



## Full wwPDB EM Validation Report ⓘ

Feb 25, 2024 – 09:27 AM EST

PDB ID : 6X62  
EMDB ID : EMD-22068  
Title : Legionella pneumophila Dot 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 : 3.50 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:

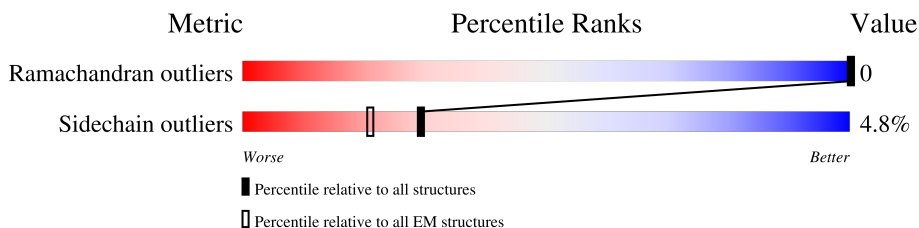
EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 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.



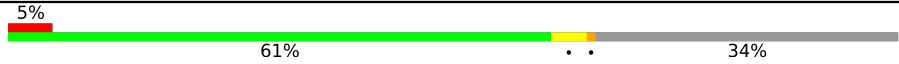

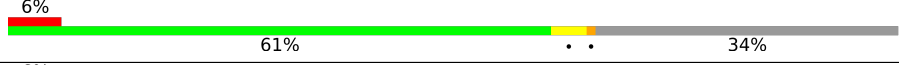

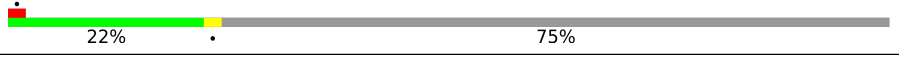

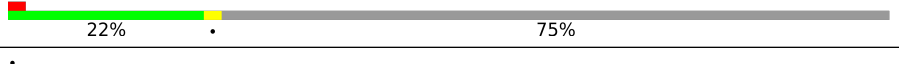







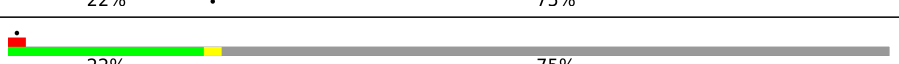

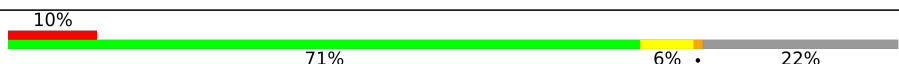
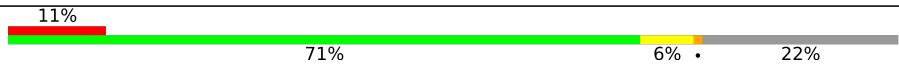
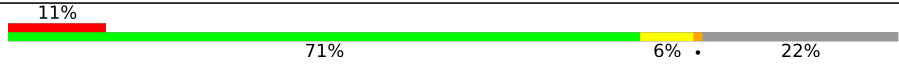


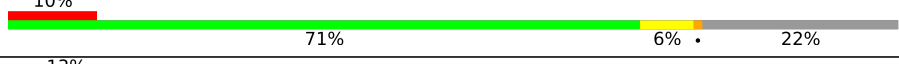
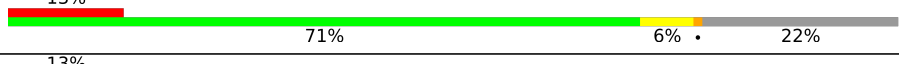


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	5% 61% 34%
1	BC	303	6% 61% 34%
1	CC	303	7% 61% 34%
1	DC	303	5% 62% 34%
1	EC	303	7% 61% 34%
1	FC	303	5% 61% 34%
1	GC	303	5% 61% 34%
1	HC	303	5% 61% 34%
1	IC	303	6% 61% 34%

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Mol	Chain	Length	Quality of chain
1	JC	303	
1	KC	303	
1	LC	303	
1	MC	303	
2	AH	361	
2	BH	361	
2	CH	361	
2	DH	361	
2	EH	361	
2	FH	361	
2	GH	361	
2	HH	361	
2	IH	361	
2	JH	361	
2	KH	361	
2	LH	361	
2	MH	361	
3	AK	189	
3	BK	189	
3	CK	189	
3	DK	189	
3	EK	189	
3	FK	189	
3	GK	189	
3	HK	189	



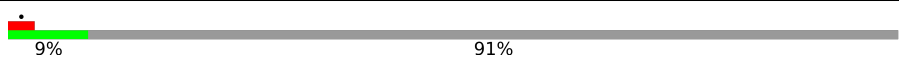
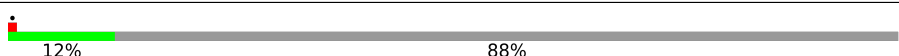
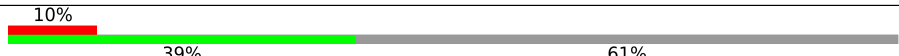

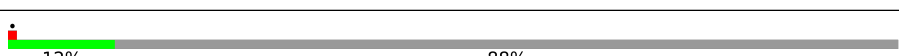


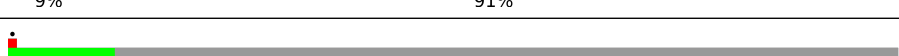

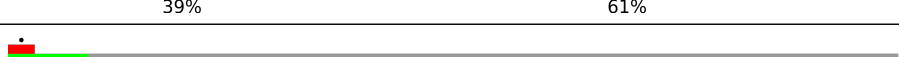
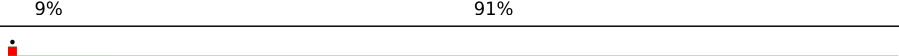
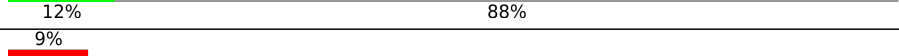
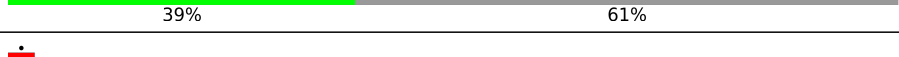
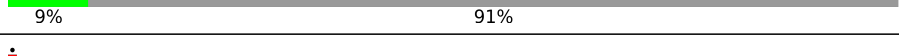


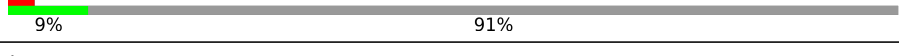


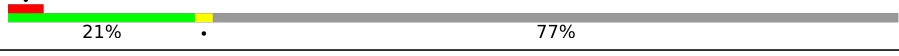



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Mol	Chain	Length	Quality of chain	
3	IK	189	12% 71% 6% • 22%	
3	JK	189	8% 71% 6% • 22%	
3	KK	189	11% 71% 6% • 22%	
3	LK	189	11% 71% 6% • 22%	
3	MK	189	9% 71% 6% • 22%	
4	AX	579	9% 39% 61%	
4	AY	579	9% 91%	
4	AZ	579	12% 88%	
4	BX	579	9% 39% 61%	
4	BY	579	9% 91%	
4	BZ	579	12% 88%	
4	CX	579	10% 39% 61%	
4	CY	579	9% 91%	
4	CZ	579	12% 88%	
4	DX	579	10% 39% 61%	
4	DY	579	9% 91%	
4	DZ	579	12% 88%	
4	EX	579	9% 39% 61%	
4	EY	579	9% 91%	
4	EZ	579	12% 88%	
4	FX	579	9% 39% 61%	
4	FY	579	9% 91%	
4	FZ	579	12% 88%	
4	GX	579	10% 39% 61%	
4	GY	579	9% 91%	

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Mol	Chain	Length	Quality of chain
4	GZ	579	 12% 88%
4	HX	579	 9% 39% 61%
4	HY	579	 9% 91%
4	HZ	579	 12% 88%
4	IX	579	 10% 39% 61%
4	IY	579	 9% 91%
4	IZ	579	 12% 88%
4	JX	579	 10% 39% 61%
4	JY	579	 9% 91%
4	JZ	579	 12% 88%
4	KX	579	 9% 39% 61%
4	KY	579	 9% 91%
4	KZ	579	 12% 88%
4	LX	579	 9% 39% 61%
4	LY	579	 9% 91%
4	LZ	579	 12% 88%
4	MX	579	 9% 39% 61%
4	MY	579	 9% 91%
4	MZ	579	 12% 88%
4	N	579	 21% 77%
4	O	579	 21% 77%
4	P	579	 21% 77%
4	Q	579	 21% 77%
4	R	579	 21% 77%
4	S	579	 21% 77%

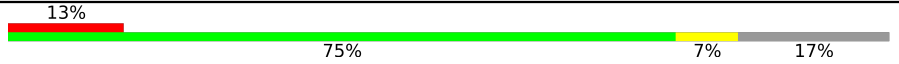
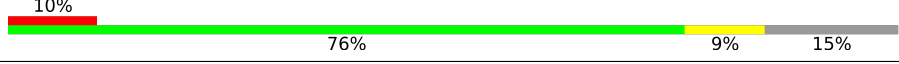
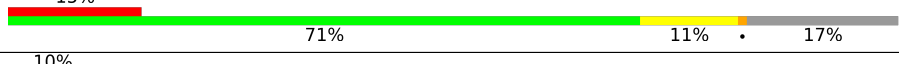


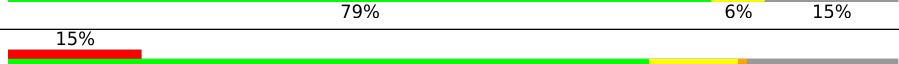
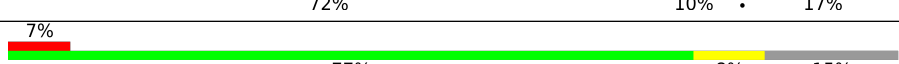
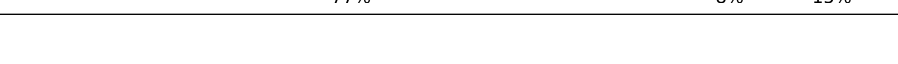
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Mol	Chain	Length	Quality of chain
4	T	579	21% 77%
4	U	579	21% 77%
4	V	579	21% 77%
4	W	579	21% 77%
4	X	579	21% 77%
4	Y	579	21% 77%
4	Z	579	21% 77%
5	AD	163	13% 72% 10% 17%
5	Ad	163	10% 75% 10% 15%
5	BD	163	17% 75% 8% 17%
5	Bd	163	9% 78% 7% 15%
5	CD	163	15% 75% 8% 17%
5	Cd	163	9% 77% 7% 15%
5	DD	163	15% 75% 7% 17%
5	Dd	163	12% 75% 10% 15%
5	ED	163	13% 74% 9% 17%
5	Ed	163	10% 77% 8% 15%
5	FD	163	16% 75% 7% 17%
5	Fd	163	11% 77% 8% 15%
5	GD	163	13% 72% 9% 17%
5	Gd	163	9% 76% 9% 15%
5	HD	163	14% 77% 6% 17%
5	Hd	163	11% 77% 8% 15%
5	ID	163	13% 77% 5% 17%
5	Id	163	9% 77% 7% 15%

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Mol	Chain	Length	Quality of chain
5	JD	163	 <p>13% 75% 7% 17%</p>
5	Jd	163	 <p>10% 76% 9% 15%</p>
5	KD	163	 <p>15% 71% 11% 17%</p>
5	Kd	163	 <p>10% 76% 9% 15%</p>
5	LD	163	 <p>15% 79% 6% 17%</p>
5	Ld	163	 <p>12% 79% 6% 15%</p>
5	MD	163	 <p>15% 72% 10% 17%</p>
5	Md	163	 <p>7% 77% 8% 15%</p>

## 2 Entry composition [i](#)

There are 5 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
			Total	C	N	O	S		
1	AC	200	1596	1016	280	295	5	0	0
1	EC	200	1596	1016	280	295	5	0	0
1	FC	200	1596	1016	280	295	5	0	0
1	GC	200	1596	1016	280	295	5	0	0
1	HC	200	1596	1016	280	295	5	0	0
1	IC	200	1596	1016	280	295	5	0	0
1	JC	200	1596	1016	280	295	5	0	0
1	KC	200	1596	1016	280	295	5	0	0
1	LC	200	1596	1016	280	295	5	0	0
1	MC	200	1596	1016	280	295	5	0	0
1	BC	200	1596	1016	280	295	5	0	0
1	CC	200	1596	1016	280	295	5	0	0
1	DC	200	1596	1016	280	295	5	0	0

- Molecule 2 is a protein called Type IV secretion protein IcmK.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	DH	89	678	432	119	123	4	0	0
2	EH	89	678	432	119	123	4	0	0

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

- Molecule 3 is a protein called Inner membrane lipoprotein YiaD.

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

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Mol	Chain	Residues	Atoms				AltConf	Trace	
3	LK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
3	MK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
3	AK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
3	BK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
3	CK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		

- Molecule 4 is a protein called Type IV secretion system unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	DX	228	Total	C	N	O	0	0
			1140	684	228	228		
4	DY	52	Total	C	N	O	0	0
			260	156	52	52		
4	DZ	70	Total	C	N	O	0	0
			350	210	70	70		
4	EX	228	Total	C	N	O	0	0
			1140	684	228	228		
4	EY	52	Total	C	N	O	0	0
			260	156	52	52		
4	EZ	70	Total	C	N	O	0	0
			350	210	70	70		
4	FX	228	Total	C	N	O	0	0
			1140	684	228	228		
4	FY	52	Total	C	N	O	0	0
			260	156	52	52		
4	FZ	70	Total	C	N	O	0	0
			350	210	70	70		
4	GX	228	Total	C	N	O	0	0
			1140	684	228	228		
4	GY	52	Total	C	N	O	0	0
			260	156	52	52		
4	GZ	70	Total	C	N	O	0	0
			350	210	70	70		
4	HX	228	Total	C	N	O	0	0
			1140	684	228	228		
4	HY	52	Total	C	N	O	0	0
			260	156	52	52		

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Mol	Chain	Residues	Atoms				AltConf	Trace	
4	HZ	70	Total	C	N	O	0	0	
			350	210	70	70			
4	IX	228	Total	C	N	O	0	0	
			1140	684	228	228			
4	IY	52	Total	C	N	O	0	0	
			260	156	52	52			
4	IZ	70	Total	C	N	O	0	0	
			350	210	70	70			
4	JX	228	Total	C	N	O	0	0	
			1140	684	228	228			
4	JY	52	Total	C	N	O	0	0	
			260	156	52	52			
4	JZ	70	Total	C	N	O	0	0	
			350	210	70	70			
4	KX	228	Total	C	N	O	0	0	
			1140	684	228	228			
4	KY	52	Total	C	N	O	0	0	
			260	156	52	52			
4	KZ	70	Total	C	N	O	0	0	
			350	210	70	70			
4	LX	228	Total	C	N	O	0	0	
			1140	684	228	228			
4	LY	52	Total	C	N	O	0	0	
			260	156	52	52			
4	LZ	70	Total	C	N	O	0	0	
			350	210	70	70			
4	MX	228	Total	C	N	O	0	0	
			1140	684	228	228			
4	MY	52	Total	C	N	O	0	0	
			260	156	52	52			
4	MZ	70	Total	C	N	O	0	0	
			350	210	70	70			
4	N	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	O	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	P	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	Q	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	R	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	T	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	U	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	V	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	W	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	X	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	Y	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	Z	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	AX	228	Total	C	N	O		0	0
			1140	684	228	228			
4	AY	52	Total	C	N	O		0	0
			260	156	52	52			
4	AZ	70	Total	C	N	O		0	0
			350	210	70	70			
4	BX	228	Total	C	N	O		0	0
			1140	684	228	228			
4	BY	52	Total	C	N	O		0	0
			260	156	52	52			
4	BZ	70	Total	C	N	O		0	0
			350	210	70	70			
4	CX	228	Total	C	N	O		0	0
			1140	684	228	228			
4	CY	52	Total	C	N	O		0	0
			260	156	52	52			
4	CZ	70	Total	C	N	O		0	0
			350	210	70	70			

- Molecule 5 is a protein called DotD.

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

*Continued on next page...*

*Continued from previous page...*

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

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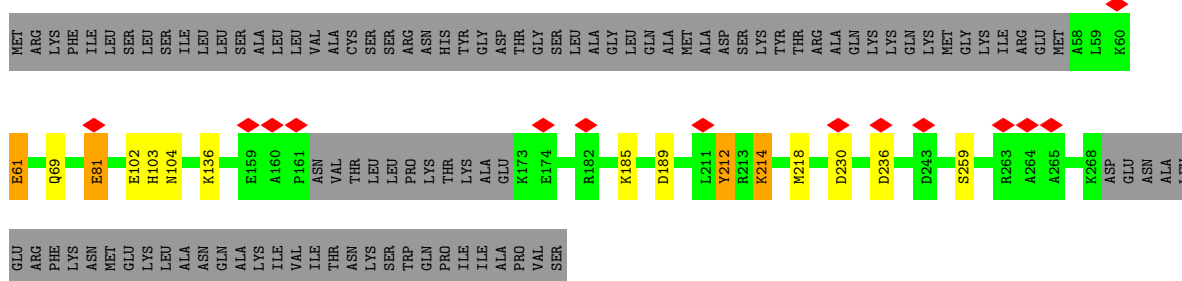
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	CD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
5	Cd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
5	DD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		

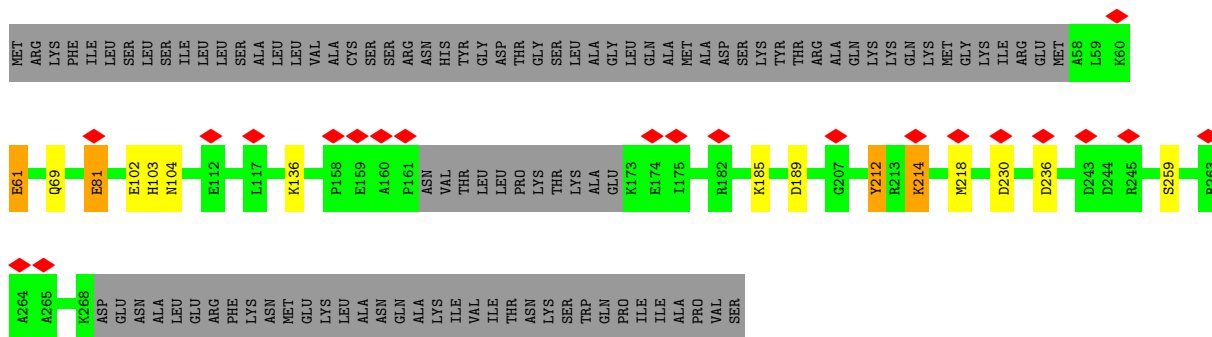
### 3 Residue-property plots [i](#)

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

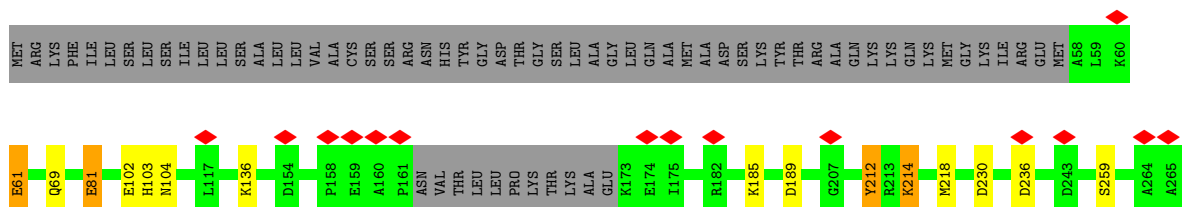
- Molecule 1: DotC



- Molecule 1: DotC

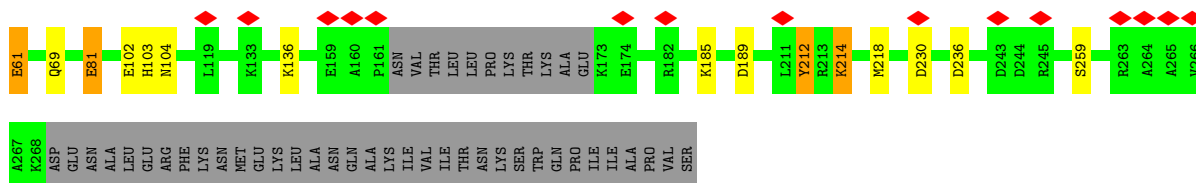


- Molecule 1: DotC

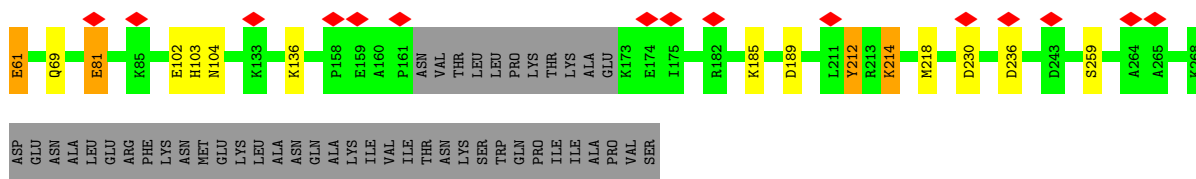
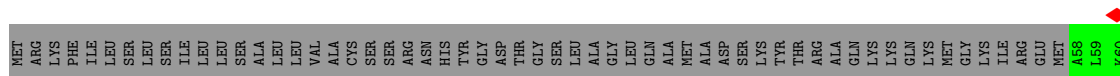




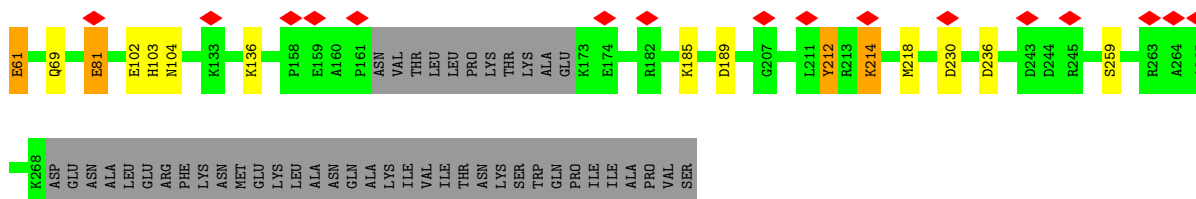
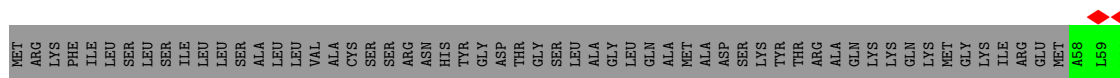




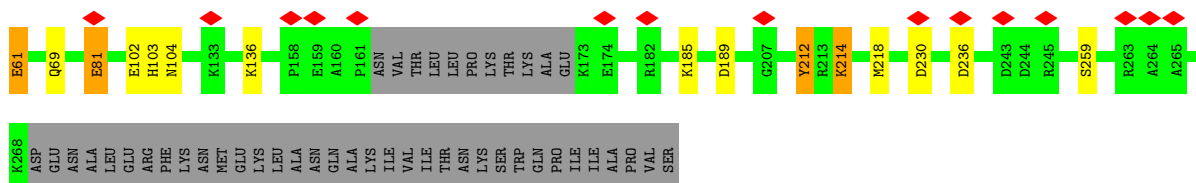
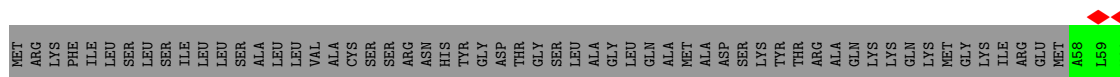
• Molecule 1: DotC



• Molecule 1: DotC



• Molecule 1: DotC



• Molecule 1: DotC



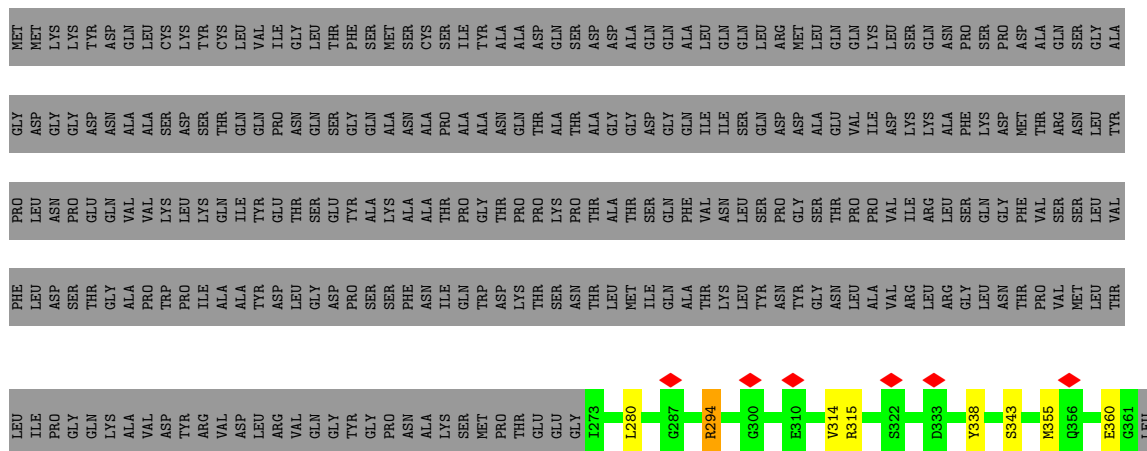




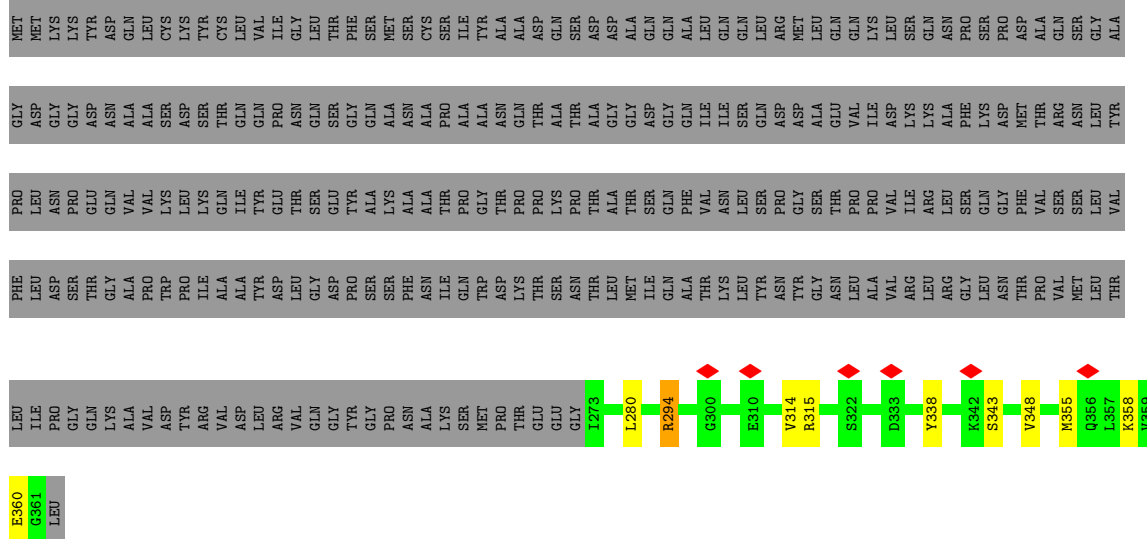




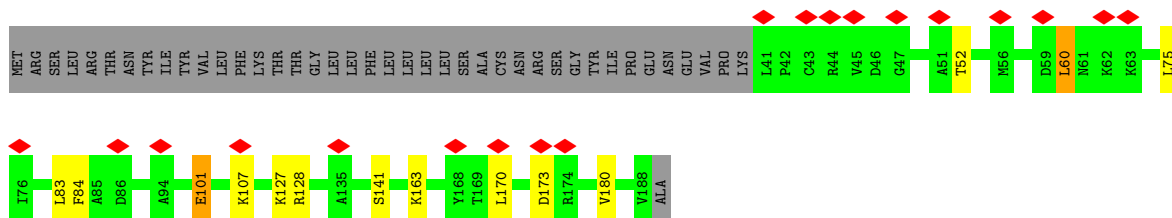
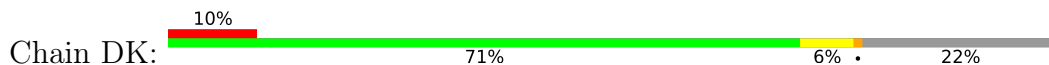




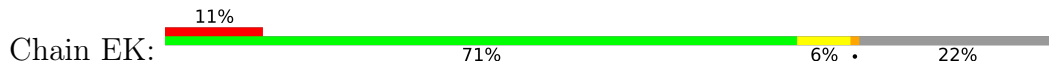
• Molecule 2: Type IV secretion protein IcmK

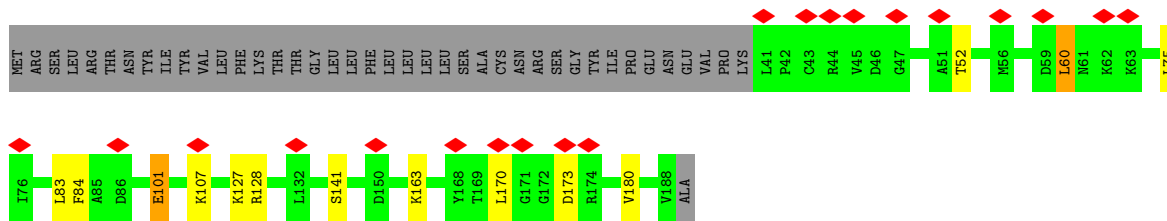


• Molecule 3: Inner membrane lipoprotein YiaD

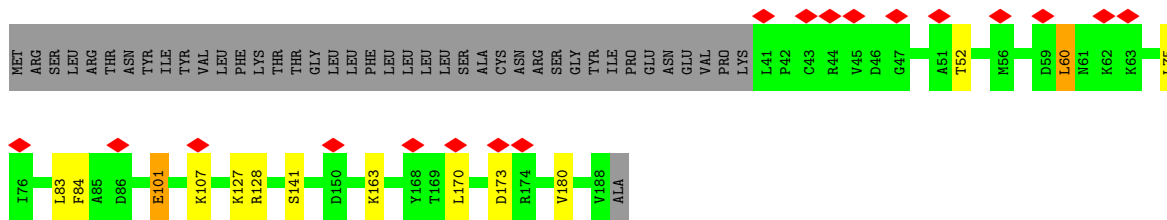
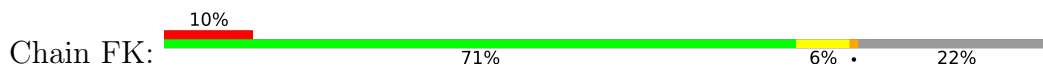


• Molecule 3: Inner membrane lipoprotein YiaD

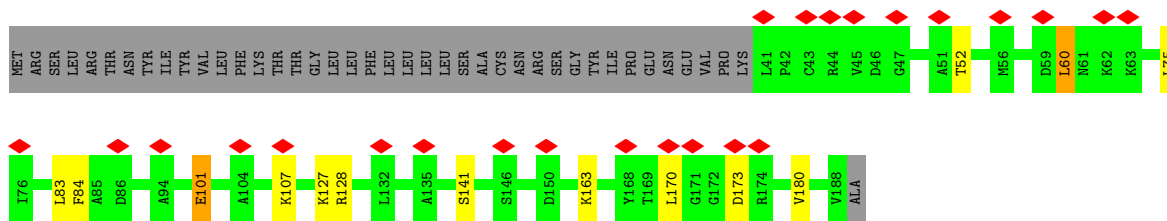
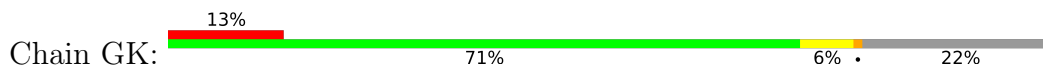




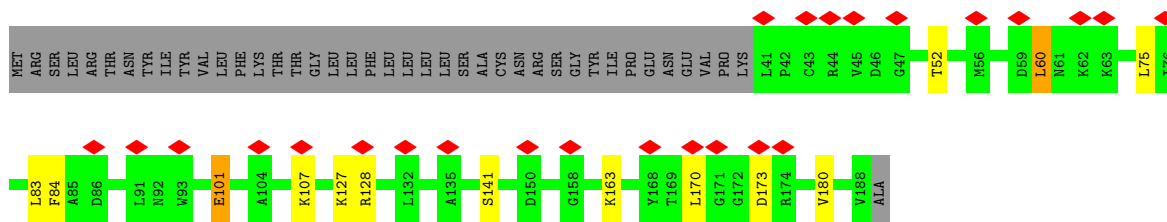
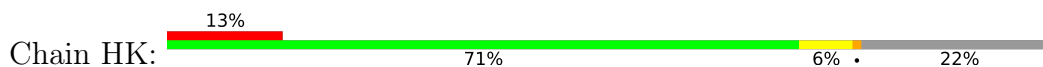
• Molecule 3: Inner membrane lipoprotein YiaD



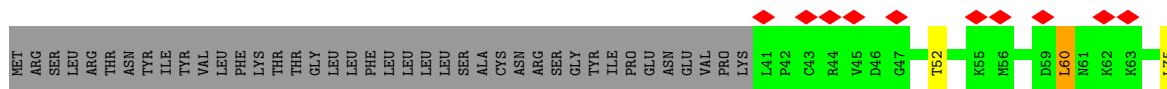
• Molecule 3: Inner membrane lipoprotein YiaD



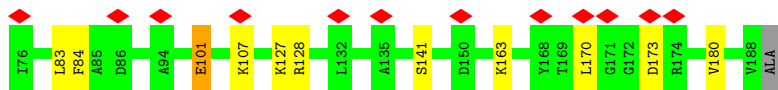
• Molecule 3: Inner membrane lipoprotein YiaD



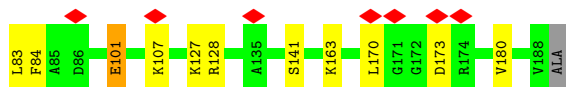
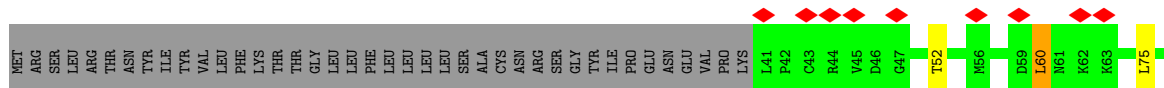
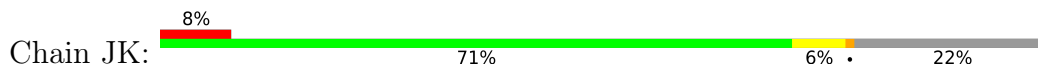
• Molecule 3: Inner membrane lipoprotein YiaD



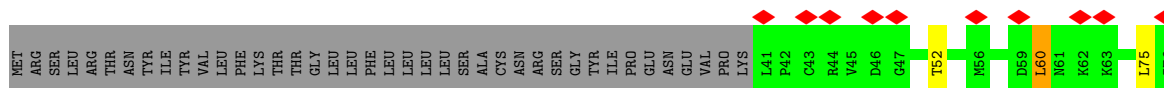
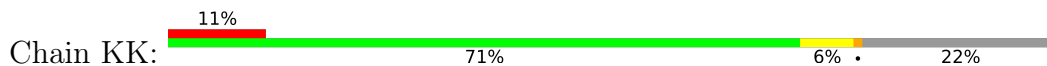




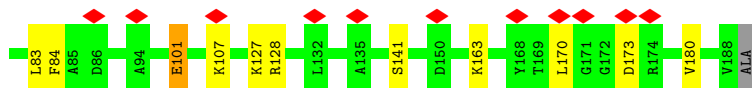
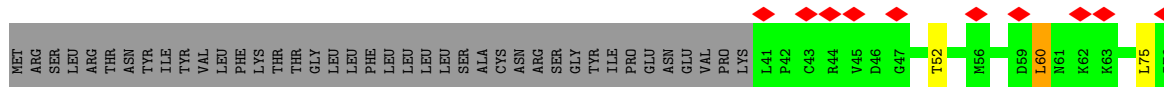
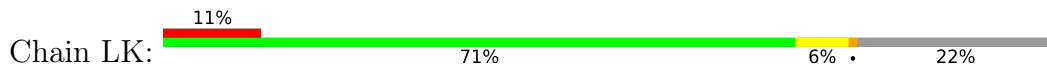
• Molecule 3: Inner membrane lipoprotein YiaD



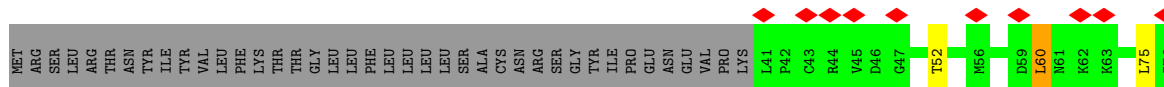
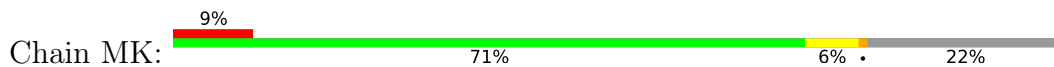
• Molecule 3: Inner membrane lipoprotein YiaD



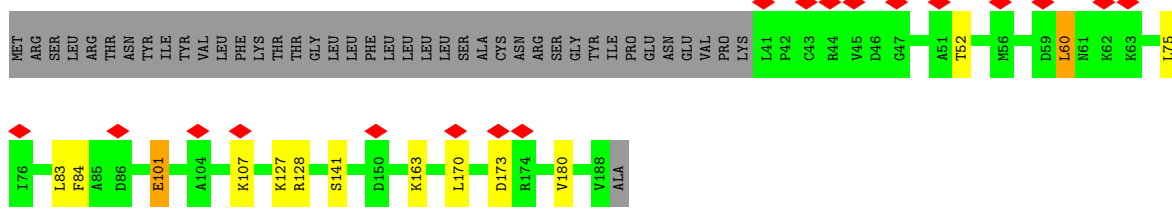
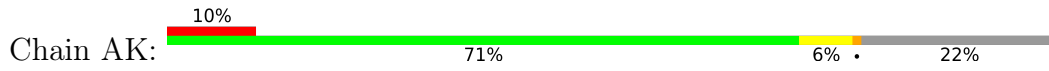
• Molecule 3: Inner membrane lipoprotein YiaD



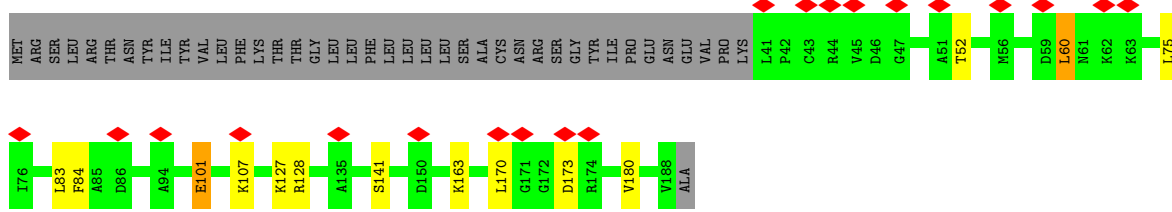
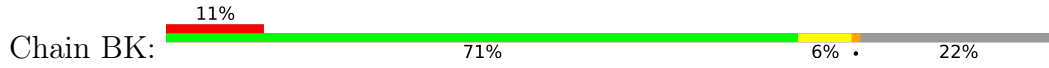
• Molecule 3: Inner membrane lipoprotein YiaD



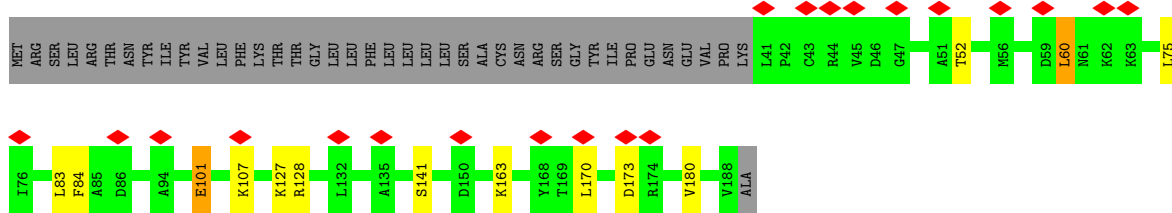
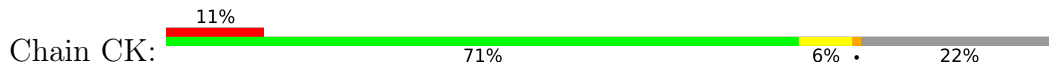
• Molecule 3: Inner membrane lipoprotein YiaD



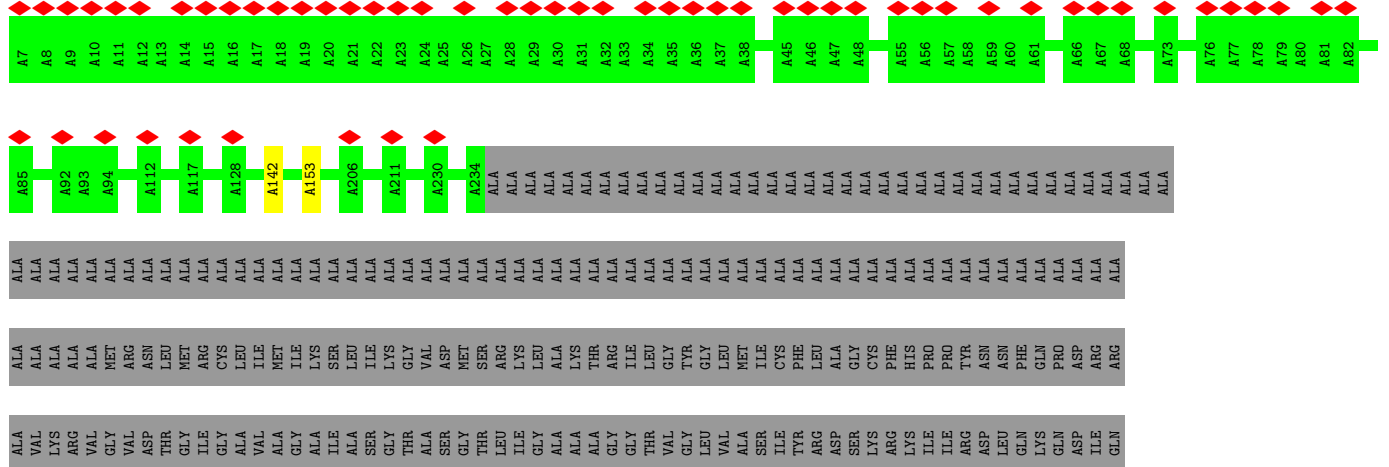
• Molecule 3: Inner membrane lipoprotein YiaD



• Molecule 3: Inner membrane lipoprotein YiaD



• Molecule 4: Type IV secretion system unknown protein fragment





















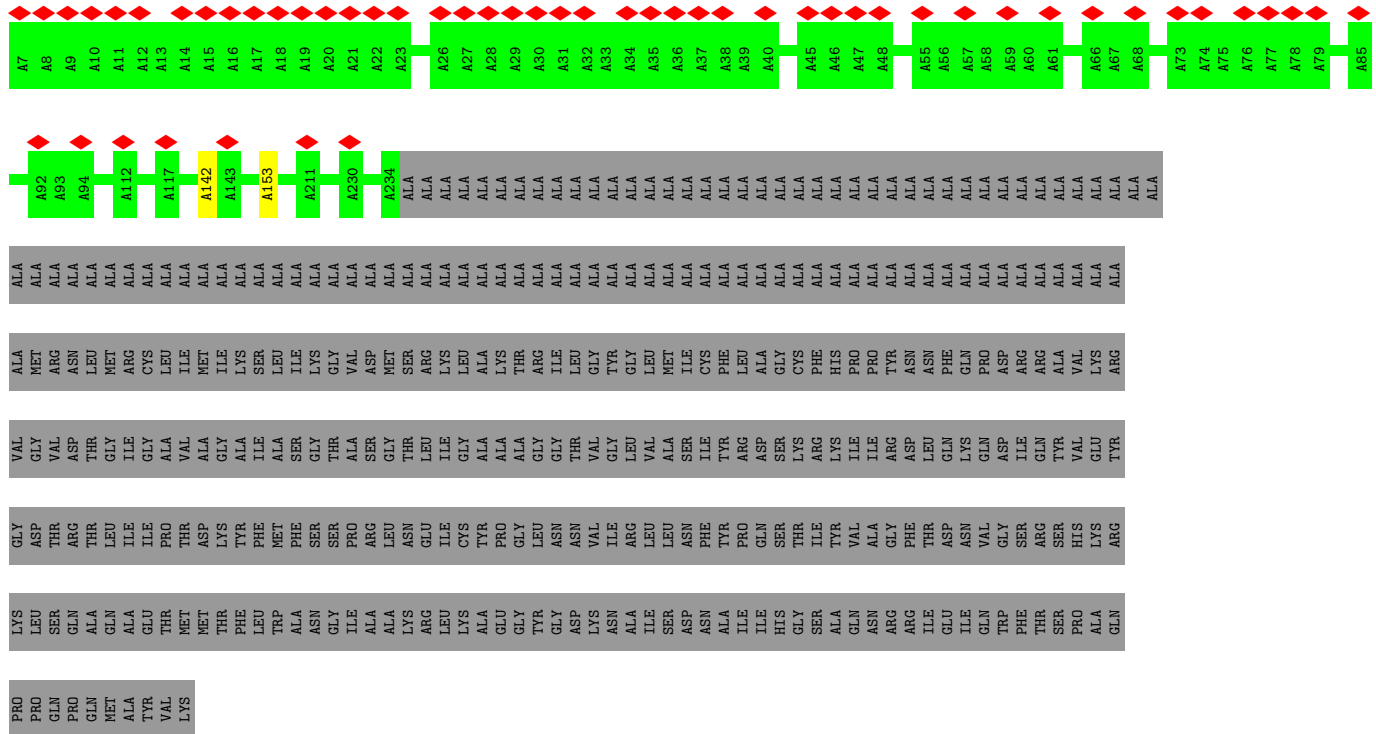






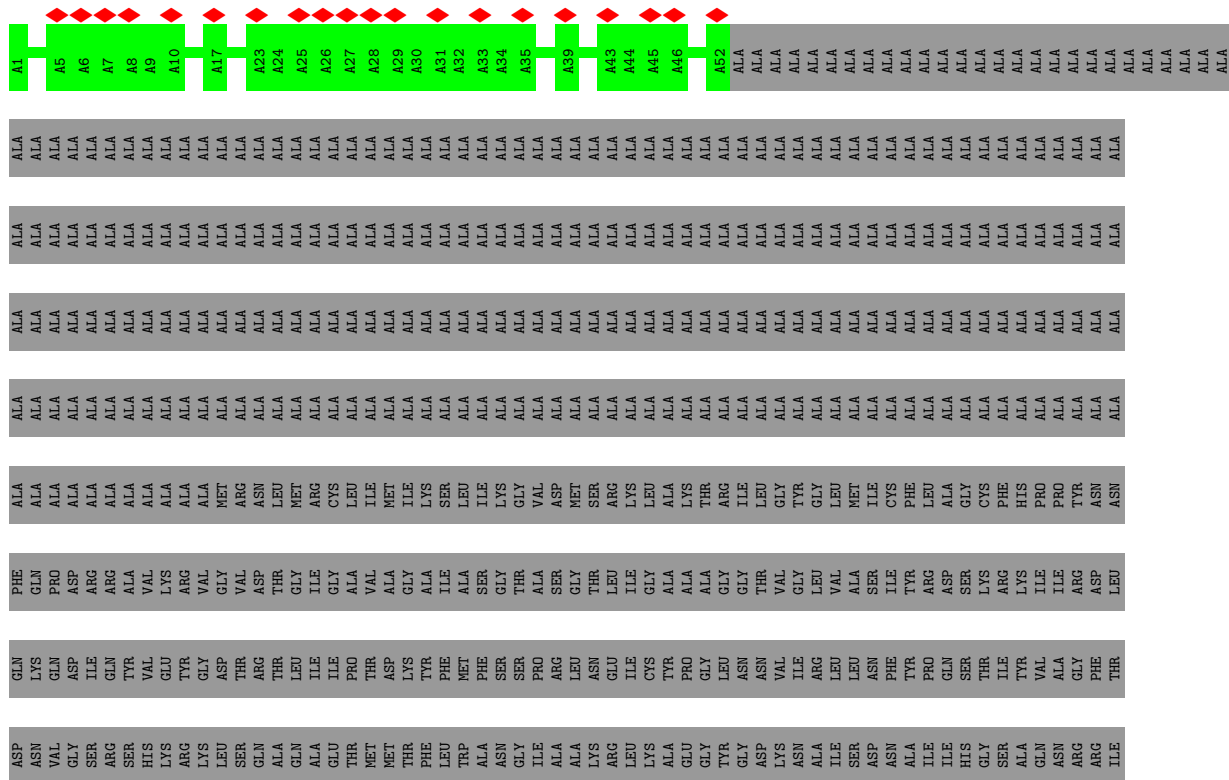






● Molecule 4: Type IV secretion system unknown protein fragment

Chain LY: 9% 91%

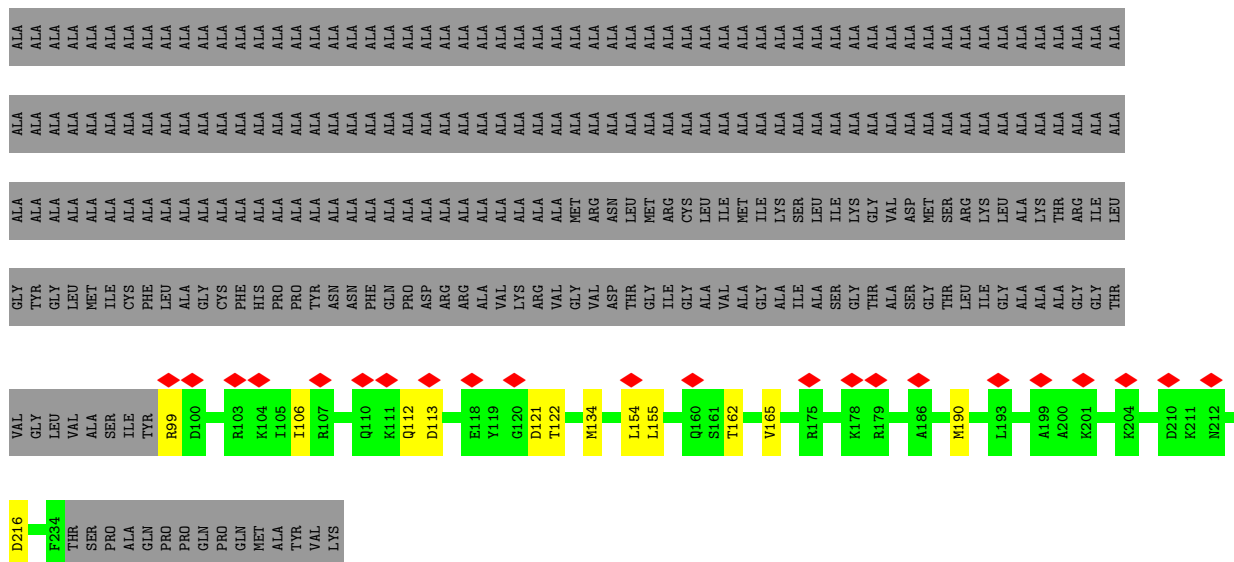




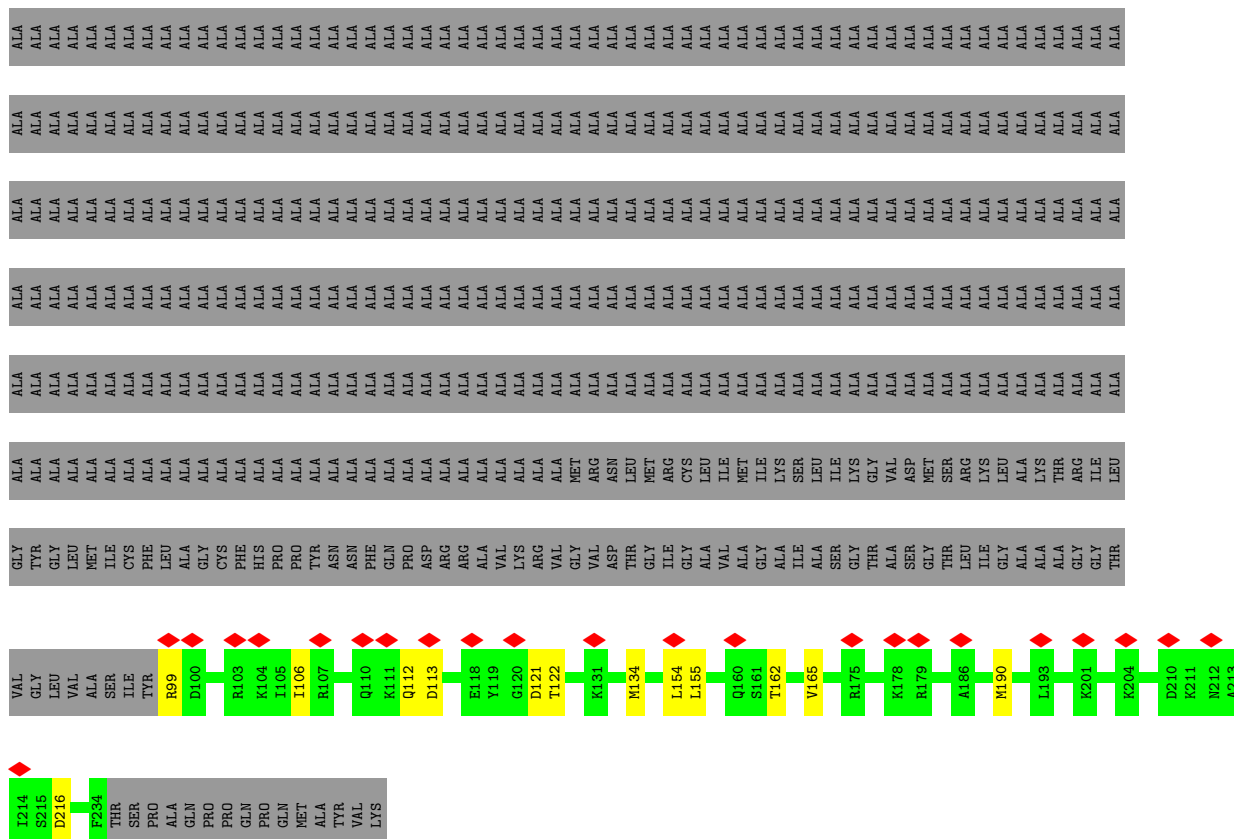






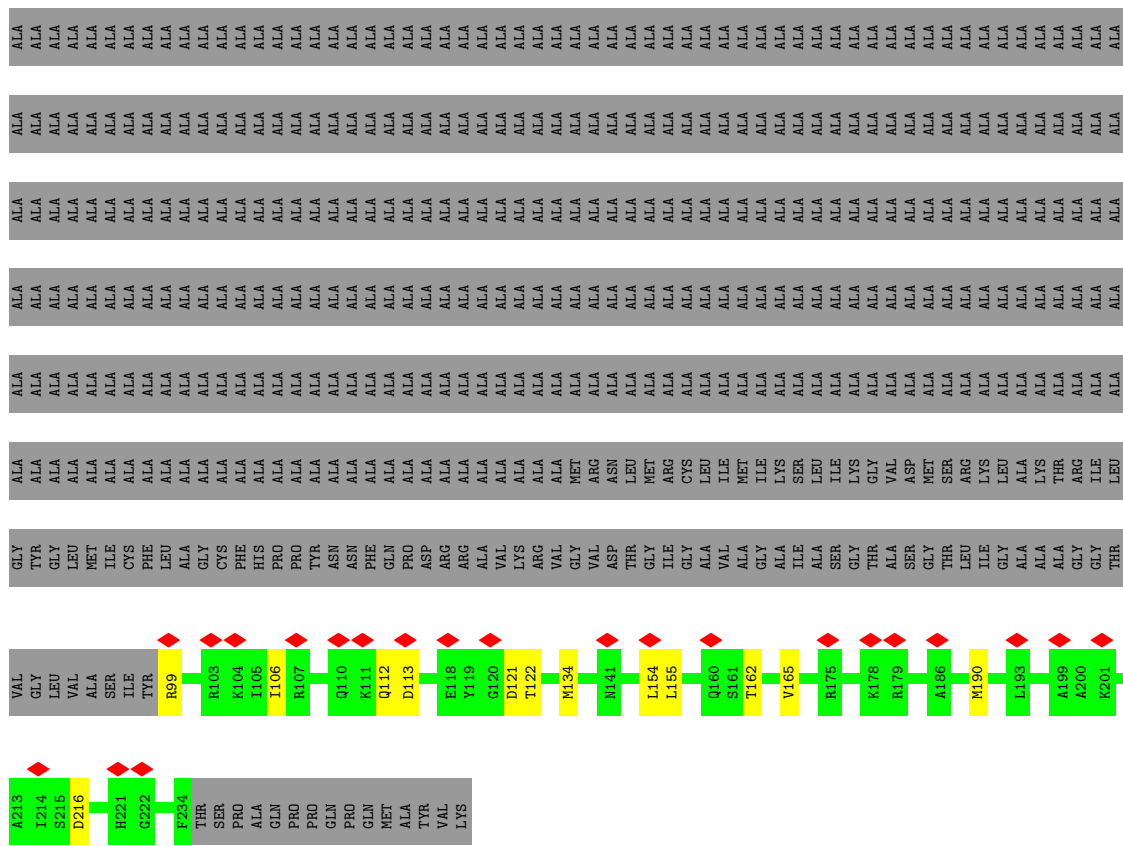


• Molecule 4: Type IV secretion system unknown protein fragment

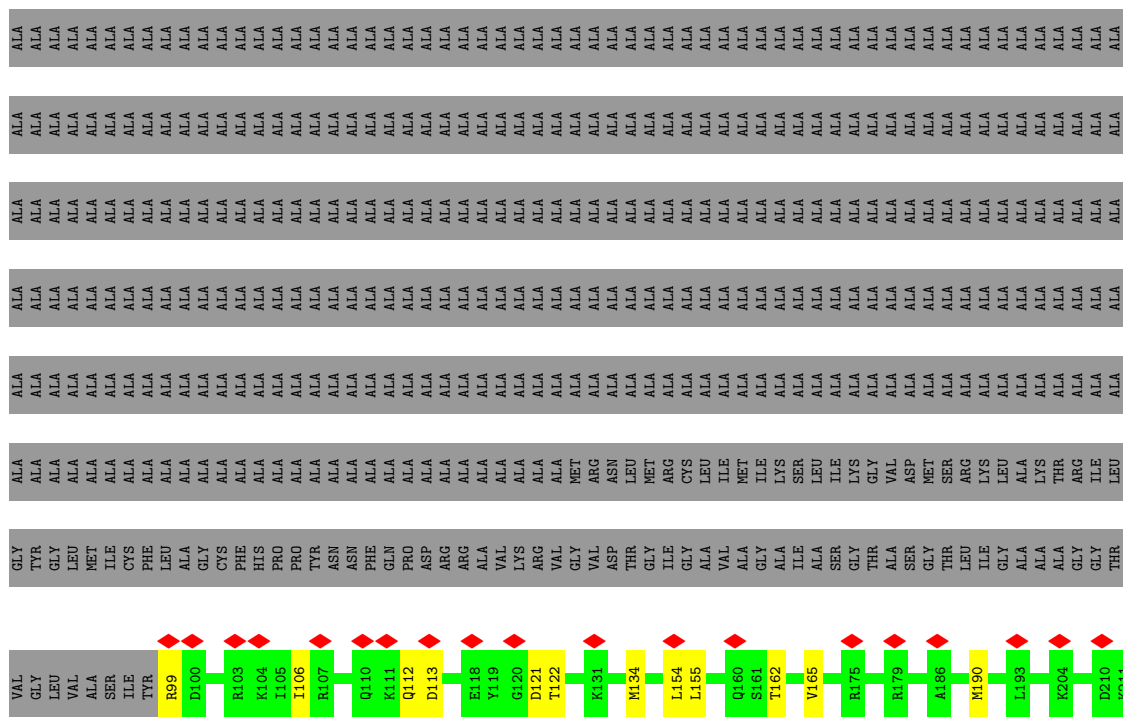


• Molecule 4: Type IV secretion system unknown protein fragment



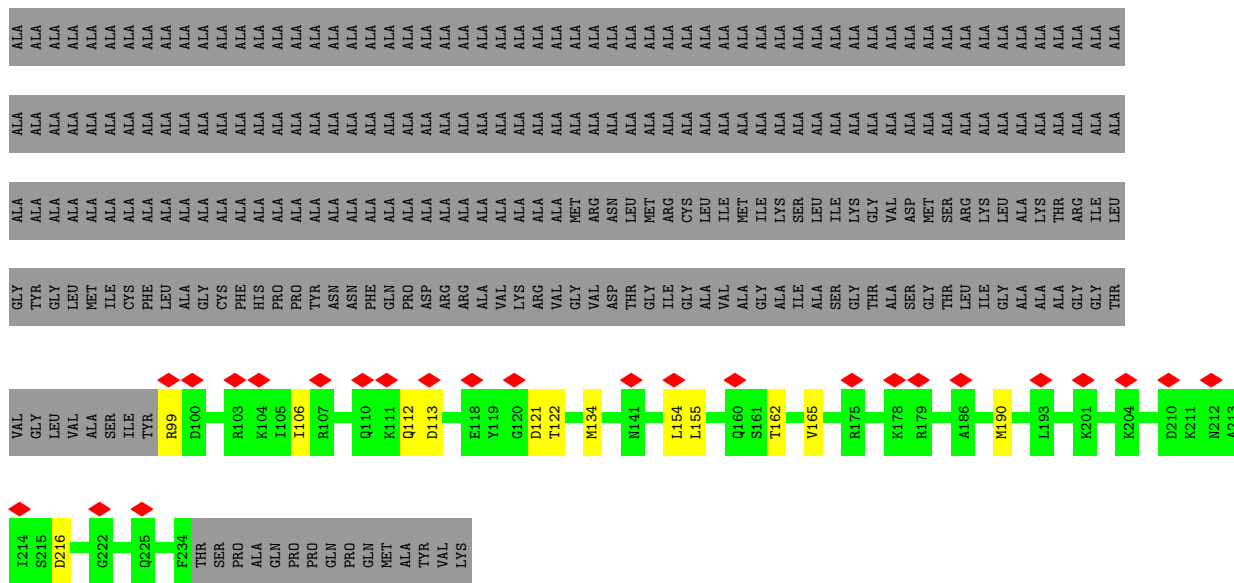


• Molecule 4: Type IV secretion system unknown protein fragment

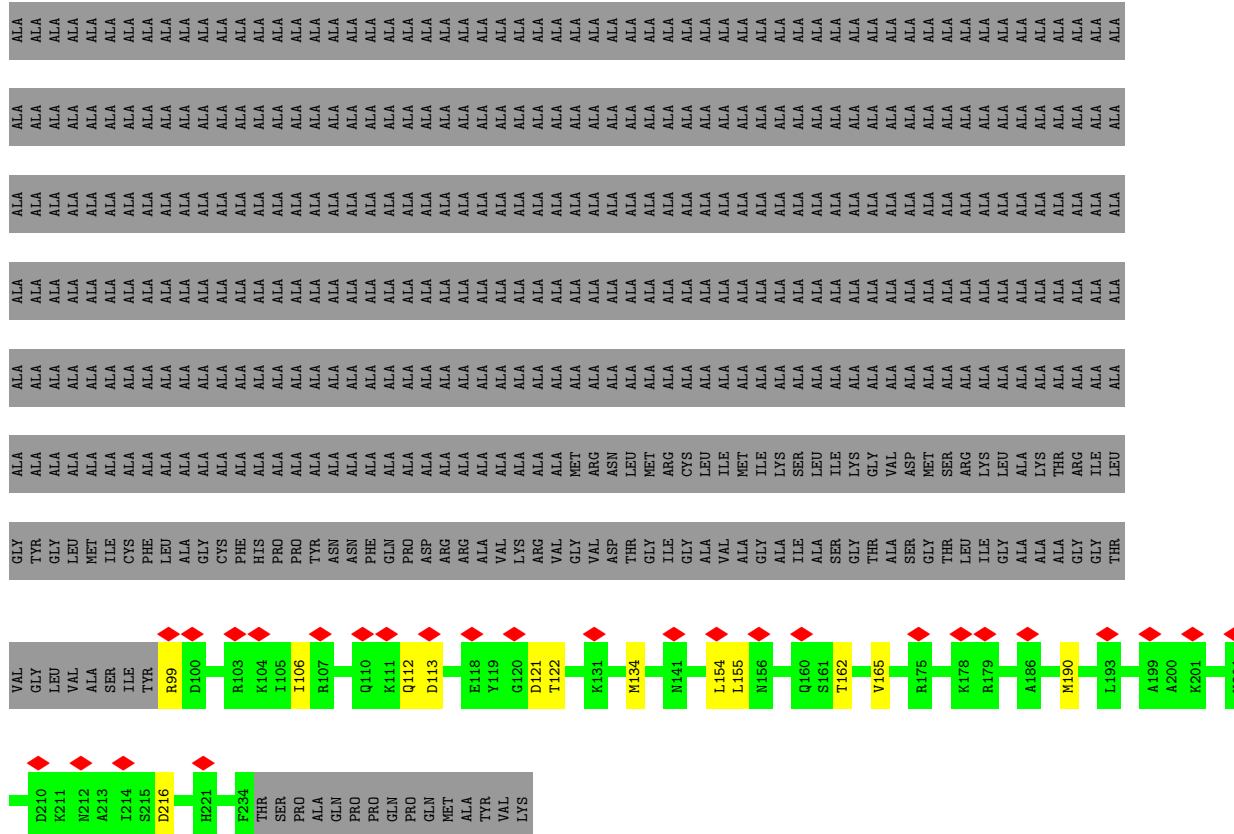








• Molecule 4: Type IV secretion system unknown protein fragment



• Molecule 4: Type IV secretion system unknown protein fragment





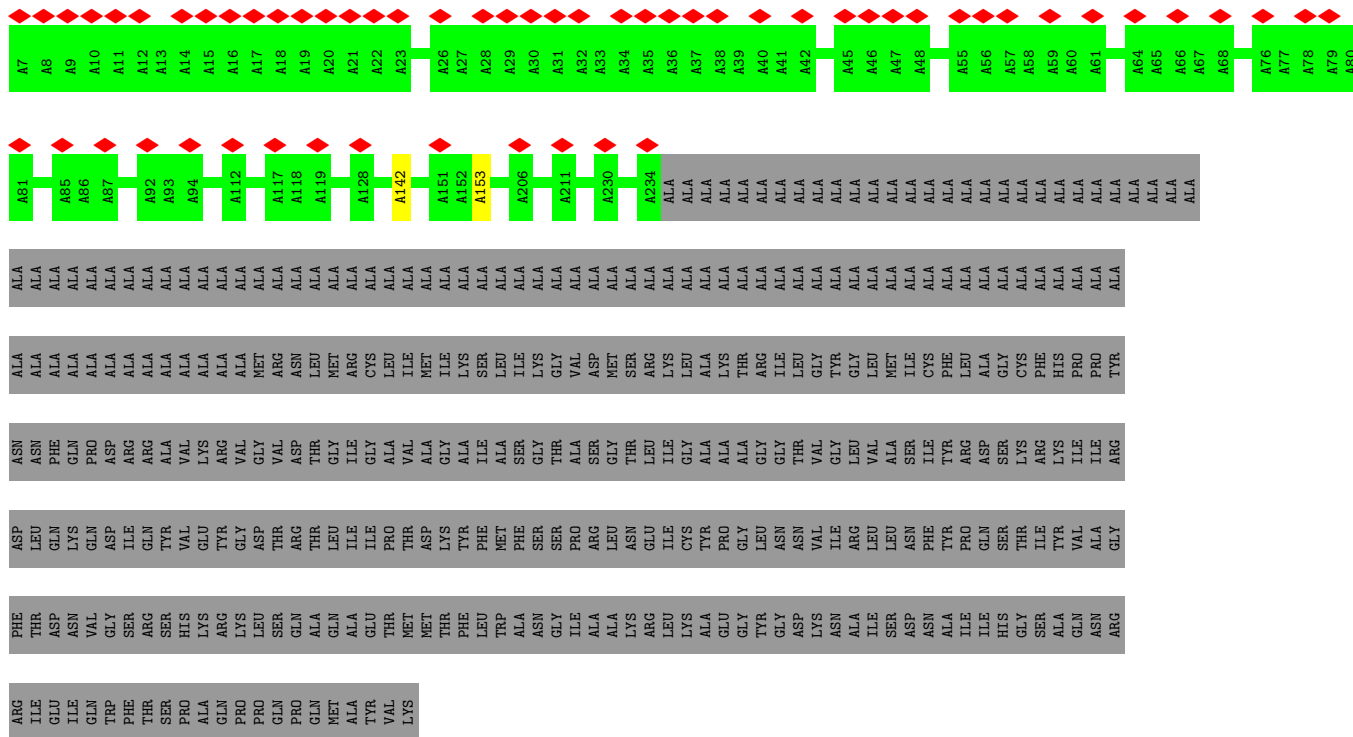






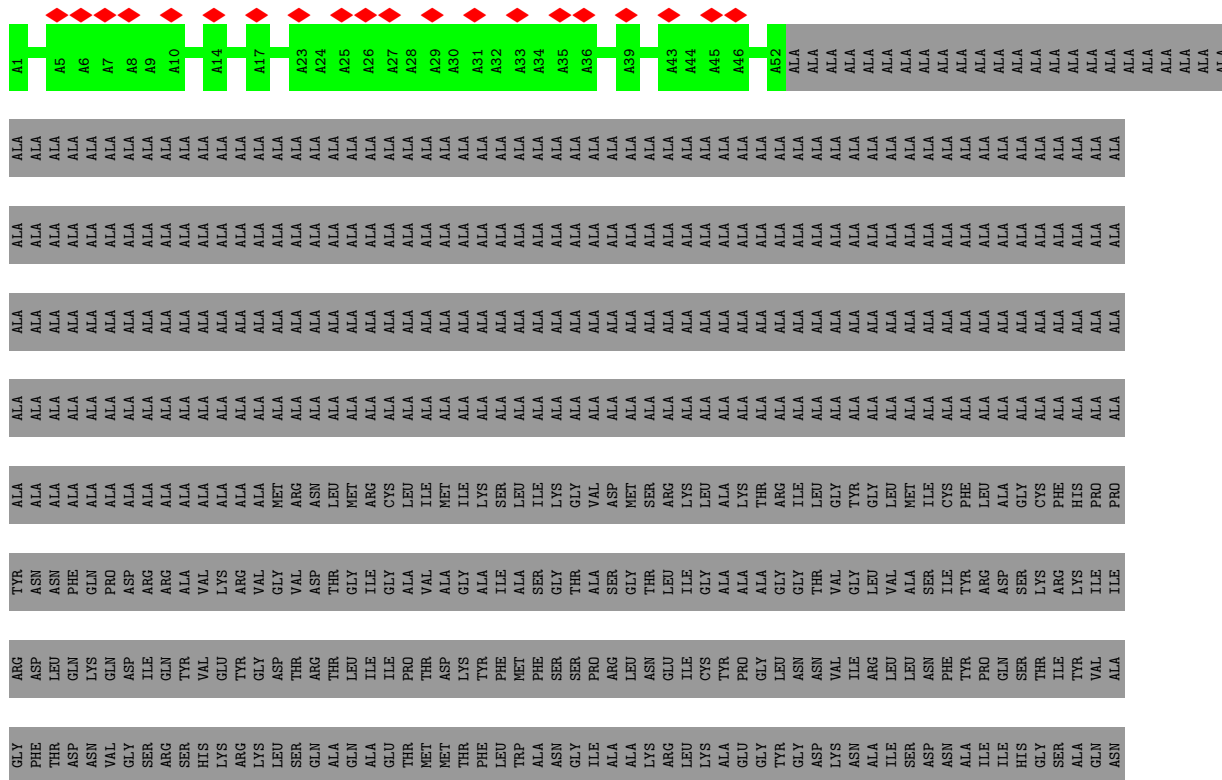




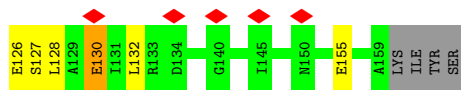


● Molecule 4: Type IV secretion system unknown protein fragment

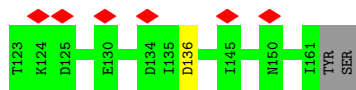
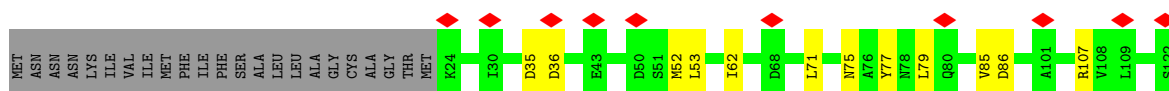
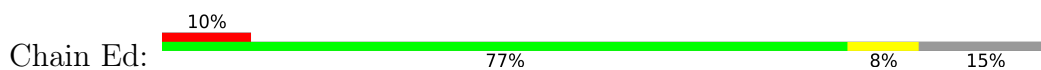
Chain CY: 9% 91%



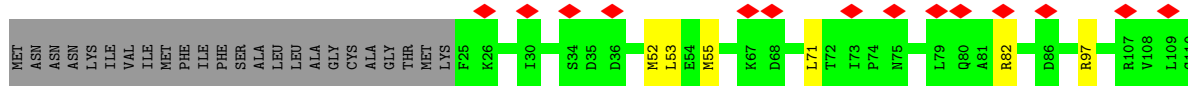
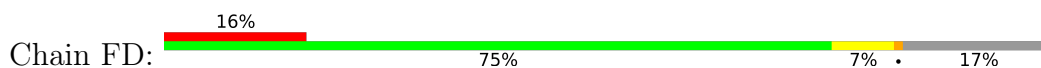




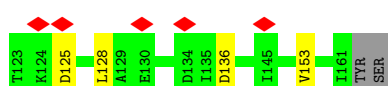
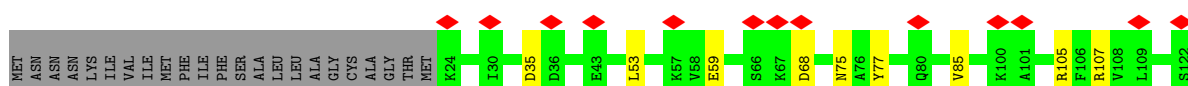
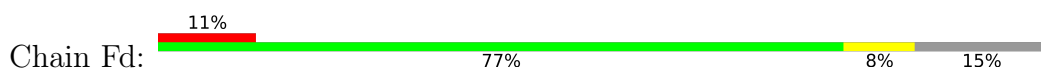
• Molecule 5: DotD



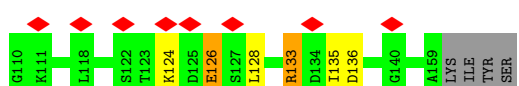
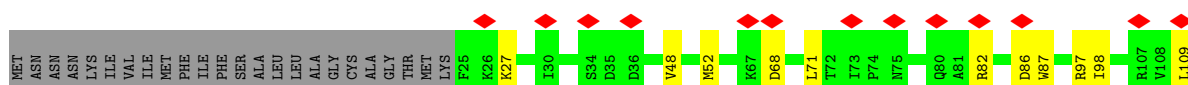
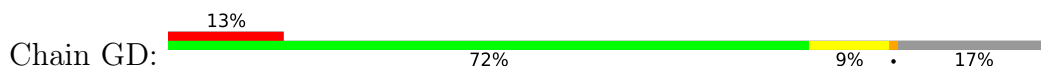
• Molecule 5: DotD



• Molecule 5: DotD

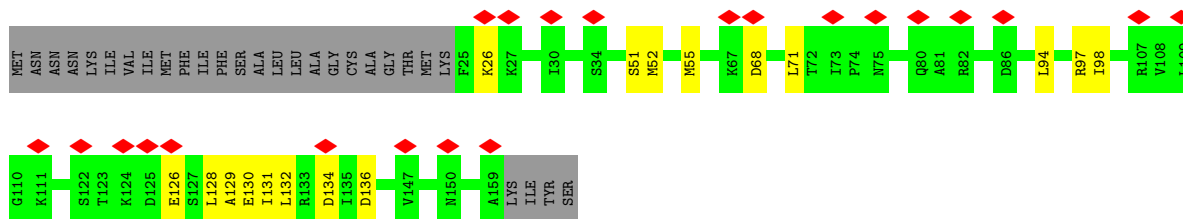
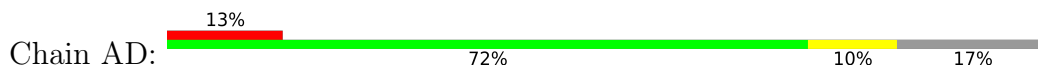


• Molecule 5: DotD

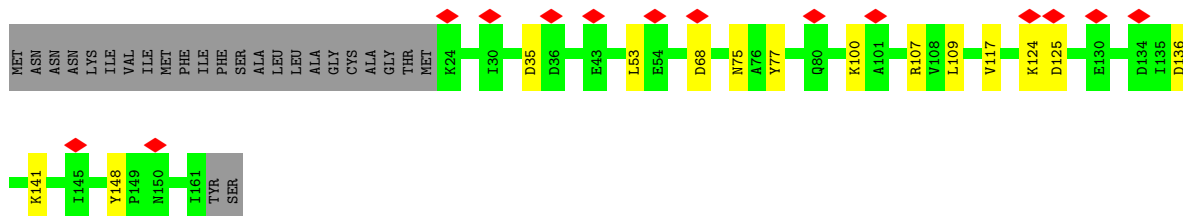
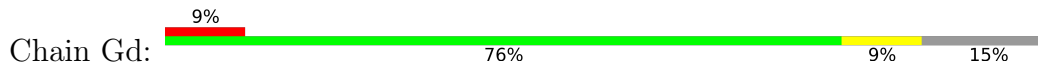


• Molecule 5: DotD

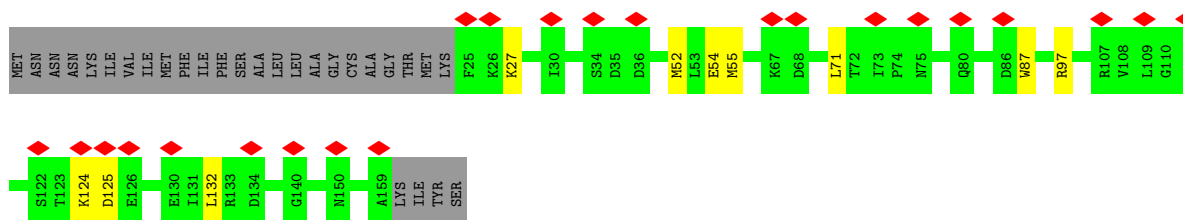
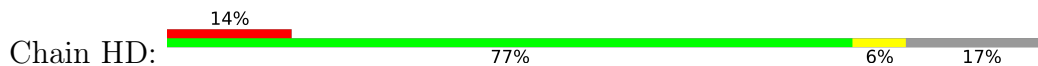




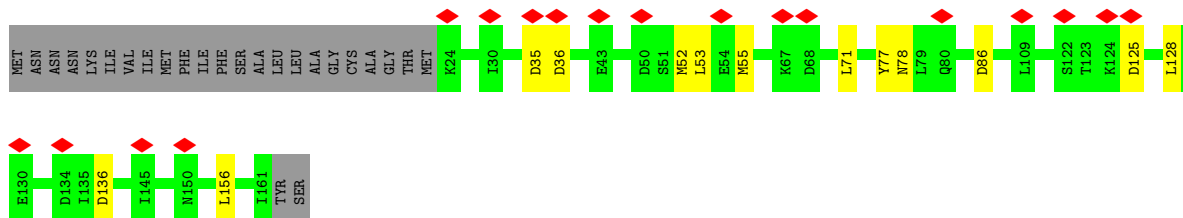
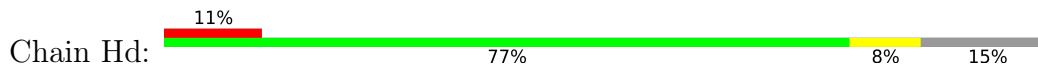
• Molecule 5: DotD



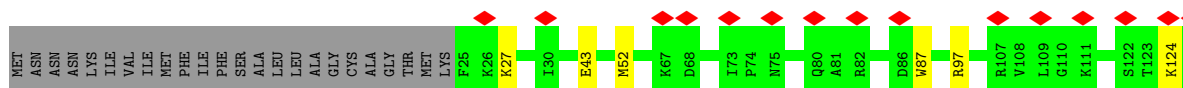
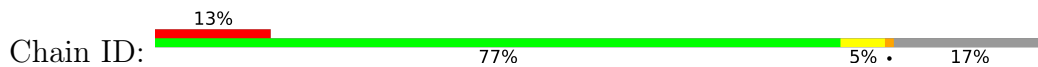
• Molecule 5: DotD

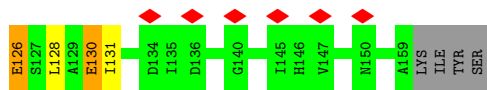


• Molecule 5: DotD

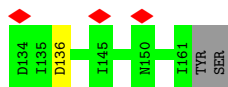
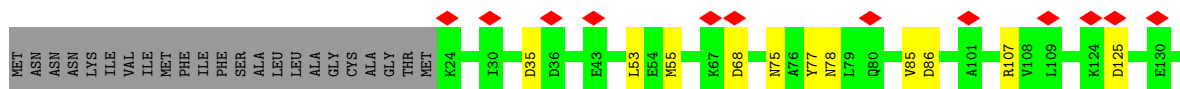
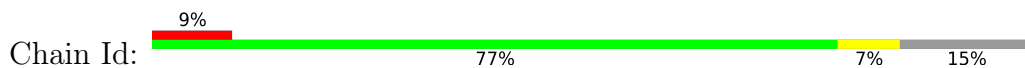


• Molecule 5: DotD

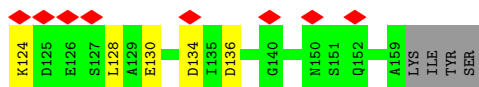
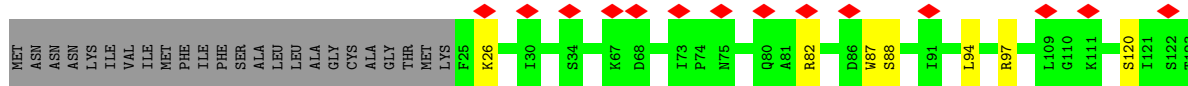
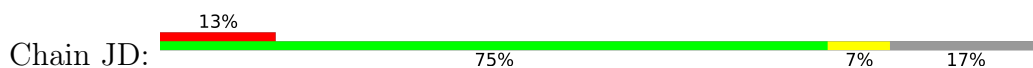




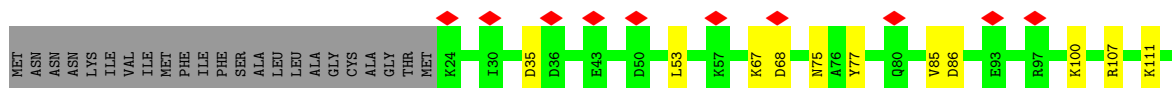
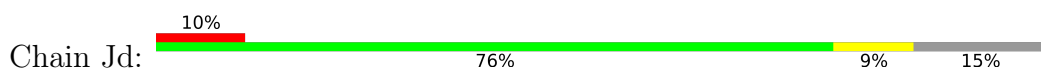
• Molecule 5: DotD



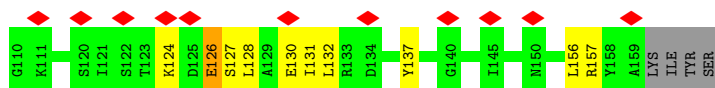
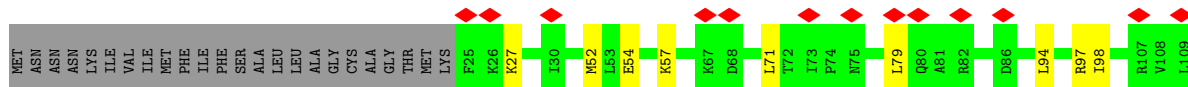
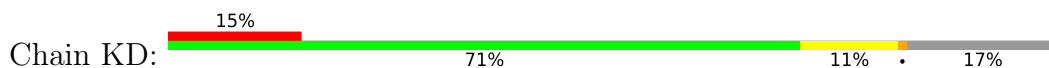
• Molecule 5: DotD



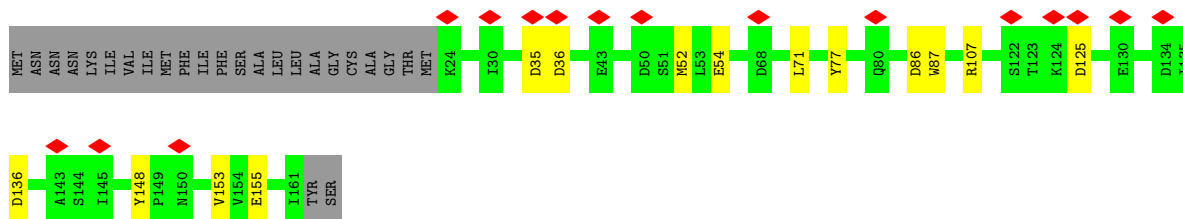
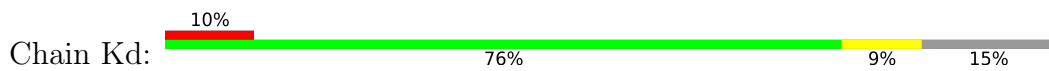
• Molecule 5: DotD



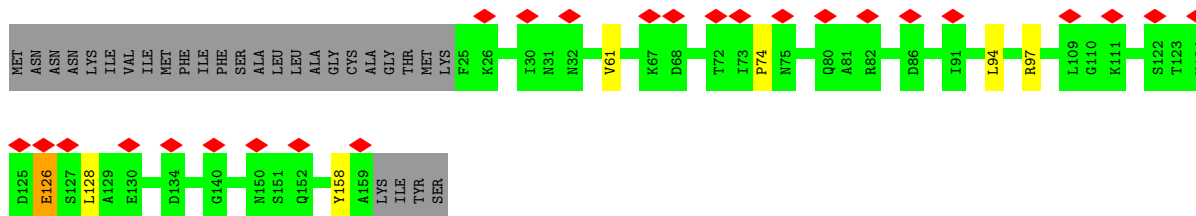
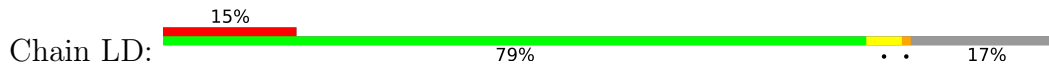
• Molecule 5: DotD



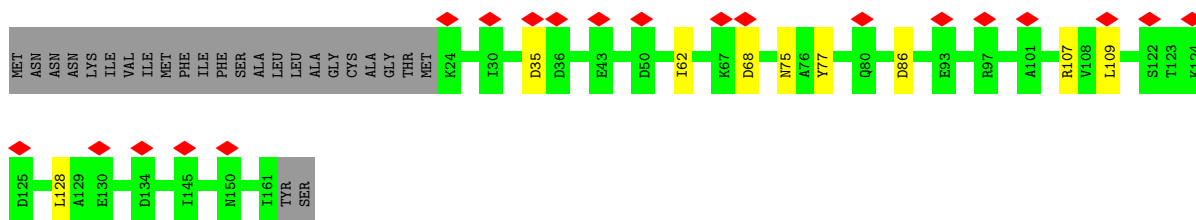
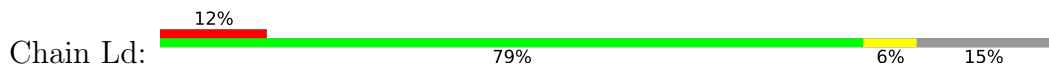
• Molecule 5: DotD



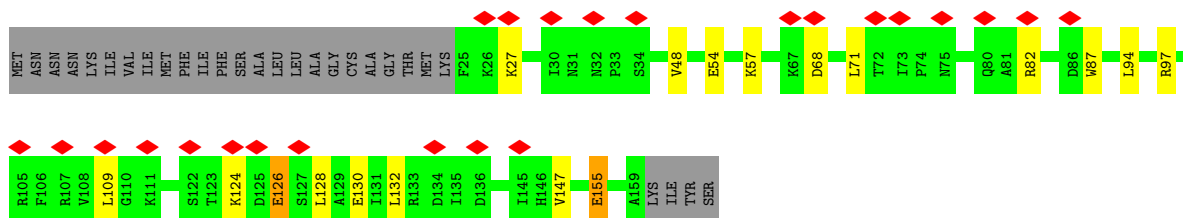
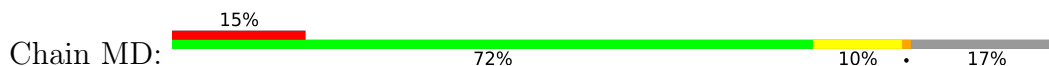
• Molecule 5: DotD



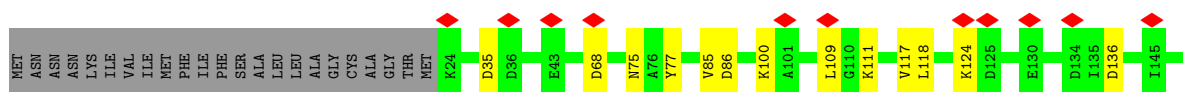
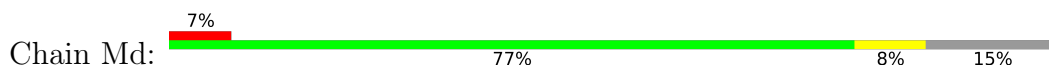
• Molecule 5: DotD

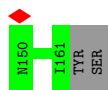


• Molecule 5: DotD

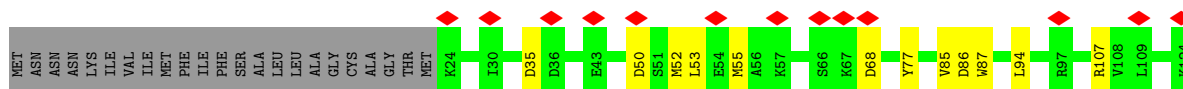
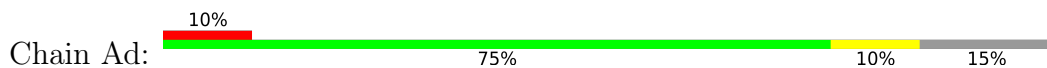


• Molecule 5: DotD

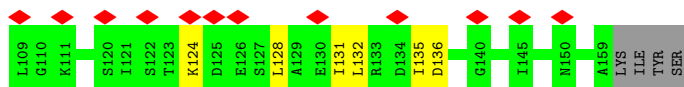
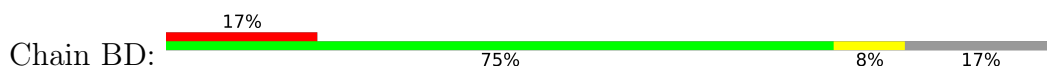




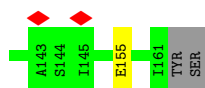
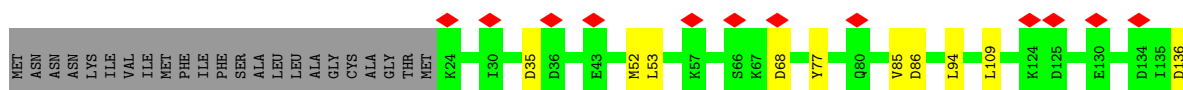
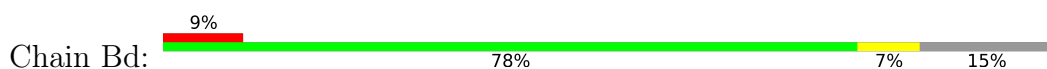
• Molecule 5: DotD



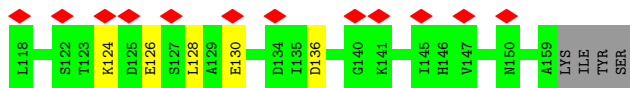
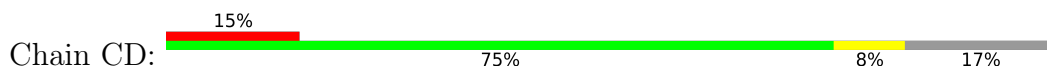
• Molecule 5: DotD



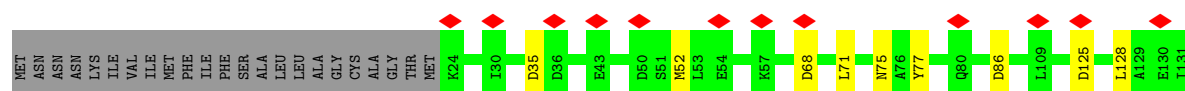
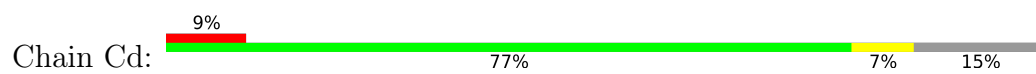
• Molecule 5: DotD



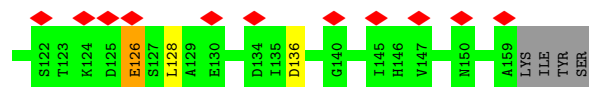
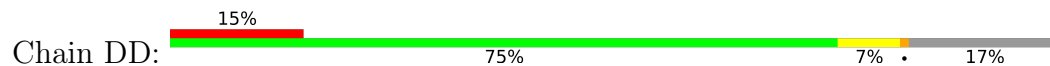
• Molecule 5: DotD



• Molecule 5: DotD



• Molecule 5: DotD



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C13	Depositor
Number of particles used	12200	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.136	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	836.39996, 836.39996, 836.39996	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.64, 1.64, 1.64	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AC	0.65	1/1629 (0.1%)	1.02	10/2214 (0.5%)
1	BC	0.65	1/1629 (0.1%)	1.02	10/2214 (0.5%)
1	CC	0.65	1/1629 (0.1%)	1.02	10/2214 (0.5%)
1	DC	0.65	1/1629 (0.1%)	1.02	10/2214 (0.5%)
1	EC	0.65	1/1629 (0.1%)	1.02	10/2214 (0.5%)
1	FC	0.65	1/1629 (0.1%)	1.02	10/2214 (0.5%)
1	GC	0.65	1/1629 (0.1%)	1.02	10/2214 (0.5%)
1	HC	0.65	1/1629 (0.1%)	1.02	10/2214 (0.5%)
1	IC	0.65	1/1629 (0.1%)	1.02	10/2214 (0.5%)
1	JC	0.65	1/1629 (0.1%)	1.02	10/2214 (0.5%)
1	KC	0.65	1/1629 (0.1%)	1.02	10/2214 (0.5%)
1	LC	0.65	1/1629 (0.1%)	1.02	10/2214 (0.5%)
1	MC	0.65	1/1629 (0.1%)	1.02	10/2214 (0.5%)
2	AH	0.69	1/695 (0.1%)	1.15	9/947 (1.0%)
2	BH	0.69	0/695	1.15	8/947 (0.8%)
2	CH	0.69	1/695 (0.1%)	1.15	8/947 (0.8%)
2	DH	0.69	1/695 (0.1%)	1.14	8/947 (0.8%)
2	EH	0.69	1/695 (0.1%)	1.14	8/947 (0.8%)
2	FH	0.69	1/695 (0.1%)	1.14	8/947 (0.8%)
2	GH	0.69	0/695	1.15	8/947 (0.8%)
2	HH	0.69	0/695	1.14	8/947 (0.8%)
2	IH	0.69	1/695 (0.1%)	1.15	8/947 (0.8%)
2	JH	0.69	0/695	1.15	8/947 (0.8%)
2	KH	0.69	0/695	1.15	8/947 (0.8%)
2	LH	0.69	1/695 (0.1%)	1.15	8/947 (0.8%)
2	MH	0.69	0/695	1.15	8/947 (0.8%)
3	AK	0.64	1/1171 (0.1%)	1.01	8/1583 (0.5%)
3	BK	0.64	1/1171 (0.1%)	1.01	8/1583 (0.5%)
3	CK	0.64	1/1171 (0.1%)	1.01	8/1583 (0.5%)
3	DK	0.64	1/1171 (0.1%)	1.01	8/1583 (0.5%)
3	EK	0.64	1/1171 (0.1%)	1.01	8/1583 (0.5%)
3	FK	0.64	1/1171 (0.1%)	1.01	8/1583 (0.5%)
3	GK	0.64	1/1171 (0.1%)	1.01	8/1583 (0.5%)
3	HK	0.64	1/1171 (0.1%)	1.01	8/1583 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	IK	0.64	1/1171 (0.1%)	1.01	8/1583 (0.5%)
3	JK	0.64	1/1171 (0.1%)	1.01	8/1583 (0.5%)
3	KK	0.64	1/1171 (0.1%)	1.01	8/1583 (0.5%)
3	LK	0.64	1/1171 (0.1%)	1.01	8/1583 (0.5%)
3	MK	0.64	1/1171 (0.1%)	1.01	8/1583 (0.5%)
4	AX	0.30	0/1139	0.68	0/1593
4	AY	0.31	0/259	0.66	0/361
4	AZ	0.30	0/349	0.69	0/487
4	BX	0.30	0/1139	0.68	0/1593
4	BY	0.31	0/259	0.66	0/361
4	BZ	0.30	0/349	0.69	0/487
4	CX	0.30	0/1139	0.68	0/1593
4	CY	0.32	0/259	0.66	0/361
4	CZ	0.30	0/349	0.69	0/487
4	DX	0.30	0/1139	0.68	0/1593
4	DY	0.32	0/259	0.66	0/361
4	DZ	0.30	0/349	0.69	0/487
4	EX	0.30	0/1139	0.68	0/1593
4	EY	0.32	0/259	0.66	0/361
4	EZ	0.30	0/349	0.69	0/487
4	FX	0.30	0/1139	0.68	0/1593
4	FY	0.32	0/259	0.66	0/361
4	FZ	0.30	0/349	0.69	0/487
4	GX	0.30	0/1139	0.68	0/1593
4	GY	0.31	0/259	0.66	0/361
4	GZ	0.30	0/349	0.69	0/487
4	HX	0.30	0/1139	0.68	0/1593
4	HY	0.32	0/259	0.66	0/361
4	HZ	0.30	0/349	0.69	0/487
4	IX	0.30	0/1139	0.68	0/1593
4	IY	0.32	0/259	0.66	0/361
4	IZ	0.30	0/349	0.69	0/487
4	JX	0.30	0/1139	0.68	0/1593
4	JY	0.31	0/259	0.66	0/361
4	JZ	0.30	0/349	0.69	0/487
4	KX	0.30	0/1139	0.68	0/1593
4	KY	0.31	0/259	0.66	0/361
4	KZ	0.30	0/349	0.69	0/487
4	LX	0.30	0/1139	0.68	0/1593
4	LY	0.32	0/259	0.66	0/361
4	LZ	0.30	0/349	0.69	0/487
4	MX	0.30	0/1139	0.68	0/1593
4	MY	0.32	0/259	0.66	0/361



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	MZ	0.30	0/349	0.69	0/487
4	N	0.56	0/1130	0.99	5/1522 (0.3%)
4	O	0.56	0/1130	0.99	5/1522 (0.3%)
4	P	0.56	0/1130	0.99	5/1522 (0.3%)
4	Q	0.56	0/1130	0.99	5/1522 (0.3%)
4	R	0.56	0/1130	0.99	5/1522 (0.3%)
4	S	0.56	0/1130	1.00	5/1522 (0.3%)
4	T	0.56	0/1130	0.99	5/1522 (0.3%)
4	U	0.56	0/1130	1.00	5/1522 (0.3%)
4	V	0.56	0/1130	0.99	5/1522 (0.3%)
4	W	0.56	0/1130	0.99	5/1522 (0.3%)
4	X	0.56	0/1130	0.99	5/1522 (0.3%)
4	Y	0.56	0/1130	1.00	5/1522 (0.3%)
4	Z	0.56	0/1130	0.99	5/1522 (0.3%)
5	AD	0.90	5/1060 (0.5%)	1.35	21/1441 (1.5%)
5	Ad	0.79	2/1086 (0.2%)	1.17	16/1474 (1.1%)
5	BD	0.73	1/1060 (0.1%)	1.21	15/1441 (1.0%)
5	Bd	0.73	0/1086	1.18	14/1474 (0.9%)
5	CD	0.89	5/1060 (0.5%)	1.18	11/1441 (0.8%)
5	Cd	0.75	0/1086	1.14	11/1474 (0.7%)
5	DD	0.93	7/1060 (0.7%)	1.54	17/1441 (1.2%)
5	Dd	0.85	2/1086 (0.2%)	1.19	15/1474 (1.0%)
5	ED	0.74	2/1060 (0.2%)	1.16	13/1441 (0.9%)
5	Ed	0.73	1/1086 (0.1%)	1.08	12/1474 (0.8%)
5	FD	1.03	6/1060 (0.6%)	1.36	16/1441 (1.1%)
5	Fd	0.77	3/1086 (0.3%)	1.14	11/1474 (0.7%)
5	GD	0.89	4/1060 (0.4%)	1.35	17/1441 (1.2%)
5	Gd	0.75	1/1086 (0.1%)	1.25	13/1474 (0.9%)
5	HD	0.78	3/1060 (0.3%)	1.34	13/1441 (0.9%)
5	Hd	0.70	0/1086	1.21	15/1474 (1.0%)
5	ID	0.84	4/1060 (0.4%)	1.10	8/1441 (0.6%)
5	Id	0.72	0/1086	1.10	9/1474 (0.6%)
5	JD	0.86	7/1060 (0.7%)	1.32	13/1441 (0.9%)
5	Jd	0.86	2/1086 (0.2%)	1.23	14/1474 (0.9%)
5	KD	1.04	6/1060 (0.6%)	1.46	21/1441 (1.5%)
5	Kd	0.86	5/1086 (0.5%)	1.12	10/1474 (0.7%)
5	LD	0.88	6/1060 (0.6%)	1.17	6/1441 (0.4%)
5	Ld	0.69	0/1086	1.04	8/1474 (0.5%)
5	MD	1.02	8/1060 (0.8%)	1.71	17/1441 (1.2%)
5	Md	0.87	3/1086 (0.3%)	1.24	10/1474 (0.7%)
All	All	0.64	116/110734 (0.1%)	1.03	750/151086 (0.5%)

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
4	AX	0	2
4	AZ	0	1
4	BX	0	2
4	BZ	0	1
4	CX	0	2
4	CZ	0	1
4	DX	0	2
4	DZ	0	1
4	EX	0	2
4	EZ	0	1
4	FX	0	2
4	FZ	0	1
4	GX	0	2
4	GZ	0	1
4	HX	0	2
4	HZ	0	1
4	IX	0	2
4	IZ	0	1
4	JX	0	2
4	JZ	0	1
4	KX	0	2
4	KZ	0	1
4	LX	0	2
4	LZ	0	1
4	MX	0	2
4	MZ	0	1
4	N	0	1
4	O	0	1
4	P	0	1
4	Q	0	1
4	R	0	1
4	S	0	1
4	T	0	1
4	U	0	1
4	V	0	1
4	W	0	1
4	X	0	1
4	Y	0	1
4	Z	0	1
5	AD	0	1

*Continued on next page...*

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	BD	0	1
5	Bd	0	1
5	CD	0	2
5	DD	0	2
5	Dd	0	1
5	ED	0	3
5	Ed	0	2
5	FD	0	2
5	Fd	0	1
5	GD	0	3
5	HD	0	2
5	ID	0	3
5	Id	0	1
5	JD	0	1
5	Jd	0	1
5	KD	0	3
5	LD	0	2
5	Ld	0	1
5	MD	0	3
5	Md	0	2
All	All	0	90

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	FD	130	GLU	CB-CG	-12.42	1.28	1.52
5	AD	26	LYS	CE-NZ	-10.38	1.23	1.49
5	FD	130	GLU	CG-CD	-10.24	1.36	1.51
5	KD	130	GLU	CG-CD	-9.87	1.37	1.51
5	Jd	111	LYS	CD-CE	-8.63	1.29	1.51
5	DD	97	ARG	CZ-NH2	-8.61	1.21	1.33
5	FD	126	GLU	CG-CD	-8.60	1.39	1.51
5	CD	97	ARG	CG-CD	-8.57	1.30	1.51
5	JD	26	LYS	CD-CE	-8.11	1.30	1.51
5	KD	27	LYS	CD-CE	-8.08	1.31	1.51
5	DD	97	ARG	CG-CD	-8.07	1.31	1.51
5	CD	48	VAL	CB-CG2	-7.86	1.36	1.52
5	MD	87	TRP	CB-CG	-7.79	1.36	1.50
5	Kd	155	GLU	CB-CG	-7.74	1.37	1.52
5	MD	97	ARG	CZ-NH2	-7.74	1.23	1.33
5	FD	97	ARG	CZ-NH2	-7.70	1.23	1.33
5	KD	97	ARG	CG-CD	-7.62	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	KD	126	GLU	CG-CD	-7.61	1.40	1.51
5	MD	130	GLU	CG-CD	-7.60	1.40	1.51
5	ID	126	GLU	CG-CD	-7.37	1.41	1.51
5	DD	126	GLU	CD-OE2	-7.24	1.17	1.25
5	Fd	59	GLU	CB-CG	-7.20	1.38	1.52
5	Jd	111	LYS	CB-CG	-7.17	1.33	1.52
5	Md	124	LYS	CD-CE	-7.14	1.33	1.51
5	AD	97	ARG	CZ-NH2	-7.00	1.24	1.33
5	MD	126	GLU	CG-CD	-6.97	1.41	1.51
5	BD	97	ARG	CG-CD	-6.82	1.34	1.51
5	CD	130	GLU	CB-CG	-6.81	1.39	1.52
5	KD	130	GLU	CB-CG	-6.74	1.39	1.52
5	HD	87	TRP	CB-CG	-6.73	1.38	1.50
5	KD	130	GLU	CD-OE1	-6.64	1.18	1.25
5	Fd	153	VAL	CB-CG2	-6.53	1.39	1.52
5	GD	87	TRP	CB-CG	-6.52	1.38	1.50
5	LD	126	GLU	CG-CD	-6.45	1.42	1.51
5	JD	130	GLU	CG-CD	-6.43	1.42	1.51
5	MD	130	GLU	CB-CG	-6.42	1.40	1.52
5	FD	97	ARG	CG-CD	-6.35	1.36	1.51
5	GD	27	LYS	CB-CG	6.34	1.69	1.52
5	DD	97	ARG	CB-CG	-6.33	1.35	1.52
5	MD	48	VAL	CB-CG2	-6.32	1.39	1.52
5	JD	130	GLU	CB-CG	-6.28	1.40	1.52
5	LD	97	ARG	CG-CD	-6.23	1.36	1.51
5	MD	147	VAL	CB-CG1	-6.21	1.39	1.52
5	ID	87	TRP	CE3-CZ3	-6.16	1.27	1.38
5	Fd	59	GLU	CG-CD	-6.11	1.42	1.51
5	Ad	155	GLU	CB-CG	-6.06	1.40	1.52
5	Kd	87	TRP	CB-CG	-6.05	1.39	1.50
5	JD	26	LYS	CG-CD	-5.98	1.32	1.52
5	Ed	107	ARG	CG-CD	-5.96	1.37	1.51
5	Kd	153	VAL	CB-CG2	-5.95	1.40	1.52
5	CD	126	GLU	CD-OE1	-5.85	1.19	1.25
5	ID	130	GLU	CG-CD	-5.83	1.43	1.51
5	JD	97	ARG	CZ-NH2	-5.80	1.25	1.33
5	LD	126	GLU	CD-OE2	-5.74	1.19	1.25
5	LD	158	TYR	CD2-CE2	-5.74	1.30	1.39
5	Md	109	LEU	CG-CD2	-5.72	1.30	1.51
5	Md	111	LYS	C-N	-5.65	1.21	1.34
1	IC	61	GLU	CB-CG	5.64	1.62	1.52
1	BC	61	GLU	CB-CG	5.63	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	LC	61	GLU	CB-CG	5.63	1.62	1.52
1	GC	61	GLU	CB-CG	5.62	1.62	1.52
5	Kd	148	TYR	CD2-CE2	-5.62	1.30	1.39
1	JC	61	GLU	CB-CG	5.62	1.62	1.52
1	DC	61	GLU	CB-CG	5.62	1.62	1.52
1	AC	61	GLU	CB-CG	5.61	1.62	1.52
1	EC	61	GLU	CB-CG	5.61	1.62	1.52
1	KC	61	GLU	CB-CG	5.60	1.62	1.52
5	DD	87	TRP	CB-CG	-5.60	1.40	1.50
1	CC	61	GLU	CB-CG	5.60	1.62	1.52
1	HC	61	GLU	CB-CG	5.60	1.62	1.52
1	FC	61	GLU	CB-CG	5.58	1.62	1.52
1	MC	61	GLU	CB-CG	5.58	1.62	1.52
5	GD	126	GLU	CG-CD	-5.57	1.43	1.51
5	LD	97	ARG	CZ-NH2	-5.48	1.25	1.33
5	Gd	148	TYR	CD2-CE2	-5.46	1.31	1.39
5	AD	130	GLU	CG-CD	-5.43	1.43	1.51
5	Dd	92	GLU	CD-OE1	-5.41	1.19	1.25
5	FD	97	ARG	CB-CG	-5.41	1.38	1.52
5	LD	97	ARG	CB-CG	-5.36	1.38	1.52
5	DD	97	ARG	CD-NE	-5.36	1.37	1.46
5	JD	88	SER	CB-OG	-5.33	1.35	1.42
3	DK	101	GLU	CD-OE1	-5.33	1.19	1.25
3	JK	101	GLU	CD-OE1	-5.31	1.19	1.25
5	HD	97	ARG	CZ-NH2	-5.31	1.26	1.33
3	AK	101	GLU	CD-OE1	-5.31	1.19	1.25
3	LK	101	GLU	CD-OE1	-5.30	1.19	1.25
5	Dd	158	TYR	CD2-CE2	-5.29	1.31	1.39
3	EK	101	GLU	CD-OE1	-5.29	1.19	1.25
3	HK	101	GLU	CD-OE1	-5.27	1.19	1.25
5	ID	27	LYS	CB-CG	-5.27	1.38	1.52
3	KK	101	GLU	CD-OE1	-5.27	1.19	1.25
3	MK	101	GLU	CD-OE1	-5.26	1.19	1.25
3	GK	101	GLU	CD-OE1	-5.26	1.19	1.25
3	CK	101	GLU	CD-OE1	-5.26	1.19	1.25
3	BK	101	GLU	CD-OE1	-5.26	1.19	1.25
3	FK	101	GLU	CD-OE1	-5.25	1.19	1.25
5	Kd	155	GLU	CG-CD	-5.22	1.44	1.51
5	JD	87	TRP	CB-CG	-5.22	1.40	1.50
3	IK	101	GLU	CD-OE1	-5.21	1.20	1.25
5	GD	27	LYS	CD-CE	-5.19	1.38	1.51
5	HD	27	LYS	CE-NZ	-5.19	1.36	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	ED	130	GLU	CB-CG	-5.16	1.42	1.52
5	MD	48	VAL	CB-CG1	-5.16	1.42	1.52
5	DD	126	GLU	CG-CD	-5.16	1.44	1.51
5	AD	26	LYS	CB-CG	-5.11	1.38	1.52
5	Ad	87	TRP	CB-CG	-5.09	1.41	1.50
2	AH	348	VAL	CB-CG2	-5.04	1.42	1.52
2	DH	348	VAL	CB-CG2	-5.04	1.42	1.52
2	LH	348	VAL	CB-CG2	-5.04	1.42	1.52
5	AD	26	LYS	CG-CD	-5.03	1.35	1.52
2	EH	348	VAL	CB-CG2	-5.02	1.42	1.52
5	CD	93	GLU	CD-OE1	-5.02	1.20	1.25
2	IH	348	VAL	CB-CG2	-5.01	1.42	1.52
2	FH	348	VAL	CB-CG2	-5.01	1.42	1.52
2	CH	348	VAL	CB-CG2	-5.01	1.42	1.52
5	ED	155	GLU	CD-OE2	-5.01	1.20	1.25

All (750) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	MD	97	ARG	NE-CZ-NH2	-27.60	106.50	120.30
5	DD	82	ARG	NE-CZ-NH1	-27.22	106.69	120.30
5	MD	57	LYS	CD-CE-NZ	-25.28	53.55	111.70
5	KD	27	LYS	CD-CE-NZ	-23.76	57.04	111.70
5	HD	27	LYS	CD-CE-NZ	23.21	165.09	111.70
5	JD	26	LYS	CD-CE-NZ	-22.05	61.00	111.70
5	MD	27	LYS	CD-CE-NZ	-19.89	65.96	111.70
5	GD	135	ILE	CG1-CB-CG2	-17.58	72.73	111.40
5	FD	97	ARG	NE-CZ-NH2	-17.57	111.52	120.30
5	AD	26	LYS	CD-CE-NZ	-16.61	73.48	111.70
5	DD	82	ARG	NE-CZ-NH2	16.47	128.53	120.30
5	LD	97	ARG	NE-CZ-NH2	-16.46	112.07	120.30
5	DD	97	ARG	NE-CZ-NH2	-16.26	112.17	120.30
5	Gd	124	LYS	CD-CE-NZ	-16.02	74.86	111.70
5	Md	124	LYS	CD-CE-NZ	-15.91	75.10	111.70
5	FD	97	ARG	NE-CZ-NH1	13.96	127.28	120.30
5	MD	97	ARG	NE-CZ-NH1	13.68	127.14	120.30
5	Bd	86	ASP	CB-CG-OD1	13.46	130.41	118.30
5	Kd	136	ASP	CB-CG-OD1	12.89	129.90	118.30
5	Gd	109	LEU	CB-CG-CD1	12.53	132.29	111.00
5	Hd	86	ASP	CB-CG-OD1	12.46	129.51	118.30
5	DD	97	ARG	CA-CB-CG	-12.40	86.12	113.40
5	Ad	35	ASP	CB-CG-OD2	12.37	129.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	MD	94	LEU	CB-CG-CD2	12.32	131.95	111.00
5	Cd	136	ASP	CB-CG-OD2	12.32	129.38	118.30
5	FD	135	ILE	CG1-CB-CG2	-12.29	84.36	111.40
5	Jd	107	ARG	NE-CZ-NH1	-12.23	114.19	120.30
3	KK	101	GLU	CA-CB-CG	11.96	139.72	113.40
3	BK	101	GLU	CA-CB-CG	11.96	139.71	113.40
3	IK	101	GLU	CA-CB-CG	11.95	139.68	113.40
3	DK	101	GLU	CA-CB-CG	11.94	139.68	113.40
3	EK	101	GLU	CA-CB-CG	11.94	139.67	113.40
3	FK	101	GLU	CA-CB-CG	11.94	139.67	113.40
3	JK	101	GLU	CA-CB-CG	11.93	139.66	113.40
3	CK	101	GLU	CA-CB-CG	11.93	139.65	113.40
3	HK	101	GLU	CA-CB-CG	11.93	139.65	113.40
3	AK	101	GLU	CA-CB-CG	11.93	139.65	113.40
5	ED	94	LEU	CB-CG-CD2	11.93	131.28	111.00
3	LK	101	GLU	CA-CB-CG	11.93	139.64	113.40
3	MK	101	GLU	CA-CB-CG	11.93	139.64	113.40
3	GK	101	GLU	CA-CB-CG	11.92	139.63	113.40
5	AD	52	MET	CA-CB-CG	11.87	133.49	113.30
5	DD	97	ARG	NE-CZ-NH1	11.70	126.15	120.30
5	CD	94	LEU	CB-CG-CD2	11.52	130.58	111.00
5	Dd	160	LYS	CD-CE-NZ	-11.30	85.70	111.70
5	Id	53	LEU	CB-CG-CD1	-11.20	91.96	111.00
5	BD	100	LYS	CD-CE-NZ	-11.04	86.30	111.70
5	HD	55	MET	CG-SD-CE	-10.87	82.81	100.20
5	Gd	35	ASP	CB-CG-OD2	10.82	128.04	118.30
5	GD	98	ILE	CG1-CB-CG2	-10.71	87.83	111.40
5	AD	97	ARG	NE-CZ-NH2	-10.69	114.96	120.30
5	Hd	52	MET	CG-SD-CE	-10.62	83.21	100.20
5	Md	136	ASP	CB-CG-OD1	10.61	127.84	118.30
5	Hd	35	ASP	CB-CG-OD1	10.44	127.69	118.30
5	Cd	160	LYS	CD-CE-NZ	-10.43	87.71	111.70
5	HD	52	MET	CG-SD-CE	10.36	116.78	100.20
5	Bd	136	ASP	CB-CG-OD1	10.25	127.53	118.30
1	MC	61	GLU	CA-CB-CG	10.20	135.83	113.40
1	FC	61	GLU	CA-CB-CG	10.19	135.82	113.40
1	JC	61	GLU	CA-CB-CG	10.19	135.81	113.40
1	GC	61	GLU	CA-CB-CG	10.18	135.80	113.40
1	HC	61	GLU	CA-CB-CG	10.18	135.79	113.40
1	KC	61	GLU	CA-CB-CG	10.18	135.79	113.40
1	EC	61	GLU	CA-CB-CG	10.18	135.79	113.40
1	CC	61	GLU	CA-CB-CG	10.17	135.78	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	IC	61	GLU	CA-CB-CG	10.17	135.77	113.40
1	BC	61	GLU	CA-CB-CG	10.17	135.78	113.40
1	DC	61	GLU	CA-CB-CG	10.17	135.78	113.40
1	LC	61	GLU	CA-CB-CG	10.17	135.77	113.40
1	AC	61	GLU	CA-CB-CG	10.16	135.74	113.40
5	HD	52	MET	CA-CB-CG	10.15	130.55	113.30
5	Ad	55	MET	CG-SD-CE	-10.10	84.04	100.20
5	FD	97	ARG	CA-CB-CG	-10.01	91.39	113.40
5	GD	133	ARG	NE-CZ-NH2	-9.94	115.33	120.30
5	GD	52	MET	CG-SD-CE	9.90	116.04	100.20
5	Jd	125	ASP	CB-CG-OD2	9.90	127.21	118.30
5	Ed	136	ASP	CB-CG-OD2	9.87	127.18	118.30
5	Fd	105	ARG	NE-CZ-NH2	-9.87	115.36	120.30
2	FH	294	ARG	CG-CD-NE	9.81	132.40	111.80
2	HH	294	ARG	CG-CD-NE	9.81	132.41	111.80
2	GH	294	ARG	CG-CD-NE	9.81	132.40	111.80
2	CH	294	ARG	CG-CD-NE	9.81	132.40	111.80
2	IH	294	ARG	CG-CD-NE	9.81	132.39	111.80
2	LH	294	ARG	CG-CD-NE	9.81	132.39	111.80
2	MH	294	ARG	CG-CD-NE	9.80	132.39	111.80
2	KH	294	ARG	CG-CD-NE	9.80	132.39	111.80
2	BH	294	ARG	CG-CD-NE	9.80	132.39	111.80
2	DH	294	ARG	CG-CD-NE	9.80	132.38	111.80
2	JH	294	ARG	CG-CD-NE	9.80	132.38	111.80
2	EH	294	ARG	CG-CD-NE	9.79	132.37	111.80
2	AH	294	ARG	CG-CD-NE	9.78	132.34	111.80
5	GD	27	LYS	CD-CE-NZ	-9.77	89.23	111.70
5	KD	98	ILE	CG1-CB-CG2	-9.72	90.02	111.40
5	AD	134	ASP	CB-CG-OD2	9.67	127.00	118.30
5	ID	97	ARG	NE-CZ-NH2	9.65	125.12	120.30
5	Fd	105	ARG	NE-CZ-NH1	9.54	125.07	120.30
4	P	155	LEU	CA-CB-CG	9.43	136.98	115.30
4	R	155	LEU	CA-CB-CG	9.43	136.98	115.30
4	N	155	LEU	CA-CB-CG	9.42	136.97	115.30
4	S	155	LEU	CA-CB-CG	9.42	136.97	115.30
4	X	155	LEU	CA-CB-CG	9.42	136.97	115.30
4	O	155	LEU	CA-CB-CG	9.42	136.97	115.30
4	T	155	LEU	CA-CB-CG	9.42	136.96	115.30
4	Z	155	LEU	CA-CB-CG	9.42	136.97	115.30
4	U	155	LEU	CA-CB-CG	9.42	136.96	115.30
4	W	155	LEU	CA-CB-CG	9.42	136.96	115.30
4	V	155	LEU	CA-CB-CG	9.41	136.95	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	155	LEU	CA-CB-CG	9.41	136.95	115.30
4	Q	155	LEU	CA-CB-CG	9.40	136.93	115.30
5	Cd	52	MET	CG-SD-CE	-9.37	85.21	100.20
5	KD	94	LEU	CB-CG-CD2	9.19	126.62	111.00
5	JD	97	ARG	NE-CZ-NH2	-9.13	115.73	120.30
5	Jd	107	ARG	NE-CZ-NH2	9.10	124.85	120.30
5	LD	97	ARG	CA-CB-CG	-9.00	93.60	113.40
5	ID	52	MET	CA-CB-CG	8.97	128.55	113.30
5	BD	135	ILE	CG1-CB-CG2	-8.95	91.72	111.40
2	LH	294	ARG	NE-CZ-NH2	8.94	124.77	120.30
2	MH	294	ARG	NE-CZ-NH2	8.91	124.76	120.30
2	CH	294	ARG	NE-CZ-NH2	8.90	124.75	120.30
1	FC	212	TYR	CB-CG-CD1	8.90	126.34	121.00
1	GC	212	TYR	CB-CG-CD1	8.89	126.33	121.00
1	EC	212	TYR	CB-CG-CD1	8.88	126.33	121.00
2	JH	294	ARG	NE-CZ-NH2	8.88	124.74	120.30
1	LC	212	TYR	CB-CG-CD1	8.88	126.33	121.00
1	MC	212	TYR	CB-CG-CD1	8.87	126.32	121.00
1	CC	212	TYR	CB-CG-CD1	8.86	126.32	121.00
2	FH	294	ARG	NE-CZ-NH2	8.85	124.72	120.30
1	KC	212	TYR	CB-CG-CD1	8.85	126.31	121.00
1	IC	212	TYR	CB-CG-CD1	8.84	126.31	121.00
1	AC	212	TYR	CB-CG-CD1	8.84	126.30	121.00
2	HH	294	ARG	NE-CZ-NH2	8.84	124.72	120.30
2	KH	294	ARG	NE-CZ-NH2	8.84	124.72	120.30
2	BH	294	ARG	NE-CZ-NH2	8.83	124.72	120.30
5	DD	94	LEU	CB-CG-CD2	8.83	126.02	111.00
1	HC	212	TYR	CB-CG-CD1	8.83	126.30	121.00
5	AD	130	GLU	CA-CB-CG	8.83	132.82	113.40
1	BC	212	TYR	CB-CG-CD1	8.82	126.29	121.00
2	EH	294	ARG	NE-CZ-NH2	8.81	124.71	120.30
2	AH	294	ARG	NE-CZ-NH2	8.81	124.71	120.30
2	IH	294	ARG	NE-CZ-NH2	8.80	124.70	120.30
1	JC	212	TYR	CB-CG-CD1	8.81	126.28	121.00
1	DC	212	TYR	CB-CG-CD1	8.79	126.28	121.00
2	GH	294	ARG	NE-CZ-NH2	8.77	124.69	120.30
2	DH	294	ARG	NE-CZ-NH2	8.76	124.68	120.30
5	FD	97	ARG	CG-CD-NE	8.70	130.07	111.80
5	HD	27	LYS	CG-CD-CE	-8.69	85.84	111.90
5	Hd	125	ASP	CB-CG-OD1	8.63	126.07	118.30
5	JD	97	ARG	CA-CB-CG	-8.60	94.49	113.40
5	Gd	109	LEU	CB-CG-CD2	-8.45	96.63	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EC	212	TYR	CB-CG-CD2	-8.40	115.96	121.00
1	GC	212	TYR	CB-CG-CD2	-8.39	115.97	121.00
1	BC	212	TYR	CB-CG-CD2	-8.38	115.97	121.00
1	DC	212	TYR	CB-CG-CD2	-8.37	115.98	121.00
1	HC	212	TYR	CB-CG-CD2	-8.34	116.00	121.00
1	CC	212	TYR	CB-CG-CD2	-8.34	116.00	121.00
1	FC	212	TYR	CB-CG-CD2	-8.34	116.00	121.00
1	MC	212	TYR	CB-CG-CD2	-8.31	116.01	121.00
1	IC	212	TYR	CB-CG-CD2	-8.30	116.02	121.00
1	KC	212	TYR	CB-CG-CD2	-8.30	116.02	121.00
1	LC	212	TYR	CB-CG-CD2	-8.30	116.02	121.00
1	JC	212	TYR	CB-CG-CD2	-8.30	116.02	121.00
5	MD	97	ARG	CA-CB-CG	-8.29	95.16	113.40
1	HC	81	GLU	CA-CB-CG	8.27	131.59	113.40
1	IC	81	GLU	CA-CB-CG	8.27	131.59	113.40
1	CC	81	GLU	CA-CB-CG	8.27	131.59	113.40
1	AC	81	GLU	CA-CB-CG	8.26	131.57	113.40
1	EC	81	GLU	CA-CB-CG	8.25	131.56	113.40
1	GC	81	GLU	CA-CB-CG	8.25	131.56	113.40
1	LC	81	GLU	CA-CB-CG	8.25	131.55	113.40
1	DC	81	GLU	CA-CB-CG	8.25	131.55	113.40
1	JC	81	GLU	CA-CB-CG	8.24	131.54	113.40
1	KC	81	GLU	CA-CB-CG	8.24	131.53	113.40
1	BC	81	GLU	CA-CB-CG	8.24	131.54	113.40
1	AC	212	TYR	CB-CG-CD2	-8.23	116.06	121.00
1	FC	81	GLU	CA-CB-CG	8.23	131.50	113.40
1	MC	81	GLU	CA-CB-CG	8.23	131.50	113.40
5	Jd	77	TYR	C-N-CA	8.19	142.18	121.70
5	ED	125	ASP	CB-CG-OD1	8.11	125.60	118.30
4	U	121	ASP	CB-CG-OD2	8.11	125.60	118.30
4	W	121	ASP	CB-CG-OD2	8.10	125.59	118.30
5	JD	82	ARG	NE-CZ-NH2	8.09	124.34	120.30
4	T	121	ASP	CB-CG-OD2	8.08	125.57	118.30
5	Fd	107	ARG	NE-CZ-NH1	-8.07	116.26	120.30
4	Y	121	ASP	CB-CG-OD2	8.07	125.56	118.30
4	V	121	ASP	CB-CG-OD2	8.06	125.55	118.30
4	Q	121	ASP	CB-CG-OD2	8.06	125.55	118.30
4	Z	121	ASP	CB-CG-OD2	8.06	125.55	118.30
5	FD	82	ARG	NE-CZ-NH2	8.05	124.33	120.30
4	O	121	ASP	CB-CG-OD2	8.05	125.55	118.30
4	P	121	ASP	CB-CG-OD2	8.05	125.54	118.30
4	N	121	ASP	CB-CG-OD2	8.04	125.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	121	ASP	CB-CG-OD2	8.04	125.54	118.30
4	R	121	ASP	CB-CG-OD2	8.02	125.52	118.30
5	Bd	109	LEU	CB-CG-CD1	-8.00	97.39	111.00
4	X	121	ASP	CB-CG-OD2	8.00	125.50	118.30
5	Md	77	TYR	C-N-CA	7.99	141.66	121.70
5	GD	128	LEU	CB-CG-CD2	7.94	124.50	111.00
5	Md	109	LEU	CB-CG-CD2	-7.94	97.50	111.00
5	CD	128	LEU	CA-CB-CG	7.93	133.53	115.30
5	Cd	68	ASP	CB-CG-OD1	7.90	125.41	118.30
5	Hd	36	ASP	CB-CG-OD1	7.89	125.40	118.30
5	BD	52	MET	CA-CB-CG	7.83	126.62	113.30
5	LD	128	LEU	CA-CB-CG	7.80	133.23	115.30
5	MD	71	LEU	CA-CB-CG	7.77	133.17	115.30
5	Fd	107	ARG	NE-CZ-NH2	7.76	124.18	120.30
5	JD	97	ARG	NE-CZ-NH1	7.75	124.18	120.30
5	Gd	125	ASP	CB-CG-OD1	7.75	125.28	118.30
5	KD	57	LYS	CD-CE-NZ	7.75	129.52	111.70
5	ED	109	LEU	CA-CB-CG	7.71	133.03	115.30
4	U	216	ASP	CB-CG-OD1	7.70	125.23	118.30
4	P	216	ASP	CB-CG-OD1	7.69	125.22	118.30
4	S	216	ASP	CB-CG-OD1	7.69	125.22	118.30
4	Z	216	ASP	CB-CG-OD1	7.68	125.21	118.30
5	BD	128	LEU	CB-CG-CD2	-7.67	97.96	111.00
4	O	216	ASP	CB-CG-OD1	7.66	125.20	118.30
4	X	216	ASP	CB-CG-OD1	7.66	125.20	118.30
4	T	216	ASP	CB-CG-OD1	7.65	125.19	118.30
4	Y	216	ASP	CB-CG-OD1	7.65	125.18	118.30
4	Q	216	ASP	CB-CG-OD1	7.65	125.18	118.30
4	R	216	ASP	CB-CG-OD1	7.65	125.18	118.30
4	W	216	ASP	CB-CG-OD1	7.65	125.18	118.30
5	GD	82	ARG	NE-CZ-NH2	7.64	124.12	120.30
4	V	216	ASP	CB-CG-OD1	7.64	125.17	118.30
5	ED	130	GLU	OE1-CD-OE2	-7.63	114.14	123.30
4	N	216	ASP	CB-CG-OD1	7.61	125.14	118.30
5	DD	136	ASP	CB-CG-OD2	7.58	125.12	118.30
5	DD	82	ARG	CD-NE-CZ	7.57	134.20	123.60
5	HD	97	ARG	NE-CZ-NH2	-7.55	116.53	120.30
5	KD	126	GLU	CG-CD-OE2	-7.55	103.20	118.30
5	Ad	77	TYR	C-N-CA	7.54	140.55	121.70
5	DD	82	ARG	CG-CD-NE	-7.54	95.97	111.80
5	HD	71	LEU	CA-CB-CG	7.52	132.60	115.30
5	Md	118	LEU	CA-CB-CG	7.51	132.57	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	JD	128	LEU	CA-CB-CG	7.50	132.56	115.30
5	DD	68	ASP	CB-CG-OD1	7.49	125.04	118.30
5	KD	57	LYS	CB-CG-CD	7.48	131.05	111.60
5	Ld	77	TYR	C-N-CA	7.47	140.38	121.70
5	HD	97	ARG	NE-CZ-NH1	7.47	124.03	120.30
5	Kd	77	TYR	C-N-CA	7.46	140.35	121.70
5	CD	52	MET	CA-CB-CG	7.46	125.97	113.30
5	Bd	94	LEU	CB-CG-CD2	-7.45	98.33	111.00
5	Ld	107	ARG	CG-CD-NE	-7.45	96.16	111.80
5	KD	131	ILE	CG1-CB-CG2	-7.43	95.05	111.40
5	Jd	107	ARG	CG-CD-NE	-7.42	96.22	111.80
5	DD	71	LEU	CA-CB-CG	7.40	132.31	115.30
5	Dd	77	TYR	C-N-CA	7.38	140.16	121.70
5	Kd	52	MET	CG-SD-CE	-7.35	88.44	100.20
5	AD	55	MET	CG-SD-CE	-7.31	88.51	100.20
1	GC	236	ASP	CB-CG-OD1	7.30	124.87	118.30
1	LC	236	ASP	CB-CG-OD1	7.30	124.87	118.30
1	HC	236	ASP	CB-CG-OD1	7.28	124.85	118.30
1	IC	236	ASP	CB-CG-OD1	7.28	124.85	118.30
1	AC	236	ASP	CB-CG-OD1	7.27	124.85	118.30
1	JC	236	ASP	CB-CG-OD1	7.27	124.84	118.30
1	KC	236	ASP	CB-CG-OD1	7.27	124.84	118.30
5	MD	82	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	BC	236	ASP	CB-CG-OD1	7.26	124.83	118.30
1	EC	236	ASP	CB-CG-OD1	7.25	124.82	118.30
1	MC	236	ASP	CB-CG-OD1	7.24	124.82	118.30
1	DC	236	ASP	CB-CG-OD1	7.24	124.81	118.30
1	FC	236	ASP	CB-CG-OD1	7.23	124.81	118.30
5	Ad	53	LEU	CB-CG-CD2	-7.22	98.73	111.00
5	AD	97	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	CC	236	ASP	CB-CG-OD1	7.20	124.78	118.30
2	IH	294	ARG	NE-CZ-NH1	-7.18	116.71	120.30
5	Bd	77	TYR	C-N-CA	7.17	139.63	121.70
2	MH	294	ARG	NE-CZ-NH1	-7.17	116.71	120.30
5	FD	71	LEU	CA-CB-CG	7.17	131.78	115.30
2	BH	294	ARG	NE-CZ-NH1	-7.16	116.72	120.30
2	LH	294	ARG	NE-CZ-NH1	-7.14	116.73	120.30
5	Dd	55	MET	CG-SD-CE	7.13	111.60	100.20
2	CH	294	ARG	NE-CZ-NH1	-7.12	116.74	120.30
2	JH	294	ARG	NE-CZ-NH1	-7.12	116.74	120.30
4	W	113	ASP	CB-CG-OD1	7.10	124.69	118.30
2	EH	294	ARG	NE-CZ-NH1	-7.09	116.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	FH	294	ARG	NE-CZ-NH1	-7.09	116.75	120.30
4	N	113	ASP	CB-CG-OD1	7.09	124.68	118.30
5	AD	98	ILE	CG1-CB-CG2	-7.08	95.82	111.40
2	KH	294	ARG	NE-CZ-NH1	-7.08	116.76	120.30
2	GH	294	ARG	NE-CZ-NH1	-7.08	116.76	120.30
4	Q	113	ASP	CB-CG-OD1	7.08	124.67	118.30
4	R	113	ASP	CB-CG-OD1	7.08	124.67	118.30
4	V	113	ASP	CB-CG-OD1	7.08	124.67	118.30
5	JD	97	ARG	CG-CD-NE	7.07	126.65	111.80
4	P	113	ASP	CB-CG-OD1	7.07	124.66	118.30
4	T	113	ASP	CB-CG-OD1	7.07	124.66	118.30
2	AH	294	ARG	CD-NE-CZ	7.07	133.49	123.60
2	DH	294	ARG	CD-NE-CZ	7.06	133.49	123.60
2	EH	294	ARG	CD-NE-CZ	7.05	133.47	123.60
2	DH	294	ARG	NE-CZ-NH1	-7.05	116.78	120.30
2	HH	294	ARG	CD-NE-CZ	7.05	133.47	123.60
2	HH	294	ARG	NE-CZ-NH1	-7.04	116.78	120.30
5	ED	97	ARG	CA-CB-CG	-7.04	97.90	113.40
2	JH	294	ARG	CD-NE-CZ	7.04	133.46	123.60
2	KH	294	ARG	CD-NE-CZ	7.04	133.46	123.60
2	GH	294	ARG	CD-NE-CZ	7.04	133.46	123.60
4	X	113	ASP	CB-CG-OD1	7.04	124.64	118.30
4	U	113	ASP	CB-CG-OD1	7.04	124.63	118.30
4	Y	113	ASP	CB-CG-OD1	7.03	124.63	118.30
2	IH	294	ARG	CD-NE-CZ	7.03	133.44	123.60
4	O	113	ASP	CB-CG-OD1	7.03	124.63	118.30
4	S	113	ASP	CB-CG-OD1	7.03	124.63	118.30
2	CH	294	ARG	CD-NE-CZ	7.03	133.44	123.60
2	AH	294	ARG	NE-CZ-NH1	-7.03	116.79	120.30
4	Z	113	ASP	CB-CG-OD1	7.02	124.62	118.30
2	FH	294	ARG	CD-NE-CZ	7.02	133.43	123.60
2	LH	294	ARG	CD-NE-CZ	7.02	133.43	123.60
2	BH	294	ARG	CD-NE-CZ	7.02	133.42	123.60
2	MH	294	ARG	CD-NE-CZ	7.01	133.42	123.60
5	Ad	94	LEU	CB-CG-CD2	7.01	122.92	111.00
5	ED	52	MET	CA-CB-CG	7.01	125.21	113.30
5	CD	97	ARG	CA-CB-CG	-7.00	97.99	113.40
5	Ed	77	TYR	C-N-CA	6.99	139.18	121.70
5	Dd	94	LEU	CB-CG-CD2	-6.96	99.16	111.00
5	CD	97	ARG	CG-CD-NE	6.96	126.41	111.80
5	Hd	77	TYR	C-N-CA	6.94	139.05	121.70
5	JD	136	ASP	CB-CG-OD2	6.93	124.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Gd	53	LEU	CB-CG-CD2	-6.92	99.23	111.00
5	BD	71	LEU	CA-CB-CG	6.90	131.18	115.30
3	LK	84	PHE	CB-CG-CD2	-6.89	115.98	120.80
5	JD	26	LYS	CA-CB-CG	6.88	128.54	113.40
3	IK	84	PHE	CB-CG-CD2	-6.87	115.99	120.80
3	GK	84	PHE	CB-CG-CD2	-6.86	116.00	120.80
3	FK	84	PHE	CB-CG-CD2	-6.86	116.00	120.80
3	KK	84	PHE	CB-CG-CD2	-6.86	116.00	120.80
3	JK	84	PHE	CB-CG-CD2	-6.86	116.00	120.80
3	DK	84	PHE	CB-CG-CD2	-6.84	116.01	120.80
5	Ad	125	ASP	CB-CG-OD1	6.84	124.45	118.30
5	JD	26	LYS	CB-CA-C	-6.84	96.73	110.40
5	KD	52	MET	CA-CB-CG	6.84	124.92	113.30
3	CK	84	PHE	CB-CG-CD2	-6.82	116.02	120.80
3	MK	84	PHE	CB-CG-CD2	-6.81	116.04	120.80
3	EK	84	PHE	CB-CG-CD2	-6.79	116.05	120.80
5	Fd	136	ASP	CB-CG-OD2	6.79	124.41	118.30
5	BD	131	ILE	CA-CB-CG1	6.79	123.90	111.00
3	HK	84	PHE	CB-CG-CD2	-6.78	116.05	120.80
3	AK	84	PHE	CB-CG-CD2	-6.77	116.06	120.80
5	JD	134	ASP	CB-CG-OD2	6.77	124.39	118.30
5	JD	94	LEU	CB-CG-CD2	6.76	122.49	111.00
3	BK	84	PHE	CB-CG-CD2	-6.75	116.07	120.80
5	GD	136	ASP	CB-CG-OD2	6.74	124.37	118.30
5	ID	52	MET	CG-SD-CE	6.72	110.95	100.20
5	Dd	136	ASP	CB-CG-OD1	6.70	124.33	118.30
5	Gd	136	ASP	CB-CG-OD2	6.70	124.33	118.30
5	CD	136	ASP	CB-CG-OD2	6.68	124.31	118.30
5	Bd	86	ASP	CB-CG-OD2	-6.63	112.33	118.30
3	CK	101	GLU	N-CA-CB	6.63	122.53	110.60
3	GK	101	GLU	N-CA-CB	6.62	122.52	110.60
3	DK	101	GLU	N-CA-CB	6.62	122.51	110.60
3	FK	101	GLU	N-CA-CB	6.62	122.51	110.60
3	IK	101	GLU	N-CA-CB	6.61	122.50	110.60
3	JK	101	GLU	N-CA-CB	6.61	122.50	110.60
5	Gd	77	TYR	C-N-CA	6.61	138.22	121.70
5	Jd	156	LEU	CB-CG-CD2	-6.61	99.77	111.00
3	LK	101	GLU	N-CA-CB	6.61	122.49	110.60
3	EK	101	GLU	N-CA-CB	6.61	122.49	110.60
3	MK	101	GLU	N-CA-CB	6.61	122.49	110.60
3	AK	101	GLU	N-CA-CB	6.60	122.49	110.60
5	AD	136	ASP	CB-CG-OD1	6.59	124.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Ad	55	MET	CB-CG-SD	6.59	132.18	112.40
3	HK	101	GLU	N-CA-CB	6.59	122.46	110.60
3	KK	101	GLU	N-CA-CB	6.59	122.45	110.60
3	BK	101	GLU	N-CA-CB	6.58	122.45	110.60
5	AD	130	GLU	N-CA-CB	-6.57	98.77	110.60
5	Ld	107	ARG	NE-CZ-NH1	-6.53	117.04	120.30
5	Ad	86	ASP	CB-CG-OD1	6.52	124.17	118.30
5	MD	155	GLU	OE1-CD-OE2	-6.52	115.47	123.30
5	ED	97	ARG	NE-CZ-NH2	-6.50	117.05	120.30
5	Id	77	TYR	C-N-CA	6.50	137.96	121.70
2	JH	355	MET	CG-SD-CE	-6.48	89.83	100.20
2	LH	355	MET	CG-SD-CE	-6.48	89.83	100.20
5	Dd	35	ASP	CB-CG-OD1	6.47	124.13	118.30
2	GH	355	MET	CG-SD-CE	-6.47	89.84	100.20
5	LD	97	ARG	NE-CZ-NH1	6.47	123.54	120.30
2	DH	355	MET	CG-SD-CE	-6.47	89.85	100.20
2	BH	355	MET	CG-SD-CE	-6.47	89.85	100.20
5	Dd	109	LEU	CA-CB-CG	6.46	130.17	115.30
2	HH	355	MET	CG-SD-CE	-6.46	89.86	100.20
2	KH	355	MET	CG-SD-CE	-6.46	89.86	100.20
2	CH	355	MET	CG-SD-CE	-6.46	89.86	100.20
2	IH	355	MET	CG-SD-CE	-6.46	89.86	100.20
2	AH	355	MET	CG-SD-CE	-6.46	89.86	100.20
5	CD	68	ASP	CB-CG-OD1	6.45	124.10	118.30
2	EH	355	MET	CG-SD-CE	-6.45	89.89	100.20
2	MH	355	MET	CG-SD-CE	-6.45	89.89	100.20
2	FH	355	MET	CG-SD-CE	-6.45	89.89	100.20
5	Bd	94	LEU	CB-CG-CD1	6.44	121.95	111.00
5	Kd	36	ASP	CB-CG-OD2	-6.44	112.51	118.30
5	Ld	35	ASP	CB-CG-OD1	6.43	124.09	118.30
5	Cd	132	LEU	CB-CG-CD2	-6.42	100.09	111.00
5	ID	128	LEU	CB-CG-CD1	-6.40	100.12	111.00
5	BD	79	LEU	CB-CA-C	-6.39	98.05	110.20
5	ID	43	GLU	OE1-CD-OE2	-6.39	115.63	123.30
5	Bd	52	MET	CG-SD-CE	-6.38	89.99	100.20
5	Cd	35	ASP	CB-CG-OD1	6.38	124.04	118.30
5	Cd	125	ASP	CB-CG-OD2	6.37	124.03	118.30
5	ED	128	LEU	CA-CB-CG	6.37	129.94	115.30
5	Id	86	ASP	CB-CG-OD1	6.35	124.02	118.30
5	HD	97	ARG	CG-CD-NE	6.35	125.13	111.80
5	Jd	35	ASP	CB-CG-OD1	6.34	124.01	118.30
5	Jd	111	LYS	CB-CG-CD	-6.33	95.16	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	KD	137	TYR	CB-CG-CD2	-6.32	117.21	121.00
5	Dd	94	LEU	CB-CG-CD1	6.31	121.73	111.00
5	Cd	86	ASP	CB-CG-OD1	6.29	123.97	118.30
1	BC	214	LYS	CD-CE-NZ	6.27	126.12	111.70
1	FC	214	LYS	CD-CE-NZ	6.27	126.12	111.70
1	LC	214	LYS	CD-CE-NZ	6.27	126.11	111.70
1	MC	214	LYS	CD-CE-NZ	6.27	126.11	111.70
1	GC	214	LYS	CD-CE-NZ	6.27	126.11	111.70
1	JC	214	LYS	CD-CE-NZ	6.26	126.11	111.70
1	KC	214	LYS	CD-CE-NZ	6.25	126.09	111.70
1	DC	214	LYS	CD-CE-NZ	6.25	126.08	111.70
1	EC	214	LYS	CD-CE-NZ	6.25	126.08	111.70
1	IC	214	LYS	CD-CE-NZ	6.25	126.08	111.70
5	Gd	107	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	AC	214	LYS	CD-CE-NZ	6.25	126.08	111.70
1	CC	214	LYS	CD-CE-NZ	6.24	126.06	111.70
1	HC	214	LYS	CD-CE-NZ	6.24	126.05	111.70
5	Md	86	ASP	CB-CG-OD1	6.23	123.91	118.30
5	GD	71	LEU	CA-CB-CG	6.22	129.62	115.30
5	Ld	86	ASP	CB-CG-OD1	6.22	123.90	118.30
5	BD	97	ARG	NE-CZ-NH1	-6.21	117.19	120.30
5	Md	117	VAL	CG1-CB-CG2	-6.21	100.97	110.90
5	ED	132	LEU	CB-CG-CD2	-6.20	100.45	111.00
2	KH	355	MET	CA-CB-CG	6.20	123.84	113.30
5	Md	109	LEU	CD1-CG-CD2	-6.20	91.90	110.50
5	FD	82	ARG	CG-CD-NE	6.20	124.81	111.80
5	Ed	71	LEU	CB-CG-CD2	-6.19	100.48	111.00
2	GH	355	MET	CA-CB-CG	6.19	123.82	113.30
2	HH	355	MET	CA-CB-CG	6.18	123.81	113.30
2	LH	355	MET	CA-CB-CG	6.18	123.81	113.30
2	AH	355	MET	CA-CB-CG	6.18	123.81	113.30
2	IH	355	MET	CA-CB-CG	6.18	123.80	113.30
5	Id	55	MET	CG-SD-CE	-6.18	90.32	100.20
5	FD	55	MET	CG-SD-CE	-6.17	90.33	100.20
2	BH	355	MET	CA-CB-CG	6.17	123.79	113.30
2	CH	355	MET	CA-CB-CG	6.17	123.79	113.30
2	MH	355	MET	CA-CB-CG	6.17	123.79	113.30
2	FH	355	MET	CA-CB-CG	6.16	123.78	113.30
5	Kd	107	ARG	NE-CZ-NH1	-6.16	117.22	120.30
2	JH	355	MET	CA-CB-CG	6.16	123.77	113.30
2	DH	355	MET	CA-CB-CG	6.16	123.76	113.30
2	EH	355	MET	CA-CB-CG	6.16	123.77	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	HD	97	ARG	CA-CB-CG	-6.14	99.90	113.40
5	Jd	86	ASP	CB-CG-OD1	6.12	123.81	118.30
5	AD	128	LEU	CA-CB-CG	6.12	129.38	115.30
5	Ad	35	ASP	CB-CG-OD1	-6.09	112.82	118.30
5	DD	82	ARG	CA-CB-CG	6.08	126.78	113.40
5	MD	132	LEU	CB-CG-CD2	-6.07	100.69	111.00
5	Kd	86	ASP	CB-CG-OD1	6.06	123.75	118.30
5	Md	118	LEU	CB-CG-CD2	-6.06	100.70	111.00
5	Ed	86	ASP	CB-CG-OD1	6.05	123.75	118.30
5	Hd	55	MET	CG-SD-CE	6.05	109.88	100.20
5	Dd	86	ASP	CB-CG-OD1	6.03	123.73	118.30
5	Bd	35	ASP	CB-CG-OD1	6.03	123.72	118.30
5	KD	71	LEU	CA-CB-CG	6.01	129.12	115.30
5	GD	128	LEU	CB-CG-CD1	-5.99	100.82	111.00
5	DD	126	GLU	OE1-CD-OE2	-5.99	116.12	123.30
5	KD	126	GLU	OE1-CD-OE2	-5.98	116.12	123.30
5	Gd	117	VAL	CG1-CB-CG2	-5.98	101.33	110.90
5	FD	53	LEU	CA-CB-CG	5.98	129.05	115.30
5	Fd	128	LEU	CB-CG-CD1	5.97	121.15	111.00
5	Ed	35	ASP	CB-CG-OD1	5.97	123.67	118.30
5	AD	68	ASP	CB-CG-OD1	5.97	123.67	118.30
5	CD	82	ARG	NE-CZ-NH2	5.96	123.28	120.30
5	GD	86	ASP	CB-CG-OD1	5.95	123.66	118.30
5	GD	97	ARG	CA-CB-CG	-5.93	100.35	113.40
5	Id	136	ASP	CB-CG-OD2	5.93	123.64	118.30
5	Dd	55	MET	CA-CB-CG	5.92	123.37	113.30
5	KD	52	MET	CG-SD-CE	5.92	109.67	100.20
5	AD	71	LEU	CA-CB-CG	5.92	128.91	115.30
5	BD	132	LEU	CA-CB-CG	-5.89	101.74	115.30
5	Fd	68	ASP	CB-CG-OD1	5.89	123.60	118.30
5	MD	147	VAL	CG1-CB-CG2	-5.89	101.48	110.90
5	FD	132	LEU	CA-CB-CG	-5.89	101.76	115.30
5	BD	136	ASP	CB-CG-OD1	5.88	123.60	118.30
5	Cd	128	LEU	CB-CG-CD1	5.87	120.98	111.00
5	Kd	35	ASP	CB-CG-OD1	5.87	123.58	118.30
5	HD	132	LEU	CA-CB-CG	5.85	128.76	115.30
5	Ed	53	LEU	CB-CG-CD2	-5.82	101.11	111.00
5	Ld	128	LEU	CB-CG-CD1	5.81	120.88	111.00
5	Id	35	ASP	CB-CG-OD1	5.80	123.52	118.30
5	DD	52	MET	CA-CB-CG	5.80	123.16	113.30
5	Kd	125	ASP	CB-CG-OD1	5.79	123.52	118.30
5	Ed	71	LEU	CA-CB-CG	5.78	128.58	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	KD	57	LYS	CA-CB-CG	5.76	126.07	113.40
5	HD	132	LEU	CB-CG-CD2	5.75	120.78	111.00
5	Id	68	ASP	CB-CG-OD1	5.75	123.48	118.30
5	CD	68	ASP	C-N-CA	5.74	136.05	121.70
5	Md	35	ASP	CB-CG-OD1	5.74	123.46	118.30
5	ID	131	ILE	CG1-CB-CG2	-5.73	98.79	111.40
5	KD	97	ARG	CA-CB-CG	-5.72	100.82	113.40
5	Dd	153	VAL	CG1-CB-CG2	-5.71	101.76	110.90
5	GD	109	LEU	CA-CB-CG	5.71	128.42	115.30
5	Kd	71	LEU	CA-CB-CG	5.69	128.39	115.30
5	BD	79	LEU	CA-CB-CG	5.69	128.38	115.30
5	Bd	155	GLU	OE1-CD-OE2	-5.68	116.48	123.30
5	DD	128	LEU	CA-CB-CG	5.66	128.32	115.30
5	Id	125	ASP	CB-CG-OD2	5.64	123.38	118.30
5	Fd	35	ASP	CB-CG-OD1	5.63	123.37	118.30
5	Hd	156	LEU	CA-CB-CG	5.63	128.24	115.30
5	AD	132	LEU	CA-CB-CG	5.61	128.20	115.30
5	Hd	36	ASP	CB-CG-OD2	-5.61	113.25	118.30
5	Hd	71	LEU	CB-CG-CD2	-5.60	101.48	111.00
5	Dd	53	LEU	CB-CG-CD2	-5.58	101.51	111.00
5	AD	126	GLU	CA-CB-CG	5.58	125.67	113.40
5	ID	97	ARG	CG-CD-NE	5.57	123.50	111.80
2	IH	338	TYR	CB-CG-CD1	-5.55	117.67	121.00
5	Ad	52	MET	CG-SD-CE	-5.54	91.34	100.20
2	AH	338	TYR	CB-CG-CD1	-5.53	117.68	121.00
2	KH	338	TYR	CB-CG-CD1	-5.53	117.68	121.00
5	Gd	68	ASP	CB-CG-OD1	5.52	123.27	118.30
5	Jd	53	LEU	CB-CG-CD2	-5.52	101.62	111.00
5	Bd	68	ASP	CB-CG-OD1	5.52	123.27	118.30
2	GH	338	TYR	CB-CG-CD1	-5.52	117.69	121.00
5	MD	54	GLU	N-CA-CB	5.51	120.52	110.60
5	Cd	77	TYR	C-N-CA	5.51	135.47	121.70
5	Fd	125	ASP	CB-CG-OD2	5.51	123.26	118.30
5	CD	126	GLU	CA-CB-CG	5.51	125.51	113.40
2	CH	338	TYR	CB-CG-CD1	-5.50	117.70	121.00
5	CD	52	MET	CG-SD-CE	5.50	109.00	100.20
2	IH	280	LEU	CB-CG-CD1	-5.50	101.65	111.00
5	MD	109	LEU	CA-CB-CG	5.50	127.95	115.30
2	LH	338	TYR	CB-CG-CD1	-5.50	117.70	121.00
2	HH	338	TYR	CB-CG-CD1	-5.50	117.70	121.00
5	Hd	86	ASP	CB-CG-OD2	-5.49	113.36	118.30
2	MH	338	TYR	CB-CG-CD1	-5.49	117.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BH	280	LEU	CB-CG-CD1	-5.49	101.67	111.00
5	Ld	68	ASP	CB-CG-OD1	5.49	123.24	118.30
2	DH	280	LEU	CB-CG-CD1	-5.48	101.68	111.00
2	LH	280	LEU	CB-CG-CD1	-5.48	101.69	111.00
5	Dd	52	MET	CB-CA-C	-5.47	99.45	110.40
2	EH	280	LEU	CB-CG-CD1	-5.47	101.69	111.00
2	CH	280	LEU	CB-CG-CD1	-5.47	101.69	111.00
5	Gd	35	ASP	CB-CG-OD1	-5.47	113.38	118.30
2	JH	280	LEU	CB-CG-CD1	-5.47	101.71	111.00
2	HH	280	LEU	CB-CG-CD1	-5.46	101.71	111.00
2	GH	280	LEU	CB-CG-CD1	-5.46	101.71	111.00
2	AH	280	LEU	CB-CG-CD1	-5.46	101.72	111.00
5	Hd	55	MET	CA-CB-CG	5.46	122.58	113.30
2	KH	280	LEU	CB-CG-CD1	-5.46	101.72	111.00
2	MH	280	LEU	CB-CG-CD1	-5.46	101.72	111.00
2	BH	338	TYR	CB-CG-CD1	-5.46	117.73	121.00
2	FH	280	LEU	CB-CG-CD1	-5.45	101.74	111.00
2	EH	338	TYR	CB-CG-CD1	-5.44	117.74	121.00
5	ID	97	ARG	CA-CB-CG	-5.44	101.44	113.40
5	AD	94	LEU	CB-CG-CD2	5.43	120.23	111.00
5	Ad	156	LEU	CA-CB-CG	5.43	127.80	115.30
2	FH	338	TYR	CB-CG-CD1	-5.43	117.74	121.00
2	JH	338	TYR	CB-CG-CD1	-5.42	117.75	121.00
2	DH	338	TYR	CB-CG-CD1	-5.42	117.75	121.00
5	MD	97	ARG	NH1-CZ-NH2	5.42	125.36	119.40
5	GD	68	ASP	C-N-CA	5.40	135.21	121.70
5	ED	126	GLU	N-CA-CB	5.40	120.32	110.60
5	Fd	53	LEU	CA-CB-CG	5.40	127.72	115.30
5	Fd	77	TYR	C-N-CA	5.40	135.19	121.70
5	GD	82	ARG	CG-CD-NE	5.40	123.13	111.80
5	Ld	109	LEU	CA-CB-CG	5.40	127.71	115.30
5	Bd	53	LEU	CB-CG-CD2	-5.39	101.83	111.00
5	GD	52	MET	CA-CB-CG	5.39	122.46	113.30
5	Hd	53	LEU	CB-CG-CD2	-5.38	101.86	111.00
5	GD	48	VAL	CG1-CB-CG2	-5.37	102.30	110.90
5	FD	126	GLU	CG-CD-OE2	-5.37	107.56	118.30
5	KD	128	LEU	CB-CG-CD1	-5.36	101.88	111.00
5	Ed	79	LEU	CA-CB-CG	5.36	127.62	115.30
5	FD	52	MET	CA-CB-CG	5.36	122.41	113.30
5	Ed	52	MET	CG-SD-CE	-5.36	91.63	100.20
1	MC	189	ASP	CB-CG-OD1	5.35	123.12	118.30
5	BD	53	LEU	CB-CG-CD2	5.35	120.10	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	GK	170	LEU	CA-CB-CG	5.34	127.59	115.30
3	BK	170	LEU	CA-CB-CG	5.34	127.59	115.30
5	Ad	68	ASP	CB-CG-OD1	5.34	123.11	118.30
3	MK	170	LEU	CA-CB-CG	5.34	127.58	115.30
3	DK	170	LEU	CA-CB-CG	5.34	127.58	115.30
3	HK	170	LEU	CA-CB-CG	5.34	127.58	115.30
3	KK	170	LEU	CA-CB-CG	5.34	127.58	115.30
5	ED	68	ASP	C-N-CA	5.34	135.04	121.70
3	FK	170	LEU	CA-CB-CG	5.33	127.56	115.30
3	JK	170	LEU	CA-CB-CG	5.33	127.56	115.30
3	LK	170	LEU	CA-CB-CG	5.33	127.55	115.30
3	AK	170	LEU	CA-CB-CG	5.32	127.54	115.30
1	CC	189	ASP	CB-CG-OD1	5.32	123.09	118.30
3	CK	170	LEU	CA-CB-CG	5.32	127.55	115.30
5	Jd	68	ASP	CB-CG-OD1	5.32	123.09	118.30
3	EK	170	LEU	CA-CB-CG	5.32	127.53	115.30
3	IK	170	LEU	CA-CB-CG	5.31	127.52	115.30
5	Kd	54	GLU	OE1-CD-OE2	5.31	129.67	123.30
5	MD	128	LEU	CA-CB-CG	5.31	127.52	115.30
5	Ad	141	LYS	CA-CB-CG	5.31	125.07	113.40
1	GC	189	ASP	CB-CG-OD1	5.30	123.07	118.30
1	DC	189	ASP	CB-CG-OD1	5.30	123.07	118.30
1	AC	189	ASP	CB-CG-OD1	5.30	123.07	118.30
1	KC	189	ASP	CB-CG-OD1	5.30	123.07	118.30
1	BC	189	ASP	CB-CG-OD1	5.29	123.07	118.30
5	HD	54	GLU	N-CA-CB	5.28	120.10	110.60
1	JC	189	ASP	CB-CG-OD1	5.28	123.05	118.30
5	Jd	67	LYS	CB-CG-CD	5.27	125.31	111.60
1	LC	189	ASP	CB-CG-OD1	5.27	123.04	118.30
3	BK	127	LYS	CA-CB-CG	5.27	124.98	113.40
3	AK	127	LYS	CA-CB-CG	5.26	124.98	113.40
1	EC	189	ASP	CB-CG-OD1	5.26	123.03	118.30
5	Ed	107	ARG	CB-CG-CD	-5.26	97.93	111.60
5	JD	120	SER	N-CA-CB	5.26	118.39	110.50
5	FD	128	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	FC	189	ASP	CB-CG-OD1	5.25	123.03	118.30
3	MK	127	LYS	CA-CB-CG	5.25	124.96	113.40
3	CK	127	LYS	CA-CB-CG	5.25	124.96	113.40
3	EK	127	LYS	CA-CB-CG	5.25	124.95	113.40
5	BD	104	PHE	CB-CG-CD2	-5.25	117.13	120.80
1	HC	189	ASP	CB-CG-OD1	5.25	123.02	118.30
3	HK	127	LYS	CA-CB-CG	5.25	124.94	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	GK	127	LYS	CA-CB-CG	5.25	124.94	113.40
3	JK	127	LYS	CA-CB-CG	5.24	124.94	113.40
3	FK	127	LYS	CA-CB-CG	5.24	124.93	113.40
1	IC	189	ASP	CB-CG-OD1	5.24	123.02	118.30
3	DK	127	LYS	CA-CB-CG	5.23	124.92	113.40
5	Hd	136	ASP	CB-CG-OD1	5.23	123.01	118.30
3	IK	127	LYS	CA-CB-CG	5.23	124.92	113.40
5	Dd	68	ASP	CB-CG-OD1	5.23	123.01	118.30
3	LK	127	LYS	CA-CB-CG	5.23	124.91	113.40
5	AD	68	ASP	C-N-CA	5.23	134.77	121.70
3	KK	127	LYS	CA-CB-CG	5.23	124.90	113.40
5	MD	68	ASP	CB-CG-OD2	5.21	122.99	118.30
5	KD	79	LEU	CB-CG-CD1	-5.21	102.14	111.00
5	AD	52	MET	CB-CA-C	-5.21	99.98	110.40
5	DD	100	LYS	CA-CB-CG	5.21	124.86	113.40
5	KD	156	LEU	CB-CG-CD2	-5.20	102.16	111.00
5	Dd	92	GLU	CB-CA-C	-5.20	100.01	110.40
5	KD	157	ARG	N-CA-CB	5.19	119.94	110.60
5	Ed	71	LEU	CB-CG-CD1	5.18	119.81	111.00
5	Jd	136	ASP	CB-CG-OD2	5.17	122.96	118.30
3	AK	75	LEU	CB-CG-CD2	-5.17	102.21	111.00
3	LK	75	LEU	CB-CG-CD2	-5.17	102.22	111.00
3	IK	75	LEU	CB-CG-CD2	-5.16	102.22	111.00
5	Ad	50	ASP	CB-CG-OD1	5.16	122.95	118.30
3	KK	75	LEU	CB-CG-CD2	-5.16	102.23	111.00
5	AD	97	ARG	CA-CB-CG	-5.16	102.06	113.40
3	HK	75	LEU	CB-CG-CD2	-5.16	102.23	111.00
3	CK	75	LEU	CB-CG-CD2	-5.16	102.24	111.00
5	ED	71	LEU	CA-CB-CG	5.15	127.16	115.30
3	EK	75	LEU	CB-CG-CD2	-5.15	102.24	111.00
3	KK	60	LEU	CA-CB-CG	5.15	127.14	115.30
3	JK	75	LEU	CB-CG-CD2	-5.15	102.25	111.00
3	AK	60	LEU	CA-CB-CG	5.15	127.14	115.30
3	DK	60	LEU	CA-CB-CG	5.15	127.14	115.30
3	DK	75	LEU	CB-CG-CD2	-5.15	102.25	111.00
3	GK	75	LEU	CB-CG-CD2	-5.14	102.26	111.00
3	HK	60	LEU	CA-CB-CG	5.14	127.13	115.30
4	N	154	LEU	CB-CG-CD1	-5.14	102.26	111.00
3	BK	60	LEU	CA-CB-CG	5.14	127.13	115.30
3	BK	75	LEU	CB-CG-CD2	-5.14	102.26	111.00
5	Bd	109	LEU	CB-CG-CD2	5.14	119.74	111.00
3	JK	60	LEU	CA-CB-CG	5.14	127.12	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	154	LEU	CB-CG-CD1	-5.14	102.26	111.00
3	FK	75	LEU	CB-CG-CD2	-5.14	102.26	111.00
3	MK	75	LEU	CB-CG-CD2	-5.14	102.26	111.00
4	T	154	LEU	CB-CG-CD1	-5.14	102.26	111.00
3	LK	60	LEU	CA-CB-CG	5.14	127.12	115.30
4	P	154	LEU	CB-CG-CD1	-5.14	102.27	111.00
4	S	154	LEU	CB-CG-CD1	-5.13	102.27	111.00
3	FK	60	LEU	CA-CB-CG	5.13	127.11	115.30
4	U	154	LEU	CB-CG-CD1	-5.13	102.27	111.00
1	LC	230	ASP	CB-CG-OD2	5.13	122.92	118.30
3	EK	60	LEU	CA-CB-CG	5.13	127.10	115.30
3	MK	60	LEU	CA-CB-CG	5.13	127.09	115.30
4	R	154	LEU	CB-CG-CD1	-5.13	102.28	111.00
3	GK	60	LEU	CA-CB-CG	5.13	127.09	115.30
4	V	154	LEU	CB-CG-CD1	-5.13	102.28	111.00
5	Cd	71	LEU	CA-CB-CG	5.13	127.09	115.30
4	Y	154	LEU	CB-CG-CD1	-5.12	102.29	111.00
4	X	154	LEU	CB-CG-CD1	-5.12	102.30	111.00
3	CK	60	LEU	CA-CB-CG	5.12	127.07	115.30
3	IK	60	LEU	CA-CB-CG	5.12	127.06	115.30
4	W	154	LEU	CB-CG-CD1	-5.12	102.30	111.00
4	Q	154	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	FC	81	GLU	N-CA-CB	5.11	119.79	110.60
4	Z	154	LEU	CB-CG-CD1	-5.11	102.32	111.00
1	MC	81	GLU	N-CA-CB	5.10	119.78	110.60
3	AK	83	LEU	CA-CB-CG	5.10	127.03	115.30
1	KC	81	GLU	N-CA-CB	5.10	119.77	110.60
5	Bd	155	GLU	CA-CB-CG	5.10	124.61	113.40
1	HC	81	GLU	N-CA-CB	5.09	119.77	110.60
1	KC	230	ASP	CB-CG-OD2	5.09	122.89	118.30
1	FC	230	ASP	CB-CG-OD2	5.09	122.88	118.30
3	FK	83	LEU	CA-CB-CG	5.09	127.01	115.30
5	AD	129	ALA	C-N-CA	5.09	134.43	121.70
5	Ad	85	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	BC	81	GLU	N-CA-CB	5.09	119.77	110.60
1	DC	81	GLU	N-CA-CB	5.09	119.76	110.60
3	CK	83	LEU	CA-CB-CG	5.09	127.00	115.30
1	JC	81	GLU	N-CA-CB	5.08	119.75	110.60
5	Jd	67	LYS	CG-CD-CE	-5.08	96.65	111.90
1	CC	61	GLU	CB-CG-CD	5.08	127.92	114.20
3	BK	83	LEU	CA-CB-CG	5.08	126.98	115.30
1	DC	230	ASP	CB-CG-OD2	5.08	122.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EC	81	GLU	N-CA-CB	5.08	119.74	110.60
1	GC	230	ASP	CB-CG-OD2	5.08	122.87	118.30
1	JC	230	ASP	CB-CG-OD2	5.08	122.87	118.30
1	LC	81	GLU	N-CA-CB	5.08	119.74	110.60
1	CC	230	ASP	CB-CG-OD2	5.08	122.87	118.30
1	AC	61	GLU	CB-CG-CD	5.08	127.90	114.20
1	GC	81	GLU	N-CA-CB	5.08	119.74	110.60
1	IC	81	GLU	N-CA-CB	5.08	119.74	110.60
3	JK	83	LEU	CA-CB-CG	5.08	126.98	115.30
3	LK	83	LEU	CA-CB-CG	5.08	126.97	115.30
1	MC	230	ASP	CB-CG-OD2	5.08	122.87	118.30
5	Gd	141	LYS	CA-CB-CG	5.07	124.56	113.40
1	KC	61	GLU	CB-CG-CD	5.07	127.90	114.20
5	LD	94	LEU	CB-CG-CD2	5.07	119.62	111.00
5	BD	53	LEU	CA-CB-CG	5.07	126.97	115.30
1	EC	61	GLU	CB-CG-CD	5.07	127.89	114.20
3	EK	83	LEU	CA-CB-CG	5.07	126.96	115.30
1	LC	61	GLU	CB-CG-CD	5.07	127.89	114.20
1	CC	81	GLU	N-CA-CB	5.07	119.73	110.60
3	DK	83	LEU	CA-CB-CG	5.07	126.96	115.30
3	IK	83	LEU	CA-CB-CG	5.07	126.96	115.30
1	AC	81	GLU	N-CA-CB	5.07	119.72	110.60
3	MK	83	LEU	CA-CB-CG	5.07	126.96	115.30
1	FC	61	GLU	CB-CG-CD	5.07	127.88	114.20
3	GK	83	LEU	CA-CB-CG	5.07	126.95	115.30
1	HC	61	GLU	CB-CG-CD	5.07	127.88	114.20
1	HC	230	ASP	CB-CG-OD2	5.07	122.86	118.30
1	JC	61	GLU	CB-CG-CD	5.07	127.88	114.20
5	KD	54	GLU	N-CA-CB	5.07	119.72	110.60
1	GC	61	GLU	CB-CG-CD	5.06	127.87	114.20
1	BC	61	GLU	CB-CG-CD	5.06	127.87	114.20
1	AC	230	ASP	CB-CG-OD2	5.06	122.85	118.30
5	Ed	36	ASP	CB-CG-OD1	5.06	122.85	118.30
1	IC	61	GLU	CB-CG-CD	5.06	127.86	114.20
3	KK	83	LEU	CA-CB-CG	5.06	126.93	115.30
1	MC	61	GLU	CB-CG-CD	5.06	127.85	114.20
1	DC	61	GLU	CB-CG-CD	5.06	127.85	114.20
3	HK	83	LEU	CA-CB-CG	5.05	126.93	115.30
5	LD	74	PRO	C-N-CA	5.05	134.34	121.70
5	AD	131	ILE	CA-CB-CG1	5.05	120.60	111.00
1	IC	230	ASP	CB-CG-OD2	5.05	122.85	118.30
5	Ad	107	ARG	CG-CD-NE	5.05	122.41	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	KD	126	GLU	CB-CA-C	5.05	120.50	110.40
5	MD	126	GLU	CG-CD-OE2	-5.05	108.20	118.30
1	BC	230	ASP	CB-CG-OD2	5.04	122.84	118.30
5	ED	74	PRO	C-N-CA	5.04	134.30	121.70
5	KD	132	LEU	CA-CB-CG	-5.03	103.72	115.30
1	EC	230	ASP	CB-CG-OD2	5.03	122.83	118.30
5	Id	107	ARG	NE-CZ-NH1	-5.02	117.79	120.30
2	AH	295	ARG	NE-CZ-NH1	5.02	122.81	120.30
5	FD	130	GLU	CB-CA-C	-5.01	100.37	110.40
5	DD	97	ARG	CG-CD-NE	5.01	122.33	111.80
5	Hd	128	LEU	CB-CG-CD1	5.01	119.51	111.00
5	FD	133	ARG	NE-CZ-NH2	-5.00	117.80	120.30
5	BD	131	ILE	CG1-CB-CG2	-5.00	100.39	111.40

There are no chirality outliers.

All (90) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AD	51	SER	Peptide
4	AX	142	ALA	Peptide
4	AX	153	ALA	Peptide
4	AZ	45	ALA	Peptide
5	BD	124	LYS	Peptide
4	BX	142	ALA	Peptide
4	BX	153	ALA	Peptide
4	BZ	45	ALA	Peptide
5	Bd	85	VAL	Peptide
5	CD	124	LYS	Peptide
5	CD	51	SER	Peptide
4	CX	142	ALA	Peptide
4	CX	153	ALA	Peptide
4	CZ	45	ALA	Peptide
5	DD	126	GLU	Sidechain
5	DD	81	ALA	Peptide
4	DX	142	ALA	Peptide
4	DX	153	ALA	Peptide
4	DZ	45	ALA	Peptide
5	Dd	85	VAL	Peptide
5	ED	124	LYS	Peptide
5	ED	127	SER	Peptide
5	ED	130	GLU	Sidechain
4	EX	142	ALA	Peptide

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Mol	Chain	Res	Type	Group
4	EX	153	ALA	Peptide
4	EZ	45	ALA	Peptide
5	Ed	62	ILE	Peptide
5	Ed	85	VAL	Peptide
5	FD	124	LYS	Peptide
5	FD	126	GLU	Sidechain
4	FX	142	ALA	Peptide
4	FX	153	ALA	Peptide
4	FZ	45	ALA	Peptide
5	Fd	85	VAL	Peptide
5	GD	124	LYS	Peptide
5	GD	126	GLU	Sidechain
5	GD	133	ARG	Sidechain
4	GX	142	ALA	Peptide
4	GX	153	ALA	Peptide
4	GZ	45	ALA	Peptide
5	HD	124	LYS	Peptide
5	HD	125	ASP	Peptide
4	HX	142	ALA	Peptide
4	HX	153	ALA	Peptide
4	HZ	45	ALA	Peptide
5	ID	124	LYS	Peptide
5	ID	126	GLU	Sidechain
5	ID	130	GLU	Peptide
4	IX	142	ALA	Peptide
4	IX	153	ALA	Peptide
4	IZ	45	ALA	Peptide
5	Id	85	VAL	Peptide
5	JD	124	LYS	Peptide
4	JX	142	ALA	Peptide
4	JX	153	ALA	Peptide
4	JZ	45	ALA	Peptide
5	Jd	85	VAL	Peptide
5	KD	124	LYS	Peptide
5	KD	126	GLU	Sidechain
5	KD	127	SER	Peptide
4	KX	142	ALA	Peptide
4	KX	153	ALA	Peptide
4	KZ	45	ALA	Peptide
5	LD	126	GLU	Sidechain
5	LD	61	VAL	Peptide
4	LX	142	ALA	Peptide

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Mol	Chain	Res	Type	Group
4	LX	153	ALA	Peptide
4	LZ	45	ALA	Peptide
5	Ld	62	ILE	Peptide
5	MD	124	LYS	Peptide
5	MD	126	GLU	Sidechain
5	MD	155	GLU	Sidechain
4	MX	142	ALA	Peptide
4	MX	153	ALA	Peptide
4	MZ	45	ALA	Peptide
5	Md	68	ASP	Peptide
5	Md	85	VAL	Peptide
4	N	134	MET	Peptide
4	O	134	MET	Peptide
4	P	134	MET	Peptide
4	Q	134	MET	Peptide
4	R	134	MET	Peptide
4	S	134	MET	Peptide
4	T	134	MET	Peptide
4	U	134	MET	Peptide
4	V	134	MET	Peptide
4	W	134	MET	Peptide
4	X	134	MET	Peptide
4	Y	134	MET	Peptide
4	Z	134	MET	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.

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	BC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	CC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	DC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	EC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	FC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	GC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	HC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	IC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	JC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	KC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	LC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	MC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
2	AH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	BH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	CH	87/361 (24%)	78 (90%)	9 (10%)	0	100	100
2	DH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	EH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	FH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	GH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	HH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	IH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	JH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	KH	87/361 (24%)	78 (90%)	9 (10%)	0	100	100
2	LH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	MH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
3	AK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	BK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	CK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	DK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	EK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	FK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	GK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	HK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	IK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	JK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	KK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	LK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	MK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
4	AX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	AY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	AZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	BX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	BY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	BZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	CX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	CY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	CZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	DX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	DY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	DZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	EX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	EY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	EZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	FX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	FY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	FZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	GX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	GY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	GZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	HX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	HY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	HZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	IX	226/579 (39%)	200 (88%)	26 (12%)	0	100	100
4	IY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	IZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	JX	226/579 (39%)	200 (88%)	26 (12%)	0	100	100
4	JY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	JZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	KX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	KY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	KZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	LX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	LY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	LZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	MX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	MY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	MZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	N	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	O	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	P	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	Q	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	R	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	S	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	T	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	U	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	V	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	W	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	X	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	Y	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	Z	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
5	AD	133/163 (82%)	120 (90%)	13 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Ad	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
5	BD	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
5	Bd	136/163 (83%)	124 (91%)	12 (9%)	0	100	100
5	CD	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
5	Cd	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
5	DD	133/163 (82%)	124 (93%)	9 (7%)	0	100	100
5	Dd	136/163 (83%)	128 (94%)	8 (6%)	0	100	100
5	ED	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
5	Ed	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
5	FD	133/163 (82%)	126 (95%)	7 (5%)	0	100	100
5	Fd	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
5	GD	133/163 (82%)	127 (96%)	6 (4%)	0	100	100
5	Gd	136/163 (83%)	125 (92%)	11 (8%)	0	100	100
5	HD	133/163 (82%)	123 (92%)	10 (8%)	0	100	100
5	Hd	136/163 (83%)	129 (95%)	7 (5%)	0	100	100
5	ID	133/163 (82%)	122 (92%)	11 (8%)	0	100	100
5	Id	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
5	JD	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
5	Jd	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
5	KD	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
5	Kd	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
5	LD	133/163 (82%)	124 (93%)	9 (7%)	0	100	100
5	Ld	136/163 (83%)	124 (91%)	12 (9%)	0	100	100
5	MD	133/163 (82%)	124 (93%)	9 (7%)	0	100	100
5	Md	136/163 (83%)	124 (91%)	12 (9%)	0	100	100
All	All	15288/45435 (34%)	13993 (92%)	1295 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AC	169/257 (66%)	157 (93%)	12 (7%)	14	46
1	BC	169/257 (66%)	157 (93%)	12 (7%)	14	46
1	CC	169/257 (66%)	157 (93%)	12 (7%)	14	46
1	DC	169/257 (66%)	159 (94%)	10 (6%)	19	53
1	EC	169/257 (66%)	157 (93%)	12 (7%)	14	46
1	FC	169/257 (66%)	157 (93%)	12 (7%)	14	46
1	GC	169/257 (66%)	157 (93%)	12 (7%)	14	46
1	HC	169/257 (66%)	158 (94%)	11 (6%)	17	50
1	IC	169/257 (66%)	157 (93%)	12 (7%)	14	46
1	JC	169/257 (66%)	157 (93%)	12 (7%)	14	46
1	KC	169/257 (66%)	157 (93%)	12 (7%)	14	46
1	LC	169/257 (66%)	157 (93%)	12 (7%)	14	46
1	MC	169/257 (66%)	157 (93%)	12 (7%)	14	46
2	AH	75/300 (25%)	70 (93%)	5 (7%)	16	48
2	BH	75/300 (25%)	70 (93%)	5 (7%)	16	48
2	CH	75/300 (25%)	69 (92%)	6 (8%)	12	41
2	DH	75/300 (25%)	69 (92%)	6 (8%)	12	41
2	EH	75/300 (25%)	69 (92%)	6 (8%)	12	41
2	FH	75/300 (25%)	69 (92%)	6 (8%)	12	41
2	GH	75/300 (25%)	69 (92%)	6 (8%)	12	41
2	HH	75/300 (25%)	69 (92%)	6 (8%)	12	41
2	IH	75/300 (25%)	70 (93%)	5 (7%)	16	48
2	JH	75/300 (25%)	69 (92%)	6 (8%)	12	41
2	KH	75/300 (25%)	69 (92%)	6 (8%)	12	41
2	LH	75/300 (25%)	69 (92%)	6 (8%)	12	41
2	MH	75/300 (25%)	69 (92%)	6 (8%)	12	41
3	AK	126/163 (77%)	117 (93%)	9 (7%)	14	46
3	BK	126/163 (77%)	117 (93%)	9 (7%)	14	46
3	CK	126/163 (77%)	117 (93%)	9 (7%)	14	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	DK	126/163 (77%)	117 (93%)	9 (7%)	14	46
3	EK	126/163 (77%)	117 (93%)	9 (7%)	14	46
3	FK	126/163 (77%)	117 (93%)	9 (7%)	14	46
3	GK	126/163 (77%)	117 (93%)	9 (7%)	14	46
3	HK	126/163 (77%)	117 (93%)	9 (7%)	14	46
3	IK	126/163 (77%)	117 (93%)	9 (7%)	14	46
3	JK	126/163 (77%)	117 (93%)	9 (7%)	14	46
3	KK	126/163 (77%)	117 (93%)	9 (7%)	14	46
3	LK	126/163 (77%)	117 (93%)	9 (7%)	14	46
3	MK	126/163 (77%)	117 (93%)	9 (7%)	14	46
4	N	118/203 (58%)	111 (94%)	7 (6%)	19	53
4	O	118/203 (58%)	111 (94%)	7 (6%)	19	53
4	P	118/203 (58%)	111 (94%)	7 (6%)	19	53
4	Q	118/203 (58%)	111 (94%)	7 (6%)	19	53
4	R	118/203 (58%)	111 (94%)	7 (6%)	19	53
4	S	118/203 (58%)	111 (94%)	7 (6%)	19	53
4	T	118/203 (58%)	111 (94%)	7 (6%)	19	53
4	U	118/203 (58%)	111 (94%)	7 (6%)	19	53
4	V	118/203 (58%)	111 (94%)	7 (6%)	19	53
4	W	118/203 (58%)	111 (94%)	7 (6%)	19	53
4	X	118/203 (58%)	111 (94%)	7 (6%)	19	53
4	Y	118/203 (58%)	111 (94%)	7 (6%)	19	53
4	Z	118/203 (58%)	111 (94%)	7 (6%)	19	53
5	AD	116/139 (84%)	116 (100%)	0	100	100
5	Ad	119/139 (86%)	119 (100%)	0	100	100
5	BD	116/139 (84%)	116 (100%)	0	100	100
5	Bd	119/139 (86%)	119 (100%)	0	100	100
5	CD	116/139 (84%)	116 (100%)	0	100	100
5	Cd	119/139 (86%)	118 (99%)	1 (1%)	81	91
5	DD	116/139 (84%)	116 (100%)	0	100	100
5	Dd	119/139 (86%)	118 (99%)	1 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	ED	116/139 (84%)	116 (100%)	0	100	100
5	Ed	119/139 (86%)	118 (99%)	1 (1%)	81	91
5	FD	116/139 (84%)	116 (100%)	0	100	100
5	Fd	119/139 (86%)	118 (99%)	1 (1%)	81	91
5	GD	116/139 (84%)	116 (100%)	0	100	100
5	Gd	119/139 (86%)	117 (98%)	2 (2%)	60	82
5	HD	116/139 (84%)	116 (100%)	0	100	100
5	Hd	119/139 (86%)	118 (99%)	1 (1%)	81	91
5	ID	116/139 (84%)	116 (100%)	0	100	100
5	Id	119/139 (86%)	117 (98%)	2 (2%)	60	82
5	JD	116/139 (84%)	116 (100%)	0	100	100
5	Jd	119/139 (86%)	117 (98%)	2 (2%)	60	82
5	KD	116/139 (84%)	116 (100%)	0	100	100
5	Kd	119/139 (86%)	119 (100%)	0	100	100
5	LD	116/139 (84%)	116 (100%)	0	100	100
5	Ld	119/139 (86%)	118 (99%)	1 (1%)	81	91
5	MD	116/139 (84%)	116 (100%)	0	100	100
5	Md	119/139 (86%)	117 (98%)	2 (2%)	60	82
All	All	9399/15613 (60%)	8949 (95%)	450 (5%)	29	60

All (450) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AC	61	GLU
1	AC	69	GLN
1	AC	81	GLU
1	AC	102	GLU
1	AC	103	HIS
1	AC	104	ASN
1	AC	136	LYS
1	AC	185	LYS
1	AC	212	TYR
1	AC	214	LYS
1	AC	218	MET
1	AC	259	SER
2	DH	294	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	DH	314	VAL
2	DH	315	ARG
2	DH	343	SER
2	DH	358	LYS
2	DH	360	GLU
3	DK	52	THR
3	DK	60	LEU
3	DK	101	GLU
3	DK	107	LYS
3	DK	128	ARG
3	DK	141	SER
3	DK	163	LYS
3	DK	173	ASP
3	DK	180	VAL
5	Dd	100	LYS
1	EC	61	GLU
1	EC	69	GLN
1	EC	81	GLU
1	EC	102	GLU
1	EC	103	HIS
1	EC	104	ASN
1	EC	136	LYS
1	EC	185	LYS
1	EC	212	TYR
1	EC	214	LYS
1	EC	218	MET
1	EC	259	SER
2	EH	294	ARG
2	EH	314	VAL
2	EH	315	ARG
2	EH	343	SER
2	EH	358	LYS
2	EH	360	GLU
3	EK	52	THR
3	EK	60	LEU
3	EK	101	GLU
3	EK	107	LYS
3	EK	128	ARG
3	EK	141	SER
3	EK	163	LYS
3	EK	173	ASP
3	EK	180	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	Ed	75	ASN
1	FC	61	GLU
1	FC	69	GLN
1	FC	81	GLU
1	FC	102	GLU
1	FC	103	HIS
1	FC	104	ASN
1	FC	136	LYS
1	FC	185	LYS
1	FC	212	TYR
1	FC	214	LYS
1	FC	218	MET
1	FC	259	SER
2	FH	294	ARG
2	FH	314	VAL
2	FH	315	ARG
2	FH	343	SER
2	FH	358	LYS
2	FH	360	GLU
3	FK	52	THR
3	FK	60	LEU
3	FK	101	GLU
3	FK	107	LYS
3	FK	128	ARG
3	FK	141	SER
3	FK	163	LYS
3	FK	173	ASP
3	FK	180	VAL
5	Fd	75	ASN
1	GC	61	GLU
1	GC	69	GLN
1	GC	81	GLU
1	GC	102	GLU
1	GC	103	HIS
1	GC	104	ASN
1	GC	136	LYS
1	GC	185	LYS
1	GC	212	TYR
1	GC	214	LYS
1	GC	218	MET
1	GC	259	SER
2	GH	294	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	GH	314	VAL
2	GH	315	ARG
2	GH	343	SER
2	GH	358	LYS
2	GH	360	GLU
3	GK	52	THR
3	GK	60	LEU
3	GK	101	GLU
3	GK	107	LYS
3	GK	128	ARG
3	GK	141	SER
3	GK	163	LYS
3	GK	173	ASP
3	GK	180	VAL
5	Gd	75	ASN
5	Gd	100	LYS
1	HC	61	GLU
1	HC	69	GLN
1	HC	81	GLU
1	HC	102	GLU
1	HC	103	HIS
1	HC	136	LYS
1	HC	185	LYS
1	HC	212	TYR
1	HC	214	LYS
1	HC	218	MET
1	HC	259	SER
2	HH	294	ARG
2	HH	314	VAL
2	HH	315	ARG
2	HH	343	SER
2	HH	358	LYS
2	HH	360	GLU
3	HK	52	THR
3	HK	60	LEU
3	HK	101	GLU
3	HK	107	LYS
3	HK	128	ARG
3	HK	141	SER
3	HK	163	LYS
3	HK	173	ASP
3	HK	180	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	Hd	78	ASN
1	IC	61	GLU
1	IC	69	GLN
1	IC	81	GLU
1	IC	102	GLU
1	IC	103	HIS
1	IC	104	ASN
1	IC	136	LYS
1	IC	185	LYS
1	IC	212	TYR
1	IC	214	LYS
1	IC	218	MET
1	IC	259	SER
2	IH	294	ARG
2	IH	314	VAL
2	IH	315	ARG
2	IH	343	SER
2	IH	360	GLU
3	IK	52	THR
3	IK	60	LEU
3	IK	101	GLU
3	IK	107	LYS
3	IK	128	ARG
3	IK	141	SER
3	IK	163	LYS
3	IK	173	ASP
3	IK	180	VAL
5	Id	75	ASN
5	Id	78	ASN
1	JC	61	GLU
1	JC	69	GLN
1	JC	81	GLU
1	JC	102	GLU
1	JC	103	HIS
1	JC	104	ASN
1	JC	136	LYS
1	JC	185	LYS
1	JC	212	TYR
1	JC	214	LYS
1	JC	218	MET
1	JC	259	SER
2	JH	294	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	JH	314	VAL
2	JH	315	ARG
2	JH	343	SER
2	JH	358	LYS
2	JH	360	GLU
3	JK	52	THR
3	JK	60	LEU
3	JK	101	GLU
3	JK	107	LYS
3	JK	128	ARG
3	JK	141	SER
3	JK	163	LYS
3	JK	173	ASP
3	JK	180	VAL
2	AH	294	ARG
2	AH	314	VAL
2	AH	315	ARG
2	AH	343	SER
2	AH	360	GLU
5	Jd	75	ASN
5	Jd	100	LYS
1	KC	61	GLU
1	KC	69	GLN
1	KC	81	GLU
1	KC	102	GLU
1	KC	103	HIS
1	KC	104	ASN
1	KC	136	LYS
1	KC	185	LYS
1	KC	212	TYR
1	KC	214	LYS
1	KC	218	MET
1	KC	259	SER
2	KH	294	ARG
2	KH	314	VAL
2	KH	315	ARG
2	KH	343	SER
2	KH	358	LYS
2	KH	360	GLU
3	KK	52	THR
3	KK	60	LEU
3	KK	101	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	KK	107	LYS
3	KK	128	ARG
3	KK	141	SER
3	KK	163	LYS
3	KK	173	ASP
3	KK	180	VAL
1	LC	61	GLU
1	LC	69	GLN
1	LC	81	GLU
1	LC	102	GLU
1	LC	103	HIS
1	LC	104	ASN
1	LC	136	LYS
1	LC	185	LYS
1	LC	212	TYR
1	LC	214	LYS
1	LC	218	MET
1	LC	259	SER
2	LH	294	ARG
2	LH	314	VAL
2	LH	315	ARG
2	LH	343	SER
2	LH	358	LYS
2	LH	360	GLU
3	LK	52	THR
3	LK	60	LEU
3	LK	101	GLU
3	LK	107	LYS
3	LK	128	ARG
3	LK	141	SER
3	LK	163	LYS
3	LK	173	ASP
3	LK	180	VAL
5	Ld	75	ASN
1	MC	61	GLU
1	MC	69	GLN
1	MC	81	GLU
1	MC	102	GLU
1	MC	103	HIS
1	MC	104	ASN
1	MC	136	LYS
1	MC	185	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	MC	212	TYR
1	MC	214	LYS
1	MC	218	MET
1	MC	259	SER
2	MH	294	ARG
2	MH	314	VAL
2	MH	315	ARG
2	MH	343	SER
2	MH	358	LYS
2	MH	360	GLU
3	MK	52	THR
3	MK	60	LEU
3	MK	101	GLU
3	MK	107	LYS
3	MK	128	ARG
3	MK	141	SER
3	MK	163	LYS
3	MK	173	ASP
3	MK	180	VAL
5	Md	75	ASN
5	Md	100	LYS
3	AK	52	THR
3	AK	60	LEU
3	AK	101	GLU
3	AK	107	LYS
3	AK	128	ARG
3	AK	141	SER
3	AK	163	LYS
3	AK	173	ASP
3	AK	180	VAL
4	N	99	ARG
4	N	106	ILE
4	N	112	GLN
4	N	122	THR
4	N	162	THR
4	N	165	VAL
4	N	190	MET
4	O	99	ARG
4	O	106	ILE
4	O	112	GLN
4	O	122	THR
4	O	162	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	O	165	VAL
4	O	190	MET
4	P	99	ARG
4	P	106	ILE
4	P	112	GLN
4	P	122	THR
4	P	162	THR
4	P	165	VAL
4	P	190	MET
4	Q	99	ARG
4	Q	106	ILE
4	Q	112	GLN
4	Q	122	THR
4	Q	162	THR
4	Q	165	VAL
4	Q	190	MET
4	R	99	ARG
4	R	106	ILE
4	R	112	GLN
4	R	122	THR
4	R	162	THR
4	R	165	VAL
4	R	190	MET
4	S	99	ARG
4	S	106	ILE
4	S	112	GLN
4	S	122	THR
4	S	162	THR
4	S	165	VAL
4	S	190	MET
4	T	99	ARG
4	T	106	ILE
4	T	112	GLN
4	T	122	THR
4	T	162	THR
4	T	165	VAL
4	T	190	MET
4	U	99	ARG
4	U	106	ILE
4	U	112	GLN
4	U	122	THR
4	U	162	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	U	165	VAL
4	U	190	MET
4	V	99	ARG
4	V	106	ILE
4	V	112	GLN
4	V	122	THR
4	V	162	THR
4	V	165	VAL
4	V	190	MET
4	W	99	ARG
4	W	106	ILE
4	W	112	GLN
4	W	122	THR
4	W	162	THR
4	W	165	VAL
4	W	190	MET
4	X	99	ARG
4	X	106	ILE
4	X	112	GLN
4	X	122	THR
4	X	162	THR
4	X	165	VAL
4	X	190	MET
4	Y	99	ARG
4	Y	106	ILE
4	Y	112	GLN
4	Y	122	THR
4	Y	162	THR
4	Y	165	VAL
4	Y	190	MET
4	Z	99	ARG
4	Z	106	ILE
4	Z	112	GLN
4	Z	122	THR
4	Z	162	THR
4	Z	165	VAL
4	Z	190	MET
1	BC	61	GLU
1	BC	69	GLN
1	BC	81	GLU
1	BC	102	GLU
1	BC	103	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	BC	104	ASN
1	BC	136	LYS
1	BC	185	LYS
1	BC	212	TYR
1	BC	214	LYS
1	BC	218	MET
1	BC	259	SER
2	BH	294	ARG
2	BH	314	VAL
2	BH	315	ARG
2	BH	343	SER
2	BH	360	GLU
3	BK	52	THR
3	BK	60	LEU
3	BK	101	GLU
3	BK	107	LYS
3	BK	128	ARG
3	BK	141	SER
3	BK	163	LYS
3	BK	173	ASP
3	BK	180	VAL
1	CC	61	GLU
1	CC	69	GLN
1	CC	81	GLU
1	CC	102	GLU
1	CC	103	HIS
1	CC	104	ASN
1	CC	136	LYS
1	CC	185	LYS
1	CC	212	TYR
1	CC	214	LYS
1	CC	218	MET
1	CC	259	SER
2	CH	294	ARG
2	CH	314	VAL
2	CH	315	ARG
2	CH	343	SER
2	CH	358	LYS
2	CH	360	GLU
3	CK	52	THR
3	CK	60	LEU
3	CK	101	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	CK	107	LYS
3	CK	128	ARG
3	CK	141	SER
3	CK	163	LYS
3	CK	173	ASP
3	CK	180	VAL
5	Cd	75	ASN
1	DC	61	GLU
1	DC	69	GLN
1	DC	81	GLU
1	DC	102	GLU
1	DC	136	LYS
1	DC	185	LYS
1	DC	212	TYR
1	DC	214	LYS
1	DC	218	MET
1	DC	259	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	DK	87	GLN
3	EK	87	GLN
5	Ed	75	ASN
3	FK	87	GLN
5	Fd	75	ASN
1	GC	103	HIS
3	GK	87	GLN
5	Gd	75	ASN
3	HK	87	GLN
5	Hd	78	ASN
3	IK	87	GLN
5	Id	75	ASN
3	JK	87	GLN
5	Jd	75	ASN
3	KK	87	GLN
3	LK	87	GLN
5	Ld	75	ASN
3	MK	87	GLN
5	Md	75	ASN
3	AK	87	GLN
4	S	150	ASN

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Mol	Chain	Res	Type
4	T	150	ASN
3	BK	87	GLN
1	CC	103	HIS
3	CK	87	GLN
5	Cd	75	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

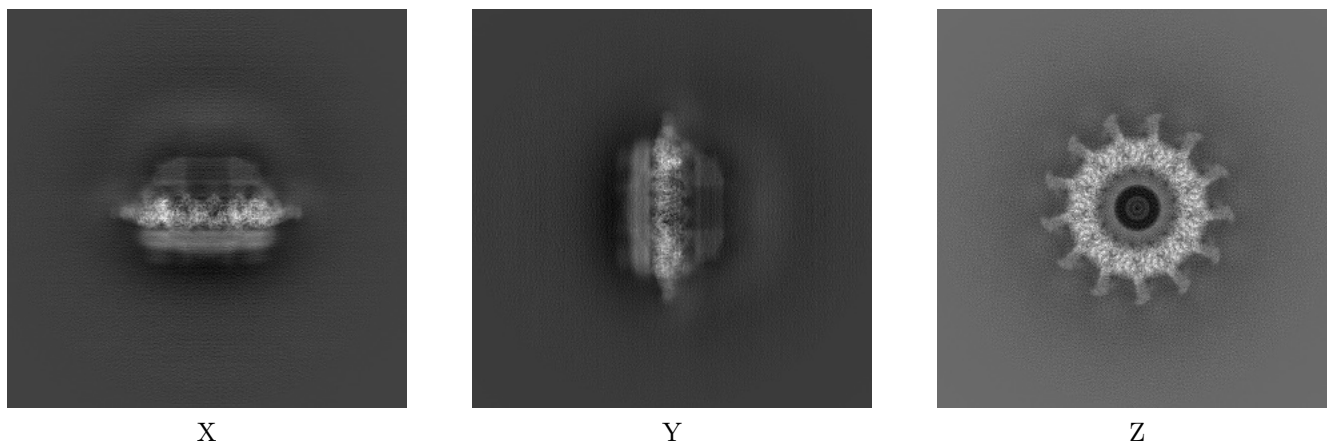
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22068. 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](#)

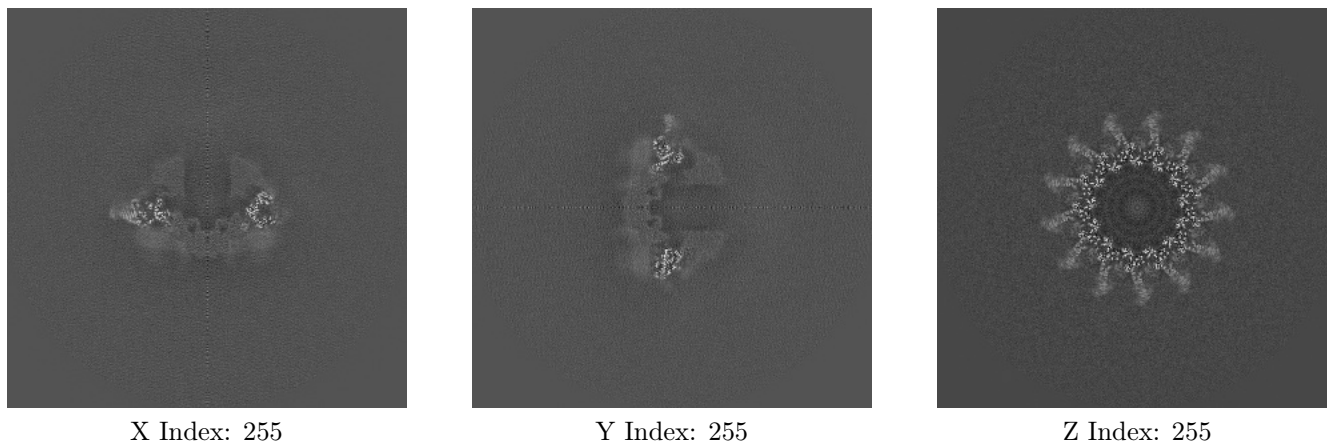
#### 6.1.1 Primary map



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

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

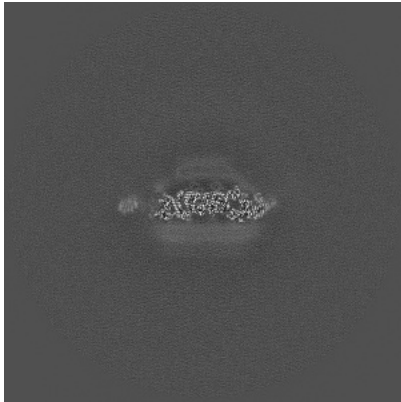
#### 6.2.1 Primary map



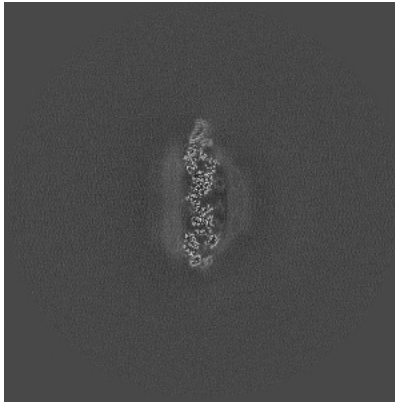
The images above show central slices of the map in three orthogonal directions.

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

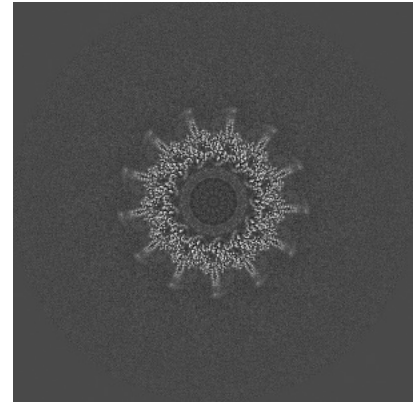
### 6.3.1 Primary map



X Index: 314



Y Index: 200

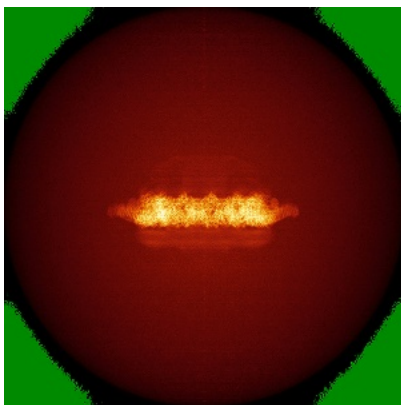


Z Index: 242

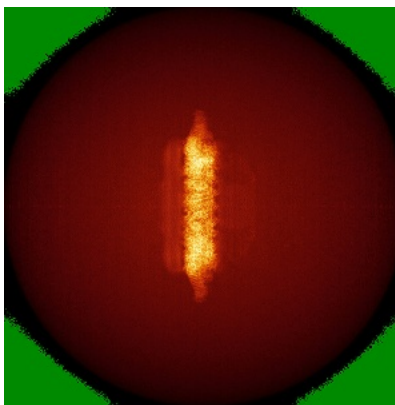
The images above show the largest variance slices of the map in three orthogonal directions.

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

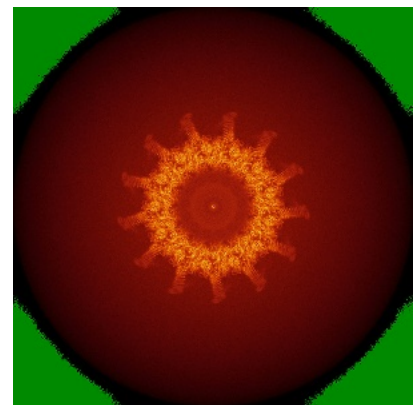
### 6.4.1 Primary map



X



Y

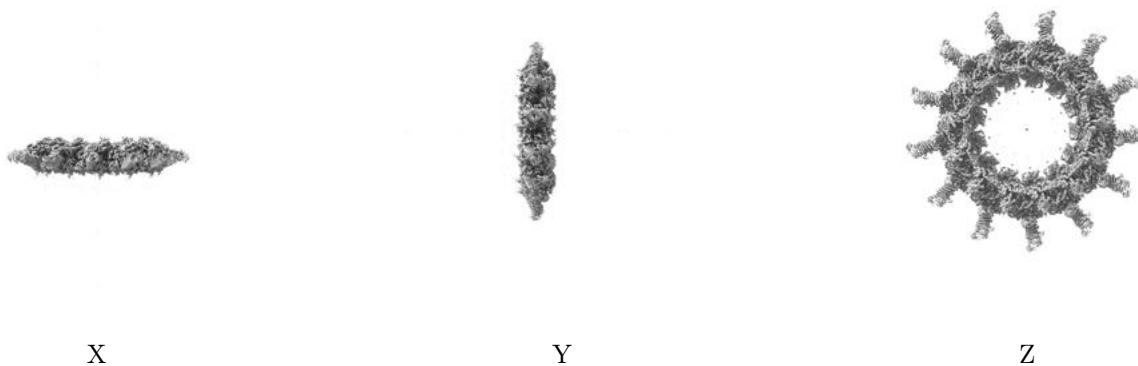


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

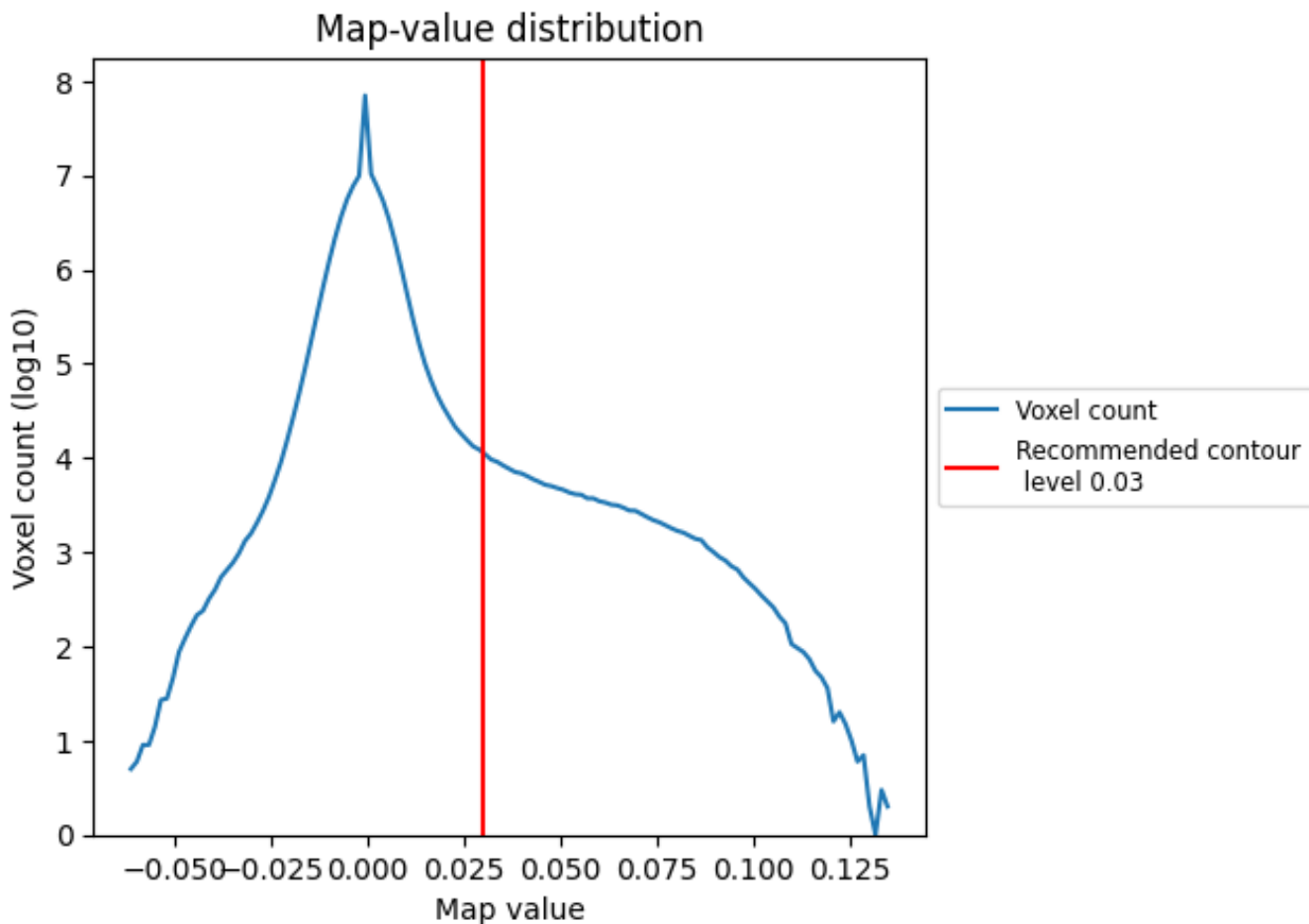
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

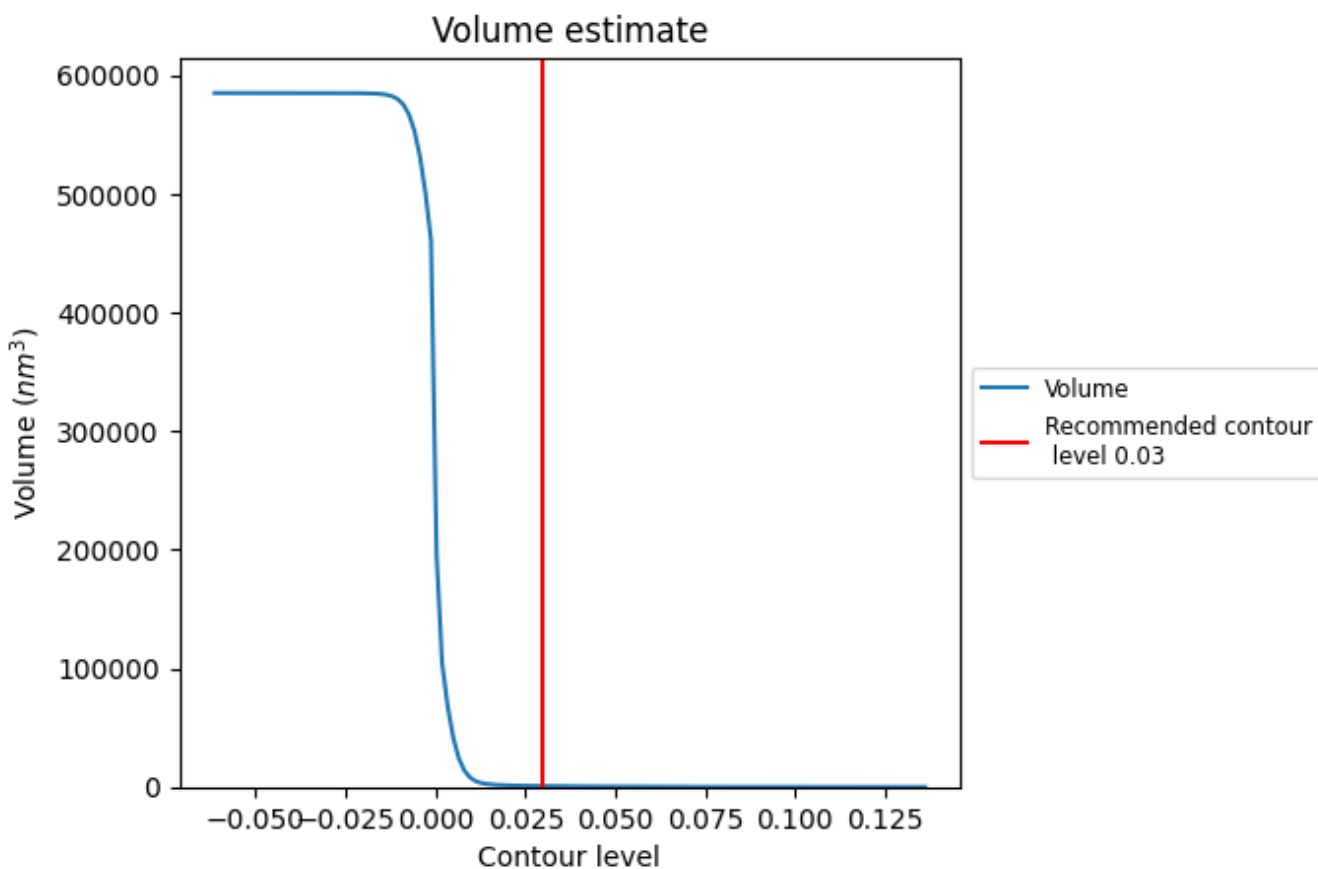
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

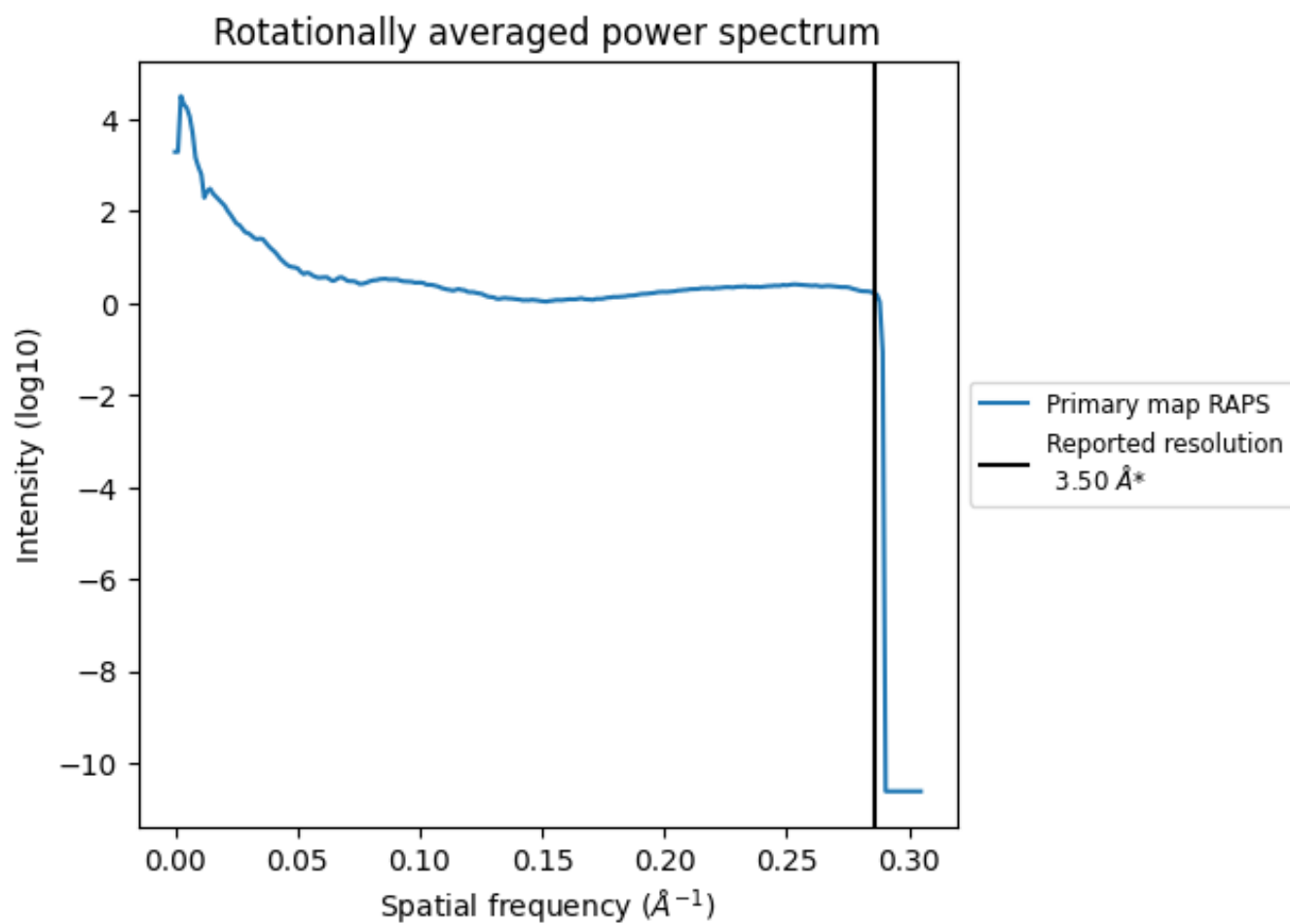
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 751 nm<sup>3</sup>; this corresponds to an approximate mass of 679 kDa.

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

### 7.3 Rotationally averaged power spectrum [\(i\)](#)

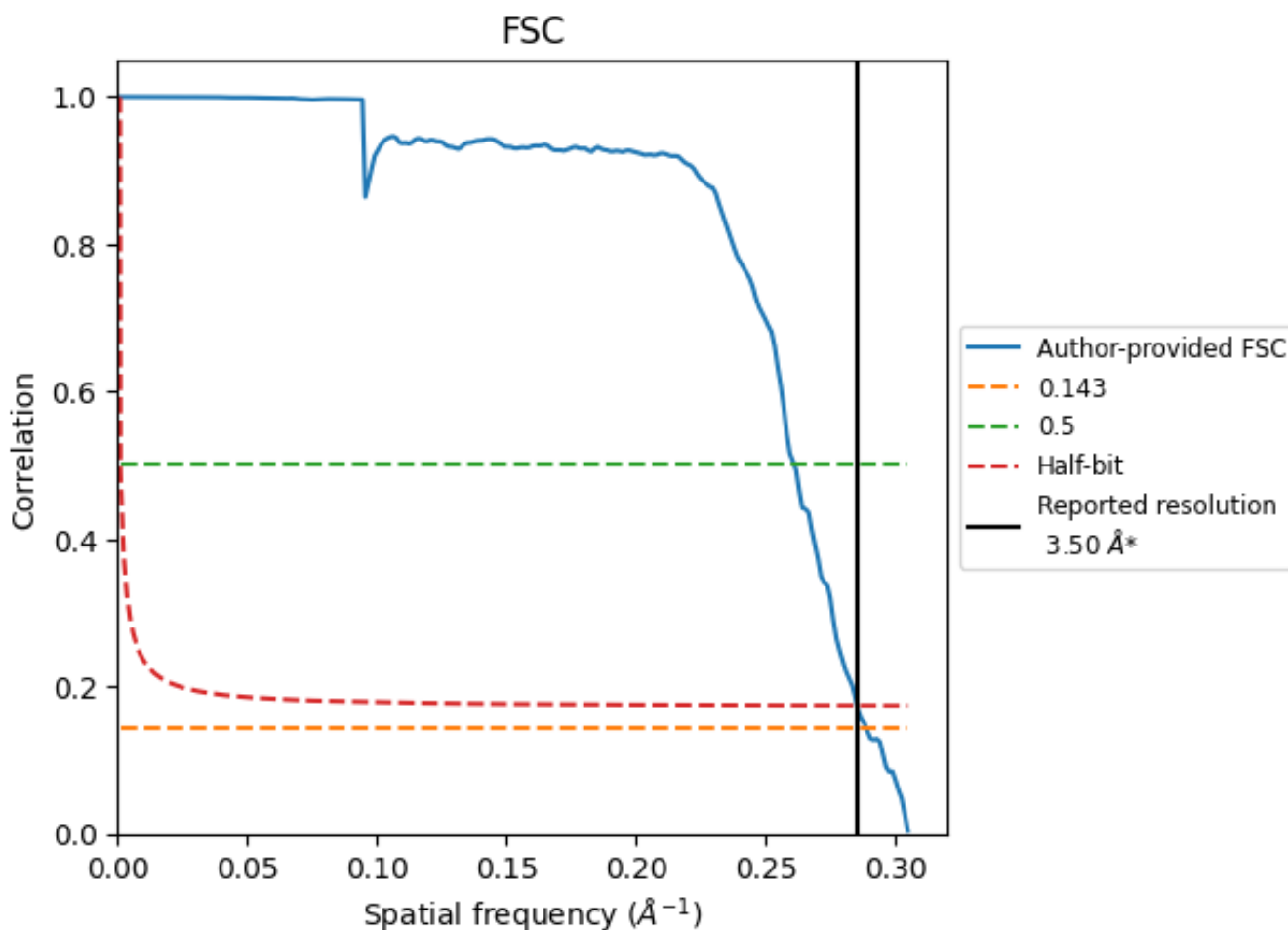


\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [\(i\)](#)

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

### 8.1 FSC [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

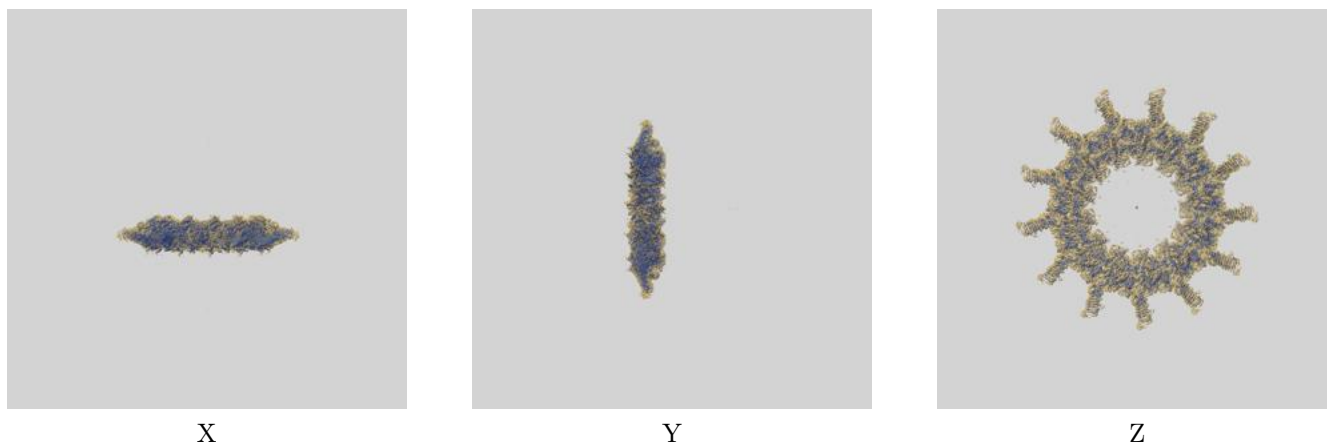
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.46	3.83	3.51
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

This section contains information regarding the fit between EMDB map EMD-22068 and PDB model 6X62. Per-residue inclusion information can be found in section 3 on page 15.

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



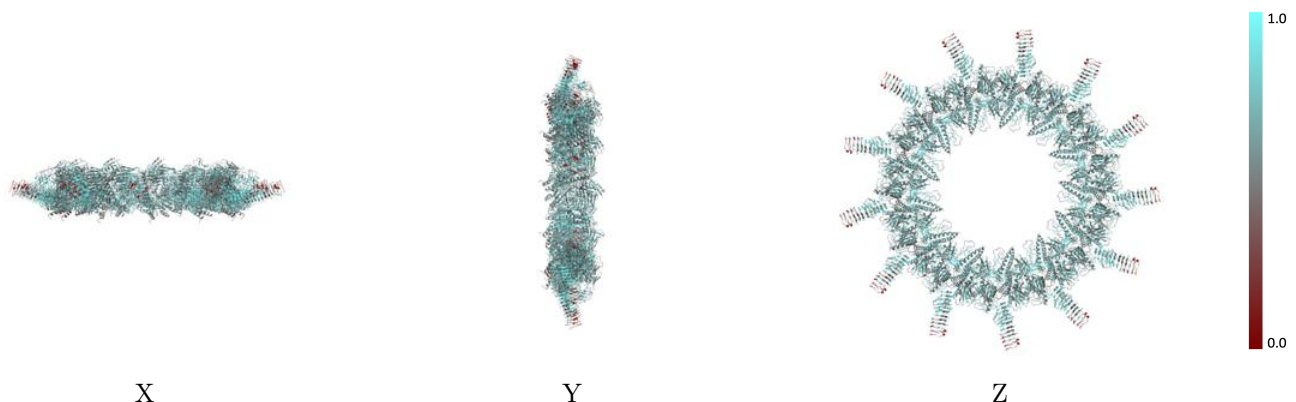
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



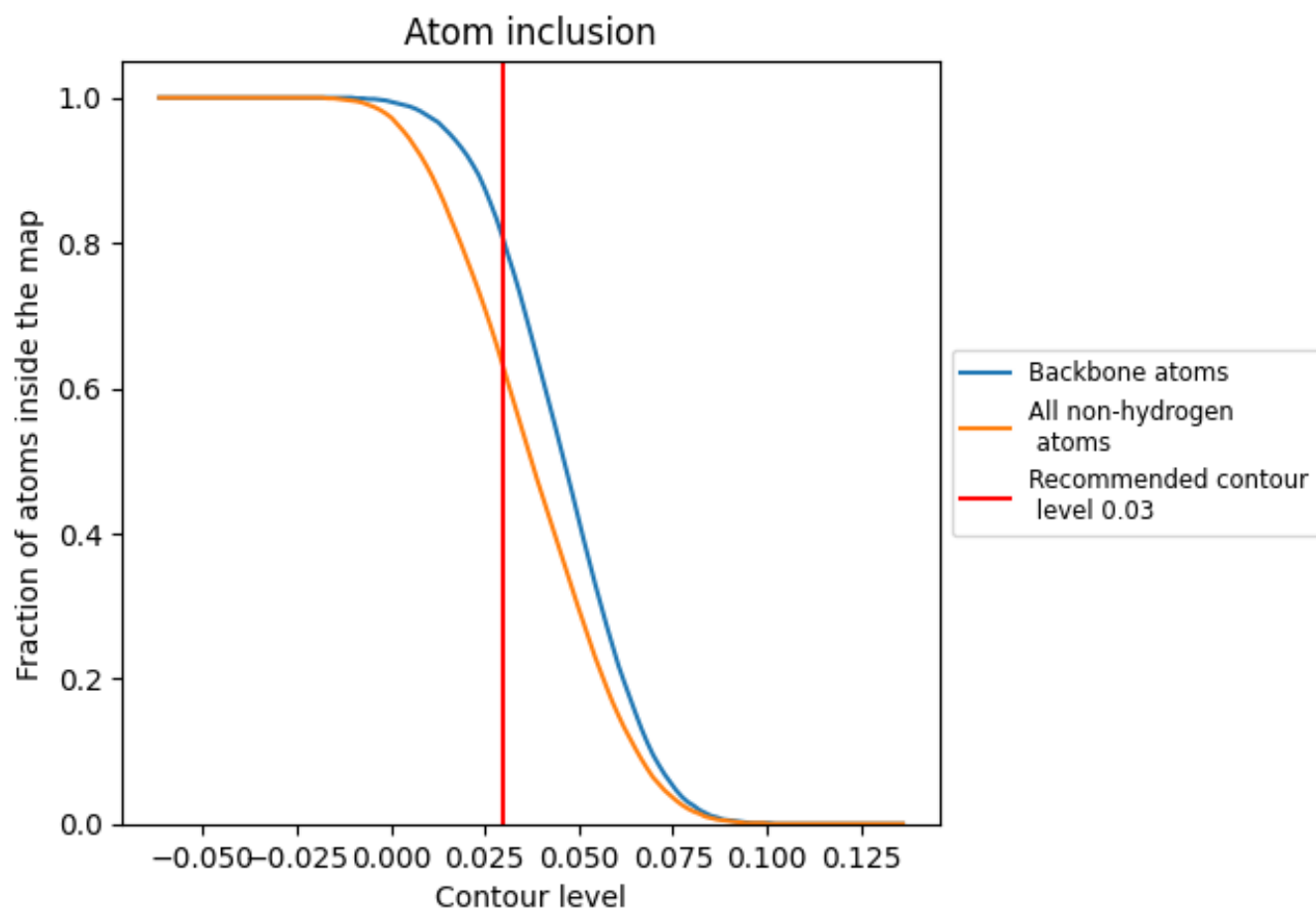
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 80% of all backbone atoms, 63% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6280	 0.3040
AC	 0.6600	 0.3360
AD	 0.5790	 0.2700
AH	 0.6480	 0.3360
AK	 0.6230	 0.2930
AX	 0.6260	 0.3080
AY	 0.5730	 0.2800
AZ	 0.7460	 0.3520
Ad	 0.6150	 0.3220
BC	 0.6450	 0.3210
BD	 0.5790	 0.2660
BH	 0.6560	 0.3380
BK	 0.6220	 0.2960
BX	 0.6370	 0.3040
BY	 0.6230	 0.3010
BZ	 0.7630	 0.3610
Bd	 0.6160	 0.3190
CC	 0.6480	 0.3160
CD	 0.5690	 0.2640
CH	 0.6630	 0.3390
CK	 0.6130	 0.2910
CX	 0.6250	 0.2930
CY	 0.6000	 0.3040
CZ	 0.7540	 0.3580
Cd	 0.6090	 0.3080
DC	 0.6550	 0.3370
DD	 0.5820	 0.2750
DH	 0.6690	 0.3450
DK	 0.6260	 0.2950
DX	 0.6360	 0.3080
DY	 0.6310	 0.3240
DZ	 0.7430	 0.3500
Dd	 0.6120	 0.3100
EC	 0.6510	 0.3200
ED	 0.5900	 0.2690





















































































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Chain	Atom inclusion	Q-score
EH	0.6630	0.3490
EK	0.6190	0.2880
EX	0.6320	0.3000
EY	0.6150	0.2940
EZ	0.7430	0.3590
Ed	0.6200	0.3140
FC	0.6640	0.3370
FD	0.5760	0.2730
FH	0.6620	0.3420
FK	0.6210	0.2890
FX	0.6440	0.3040
FY	0.6120	0.2990
FZ	0.7460	0.3630
Fd	0.6090	0.3120
GC	0.6570	0.3310
GD	0.5830	0.2740
GH	0.6530	0.3360
GK	0.6050	0.2840
GX	0.6320	0.3030
GY	0.6150	0.3110
GZ	0.7430	0.3640
Gd	0.6240	0.3210
HC	0.6520	0.3330
HD	0.5840	0.2740
HH	0.6500	0.3340
HK	0.6080	0.2890
HX	0.6320	0.3050
HY	0.5920	0.2880
HZ	0.7510	0.3680
Hd	0.6090	0.3120
IC	0.6520	0.3250
ID	0.5850	0.2630
IH	0.6540	0.3340
IK	0.6140	0.2900
IX	0.6370	0.2930
IY	0.6080	0.2840
IZ	0.7430	0.3570
Id	0.6140	0.3070
JC	0.6490	0.3190
JD	0.5880	0.2730
JH	0.6510	0.3450
JK	0.6220	0.3000

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Chain	Atom inclusion	Q-score
JX	 0.6310	 0.2940
JY	 0.6000	 0.3000
JZ	 0.7510	 0.3650
Jd	 0.6120	 0.3110
KC	 0.6510	 0.3270
KD	 0.5680	 0.2710
KH	 0.6540	 0.3400
KK	 0.6210	 0.2970
KX	 0.6260	 0.3010
KY	 0.6000	 0.2900
KZ	 0.7570	 0.3600
Kd	 0.6080	 0.3120
LC	 0.6450	 0.3270
LD	 0.5860	 0.2700
LH	 0.6530	 0.3320
LK	 0.6160	 0.2920
LX	 0.6370	 0.2960
LY	 0.6120	 0.2840
LZ	 0.7630	 0.3620
Ld	 0.6070	 0.3170
MC	 0.6550	 0.3310
MD	 0.5690	 0.2640
MH	 0.6570	 0.3310
MK	 0.6210	 0.2910
MX	 0.6390	 0.2960
MY	 0.5890	 0.2740
MZ	 0.7430	 0.3680
Md	 0.6290	 0.3140
N	 0.6120	 0.2790
O	 0.6130	 0.2750
P	 0.6110	 0.2770
Q	 0.6090	 0.2740
R	 0.6030	 0.2780
S	 0.6090	 0.2800
T	 0.6110	 0.2790
U	 0.6050	 0.2760
V	 0.6000	 0.2690
W	 0.5990	 0.2700
X	 0.6040	 0.2740
Y	 0.6130	 0.2750
Z	 0.6010	 0.2760