



wwPDB EM Validation Summary Report ⓘ

Feb 25, 2024 – 09:18 AM EST

PDB ID : 6X65
EMDB ID : EMD-22070
Title : Legionella pneumophila Dot/Icm T4SS
Authors : Durie, C.L.; Sheedlo, M.J.; Chung, J.M.; Byrne, B.G.; Su, M.; Knight, T.; Swanson, M.S.; Lacy, D.B.; Ohi, M.D.
Deposited on : 2020-05-27
Resolution : 3.70 Å(reported)

This is a wwPDB EM Validation Summary 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:

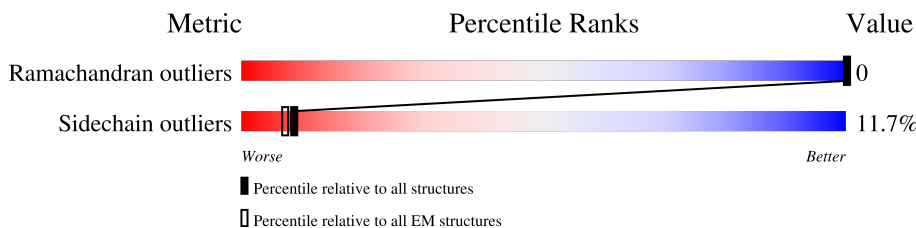
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.70 Å.

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






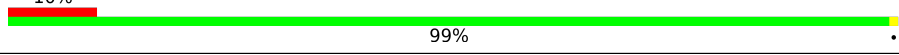




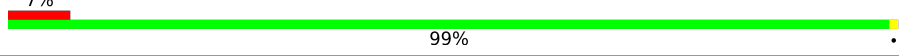




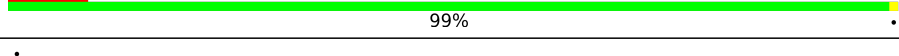




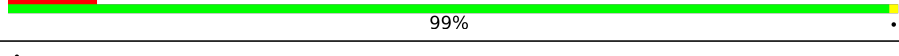




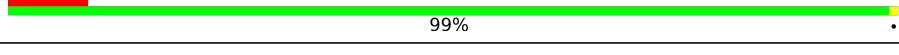

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	AV	228	63% 37%
1	AW	228	14% 86%
1	AX	228	9% 99%
1	AY	228	23% 77%
1	AZ	228	30% 69%
1	BV	228	62% 37%
1	BW	228	14% 86%
1	BX	228	9% 99%
1	BY	228	23% 77%




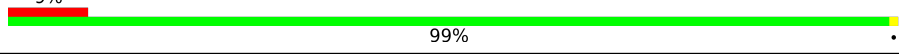

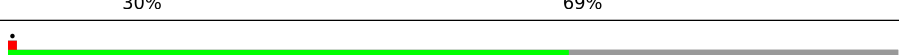

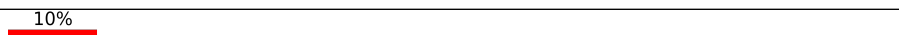
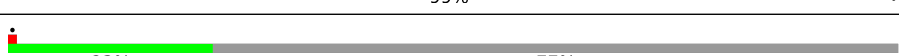



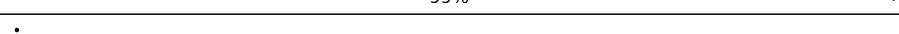

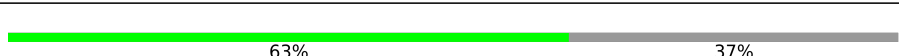

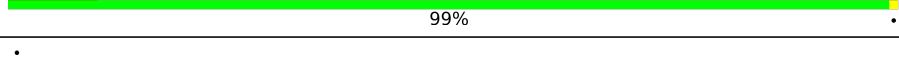
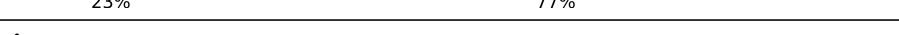


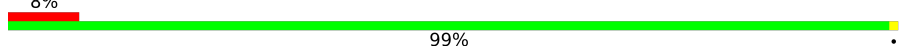




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Mol	Chain	Length	Quality of chain
1	BZ	228	
1	CV	228	
1	CW	228	
1	CX	228	
1	CY	228	
1	CZ	228	
1	DV	228	
1	DW	228	
1	DX	228	
1	DY	228	
1	DZ	228	
1	EV	228	
1	EW	228	
1	EX	228	
1	EY	228	
1	EZ	228	
1	FV	228	
1	FW	228	
1	FX	228	
1	FY	228	
1	FZ	228	
1	GV	228	
1	GW	228	
1	GX	228	
1	GY	228	




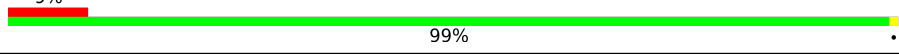

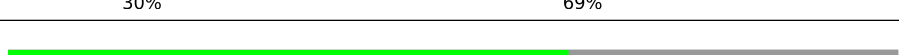

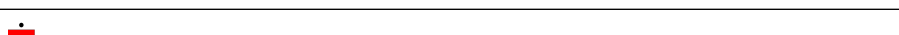



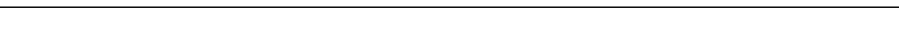
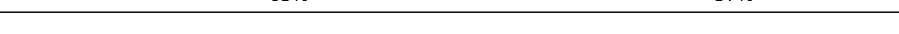












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Mol	Chain	Length	Quality of chain
1	GZ	228	
1	HV	228	
1	HW	228	
1	HX	228	
1	HY	228	
1	HZ	228	
1	IV	228	
1	IW	228	
1	IX	228	
1	IY	228	
1	IZ	228	
1	JV	228	
1	JW	228	
1	JX	228	
1	JY	228	
1	JZ	228	
1	KV	228	
1	KW	228	
1	KX	228	
1	KY	228	
1	KZ	228	
1	LV	228	
1	LW	228	
1	LX	228	
1	LY	228	




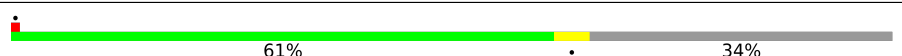
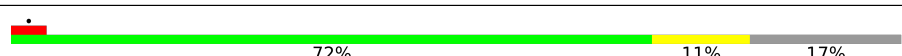
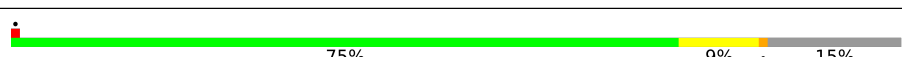
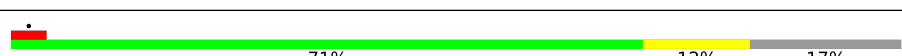
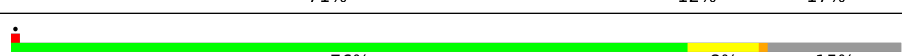
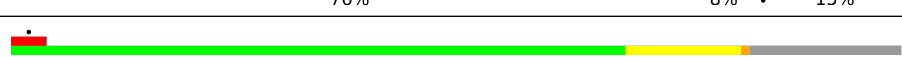

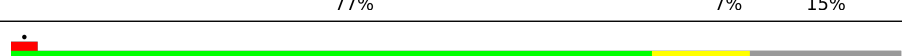
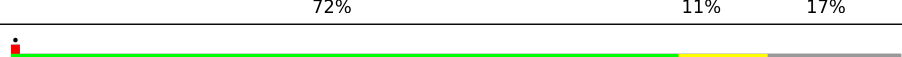

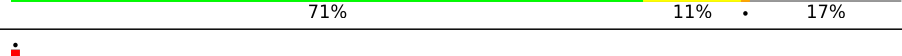
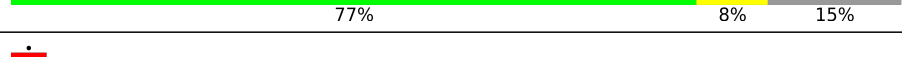




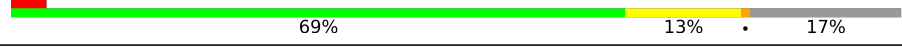

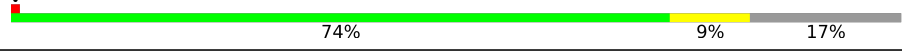



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Mol	Chain	Length	Quality of chain
1	LZ	228	
1	MV	228	
1	MW	228	
1	MX	228	
1	MY	228	
1	MZ	228	
1	NV	228	
1	NW	228	
1	OV	228	
1	OW	228	
1	PV	228	
1	PW	228	
1	QV	228	
1	QW	228	
1	RV	228	
1	RW	228	
2	AC	303	
2	BC	303	
2	CC	303	
2	DC	303	
2	EC	303	
2	FC	303	
2	GC	303	
2	HC	303	
2	IC	303	




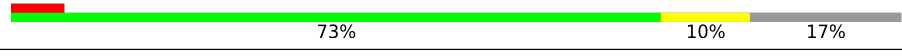
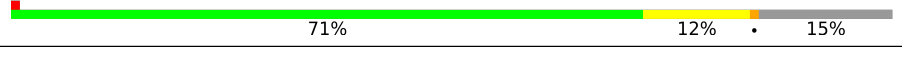



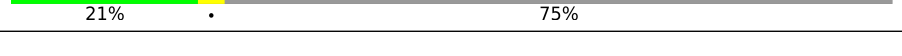
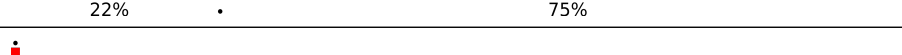
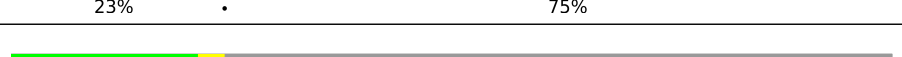
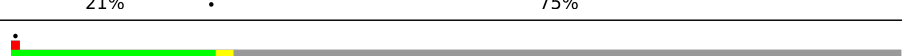

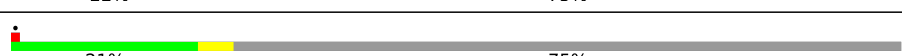


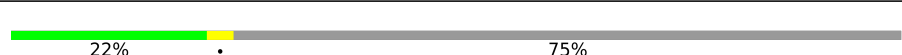




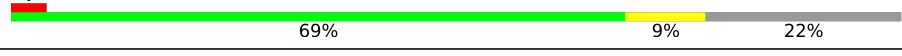

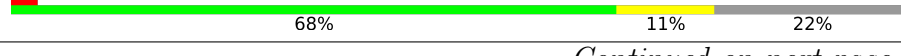

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Mol	Chain	Length	Quality of chain
2	JC	303	
2	KC	303	
2	LC	303	
2	MC	303	
3	AD	163	
3	Ad	163	
3	BD	163	
3	Bd	163	
3	CD	163	
3	Cd	163	
3	DD	163	
3	Dd	163	
3	ED	163	
3	Ed	163	
3	FD	163	
3	Fd	163	
3	GD	163	
3	Gd	163	
3	HD	163	
3	Hd	163	
3	ID	163	
3	Id	163	
3	JD	163	
3	Jd	163	
3	KD	163	




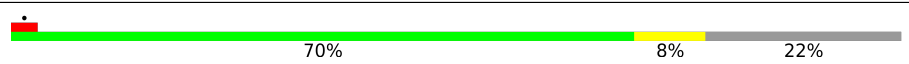
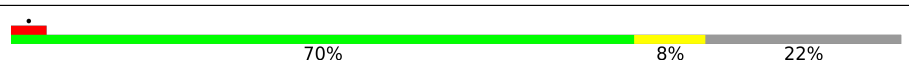
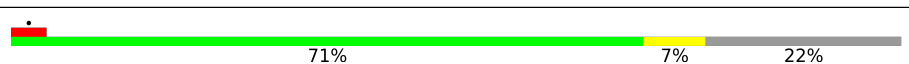
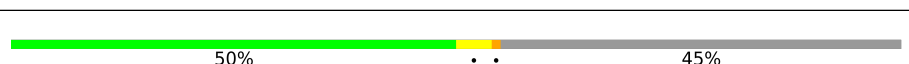
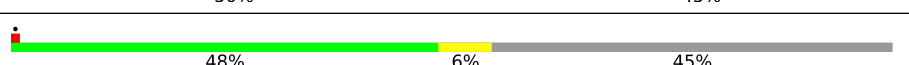
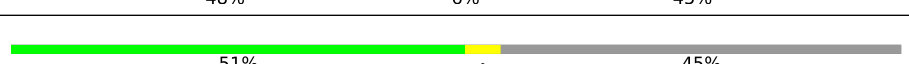
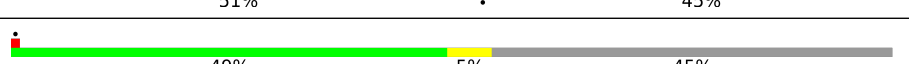
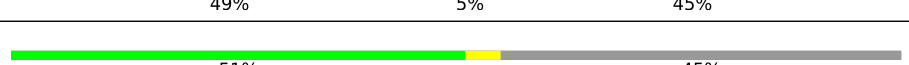

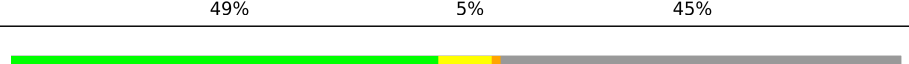
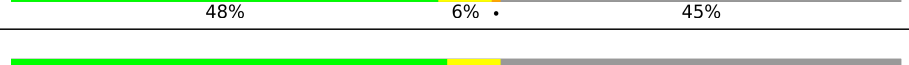
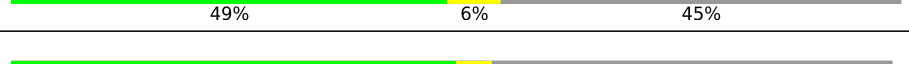


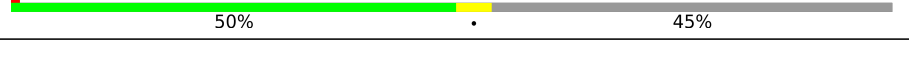
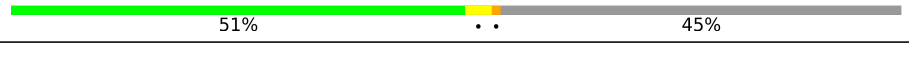
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Mol	Chain	Length	Quality of chain
3	Kd	163	 72% 12% 15%
3	LD	163	 72% 11% 17%
3	Ld	163	 74% 10% 15%
3	MD	163	 6% 73% 10% 17%
3	Md	163	 71% 12% 15%
4	AH	361	 22% 75%
4	BH	361	 21% 75%
4	CH	361	 22% 75%
4	DH	361	 21% 75%
4	EH	361	 22% 75%
4	FH	361	 23% 75%
4	GH	361	 21% 75%
4	HH	361	 23% 75%
4	IH	361	 22% 75%
4	JH	361	 21% 75%
4	KH	361	 22% 75%
4	LH	361	 21% 75%
4	MH	361	 22% 75%
5	AK	189	 69% 10% 22%
5	BK	189	 68% 10% 22%
5	CK	189	 66% 12% 22%
5	DK	189	 69% 10% 22%
5	EK	189	 69% 9% 22%
5	FK	189	 66% 13% 22%
5	GK	189	 68% 11% 22%

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Mol	Chain	Length	Quality of chain
5	HK	189	 67% 12% 22%
5	IK	189	 71% 7% 22%
5	JK	189	 69% 9% 22%
5	KK	189	 70% 8% 22%
5	LK	189	 70% 8% 22%
5	MK	189	 71% 7% 22%
6	N	249	 50% 45%
6	O	249	 48% 6% 45%
6	P	249	 51% 45%
6	Q	249	 49% 5% 45%
6	R	249	 51% 45%
6	S	249	 49% 5% 45%
6	T	249	 48% 6% 45%
6	U	249	 49% 6% 45%
6	V	249	 50% 45%
6	W	249	 50% 45%
6	X	249	 50% 45%
6	Y	249	 51% 45%
6	Z	249	 49% 5% 45%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 124910 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 Type IV secretion system unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	AV	144	720	432	144	144	0	0
1	AW	32	160	96	32	32	0	0
1	BV	144	720	432	144	144	0	0
1	BW	32	160	96	32	32	0	0
1	CV	144	720	432	144	144	0	0
1	CW	32	160	96	32	32	0	0
1	DV	144	720	432	144	144	0	0
1	DW	32	160	96	32	32	0	0
1	EV	144	720	432	144	144	0	0
1	EW	32	160	96	32	32	0	0
1	FV	144	720	432	144	144	0	0
1	FW	32	160	96	32	32	0	0
1	GV	144	720	432	144	144	0	0
1	GW	32	160	96	32	32	0	0
1	HV	144	720	432	144	144	0	0
1	HW	32	160	96	32	32	0	0
1	IV	144	720	432	144	144	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	IW	32	Total	C	N	O	0	0
			160	96	32	32		
1	JV	144	Total	C	N	O	0	0
			720	432	144	144		
1	JW	32	Total	C	N	O	0	0
			160	96	32	32		
1	KV	144	Total	C	N	O	0	0
			720	432	144	144		
1	KW	32	Total	C	N	O	0	0
			160	96	32	32		
1	LV	144	Total	C	N	O	0	0
			720	432	144	144		
1	LW	32	Total	C	N	O	0	0
			160	96	32	32		
1	MV	144	Total	C	N	O	0	0
			720	432	144	144		
1	MW	32	Total	C	N	O	0	0
			160	96	32	32		
1	NV	144	Total	C	N	O	0	0
			720	432	144	144		
1	NW	32	Total	C	N	O	0	0
			160	96	32	32		
1	OV	144	Total	C	N	O	0	0
			720	432	144	144		
1	OW	32	Total	C	N	O	0	0
			160	96	32	32		
1	PV	144	Total	C	N	O	0	0
			720	432	144	144		
1	PW	32	Total	C	N	O	0	0
			160	96	32	32		
1	QV	144	Total	C	N	O	0	0
			720	432	144	144		
1	QW	32	Total	C	N	O	0	0
			160	96	32	32		
1	RV	144	Total	C	N	O	0	0
			720	432	144	144		
1	RW	32	Total	C	N	O	0	0
			160	96	32	32		
1	AX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	AY	52	Total	C	N	O	0	0
			260	156	52	52		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	AZ	70	Total 350	C 210	N 70	O 70	0	0
1	BX	228	Total 1140	C 684	N 228	O 228	0	0
1	BY	52	Total 260	C 156	N 52	O 52	0	0
1	BZ	70	Total 350	C 210	N 70	O 70	0	0
1	CX	228	Total 1140	C 684	N 228	O 228	0	0
1	CY	52	Total 260	C 156	N 52	O 52	0	0
1	CZ	70	Total 350	C 210	N 70	O 70	0	0
1	DX	228	Total 1140	C 684	N 228	O 228	0	0
1	DY	52	Total 260	C 156	N 52	O 52	0	0
1	DZ	70	Total 350	C 210	N 70	O 70	0	0
1	EX	228	Total 1140	C 684	N 228	O 228	0	0
1	EY	52	Total 260	C 156	N 52	O 52	0	0
1	EZ	70	Total 350	C 210	N 70	O 70	0	0
1	FX	228	Total 1140	C 684	N 228	O 228	0	0
1	FY	52	Total 260	C 156	N 52	O 52	0	0
1	FZ	70	Total 350	C 210	N 70	O 70	0	0
1	GX	228	Total 1140	C 684	N 228	O 228	0	0
1	GY	52	Total 260	C 156	N 52	O 52	0	0
1	GZ	70	Total 350	C 210	N 70	O 70	0	0
1	HX	228	Total 1140	C 684	N 228	O 228	0	0
1	HY	52	Total 260	C 156	N 52	O 52	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	HZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	IX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	IY	52	Total	C	N	O	0	0
			260	156	52	52		
1	IZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	JX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	JY	52	Total	C	N	O	0	0
			260	156	52	52		
1	JZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	KX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	KY	52	Total	C	N	O	0	0
			260	156	52	52		
1	KZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	LX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	LY	52	Total	C	N	O	0	0
			260	156	52	52		
1	LZ	70	Total	C	N	O	0	0
			350	210	70	70		
1	MX	228	Total	C	N	O	0	0
			1140	684	228	228		
1	MY	52	Total	C	N	O	0	0
			260	156	52	52		
1	MZ	70	Total	C	N	O	0	0
			350	210	70	70		

- Molecule 2 is a protein called DotC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	BC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	CC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	DC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	EC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	FC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	GC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	HC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	IC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	JC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	KC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	LC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
2	MC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		

- Molecule 3 is a protein called DotD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Ad	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	BD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Bd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	CD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Cd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	DD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Dd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	ED	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ed	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	FD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Fd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	GD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Gd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	HD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Hd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	ID	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Id	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	JD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Jd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	KD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Kd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	LD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Ld	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
3	MD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
3	Md	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		

- Molecule 4 is a protein called Type IV secretion protein IcmK.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
4	BH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	CH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
4	DH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
4	EH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
4	FH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
4	GH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
4	HH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
4	IH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
4	JH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
4	KH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
4	LH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
4	MH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		

- Molecule 5 is a protein called Inner membrane lipoprotein YiaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
5	BK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
5	CK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
5	DK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
5	EK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
5	FK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
5	GK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
5	HK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	IK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
5	JK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
5	KK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
5	LK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
5	MK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		

- Molecule 6 is a protein called Outer membrane protein, OmpA family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	O	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	P	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	Q	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	R	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	S	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	T	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	U	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	V	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	W	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	X	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	Y	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	Z	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		

3 Residue-property plots [i](#)

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

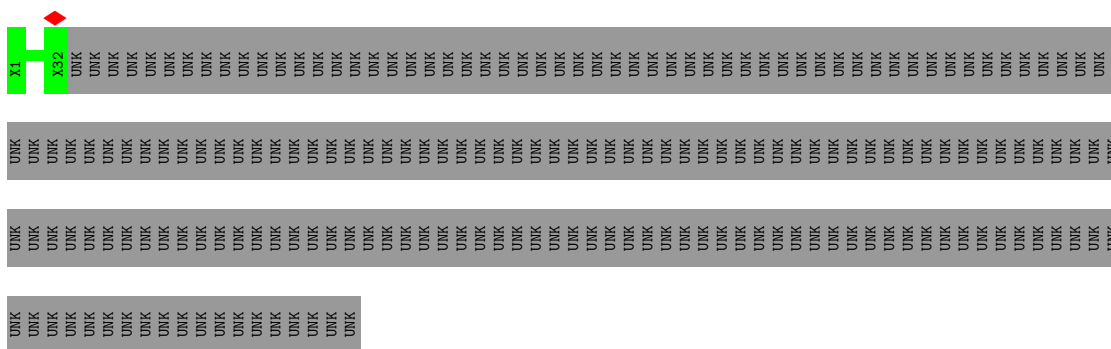
- Molecule 1: Type IV secretion system unknown protein fragment

Chain AV:  63% 37%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain AW:  14% 86%



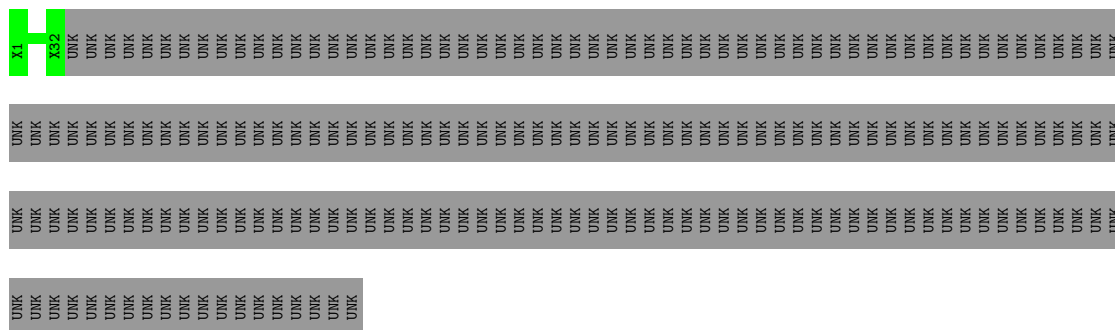
- Molecule 1: Type IV secretion system unknown protein fragment

Chain BV:  62% 37%

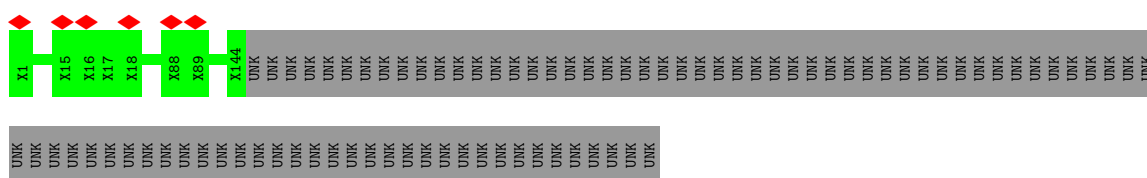


- Molecule 1: Type IV secretion system unknown protein fragment

Chain BW:  14% 86%



• Molecule 1: Type IV secretion system unknown protein fragment



• Molecule 1: Type IV secretion system unknown protein fragment

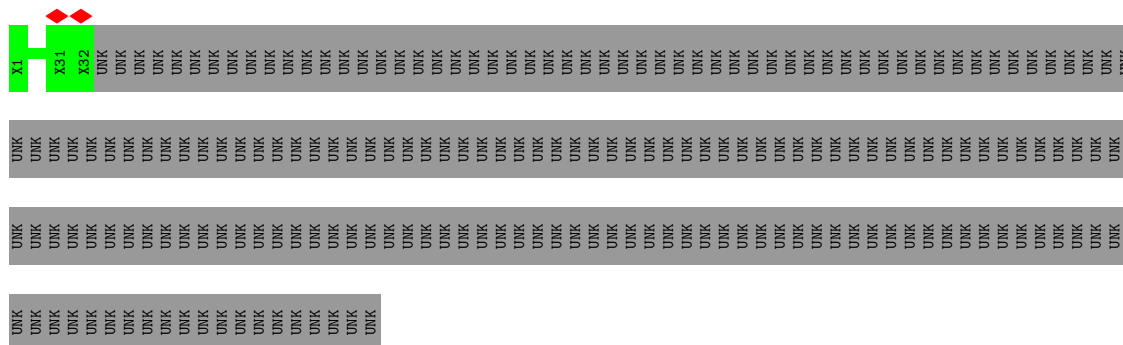


• Molecule 1: Type IV secretion system unknown protein fragment



• Molecule 1: Type IV secretion system unknown protein fragment

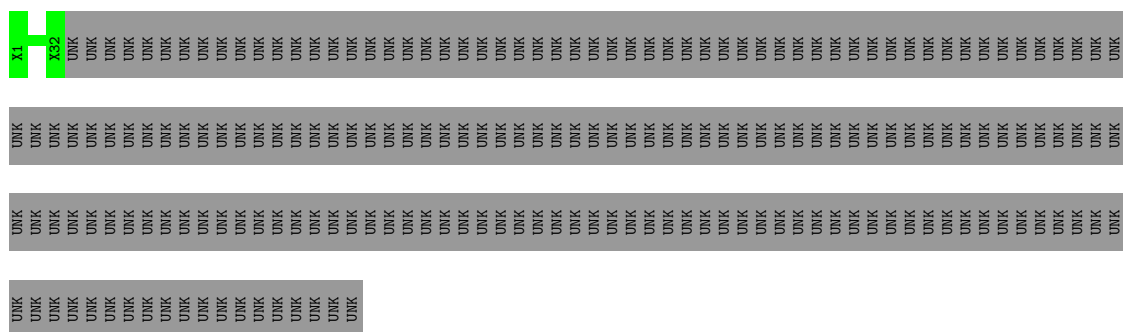




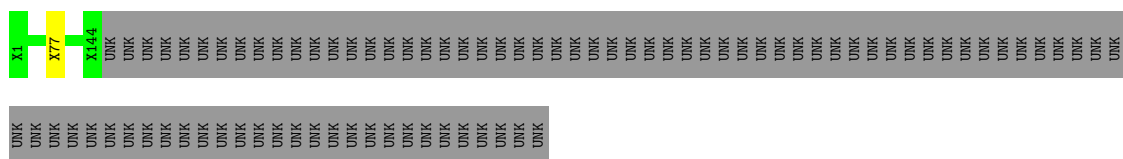
• Molecule 1: Type IV secretion system unknown protein fragment



• Molecule 1: Type IV secretion system unknown protein fragment

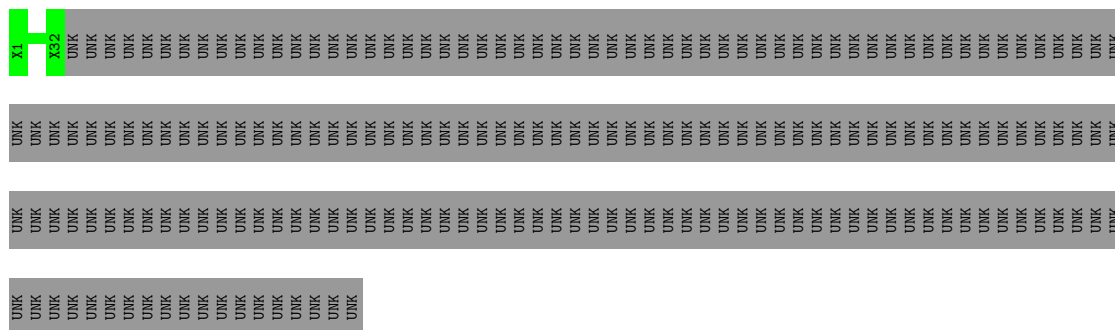


• Molecule 1: Type IV secretion system unknown protein fragment

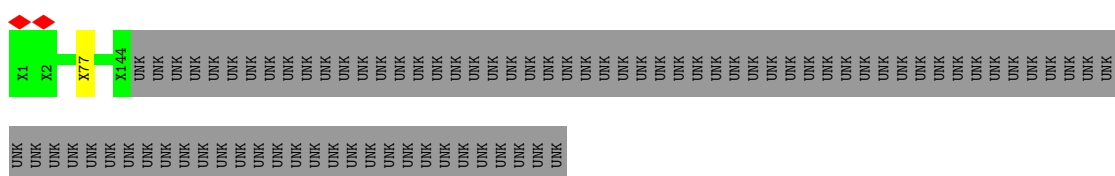


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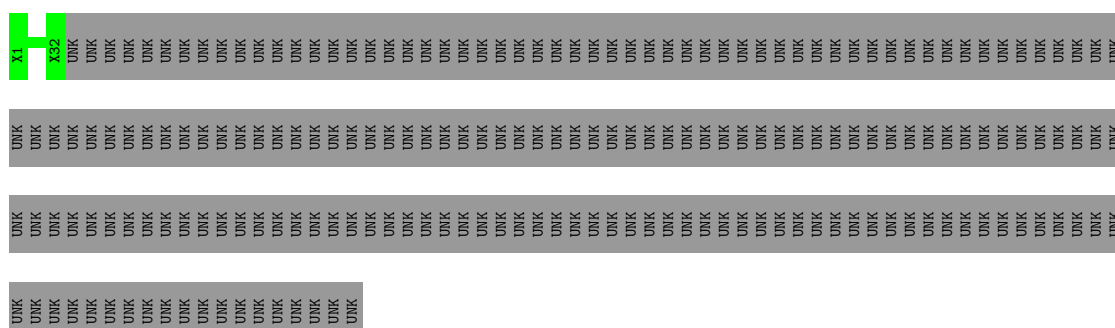




• Molecule 1: Type IV secretion system unknown protein fragment



• Molecule 1: Type IV secretion system unknown protein fragment

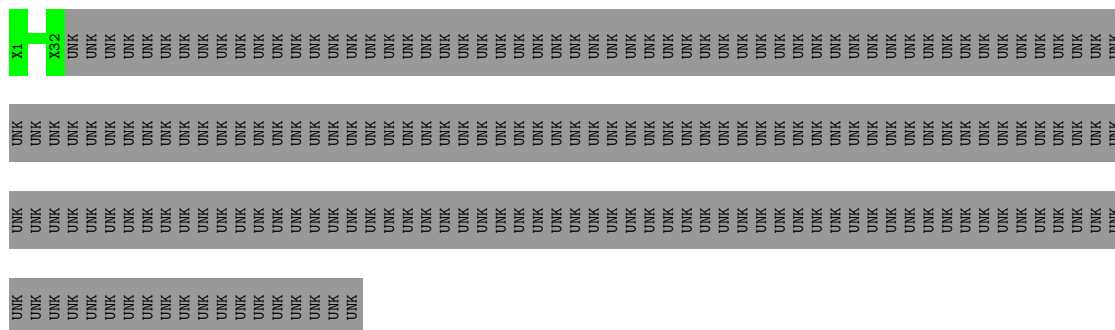


• Molecule 1: Type IV secretion system unknown protein fragment



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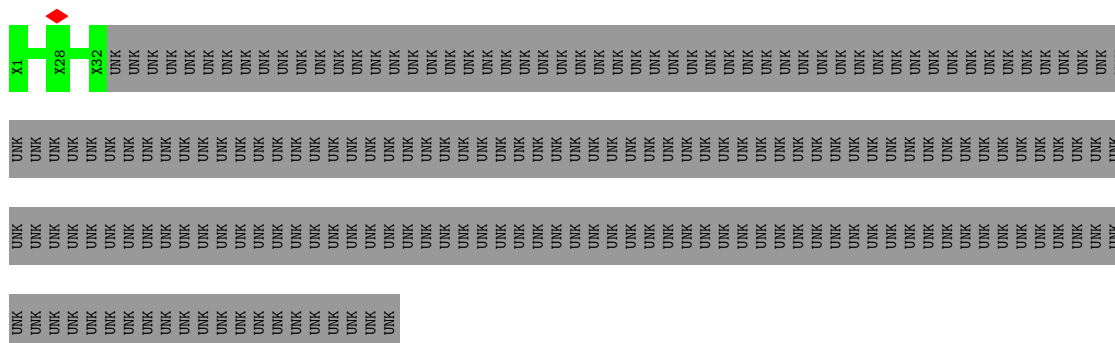




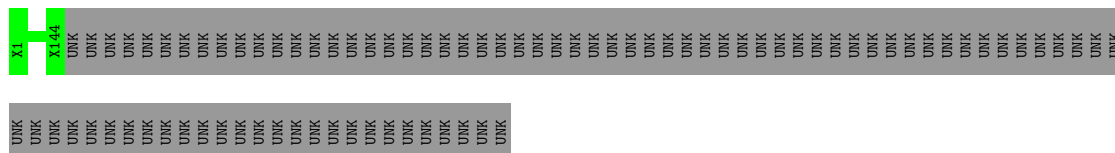
• Molecule 1: Type IV secretion system unknown protein fragment



• Molecule 1: Type IV secretion system unknown protein fragment

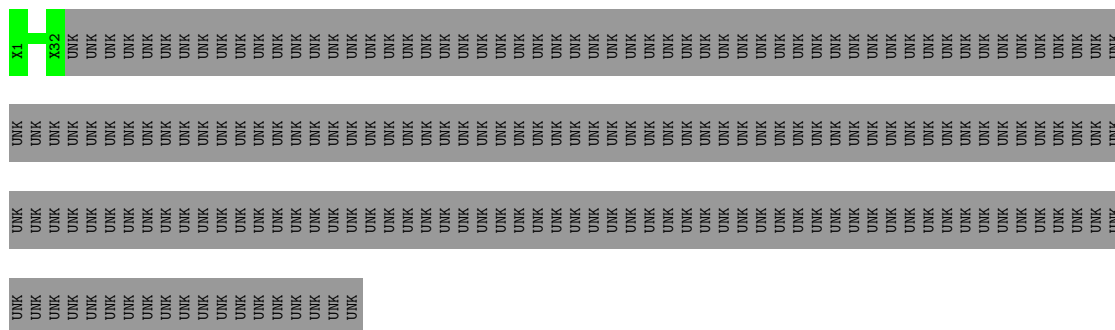


• Molecule 1: Type IV secretion system unknown protein fragment



• Molecule 1: Type IV secretion system unknown protein fragment

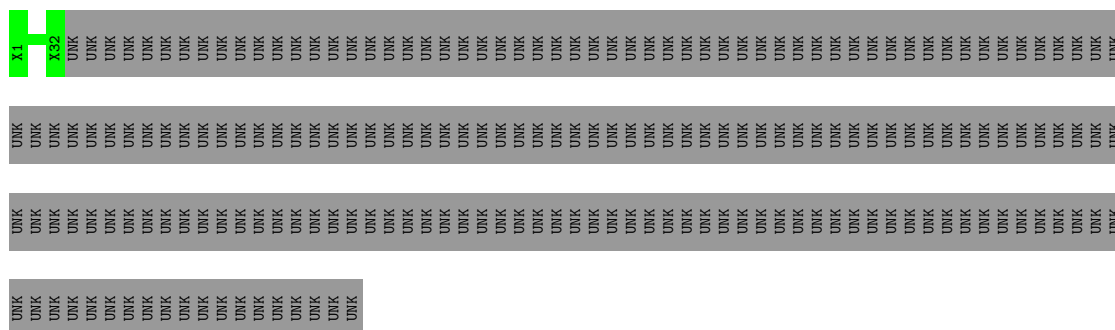




• Molecule 1: Type IV secretion system unknown protein fragment



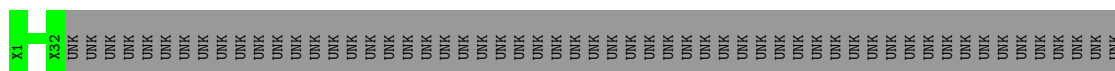
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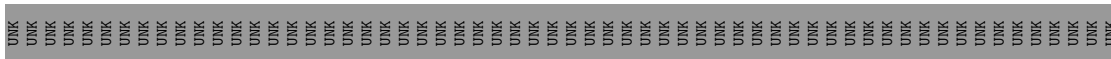


• Molecule 1: Type IV secretion system unknown protein fragment



• Molecule 1: Type IV secretion system unknown protein fragment

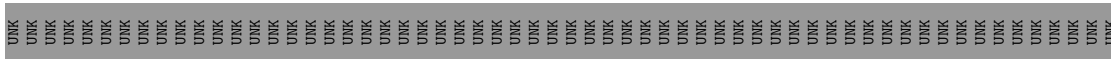




- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment



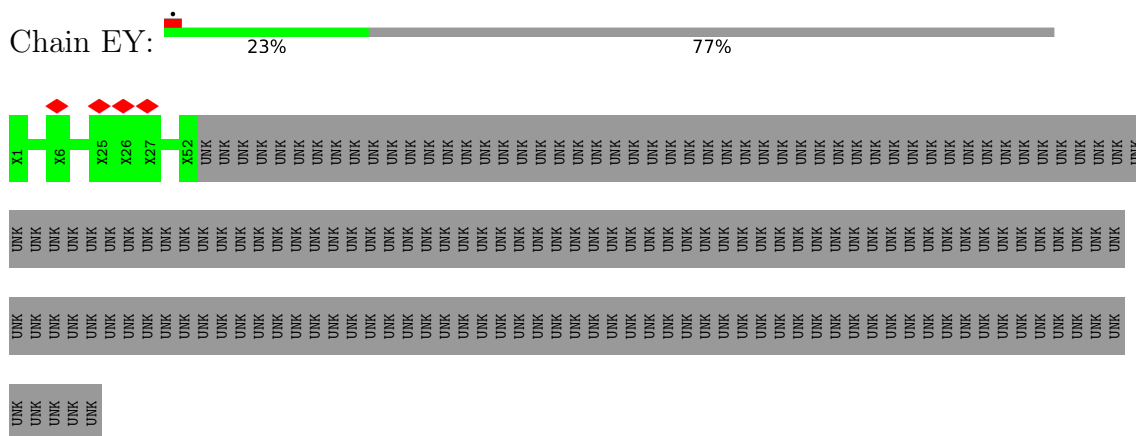
- Molecule 1: Type IV secretion system unknown protein fragment



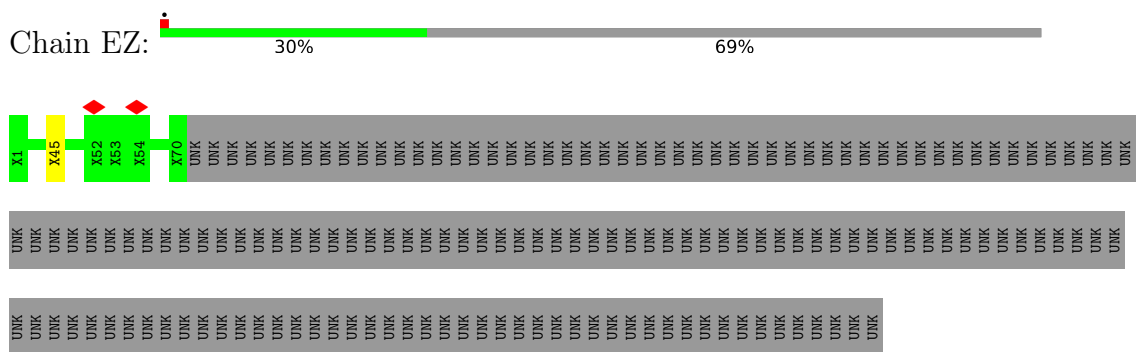
- Molecule 1: Type IV secretion system unknown protein fragment



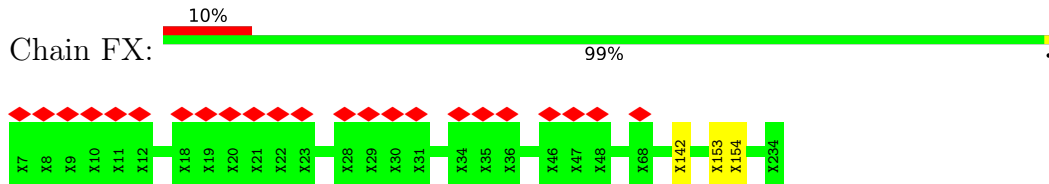
• Molecule 1: Type IV secretion system unknown protein fragment



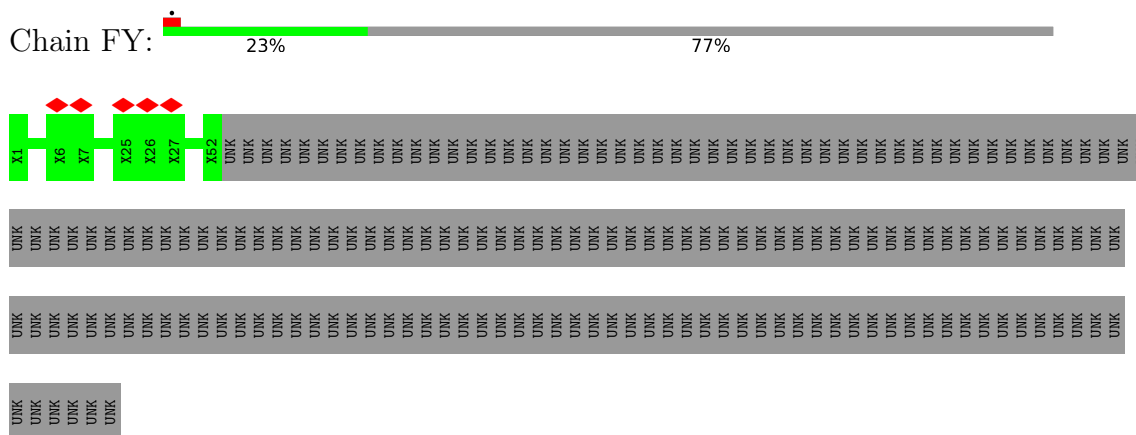
• Molecule 1: Type IV secretion system unknown protein fragment



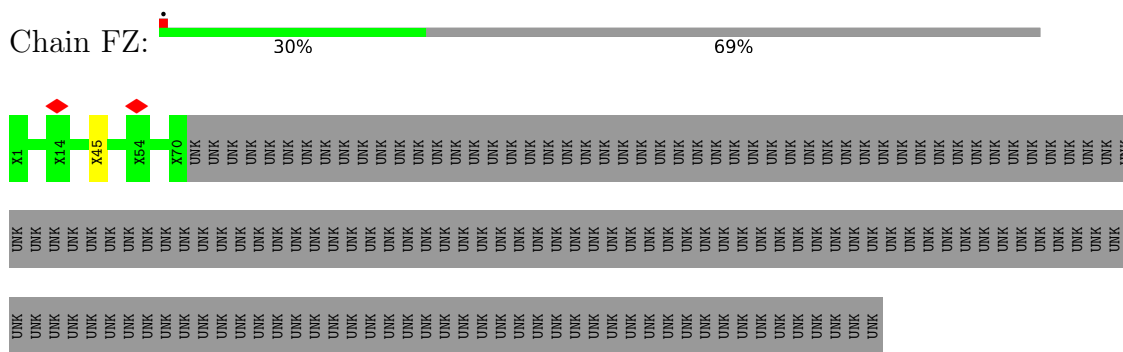
• Molecule 1: Type IV secretion system unknown protein fragment



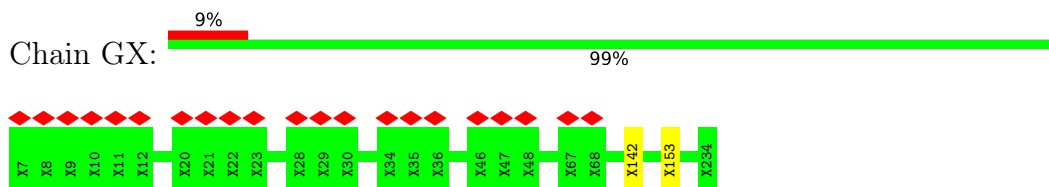
• Molecule 1: Type IV secretion system unknown protein fragment



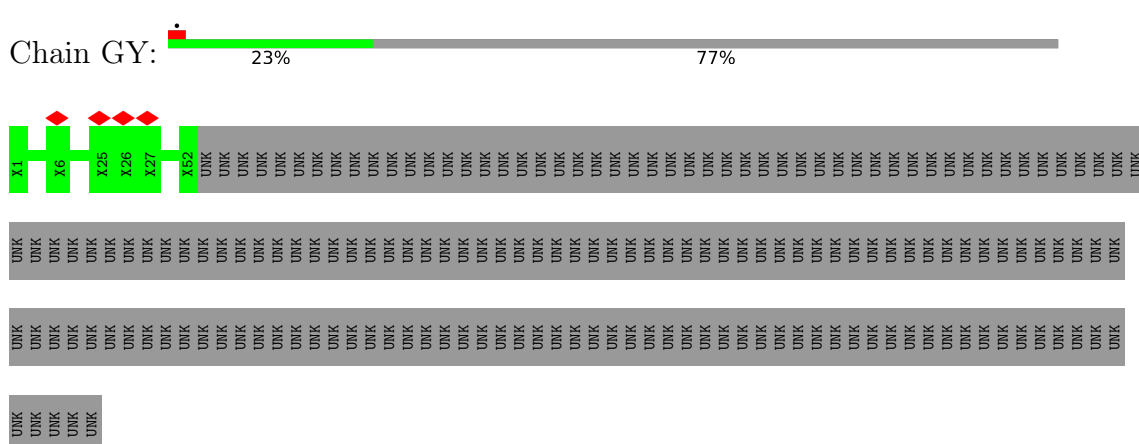
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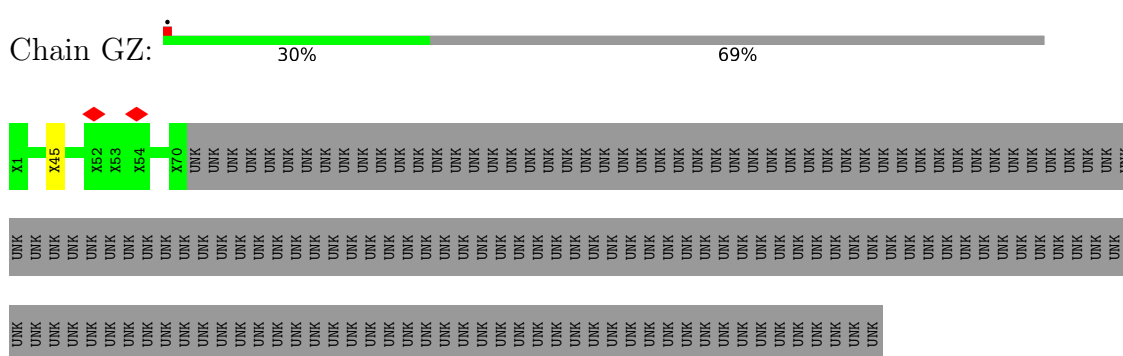
• Molecule 1: Type IV secretion system unknown protein fragment



• Molecule 1: Type IV secretion system unknown protein fragment

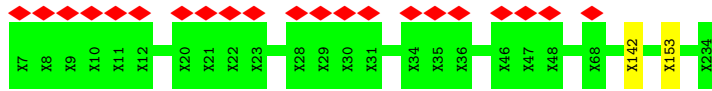


• Molecule 1: Type IV secretion system unknown protein fragment

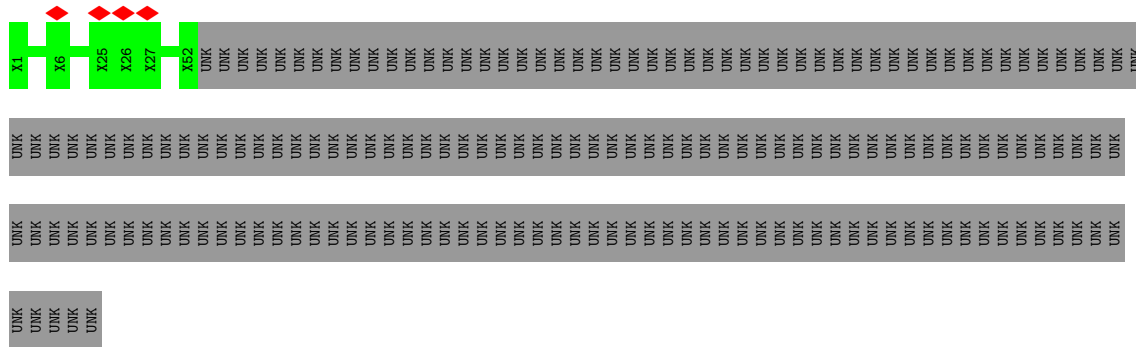


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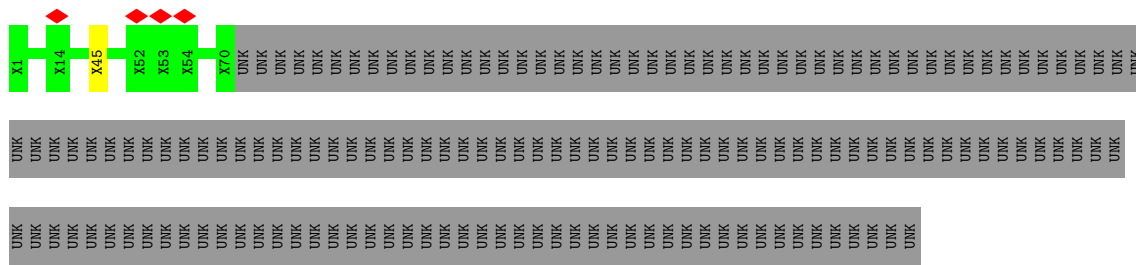




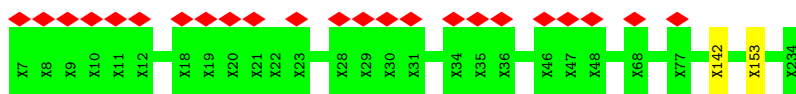
- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment

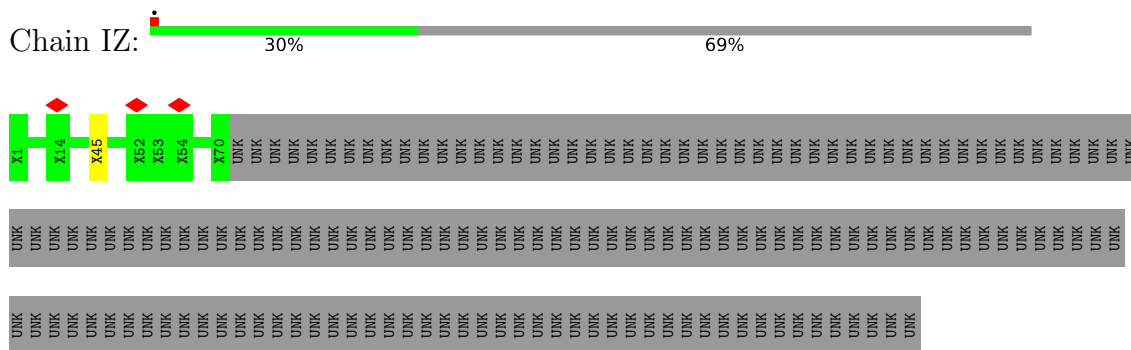


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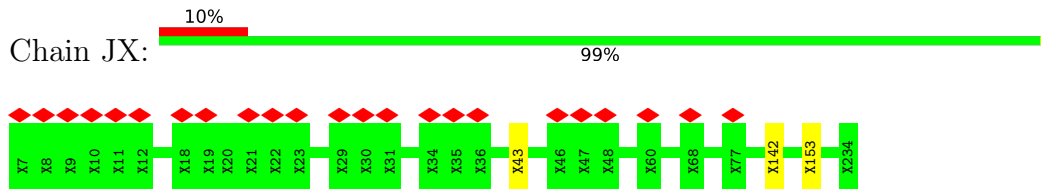


UNK
UNK
UNK

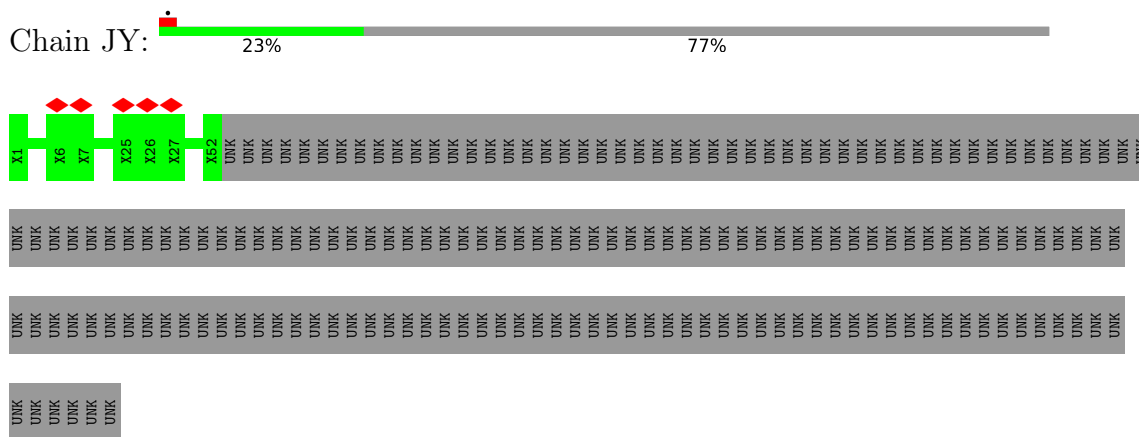
• Molecule 1: Type IV secretion system unknown protein fragment



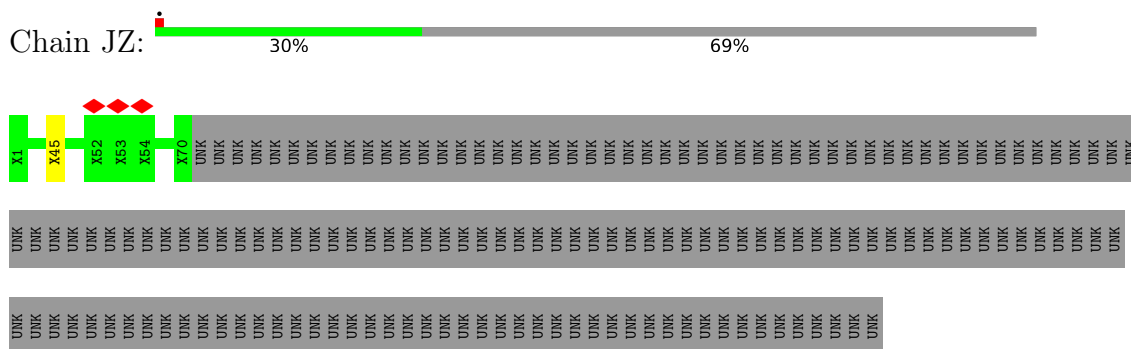
• Molecule 1: Type IV secretion system unknown protein fragment



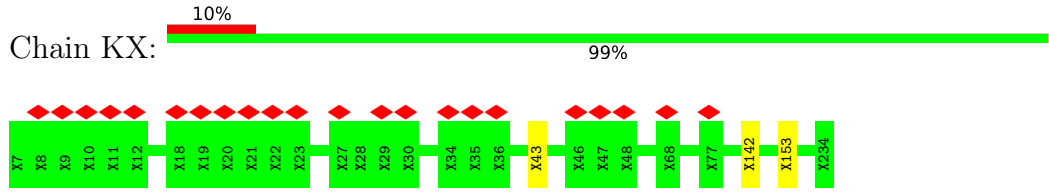
• Molecule 1: Type IV secretion system unknown protein fragment



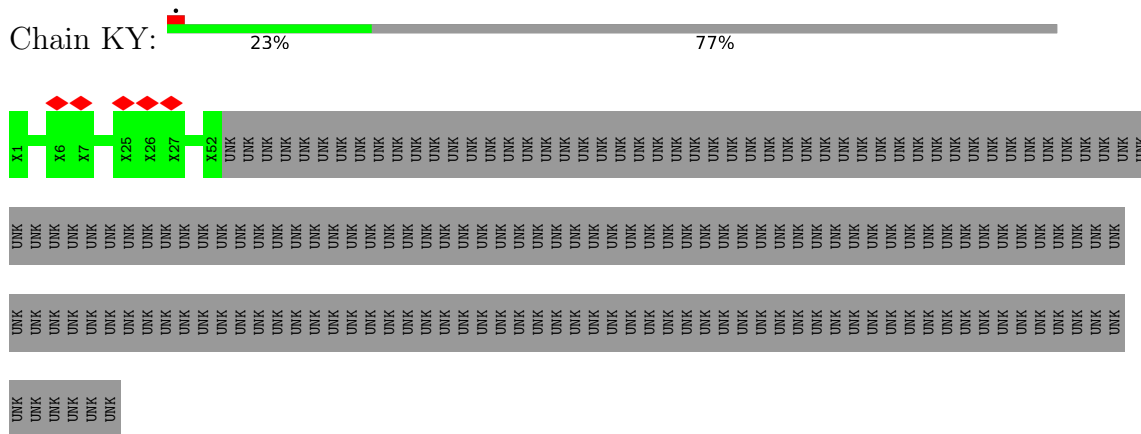
• Molecule 1: Type IV secretion system unknown protein fragment



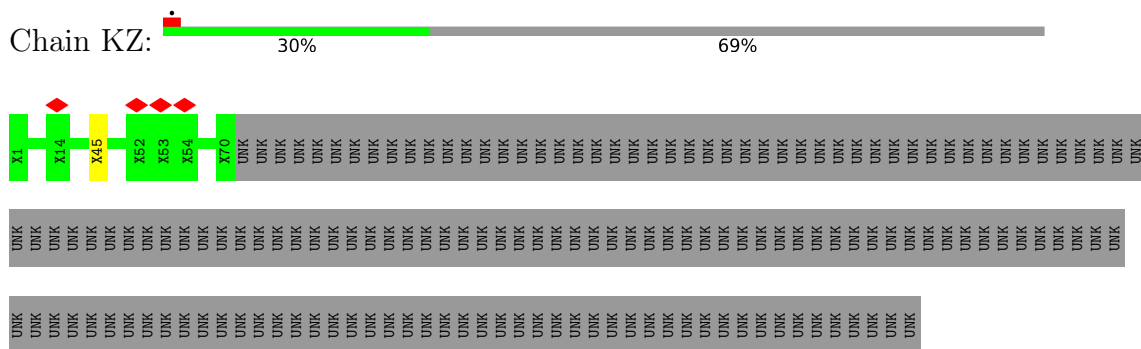
- Molecule 1: Type IV secretion system unknown protein fragment



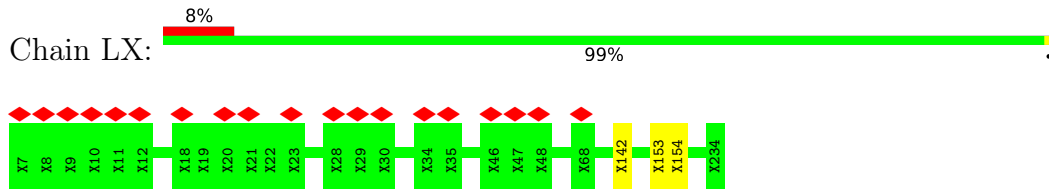
- Molecule 1: Type IV secretion system unknown protein fragment



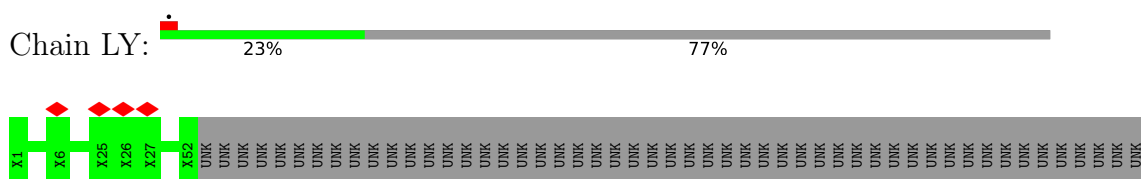
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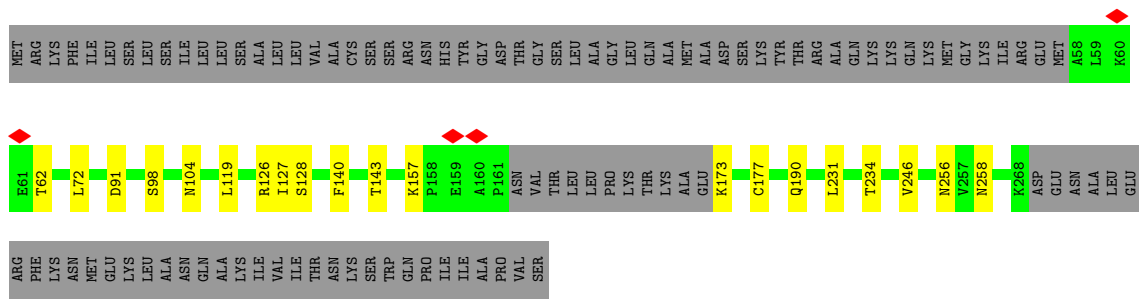


- Molecule 1: Type IV secretion system unknown protein fragment

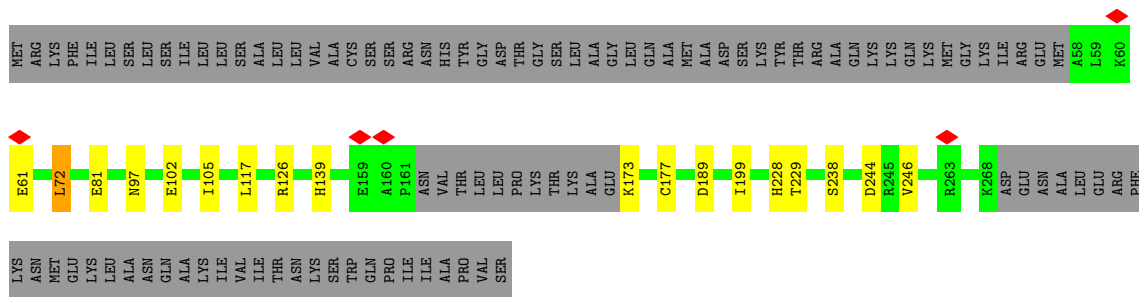


- Molecule 1: Type IV secretion system unknown protein fragment

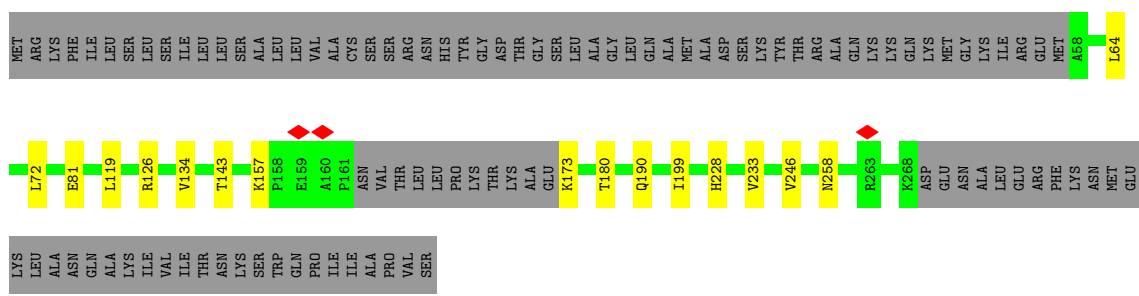




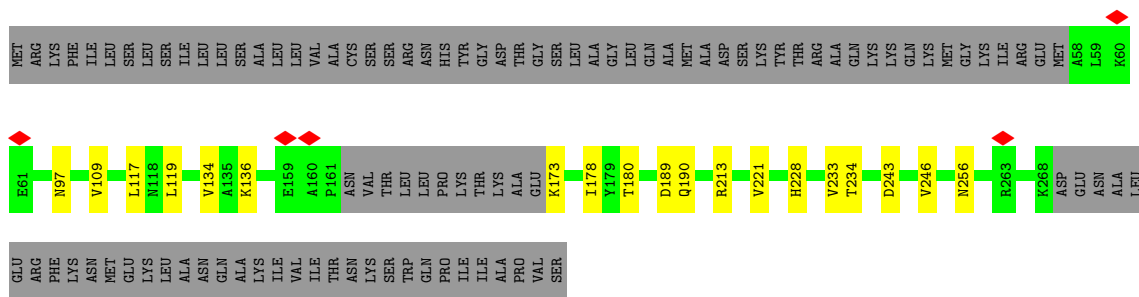
• Molecule 2: DotC



• Molecule 2: DotC



• Molecule 2: DotC



• Molecule 2: DotC

ASN MET GLU LYS LEU ALA ASN GLN ALA ILE VAL ILE THR ASN LYS SER TRP GLN PRO ILE ILE ALA ALA VAL SER

• Molecule 2: DotC



MET ARG LYS PHE ILE LEU SER LEU SER ILE LEU LEU VAL SER ALA LEU LEU VAL ALA CYS SER SER ARG ASN HIS TYR GLY ASP THR GLY SER LEU ALA GLY GLN MET MET ASP SER LYS TYR THR ARG ALA GLN LYS LYS LYS MET GLY ILE LYS ARG ARG ILE ILE ARG LYS ASN MET MET A58 E61

E81 N104 T116 V134 M153 E189 A160 P161 ASN VAL THR LEU LEU PRO LYS THR LYS ALA TYR GLY K173 C177 T180 D189 V221 H228 T229 D243 D244 E245 V246 N256 K268 ASP GLU ASN ALA LEU LEU ARG PHE LYS ASN MET MET GLU LYS LEU

ALA ASN GLN ALA LYS ILE VAL THR ASN LYS SER TRP GLN PRO ILE ILE ALA ALA CYS SER SER ARG ASN HIS TYR GLY ASP THR GLY SER LEU ALA GLY GLN MET MET ASP SER LYS TYR THR ARG ALA GLN LYS LYS LYS MET GLY ILE LYS ARG ARG ILE ILE ARG LYS ASN MET MET A58 E61

• Molecule 2: DotC

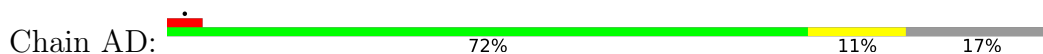


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L72 D91 E112 R126 V134 T143 E159 A160 P161 VAL THR LEU LEU PRO LYS THR LYS ALA TYR GLY K173 C177 L211 H228 T229 D243 V246 L255 N258 K268 ASP GLU ASN ALA LEU LEU ARG PHE LYS ASN MET MET GLU LYS LEU ALA

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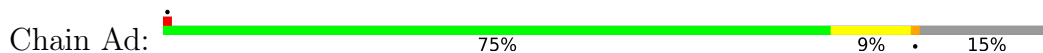
• Molecule 3: DotD



MET ASN ASN LYS VAL MET PHE PHE SER ALA LEU LEU LEU GLY CYS ALA ALA GLY THR MET MET LYS F25 N31 S47 D50 V58 V61 A62 T63 N69 T70 I73 P74 N75 D86 L94 V108 K111 S114 V115 P116 V117 T123 K124

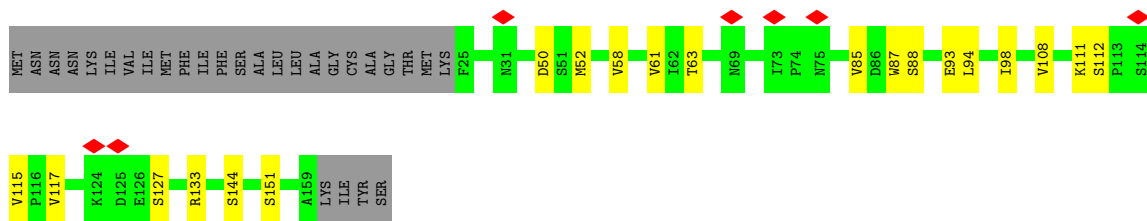
B125 E126 S127 L128 K141 R157 Y158 A159 LYS ILE TYR SER

• Molecule 3: DotD

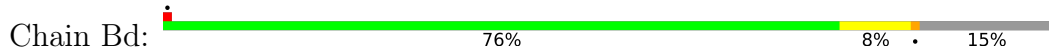


MET ASN ASN LYS VAL ILE MET PHE PHE SER ALA LEU LEU LEU GLY CYS ALA ALA GLY THR MET MET K24 T38 E43 M65 T63 K67 N75 A76 Y77 N78 V85 E93 L94 T95 K111 V117 S127 E130 I131 I161 TYR SER

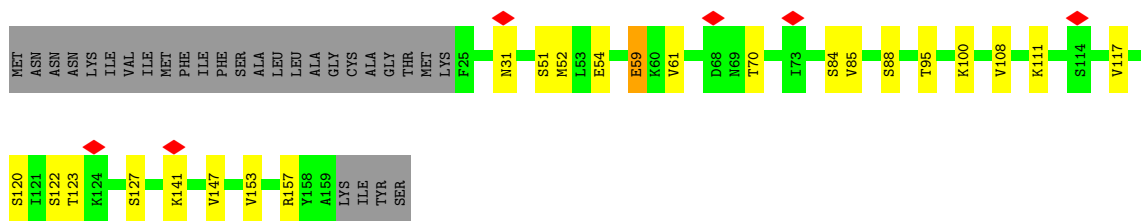
• Molecule 3: DotD



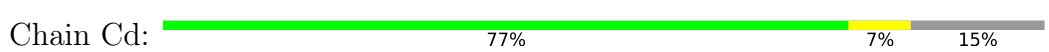
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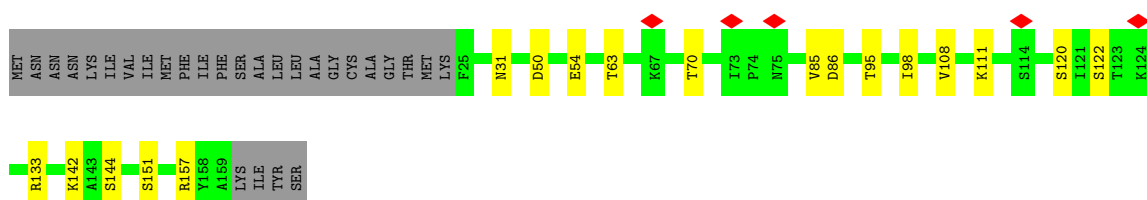
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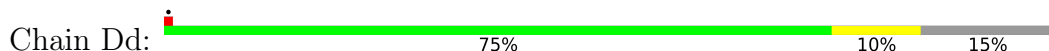
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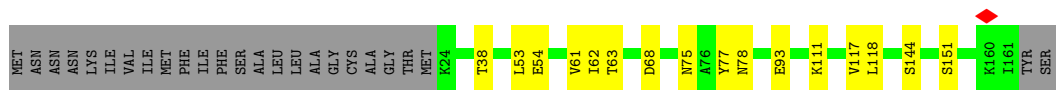


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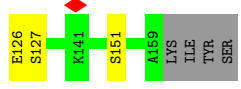
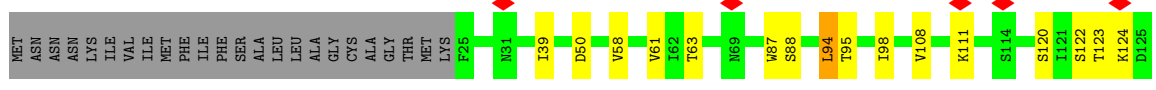


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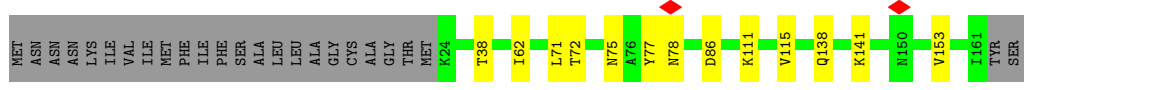
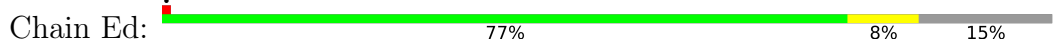




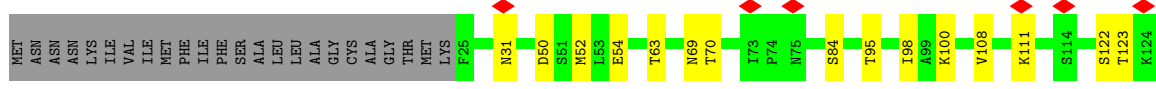
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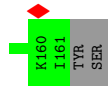
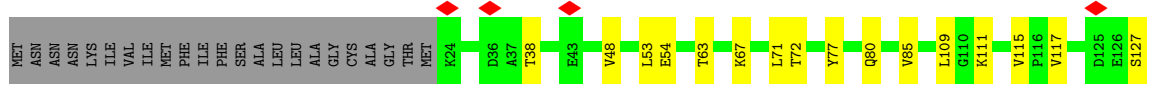
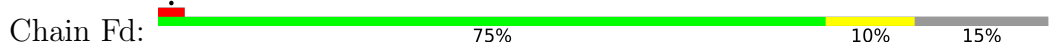
• Molecule 3: DotD



• Molecule 3: DotD

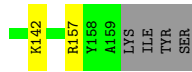


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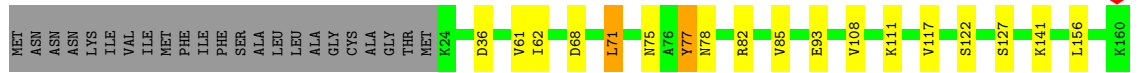
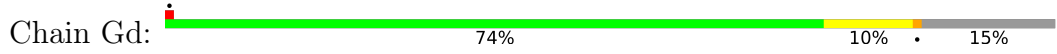


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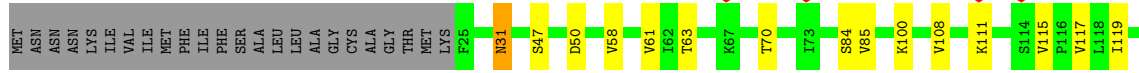




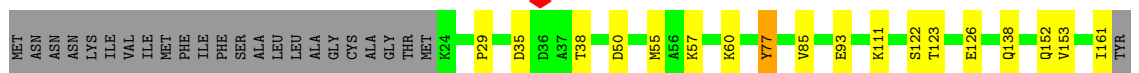
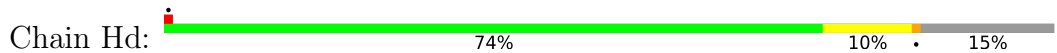
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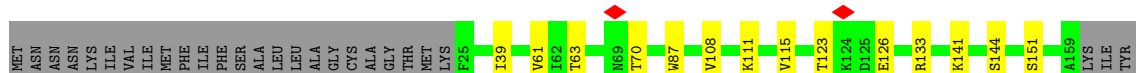
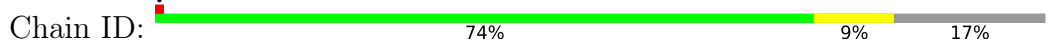
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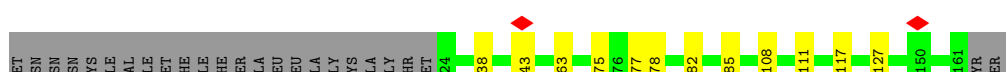
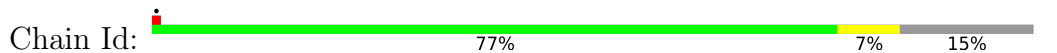
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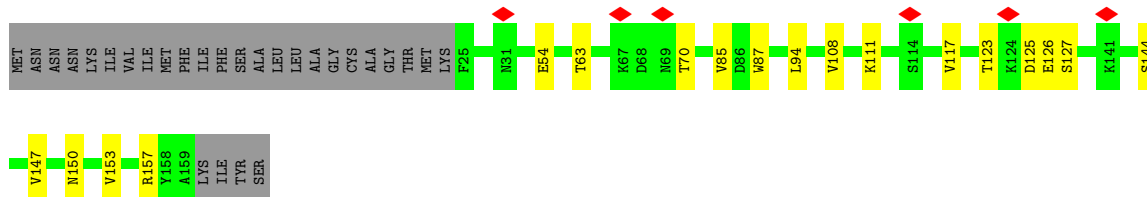
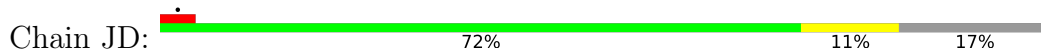
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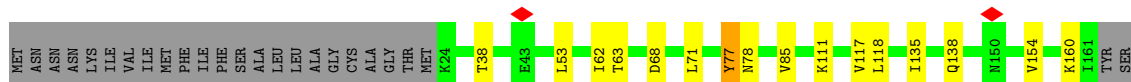
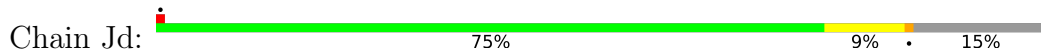
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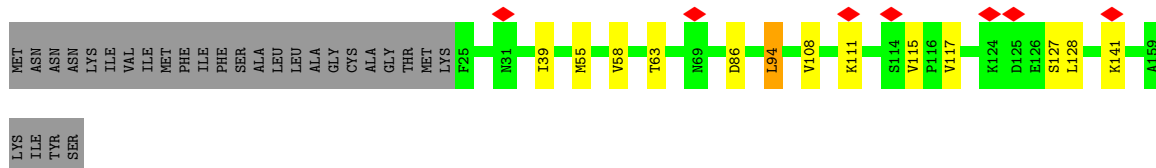
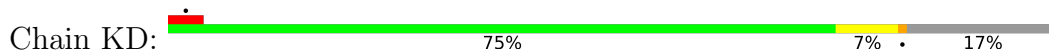
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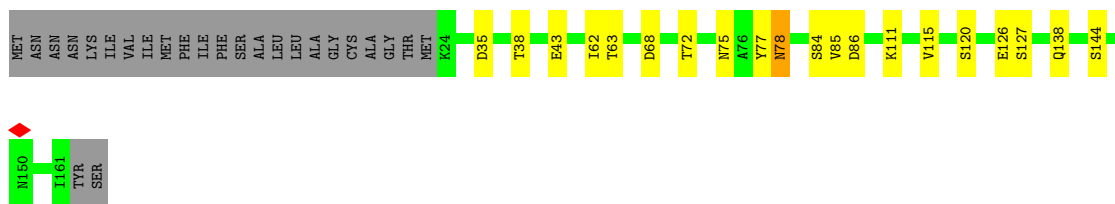
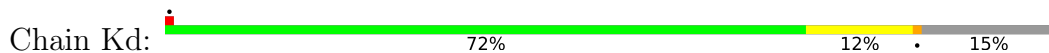
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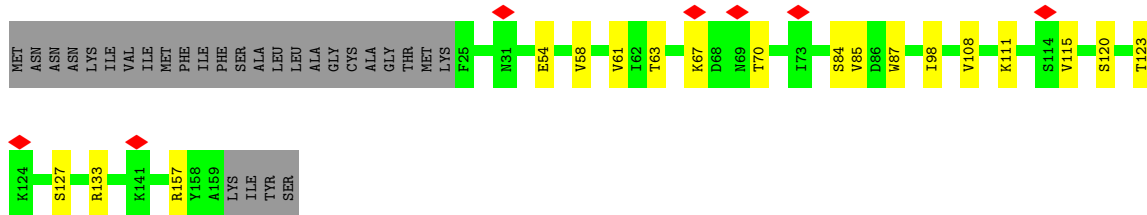
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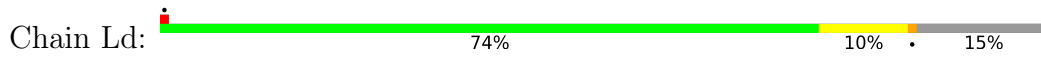
• Molecule 3: DotD



• Molecule 3: DotD

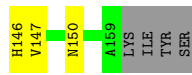
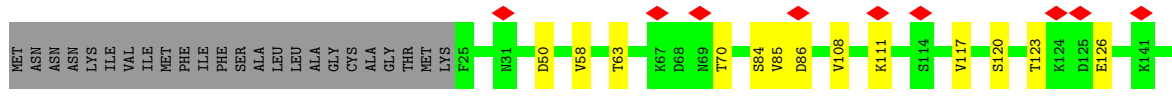
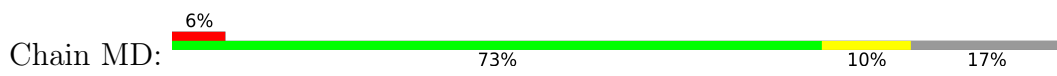


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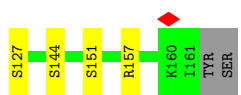
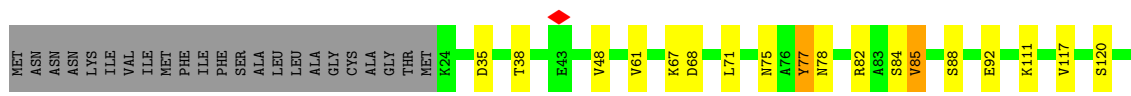
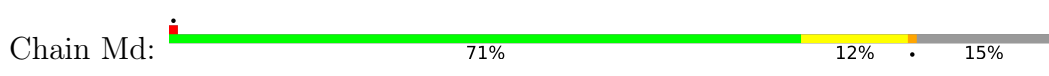


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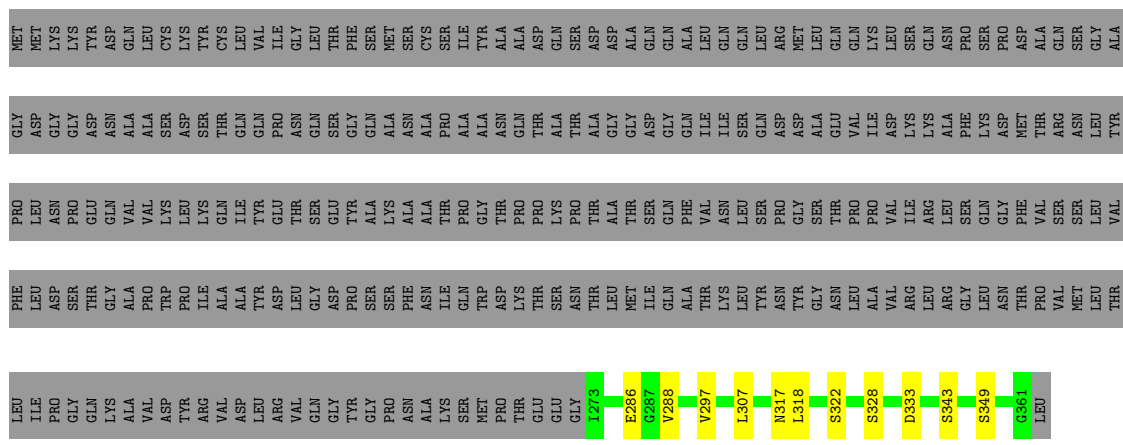
• Molecule 3: DotD



• Molecule 3: DotD

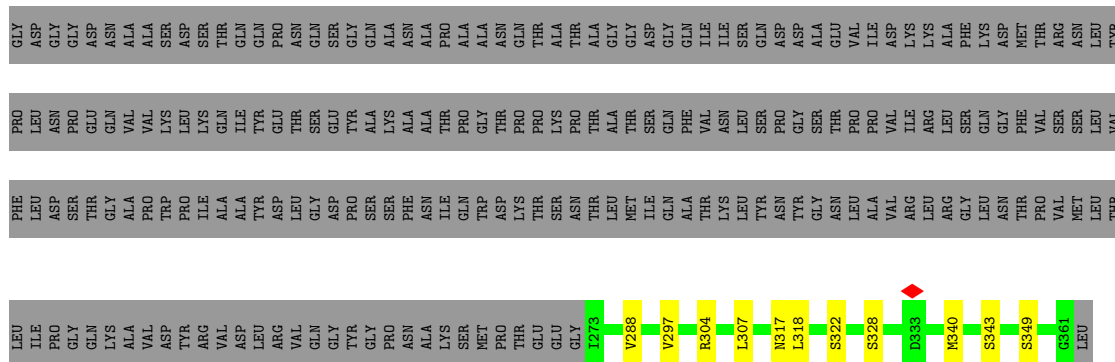


• Molecule 4: Type IV secretion protein IcmK

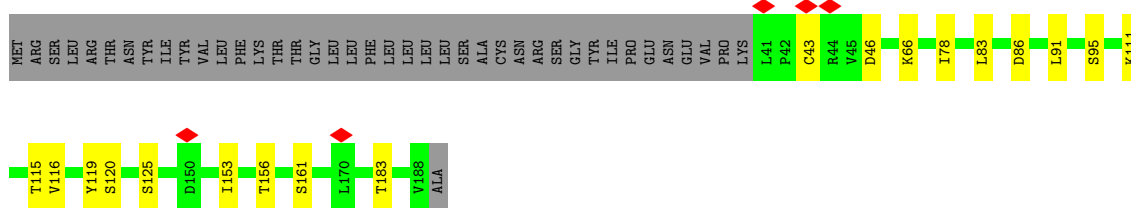


• Molecule 4: Type IV secretion protein IcmK

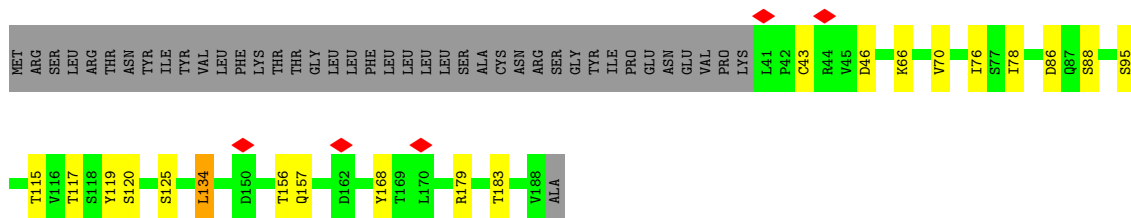




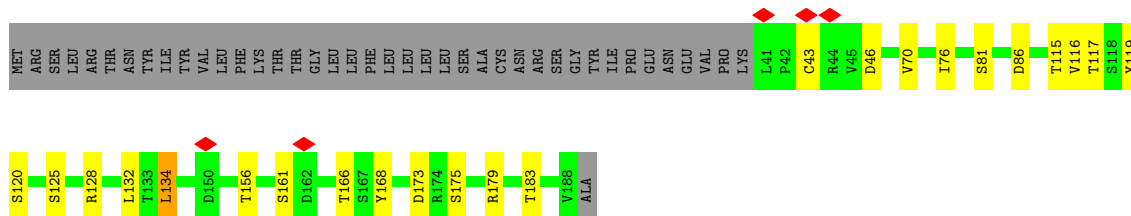
• Molecule 5: Inner membrane lipoprotein YiaD



• Molecule 5: Inner membrane lipoprotein YiaD

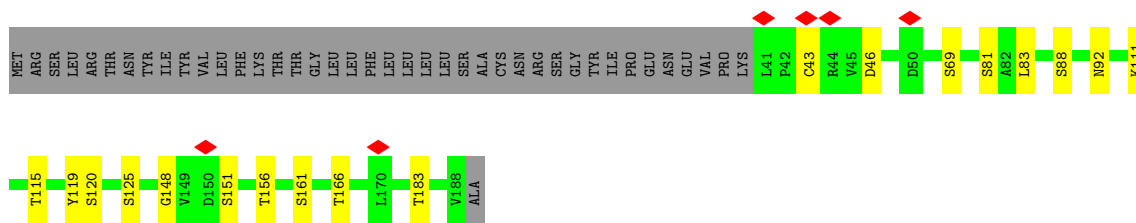


• Molecule 5: Inner membrane lipoprotein YiaD

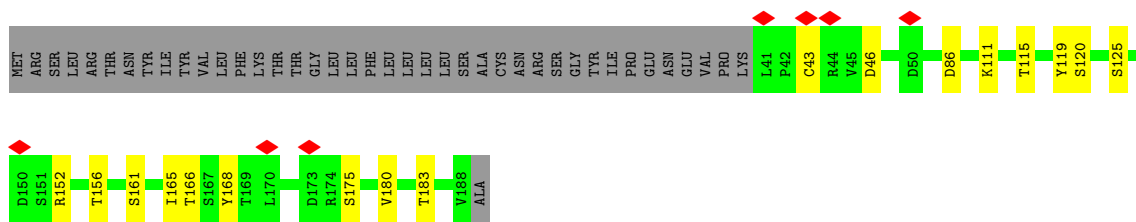


• Molecule 5: Inner membrane lipoprotein YiaD

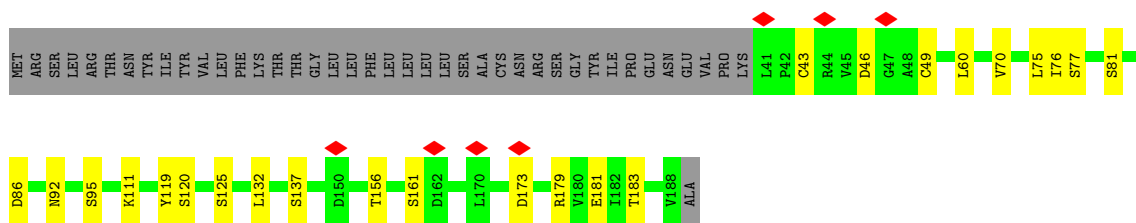




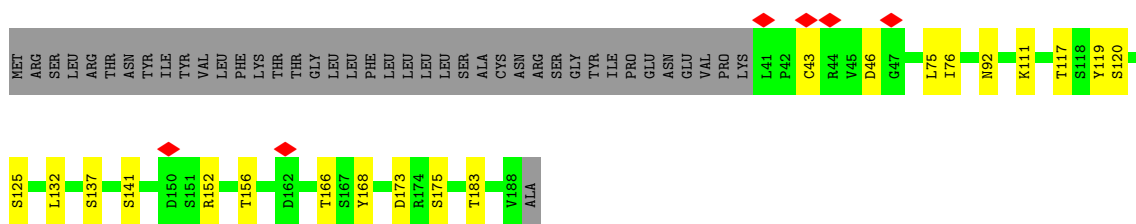
• Molecule 5: Inner membrane lipoprotein YiaD



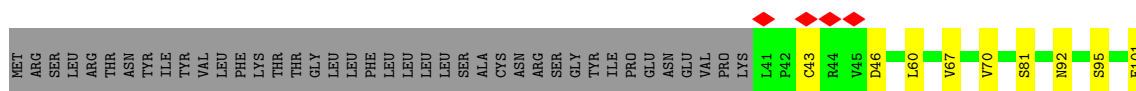
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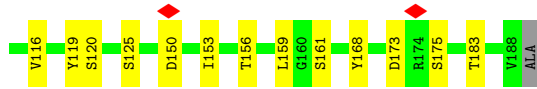


• Molecule 5: Inner membrane lipoprotein YiaD

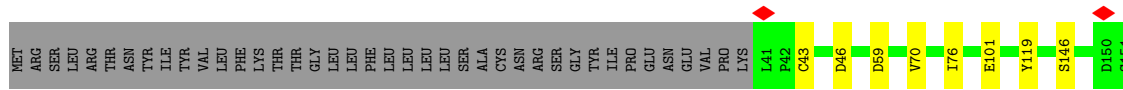


• Molecule 5: Inner membrane lipoprotein YiaD

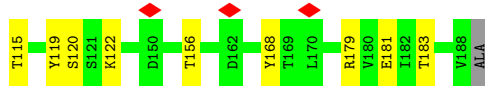
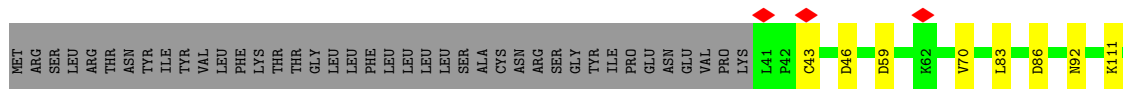




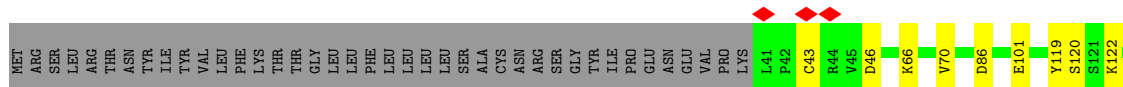
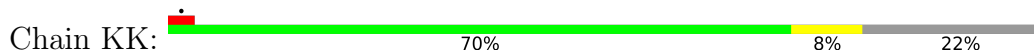
- Molecule 5: Inner membrane lipoprotein YiaD



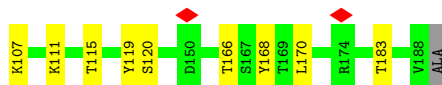
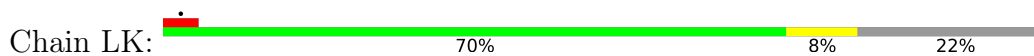
- Molecule 5: Inner membrane lipoprotein YiaD



- Molecule 5: Inner membrane lipoprotein YiaD



- Molecule 5: Inner membrane lipoprotein YiaD



- Molecule 5: Inner membrane lipoprotein YiaD

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12200	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	42.385	Depositor
Minimum map value	-19.636	Depositor
Average map value	0.017	Depositor
Map value standard deviation	1.109	Depositor
Recommended contour level	9.0	Depositor
Map size (\AA)	836.39996, 836.39996, 836.39996	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.64, 1.64, 1.64	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	AC	0.51	0/1629	0.67	0/2214
2	BC	0.51	0/1629	0.70	1/2214 (0.0%)
2	CC	0.52	0/1629	0.73	2/2214 (0.1%)
2	DC	0.49	0/1629	0.67	0/2214
2	EC	0.53	0/1629	0.74	2/2214 (0.1%)
2	FC	0.52	0/1629	0.71	2/2214 (0.1%)
2	GC	0.52	0/1629	0.78	3/2214 (0.1%)
2	HC	0.52	0/1629	0.79	3/2214 (0.1%)
2	IC	0.52	0/1629	0.74	2/2214 (0.1%)
2	JC	0.51	0/1629	0.74	2/2214 (0.1%)
2	KC	0.53	0/1629	0.75	1/2214 (0.0%)
2	LC	0.53	0/1629	0.71	1/2214 (0.0%)
2	MC	0.53	0/1629	0.73	3/2214 (0.1%)
3	AD	0.49	0/1060	0.76	3/1441 (0.2%)
3	Ad	0.50	0/1086	0.81	2/1474 (0.1%)
3	BD	0.50	0/1060	0.80	3/1441 (0.2%)
3	Bd	0.52	0/1086	0.78	1/1474 (0.1%)
3	CD	0.50	0/1060	0.80	1/1441 (0.1%)
3	Cd	0.53	1/1086 (0.1%)	0.82	2/1474 (0.1%)
3	DD	0.50	0/1060	0.78	2/1441 (0.1%)
3	Dd	0.53	0/1086	0.80	1/1474 (0.1%)
3	ED	0.52	0/1060	0.77	2/1441 (0.1%)
3	Ed	0.51	0/1086	0.77	1/1474 (0.1%)
3	FD	0.52	0/1060	0.75	1/1441 (0.1%)
3	Fd	0.55	0/1086	0.78	2/1474 (0.1%)
3	GD	0.50	0/1060	0.79	2/1441 (0.1%)
3	Gd	0.49	0/1086	0.78	2/1474 (0.1%)
3	HD	0.56	1/1060 (0.1%)	0.78	1/1441 (0.1%)
3	Hd	0.53	0/1086	0.82	2/1474 (0.1%)
3	ID	0.49	0/1060	0.76	0/1441
3	Id	0.52	0/1086	0.82	2/1474 (0.1%)
3	JD	0.49	0/1060	0.75	2/1441 (0.1%)
3	Jd	0.54	0/1086	0.82	2/1474 (0.1%)
3	KD	0.51	0/1060	0.77	3/1441 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	Kd	0.52	0/1086	0.77	1/1474 (0.1%)
3	LD	0.55	0/1060	0.80	1/1441 (0.1%)
3	Ld	0.51	0/1086	0.77	2/1474 (0.1%)
3	MD	0.51	0/1060	0.76	2/1441 (0.1%)
3	Md	0.53	0/1086	0.77	1/1474 (0.1%)
4	AH	0.61	0/695	0.79	0/947
4	BH	0.59	0/695	0.82	0/947
4	CH	0.59	0/695	0.78	0/947
4	DH	0.57	0/695	0.77	0/947
4	EH	0.61	0/695	0.79	1/947 (0.1%)
4	FH	0.59	0/695	0.76	0/947
4	GH	0.58	0/695	0.77	2/947 (0.2%)
4	HH	0.55	0/695	0.72	0/947
4	IH	0.57	0/695	0.76	1/947 (0.1%)
4	JH	0.64	0/695	0.79	1/947 (0.1%)
4	KH	0.59	0/695	0.81	1/947 (0.1%)
4	LH	0.62	0/695	0.80	1/947 (0.1%)
4	MH	0.59	0/695	0.78	0/947
5	AK	0.54	0/1171	0.70	0/1583
5	BK	0.52	0/1171	0.73	1/1583 (0.1%)
5	CK	0.52	0/1171	0.75	3/1583 (0.2%)
5	DK	0.53	0/1171	0.70	1/1583 (0.1%)
5	EK	0.53	0/1171	0.71	0/1583
5	FK	0.51	0/1171	0.73	1/1583 (0.1%)
5	GK	0.54	0/1171	0.74	1/1583 (0.1%)
5	HK	0.52	0/1171	0.70	0/1583
5	IK	0.53	0/1171	0.71	1/1583 (0.1%)
5	JK	0.53	0/1171	0.76	1/1583 (0.1%)
5	KK	0.53	0/1171	0.71	1/1583 (0.1%)
5	LK	0.53	0/1171	0.68	1/1583 (0.1%)
5	MK	0.50	0/1171	0.69	0/1583
6	N	0.52	0/1130	0.75	2/1522 (0.1%)
6	O	0.52	0/1130	0.71	0/1522
6	P	0.52	0/1130	0.74	0/1522
6	Q	0.49	0/1130	0.69	0/1522
6	R	0.50	0/1130	0.77	1/1522 (0.1%)
6	S	0.51	0/1130	0.71	0/1522
6	T	0.54	0/1130	0.74	1/1522 (0.1%)
6	U	0.49	0/1130	0.74	2/1522 (0.1%)
6	V	0.51	0/1130	0.77	1/1522 (0.1%)
6	W	0.52	0/1130	0.71	0/1522
6	X	0.53	0/1130	0.75	1/1522 (0.1%)
6	Y	0.54	0/1130	0.74	2/1522 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	Z	0.50	0/1130	0.69	0/1522
All	All	0.53	2/88023 (0.0%)	0.75	94/119353 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AX	0	2
1	AZ	0	2
1	BV	0	2
1	BX	0	2
1	BZ	0	2
1	CV	0	1
1	CX	0	2
1	CZ	0	1
1	DX	0	3
1	DZ	0	2
1	EX	0	3
1	EZ	0	1
1	FV	0	1
1	FX	0	3
1	FZ	0	1
1	GV	0	1
1	GX	0	2
1	GZ	0	1
1	HV	0	1
1	HX	0	2
1	HZ	0	1
1	IV	0	1
1	IX	0	2
1	IZ	0	1
1	JX	0	3
1	JZ	0	1
1	KV	0	1
1	KX	0	3
1	KZ	0	1
1	LX	0	3
1	LZ	0	2
1	MX	0	3
1	MZ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	NV	0	1
1	OV	0	2
1	PV	0	1
1	RV	0	1
2	BC	0	1
3	Bd	0	1
3	Ed	0	1
3	Fd	0	1
3	Id	0	1
3	Jd	0	1
3	Kd	0	1
3	Md	0	1
4	AH	0	1
4	BH	0	1
4	DH	0	2
4	EH	0	1
4	FH	0	1
4	GH	0	1
4	HH	0	1
4	IH	0	1
4	JH	0	1
4	KH	0	1
4	LH	0	1
5	DK	0	1
6	N	0	2
6	O	0	2
6	Q	0	2
6	T	0	1
6	V	0	2
6	W	0	1
6	X	0	1
6	Z	0	1
All	All	0	96

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Cd	58	VAL	CB-CG1	-5.97	1.40	1.52
3	HD	31	ASN	C-N	-5.41	1.21	1.34

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	JK	59	ASP	CB-CG-OD2	10.30	127.58	118.30
2	HC	117	LEU	CA-CB-CG	10.27	138.92	115.30
6	X	155	LEU	CA-CB-CG	9.98	138.26	115.30
6	V	113	ASP	CB-CG-OD1	9.90	127.21	118.30
2	GC	117	LEU	CA-CB-CG	9.13	136.30	115.30

There are no chirality outliers.

5 of 96 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BV	42	UNK	Peptide
1	BV	46	UNK	Peptide
1	CV	77	UNK	Peptide
1	FV	42	UNK	Peptide
1	GV	77	UNK	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AC	196/303 (65%)	190 (97%)	6 (3%)	0	100	100
2	BC	196/303 (65%)	189 (96%)	7 (4%)	0	100	100
2	CC	196/303 (65%)	189 (96%)	7 (4%)	0	100	100
2	DC	196/303 (65%)	187 (95%)	9 (5%)	0	100	100
2	EC	196/303 (65%)	187 (95%)	9 (5%)	0	100	100
2	FC	196/303 (65%)	187 (95%)	9 (5%)	0	100	100
2	GC	196/303 (65%)	189 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	HC	196/303 (65%)	190 (97%)	6 (3%)	0	100	100
2	IC	196/303 (65%)	191 (97%)	5 (3%)	0	100	100
2	JC	196/303 (65%)	187 (95%)	9 (5%)	0	100	100
2	KC	196/303 (65%)	189 (96%)	7 (4%)	0	100	100
2	LC	196/303 (65%)	188 (96%)	8 (4%)	0	100	100
2	MC	196/303 (65%)	191 (97%)	5 (3%)	0	100	100
3	AD	133/163 (82%)	127 (96%)	6 (4%)	0	100	100
3	Ad	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	BD	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
3	Bd	136/163 (83%)	125 (92%)	11 (8%)	0	100	100
3	CD	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
3	Cd	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	DD	133/163 (82%)	126 (95%)	7 (5%)	0	100	100
3	Dd	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
3	ED	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
3	Ed	136/163 (83%)	129 (95%)	7 (5%)	0	100	100
3	FD	133/163 (82%)	126 (95%)	7 (5%)	0	100	100
3	Fd	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	GD	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
3	Gd	136/163 (83%)	128 (94%)	8 (6%)	0	100	100
3	HD	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
3	Hd	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	ID	133/163 (82%)	129 (97%)	4 (3%)	0	100	100
3	Id	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	JD	133/163 (82%)	126 (95%)	7 (5%)	0	100	100
3	Jd	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
3	KD	133/163 (82%)	127 (96%)	6 (4%)	0	100	100
3	Kd	136/163 (83%)	130 (96%)	6 (4%)	0	100	100
3	LD	133/163 (82%)	126 (95%)	7 (5%)	0	100	100
3	Ld	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	MD	133/163 (82%)	128 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Md	136/163 (83%)	129 (95%)	7 (5%)	0	100	100
4	AH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	BH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	CH	87/361 (24%)	77 (88%)	10 (12%)	0	100	100
4	DH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	EH	87/361 (24%)	76 (87%)	11 (13%)	0	100	100
4	FH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	GH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	HH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	IH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	JH	87/361 (24%)	78 (90%)	9 (10%)	0	100	100
4	KH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	LH	87/361 (24%)	77 (88%)	10 (12%)	0	100	100
4	MH	87/361 (24%)	78 (90%)	9 (10%)	0	100	100
5	AK	146/189 (77%)	142 (97%)	4 (3%)	0	100	100
5	BK	146/189 (77%)	138 (94%)	8 (6%)	0	100	100
5	CK	146/189 (77%)	138 (94%)	8 (6%)	0	100	100
5	DK	146/189 (77%)	138 (94%)	8 (6%)	0	100	100
5	EK	146/189 (77%)	139 (95%)	7 (5%)	0	100	100
5	FK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
5	GK	146/189 (77%)	140 (96%)	6 (4%)	0	100	100
5	HK	146/189 (77%)	138 (94%)	8 (6%)	0	100	100
5	IK	146/189 (77%)	140 (96%)	6 (4%)	0	100	100
5	JK	146/189 (77%)	141 (97%)	5 (3%)	0	100	100
5	KK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
5	LK	146/189 (77%)	139 (95%)	7 (5%)	0	100	100
5	MK	146/189 (77%)	136 (93%)	10 (7%)	0	100	100
6	N	134/249 (54%)	123 (92%)	11 (8%)	0	100	100
6	O	134/249 (54%)	124 (92%)	10 (8%)	0	100	100
6	P	134/249 (54%)	126 (94%)	8 (6%)	0	100	100
6	Q	134/249 (54%)	127 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	R	134/249 (54%)	126 (94%)	8 (6%)	0	100	100
6	S	134/249 (54%)	127 (95%)	7 (5%)	0	100	100
6	T	134/249 (54%)	126 (94%)	8 (6%)	0	100	100
6	U	134/249 (54%)	128 (96%)	6 (4%)	0	100	100
6	V	134/249 (54%)	126 (94%)	8 (6%)	0	100	100
6	W	134/249 (54%)	124 (92%)	10 (8%)	0	100	100
6	X	134/249 (54%)	125 (93%)	9 (7%)	0	100	100
6	Y	134/249 (54%)	125 (93%)	9 (7%)	0	100	100
6	Z	134/249 (54%)	126 (94%)	8 (6%)	0	100	100
All	All	10816/18564 (58%)	10205 (94%)	611 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	169/257 (66%)	157 (93%)	12 (7%)	14	45
2	BC	169/257 (66%)	153 (90%)	16 (10%)	8	34
2	CC	169/257 (66%)	154 (91%)	15 (9%)	9	37
2	DC	169/257 (66%)	149 (88%)	20 (12%)	5	26
2	EC	169/257 (66%)	152 (90%)	17 (10%)	7	31
2	FC	169/257 (66%)	155 (92%)	14 (8%)	11	40
2	GC	169/257 (66%)	153 (90%)	16 (10%)	8	34
2	HC	169/257 (66%)	156 (92%)	13 (8%)	13	43
2	IC	169/257 (66%)	152 (90%)	17 (10%)	7	31
2	JC	169/257 (66%)	156 (92%)	13 (8%)	13	43
2	KC	169/257 (66%)	154 (91%)	15 (9%)	9	37
2	LC	169/257 (66%)	154 (91%)	15 (9%)	9	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	MC	169/257 (66%)	157 (93%)	12 (7%)	14	45
3	AD	116/139 (84%)	101 (87%)	15 (13%)	4	22
3	Ad	119/139 (86%)	105 (88%)	14 (12%)	5	26
3	BD	116/139 (84%)	99 (85%)	17 (15%)	3	18
3	Bd	119/139 (86%)	106 (89%)	13 (11%)	6	29
3	CD	116/139 (84%)	93 (80%)	23 (20%)	1	8
3	Cd	119/139 (86%)	109 (92%)	10 (8%)	11	40
3	DD	116/139 (84%)	100 (86%)	16 (14%)	3	21
3	Dd	119/139 (86%)	104 (87%)	15 (13%)	4	23
3	ED	116/139 (84%)	98 (84%)	18 (16%)	2	17
3	Ed	119/139 (86%)	108 (91%)	11 (9%)	9	36
3	FD	116/139 (84%)	98 (84%)	18 (16%)	2	17
3	Fd	119/139 (86%)	106 (89%)	13 (11%)	6	29
3	GD	116/139 (84%)	101 (87%)	15 (13%)	4	22
3	Gd	119/139 (86%)	101 (85%)	18 (15%)	3	17
3	HD	116/139 (84%)	95 (82%)	21 (18%)	1	11
3	Hd	119/139 (86%)	102 (86%)	17 (14%)	3	19
3	ID	116/139 (84%)	102 (88%)	14 (12%)	5	24
3	Id	119/139 (86%)	110 (92%)	9 (8%)	13	43
3	JD	116/139 (84%)	100 (86%)	16 (14%)	3	21
3	Jd	119/139 (86%)	105 (88%)	14 (12%)	5	26
3	KD	116/139 (84%)	105 (90%)	11 (10%)	8	34
3	Kd	119/139 (86%)	100 (84%)	19 (16%)	2	15
3	LD	116/139 (84%)	99 (85%)	17 (15%)	3	18
3	Ld	119/139 (86%)	103 (87%)	16 (13%)	4	21
3	MD	116/139 (84%)	102 (88%)	14 (12%)	5	24
3	Md	119/139 (86%)	97 (82%)	22 (18%)	1	10
4	AH	75/300 (25%)	65 (87%)	10 (13%)	4	22
4	BH	75/300 (25%)	64 (85%)	11 (15%)	3	18
4	CH	75/300 (25%)	67 (89%)	8 (11%)	6	30
4	DH	75/300 (25%)	65 (87%)	10 (13%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	EH	75/300 (25%)	65 (87%)	10 (13%)	4	22
4	FH	75/300 (25%)	69 (92%)	6 (8%)	12	42
4	GH	75/300 (25%)	66 (88%)	9 (12%)	5	25
4	HH	75/300 (25%)	69 (92%)	6 (8%)	12	42
4	IH	75/300 (25%)	65 (87%)	10 (13%)	4	22
4	JH	75/300 (25%)	64 (85%)	11 (15%)	3	18
4	KH	75/300 (25%)	67 (89%)	8 (11%)	6	30
4	LH	75/300 (25%)	64 (85%)	11 (15%)	3	18
4	MH	75/300 (25%)	64 (85%)	11 (15%)	3	18
5	AK	126/163 (77%)	108 (86%)	18 (14%)	3	19
5	BK	126/163 (77%)	106 (84%)	20 (16%)	2	16
5	CK	126/163 (77%)	105 (83%)	21 (17%)	2	14
5	DK	126/163 (77%)	110 (87%)	16 (13%)	4	23
5	EK	126/163 (77%)	109 (86%)	17 (14%)	4	21
5	FK	126/163 (77%)	103 (82%)	23 (18%)	1	10
5	GK	126/163 (77%)	107 (85%)	19 (15%)	3	17
5	HK	126/163 (77%)	104 (82%)	22 (18%)	2	12
5	IK	126/163 (77%)	114 (90%)	12 (10%)	8	34
5	JK	126/163 (77%)	110 (87%)	16 (13%)	4	23
5	KK	126/163 (77%)	112 (89%)	14 (11%)	6	28
5	LK	126/163 (77%)	111 (88%)	15 (12%)	5	25
5	MK	126/163 (77%)	112 (89%)	14 (11%)	6	28
6	N	118/203 (58%)	108 (92%)	10 (8%)	10	40
6	O	118/203 (58%)	104 (88%)	14 (12%)	5	25
6	P	118/203 (58%)	108 (92%)	10 (8%)	10	40
6	Q	118/203 (58%)	107 (91%)	11 (9%)	9	35
6	R	118/203 (58%)	108 (92%)	10 (8%)	10	40
6	S	118/203 (58%)	105 (89%)	13 (11%)	6	29
6	T	118/203 (58%)	102 (86%)	16 (14%)	3	21
6	U	118/203 (58%)	104 (88%)	14 (12%)	5	25
6	V	118/203 (58%)	108 (92%)	10 (8%)	10	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	W	118/203 (58%)	108 (92%)	10 (8%)	10	40
6	X	118/203 (58%)	109 (92%)	9 (8%)	13	43
6	Y	118/203 (58%)	108 (92%)	10 (8%)	10	40
6	Z	118/203 (58%)	106 (90%)	12 (10%)	7	31
All	All	9399/15613 (60%)	8301 (88%)	1098 (12%)	9	26

5 of 1098 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	MK	183	THR
6	N	119	TYR
5	MK	173	ASP
6	U	143	ILE
3	FD	52	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
6	V	212	ASN
6	W	177	HIS
6	Z	112	GLN
2	JC	241	HIS
2	JC	103	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

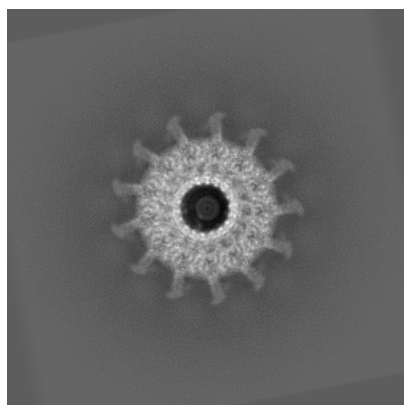
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22070. These allow visual inspection of the internal detail of the map and identification of artifacts.

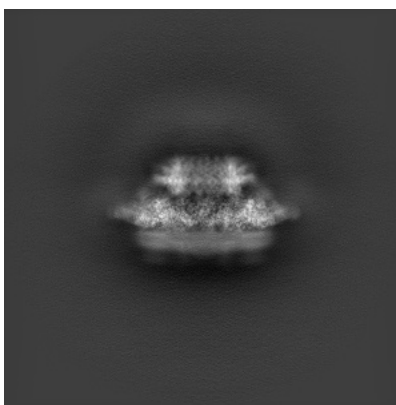
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

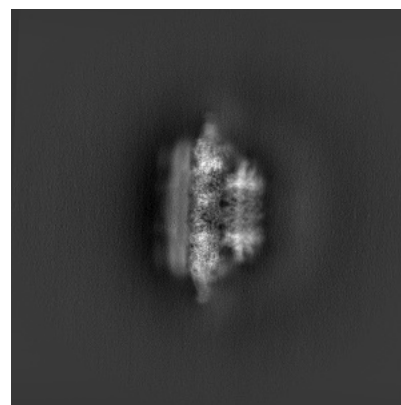
6.1.1 Primary map



X



Y

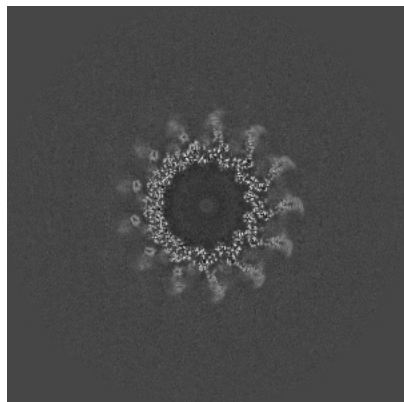


Z

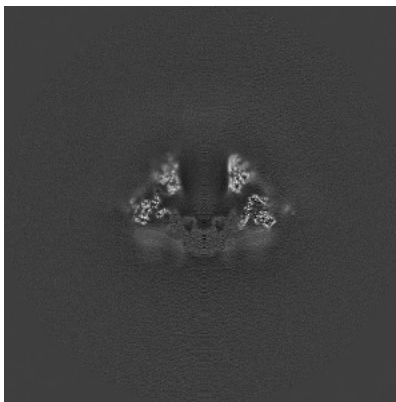
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

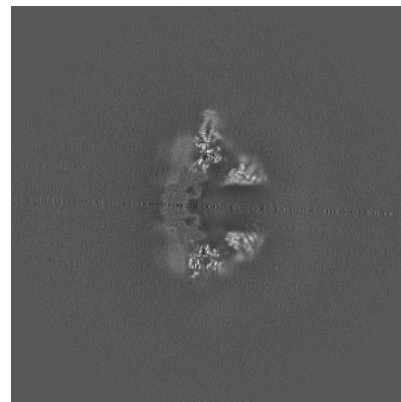
6.2.1 Primary map



X Index: 255



Y Index: 255

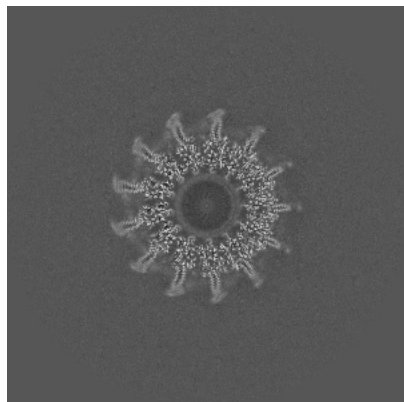


Z Index: 255

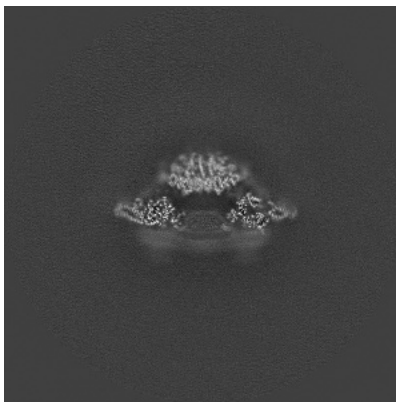
The images above show central slices of the map in three orthogonal directions.

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

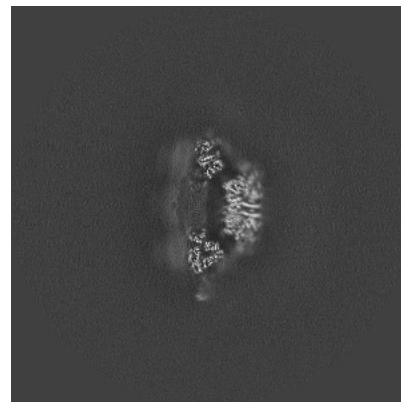
6.3.1 Primary map



X Index: 245



Y Index: 218

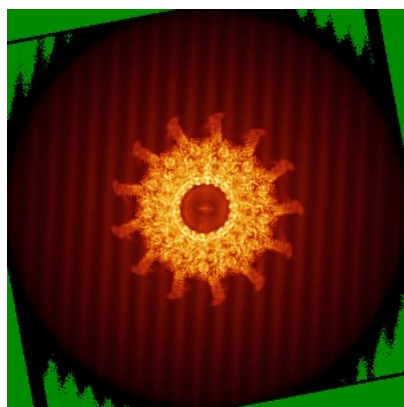


Z Index: 288

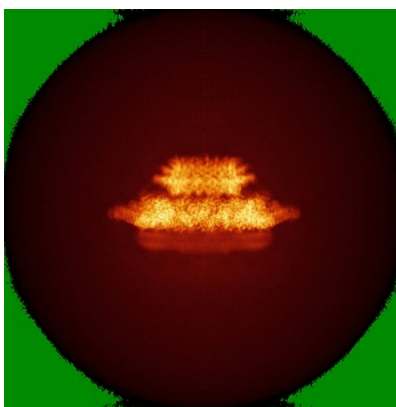
The images above show the largest variance slices of the map in three orthogonal directions.

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

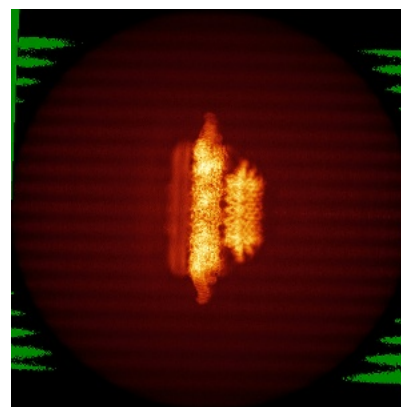
6.4.1 Primary map



X



Y

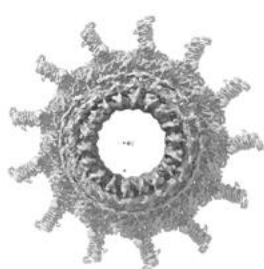


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 9.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

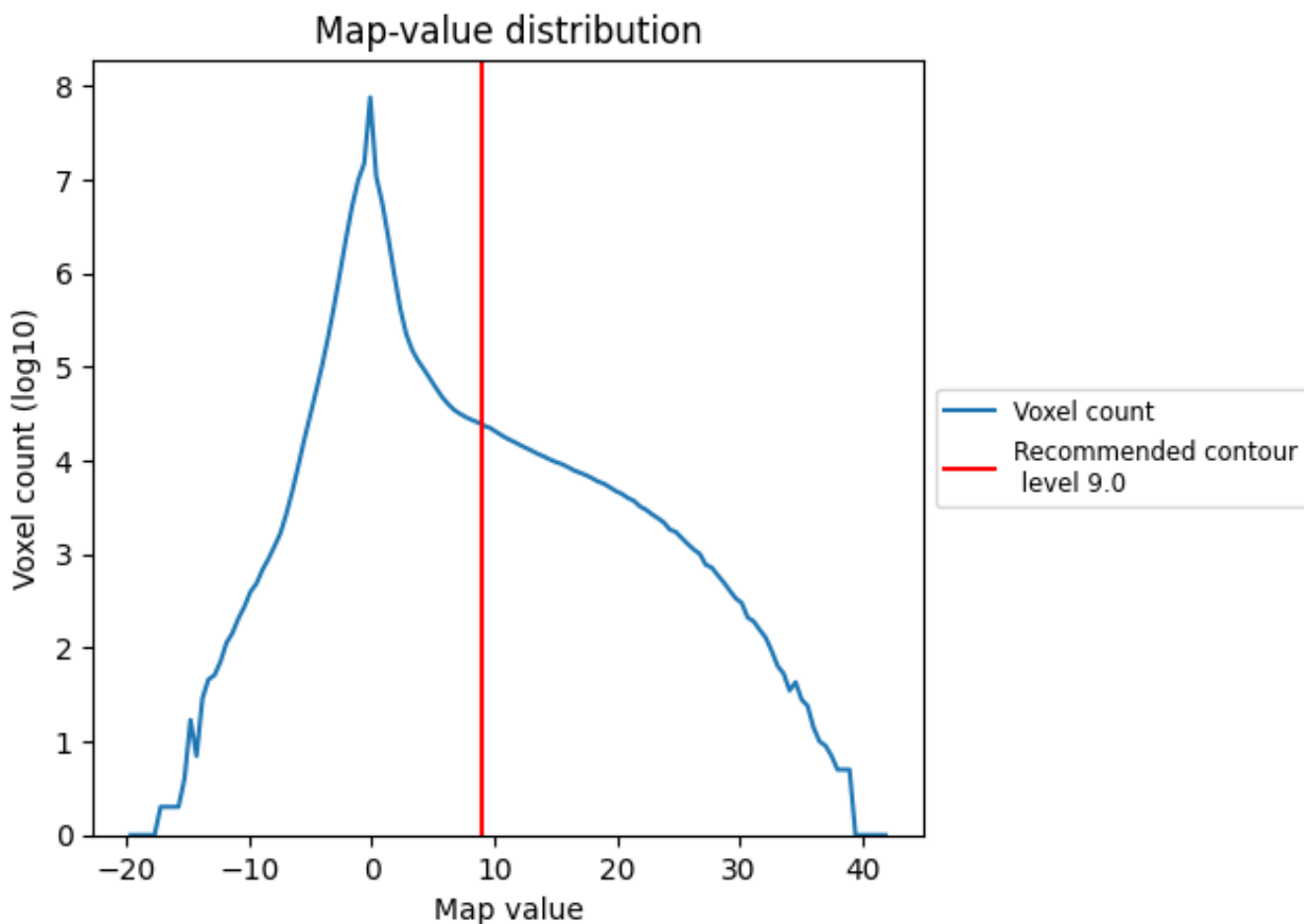
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

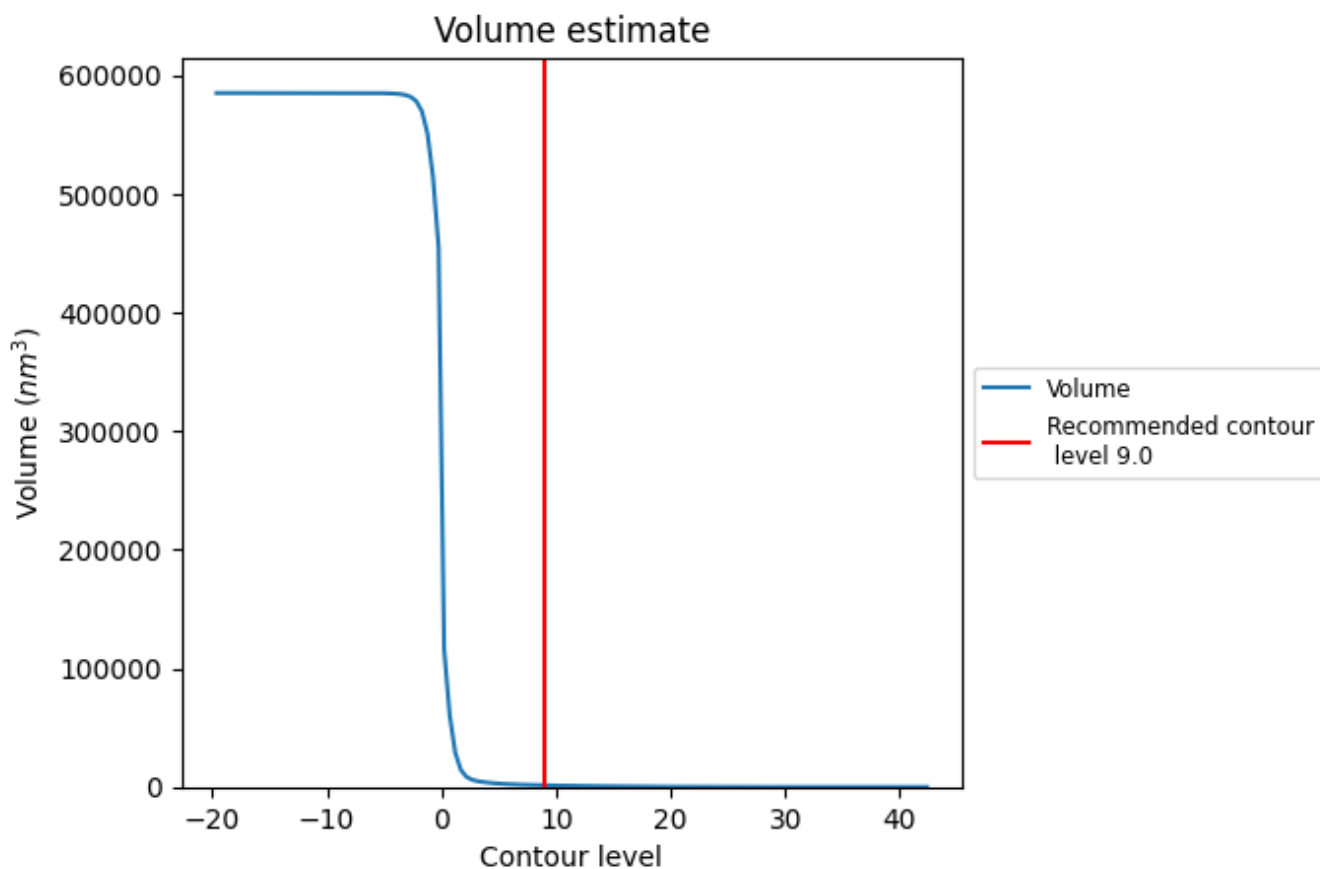
This section contains the results of statistical analysis of the map.

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.

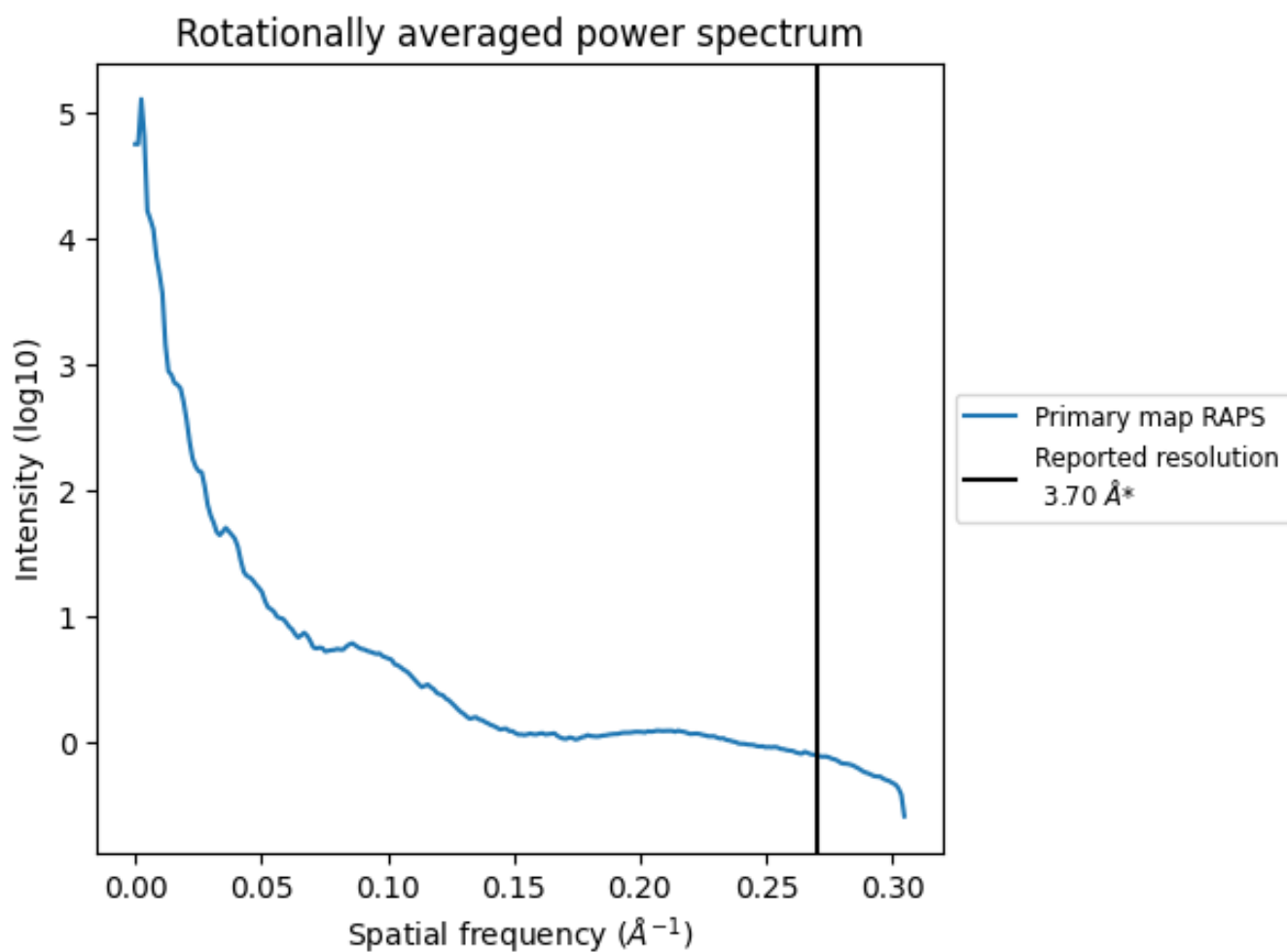
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1402 nm³; this corresponds to an approximate mass of 1266 kDa.

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

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

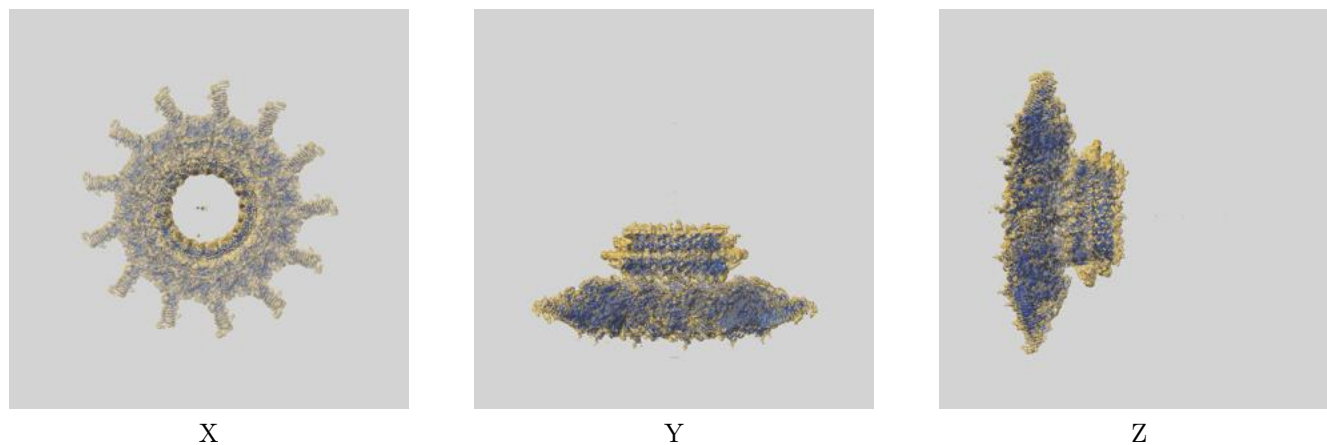
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

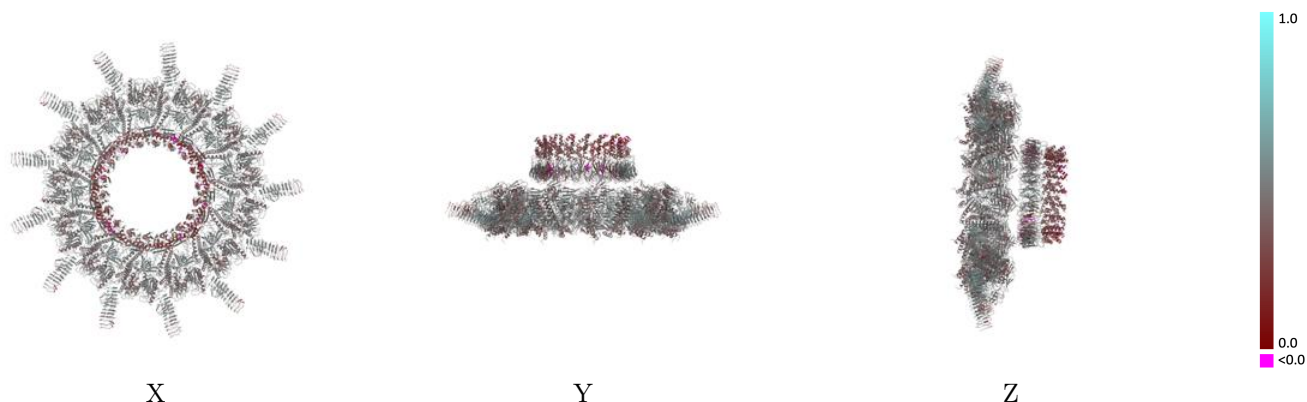
This section contains information regarding the fit between EMDB map EMD-22070 and PDB model 6X65. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



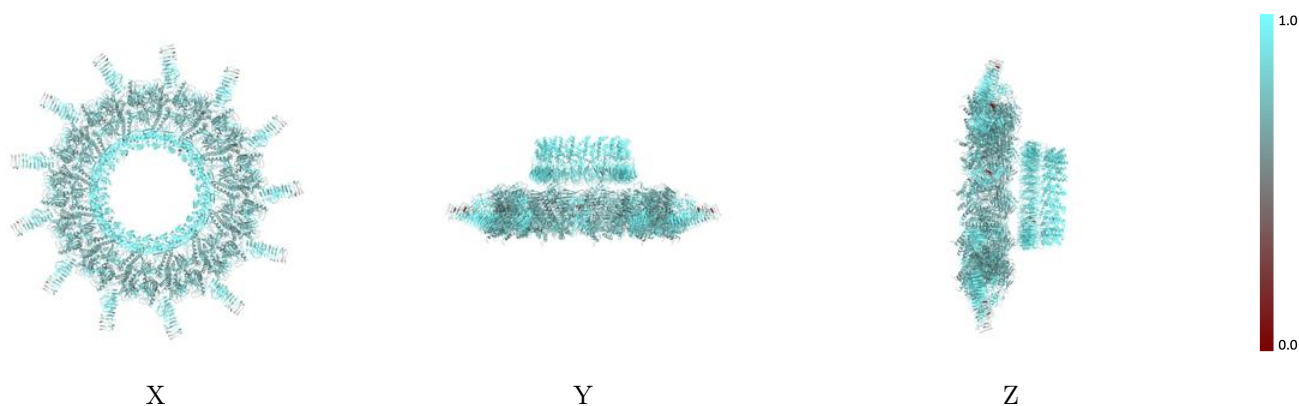
The images above show the 3D surface view of the map at the recommended contour level 9.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



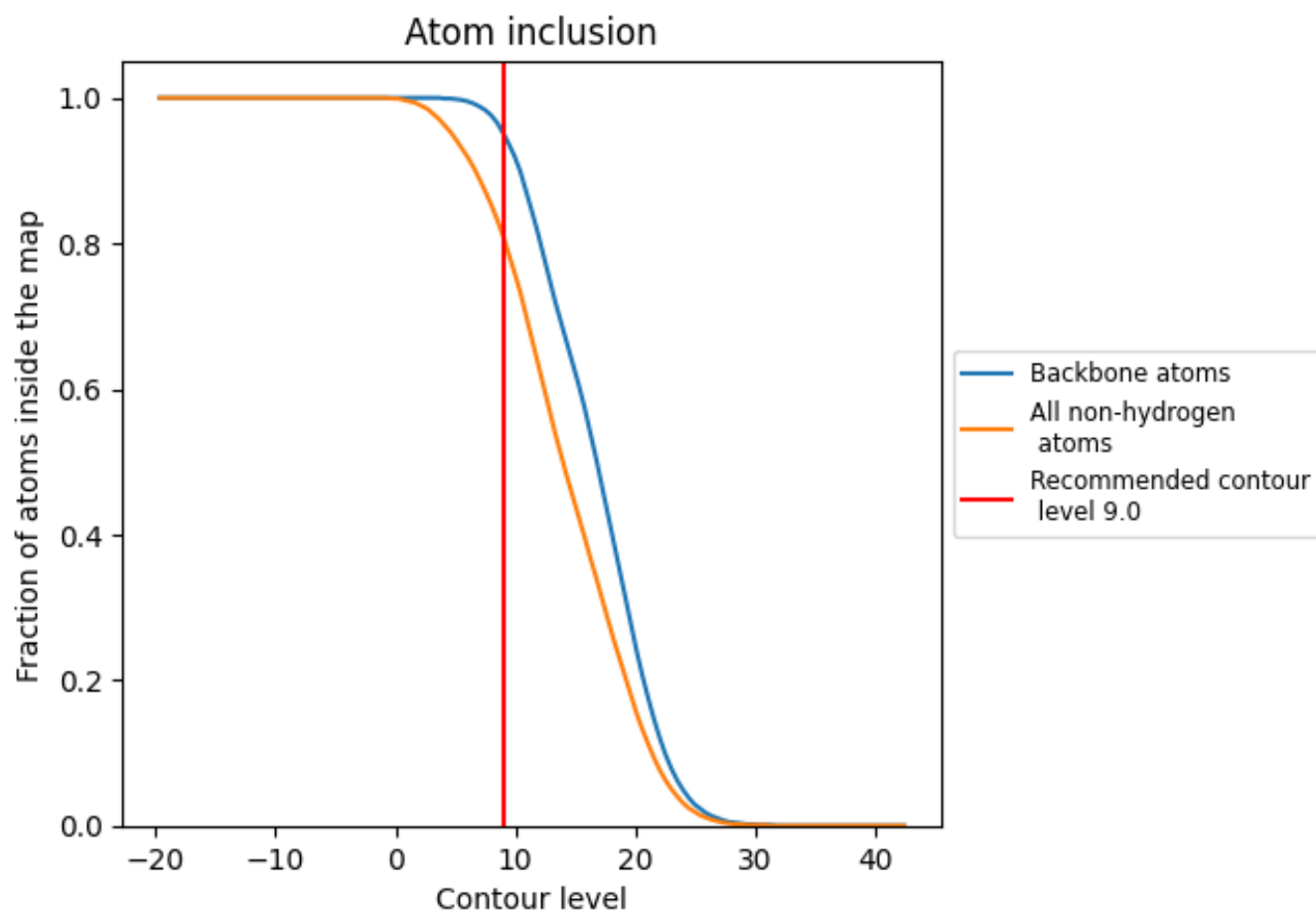
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (9.0).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 81% 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 (9.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.4470
AC	0.7620	0.4530
AD	0.7180	0.4220
AH	0.8070	0.5070
AK	0.7700	0.4580
AV	0.9760	0.3580
AW	0.9810	0.3400
AX	0.8610	0.4630
AY	0.8460	0.4500
AZ	0.8860	0.5180
Ad	0.7510	0.4540
BC	0.7660	0.4570
BD	0.7250	0.4290
BH	0.8150	0.5090
BK	0.7620	0.4450
BV	0.9610	0.2800
BW	0.9630	0.3040
BX	0.8580	0.4760
BY	0.8420	0.4470
BZ	0.8970	0.5160
Bd	0.7500	0.4560
CC	0.7700	0.4530
CD	0.7230	0.4170
CH	0.7950	0.5060
CK	0.7660	0.4510
CV	0.9810	0.3860
CW	0.9750	0.3280
CX	0.8590	0.4620
CY	0.8580	0.4410
CZ	0.8910	0.5130
Cd	0.7430	0.4470
DC	0.7690	0.4560
DD	0.7290	0.4350
DH	0.8070	0.5020
DK	0.7620	0.4540























































































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Chain	Atom inclusion	Q-score
DV	 0.9820	 0.3910
DW	 0.9380	 0.3030
DX	 0.8540	 0.4700
DY	 0.8500	 0.4410
DZ	 0.9030	 0.5150
Dd	 0.7640	 0.4570
EC	 0.7670	 0.4590
ED	 0.7260	 0.4310
EH	 0.7970	 0.4990
EK	 0.7700	 0.4520
EV	 0.9390	 0.2740
EW	 0.9690	 0.3310
EX	 0.8590	 0.4730
EY	 0.8500	 0.4540
EZ	 0.9090	 0.5190
Ed	 0.7430	 0.4570
FC	 0.7760	 0.4610
FD	 0.7150	 0.4230
FH	 0.7980	 0.5080
FK	 0.7700	 0.4530
FV	 0.9360	 0.2930
FW	 0.8750	 0.2360
FX	 0.8500	 0.4730
FY	 0.8350	 0.4580
FZ	 0.9060	 0.5080
Fd	 0.7460	 0.4580
GC	 0.7720	 0.4620
GD	 0.7200	 0.4230
GH	 0.7980	 0.5090
GK	 0.7740	 0.4550
GV	 0.9960	 0.4300
GW	 0.9560	 0.2900
GX	 0.8500	 0.4690
GY	 0.8460	 0.4480
GZ	 0.8860	 0.5140
Gd	 0.7550	 0.4670
HC	 0.7700	 0.4600
HD	 0.7350	 0.4330
HH	 0.8040	 0.5030
HK	 0.7660	 0.4490
HV	 0.9960	 0.4550
HW	 0.9440	 0.3390







































































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Chain	Atom inclusion	Q-score
HX	 0.8570	 0.4730
HY	 0.8540	 0.4360
HZ	 0.8890	 0.5010
Hd	 0.7470	 0.4510
IC	 0.7680	 0.4600
ID	 0.7170	 0.4300
IH	 0.7950	 0.4980
IK	 0.7720	 0.4530
IV	 0.9860	 0.4410
IW	 0.9940	 0.3720
IX	 0.8580	 0.4700
IY	 0.8540	 0.4480
IZ	 0.8860	 0.5150
Id	 0.7450	 0.4550
JC	 0.7660	 0.4510
JD	 0.7270	 0.4290
JH	 0.8010	 0.5050
JK	 0.7570	 0.4510
JV	 0.9460	 0.2930
JW	 0.9750	 0.3670
JX	 0.8490	 0.4680
JY	 0.8390	 0.4440
JZ	 0.8910	 0.5080
Jd	 0.7560	 0.4580
KC	 0.7680	 0.4570
KD	 0.7250	 0.4320
KH	 0.7980	 0.5070
KK	 0.7640	 0.4470
KV	 0.9690	 0.3160
KW	 0.9500	 0.3300
KX	 0.8580	 0.4710
KY	 0.8310	 0.4380
KZ	 0.9030	 0.5180
Kd	 0.7460	 0.4560
LC	 0.7750	 0.4550
LD	 0.7210	 0.4250
LH	 0.8060	 0.5050
LK	 0.7590	 0.4500
LV	 0.9940	 0.3760
LW	 0.9690	 0.3240
LX	 0.8610	 0.4700
LY	 0.8460	 0.4470

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Chain	Atom inclusion	Q-score
LZ	 0.8890	 0.5160
Ld	 0.7420	 0.4470
MC	 0.7610	 0.4620
MD	 0.7200	 0.4260
MH	 0.8150	 0.5050
MK	 0.7590	 0.4450
MV	 0.9960	 0.4090
MW	 0.9690	 0.3240
MX	 0.8550	 0.4660
MY	 0.8690	 0.4590
MZ	 0.8970	 0.5130
Md	 0.7490	 0.4500
N	 0.7830	 0.4560
NV	 0.9890	 0.3740
NW	 0.9500	 0.2530
O	 0.7820	 0.4500
OV	 0.9360	 0.3130
OW	 0.8870	 0.2990
P	 0.7900	 0.4660
PV	 0.9930	 0.4050
PW	 0.9560	 0.3400
Q	 0.7850	 0.4570
QV	 0.9970	 0.4140
QW	 0.9940	 0.3590
R	 0.7810	 0.4480
RV	 0.9960	 0.4260
RW	 0.9880	 0.3870
S	 0.7710	 0.4430
T	 0.7790	 0.4540
U	 0.7700	 0.4440
V	 0.7710	 0.4440
W	 0.7870	 0.4550
X	 0.7810	 0.4560
Y	 0.7880	 0.4600
Z	 0.7740	 0.4420