 0.1200
GB	 0.9350	 0.1210
GC	 0.9980	 0.0960
GD	 0.8370	 0.1200
GE	 0.9450	 0.2070
GF	 1.0000	 0.2470
GG	 0.8650	 0.1650
H	 1.0000	 0.2310
HA	 0.9830	 0.1470
HB	 1.0000	 0.1020
HC	 0.2940	 0.1380
HD	 0.9510	 0.1410
HE	 1.0000	 0.1840
HF	 0.3060	 0.1350
HG	 0.9950	 0.2530
I	 0.3320	 0.1410
IA	 0.9550	 0.1500
IB	 1.0000	 0.1140
IC	 0.8350	 0.1060
ID	 0.9350	 0.1700
IE	 1.0000	 0.2020
IF	 0.8610	 0.1670
IG	 0.9790	 0.2260
J	 0.8600	 0.1390
JA	 1.0000	 0.1400
JB	 0.3110	 0.1450
JC	 0.9480	 0.1150

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Chain	Atom inclusion	Q-score
JD	 0.9950	 0.1230
JE	 0.2940	 0.1280
JF	 0.9900	 0.2500
JG	 1.0000	 0.2580
K	 0.9920	 0.1860
KA	 1.0000	 0.1640
KB	 0.8410	 0.1060
KC	 0.9310	 0.1270
KD	 0.9980	 0.1340
KE	 0.8510	 0.1500
KF	 0.9710	 0.2360
KG	 1.0000	 0.2690
L	 0.9640	 0.1790
LA	 0.3230	 0.1470
LB	 0.9550	 0.1110
LC	 0.9950	 0.0940
LD	 0.2890	 0.1280
LE	 0.9790	 0.2070
LF	 1.0000	 0.2560
LG	 0.3190	 0.1410
M	 0.9950	 0.2190
MA	 0.8490	 0.1160
MB	 0.9350	 0.1210
MC	 0.9980	 0.1070
MD	 0.8390	 0.1260
ME	 0.9520	 0.2170
MF	 1.0000	 0.2510
MG	 0.8610	 0.1620
N	 0.9740	 0.2010
NA	 0.9780	 0.1360
NB	 1.0000	 0.0940
NC	 0.2940	 0.1340
ND	 0.9570	 0.1530
NE	 1.0000	 0.2050
NF	 0.3150	 0.1330
NG	 0.9960	 0.2440
O	 1.0000	 0.1860
OA	 0.9500	 0.1410
OB	 0.9980	 0.1110
OC	 0.8340	 0.1090
OD	 0.9380	 0.1790
OE	 1.0000	 0.2150

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Chain	Atom inclusion	Q-score
OF	 0.8620	 0.1700
OG	 0.9790	 0.2190
P	 1.0000	 0.2150
PA	 1.0000	 0.1280
PB	 0.3110	 0.1460
PC	 0.9460	 0.1230
PD	 0.9980	 0.1370
PE	 0.2980	 0.1260
PF	 0.9920	 0.2550
PG	 1.0000	 0.2500
Q	 1.0000	 0.2420
QA	 1.0000	 0.1450
QB	 0.8400	 0.1020
QC	 0.9280	 0.1400
QD	 0.9980	 0.1430
QE	 0.8560	 0.1550
QF	 0.9790	 0.2420
QG	 1.0000	 0.2590
R	 1.0000	 0.2160
RA	 0.3230	 0.1490
RB	 0.9500	 0.1040
RC	 0.9950	 0.1040
RD	 0.2940	 0.1230
RE	 0.9830	 0.2210
RF	 1.0000	 0.2630
RG	 0.3280	 0.1440
S	 0.3360	 0.1420
SA	 0.8460	 0.1100
SB	 0.9330	 0.1150
SC	 0.9980	 0.1100
SD	 0.8420	 0.1310
SE	 0.9570	 0.2270
SF	 1.0000	 0.2610
SG	 0.8630	 0.1590
T	 0.8570	 0.1340
TA	 0.9720	 0.1200
TB	 1.0000	 0.0840
TC	 0.2940	 0.1310
TD	 0.9650	 0.1650
TE	 1.0000	 0.2200
TF	 0.3150	 0.1390
TG	 0.9940	 0.2310

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Chain	Atom inclusion	Q-score
UA	 0.9400	 0.1310
UB	 0.9980	 0.1000
UC	 0.8320	 0.1110
UD	 0.9380	 0.1940
UE	 1.0000	 0.2290
UF	 0.8640	 0.1700
UG	 0.9760	 0.2120
V	 0.9910	 0.1750
VA	 1.0000	 0.1130
VB	 0.3060	 0.1430
VC	 0.9450	 0.1240
VD	 1.0000	 0.1560
VE	 0.3020	 0.1270
VF	 0.9930	 0.2590
VG	 1.0000	 0.2300
W	 0.9590	 0.1690
WA	 1.0000	 0.1320
WB	 0.8370	 0.1030
WC	 0.9310	 0.1490
WD	 1.0000	 0.1600
WE	 0.8580	 0.1590
WF	 0.9790	 0.2360
WG	 1.0000	 0.2520
X	 1.0000	 0.1720
XA	 0.3230	 0.1440
XB	 0.9480	 0.1100
XC	 0.9930	 0.1040
XD	 0.2940	 0.1310
XE	 0.9870	 0.2330
XF	 1.0000	 0.2690
Y	 1.0000	 0.2020
YA	 0.8410	 0.1080
YB	 0.9310	 0.1190
YC	 0.9980	 0.1100
YD	 0.8460	 0.1370
YE	 0.9640	 0.2290
YF	 1.0000	 0.2650
Z	 0.3360	 0.1490
ZA	 0.9660	 0.1130
ZB	 0.9980	 0.0890
ZC	 0.2940	 0.1360
ZD	 0.9680	 0.1800

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Chain	Atom inclusion	Q-score
ZE	 1.0000	 0.2320
ZF	 0.3150	 0.1410