



## Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 07:06 PM EST

PDB ID : 6X66  
EMDB ID : EMD-22071  
Title : Legionella pneumophila dDot T4SS OMC  
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 : 4.20 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](mailto: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>.

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

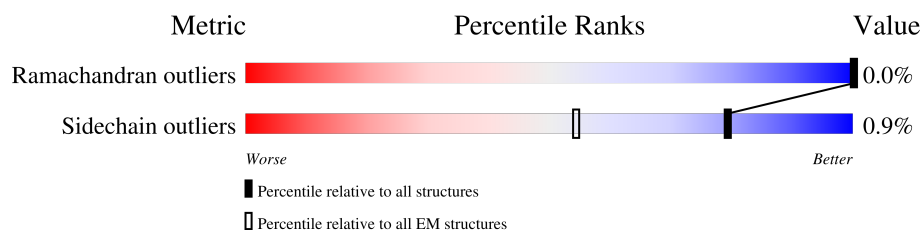
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP)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

# 1 Overall quality at a glance

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



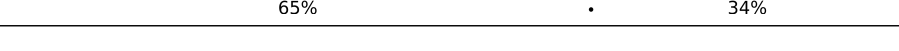



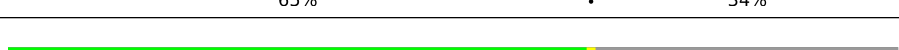


The reported resolution of this entry is 4.20 Å.

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.













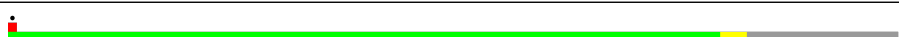


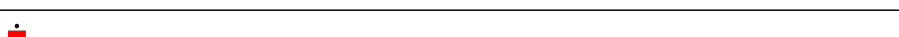
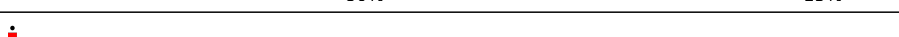
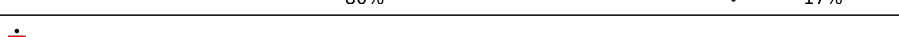



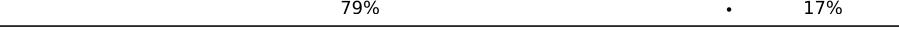





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	AC	303	 65%                      34%
1	BC	303	 65%                      34%
1	CC	303	 65%                      34%
1	DC	303	 65%                      34%
1	EC	303	 65%                      34%
1	FC	303	 65%                      34%
1	GC	303	 65%                      34%
1	HC	303	 65%                      34%
1	IC	303	 65%                      34%






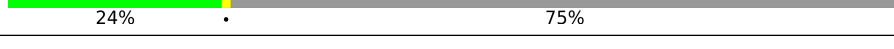

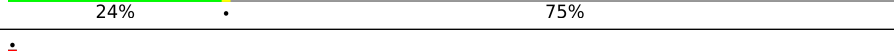
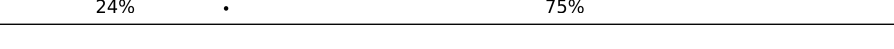
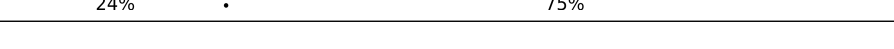










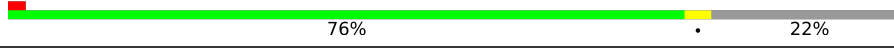
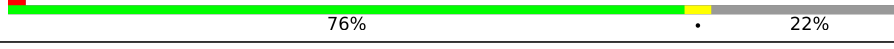



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Mol	Chain	Length	Quality of chain
1	JC	303	
1	KC	303	
1	LC	303	
1	MC	303	
2	AD	163	
2	Ad	163	
2	BD	163	
2	Bd	163	
2	CD	163	
2	Cd	163	
2	DD	163	
2	Dd	163	
2	ED	163	
2	Ed	163	
2	FD	163	
2	Fd	163	
2	GD	163	
2	Gd	163	
2	HD	163	
2	Hd	163	
2	ID	163	
2	Id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


























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Mol	Chain	Length	Quality of chain
2	Kd	163	
2	LD	163	
2	Ld	163	
2	MD	163	
2	Md	163	
3	AH	361	
3	BH	361	
3	CH	361	
3	DH	361	
3	EH	361	
3	FH	361	
3	GH	361	
3	HH	361	
3	IH	361	
3	JH	361	
3	KH	361	
3	LH	361	
3	MH	361	
4	AK	189	
4	BK	189	
4	CK	189	
4	DK	189	
4	EK	189	
4	FK	189	
4	GK	189	




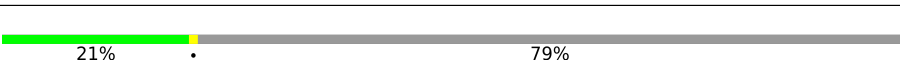


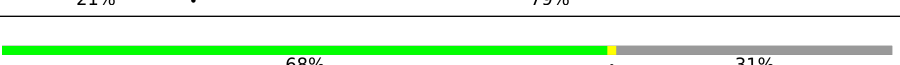



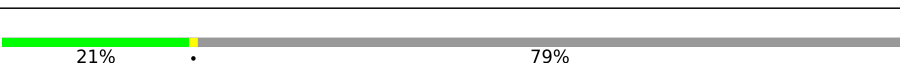


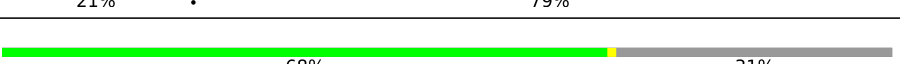



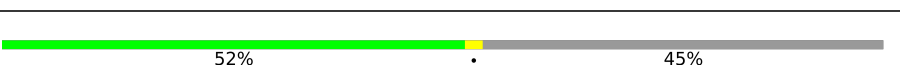
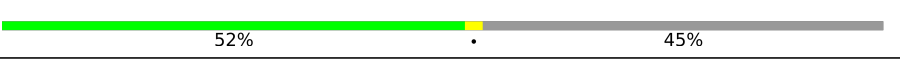
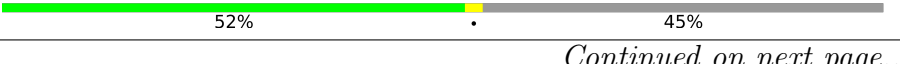



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Mol	Chain	Length	Quality of chain
4	HK	189	
4	IK	189	
4	JK	189	
4	KK	189	
4	LK	189	
4	MK	189	
5	AX	330	
5	AY	330	
5	AZ	330	
5	BX	330	
5	BY	330	
5	BZ	330	
5	CX	330	
5	CY	330	
5	CZ	330	
5	DX	330	
5	DY	330	
5	DZ	330	
5	EX	330	
5	EY	330	
5	EZ	330	
5	FX	330	
5	FY	330	
5	FZ	330	
5	GX	330	









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Mol	Chain	Length	Quality of chain
5	GY	330	
5	GZ	330	
5	HX	330	
5	HY	330	
5	HZ	330	
5	IX	330	
5	IY	330	
5	IZ	330	
5	JX	330	
5	JY	330	
5	JZ	330	
5	KX	330	
5	KY	330	
5	KZ	330	
5	LX	330	
5	LY	330	
5	LZ	330	
5	MX	330	
5	MY	330	
5	MZ	330	
6	AA	249	
6	BA	249	
6	CA	249	
6	DA	249	
6	EA	249	

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Mol	Chain	Length	Quality of chain
6	FA	249	 52% . 45%
6	GA	249	 52% . 45%
6	HA	249	 52% . 45%
6	IA	249	 52% . 45%
6	JA	249	 52% . 45%
6	KA	249	 52% . 45%
6	LA	249	 52% . 45%
6	QA	249	 52% . 45%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 109070 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 DotC.

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

- Molecule 2 is a protein called DotD.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Ad	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Bd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	CD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Cd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	DD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Dd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	ED	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Ed	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	FD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Fd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	GD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Gd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	HD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Hd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	ID	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Id	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	JD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Jd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	KD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Kd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	LD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ld	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	MD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Md	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		

- Molecule 3 is a protein called Type IV secretion protein IcmK.

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

- Molecule 4 is a protein called Inner membrane lipoprotein YiaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	BK	148	Total 1152	C 731	N 205	O 212	S 4	0 0
4	CK	148	Total 1152	C 731	N 205	O 212	S 4	0 0
4	DK	148	Total 1152	C 731	N 205	O 212	S 4	0 0
4	EK	148	Total 1152	C 731	N 205	O 212	S 4	0 0
4	FK	148	Total 1152	C 731	N 205	O 212	S 4	0 0
4	GK	148	Total 1152	C 731	N 205	O 212	S 4	0 0
4	HK	148	Total 1152	C 731	N 205	O 212	S 4	0 0
4	IK	148	Total 1152	C 731	N 205	O 212	S 4	0 0
4	JK	148	Total 1152	C 731	N 205	O 212	S 4	0 0
4	KK	148	Total 1152	C 731	N 205	O 212	S 4	0 0
4	LK	148	Total 1152	C 731	N 205	O 212	S 4	0 0
4	MK	148	Total 1152	C 731	N 205	O 212	S 4	0 0

- Molecule 5 is a protein called Type IV secretion system unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AX	228	Total 1140	C 684	N 228	O 228	0	0
5	AY	52	Total 260	C 156	N 52	O 52	0	0
5	AZ	70	Total 350	C 210	N 70	O 70	0	0
5	BX	228	Total 1140	C 684	N 228	O 228	0	0
5	BY	52	Total 260	C 156	N 52	O 52	0	0
5	BZ	70	Total 350	C 210	N 70	O 70	0	0
5	CX	228	Total 1140	C 684	N 228	O 228	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	CY	52	Total	C	N	O	0	0
			260	156	52	52		
5	CZ	70	Total	C	N	O	0	0
			350	210	70	70		
5	DX	228	Total	C	N	O	0	0
			1140	684	228	228		
5	DY	52	Total	C	N	O	0	0
			260	156	52	52		
5	DZ	70	Total	C	N	O	0	0
			350	210	70	70		
5	EX	228	Total	C	N	O	0	0
			1140	684	228	228		
5	EY	52	Total	C	N	O	0	0
			260	156	52	52		
5	EZ	70	Total	C	N	O	0	0
			350	210	70	70		
5	FX	228	Total	C	N	O	0	0
			1140	684	228	228		
5	FY	52	Total	C	N	O	0	0
			260	156	52	52		
5	FZ	70	Total	C	N	O	0	0
			350	210	70	70		
5	GX	228	Total	C	N	O	0	0
			1140	684	228	228		
5	GY	52	Total	C	N	O	0	0
			260	156	52	52		
5	GZ	70	Total	C	N	O	0	0
			350	210	70	70		
5	HX	228	Total	C	N	O	0	0
			1140	684	228	228		
5	HY	52	Total	C	N	O	0	0
			260	156	52	52		
5	HZ	70	Total	C	N	O	0	0
			350	210	70	70		
5	IX	228	Total	C	N	O	0	0
			1140	684	228	228		
5	IY	52	Total	C	N	O	0	0
			260	156	52	52		
5	IZ	70	Total	C	N	O	0	0
			350	210	70	70		
5	JX	228	Total	C	N	O	0	0
			1140	684	228	228		

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

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

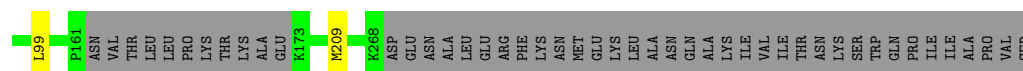
Mol	Chain	Residues	Atoms					AltConf	Trace
6	AA	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	BA	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	CA	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	DA	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	EA	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	FA	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	GA	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	HA	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		

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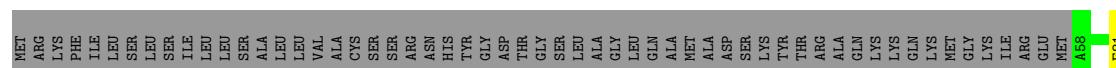
Mol	Chain	Residues	Atoms					AltConf	Trace
6	IA	136	Total 1108	C 701	N 201	O 202	S 4	0	0
6	JA	136	Total 1108	C 701	N 201	O 202	S 4	0	0
6	KA	136	Total 1108	C 701	N 201	O 202	S 4	0	0
6	LA	136	Total 1108	C 701	N 201	O 202	S 4	0	0
6	QA	136	Total 1108	C 701	N 201	O 202	S 4	0	0





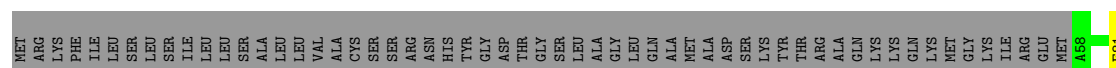
- Molecule 1: DotC

Chain EC:   
65% 34%



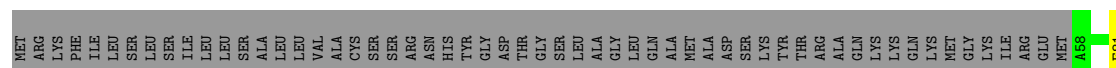
- Molecule 1: DotC

Chain FC:   
65% 34%



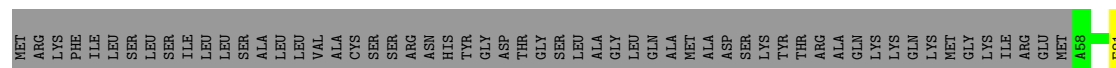
- Molecule 1: DotC

Chain GC:   
65% 34%



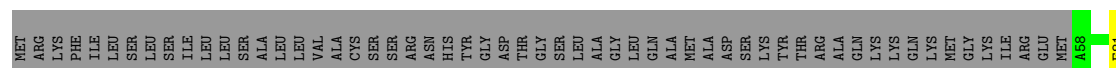
- Molecule 1: DotC

Chain HC:   
65% 34%

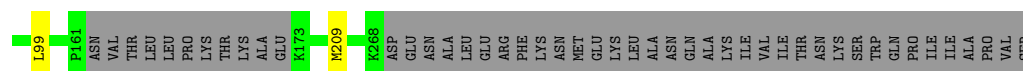


- Molecule 1: DotC

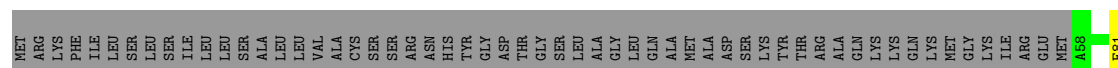
Chain IC:   
65% 34%



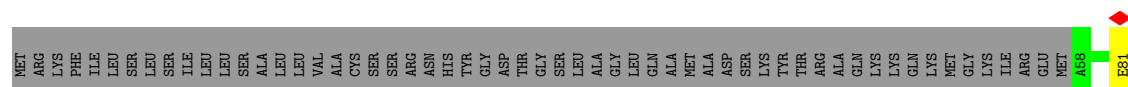




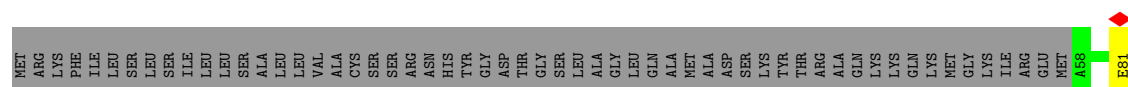
- Molecule 1: DotC



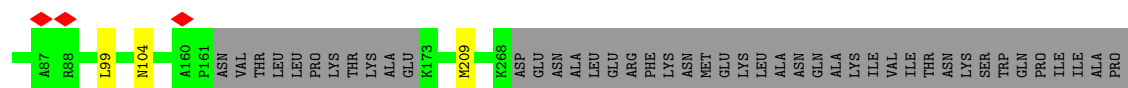
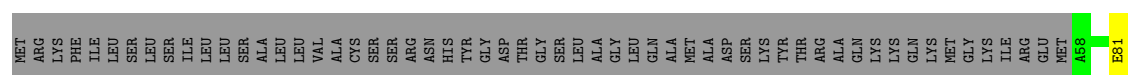
- Molecule 1: DotC




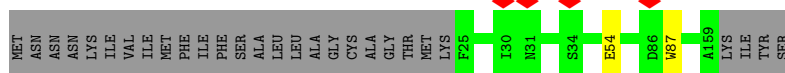
- Molecule 1: DotC




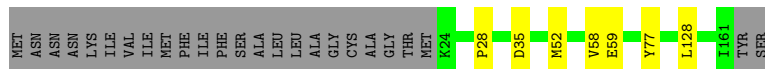
- Molecule 1: DotC




## • Molecule 2: DotD

Chain AD:  82% 17%


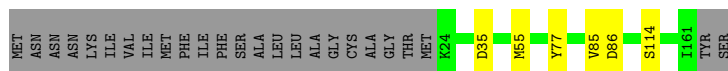
## • Molecule 2: DotD

Chain Ad:  80% 15%


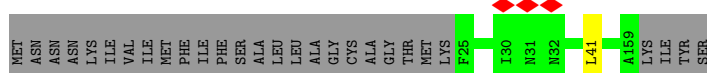
## • Molecule 2: DotD

Chain BD:  78% 5% 17%


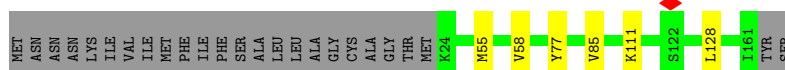
## • Molecule 2: DotD

Chain Bd:  81% 15%


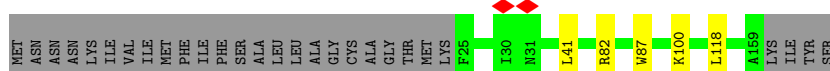
## • Molecule 2: DotD

Chain CD:  82% 17%


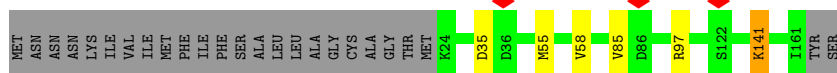
## • Molecule 2: DotD

Chain Cd:  81% 15%


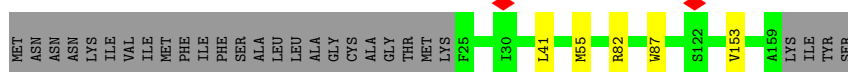
## • Molecule 2: DotD

Chain DD:  80% 17%


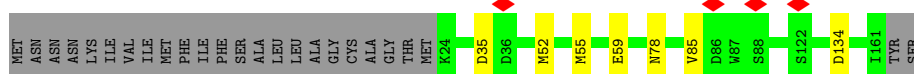
## ● Molecule 2: DotD

Chain Dd:  81% 15%


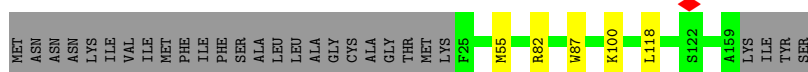
## ● Molecule 2: DotD

Chain ED:  80% 17%


## ● Molecule 2: DotD

Chain Ed:  80% 15%


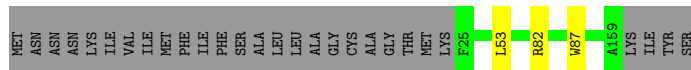
## ● Molecule 2: DotD

Chain FD:  80% 17%


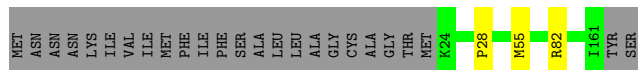
## ● Molecule 2: DotD

Chain Fd:  81% 15%


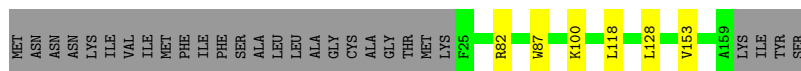
## ● Molecule 2: DotD

Chain GD:  81% 17%


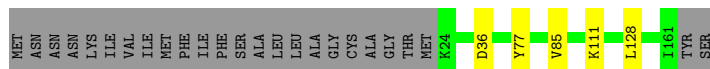
## ● Molecule 2: DotD

Chain Gd:  83% 15%


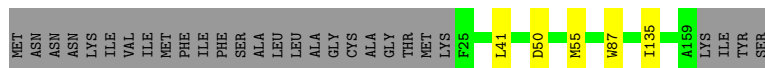
## ● Molecule 2: DotD

Chain HD:  79% 17%


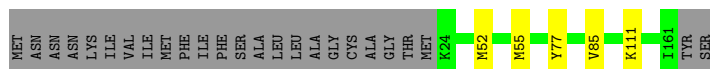
## ● Molecule 2: DotD

Chain Hd:  82% 15%


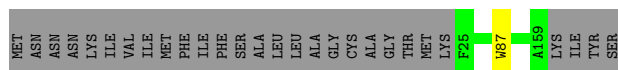
## ● Molecule 2: DotD

Chain ID:  80% 17%


## ● Molecule 2: DotD

Chain Id:  82% 15%


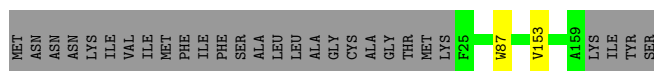
## ● Molecule 2: DotD

Chain JD:  82% 17%

## ● Molecule 2: DotD

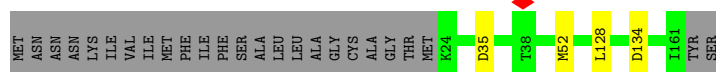
Chain Jd:  79% 15%

## ● Molecule 2: DotD


Chain KD:  82% 17%

## ● Molecule 2: DotD

Chain Kd:  82% 15%



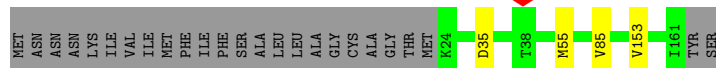
- Molecule 2: DotD

Chain LD: 

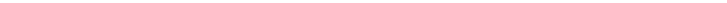


- Molecule 2: DotD

Chain Ld: 82% 15%




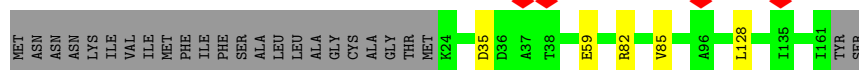
- Molecule 2: DotD

Chain MD:  80% 17%



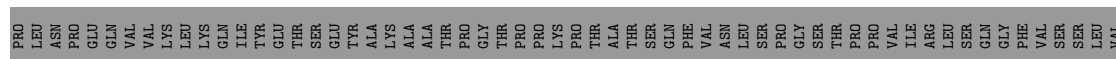
- Molecule 2: DotD

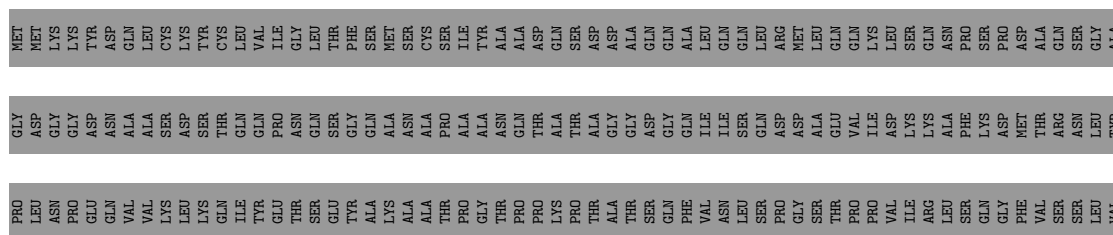
Chain Md:  82% 15%



- Molecule 3: Type IV secretion protein IcmK

Chain AH:  24% 75%

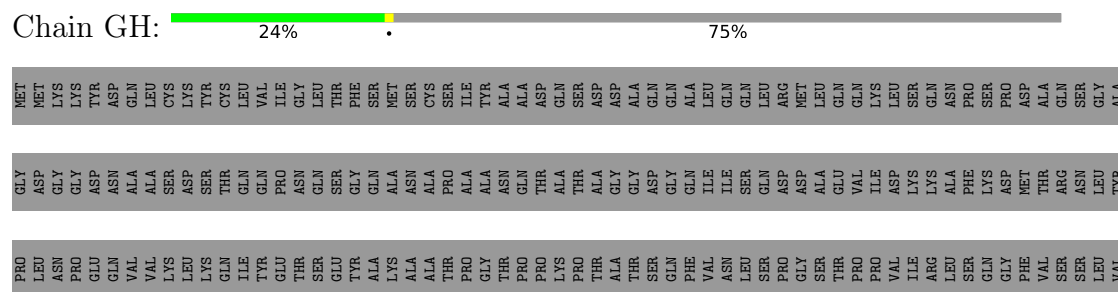




- Molecule 3: Type IV secretion protein IcmK

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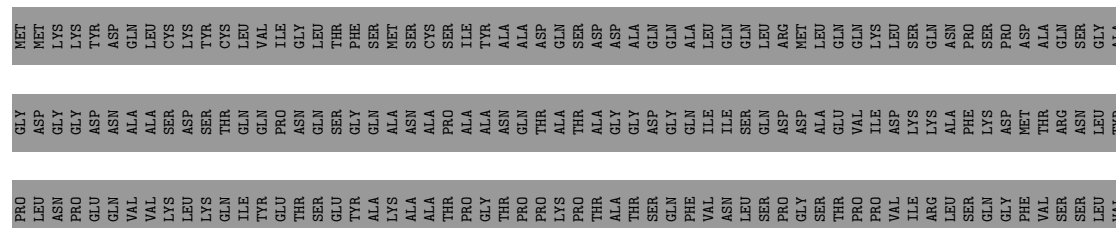
Chain HH:  24% . 75%

- Molecule 3: Type IV secretion protein IcmK

Chain IH:  24% . 75%

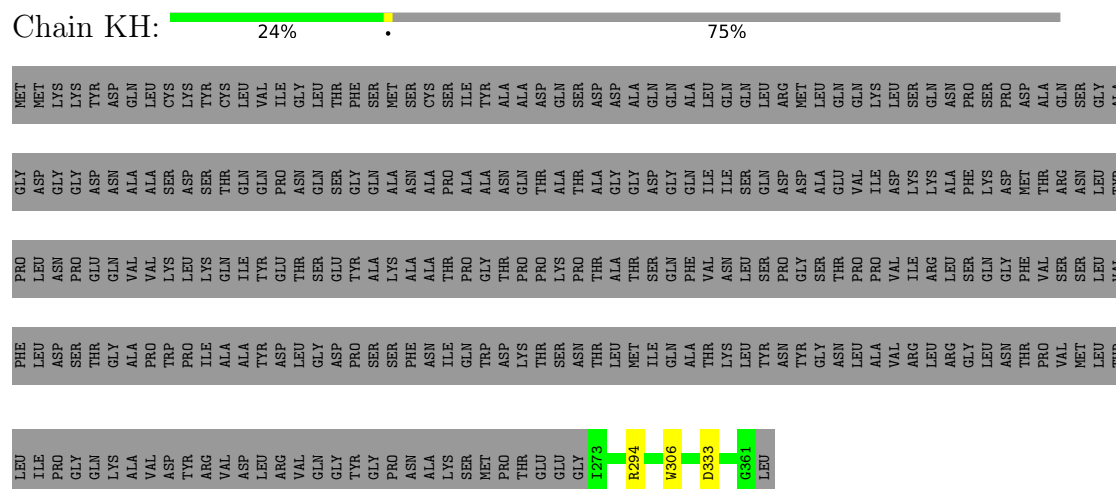
- Molecule 3: Type IV secretion protein IcmK

Chain JH:  24% . 75%

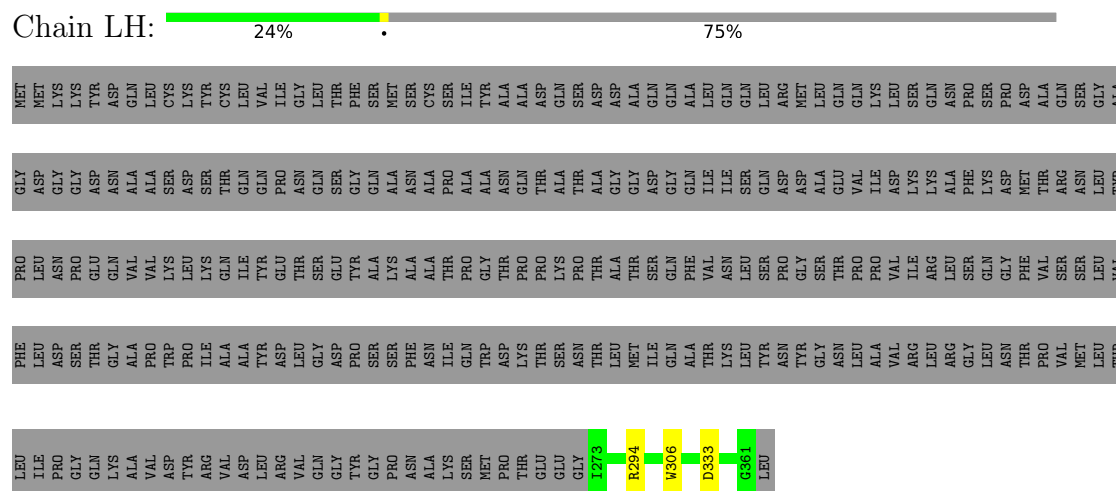




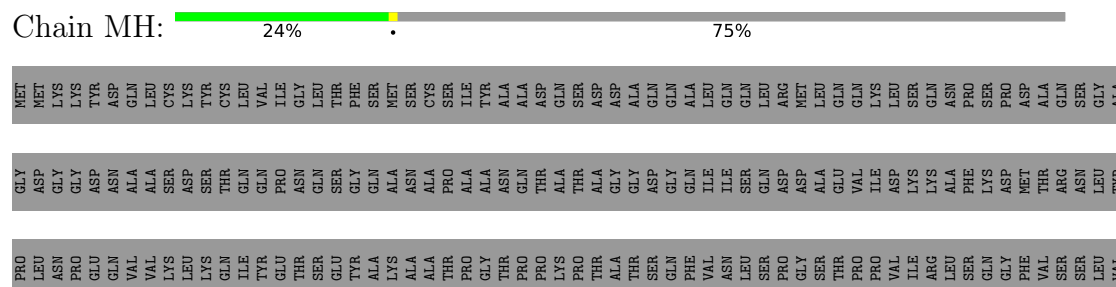
- Molecule 3: Type IV secretion protein IcmK

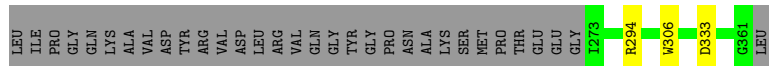



- Molecule 3: Type IV secretion protein IcmK

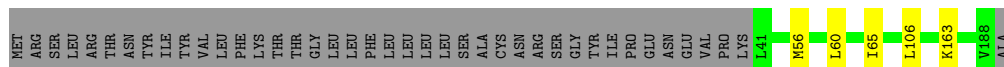


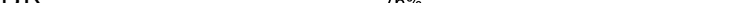
- Molecule 3: Type IV secretion protein IcmK

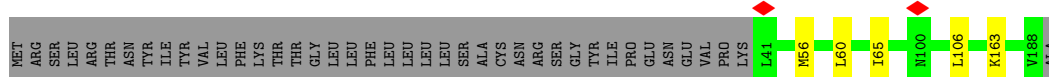


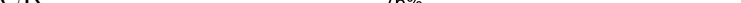


- Chain AK:  76% 22%



- Chain BK:  76% 2% 22%

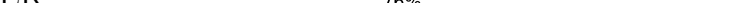


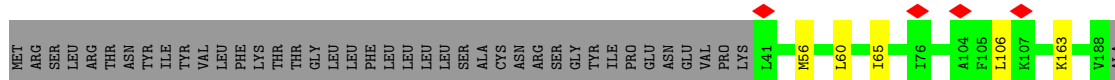
- Chain CK:  76% 22%

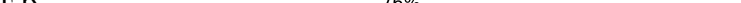


- Chain DK:  76% 2% 22%




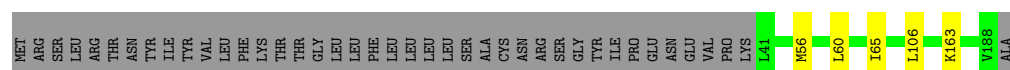
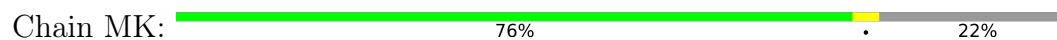
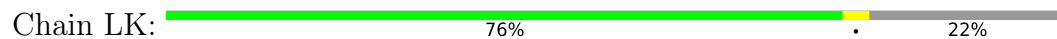
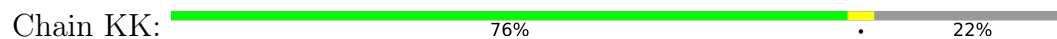
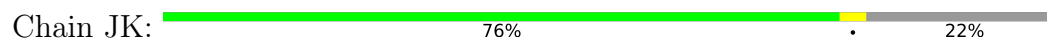
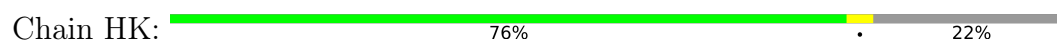
- Chain EK:  76% 22%



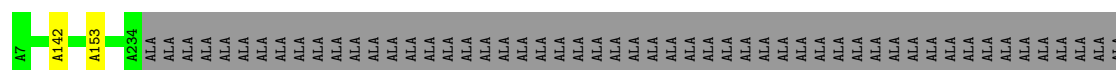
- Chain FK:  76% 2% 22%

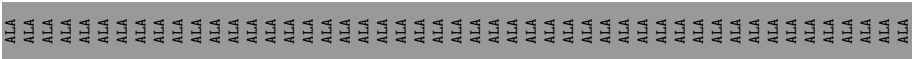


- Chain GK:  76% 22%

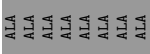
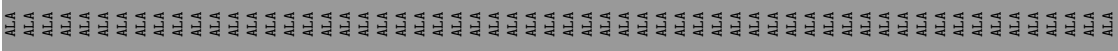
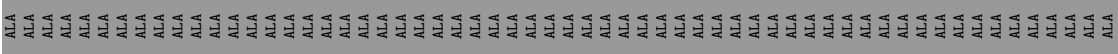
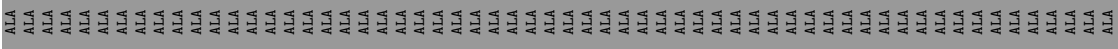
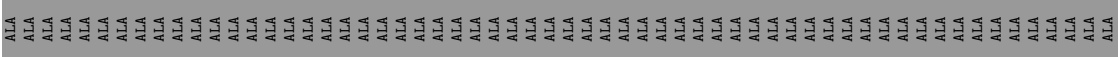
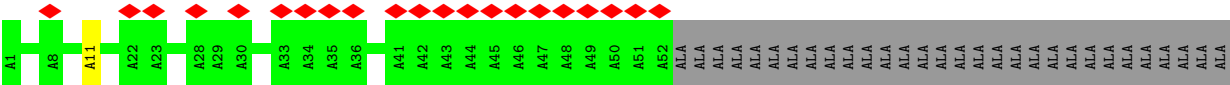


- Chain BX:  68% 31%

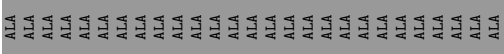
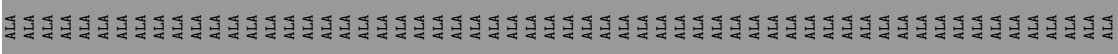
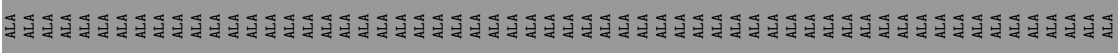
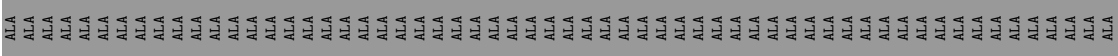




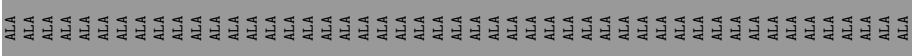
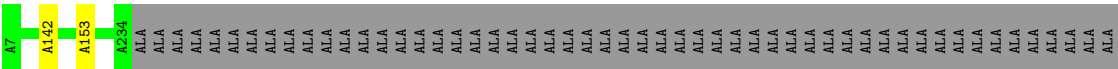
• Molecule 5: Type IV secretion system unknown protein fragment



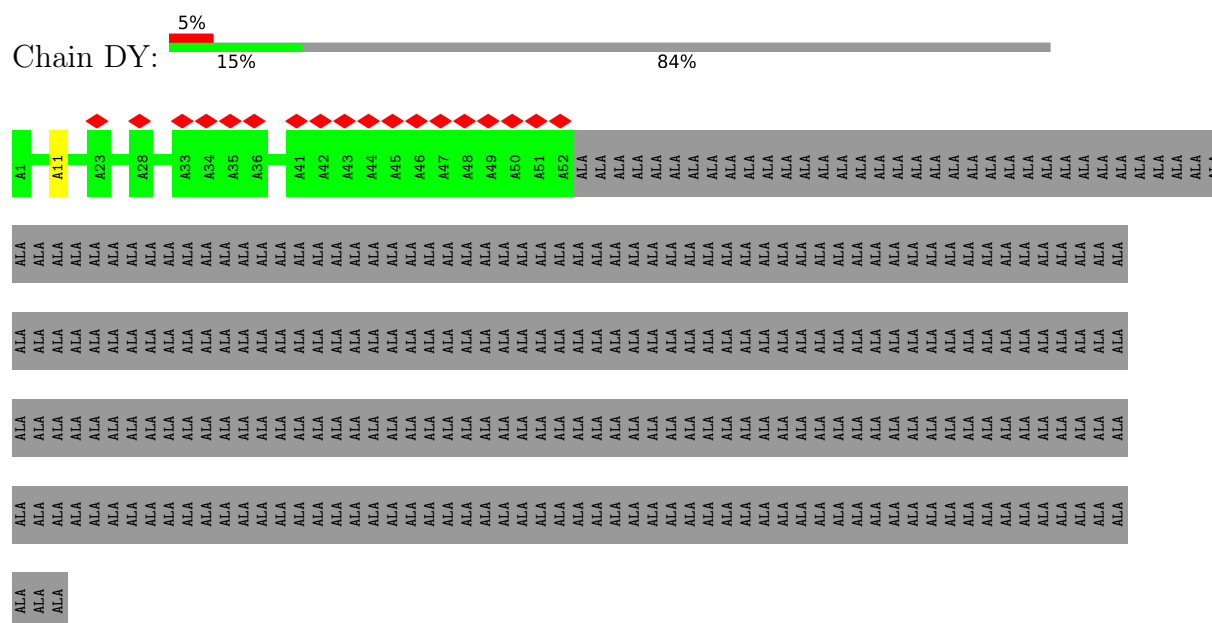
• Molecule 5: Type IV secretion system unknown protein fragment



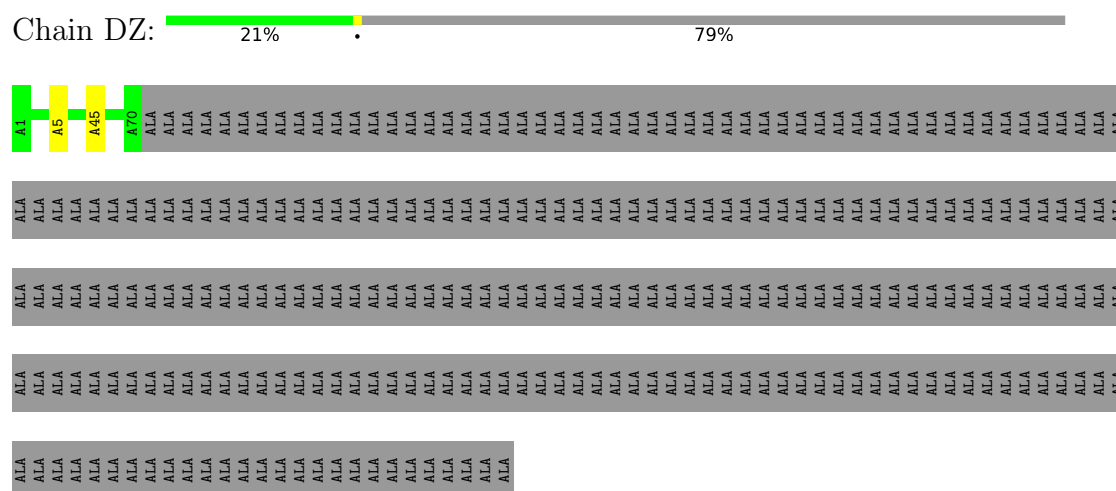
• Molecule 5: Type IV secretion system unknown protein fragment



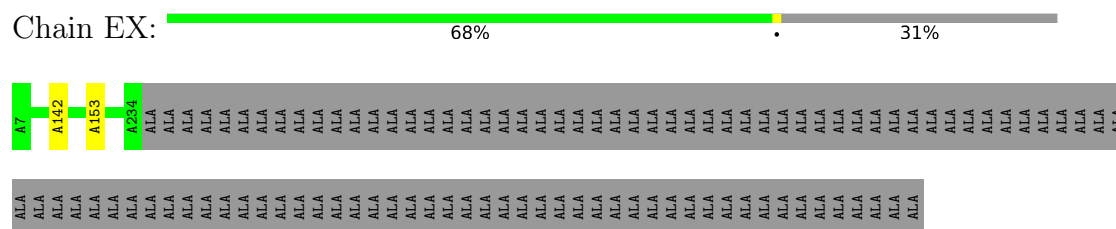
• Molecule 5: Type IV secretion system unknown protein fragment



- Molecule 5: Type IV secretion system unknown protein fragment

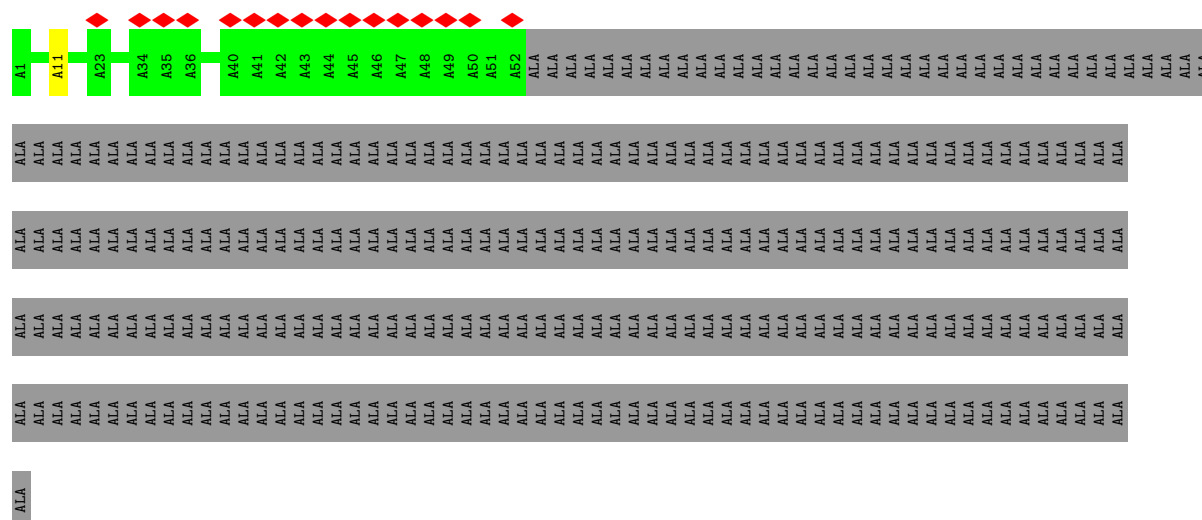


- Molecule 5: Type IV secretion system unknown protein fragment



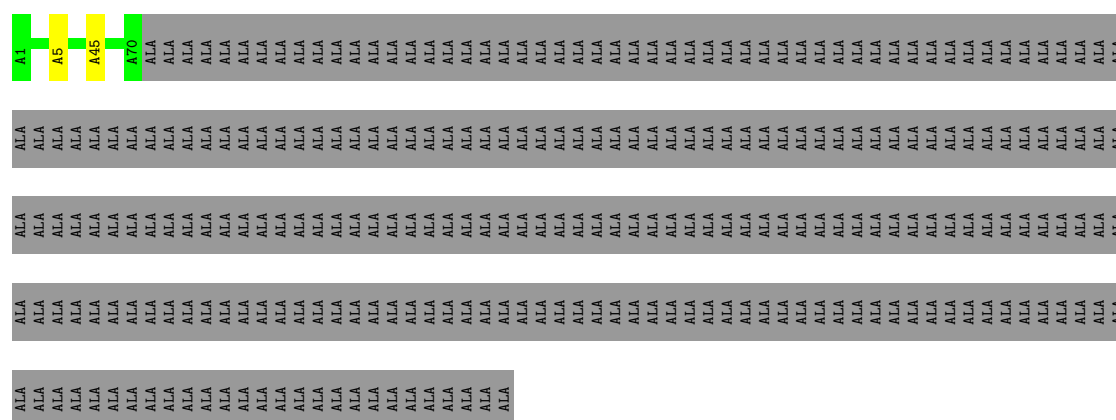
- Molecule 5: Type IV secretion system unknown protein fragment





- Molecule 5: Type IV secretion system unknown protein fragment

Chain EZ: 21% 79%



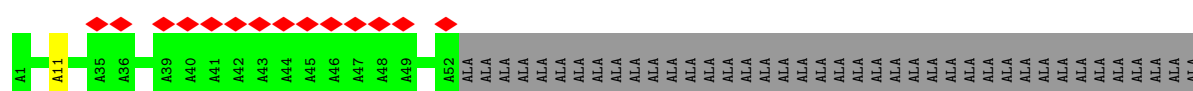
- Molecule 5: Type IV secretion system unknown protein fragment

Chain FX: 68% 31%

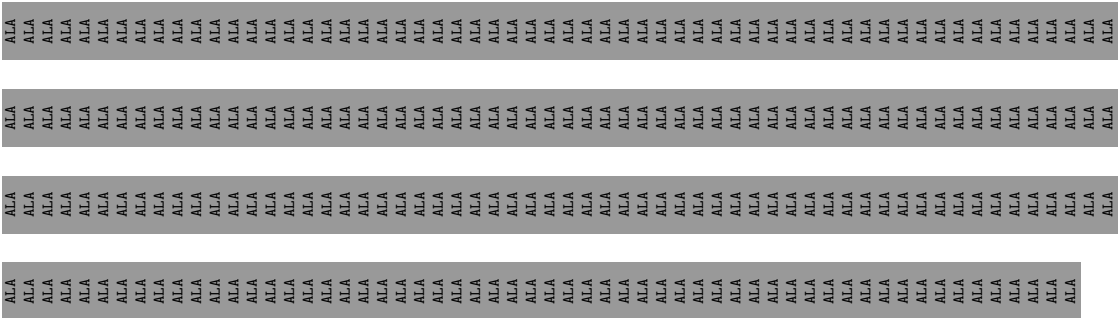


- Molecule 5: Type IV secretion system unknown protein fragment

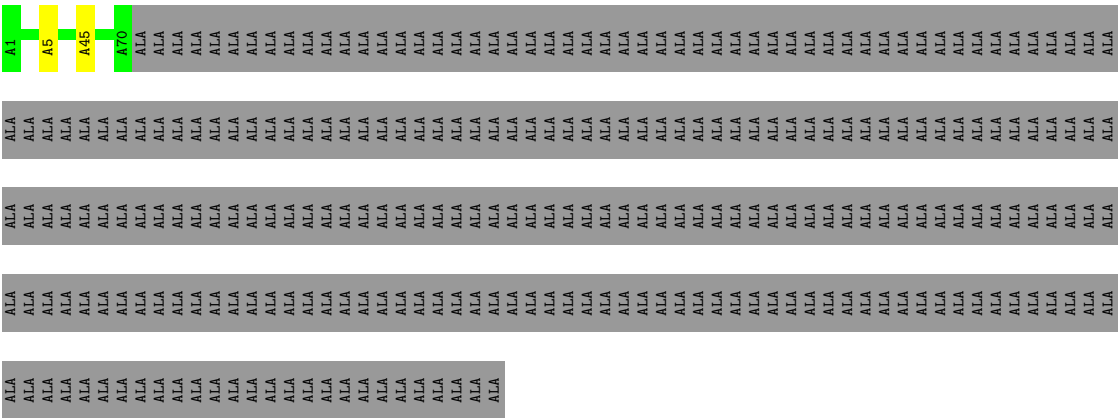
Chain FY: 15% 84%



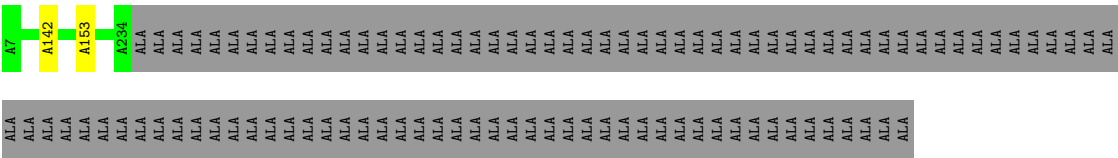




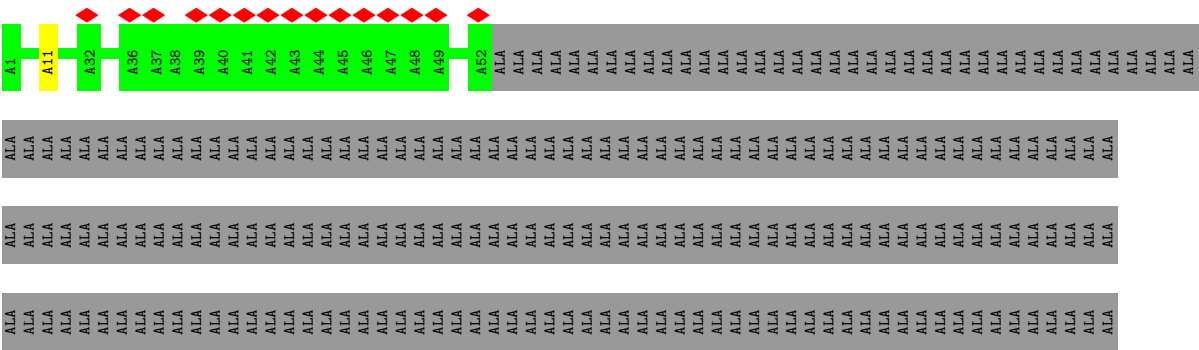
● Molecule 5: Type IV secretion system unknown protein fragment



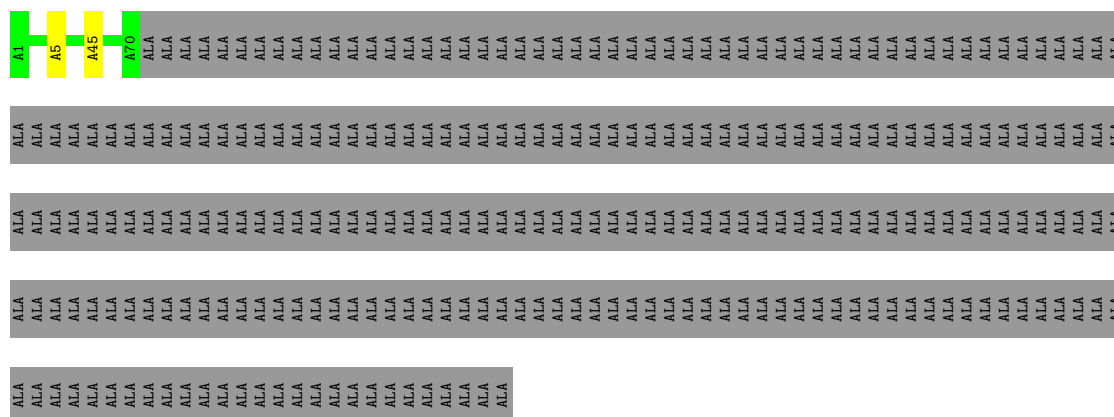
● Molecule 5: Type IV secretion system unknown protein fragment



● Molecule 5: Type IV secretion system unknown protein fragment

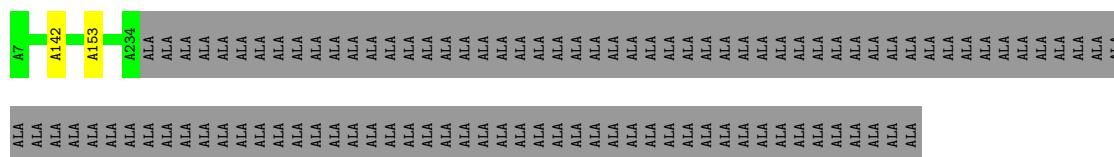


Chain HZ:  21% 79%



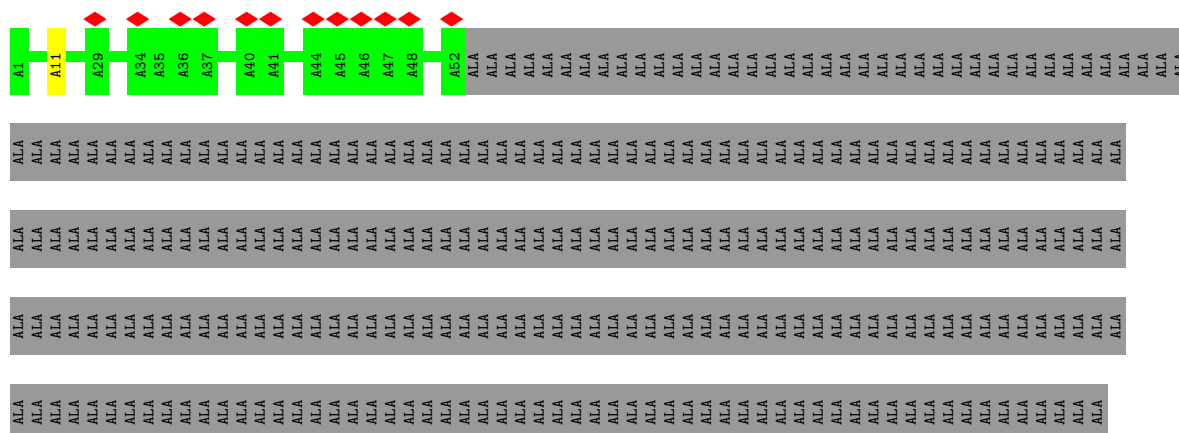
- Molecule 5: Type IV secretion system unknown protein fragment

Chain IX: 68% 31%



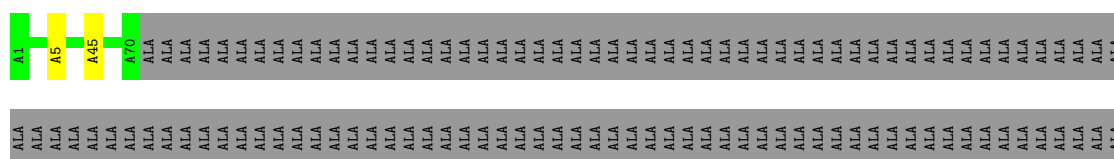
- Molecule 5: Type IV secretion system unknown protein fragment

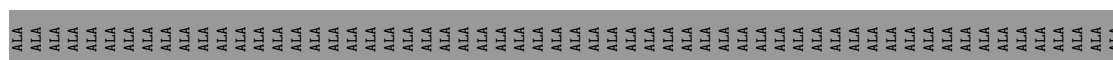
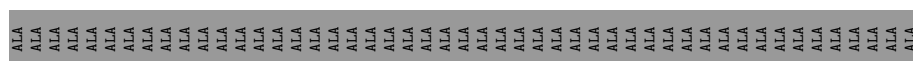
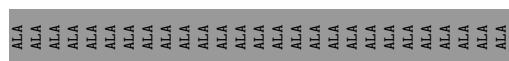
Chain IV: 15% 84%

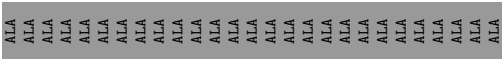


- Molecule 5: Type IV secretion system unknown protein fragment

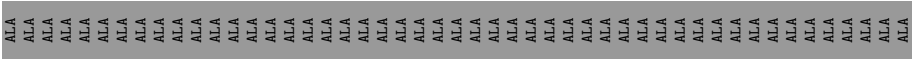
Chain IZ: 21% 79%



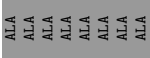
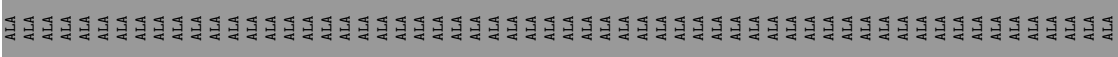
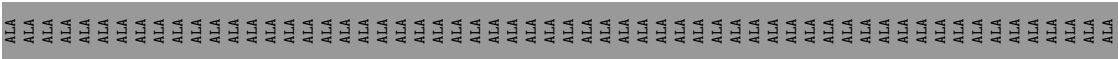
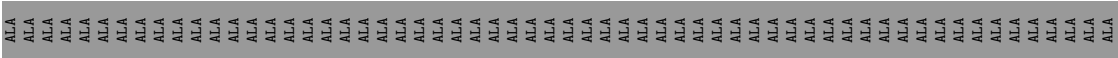
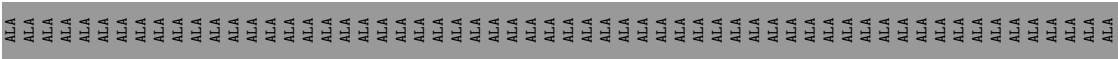
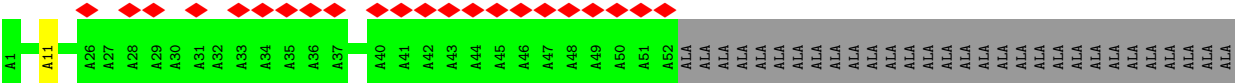




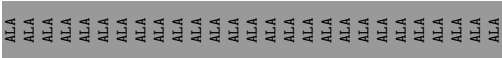
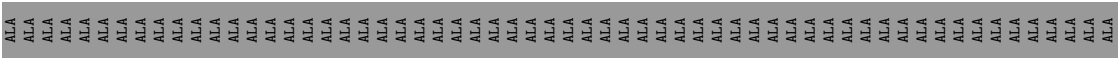
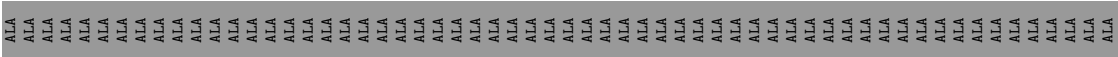
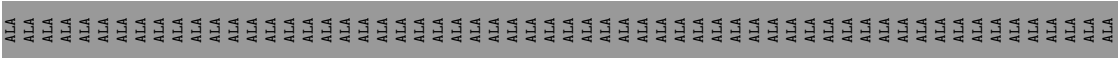
• Molecule 5: Type IV secretion system unknown protein fragment



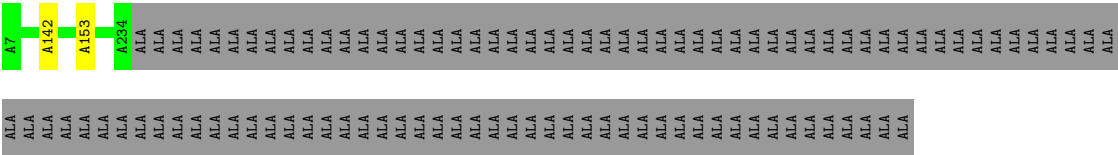
• Molecule 5: Type IV secretion system unknown protein fragment



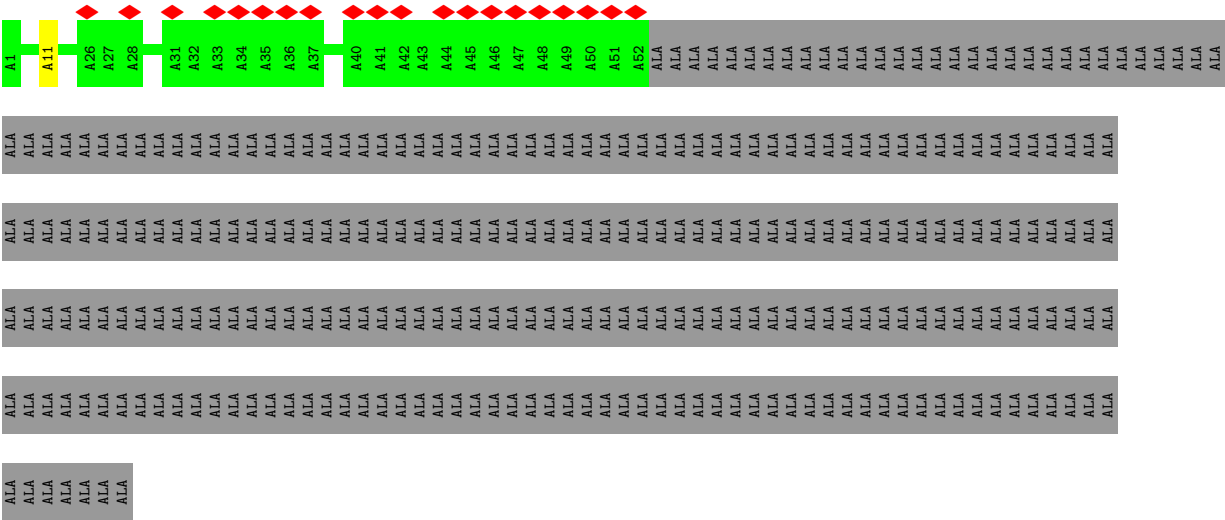
• Molecule 5: Type IV secretion system unknown protein fragment



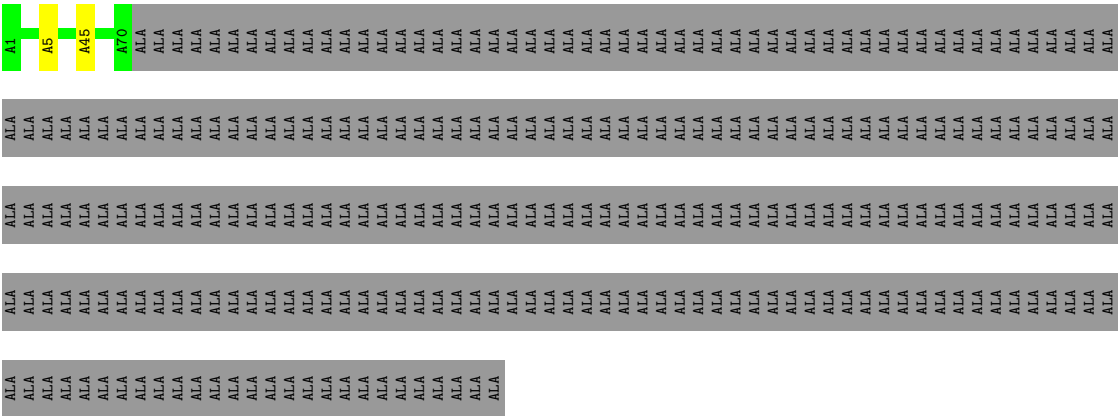
• Molecule 5: Type IV secretion system unknown protein fragment



• Molecule 5: Type IV secretion system unknown protein fragment

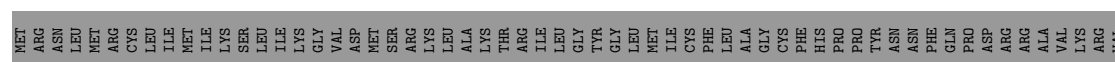


• Molecule 5: Type IV secretion system unknown protein fragment

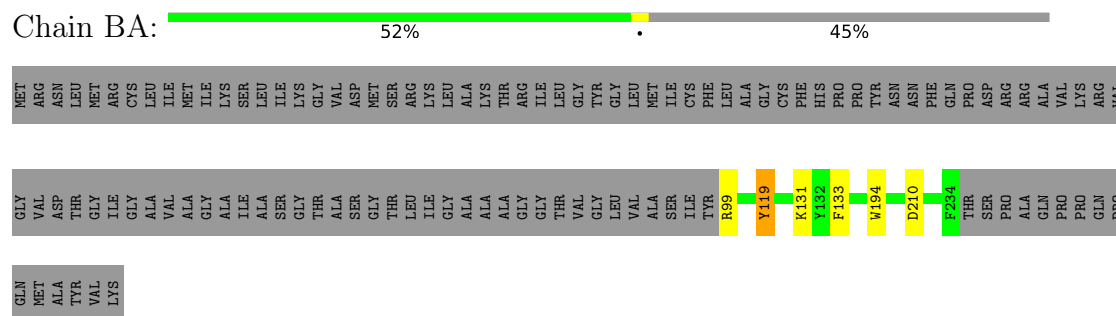


• Molecule 5: Type IV secretion system unknown protein fragment

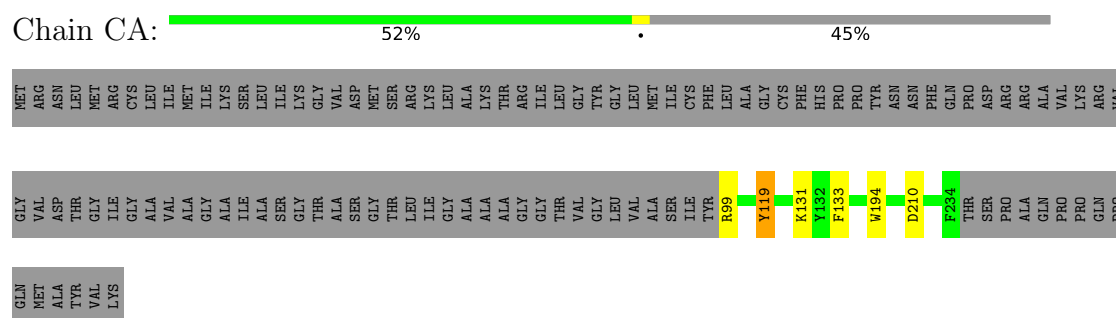




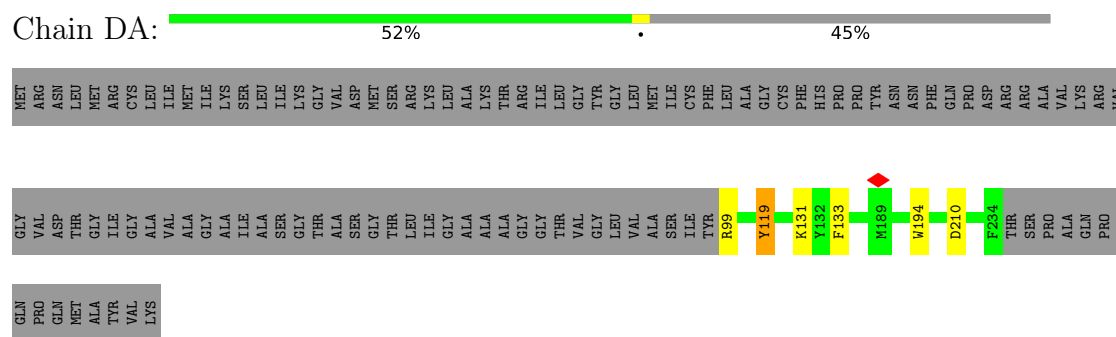
- Molecule 6: Outer membrane protein, OmpA family protein



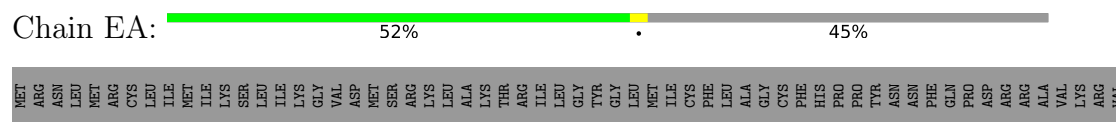
- Molecule 6: Outer membrane protein, OmpA family protein



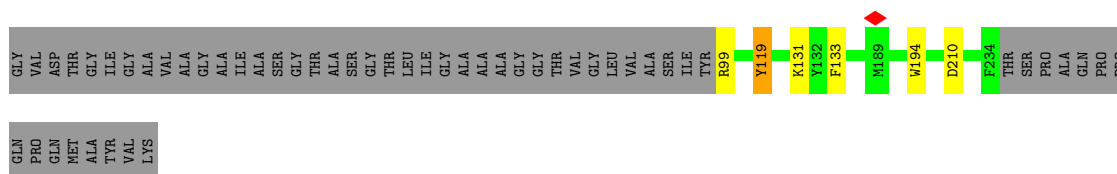
- Molecule 6: Outer membrane protein, OmpA family protein



- Molecule 6: Outer membrane protein, OmpA family protein

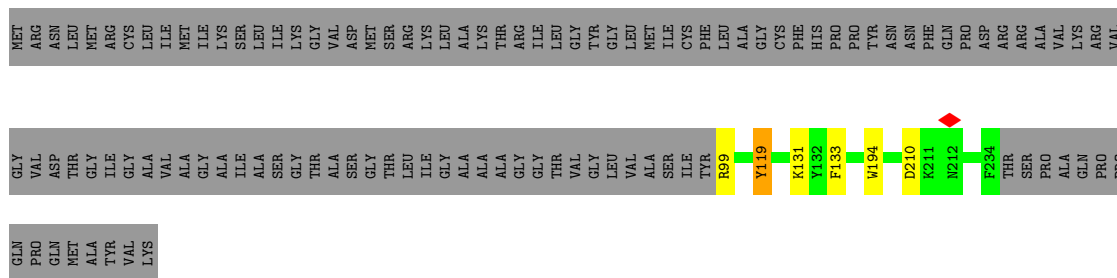






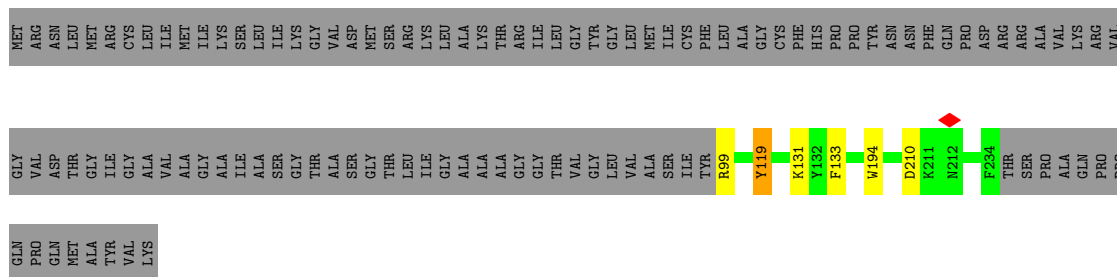
- Molecule 6: Outer membrane protein, OmpA family protein

Chain FA: 52% 45%



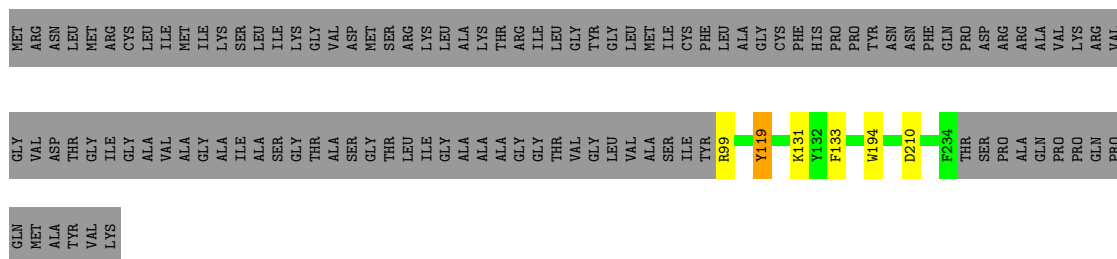
- Molecule 6: Outer membrane protein, OmpA family protein

Chain GA: 52% 45%



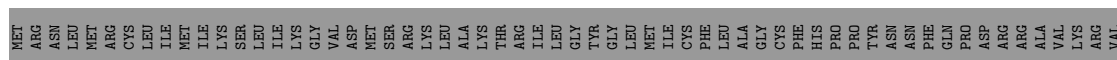
- Molecule 6: Outer membrane protein, OmpA family protein

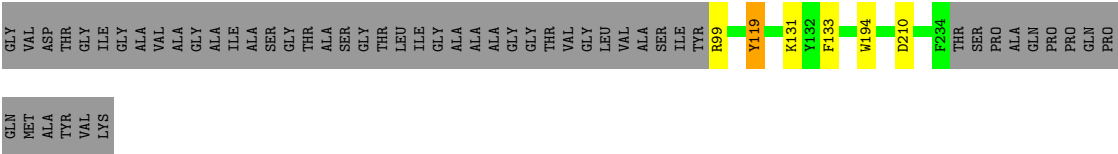
Chain HA: 52% 45%



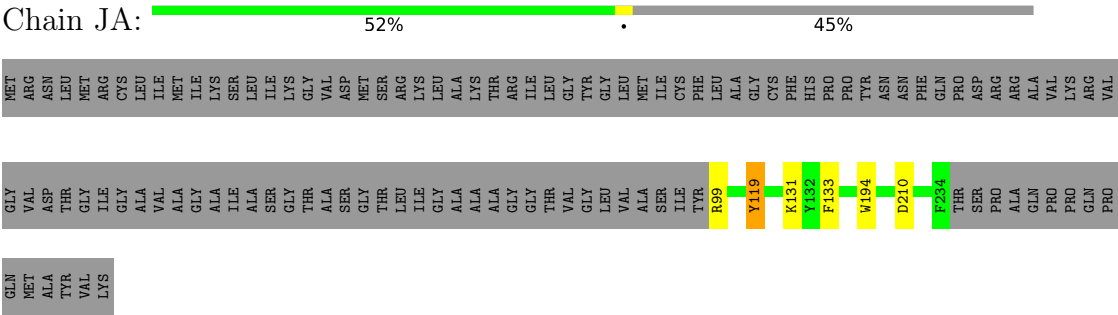
- Molecule 6: Outer membrane protein, OmpA family protein

Chain IA: 52% 45%

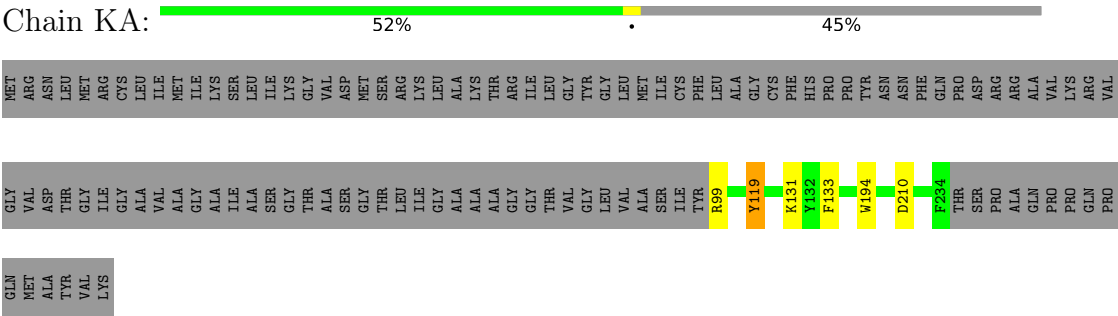




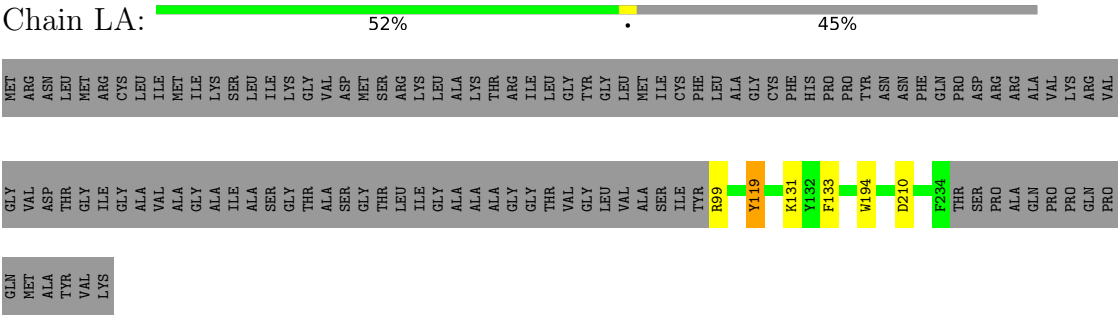
• Molecule 6: Outer membrane protein, OmpA family protein



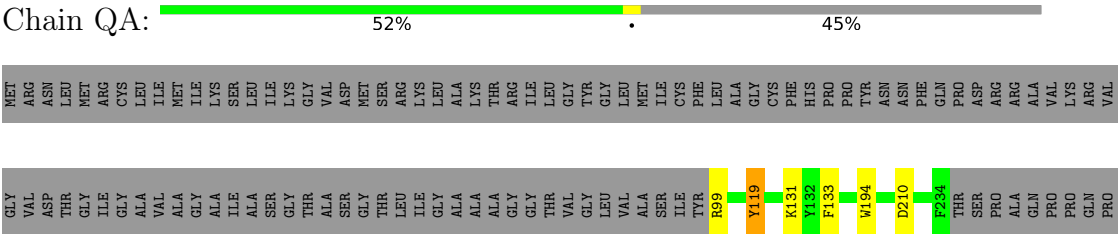
• Molecule 6: Outer membrane protein, OmpA family protein



• Molecule 6: Outer membrane protein, OmpA family protein



• Molecule 6: Outer membrane protein, OmpA family protein



GLN  
MET  
ALA  
TYR  
VAL  
LYS

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6342	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 ( $e^-/\text{\AA}^2$ )	65.0	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	0.955	Depositor
Minimum map value	-0.292	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.129	Depositor
Map size (Å)	688.5, 688.5, 688.5	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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	AC	0.89	0/1629	0.99	3/2214 (0.1%)
1	BC	0.89	0/1629	0.99	3/2214 (0.1%)
1	CC	0.89	0/1629	0.99	3/2214 (0.1%)
1	DC	0.89	0/1629	0.99	3/2214 (0.1%)
1	EC	0.89	0/1629	0.99	3/2214 (0.1%)
1	FC	0.89	0/1629	0.99	3/2214 (0.1%)
1	GC	0.89	0/1629	0.99	3/2214 (0.1%)
1	HC	0.89	0/1629	0.99	3/2214 (0.1%)
1	IC	0.89	0/1629	0.99	3/2214 (0.1%)
1	JC	0.89	0/1629	0.99	3/2214 (0.1%)
1	KC	0.89	0/1629	0.99	3/2214 (0.1%)
1	LC	0.89	0/1629	0.99	3/2214 (0.1%)
1	MC	0.89	0/1629	0.99	3/2214 (0.1%)
2	AD	0.78	2/1060 (0.2%)	0.83	0/1441
2	Ad	0.84	2/1086 (0.2%)	0.94	4/1474 (0.3%)
2	BD	0.81	2/1060 (0.2%)	0.91	5/1441 (0.3%)
2	Bd	0.83	1/1086 (0.1%)	0.97	4/1474 (0.3%)
2	CD	0.76	0/1060	0.81	1/1441 (0.1%)
2	Cd	0.82	1/1086 (0.1%)	0.94	3/1474 (0.2%)
2	DD	0.73	1/1060 (0.1%)	0.84	3/1441 (0.2%)
2	Dd	0.85	1/1086 (0.1%)	0.97	5/1474 (0.3%)
2	ED	0.74	1/1060 (0.1%)	0.89	6/1441 (0.4%)
2	Ed	0.84	1/1086 (0.1%)	0.94	5/1474 (0.3%)
2	FD	0.75	1/1060 (0.1%)	0.87	3/1441 (0.2%)
2	Fd	0.86	1/1086 (0.1%)	0.95	3/1474 (0.2%)
2	GD	0.75	1/1060 (0.1%)	0.84	1/1441 (0.1%)
2	Gd	0.83	1/1086 (0.1%)	0.96	2/1474 (0.1%)
2	HD	0.76	1/1060 (0.1%)	0.87	3/1441 (0.2%)
2	Hd	0.84	0/1086	0.88	3/1474 (0.2%)
2	ID	0.84	1/1060 (0.1%)	0.88	4/1441 (0.3%)
2	Id	0.83	0/1086	0.96	4/1474 (0.3%)
2	JD	0.78	1/1060 (0.1%)	0.86	0/1441
2	Jd	0.88	1/1086 (0.1%)	0.98	6/1474 (0.4%)
2	KD	0.74	1/1060 (0.1%)	0.81	1/1441 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	Kd	0.80	0/1086	0.98	4/1474 (0.3%)
2	LD	0.76	1/1060 (0.1%)	0.91	5/1441 (0.3%)
2	Ld	0.80	0/1086	0.89	2/1474 (0.1%)
2	MD	0.75	1/1060 (0.1%)	0.87	3/1441 (0.2%)
2	Md	0.83	1/1086 (0.1%)	0.90	4/1474 (0.3%)
3	AH	0.88	1/695 (0.1%)	1.07	1/947 (0.1%)
3	BH	0.88	1/695 (0.1%)	1.07	1/947 (0.1%)
3	CH	0.88	1/695 (0.1%)	1.07	1/947 (0.1%)
3	DH	0.88	1/695 (0.1%)	1.07	1/947 (0.1%)
3	EH	0.88	1/695 (0.1%)	1.07	1/947 (0.1%)
3	FH	0.88	1/695 (0.1%)	1.07	1/947 (0.1%)
3	GH	0.88	1/695 (0.1%)	1.07	1/947 (0.1%)
3	HH	0.88	1/695 (0.1%)	1.07	1/947 (0.1%)
3	IH	0.88	1/695 (0.1%)	1.07	1/947 (0.1%)
3	JH	0.88	1/695 (0.1%)	1.07	1/947 (0.1%)
3	KH	0.88	1/695 (0.1%)	1.07	1/947 (0.1%)
3	LH	0.88	1/695 (0.1%)	1.07	1/947 (0.1%)
3	MH	0.88	1/695 (0.1%)	1.07	1/947 (0.1%)
4	AK	0.83	0/1171	0.98	6/1583 (0.4%)
4	BK	0.83	0/1171	0.98	6/1583 (0.4%)
4	CK	0.83	0/1171	0.98	6/1583 (0.4%)
4	DK	0.83	0/1171	0.98	6/1583 (0.4%)
4	EK	0.83	0/1171	0.98	6/1583 (0.4%)
4	FK	0.83	0/1171	0.98	6/1583 (0.4%)
4	GK	0.83	0/1171	0.98	6/1583 (0.4%)
4	HK	0.83	0/1171	0.98	6/1583 (0.4%)
4	IK	0.83	0/1171	0.98	6/1583 (0.4%)
4	JK	0.83	0/1171	0.98	6/1583 (0.4%)
4	KK	0.83	0/1171	0.98	6/1583 (0.4%)
4	LK	0.83	0/1171	0.98	6/1583 (0.4%)
4	MK	0.83	0/1171	0.98	6/1583 (0.4%)
5	AX	0.36	0/1139	0.71	0/1593
5	AY	0.32	0/259	0.68	0/361
5	AZ	0.38	0/349	0.69	0/487
5	BX	0.36	0/1139	0.71	0/1593
5	BY	0.32	0/259	0.68	0/361
5	BZ	0.38	0/349	0.69	0/487
5	CX	0.36	0/1139	0.71	0/1593
5	CY	0.32	0/259	0.68	0/361
5	CZ	0.38	0/349	0.69	0/487
5	DX	0.36	0/1139	0.71	0/1593
5	DY	0.32	0/259	0.68	0/361
5	DZ	0.38	0/349	0.69	0/487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
5	EX	0.36	0/1139	0.71	0/1593
5	EY	0.32	0/259	0.68	0/361
5	EZ	0.38	0/349	0.69	0/487
5	FX	0.36	0/1139	0.71	0/1593
5	FY	0.32	0/259	0.68	0/361
5	FZ	0.38	0/349	0.69	0/487
5	GX	0.36	0/1139	0.71	0/1593
5	GY	0.32	0/259	0.68	0/361
5	GZ	0.38	0/349	0.69	0/487
5	HX	0.36	0/1139	0.71	0/1593
5	HY	0.32	0/259	0.68	0/361
5	HZ	0.38	0/349	0.69	0/487
5	IX	0.36	0/1139	0.71	0/1593
5	IY	0.32	0/259	0.68	0/361
5	IZ	0.38	0/349	0.69	0/487
5	JX	0.36	0/1139	0.71	0/1593
5	JY	0.32	0/259	0.68	0/361
5	JZ	0.38	0/349	0.69	0/487
5	KX	0.36	0/1139	0.71	0/1593
5	KY	0.32	0/259	0.68	0/361
5	KZ	0.38	0/349	0.69	0/487
5	LX	0.36	0/1139	0.71	0/1593
5	LY	0.32	0/259	0.68	0/361
5	LZ	0.38	0/349	0.69	0/487
5	MX	0.36	0/1139	0.71	0/1593
5	MY	0.32	0/259	0.68	0/361
5	MZ	0.38	0/349	0.69	0/487
6	AA	0.85	1/1130 (0.1%)	0.96	2/1522 (0.1%)
6	BA	0.85	1/1130 (0.1%)	0.96	2/1522 (0.1%)
6	CA	0.85	1/1130 (0.1%)	0.96	2/1522 (0.1%)
6	DA	0.85	1/1130 (0.1%)	0.96	2/1522 (0.1%)
6	EA	0.85	1/1130 (0.1%)	0.96	2/1522 (0.1%)
6	FA	0.85	1/1130 (0.1%)	0.96	2/1522 (0.1%)
6	GA	0.85	1/1130 (0.1%)	0.96	2/1522 (0.1%)
6	HA	0.85	1/1130 (0.1%)	0.96	2/1522 (0.1%)
6	IA	0.85	1/1130 (0.1%)	0.96	2/1522 (0.1%)
6	JA	0.85	1/1130 (0.1%)	0.96	2/1522 (0.1%)
6	KA	0.85	1/1130 (0.1%)	0.96	2/1522 (0.1%)
6	LA	0.85	1/1130 (0.1%)	0.96	2/1522 (0.1%)
6	QA	0.85	1/1130 (0.1%)	0.96	2/1522 (0.1%)
All	All	0.77	50/110734 (0.0%)	0.91	240/151086 (0.2%)

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
2	Bd	0	1
2	Cd	0	1
2	Dd	0	1
2	Ed	0	2
2	Fd	0	1
2	Hd	0	1
2	Id	0	1
2	Jd	0	1
2	Ld	0	2
2	Md	0	1
4	AK	0	1
4	BK	0	1
4	CK	0	1
4	DK	0	1
4	EK	0	1
4	FK	0	1
4	GK	0	1
4	HK	0	1
4	IK	0	1
4	JK	0	1
4	KK	0	1
4	LK	0	1
4	MK	0	1
5	AX	0	2
5	AY	0	1
5	AZ	0	2
5	BX	0	2
5	BY	0	1
5	BZ	0	2
5	CX	0	2
5	CY	0	1
5	CZ	0	2
5	DX	0	2
5	DY	0	1
5	DZ	0	2
5	EX	0	2
5	EY	0	1
5	EZ	0	2
5	FX	0	2
5	FY	0	1

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*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
5	FZ	0	2
5	GX	0	2
5	GY	0	1
5	GZ	0	2
5	HX	0	2
5	HY	0	1
5	HZ	0	2
5	IX	0	2
5	IY	0	1
5	IZ	0	2
5	JX	0	2
5	JY	0	1
5	JZ	0	2
5	KX	0	2
5	KY	0	1
5	KZ	0	2
5	LX	0	2
5	LY	0	1
5	LZ	0	2
5	MX	0	2
5	MY	0	1
5	MZ	0	2
6	AA	0	1
6	BA	0	1
6	CA	0	1
6	DA	0	1
6	EA	0	1
6	FA	0	1
6	GA	0	1
6	HA	0	1
6	IA	0	1
6	JA	0	1
6	KA	0	1
6	LA	0	1
6	QA	0	1
All	All	0	103

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	ID	87	TRP	CB-CG	-9.55	1.33	1.50
2	GD	87	TRP	CB-CG	-7.47	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Dd	58	VAL	CB-CG1	-7.36	1.37	1.52
2	Cd	58	VAL	CB-CG1	-7.14	1.37	1.52
2	BD	87	TRP	CB-CG	-7.05	1.37	1.50
2	AD	54	GLU	CB-CG	-6.99	1.38	1.52
2	Md	59	GLU	CG-CD	-6.87	1.41	1.51
2	DD	87	TRP	CB-CG	-6.72	1.38	1.50
2	JD	87	TRP	CB-CG	-6.48	1.38	1.50
2	FD	87	TRP	CB-CG	-6.42	1.38	1.50
2	Jd	152	GLN	CA-CB	-6.39	1.39	1.53
2	MD	87	TRP	CB-CG	-6.30	1.39	1.50
2	Gd	82	ARG	CZ-NH1	-6.24	1.25	1.33
2	Ed	59	GLU	CG-CD	-6.12	1.42	1.51
2	HD	87	TRP	CB-CG	-6.07	1.39	1.50
2	Ad	58	VAL	CB-CG1	-5.89	1.40	1.52
2	AD	87	TRP	CB-CG	-5.87	1.39	1.50
2	Fd	152	GLN	CA-CB	-5.64	1.41	1.53
3	MH	306	TRP	CB-CG	-5.53	1.40	1.50
2	KD	87	TRP	CB-CG	-5.53	1.40	1.50
3	AH	306	TRP	CB-CG	-5.53	1.40	1.50
3	HH	306	TRP	CB-CG	-5.51	1.40	1.50
3	JH	306	TRP	CB-CG	-5.51	1.40	1.50
3	GH	306	TRP	CB-CG	-5.51	1.40	1.50
3	BH	306	TRP	CB-CG	-5.51	1.40	1.50
3	EH	306	TRP	CB-CG	-5.51	1.40	1.50
3	IH	306	TRP	CB-CG	-5.51	1.40	1.50
3	LH	306	TRP	CB-CG	-5.51	1.40	1.50
3	KH	306	TRP	CB-CG	-5.50	1.40	1.50
3	FH	306	TRP	CB-CG	-5.49	1.40	1.50
2	BD	126	GLU	CG-CD	-5.49	1.43	1.51
2	Ad	59	GLU	CG-CD	-5.47	1.43	1.51
3	CH	306	TRP	CB-CG	-5.47	1.40	1.50
3	DH	306	TRP	CB-CG	-5.47	1.40	1.50
2	ED	87	TRP	CB-CG	-5.41	1.40	1.50
2	LD	87	TRP	CB-CG	-5.15	1.41	1.50
6	KA	194	TRP	CB-CG	-5.12	1.41	1.50
2	Bd	114	SER	CB-OG	-5.11	1.35	1.42
6	AA	194	TRP	CB-CG	-5.09	1.41	1.50
6	LA	194	TRP	CB-CG	-5.09	1.41	1.50
6	CA	194	TRP	CB-CG	-5.07	1.41	1.50
6	QA	194	TRP	CB-CG	-5.07	1.41	1.50
6	BA	194	TRP	CB-CG	-5.07	1.41	1.50
6	DA	194	TRP	CB-CG	-5.06	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	JA	194	TRP	CB-CG	-5.06	1.41	1.50
6	FA	194	TRP	CB-CG	-5.05	1.41	1.50
6	HA	194	TRP	CB-CG	-5.05	1.41	1.50
6	EA	194	TRP	CB-CG	-5.05	1.41	1.50
6	GA	194	TRP	CB-CG	-5.05	1.41	1.50
6	IA	194	TRP	CB-CG	-5.04	1.41	1.50

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Kd	52	MET	CG-SD-CE	10.92	117.67	100.20
2	Bd	86	ASP	CB-CG-OD2	10.73	127.96	118.30
6	JA	210	ASP	CB-CG-OD1	10.45	127.70	118.30
6	AA	210	ASP	CB-CG-OD1	10.43	127.69	118.30
6	CA	210	ASP	CB-CG-OD1	10.43	127.69	118.30
6	LA	210	ASP	CB-CG-OD1	10.43	127.69	118.30
6	QA	210	ASP	CB-CG-OD1	10.42	127.68	118.30
6	FA	210	ASP	CB-CG-OD1	10.40	127.66	118.30
6	BA	210	ASP	CB-CG-OD1	10.39	127.65	118.30
6	IA	210	ASP	CB-CG-OD1	10.39	127.65	118.30
6	GA	210	ASP	CB-CG-OD1	10.38	127.65	118.30
6	HA	210	ASP	CB-CG-OD1	10.37	127.63	118.30
6	KA	210	ASP	CB-CG-OD1	10.37	127.63	118.30
6	EA	210	ASP	CB-CG-OD1	10.36	127.63	118.30
6	DA	210	ASP	CB-CG-OD1	10.35	127.61	118.30
2	Dd	141	LYS	CD-CE-NZ	-9.40	90.07	111.70
2	Fd	55	MET	CG-SD-CE	-8.78	86.16	100.20
2	Kd	134	ASP	CB-CG-OD1	8.71	126.14	118.30
2	Jd	55	MET	CG-SD-CE	-8.38	86.79	100.20
2	ED	55	MET	CA-CB-CG	8.37	127.52	113.30
2	Id	55	MET	CG-SD-CE	-8.29	86.94	100.20
2	Id	52	MET	CA-CB-CG	8.19	127.22	113.30
2	BD	135	ILE	CG1-CB-CG2	-7.99	93.83	111.40
2	BD	53	LEU	CA-CB-CG	7.98	133.66	115.30
2	Bd	55	MET	CG-SD-CE	-7.80	87.72	100.20
2	Ld	55	MET	CG-SD-CE	-7.43	88.32	100.20
2	LD	52	MET	CG-SD-CE	-7.30	88.51	100.20
2	Cd	128	LEU	CA-CB-CG	-7.17	98.81	115.30
2	Cd	55	MET	CG-SD-CE	-6.90	89.17	100.20
2	MD	55	MET	CB-CG-SD	6.81	132.83	112.40
2	ED	55	MET	CB-CG-SD	6.77	132.70	112.40
2	ED	41	LEU	CB-CG-CD1	-6.73	99.56	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Dd	35	ASP	CB-CG-OD1	6.60	124.24	118.30
4	GK	56	MET	CG-SD-CE	-6.57	89.70	100.20
4	BK	56	MET	CG-SD-CE	-6.55	89.72	100.20
4	JK	56	MET	CG-SD-CE	-6.55	89.72	100.20
4	EK	56	MET	CG-SD-CE	-6.55	89.72	100.20
4	KK	56	MET	CG-SD-CE	-6.55	89.72	100.20
4	FK	56	MET	CG-SD-CE	-6.54	89.73	100.20
4	IK	56	MET	CG-SD-CE	-6.54	89.74	100.20
4	CK	56	MET	CG-SD-CE	-6.54	89.74	100.20
4	LK	56	MET	CG-SD-CE	-6.54	89.74	100.20
4	DK	56	MET	CG-SD-CE	-6.53	89.75	100.20
4	HK	56	MET	CG-SD-CE	-6.53	89.75	100.20
4	AK	56	MET	CG-SD-CE	-6.52	89.77	100.20
4	MK	56	MET	CG-SD-CE	-6.52	89.77	100.20
2	Md	35	ASP	CB-CG-OD1	6.51	124.16	118.30
2	Jd	128	LEU	CA-CB-CG	-6.51	100.33	115.30
2	Kd	35	ASP	CB-CG-OD1	6.48	124.13	118.30
2	Gd	55	MET	CG-SD-CE	-6.46	89.87	100.20
6	AA	119	TYR	CB-CG-CD1	6.37	124.82	121.00
4	JK	56	MET	CA-CB-CG	-6.36	102.48	113.30
2	DD	41	LEU	CB-CG-CD1	-6.36	100.19	111.00
4	DK	56	MET	CA-CB-CG	-6.36	102.49	113.30
2	Ed	52	MET	CG-SD-CE	6.35	110.36	100.20
4	IK	56	MET	CA-CB-CG	-6.35	102.50	113.30
4	AK	56	MET	CA-CB-CG	-6.35	102.51	113.30
4	FK	56	MET	CA-CB-CG	-6.35	102.51	113.30
4	CK	56	MET	CA-CB-CG	-6.34	102.51	113.30
4	EK	56	MET	CA-CB-CG	-6.34	102.52	113.30
4	BK	56	MET	CA-CB-CG	-6.33	102.53	113.30
4	LK	56	MET	CA-CB-CG	-6.33	102.53	113.30
4	MK	56	MET	CA-CB-CG	-6.33	102.53	113.30
4	HK	56	MET	CA-CB-CG	-6.33	102.54	113.30
4	GK	56	MET	CA-CB-CG	-6.33	102.54	113.30
4	KK	56	MET	CA-CB-CG	-6.32	102.56	113.30
6	HA	119	TYR	CB-CG-CD1	6.32	124.79	121.00
6	FA	119	TYR	CB-CG-CD1	6.31	124.79	121.00
6	KA	119	TYR	CB-CG-CD1	6.31	124.79	121.00
2	Ld	35	ASP	CB-CG-OD1	6.31	123.98	118.30
6	DA	119	TYR	CB-CG-CD1	6.30	124.78	121.00
6	BA	119	TYR	CB-CG-CD1	6.30	124.78	121.00
6	IA	119	TYR	CB-CG-CD1	6.29	124.78	121.00
6	QA	119	TYR	CB-CG-CD1	6.27	124.76	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	GA	119	TYR	CB-CG-CD1	6.26	124.76	121.00
6	JA	119	TYR	CB-CG-CD1	6.25	124.75	121.00
2	Ad	128	LEU	CA-CB-CG	-6.24	100.95	115.30
2	Kd	128	LEU	CA-CB-CG	-6.23	100.97	115.30
2	Ed	35	ASP	CB-CG-OD1	6.23	123.90	118.30
6	LA	119	TYR	CB-CG-CD1	6.23	124.74	121.00
2	LD	118	LEU	CA-CB-CG	-6.23	100.98	115.30
6	CA	119	TYR	CB-CG-CD1	6.23	124.74	121.00
6	EA	119	TYR	CB-CG-CD1	6.22	124.73	121.00
2	Dd	55	MET	CG-SD-CE	-6.10	90.43	100.20
2	Ad	52	MET	CG-SD-CE	6.09	109.95	100.20
2	HD	118	LEU	CA-CB-CG	-6.06	101.36	115.30
2	Hd	128	LEU	CA-CB-CG	-6.04	101.42	115.30
2	ID	135	ILE	CG1-CB-CG2	-6.03	98.13	111.40
2	LD	135	ILE	CG1-CB-CG2	-6.02	98.15	111.40
2	GD	53	LEU	CA-CB-CG	5.97	129.04	115.30
2	Jd	35	ASP	CB-CG-OD1	5.96	123.67	118.30
2	Jd	132	LEU	CB-CG-CD2	-5.95	100.89	111.00
1	LC	209	MET	CG-SD-CE	5.92	109.67	100.20
1	HC	209	MET	CG-SD-CE	5.90	109.65	100.20
1	DC	209	MET	CG-SD-CE	5.90	109.64	100.20
1	EC	209	MET	CG-SD-CE	5.90	109.64	100.20
1	JC	209	MET	CG-SD-CE	5.90	109.64	100.20
1	KC	209	MET	CG-SD-CE	5.90	109.64	100.20
1	AC	209	MET	CG-SD-CE	5.90	109.64	100.20
1	BC	209	MET	CG-SD-CE	5.89	109.63	100.20
1	GC	209	MET	CG-SD-CE	5.89	109.62	100.20
2	FD	55	MET	CG-SD-CE	-5.89	90.78	100.20
1	MC	209	MET	CG-SD-CE	5.89	109.62	100.20
2	ED	82	ARG	NE-CZ-NH1	-5.89	117.36	120.30
1	CC	209	MET	CG-SD-CE	5.88	109.61	100.20
1	FC	209	MET	CG-SD-CE	5.88	109.61	100.20
4	HK	60	LEU	CB-CG-CD1	5.88	120.99	111.00
4	FK	60	LEU	CB-CG-CD1	5.88	120.99	111.00
1	IC	209	MET	CG-SD-CE	5.88	109.60	100.20
4	CK	60	LEU	CB-CG-CD1	5.87	120.98	111.00
4	MK	60	LEU	CB-CG-CD1	5.87	120.98	111.00
4	EK	60	LEU	CB-CG-CD1	5.87	120.98	111.00
2	Ed	134	ASP	CB-CG-OD1	5.87	123.58	118.30
4	KK	60	LEU	CB-CG-CD1	5.87	120.97	111.00
4	DK	60	LEU	CB-CG-CD1	5.86	120.96	111.00
4	IK	60	LEU	CB-CG-CD1	5.85	120.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	JK	60	LEU	CB-CG-CD1	5.85	120.95	111.00
4	LK	60	LEU	CB-CG-CD1	5.85	120.95	111.00
4	AK	60	LEU	CB-CG-CD1	5.85	120.95	111.00
4	BK	60	LEU	CB-CG-CD1	5.85	120.95	111.00
4	GK	60	LEU	CB-CG-CD1	5.84	120.93	111.00
2	Jd	109	LEU	CB-CG-CD1	-5.84	101.07	111.00
2	Gd	82	ARG	CD-NE-CZ	5.83	131.76	123.60
2	DD	118	LEU	CA-CB-CG	-5.75	102.08	115.30
2	Ad	35	ASP	CB-CG-OD1	5.74	123.47	118.30
2	ED	55	MET	CG-SD-CE	-5.72	91.05	100.20
2	FD	82	ARG	NE-CZ-NH1	-5.66	117.47	120.30
2	ED	153	VAL	CG1-CB-CG2	-5.65	101.86	110.90
2	Fd	128	LEU	CA-CB-CG	-5.63	102.34	115.30
2	MD	50	ASP	CB-CG-OD1	5.61	123.35	118.30
2	Dd	97	ARG	NE-CZ-NH1	-5.55	117.53	120.30
2	ID	55	MET	CG-SD-CE	5.55	109.08	100.20
1	KC	81	GLU	N-CA-CB	5.52	120.54	110.60
1	EC	81	GLU	N-CA-CB	5.52	120.54	110.60
1	CC	81	GLU	N-CA-CB	5.52	120.53	110.60
1	MC	81	GLU	N-CA-CB	5.52	120.53	110.60
1	HC	81	GLU	N-CA-CB	5.51	120.52	110.60
1	BC	81	GLU	N-CA-CB	5.51	120.51	110.60
1	AC	81	GLU	N-CA-CB	5.51	120.51	110.60
1	DC	81	GLU	N-CA-CB	5.50	120.51	110.60
1	JC	81	GLU	N-CA-CB	5.50	120.51	110.60
1	LC	81	GLU	N-CA-CB	5.50	120.50	110.60
1	FC	81	GLU	N-CA-CB	5.50	120.49	110.60
1	GC	81	GLU	N-CA-CB	5.49	120.49	110.60
1	IC	81	GLU	N-CA-CB	5.49	120.48	110.60
2	ID	50	ASP	CB-CG-OD1	5.48	123.23	118.30
2	FD	118	LEU	CA-CB-CG	-5.48	102.70	115.30
4	MK	56	MET	CB-CA-C	-5.46	99.47	110.40
2	HD	128	LEU	CA-CB-CG	5.46	127.86	115.30
4	GK	56	MET	CB-CA-C	-5.45	99.49	110.40
4	CK	56	MET	CB-CA-C	-5.45	99.50	110.40
4	FK	56	MET	CB-CA-C	-5.45	99.50	110.40
4	JK	56	MET	CB-CA-C	-5.44	99.51	110.40
4	EK	56	MET	CB-CA-C	-5.44	99.51	110.40
4	IK	56	MET	CB-CA-C	-5.44	99.52	110.40
4	LK	56	MET	CB-CA-C	-5.44	99.52	110.40
4	BK	56	MET	CB-CA-C	-5.43	99.53	110.40
4	DK	106	LEU	CA-CB-CG	-5.43	102.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	HK	106	LEU	CA-CB-CG	-5.43	102.80	115.30
2	Md	128	LEU	CA-CB-CG	-5.43	102.80	115.30
4	AK	56	MET	CB-CA-C	-5.43	99.54	110.40
4	IK	106	LEU	CA-CB-CG	-5.43	102.81	115.30
2	BD	117	VAL	CG1-CB-CG2	-5.43	102.22	110.90
4	AK	106	LEU	CA-CB-CG	-5.43	102.82	115.30
4	DK	56	MET	CB-CA-C	-5.43	99.55	110.40
4	EK	106	LEU	CA-CB-CG	-5.43	102.82	115.30
4	KK	56	MET	CB-CA-C	-5.43	99.55	110.40
4	GK	106	LEU	CA-CB-CG	-5.42	102.83	115.30
4	LK	106	LEU	CA-CB-CG	-5.42	102.83	115.30
4	KK	106	LEU	CA-CB-CG	-5.42	102.84	115.30
4	HK	56	MET	CB-CA-C	-5.41	99.57	110.40
4	BK	106	LEU	CA-CB-CG	-5.41	102.86	115.30
4	CK	106	LEU	CA-CB-CG	-5.41	102.86	115.30
4	FK	106	LEU	CA-CB-CG	-5.41	102.86	115.30
4	MK	106	LEU	CA-CB-CG	-5.41	102.86	115.30
4	JK	106	LEU	CA-CB-CG	-5.40	102.88	115.30
2	Id	52	MET	N-CA-CB	-5.35	100.97	110.60
2	Ed	59	GLU	OE1-CD-OE2	5.34	129.72	123.30
2	CD	41	LEU	CB-CG-CD1	-5.32	101.95	111.00
3	FH	333	ASP	CB-CG-OD1	5.31	123.08	118.30
3	KH	333	ASP	CB-CG-OD1	5.31	123.08	118.30
3	IH	333	ASP	CB-CG-OD1	5.30	123.07	118.30
3	MH	333	ASP	CB-CG-OD1	5.29	123.06	118.30
3	CH	333	ASP	CB-CG-OD1	5.29	123.06	118.30
2	HD	153	VAL	CG1-CB-CG2	-5.29	102.44	110.90
3	GH	333	ASP	CB-CG-OD1	5.28	123.06	118.30
3	JH	333	ASP	CB-CG-OD1	5.28	123.06	118.30
2	BD	134	ASP	CB-CG-OD1	5.28	123.05	118.30
3	AH	333	ASP	CB-CG-OD1	5.27	123.04	118.30
3	BH	333	ASP	CB-CG-OD1	5.27	123.04	118.30
3	EH	333	ASP	CB-CG-OD1	5.27	123.04	118.30
3	DH	333	ASP	CB-CG-OD1	5.25	123.03	118.30
3	HH	333	ASP	CB-CG-OD1	5.24	123.01	118.30
2	LD	53	LEU	CA-CB-CG	5.22	127.32	115.30
3	LH	333	ASP	CB-CG-OD1	5.22	123.00	118.30
2	ID	41	LEU	CB-CG-CD1	-5.20	102.16	111.00
2	LD	94	LEU	CB-CG-CD2	5.18	119.81	111.00
1	FC	99	LEU	CA-CB-CG	-5.17	103.40	115.30
1	HC	99	LEU	CA-CB-CG	-5.17	103.40	115.30
1	IC	99	LEU	CA-CB-CG	-5.17	103.41	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	MC	99	LEU	CA-CB-CG	-5.17	103.41	115.30
1	BC	99	LEU	CA-CB-CG	-5.16	103.43	115.30
1	CC	99	LEU	CA-CB-CG	-5.16	103.42	115.30
1	GC	99	LEU	CA-CB-CG	-5.16	103.42	115.30
1	AC	99	LEU	CA-CB-CG	-5.16	103.43	115.30
1	JC	99	LEU	CA-CB-CG	-5.16	103.43	115.30
1	EC	99	LEU	CA-CB-CG	-5.16	103.43	115.30
1	LC	99	LEU	CA-CB-CG	-5.16	103.44	115.30
1	DC	99	LEU	CA-CB-CG	-5.16	103.44	115.30
2	Fd	53	LEU	CA-CB-CG	5.15	127.15	115.30
1	KC	99	LEU	CA-CB-CG	-5.15	103.45	115.30
4	EK	56	MET	CB-CG-SD	5.14	127.83	112.40
2	Cd	77	TYR	C-N-CA	5.14	134.55	121.70
4	CK	56	MET	CB-CG-SD	5.14	127.81	112.40
4	GK	56	MET	CB-CG-SD	5.14	127.81	112.40
4	HK	56	MET	CB-CG-SD	5.14	127.81	112.40
4	KK	56	MET	CB-CG-SD	5.14	127.81	112.40
4	LK	56	MET	CB-CG-SD	5.13	127.80	112.40
4	MK	56	MET	CB-CG-SD	5.13	127.79	112.40
4	BK	56	MET	CB-CG-SD	5.13	127.78	112.40
4	FK	56	MET	CB-CG-SD	5.13	127.78	112.40
4	DK	56	MET	CB-CG-SD	5.12	127.77	112.40
4	JK	56	MET	CB-CG-SD	5.12	127.77	112.40
2	MD	55	MET	CA-CB-CG	5.12	122.01	113.30
4	IK	56	MET	CB-CG-SD	5.12	127.77	112.40
4	AK	56	MET	CB-CG-SD	5.12	127.75	112.40
2	Id	77	TYR	C-N-CA	5.12	134.50	121.70
2	Jd	77	TYR	C-N-CA	5.11	134.49	121.70
2	Bd	77	TYR	C-N-CA	5.11	134.47	121.70
2	Md	59	GLU	OE1-CD-OE2	5.09	129.41	123.30
2	Dd	58	VAL	CG1-CB-CG2	-5.08	102.76	110.90
2	Hd	77	TYR	C-N-CA	5.06	134.36	121.70
2	Md	82	ARG	CG-CD-NE	-5.04	101.22	111.80
2	Ad	77	TYR	C-N-CA	5.04	134.29	121.70
2	Hd	36	ASP	CB-CG-OD1	5.04	122.83	118.30
2	Ed	55	MET	CG-SD-CE	-5.03	92.16	100.20
2	BD	132	LEU	CA-CB-CG	-5.02	103.75	115.30
2	KD	153	VAL	CG1-CB-CG2	-5.02	102.88	110.90
2	DD	82	ARG	NE-CZ-NH1	-5.01	117.79	120.30
2	Bd	35	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.



All (103) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	AA	133	PHE	Peptide
4	AK	65	ILE	Peptide
5	AX	142	ALA	Peptide
5	AX	153	ALA	Peptide
5	AY	11	ALA	Peptide
5	AZ	45	ALA	Peptide
5	AZ	5	ALA	Peptide
6	BA	133	PHE	Peptide
4	BK	65	ILE	Peptide
5	BX	142	ALA	Peptide
5	BX	153	ALA	Peptide
5	BY	11	ALA	Peptide
5	BZ	45	ALA	Peptide
5	BZ	5	ALA	Peptide
2	Bd	85	VAL	Peptide
6	CA	133	PHE	Peptide
4	CK	65	ILE	Peptide
5	CX	142	ALA	Peptide
5	CX	153	ALA	Peptide
5	CY	11	ALA	Peptide
5	CZ	45	ALA	Peptide
5	CZ	5	ALA	Peptide
2	Cd	85	VAL	Peptide
6	DA	133	PHE	Peptide
4	DK	65	ILE	Peptide
5	DX	142	ALA	Peptide
5	DX	153	ALA	Peptide
5	DY	11	ALA	Peptide
5	DZ	45	ALA	Peptide
5	DZ	5	ALA	Peptide
2	Dd	85	VAL	Peptide
6	EA	133	PHE	Peptide
4	EK	65	ILE	Peptide
5	EX	142	ALA	Peptide
5	EX	153	ALA	Peptide
5	EY	11	ALA	Peptide
5	EZ	45	ALA	Peptide
5	EZ	5	ALA	Peptide
2	Ed	78	ASN	Peptide
2	Ed	85	VAL	Peptide
6	FA	133	PHE	Peptide
4	FK	65	ILE	Peptide

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Mol	Chain	Res	Type	Group
5	FX	142	ALA	Peptide
5	FX	153	ALA	Peptide
5	FY	11	ALA	Peptide
5	FZ	45	ALA	Peptide
5	FZ	5	ALA	Peptide
2	Fd	85	VAL	Peptide
6	GA	133	PHE	Peptide
4	GK	65	ILE	Peptide
5	GX	142	ALA	Peptide
5	GX	153	ALA	Peptide
5	GY	11	ALA	Peptide
5	GZ	45	ALA	Peptide
5	GZ	5	ALA	Peptide
6	HA	133	PHE	Peptide
4	HK	65	ILE	Peptide
5	HX	142	ALA	Peptide
5	HX	153	ALA	Peptide
5	HY	11	ALA	Peptide
5	HZ	45	ALA	Peptide
5	HZ	5	ALA	Peptide
2	Hd	85	VAL	Peptide
6	IA	133	PHE	Peptide
4	IK	65	ILE	Peptide
5	IX	142	ALA	Peptide
5	IX	153	ALA	Peptide
5	IY	11	ALA	Peptide
5	IZ	45	ALA	Peptide
5	IZ	5	ALA	Peptide
2	Id	85	VAL	Peptide
6	JA	133	PHE	Peptide
4	JK	65	ILE	Peptide
5	JX	142	ALA	Peptide
5	JX	153	ALA	Peptide
5	JY	11	ALA	Peptide
5	JZ	45	ALA	Peptide
5	JZ	5	ALA	Peptide
2	Jd	85	VAL	Peptide
6	KA	133	PHE	Peptide
4	KK	65	ILE	Peptide
5	KX	142	ALA	Peptide
5	KX	153	ALA	Peptide
5	KY	11	ALA	Peptide

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Mol	Chain	Res	Type	Group
5	KZ	45	ALA	Peptide
5	KZ	5	ALA	Peptide
6	LA	133	PHE	Peptide
4	LK	65	ILE	Peptide
5	LX	142	ALA	Peptide
5	LX	153	ALA	Peptide
5	LY	11	ALA	Peptide
5	LZ	45	ALA	Peptide
5	LZ	5	ALA	Peptide
2	Ld	153	VAL	Peptide
2	Ld	85	VAL	Peptide
4	MK	65	ILE	Peptide
5	MX	142	ALA	Peptide
5	MX	153	ALA	Peptide
5	MY	11	ALA	Peptide
5	MZ	45	ALA	Peptide
5	MZ	5	ALA	Peptide
2	Md	85	VAL	Peptide
6	QA	133	PHE	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	
1	AC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	BC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	CC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	DC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	FC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	GC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	HC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	IC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	JC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	KC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	LC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	MC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
2	AD	133/163 (82%)	131 (98%)	2 (2%)	0	100	100
2	Ad	136/163 (83%)	129 (95%)	6 (4%)	1 (1%)	22	62
2	BD	133/163 (82%)	129 (97%)	4 (3%)	0	100	100
2	Bd	136/163 (83%)	124 (91%)	12 (9%)	0	100	100
2	CD	133/163 (82%)	126 (95%)	7 (5%)	0	100	100
2	Cd	136/163 (83%)	121 (89%)	15 (11%)	0	100	100
2	DD	133/163 (82%)	127 (96%)	6 (4%)	0	100	100
2	Dd	136/163 (83%)	125 (92%)	11 (8%)	0	100	100
2	ED	133/163 (82%)	124 (93%)	9 (7%)	0	100	100
2	Ed	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
2	FD	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
2	Fd	136/163 (83%)	124 (91%)	12 (9%)	0	100	100
2	GD	133/163 (82%)	129 (97%)	4 (3%)	0	100	100
2	Gd	136/163 (83%)	122 (90%)	13 (10%)	1 (1%)	22	62
2	HD	133/163 (82%)	129 (97%)	4 (3%)	0	100	100
2	Hd	136/163 (83%)	121 (89%)	15 (11%)	0	100	100
2	ID	133/163 (82%)	131 (98%)	2 (2%)	0	100	100
2	Id	136/163 (83%)	125 (92%)	11 (8%)	0	100	100
2	JD	133/163 (82%)	127 (96%)	6 (4%)	0	100	100
2	Jd	136/163 (83%)	125 (92%)	11 (8%)	0	100	100
2	KD	133/163 (82%)	127 (96%)	6 (4%)	0	100	100
2	Kd	136/163 (83%)	122 (90%)	14 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	LD	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
2	Ld	136/163 (83%)	124 (91%)	12 (9%)	0	100	100
2	MD	133/163 (82%)	129 (97%)	4 (3%)	0	100	100
2	Md	136/163 (83%)	125 (92%)	11 (8%)	0	100	100
3	AH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	BH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	CH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	DH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	EH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	FH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	GH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	HH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	IH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	JH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	KH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	LH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	MH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
4	AK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	BK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	CK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	DK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	EK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	FK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	GK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	HK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	IK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	JK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	KK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	LK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	MK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
5	AX	226/330 (68%)	184 (81%)	42 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AY	50/330 (15%)	36 (72%)	14 (28%)	0	100	100
5	AZ	68/330 (21%)	55 (81%)	13 (19%)	0	100	100
5	BX	226/330 (68%)	184 (81%)	42 (19%)	0	100	100
5	BY	50/330 (15%)	36 (72%)	14 (28%)	0	100	100
5	BZ	68/330 (21%)	55 (81%)	13 (19%)	0	100	100
5	CX	226/330 (68%)	184 (81%)	42 (19%)	0	100	100
5	CY	50/330 (15%)	36 (72%)	14 (28%)	0	100	100
5	CZ	68/330 (21%)	55 (81%)	13 (19%)	0	100	100
5	DX	226/330 (68%)	184 (81%)	42 (19%)	0	100	100
5	DY	50/330 (15%)	36 (72%)	14 (28%)	0	100	100
5	DZ	68/330 (21%)	55 (81%)	13 (19%)	0	100	100
5	EX	226/330 (68%)	184 (81%)	42 (19%)	0	100	100
5	EY	50/330 (15%)	36 (72%)	14 (28%)	0	100	100
5	EZ	68/330 (21%)	55 (81%)	13 (19%)	0	100	100
5	FX	226/330 (68%)	184 (81%)	42 (19%)	0	100	100
5	FY	50/330 (15%)	36 (72%)	14 (28%)	0	100	100
5	FZ	68/330 (21%)	55 (81%)	13 (19%)	0	100	100
5	GX	226/330 (68%)	184 (81%)	42 (19%)	0	100	100
5	GY	50/330 (15%)	36 (72%)	14 (28%)	0	100	100
5	GZ	68/330 (21%)	55 (81%)	13 (19%)	0	100	100
5	HX	226/330 (68%)	184 (81%)	42 (19%)	0	100	100
5	HY	50/330 (15%)	36 (72%)	14 (28%)	0	100	100
5	HZ	68/330 (21%)	55 (81%)	13 (19%)	0	100	100
5	IX	226/330 (68%)	184 (81%)	42 (19%)	0	100	100
5	IY	50/330 (15%)	36 (72%)	14 (28%)	0	100	100
5	IZ	68/330 (21%)	55 (81%)	13 (19%)	0	100	100
5	JX	226/330 (68%)	184 (81%)	42 (19%)	0	100	100
5	JY	50/330 (15%)	36 (72%)	14 (28%)	0	100	100
5	JZ	68/330 (21%)	55 (81%)	13 (19%)	0	100	100
5	KX	226/330 (68%)	184 (81%)	42 (19%)	0	100	100
5	KY	50/330 (15%)	36 (72%)	14 (28%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	KZ	68/330 (21%)	55 (81%)	13 (19%)	0	100	100
5	LX	226/330 (68%)	184 (81%)	42 (19%)	0	100	100
5	LY	50/330 (15%)	36 (72%)	14 (28%)	0	100	100
5	LZ	68/330 (21%)	55 (81%)	13 (19%)	0	100	100
5	MX	226/330 (68%)	184 (81%)	42 (19%)	0	100	100
5	MY	50/330 (15%)	36 (72%)	14 (28%)	0	100	100
5	MZ	68/330 (21%)	55 (81%)	13 (19%)	0	100	100
6	AA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	BA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	CA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	DA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	EA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	FA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	GA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	HA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	IA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	JA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	KA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	LA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	QA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
All	All	15288/31434 (49%)	13406 (88%)	1880 (12%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Ad	28	PRO
2	Gd	28	PRO

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AC	169/257 (66%)	168 (99%)	1 (1%)	86	92
1	BC	169/257 (66%)	168 (99%)	1 (1%)	86	92
1	CC	169/257 (66%)	168 (99%)	1 (1%)	86	92
1	DC	169/257 (66%)	169 (100%)	0	100	100
1	EC	169/257 (66%)	168 (99%)	1 (1%)	86	92
1	FC	169/257 (66%)	168 (99%)	1 (1%)	86	92
1	GC	169/257 (66%)	168 (99%)	1 (1%)	86	92
1	HC	169/257 (66%)	168 (99%)	1 (1%)	86	92
1	IC	169/257 (66%)	169 (100%)	0	100	100
1	JC	169/257 (66%)	169 (100%)	0	100	100
1	KC	169/257 (66%)	168 (99%)	1 (1%)	86	92
1	LC	169/257 (66%)	168 (99%)	1 (1%)	86	92
1	MC	169/257 (66%)	168 (99%)	1 (1%)	86	92
2	AD	116/139 (84%)	116 (100%)	0	100	100
2	Ad	119/139 (86%)	119 (100%)	0	100	100
2	BD	116/139 (84%)	115 (99%)	1 (1%)	78	87
2	Bd	119/139 (86%)	119 (100%)	0	100	100
2	CD	116/139 (84%)	116 (100%)	0	100	100
2	Cd	119/139 (86%)	118 (99%)	1 (1%)	81	89
2	DD	116/139 (84%)	115 (99%)	1 (1%)	78	87
2	Dd	119/139 (86%)	118 (99%)	1 (1%)	81	89
2	ED	116/139 (84%)	116 (100%)	0	100	100
2	Ed	119/139 (86%)	119 (100%)	0	100	100
2	FD	116/139 (84%)	115 (99%)	1 (1%)	78	87
2	Fd	119/139 (86%)	118 (99%)	1 (1%)	81	89
2	GD	116/139 (84%)	115 (99%)	1 (1%)	78	87
2	Gd	119/139 (86%)	119 (100%)	0	100	100
2	HD	116/139 (84%)	114 (98%)	2 (2%)	60	78
2	Hd	119/139 (86%)	118 (99%)	1 (1%)	81	89
2	ID	116/139 (84%)	116 (100%)	0	100	100
2	Id	119/139 (86%)	118 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	JD	116/139 (84%)	116 (100%)	0	100	100
2	Jd	119/139 (86%)	118 (99%)	1 (1%)	81	89
2	KD	116/139 (84%)	116 (100%)	0	100	100
2	Kd	119/139 (86%)	119 (100%)	0	100	100
2	LD	116/139 (84%)	116 (100%)	0	100	100
2	Ld	119/139 (86%)	119 (100%)	0	100	100
2	MD	116/139 (84%)	115 (99%)	1 (1%)	78	87
2	Md	119/139 (86%)	119 (100%)	0	100	100
3	AH	75/300 (25%)	74 (99%)	1 (1%)	69	82
3	BH	75/300 (25%)	74 (99%)	1 (1%)	69	82
3	CH	75/300 (25%)	74 (99%)	1 (1%)	69	82
3	DH	75/300 (25%)	74 (99%)	1 (1%)	69	82
3	EH	75/300 (25%)	74 (99%)	1 (1%)	69	82
3	FH	75/300 (25%)	74 (99%)	1 (1%)	69	82
3	GH	75/300 (25%)	74 (99%)	1 (1%)	69	82
3	HH	75/300 (25%)	74 (99%)	1 (1%)	69	82
3	IH	75/300 (25%)	74 (99%)	1 (1%)	69	82
3	JH	75/300 (25%)	74 (99%)	1 (1%)	69	82
3	KH	75/300 (25%)	74 (99%)	1 (1%)	69	82
3	LH	75/300 (25%)	74 (99%)	1 (1%)	69	82
3	MH	75/300 (25%)	74 (99%)	1 (1%)	69	82
4	AK	126/163 (77%)	125 (99%)	1 (1%)	81	89
4	BK	126/163 (77%)	125 (99%)	1 (1%)	81	89
4	CK	126/163 (77%)	125 (99%)	1 (1%)	81	89
4	DK	126/163 (77%)	125 (99%)	1 (1%)	81	89
4	EK	126/163 (77%)	125 (99%)	1 (1%)	81	89
4	FK	126/163 (77%)	125 (99%)	1 (1%)	81	89
4	GK	126/163 (77%)	125 (99%)	1 (1%)	81	89
4	HK	126/163 (77%)	125 (99%)	1 (1%)	81	89
4	IK	126/163 (77%)	125 (99%)	1 (1%)	81	89
4	JK	126/163 (77%)	125 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	KK	126/163 (77%)	125 (99%)	1 (1%)	81	89
4	LK	126/163 (77%)	125 (99%)	1 (1%)	81	89
4	MK	126/163 (77%)	125 (99%)	1 (1%)	81	89
6	AA	118/203 (58%)	115 (98%)	3 (2%)	47	68
6	BA	118/203 (58%)	115 (98%)	3 (2%)	47	68
6	CA	118/203 (58%)	115 (98%)	3 (2%)	47	68
6	DA	118/203 (58%)	115 (98%)	3 (2%)	47	68
6	EA	118/203 (58%)	115 (98%)	3 (2%)	47	68
6	FA	118/203 (58%)	115 (98%)	3 (2%)	47	68
6	GA	118/203 (58%)	115 (98%)	3 (2%)	47	68
6	HA	118/203 (58%)	115 (98%)	3 (2%)	47	68
6	IA	118/203 (58%)	115 (98%)	3 (2%)	47	68
6	JA	118/203 (58%)	115 (98%)	3 (2%)	47	68
6	KA	118/203 (58%)	115 (98%)	3 (2%)	47	68
6	LA	118/203 (58%)	115 (98%)	3 (2%)	47	68
6	QA	118/203 (58%)	115 (98%)	3 (2%)	47	68
All	All	9399/15613 (60%)	9311 (99%)	88 (1%)	79	87

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AC	104	ASN
3	AH	294	ARG
4	AK	163	LYS
1	BC	104	ASN
2	BD	100	LYS
3	BH	294	ARG
4	BK	163	LYS
1	CC	104	ASN
3	CH	294	ARG
4	CK	163	LYS
2	Cd	111	LYS
2	DD	100	LYS
3	DH	294	ARG
4	DK	163	LYS
2	Dd	141	LYS

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Mol	Chain	Res	Type
1	EC	104	ASN
3	EH	294	ARG
4	EK	163	LYS
1	FC	104	ASN
2	FD	100	LYS
3	FH	294	ARG
4	FK	163	LYS
2	Fd	111	LYS
1	GC	104	ASN
2	GD	82	ARG
3	GH	294	ARG
4	GK	163	LYS
1	HC	104	ASN
2	HD	82	ARG
2	HD	100	LYS
3	HH	294	ARG
4	HK	163	LYS
2	Hd	111	LYS
3	IH	294	ARG
4	IK	163	LYS
2	Id	111	LYS
3	JH	294	ARG
4	JK	163	LYS
2	Jd	111	LYS
1	KC	104	ASN
3	KH	294	ARG
4	KK	163	LYS
1	LC	104	ASN
3	LH	294	ARG
4	LK	163	LYS
1	MC	104	ASN
2	MD	107	ARG
3	MH	294	ARG
4	MK	163	LYS
6	AA	99	ARG
6	AA	119	TYR
6	AA	131	LYS
6	BA	99	ARG
6	BA	119	TYR
6	BA	131	LYS
6	CA	99	ARG
6	CA	119	TYR

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Mol	Chain	Res	Type
6	CA	131	LYS
6	DA	99	ARG
6	DA	119	TYR
6	DA	131	LYS
6	EA	99	ARG
6	EA	119	TYR
6	EA	131	LYS
6	FA	99	ARG
6	FA	119	TYR
6	FA	131	LYS
6	GA	99	ARG
6	GA	119	TYR
6	GA	131	LYS
6	HA	99	ARG
6	HA	119	TYR
6	HA	131	LYS
6	IA	99	ARG
6	IA	119	TYR
6	IA	131	LYS
6	JA	99	ARG
6	JA	119	TYR
6	JA	131	LYS
6	KA	99	ARG
6	KA	119	TYR
6	KA	131	LYS
6	LA	99	ARG
6	LA	119	TYR
6	LA	131	LYS
6	QA	99	ARG
6	QA	119	TYR
6	QA	131	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	AC	104	ASN
1	AC	149	GLN
2	Ad	32	ASN
1	BC	104	ASN
1	BC	149	GLN
1	CC	104	ASN
1	CC	149	GLN

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Mol	Chain	Res	Type
1	DC	149	GLN
1	EC	104	ASN
1	EC	149	GLN
1	FC	104	ASN
1	FC	149	GLN
2	FD	78	ASN
2	FD	103	HIS
1	GC	104	ASN
1	GC	149	GLN
1	HC	104	ASN
1	HC	149	GLN
1	IC	149	GLN
2	Id	80	GLN
1	JC	149	GLN
1	KC	104	ASN
1	KC	149	GLN
1	LC	104	ASN
1	LC	149	GLN
1	MC	104	ASN
1	MC	149	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

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.

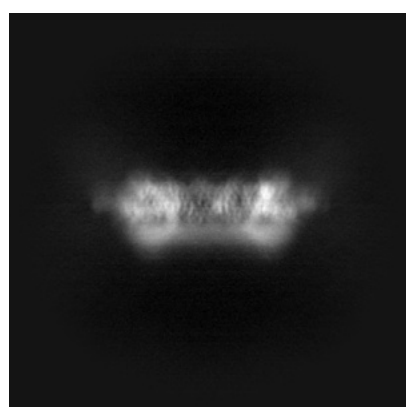
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22071. These allow visual inspection of the internal detail of the map and identification of artifacts.

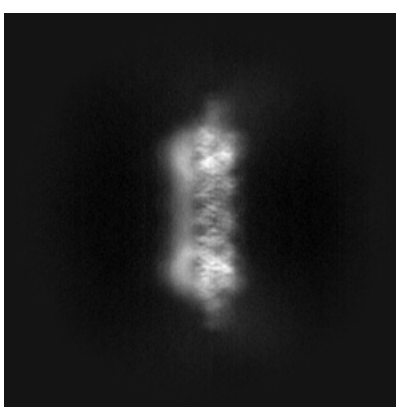
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

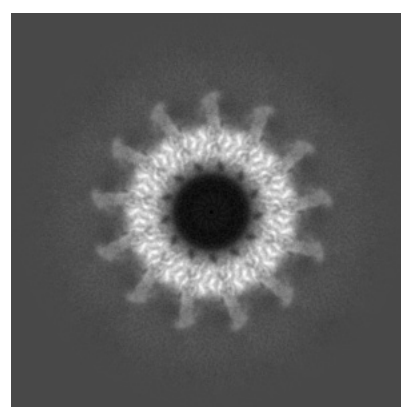
#### 6.1.1 Primary map



X



Y

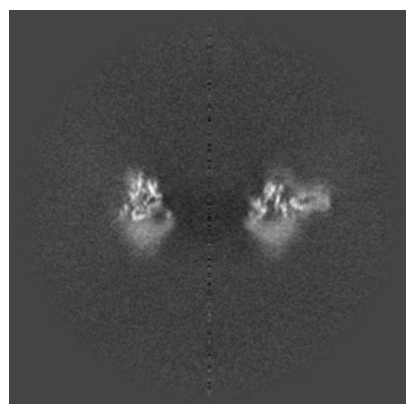


Z

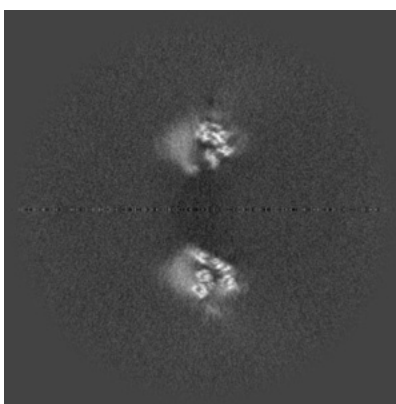
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

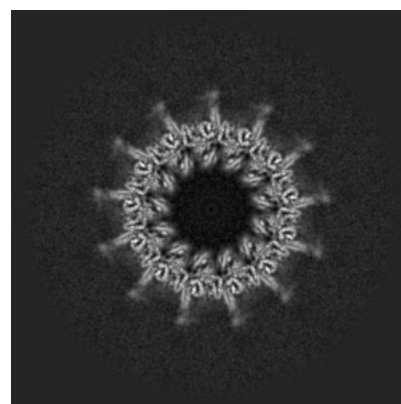
#### 6.2.1 Primary map



X Index: 255



Y Index: 255

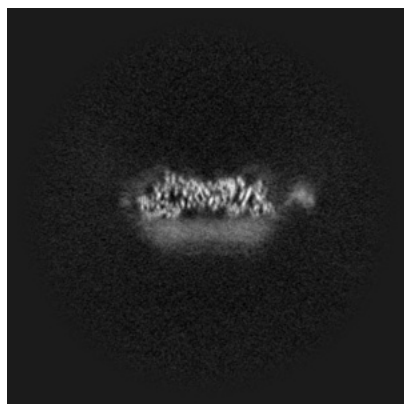


Z Index: 255

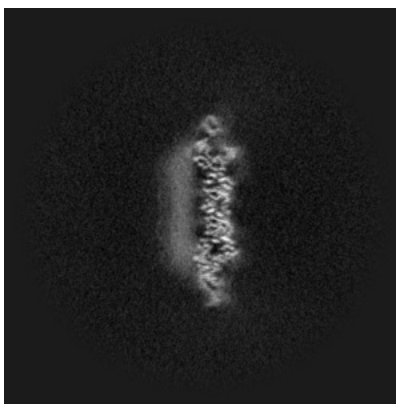
The images above show central slices of the map in three orthogonal directions.

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

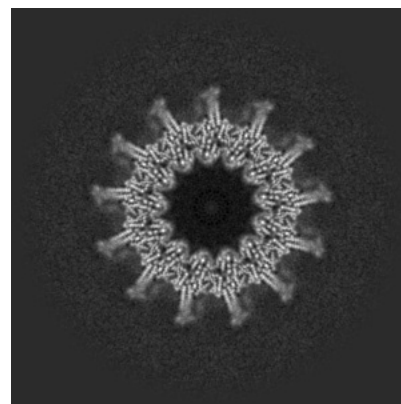
### 6.3.1 Primary map



X Index: 184



Y Index: 326

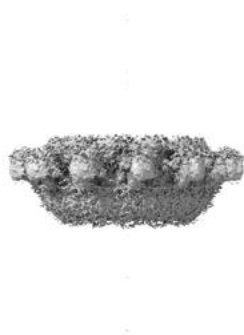


Z Index: 258

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

## 6.4 Orthogonal surface views [i](#)

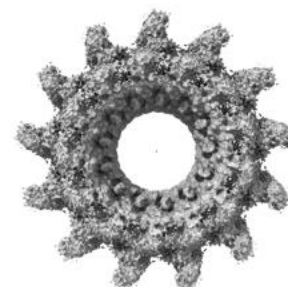
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.129. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



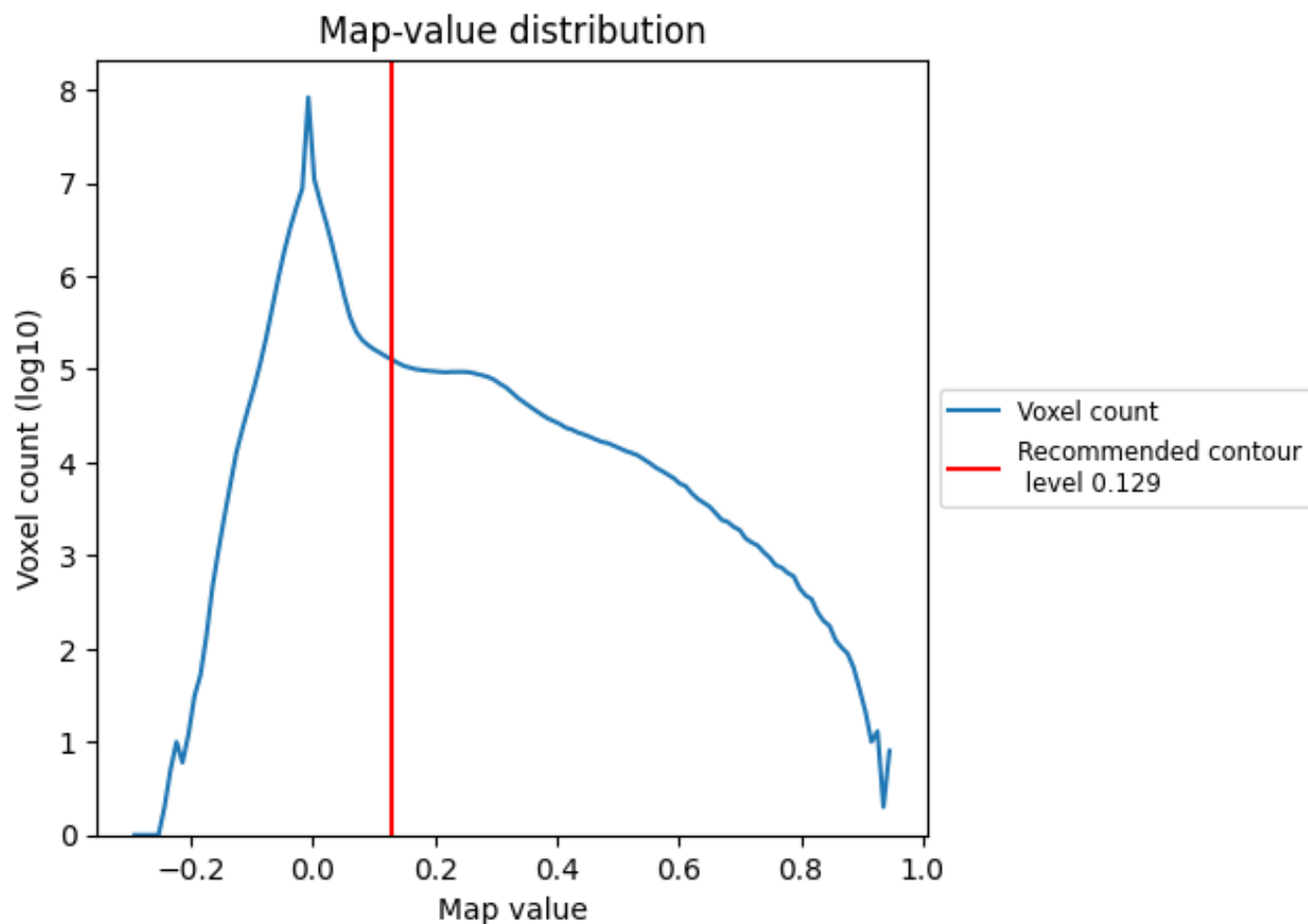
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

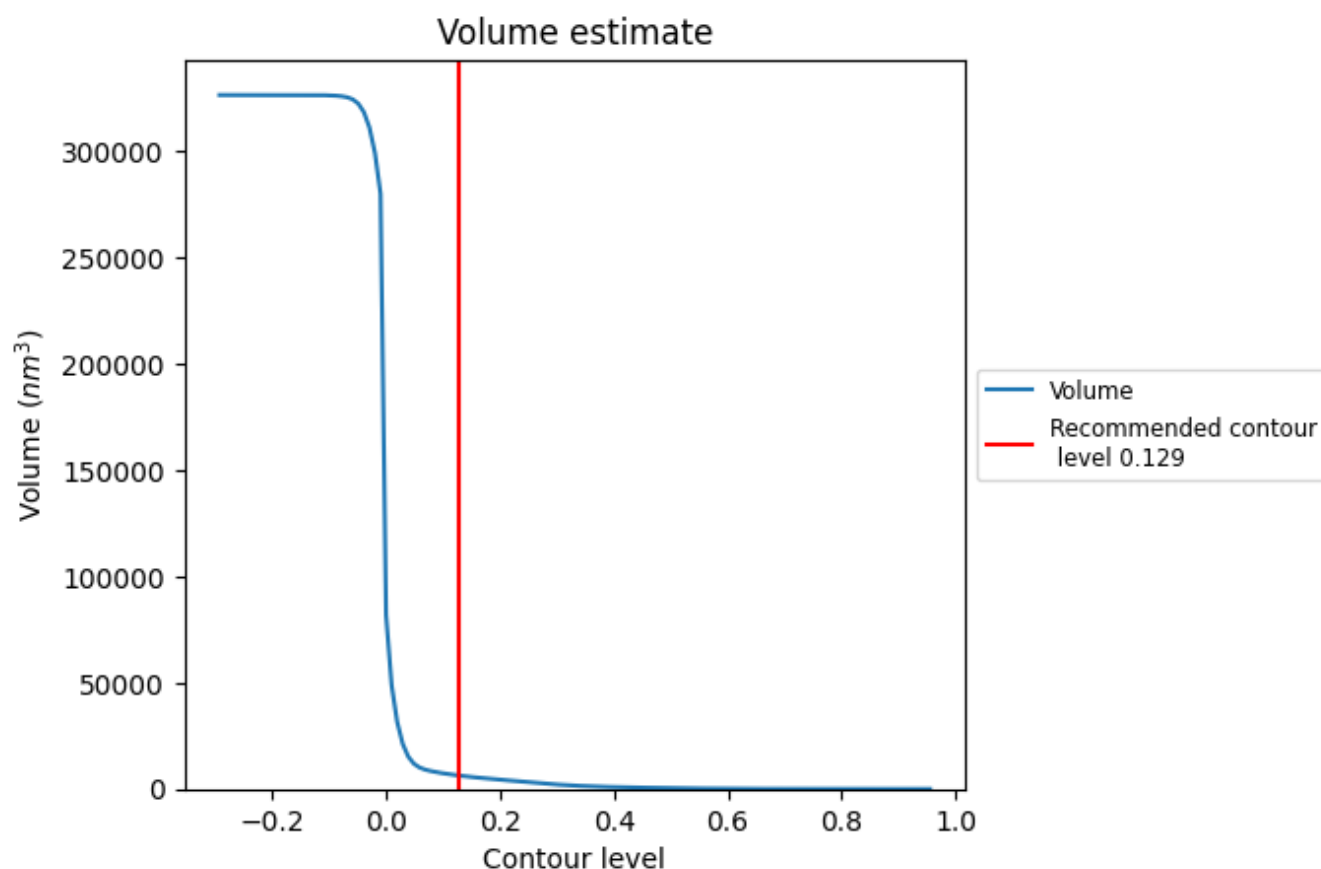
This section contains the results of statistical analysis of the map.

### 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.

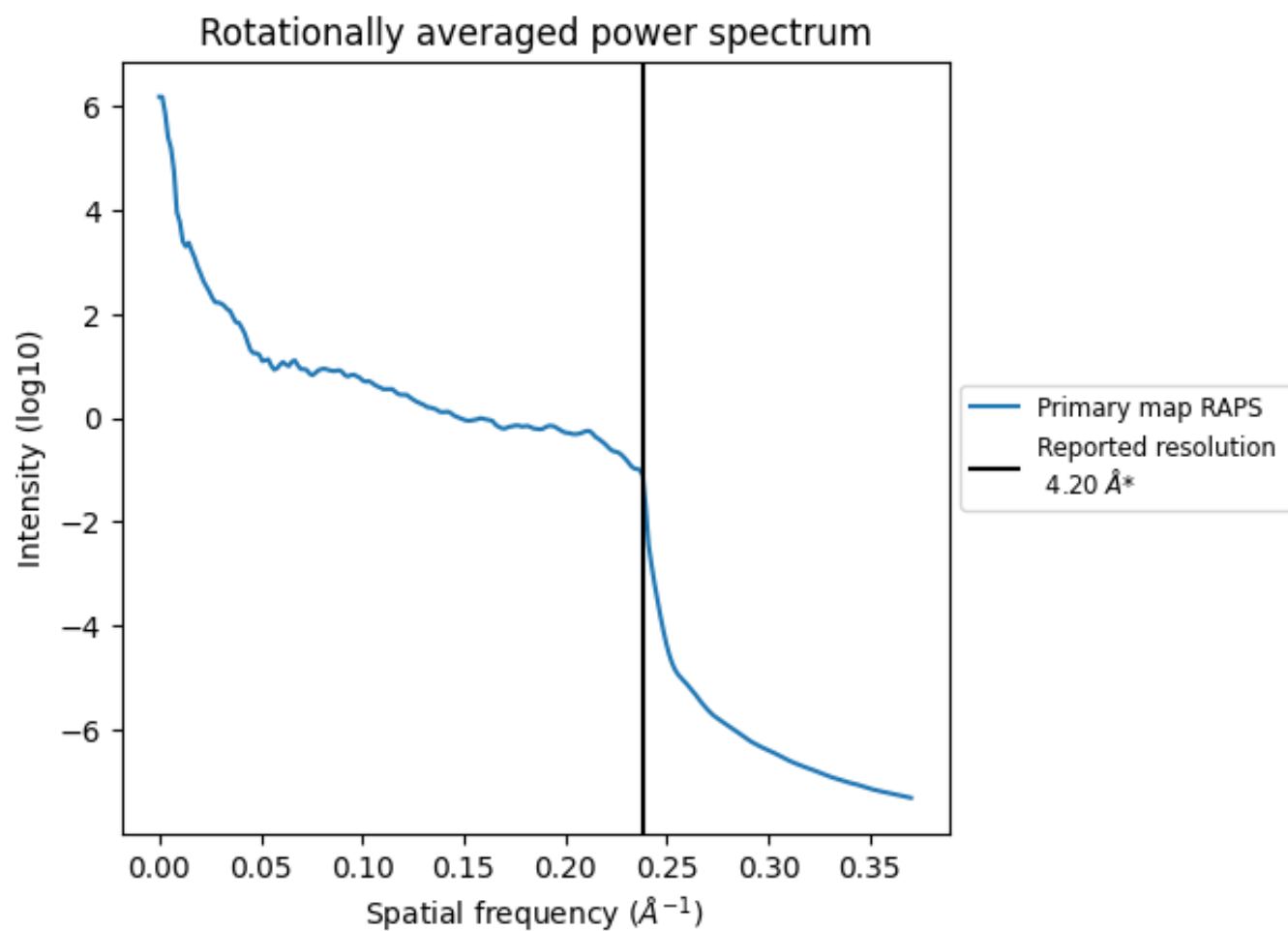
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6278  $\text{nm}^3$ ; this corresponds to an approximate mass of 5671 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 0.238 Å<sup>-1</sup>

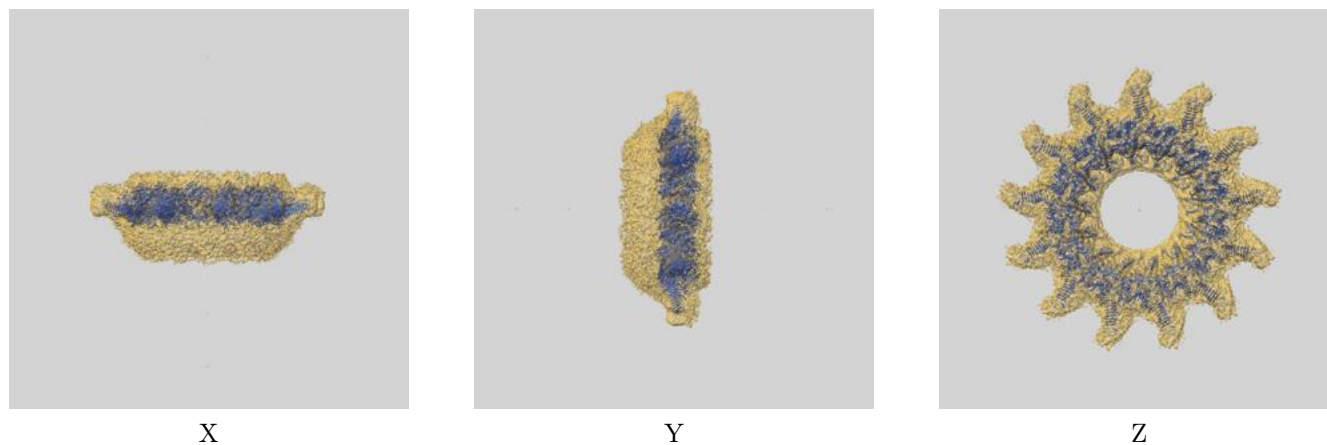
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

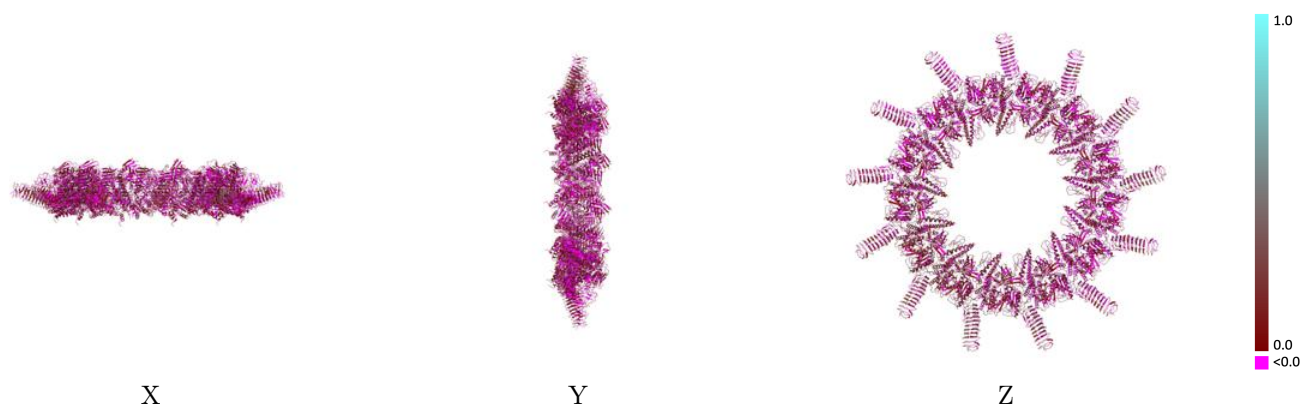
This section contains information regarding the fit between EMDB map EMD-22071 and PDB model 6X66. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

### 9.1 Map-model overlay [i](#)



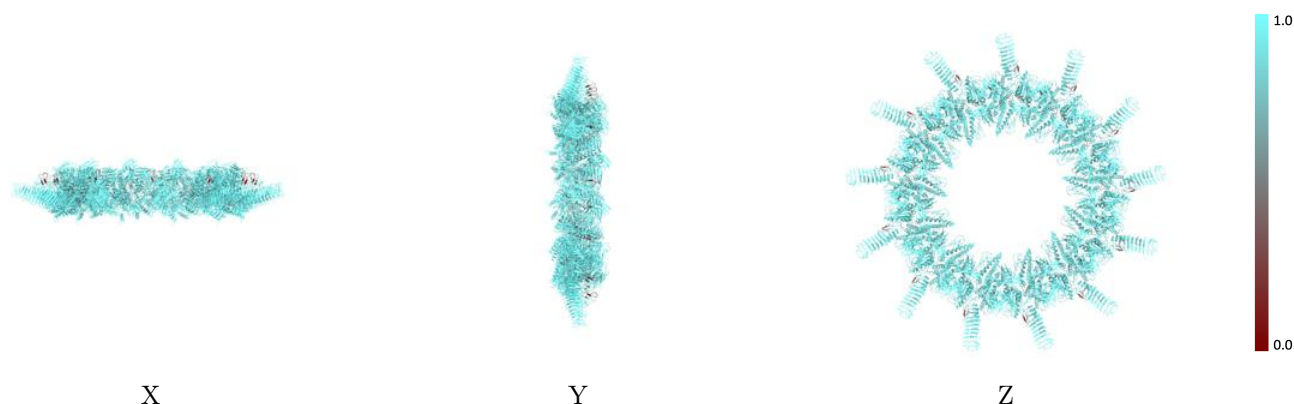
The images above show the 3D surface view of the map at the recommended contour level 0.129 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



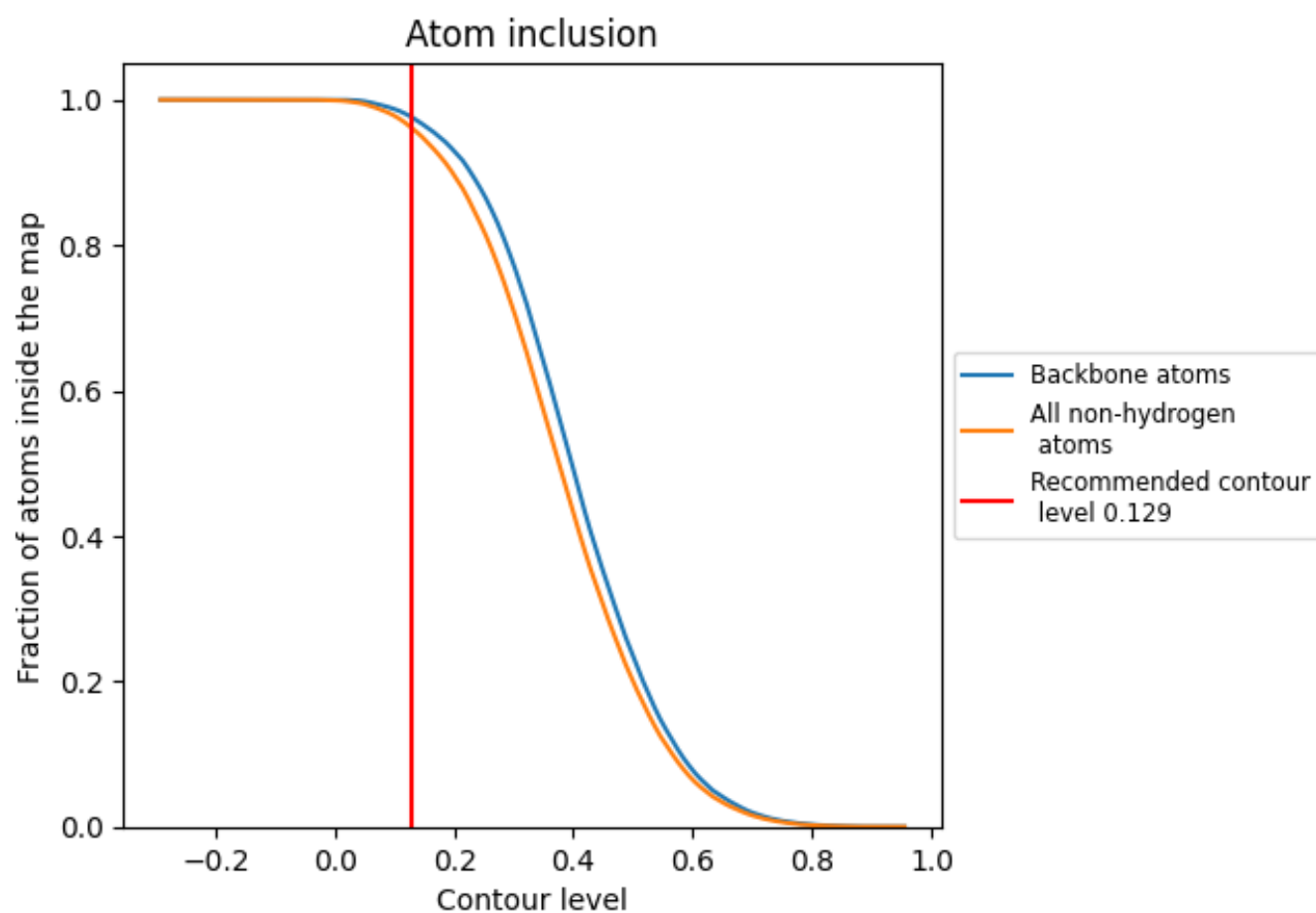
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.129).

## 9.4 Atom inclusion ⓘ









































































At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.129) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9613	 0.0690
AA	 0.9768	 0.0470
AC	 0.9782	 0.0500
AD	 0.9404	 0.0030
AH	 0.9549	 0.0490
AK	 0.9714	 0.0520
AX	 0.9921	 0.1080
AY	 0.6115	 0.0340
AZ	 0.9514	 0.1000
Ad	 0.9514	 0.0310
BA	 0.9749	 0.0560
BC	 0.9795	 0.0670
BD	 0.9413	 0.0240
BH	 0.9534	 0.0670
BK	 0.9652	 0.0620
BX	 0.9921	 0.1080
BY	 0.6269	 -0.0210
BZ	 0.9657	 0.1110
Bd	 0.9552	 0.0370
CA	 0.9694	 0.0540
CC	 0.9788	 0.0720
CD	 0.9580	 0.0580
CH	 0.9429	 0.0610
CK	 0.9518	 0.0490
CX	 0.9947	 0.0350
CY	 0.6000	 -0.0600
CZ	 0.9714	 0.1010
Cd	 0.9657	 0.0470
DA	 0.9684	 0.0420
DC	 0.9763	 0.0650
DD	 0.9599	 0.0780
DH	 0.9323	 0.0470
DK	 0.9429	 0.0320
DX	 0.9895	 -0.0110
DY	 0.6385	 -0.0340





















































































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Chain	Atom inclusion	Q-score
DZ	 0.9829	 0.1030
Dd	 0.9428	 0.0460
EA	 0.9712	 0.0300
EC	 0.9750	 0.0570
ED	 0.9638	 0.0750
EH	 0.9489	 0.0420
EK	 0.9464	 0.0200
EX	 0.9877	 0.0320
EY	 0.6923	 -0.0170
EZ	 0.9971	 0.1040
Ed	 0.9295	 0.0380
FA	 0.9712	 0.0450
FC	 0.9660	 0.0660
FD	 0.9707	 0.0670
FH	 0.9519	 0.0360
FK	 0.9580	 0.0340
FX	 0.9930	 0.0520
FY	 0.7231	 -0.0370
FZ	 0.9914	 0.0780
Fd	 0.9276	 0.0400
GA	 0.9879	 0.0830
GC	 0.9666	 0.0870
GD	 0.9687	 0.0760
GH	 0.9609	 0.0440
GK	 0.9696	 0.0810
GX	 0.9956	 0.0550
GY	 0.7231	 -0.0310
GZ	 0.9886	 0.0780
Gd	 0.9333	 0.0540
HA	 0.9944	 0.1260
HC	 0.9666	 0.1100
HD	 0.9687	 0.0920
HH	 0.9684	 0.0780
HK	 0.9839	 0.1240
HX	 0.9991	 0.0940
HY	 0.7385	 -0.0200
HZ	 0.9886	 0.0990
Hd	 0.9581	 0.0870
IA	 0.9861	 0.1260
IC	 0.9763	 0.1140
ID	 0.9824	 0.1250
IH	 0.9699	 0.1150

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Chain	Atom inclusion	Q-score
IK	 0.9893	 0.1330
IX	 1.0000	 0.1570
IY	 0.7192	 -0.0220
IZ	 0.9886	 0.1280
Id	 0.9847	 0.1270
JA	 0.9777	 0.0840
JC	 0.9795	 0.0990
JD	 0.9795	 0.1420
JH	 0.9744	 0.1160
JK	 0.9848	 0.1070
JX	 1.0000	 0.1980
JY	 0.6731	 -0.0200
JZ	 0.9943	 0.1360
Jd	 0.9819	 0.1100
KA	 0.9786	 0.0560
KC	 0.9699	 0.0750
KD	 0.9736	 0.1220
KH	 0.9624	 0.0850
KK	 0.9804	 0.0760
KX	 0.9991	 0.1460
KY	 0.6000	 -0.0060
KZ	 1.0000	 0.1190
Kd	 0.9685	 0.0700
LA	 0.9749	 0.0430
LC	 0.9660	 0.0570
LD	 0.9550	 0.0730
LH	 0.9579	 0.0570
LK	 0.9777	 0.0560
LX	 0.9956	 0.0440
LY	 0.6308	 0.0210
LZ	 0.9800	 0.0890
Ld	 0.9542	 0.0490
MC	 0.9724	 0.0470
MD	 0.9374	 0.0150
MH	 0.9579	 0.0440
MK	 0.9705	 0.0510
MX	 0.9930	 0.0460
MY	 0.6077	 0.0550
MZ	 0.9657	 0.0800
Md	 0.9399	 0.0440
QA	 0.9731	 0.0410