



## Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 12:13 AM EST

PDB ID : 7MUW  
EMDB ID : EMD-24024  
Title : Reconstruction of the Legionella pneumophila Dot/Icm T4SS 3DVA Map 4  
Authors : Sheedlo, M.J.; Durie, C.L.; Swanson, M.; Lacy, D.B.; Ohi, M.D.  
Deposited on : 2021-05-14  
Resolution : 4.60 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

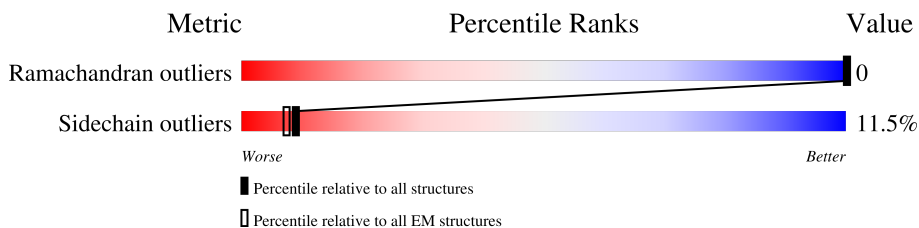
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 4.60 Å.

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



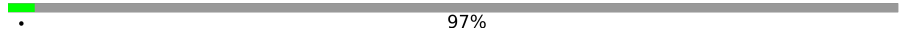

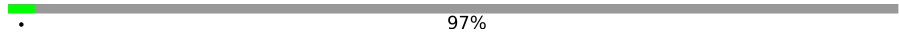

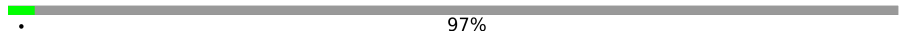

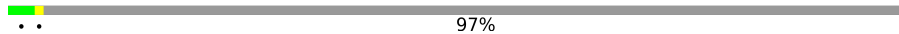

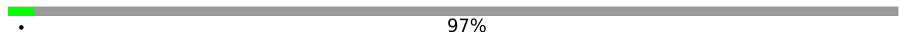

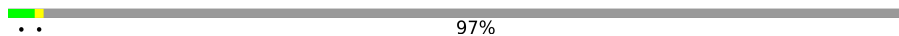

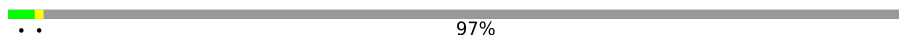

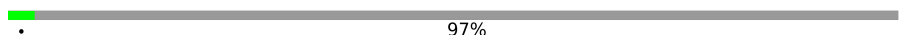

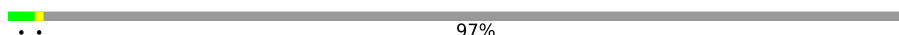



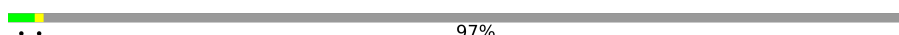
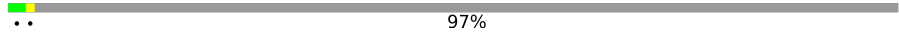
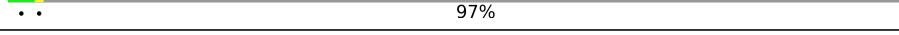
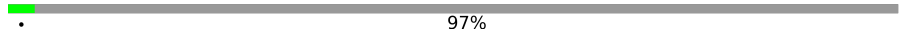
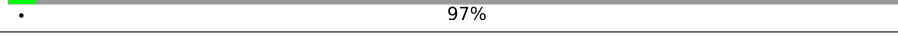
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	AG	1048	14% 84%
1	Ag	1048	97%
1	BG	1048	14% 84%
1	Bg	1048	97%
1	CG	1048	14% 84%
1	Cg	1048	97%
1	DG	1048	14% 84%
1	Dg	1048	97%
1	EG	1048	14% 84%







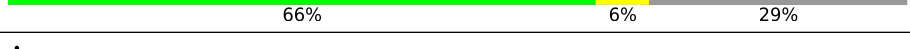
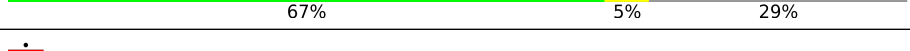
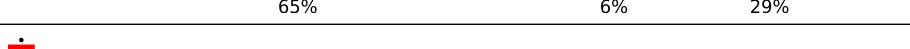
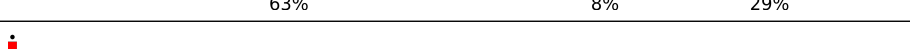
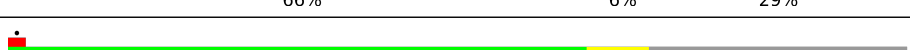

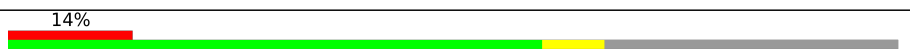

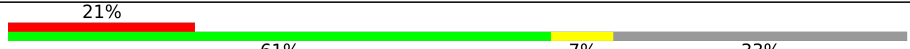





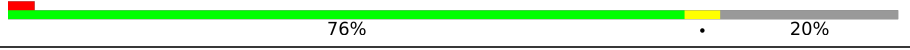
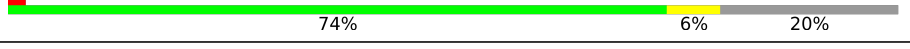



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Mol	Chain	Length	Quality of chain
1	Eg	1048	 97%
1	FG	1048	 14% 84%
1	Fg	1048	 97%
1	GG	1048	 14% 84%
1	Gg	1048	 97%
1	HG	1048	 14% 84%
1	Hg	1048	 97%
1	IG	1048	 14% 84%
1	Ig	1048	 97%
1	JG	1048	 15% 84%
1	Jg	1048	 97%
1	KG	1048	 15% 84%
1	Kg	1048	 97%
1	LG	1048	 14% 84%
1	Lg	1048	 97%
1	MG	1048	 14% 84%
1	Mg	1048	 97%
1	NG	1048	 14% 84%
1	OG	1048	 14% 84%
1	PG	1048	 14% 84%
1	VG	1048	 97%
1	WG	1048	 97%
1	XG	1048	 97%
1	YG	1048	 97%
1	ZG	1048	 97%




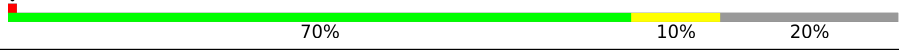
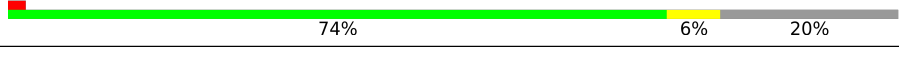



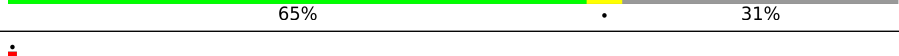
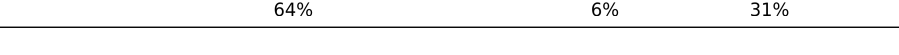
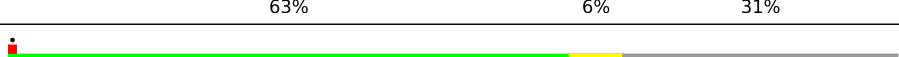
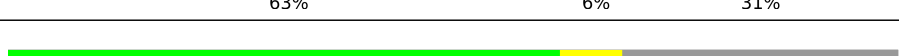

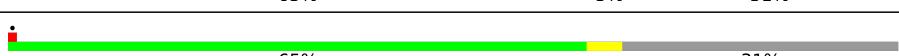
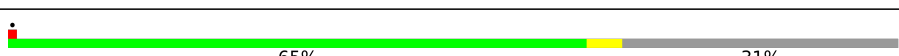
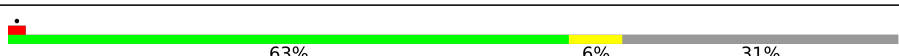





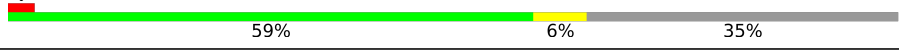

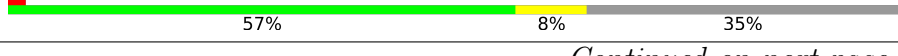

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Mol	Chain	Length	Quality of chain
2	AH	361	 64% 8% 29%
2	BH	361	 64% 7% 29%
2	CH	361	 65% 6% 29%
2	DH	361	 65% 7% 29%
2	EH	361	 63% 8% 29%
2	FH	361	 64% 7% 29%
2	GH	361	 66% 6% 29%
2	HH	361	 67% 5% 29%
2	IH	361	 65% 6% 29%
2	JH	361	 63% 8% 29%
2	KH	361	 66% 6% 29%
2	LH	361	 65% 7% 29%
2	MH	361	 64% 8% 29%
2	VH	361	 14% 60% 7% 33%
2	WH	361	 18% 60% 7% 33%
2	XH	361	 21% 61% 7% 33%
2	YH	361	 10% 60% 7% 33%
2	ZH	361	 23% 60% 8% 33%
3	AK	189	 72% 8% 20%
3	BK	189	 71% 9% 20%
3	CK	189	 72% 8% 20%
3	DK	189	 76% 6% 20%
3	EK	189	 74% 6% 20%
3	FK	189	 74% 6% 20%
3	GK	189	 74% 6% 20%













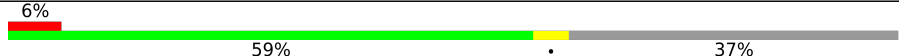
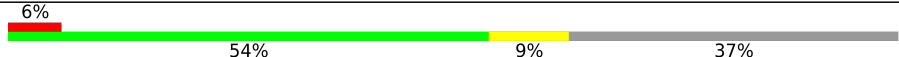
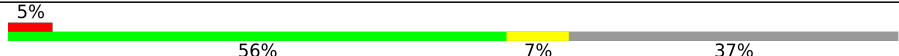

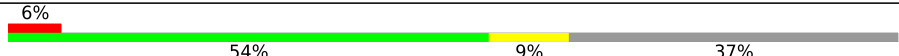
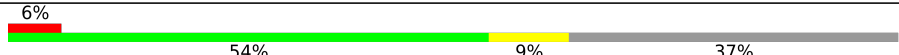
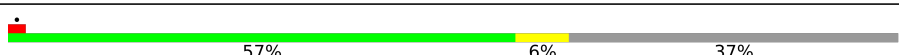
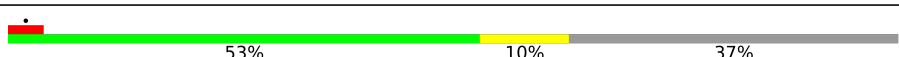
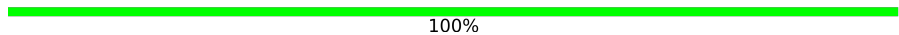
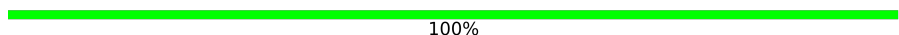
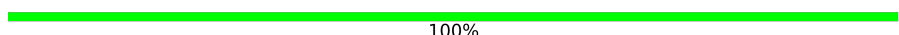
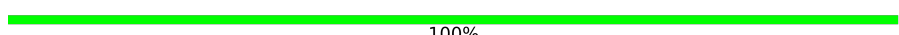
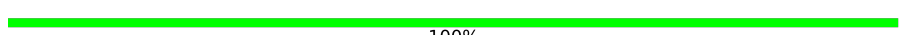
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Mol	Chain	Length	Quality of chain
3	HK	189	 74% 6% 20%
3	IK	189	 74% 6% 20%
3	JK	189	 73% 7% 20%
3	KK	189	 70% 10% 20%
3	LK	189	 74% 6% 20%
3	MK	189	 70% 10% 20%
4	AL	249	 65% 0% 31%
4	BL	249	 62% 8% 31%
4	CL	249	 65% 0% 31%
4	DL	249	 64% 6% 31%
4	EL	249	 63% 6% 31%
4	FL	249	 63% 6% 31%
4	GL	249	 62% 7% 31%
4	HL	249	 65% 5% 31%
4	IL	249	 65% 0% 31%
4	JL	249	 65% 0% 31%
4	KL	249	 63% 6% 31%
4	LL	249	 66% 0% 31%
4	ML	249	 65% 0% 31%
5	AM	320	 55% 10% 35%
5	BM	320	 59% 6% 35%
5	CM	320	 57% 8% 35%
5	DM	320	 59% 6% 35%
5	EM	320	 58% 7% 35%
5	FM	320	 57% 8% 35%

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Mol	Chain	Length	Quality of chain
5	GM	320	 55% 10% 35%
5	HM	320	 58% 7% 35%
5	IM	320	 60% 5% 35%
5	JM	320	 57% 8% 35%
5	KM	320	 58% 7% 35%
5	LM	320	 59% 6% 35%
5	MM	320	 59% 6% 35%
6	AN	124	 6% 54% 9% 37%
6	BN	124	 8% 52% 10% 37%
6	CN	124	 8% 53% 10% 37%
6	DN	124	 55% 8% 37%
6	EN	124	 56% 6% 37%
6	FN	124	 6% 59% 37%
6	GN	124	 6% 54% 9% 37%
6	HN	124	 5% 56% 7% 37%
6	IN	124	 6% 55% 8% 37%
6	JN	124	 6% 54% 9% 37%
6	KN	124	 6% 54% 9% 37%
6	LN	124	 57% 6% 37%
6	MN	124	 6% 53% 10% 37%
7	AU	9	 100%
7	BU	9	 100%
7	CU	9	 100%
7	DU	9	 100%
7	EU	9	 100%

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Mol	Chain	Length	Quality of chain
7	FU	9	100%
7	GU	9	100%
7	HU	9	100%
7	IU	9	100%
7	JU	9	100%
7	KU	9	100%
7	LU	9	100%
7	MU	9	100%
8	AX	48	29% 100%
8	BX	48	42% 100%
8	CX	48	38% 100%
8	DX	48	23% 100%
8	EX	48	38% 100%
8	FX	48	21% 100%
8	GX	48	54% 100%
8	HX	48	38% 100%
8	IX	48	29% 100%
8	JX	48	33% 100%
8	KX	48	46% 100%
8	LX	48	46% 100%
8	MX	48	40% 100%
8	VX	48	33% 100%
8	WX	48	31% 100%
8	XX	48	29% 100%
8	YX	48	33% 100%

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Mol	Chain	Length	Quality of chain
8	ZX	48	
9	AD	163	
9	Ad	163	
9	BD	163	
9	Bd	163	
9	CD	163	
9	Cd	163	
9	DD	163	
9	Dd	163	
9	ED	163	
9	Ed	163	
9	FD	163	
9	Fd	163	
9	GD	163	
9	Gd	163	
9	HD	163	
9	Hd	163	
9	ID	163	
9	Id	163	
9	JD	163	
9	Jd	163	
9	KD	163	
9	Kd	163	
9	LD	163	
9	Ld	163	

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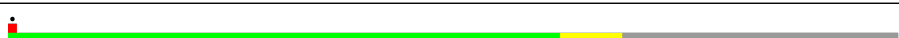

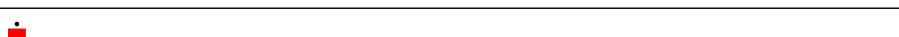
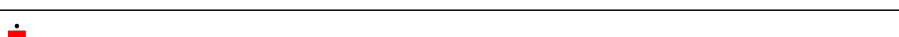
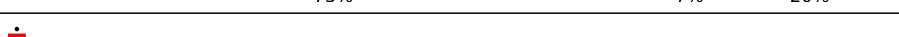
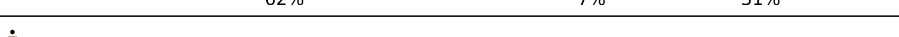

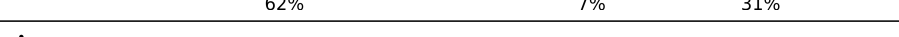

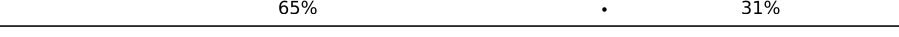
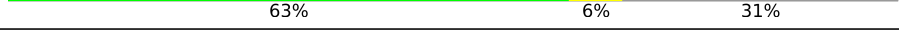


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Mol	Chain	Length	Quality of chain
9	MD	163	82% 14%
9	Md	163	74% 10% 16%
10	AF	269	21% 77%
10	Af	269	20% 78%
10	BF	269	21% 77%
10	Bf	269	20% 78%
10	CF	269	21% 77%
10	Cf	269	19% 78%
10	DF	269	21% 77%
10	Df	269	19% 78%
10	EF	269	20% 77%
10	Ef	269	20% 78%
10	FF	269	21% 77%
10	Ff	269	19% 78%
10	GF	269	22% 77%
10	Gf	269	20% 78%
10	HF	269	21% 77%
10	Hf	269	21% 78%
10	IF	269	22% 77%
10	If	269	20% 78%
10	JF	269	22% 77%
10	Jf	269	20% 78%
10	KF	269	20% 77%
10	Kf	269	20% 78%
10	LF	269	21% 77%

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Mol	Chain	Length	Quality of chain
10	Lf	269	 21% 78%
10	MF	269	 21% 77%
10	Mf	269	 19% 78%
10	VF	269	 22% 77%
10	WF	269	 21% 77%
10	XF	269	 21% 77%
10	YF	269	 21% 77%
10	ZF	269	 22% 77%
11	AC	303	 73% 7% 20%
11	BC	303	 6% 73% 8% 20%
11	CC	303	 62% 7% 31%
11	DC	303	 62% 7% 31%
11	EC	303	 62% 7% 31%
11	FC	303	 73% 7% 20%
11	GC	303	 62% 7% 31%
11	HC	303	 61% 8% 31%
11	IC	303	 62% 7% 31%
11	JC	303	 71% 9% 20%
11	KC	303	 65% 31%
11	LC	303	 63% 6% 31%
11	MC	303	 60% 9% 31%

## 2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 192116 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 IcmE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AG	165	1229	780	203	242	4	0	0
1	Fg	34	276	168	47	60	1	0	0
1	Gg	34	276	168	47	60	1	0	0
1	BG	165	1229	780	203	242	4	0	0
1	Hg	34	276	168	47	60	1	0	0
1	Bg	34	276	168	47	60	1	0	0
1	Ig	34	276	168	47	60	1	0	0
1	CG	165	1229	780	203	242	4	0	0
1	Jg	34	276	168	47	60	1	0	0
1	Kg	34	276	168	47	60	1	0	0
1	DG	165	1229	780	203	242	4	0	0
1	Lg	34	276	168	47	60	1	0	0
1	Mg	34	276	168	47	60	1	0	0
1	EG	165	1229	780	203	242	4	0	0
1	VG	34	276	168	47	60	1	0	0
1	WG	34	276	168	47	60	1	0	0
1	XG	34	276	168	47	60	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	YG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	FG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	ZG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	Cg	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	GG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	Dg	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	HG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	IG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	JG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	KG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	LG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	MG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	NG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	OG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	PG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	Ag	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	Eg	34	Total	C	N	O	S	0	0
			276	168	47	60	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	EH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
2	FH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	GH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
2	HH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
2	IH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
2	JH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
2	AH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
2	KH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
2	LH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
2	MH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
2	VH	243	Total	C	N	O	S	0	0
			1875	1201	319	348	7		
2	WH	243	Total	C	N	O	S	0	0
			1875	1201	319	348	7		
2	XH	243	Total	C	N	O	S	0	0
			1875	1201	319	348	7		
2	YH	243	Total	C	N	O	S	0	0
			1875	1201	319	348	7		
2	ZH	243	Total	C	N	O	S	0	0
			1875	1201	319	348	7		
2	BH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
2	CH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
2	DH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	EK	151	Total	C	N	O	S	0	0
			1175	747	209	215	4		
3	FK	151	Total	C	N	O	S	0	0
			1175	747	209	215	4		
3	GK	151	Total	C	N	O	S	0	0
			1175	747	209	215	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	HK	151	Total 1175	C 747	N 209	O 215	S 4	0	0
3	IK	151	Total 1175	C 747	N 209	O 215	S 4	0	0
3	JK	151	Total 1175	C 747	N 209	O 215	S 4	0	0
3	KK	151	Total 1175	C 747	N 209	O 215	S 4	0	0
3	LK	151	Total 1175	C 747	N 209	O 215	S 4	0	0
3	AK	151	Total 1175	C 747	N 209	O 215	S 4	0	0
3	MK	151	Total 1175	C 747	N 209	O 215	S 4	0	0
3	BK	151	Total 1175	C 747	N 209	O 215	S 4	0	0
3	CK	151	Total 1175	C 747	N 209	O 215	S 4	0	0
3	DK	151	Total 1175	C 747	N 209	O 215	S 4	0	0

- Molecule 4 is a protein called Outer membrane protein, OmpA family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	EL	173	Total 1388	C 877	N 253	O 253	S 5	0	0
4	FL	173	Total 1388	C 877	N 253	O 253	S 5	0	0
4	GL	173	Total 1388	C 877	N 253	O 253	S 5	0	0
4	HL	173	Total 1388	C 877	N 253	O 253	S 5	0	0
4	IL	173	Total 1388	C 877	N 253	O 253	S 5	0	0
4	JL	173	Total 1388	C 877	N 253	O 253	S 5	0	0
4	KL	173	Total 1388	C 877	N 253	O 253	S 5	0	0
4	LL	173	Total 1388	C 877	N 253	O 253	S 5	0	0
4	ML	173	Total 1388	C 877	N 253	O 253	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	AL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		
4	BL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		
4	CL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		
4	DL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		

- Molecule 5 is a protein called DUF2807 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	EM	208	Total	C	N	O	S	0	0
			1650	1046	293	308	3		
5	FM	208	Total	C	N	O	S	0	0
			1650	1046	293	308	3		
5	GM	208	Total	C	N	O	S	0	0
			1650	1046	293	308	3		
5	HM	208	Total	C	N	O	S	0	0
			1650	1046	293	308	3		
5	IM	208	Total	C	N	O	S	0	0
			1650	1046	293	308	3		
5	JM	208	Total	C	N	O	S	0	0
			1650	1046	293	308	3		
5	KM	208	Total	C	N	O	S	0	0
			1650	1046	293	308	3		
5	LM	208	Total	C	N	O	S	0	0
			1650	1046	293	308	3		
5	MM	208	Total	C	N	O	S	0	0
			1650	1046	293	308	3		
5	AM	208	Total	C	N	O	S	0	0
			1650	1046	293	308	3		
5	BM	208	Total	C	N	O	S	0	0
			1650	1046	293	308	3		
5	CM	208	Total	C	N	O	S	0	0
			1650	1046	293	308	3		
5	DM	208	Total	C	N	O	S	0	0
			1650	1046	293	308	3		

- Molecule 6 is a protein called Neurogenic locus notch.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	EN	78	Total	C	N	O	S	0	0
			582	357	99	113	13		
6	FN	78	Total	C	N	O	S	0	0
			582	357	99	113	13		
6	GN	78	Total	C	N	O	S	0	0
			582	357	99	113	13		
6	HN	78	Total	C	N	O	S	0	0
			582	357	99	113	13		
6	IN	78	Total	C	N	O	S	0	0
			582	357	99	113	13		
6	JN	78	Total	C	N	O	S	0	0
			582	357	99	113	13		
6	KN	78	Total	C	N	O	S	0	0
			582	357	99	113	13		
6	LN	78	Total	C	N	O	S	0	0
			582	357	99	113	13		
6	MN	78	Total	C	N	O	S	0	0
			582	357	99	113	13		
6	AN	78	Total	C	N	O	S	0	0
			582	357	99	113	13		
6	BN	78	Total	C	N	O	S	0	0
			582	357	99	113	13		
6	CN	78	Total	C	N	O	S	0	0
			582	357	99	113	13		
6	DN	78	Total	C	N	O	S	0	0
			582	357	99	113	13		

- Molecule 7 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	EU	9	Total	C	N	O	0	0
			45	27	9	9		
7	FU	9	Total	C	N	O	0	0
			45	27	9	9		
7	GU	9	Total	C	N	O	0	0
			45	27	9	9		
7	HU	9	Total	C	N	O	0	0
			45	27	9	9		
7	IU	9	Total	C	N	O	0	0
			45	27	9	9		
7	JU	9	Total	C	N	O	0	0
			45	27	9	9		
7	KU	9	Total	C	N	O	0	0
			45	27	9	9		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	LU	9	Total 45	C 27	N 9	O 9	0	0
7	MU	9	Total 45	C 27	N 9	O 9	0	0
7	AU	9	Total 45	C 27	N 9	O 9	0	0
7	BU	9	Total 45	C 27	N 9	O 9	0	0
7	CU	9	Total 45	C 27	N 9	O 9	0	0
7	DU	9	Total 45	C 27	N 9	O 9	0	0

- Molecule 8 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	EX	48	Total 240	C 144	N 48	O 48	0	0
8	FX	48	Total 240	C 144	N 48	O 48	0	0
8	GX	48	Total 240	C 144	N 48	O 48	0	0
8	HX	48	Total 240	C 144	N 48	O 48	0	0
8	IX	48	Total 240	C 144	N 48	O 48	0	0
8	JX	48	Total 240	C 144	N 48	O 48	0	0
8	KX	48	Total 240	C 144	N 48	O 48	0	0
8	LX	48	Total 240	C 144	N 48	O 48	0	0
8	MX	48	Total 240	C 144	N 48	O 48	0	0
8	VX	48	Total 240	C 144	N 48	O 48	0	0
8	WX	48	Total 240	C 144	N 48	O 48	0	0
8	XX	48	Total 240	C 144	N 48	O 48	0	0
8	YX	48	Total 240	C 144	N 48	O 48	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	ZX	48	Total	C	N	O	0	0
			240	144	48	48		
8	AX	48	Total	C	N	O	0	0
			240	144	48	48		
8	BX	48	Total	C	N	O	0	0
			240	144	48	48		
8	CX	48	Total	C	N	O	0	0
			240	144	48	48		
8	DX	48	Total	C	N	O	0	0
			240	144	48	48		

- Molecule 9 is a protein called DotD.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ed	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		
9	FD	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		
9	Fd	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		
9	GD	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		
9	Gd	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		
9	HD	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		
9	Hd	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		
9	ID	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		
9	Id	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		
9	JD	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		
9	Jd	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		
9	KD	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		
9	Kd	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		
9	CD	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	LD	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		
9	Ld	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		
9	MD	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		
9	Md	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		
9	Ad	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		
9	BD	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		
9	Bd	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		
9	Cd	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		
9	DD	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		
9	Dd	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		
9	AD	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		
9	ED	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		

- Molecule 10 is a protein called DotF.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Ef	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
10	FF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
10	Ff	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
10	AF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
10	GF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
10	Gf	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
10	HF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Hf	59	449	290	77	81	1	0	0
10	IF	63	483	308	84	90	1	0	0
10	If	59	449	290	77	81	1	0	0
10	JF	63	483	308	84	90	1	0	0
10	Jf	59	449	290	77	81	1	0	0
10	KF	63	483	308	84	90	1	0	0
10	Kf	59	449	290	77	81	1	0	0
10	LF	63	483	308	84	90	1	0	0
10	Lf	59	449	290	77	81	1	0	0
10	MF	63	483	308	84	90	1	0	0
10	CF	63	483	308	84	90	1	0	0
10	Mf	59	449	290	77	81	1	0	0
10	VF	63	483	308	84	90	1	0	0
10	WF	63	483	308	84	90	1	0	0
10	XF	63	483	308	84	90	1	0	0
10	YF	63	483	308	84	90	1	0	0
10	ZF	63	483	308	84	90	1	0	0
10	Af	59	449	290	77	81	1	0	0
10	BF	63	483	308	84	90	1	0	0
10	Bf	59	449	290	77	81	1	0	0
10	Cf	59	449	290	77	81	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	DF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
10	Df	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
10	EF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		

- Molecule 11 is a protein called DotC.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BC	243	Total	C	N	O	S	0	0
			1921	1216	340	357	8		
11	CC	209	Total	C	N	O	S	0	0
			1667	1061	292	309	5		
11	DC	209	Total	C	N	O	S	0	0
			1667	1061	292	309	5		
11	EC	209	Total	C	N	O	S	0	0
			1667	1061	292	309	5		
11	FC	243	Total	C	N	O	S	0	0
			1921	1216	340	357	8		
11	GC	209	Total	C	N	O	S	0	0
			1667	1061	292	309	5		
11	HC	209	Total	C	N	O	S	0	0
			1667	1061	292	309	5		
11	IC	209	Total	C	N	O	S	0	0
			1667	1061	292	309	5		
11	JC	243	Total	C	N	O	S	0	0
			1921	1216	340	357	8		
11	KC	209	Total	C	N	O	S	0	0
			1667	1061	292	309	5		
11	LC	209	Total	C	N	O	S	0	0
			1667	1061	292	309	5		
11	MC	209	Total	C	N	O	S	0	0
			1667	1061	292	309	5		
11	AC	243	Total	C	N	O	S	0	0
			1921	1216	340	357	8		















































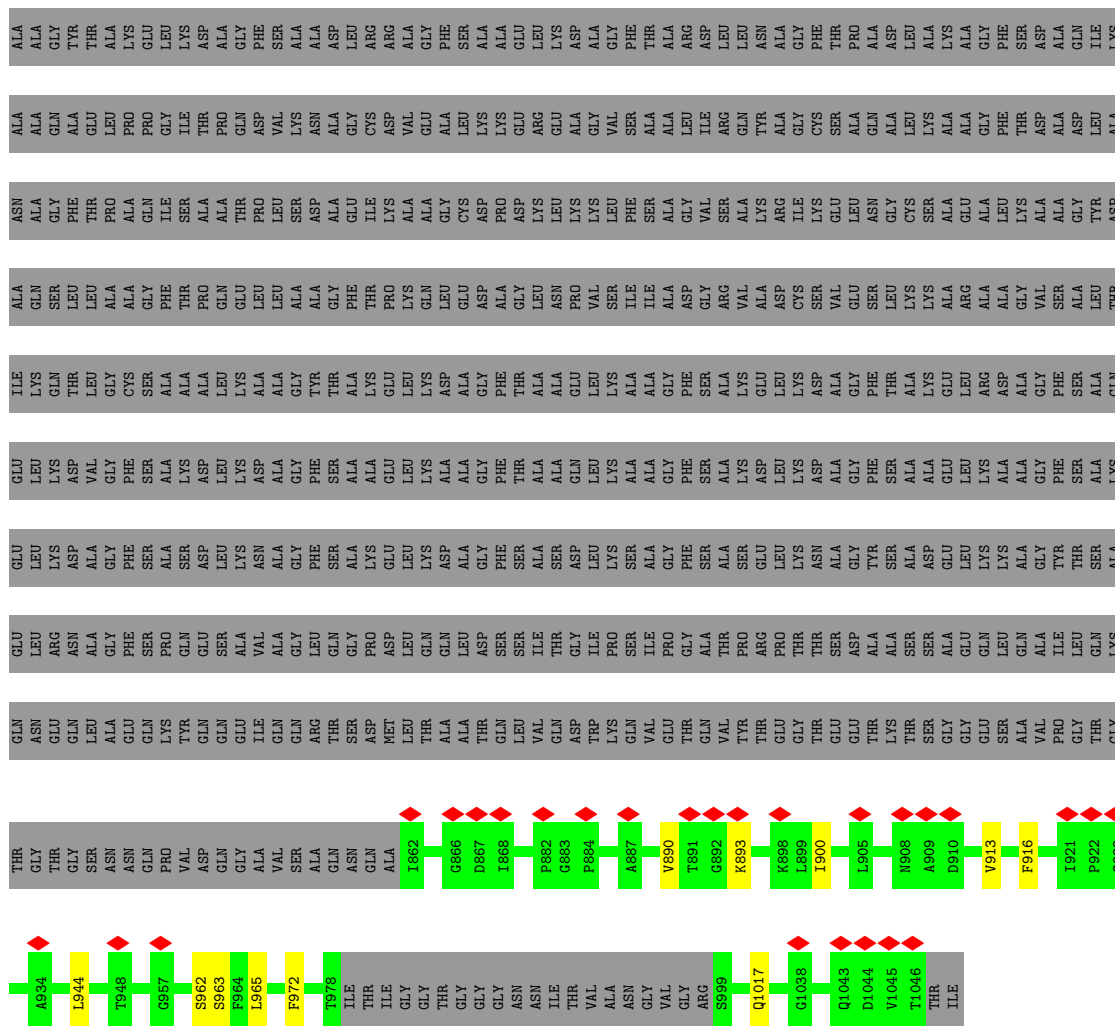




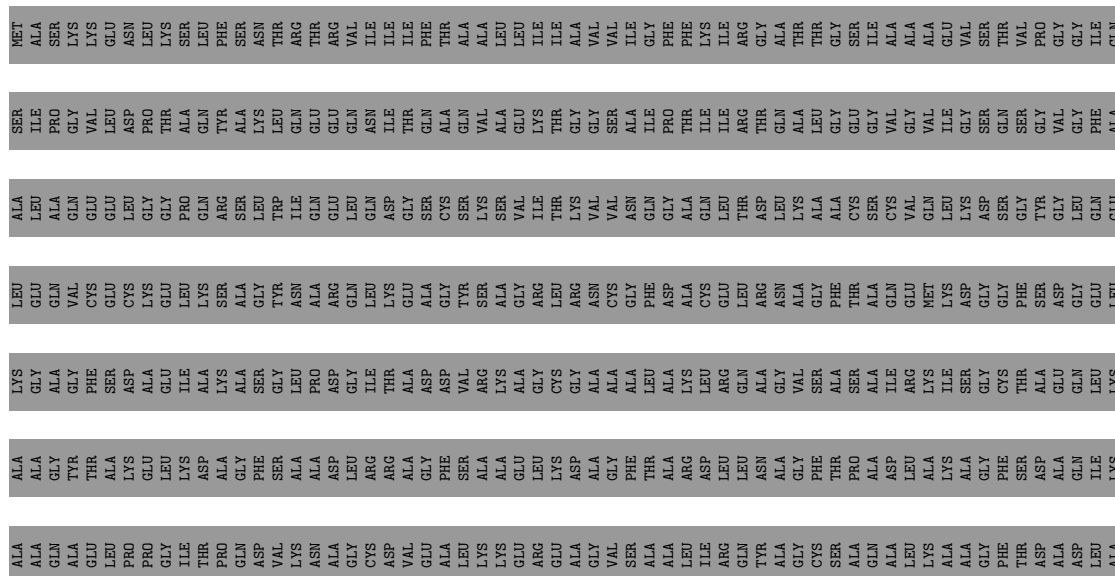


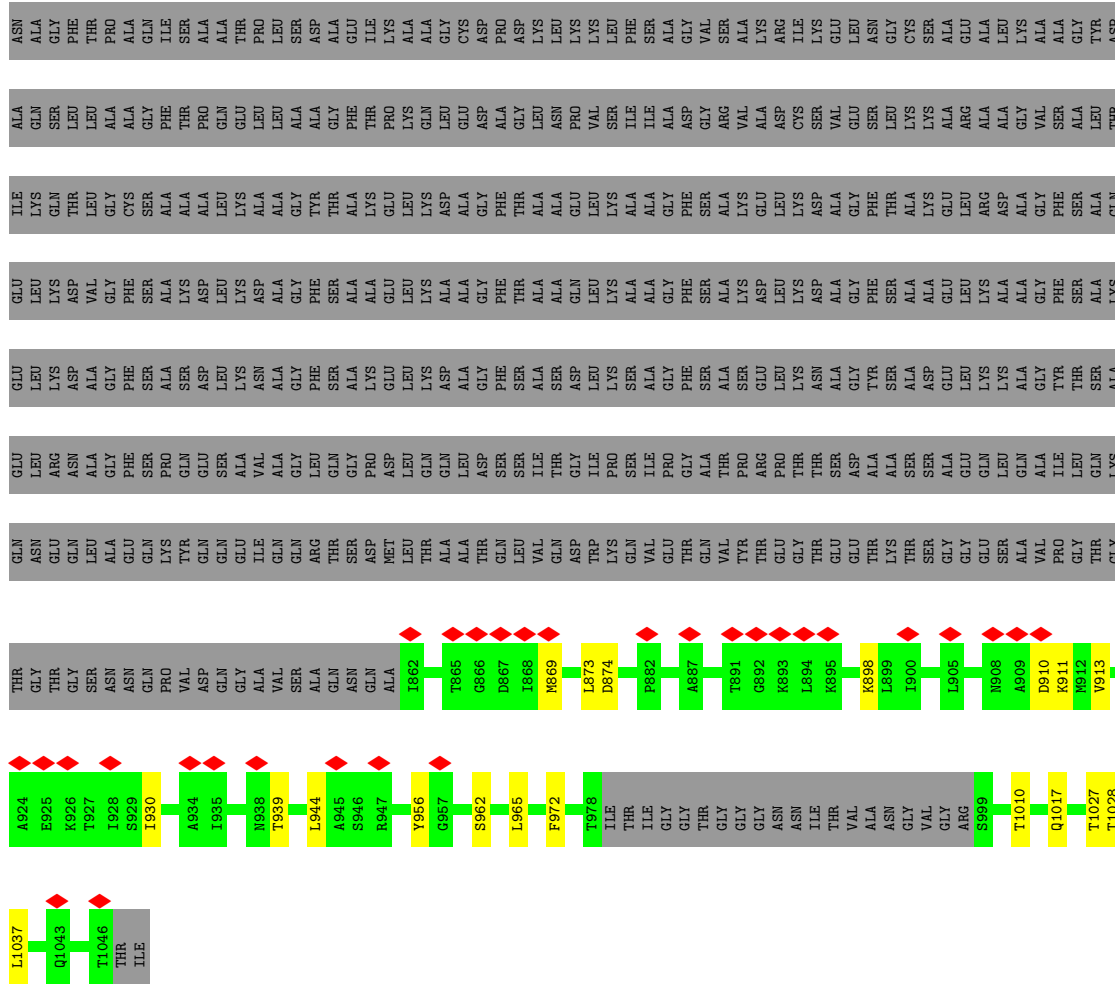




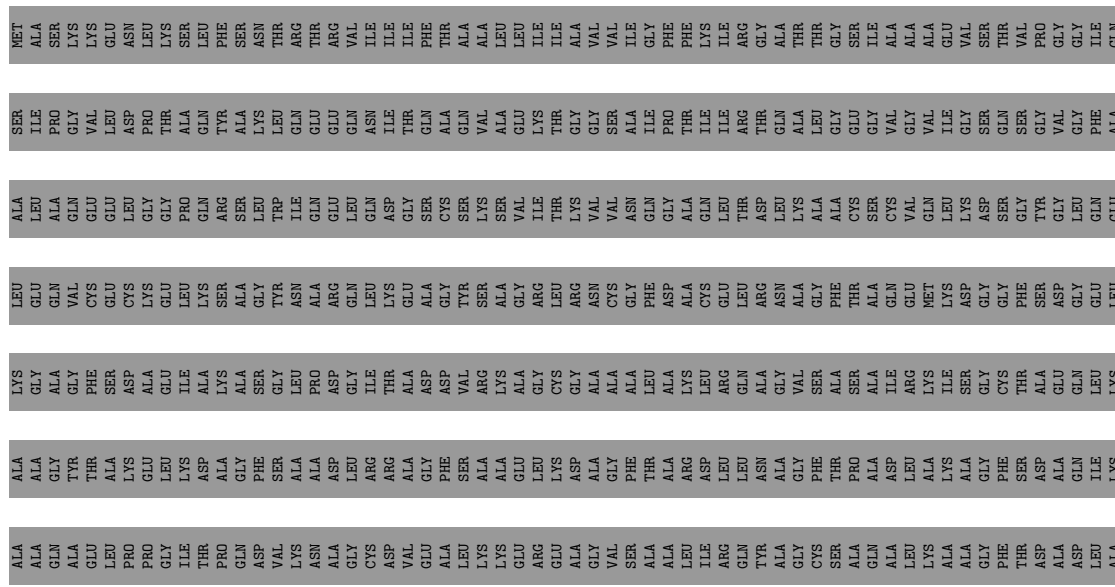


Molecule 1: IcmE protein





● Molecule 1: IcmE protein







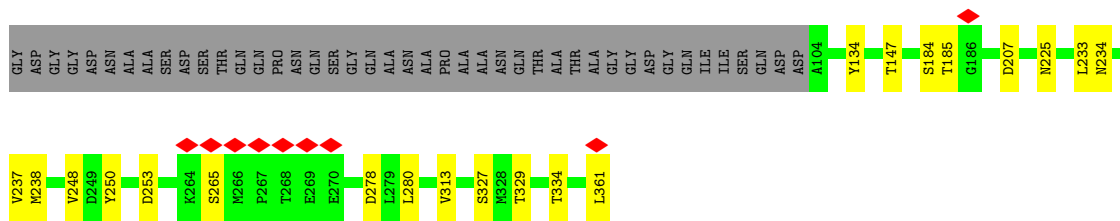




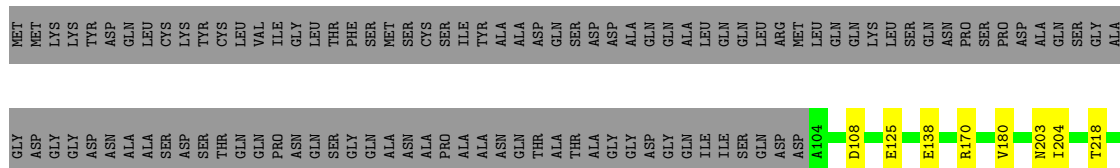




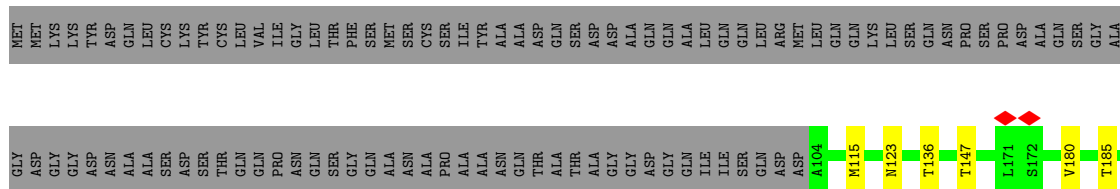




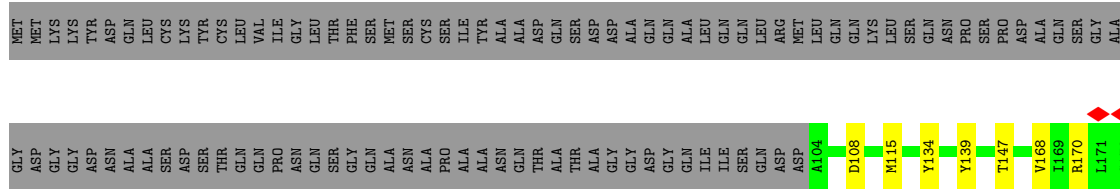
• Molecule 2: Type IV secretion protein IcmK



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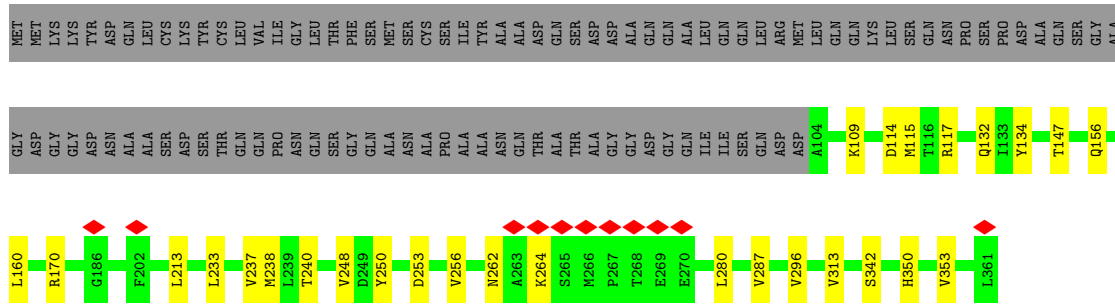


• Molecule 2: Type IV secretion protein IcmK



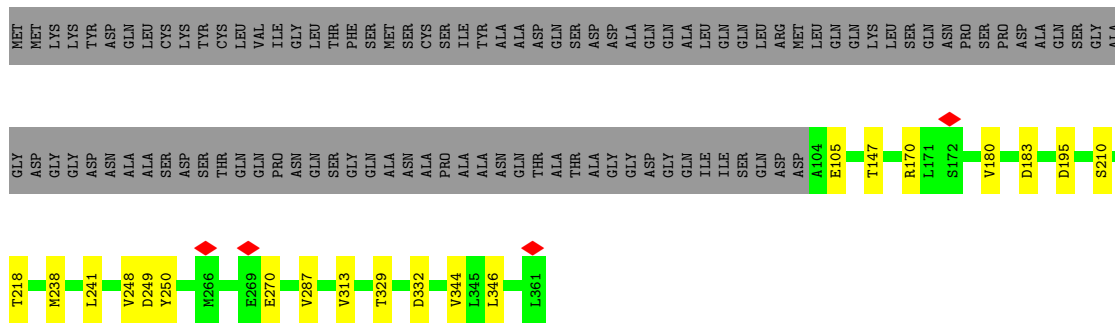
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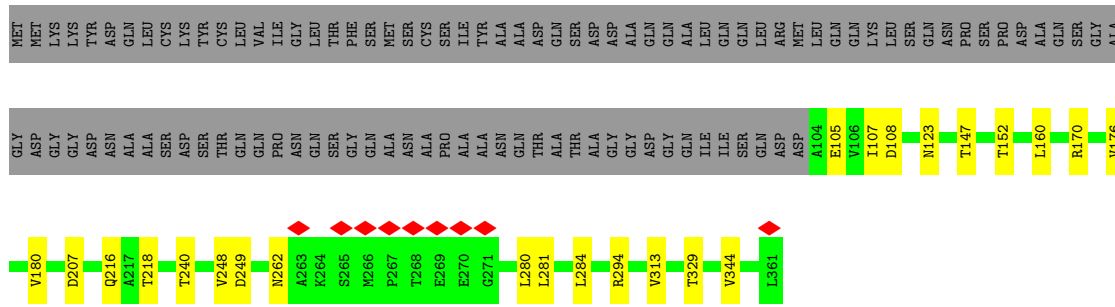
- Molecule 2: Type IV secretion protein IcmK

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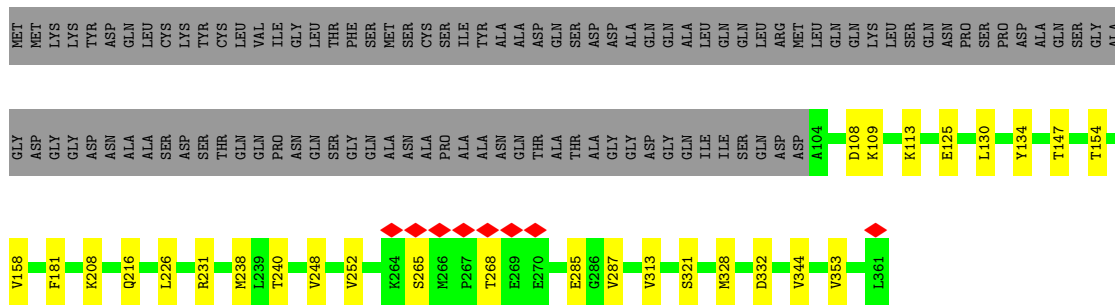
- Molecule 2: Type IV secretion protein IcmK

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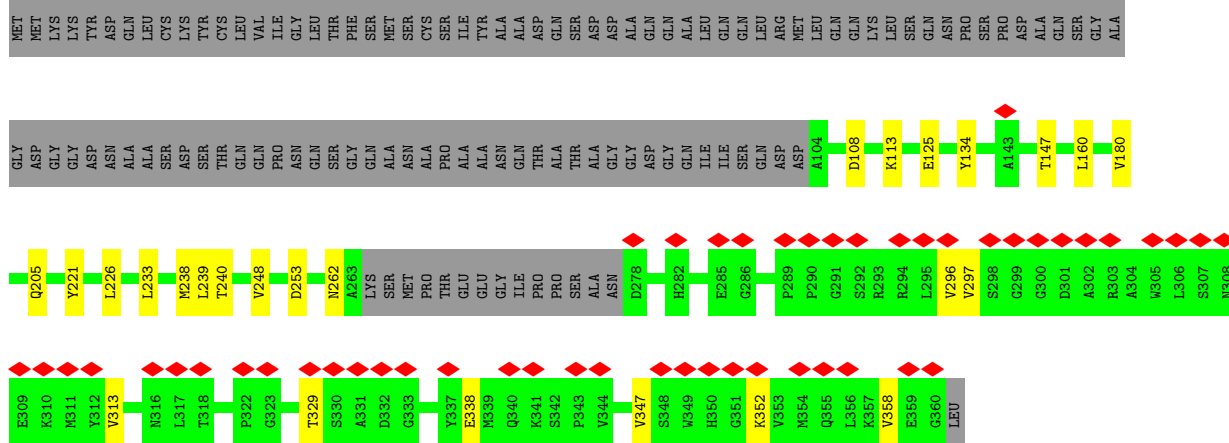
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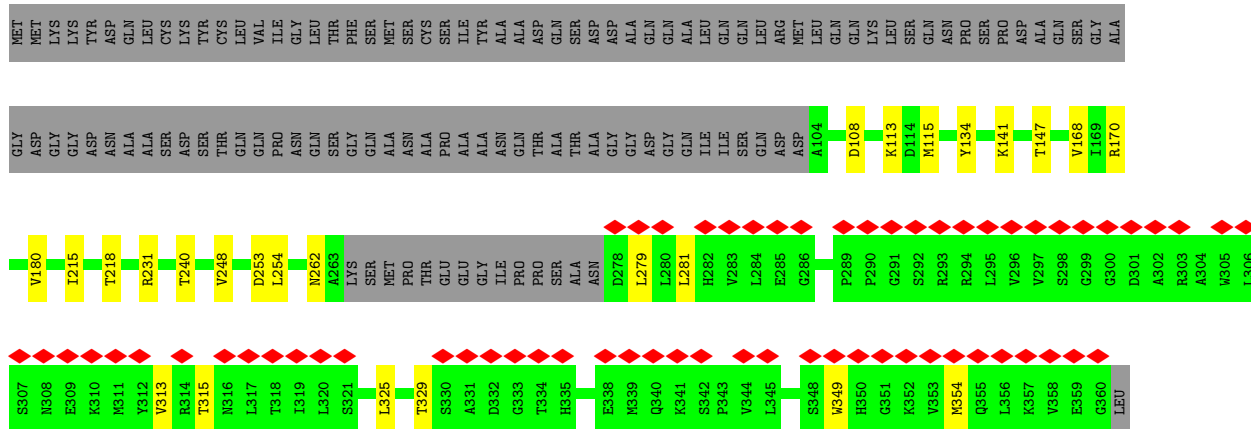




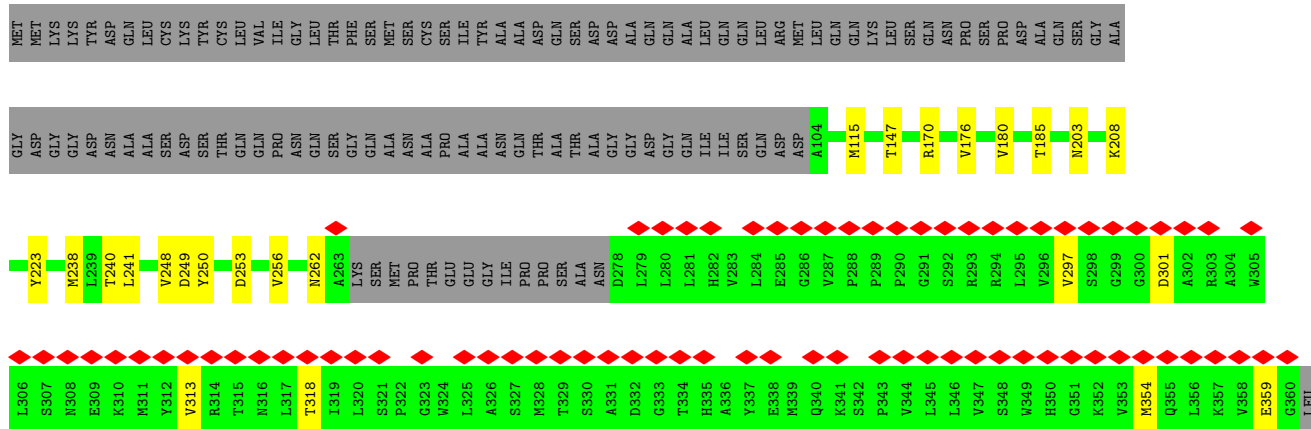
• Molecule 2: Type IV secretion protein IcmK



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GLY ASP GLY TYR ASN ALA SER ASP THR GLN PRO ASN LEU SER GLY GLN MET ALA ALA PRO THR ALA ALA THR ASN THR ASP GLY GLN ILE SER SER ARG ASP ASP K104 K109 K113 D114 M115 Y134 T147 L160 R170 F175

V176 V180 V186 T185 L204 T240 V248 D249 Y250 D253 A263 L283 SER MET SER THR V1313 N316 L317 T318 S321 S330 A331 D332 G333 M339 Q340 K341 L345 S348 W349 H350 G351 K352 V353 M354 Q355 K357 V358 G359 G360 LEU P288 P289 P290 G291 S292 R293 R294 L295 V296 V297 S298 G299 D300 D301 A302 R303 A304 E309 K310 M311 Y312 D278 H282 V283 L284 E285 P288 P289 P290 G291 S292 R293 R294 L295 V296 V297 S298 G299 D300 D301 A302 R303 A304 E309 K310 M311 Y312

• Molecule 2: Type IV secretion protein IcmK



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GLY ASP GLY TYR ASN ALA SER ASP THR GLN PRO ASN LEU SER GLY GLN MET ALA ALA PRO THR ALA ALA THR ASN THR ASP GLY GLN ILE SER SER ARG ASP ASP E105 D108 M115 L130 T136 T147 V180 D183

L213 Y221 L233 M238 L239 T240 V248 D253 A263 L283 SER MET SER THR V1313 N316 L317 T318 S321 S330 A331 D332 G333 M339 Q340 K341 L345 S348 W349 H350 G351 K352 V358 G359 G360 LEU L213 Y221 L233 M238 L239 T240 V248 D253 A263 L283 SER MET SER THR V1313 N316 L317 T318 S321 S330 A331 D332 G333 M339 Q340 K341 L345 S348 W349 H350 G351 K352 V358 G359 G360 LEU P288 P289 P290 G291 S292 R293 R294 L295 V296 V297 S298 G299 D300 D301 A302 R303 A304 E309 K310 M311 Y312

• Molecule 2: Type IV secretion protein IcmK



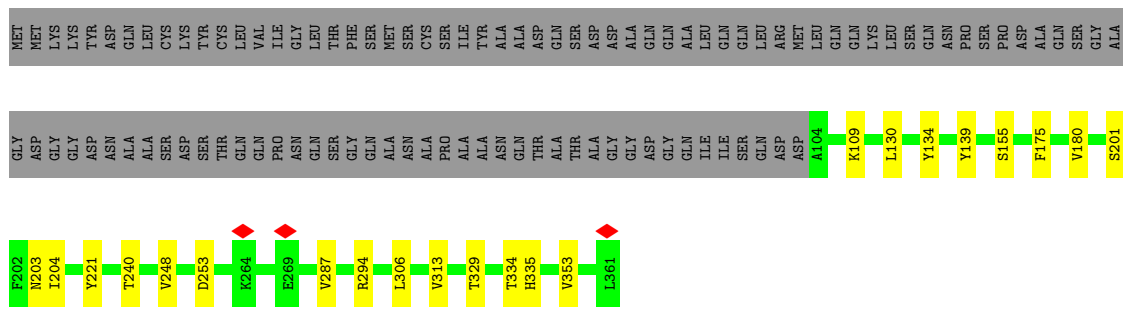
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GLY ASP GLY TYR ASN ALA SER ASP THR GLN PRO ASN LEU SER GLY GLN MET ALA ALA PRO THR ALA ALA THR ASN THR ASP GLY GLN ILE SER SER ARG ASP ASP A104 I107 D108 K109 T147 L160 R170 L171 F175 V176 V180

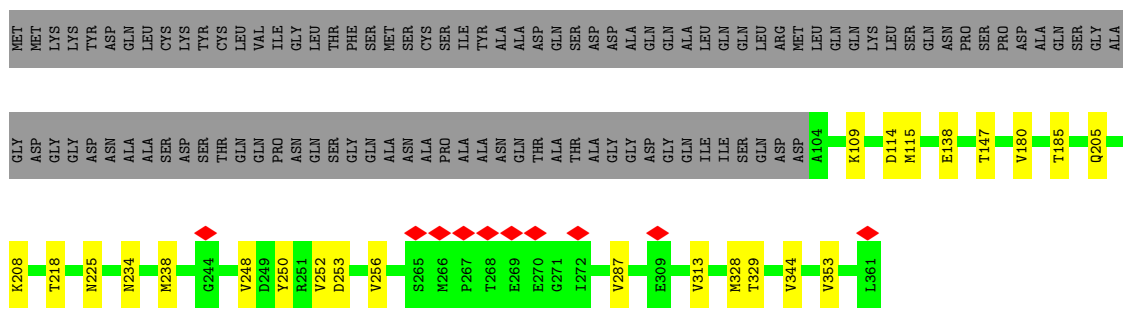
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• Molecule 2: Type IV secretion protein IcmK

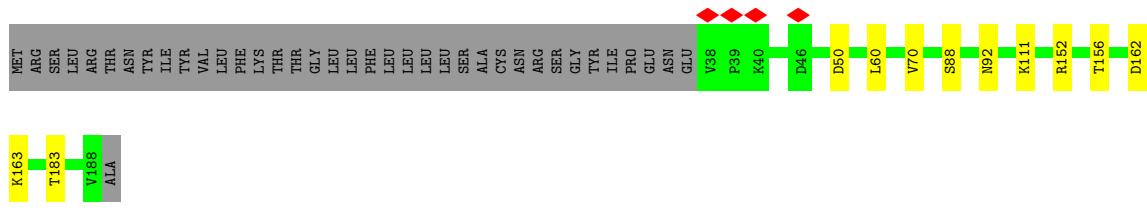
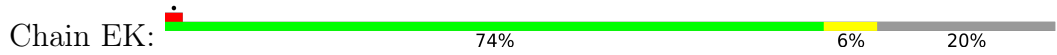




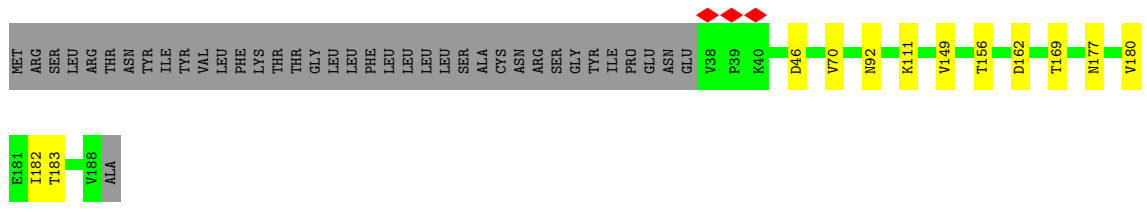
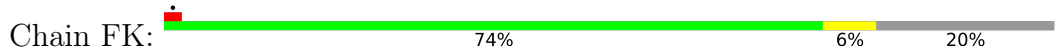
• Molecule 2: Type IV secretion protein IcmK



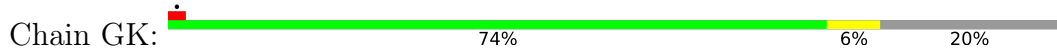
• Molecule 3: Inner membrane lipoprotein YiaD

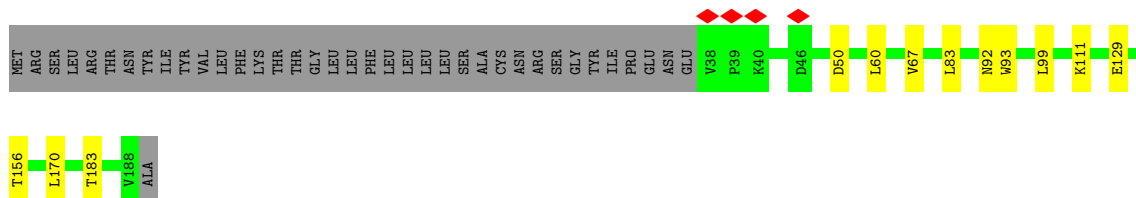


• Molecule 3: Inner membrane lipoprotein YiaD

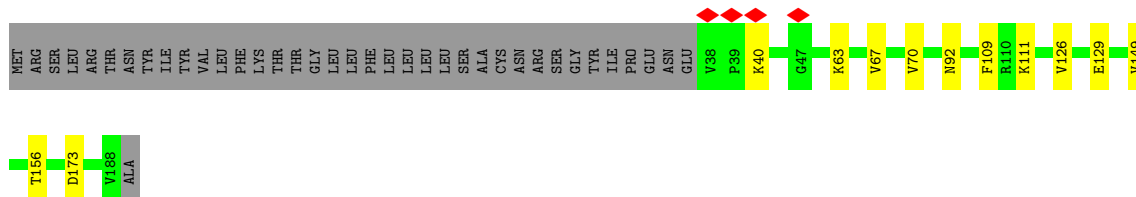
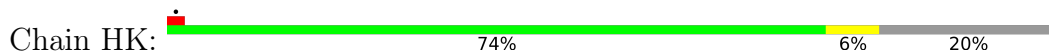


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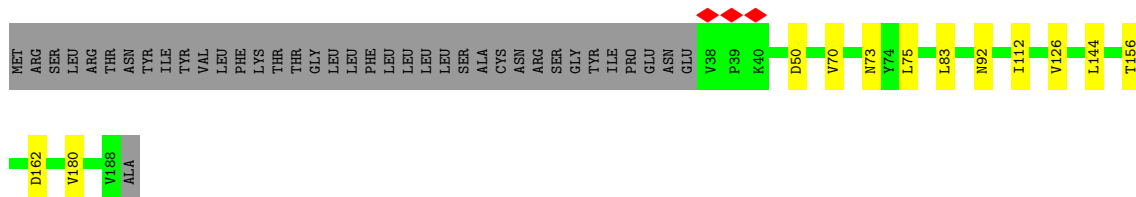
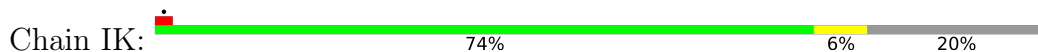




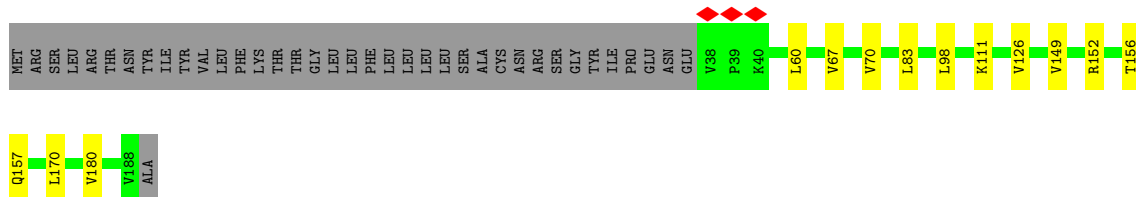
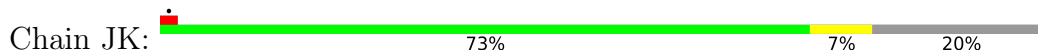
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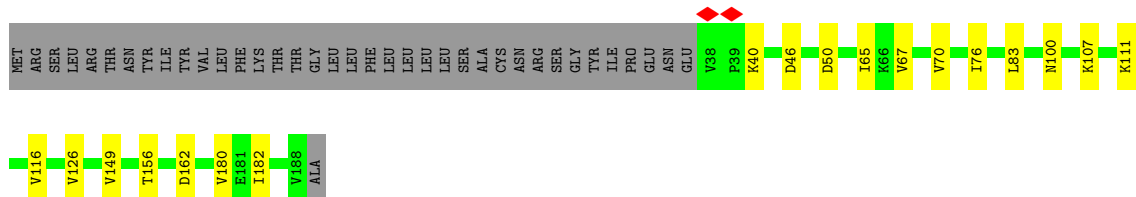
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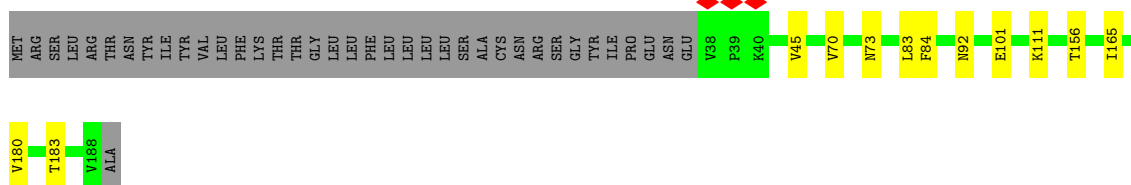
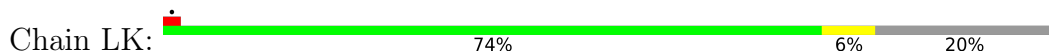
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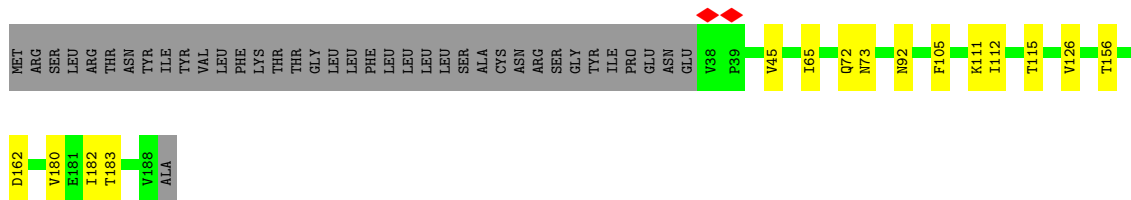
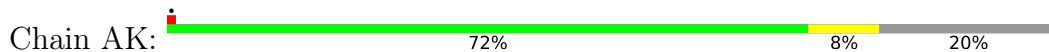
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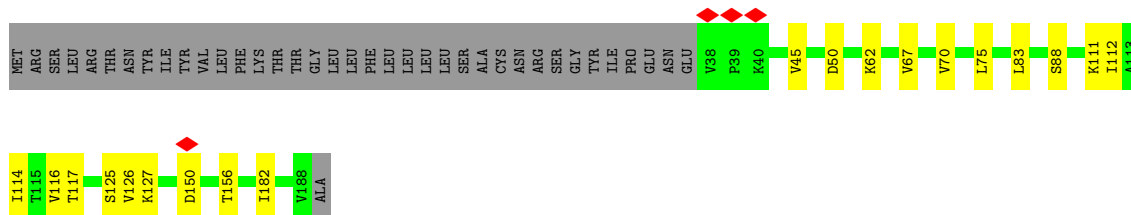
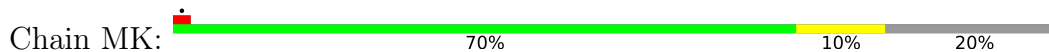
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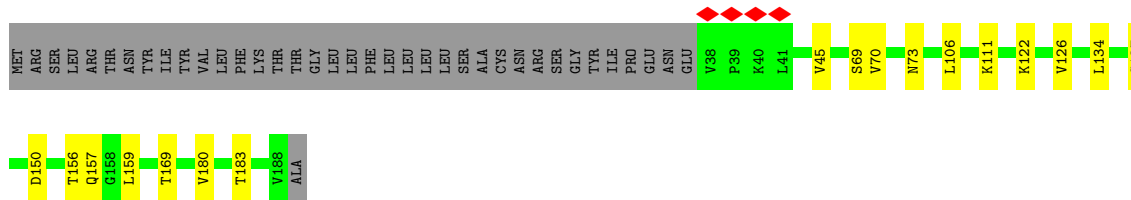
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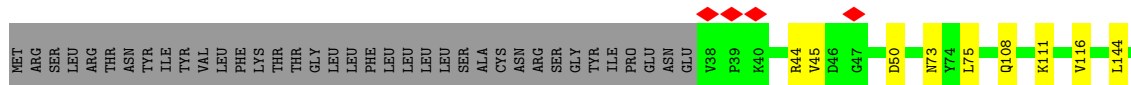
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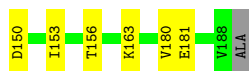


- Molecule 3: Inner membrane lipoprotein YiaD

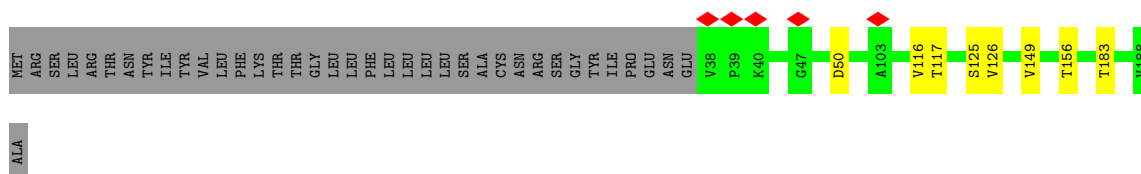
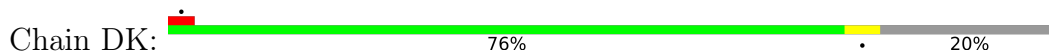


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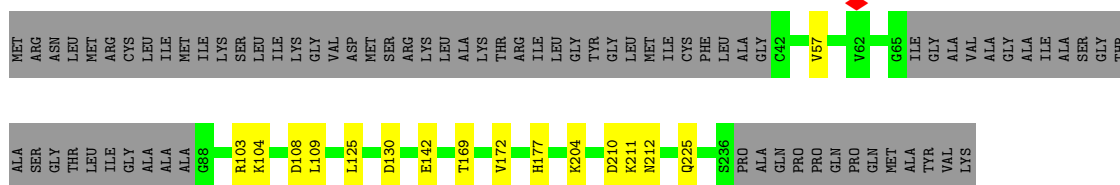




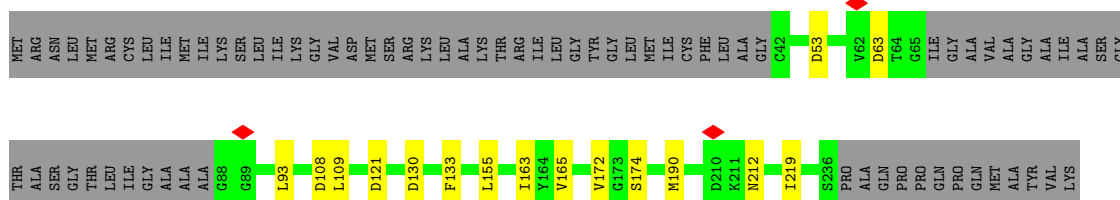
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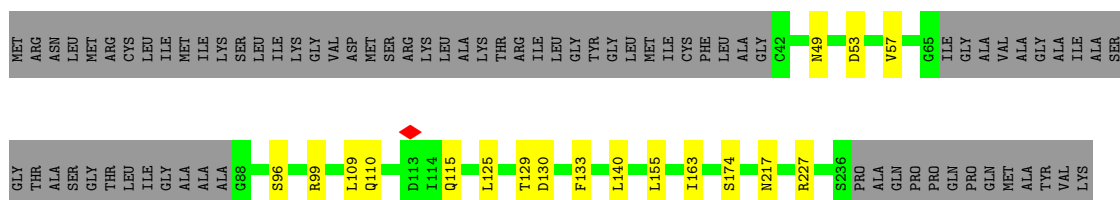
- Molecule 4: Outer membrane protein, OmpA family protein



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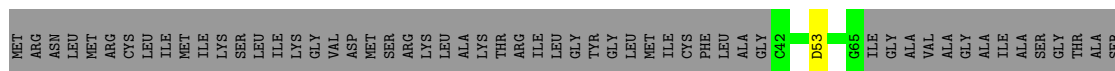


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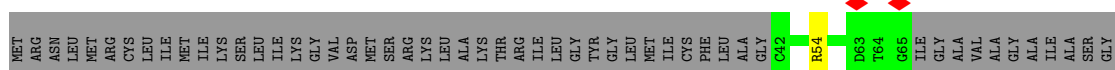


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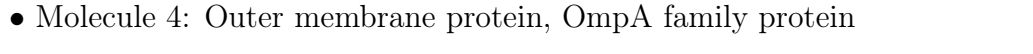
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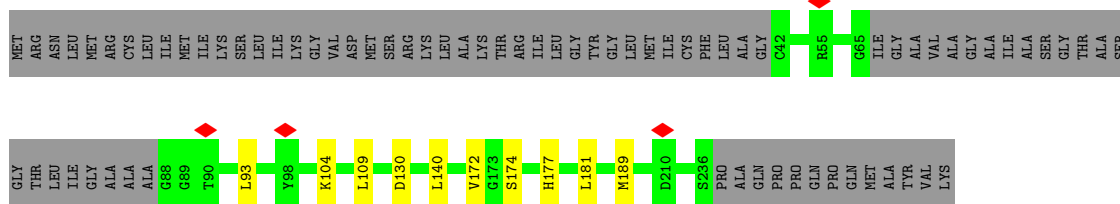
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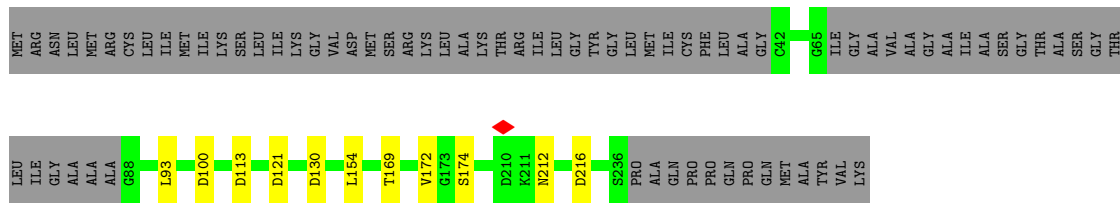
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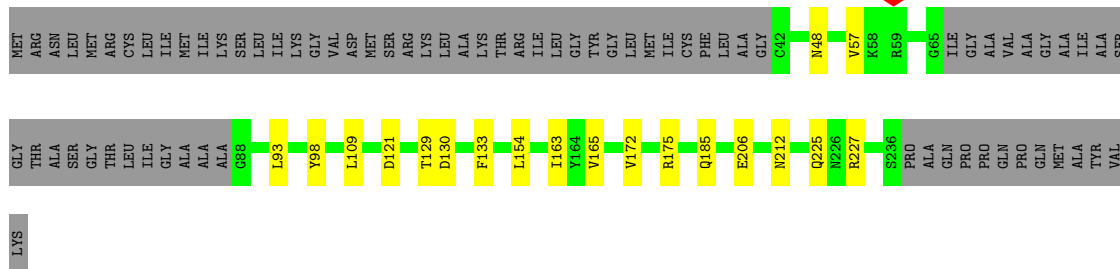
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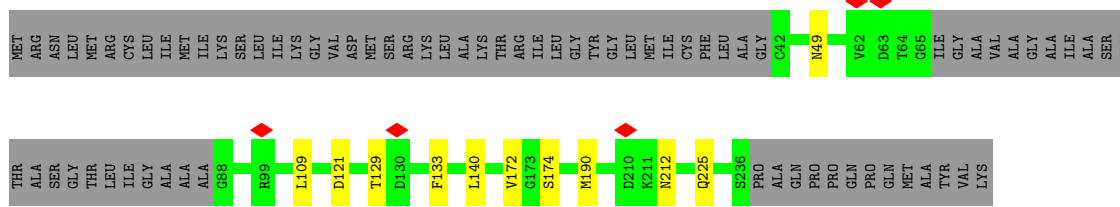
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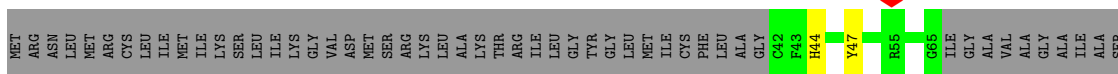
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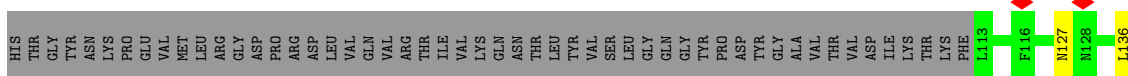
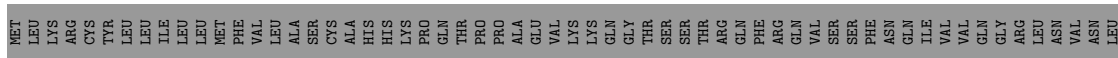
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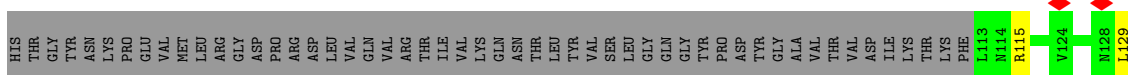
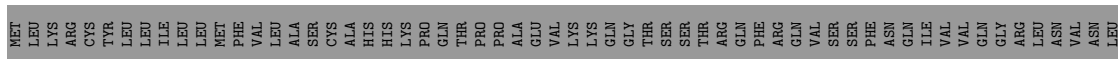




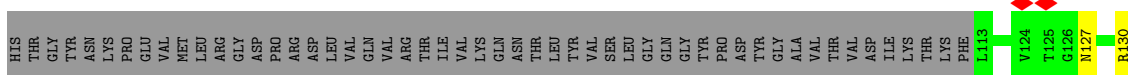
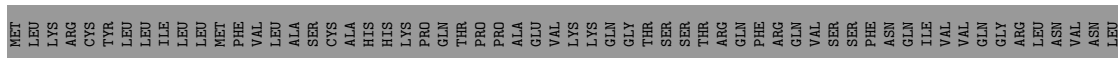
• Molecule 5: DUF2807 domain-containing protein



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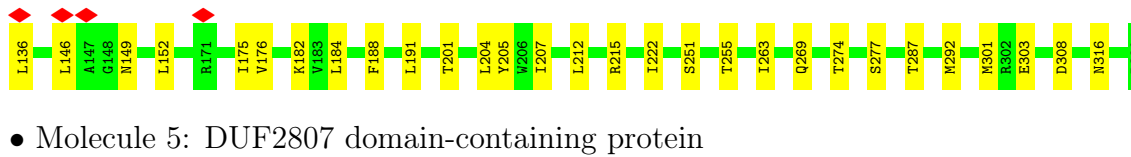
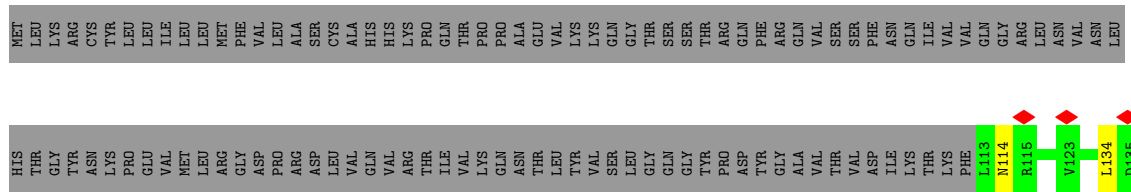
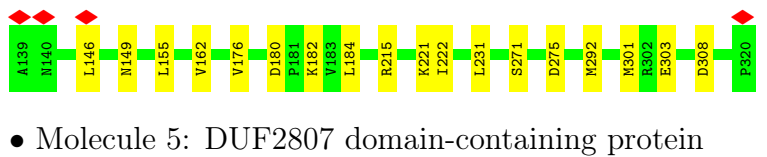
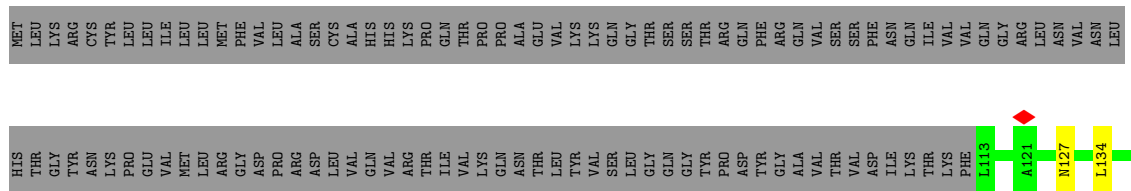
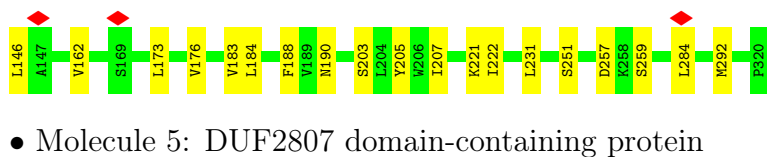
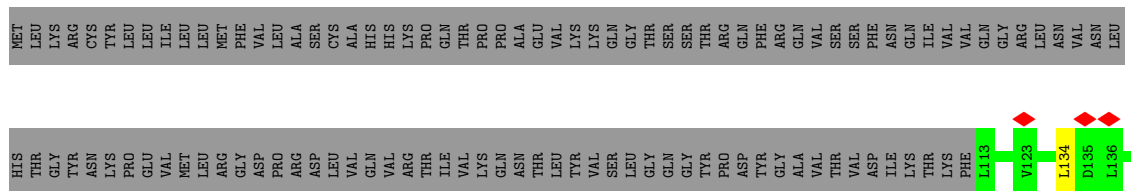
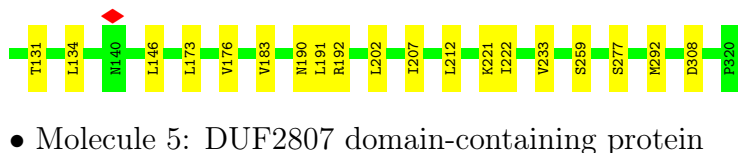


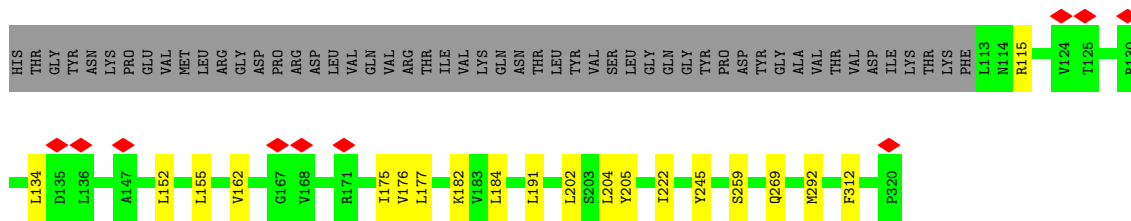
• Molecule 5: DUF2807 domain-containing protein



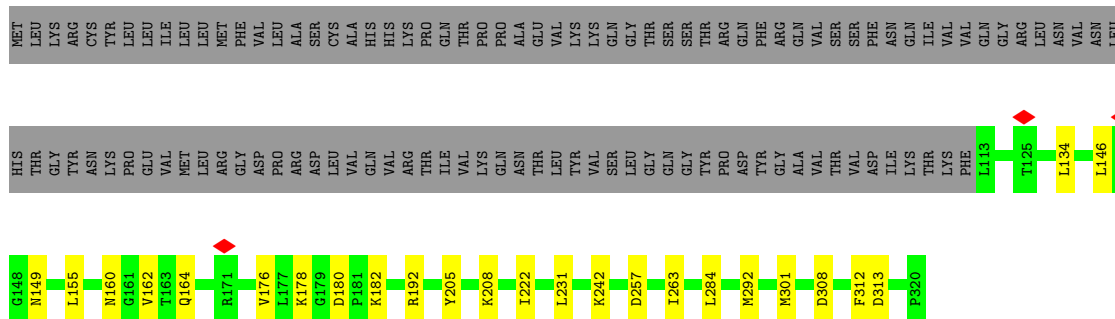
• Molecule 5: DUF2807 domain-containing protein



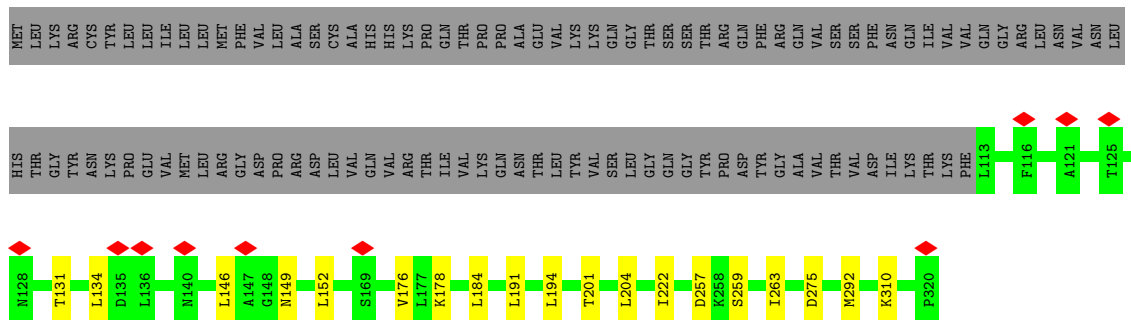




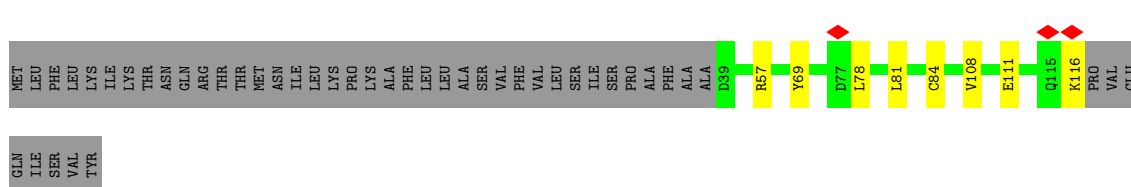
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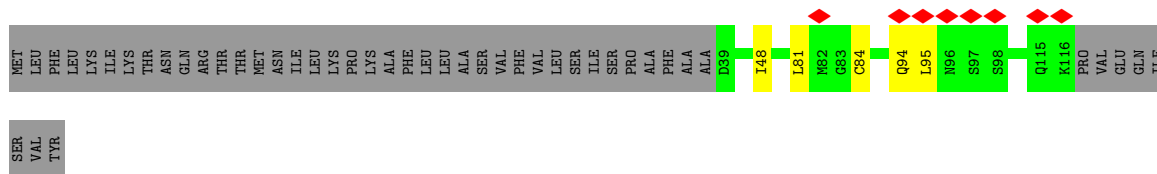


• Molecule 6: Neurogenic locus notch

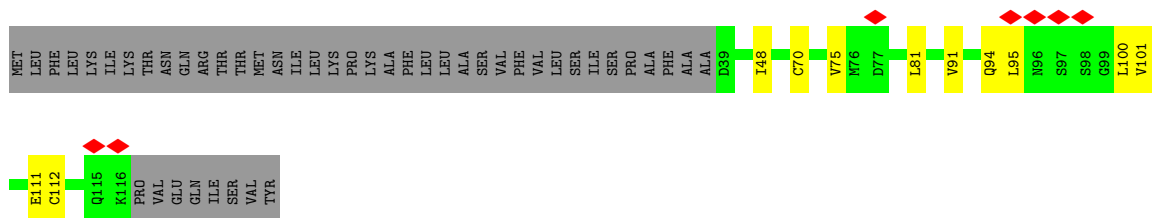


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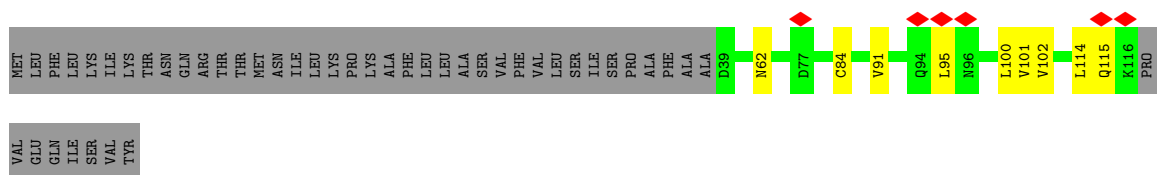




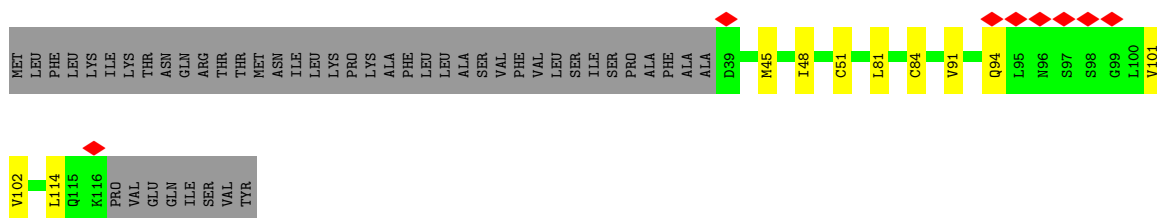
• Molecule 6: Neurogenic locus notch



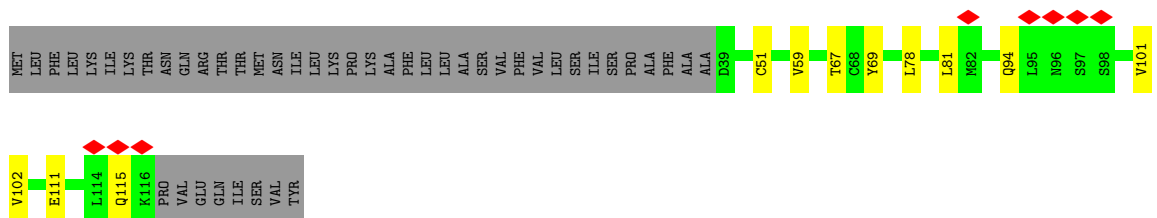
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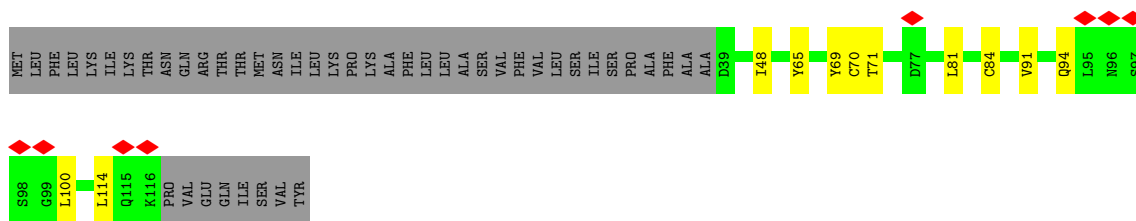
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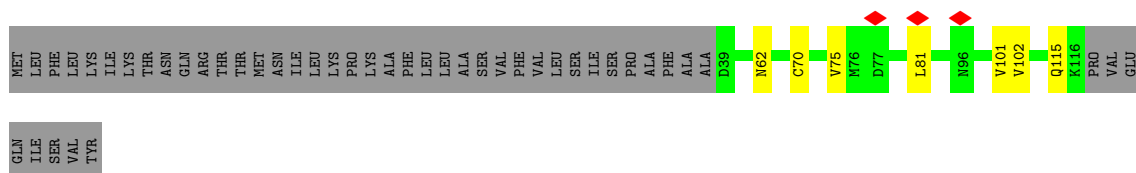
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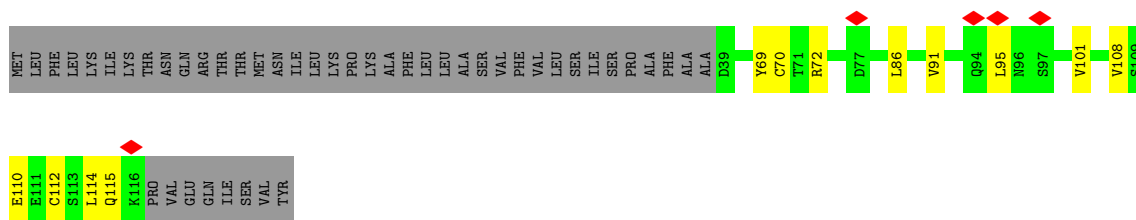
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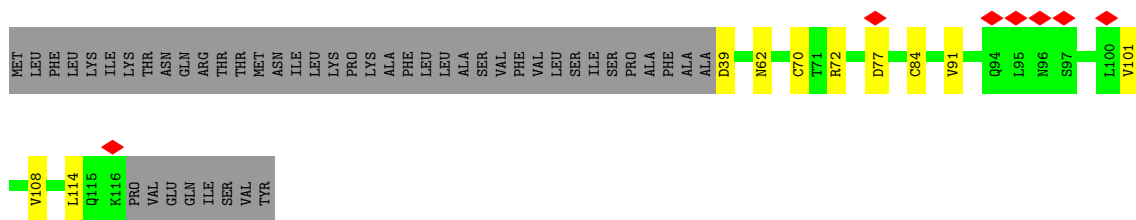
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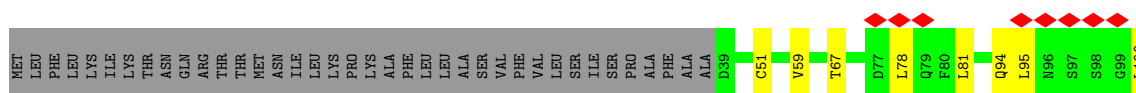
• Molecule 6: Neurogenic locus notch



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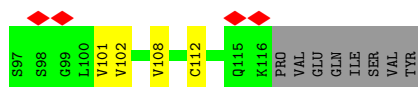
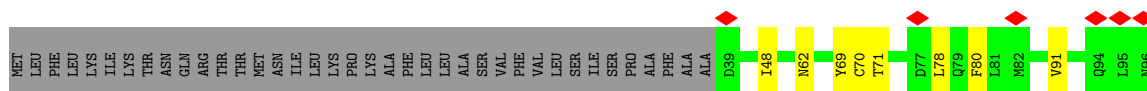


• Molecule 6: Neurogenic locus notch

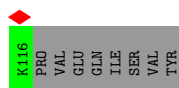
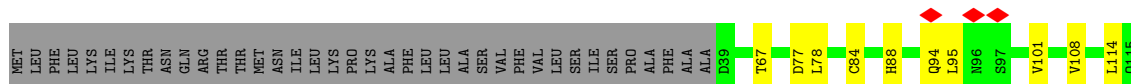




- Molecule 6: Neurogenic locus notch



- Molecule 6: Neurogenic locus notch



- Molecule 7: Unknown protein fragment



There are no outlier residues recorded for this chain.

- Molecule 7: Unknown protein fragment



There are no outlier residues recorded for this chain.

- Molecule 7: Unknown protein fragment



There are no outlier residues recorded for this chain.

- Molecule 7: Unknown protein fragment



There are no outlier residues recorded for this chain.

- Molecule 7: Unknown protein fragment

Chain IU:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Unknown protein fragment

Chain JU:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Unknown protein fragment

Chain KU:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Unknown protein fragment

Chain LU:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Unknown protein fragment

Chain MU:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Unknown protein fragment

Chain AU:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Unknown protein fragment

Chain BU:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Unknown protein fragment

Chain CU:  100%

There are no outlier residues recorded for this chain.

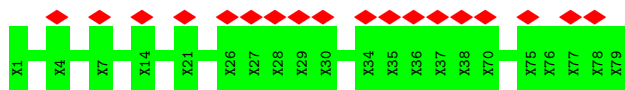
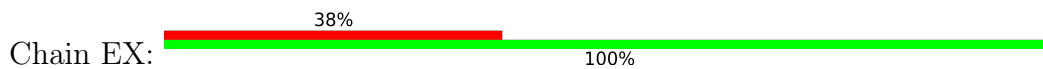
- Molecule 7: Unknown protein fragment

Chain DU:  100%

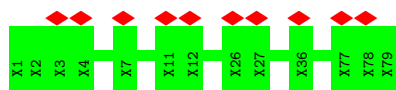
There are no outlier residues recorded for this chain.

- Molecule 8: Unknown protein fragment

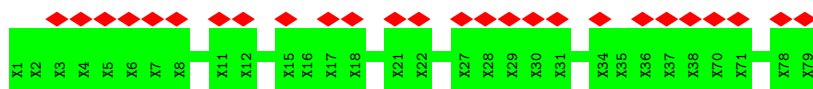




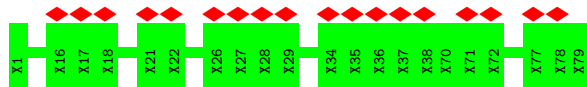
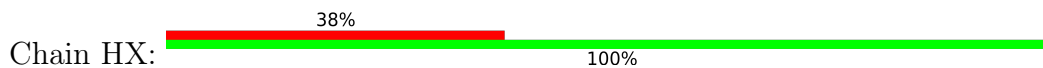
• Molecule 8: Unknown protein fragment



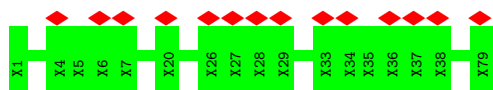
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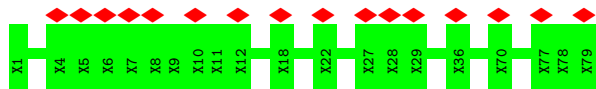
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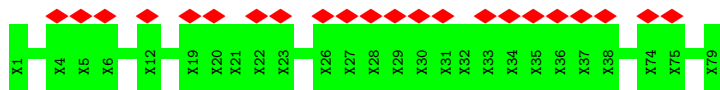
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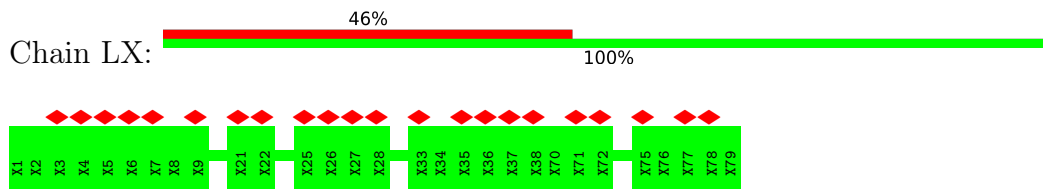
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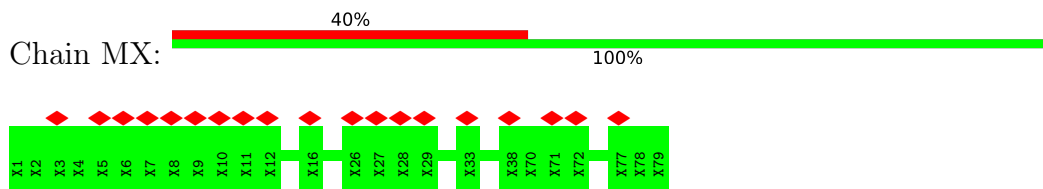
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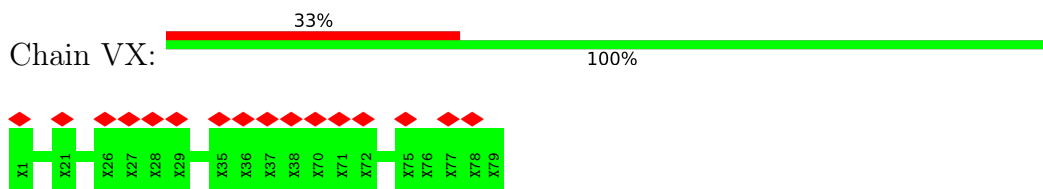
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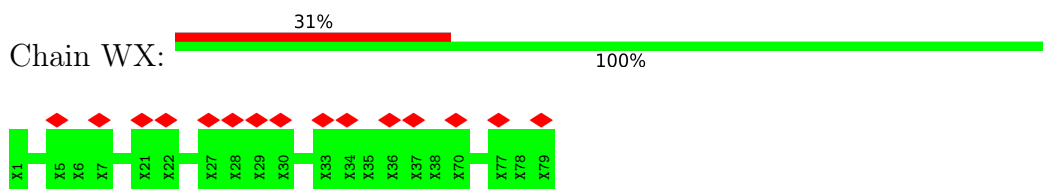
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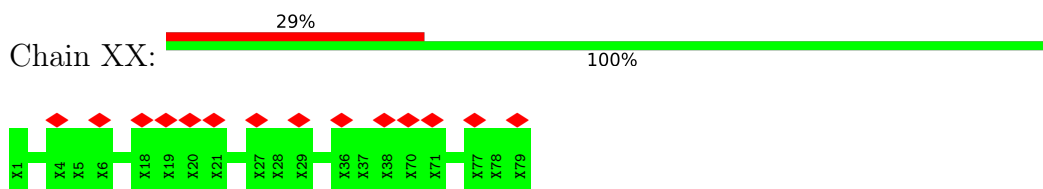
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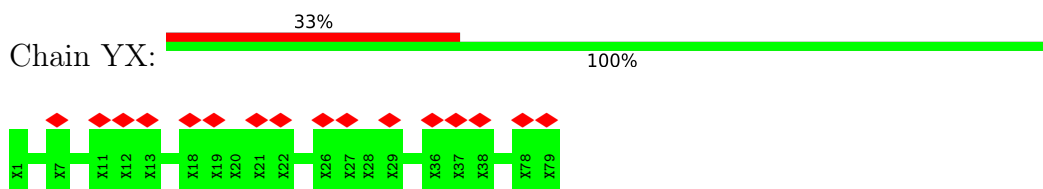
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- Molecule 8: Unknown protein fragment

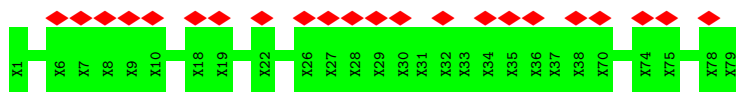


- Molecule 8: Unknown protein fragment

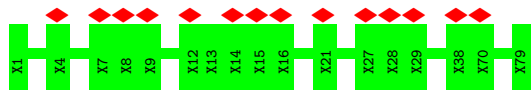


- Molecule 8: Unknown protein fragment

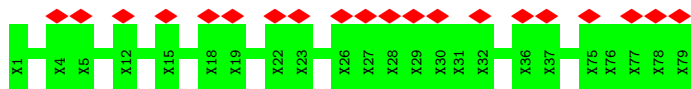
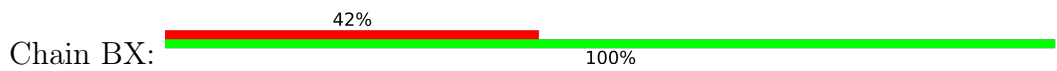




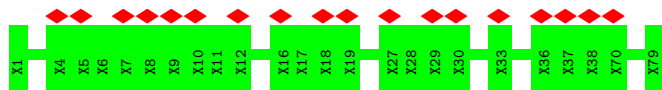
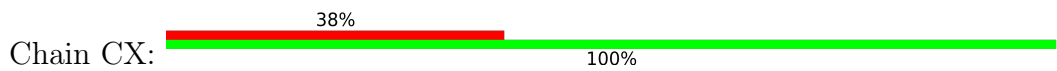
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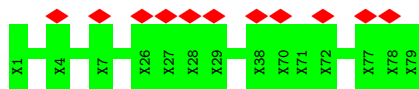
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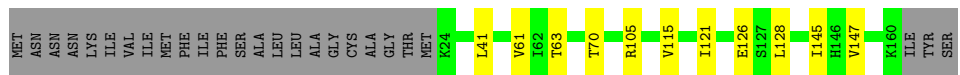
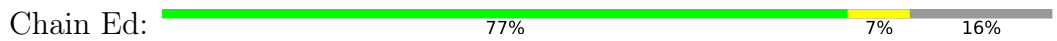
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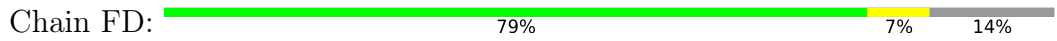
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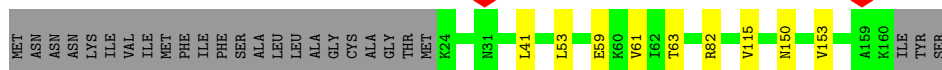
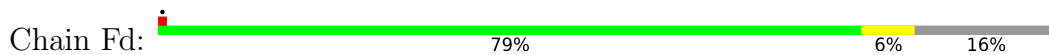
• Molecule 9: DotD



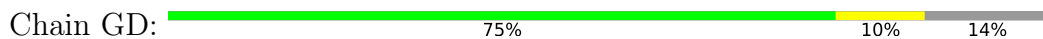
• Molecule 9: DotD



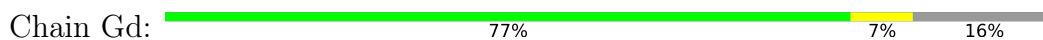
• Molecule 9: DotD



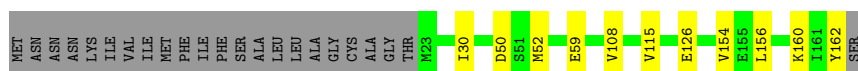
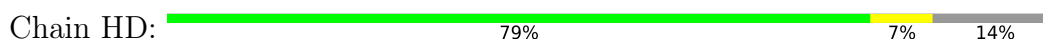
● Molecule 9: DotD



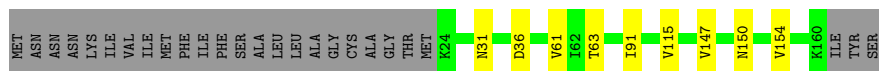
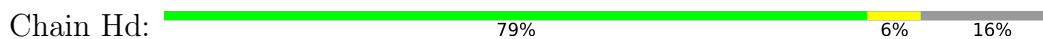
● Molecule 9: DotD



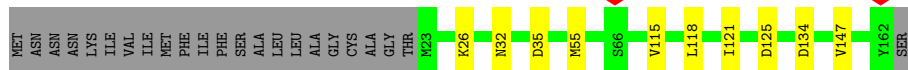
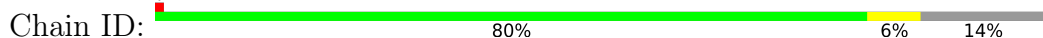
● Molecule 9: DotD



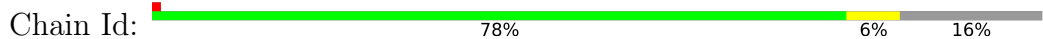
● Molecule 9: DotD



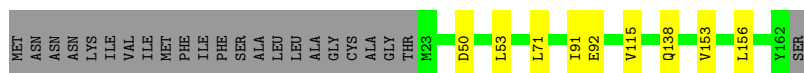
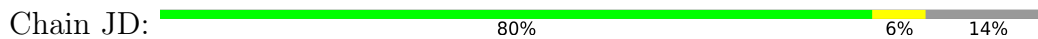
● Molecule 9: DotD



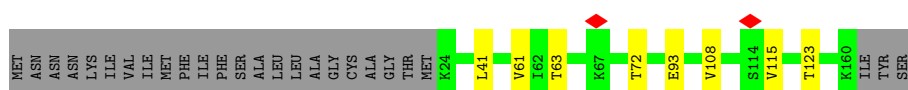
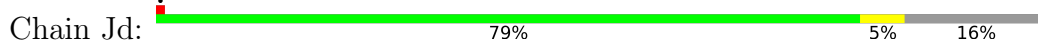
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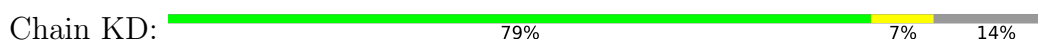
● Molecule 9: DotD



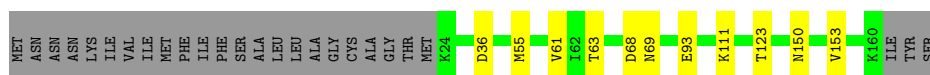
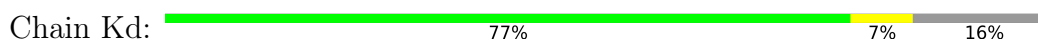
● Molecule 9: DotD



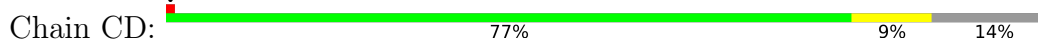
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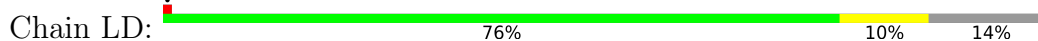
● Molecule 9: DotD



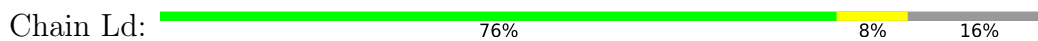
● Molecule 9: DotD



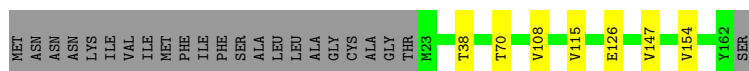
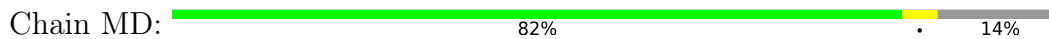
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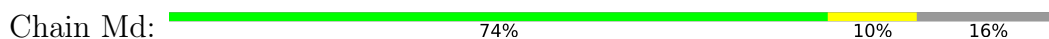
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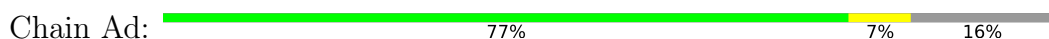
● Molecule 9: DotD



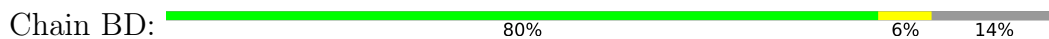
● Molecule 9: DotD



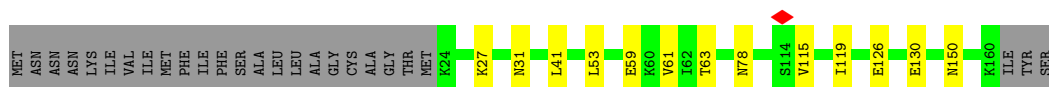
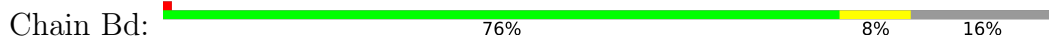
● Molecule 9: DotD



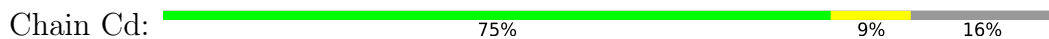
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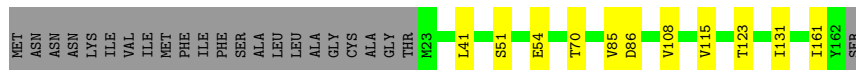
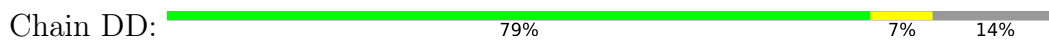
● Molecule 9: DotD



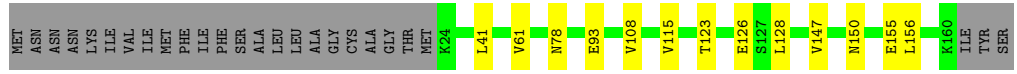
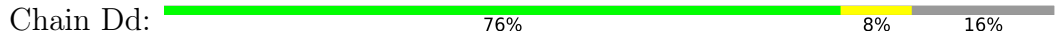
● Molecule 9: DotD



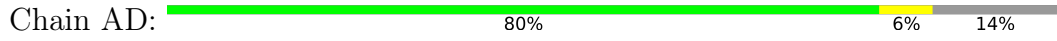
● Molecule 9: DotD



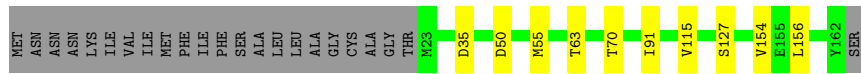
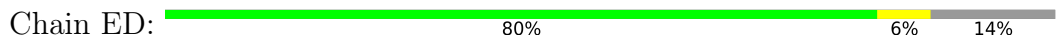
● Molecule 9: DotD



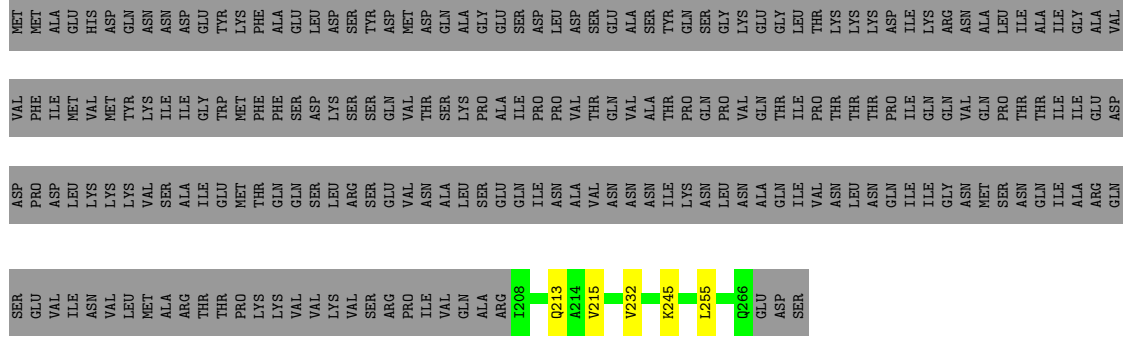
● Molecule 9: DotD



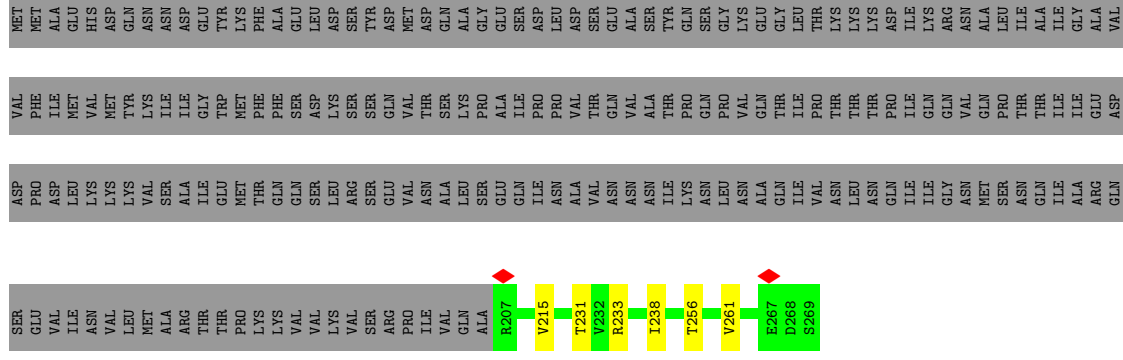
● Molecule 9: DotD



● Molecule 10: DotF



● Molecule 10: DotF



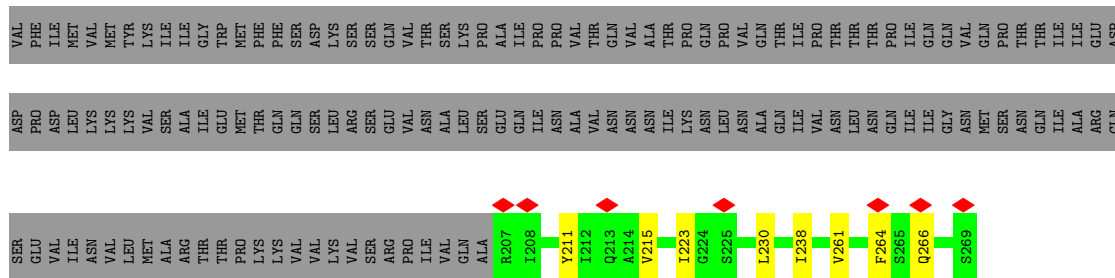
● Molecule 10: DotF





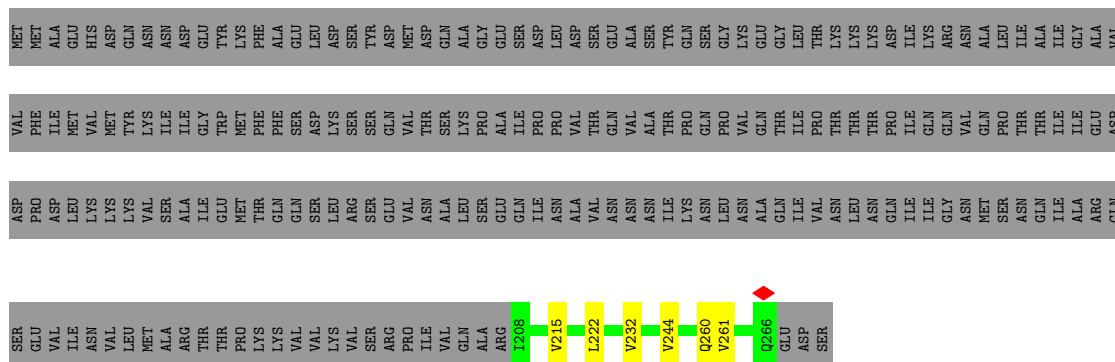






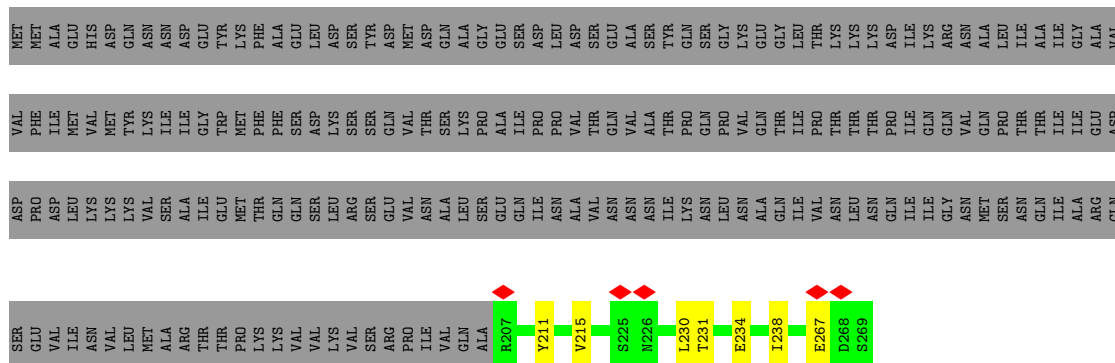
Molecule 10: DotF

Chain Kf: 20% . 78%



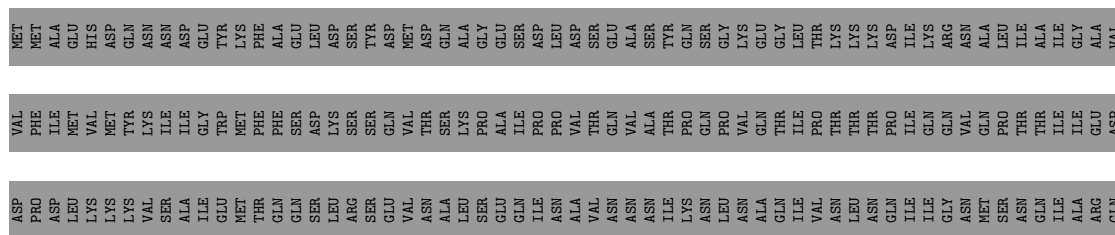
Molecule 10: DotF

Chain LF: 21% . 77%



Molecule 10: DotF

Chain Lf: 21% . 78%





Chain VF: 22% 77%

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

SER	GLU	VAL	ILE	ASN	VAL	LEU	MET	ALA	ARG	THR	THR	PRO	LYS	LYS	VAL	VAL	LEU	LYS	VAL	SER	SER	ARG	ARG	PRO	PRO	ILE	ALA	VAL	GLN	ALA	R207	V215	L230	T231	K245	D248	T256	V261	E267	D268	S269
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• Molecule 10: DotF

Chain WF: 21% 77%

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

SER	GLU	VAL	ILE	ASN	VAL	LEU	MET	ALA	ARG	THR	THR	PRO	LYS	LYS	VAL	VAL	LEU	LYS	VAL	SER	SER	ARG	ARG	PRO	PRO	ILE	ALA	VAL	GLN	ALA	R207	V215	T231	I238	K245	D251	T256	V261	F264	S269
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• Molecule 10: DotF

Chain XF: 21% 77%

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

SER	GLU	VAL	ILE	ASN	VAL	LEU	MET	ALA	ARG	THR	THR	PRO	LYS	LYS	VAL	VAL	LEU	LYS	VAL	SER	SER	ARG	ARG	PRO	PRO	ILE	ALA	VAL	GLN	ALA	R207	I208	V215	S225	L230	T231	V232	R233	L246	I247	D248	S249	T256	V261	E267	D268	S269
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

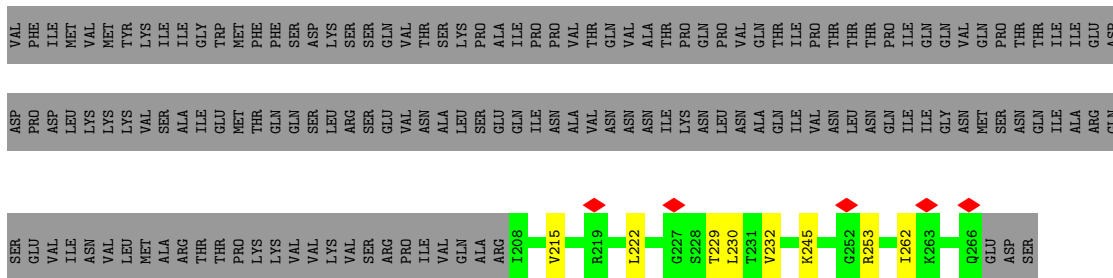
• Molecule 10: DotF

Chain YF: 21% 77%

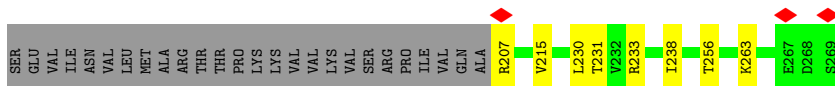
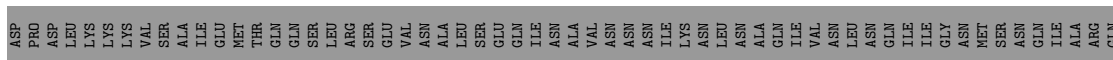
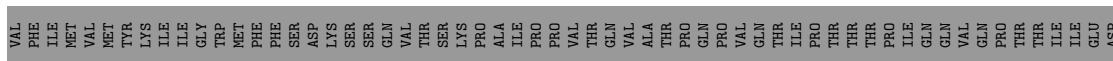
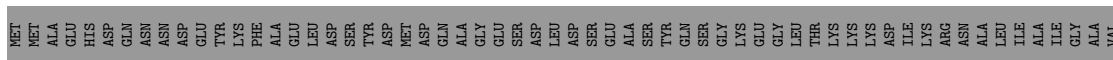
MET	MET	ALA	GLU	HIS	ASP	GLN	ASN	ASN	ASP	GLU	TYR	PHE	ALA	GLU	LEU	ASP	ASP	SER	TYR	ASP	GLN	MET	ASP	GLN	ASP	GLN	ALA	GLY	GLU	GLU	SER	ASP	LEU	ASP	GLN	LEU	ASP	SER	TYR	ASP	GLN	GLN	GLN	GLY	VAL			
VAL	PHE	ILE	LEU	MET	VAL	TYR	LYS	ILE	GLY	TRP	MET	PHE	PHE	ALA	GLN	ASP	VAL	SER	SER	SER	GLN	VAL	VAL	THR	THR	SER	VAL	PRO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



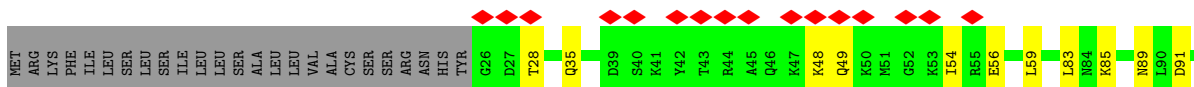
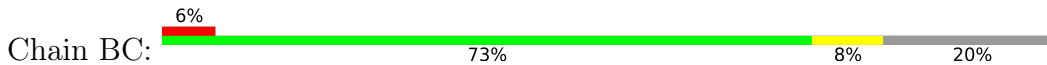




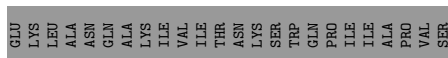
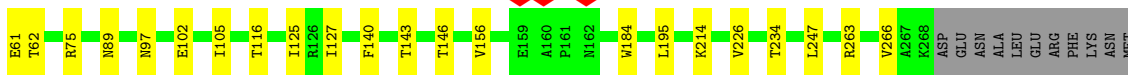
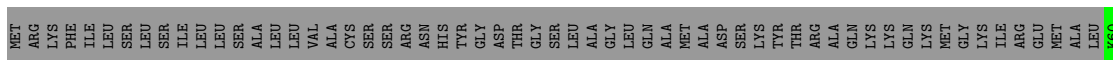
• Molecule 10: DotF



• Molecule 11: DotC



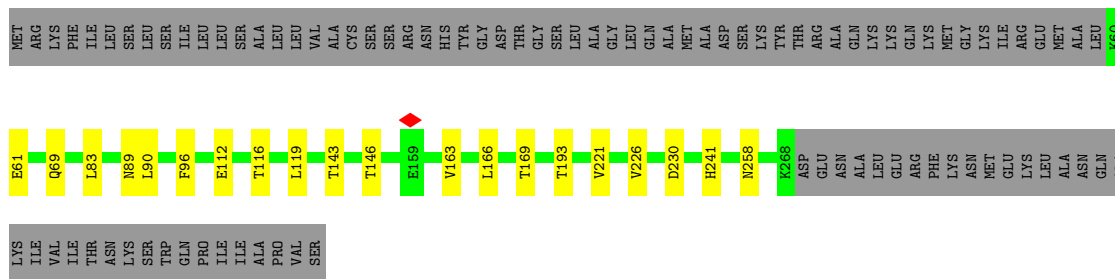
• Molecule 11: DotC



• Molecule 11: DotC

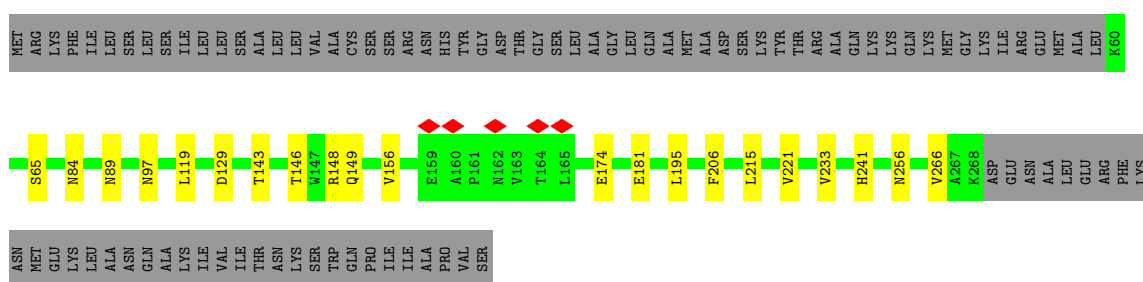


Chain DC: 62% 7% 31%



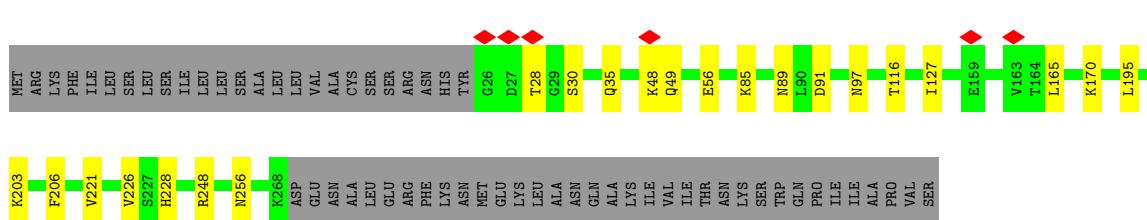
• Molecule 11: DotC

Chain EC: 62% 7% 31%



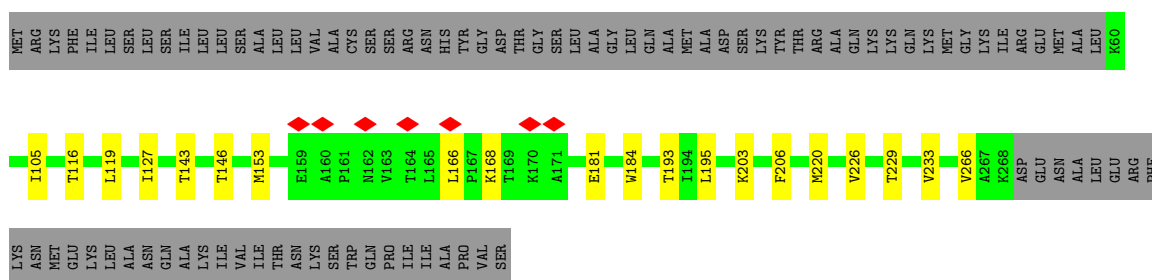
• Molecule 11: DotC

Chain FC: 73% 7% 20%



• Molecule 11: DotC

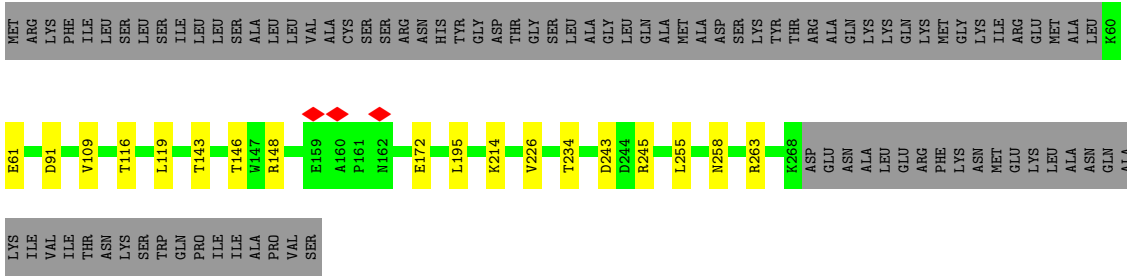
Chain GC: 62% 7% 31%



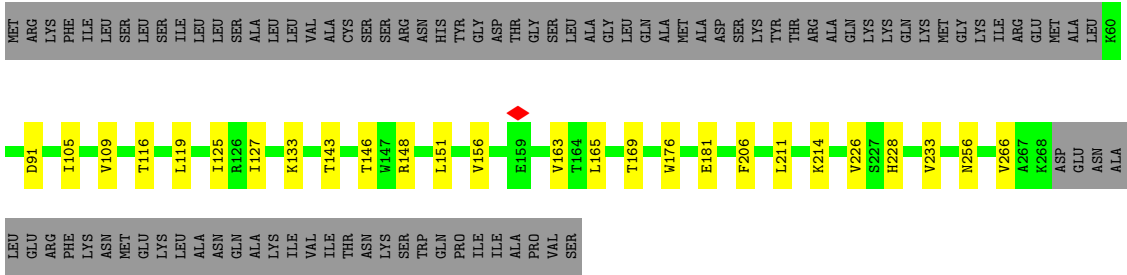
• Molecule 11: DotC

Chain HC: 61% 8% 31%

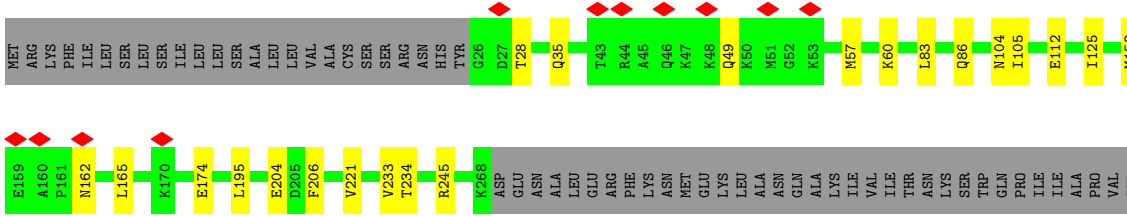




• Molecule 11: DotC



• Molecule 11: DotC



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42013	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.809	Depositor
Minimum map value	-3.314	Depositor
Average map value	0.095	Depositor
Map value standard deviation	0.541	Depositor
Recommended contour level	2.25	Depositor
Map size (Å)	561.0, 561.0, 561.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.244, 2.244, 2.244	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	AG	0.30	0/1250	0.54	0/1699
1	Ag	0.25	0/278	0.45	0/377
1	BG	0.29	0/1250	0.55	0/1699
1	Bg	0.28	0/278	0.46	0/377
1	CG	0.29	0/1250	0.55	0/1699
1	Cg	0.26	0/278	0.44	0/377
1	DG	0.29	0/1250	0.56	0/1699
1	Dg	0.28	0/278	0.50	0/377
1	EG	0.30	0/1250	0.54	0/1699
1	Eg	0.25	0/278	0.47	0/377
1	FG	0.29	0/1250	0.55	0/1699
1	Fg	0.26	0/278	0.46	0/377
1	GG	0.30	0/1250	0.55	0/1699
1	Gg	0.26	0/278	0.49	0/377
1	HG	0.29	0/1250	0.55	0/1699
1	Hg	0.26	0/278	0.46	0/377
1	IG	0.29	0/1250	0.56	0/1699
1	Ig	0.25	0/278	0.44	0/377
1	JG	0.29	0/1250	0.54	0/1699
1	Jg	0.26	0/278	0.46	0/377
1	KG	0.30	0/1250	0.56	0/1699
1	Kg	0.26	0/278	0.46	0/377
1	LG	0.29	0/1250	0.56	0/1699
1	Lg	0.25	0/278	0.45	0/377
1	MG	0.28	0/1250	0.55	0/1699
1	Mg	0.26	0/278	0.47	0/377
1	NG	0.28	0/1250	0.57	1/1699 (0.1%)
1	OG	0.29	0/1250	0.56	1/1699 (0.1%)
1	PG	0.29	0/1250	0.55	0/1699
1	VG	0.26	0/278	0.53	0/377
1	WG	0.27	0/278	0.46	0/377
1	XG	0.26	0/278	0.55	0/377
1	YG	0.28	0/278	0.50	0/377
1	ZG	0.28	0/278	0.53	0/377

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	AH	0.29	0/2033	0.53	0/2775
2	BH	0.29	0/2033	0.53	0/2775
2	CH	0.29	0/2033	0.52	0/2775
2	DH	0.29	0/2033	0.52	0/2775
2	EH	0.28	0/2033	0.52	0/2775
2	FH	0.28	0/2033	0.51	0/2775
2	GH	0.29	0/2033	0.53	0/2775
2	HH	0.29	0/2033	0.51	0/2775
2	IH	0.28	0/2033	0.52	0/2775
2	JH	0.28	0/2033	0.51	0/2775
2	KH	0.29	0/2033	0.53	0/2775
2	LH	0.30	0/2033	0.55	0/2775
2	MH	0.28	0/2033	0.51	0/2775
2	VH	0.27	0/1921	0.53	0/2620
2	WH	0.28	0/1921	0.52	0/2620
2	XH	0.28	0/1921	0.53	0/2620
2	YH	0.27	0/1921	0.52	0/2620
2	ZH	0.27	0/1921	0.54	0/2620
3	AK	0.29	0/1195	0.54	0/1616
3	BK	0.29	0/1195	0.55	0/1616
3	CK	0.31	0/1195	0.53	0/1616
3	DK	0.29	0/1195	0.53	0/1616
3	EK	0.29	0/1195	0.53	0/1616
3	FK	0.30	0/1195	0.53	0/1616
3	GK	0.30	0/1195	0.54	0/1616
3	HK	0.29	0/1195	0.52	0/1616
3	IK	0.30	0/1195	0.55	0/1616
3	JK	0.30	0/1195	0.54	0/1616
3	KK	0.30	0/1195	0.53	0/1616
3	LK	0.30	0/1195	0.54	0/1616
3	MK	0.29	0/1195	0.52	0/1616
4	AL	0.30	0/1417	0.54	0/1912
4	BL	0.30	0/1417	0.54	0/1912
4	CL	0.30	0/1417	0.53	0/1912
4	DL	0.30	0/1417	0.55	0/1912
4	EL	0.29	0/1417	0.55	0/1912
4	FL	0.29	0/1417	0.54	0/1912
4	GL	0.30	0/1417	0.55	0/1912
4	HL	0.29	0/1417	0.55	0/1912
4	IL	0.29	0/1417	0.55	0/1912
4	JL	0.29	0/1417	0.54	0/1912
4	KL	0.29	0/1417	0.54	0/1912
4	LL	0.30	0/1417	0.54	0/1912

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	ML	0.30	0/1417	0.54	0/1912
5	AM	0.28	0/1678	0.57	0/2262
5	BM	0.28	0/1678	0.56	0/2262
5	CM	0.29	0/1678	0.58	0/2262
5	DM	0.29	0/1678	0.56	0/2262
5	EM	0.29	0/1678	0.56	0/2262
5	FM	0.29	0/1678	0.57	0/2262
5	GM	0.28	0/1678	0.55	0/2262
5	HM	0.28	0/1678	0.57	0/2262
5	IM	0.29	0/1678	0.60	0/2262
5	JM	0.28	0/1678	0.59	0/2262
5	KM	0.29	0/1678	0.58	0/2262
5	LM	0.28	0/1678	0.57	0/2262
5	MM	0.28	0/1678	0.57	0/2262
6	AN	0.32	0/593	0.51	0/799
6	BN	0.31	0/593	0.52	0/799
6	CN	0.30	0/593	0.50	0/799
6	DN	0.30	0/593	0.51	0/799
6	EN	0.31	0/593	0.53	0/799
6	FN	0.31	0/593	0.51	0/799
6	GN	0.30	0/593	0.52	0/799
6	HN	0.30	0/593	0.50	0/799
6	IN	0.31	0/593	0.53	0/799
6	JN	0.30	0/593	0.53	0/799
6	KN	0.32	0/593	0.53	0/799
6	LN	0.32	0/593	0.52	0/799
6	MN	0.30	0/593	0.54	0/799
9	AD	0.32	0/1107	0.53	0/1502
9	Ad	0.28	0/1078	0.49	0/1463
9	BD	0.28	0/1107	0.51	0/1502
9	Bd	0.28	0/1078	0.50	0/1463
9	CD	0.29	0/1107	0.52	0/1502
9	Cd	0.28	0/1078	0.48	0/1463
9	DD	0.30	0/1107	0.52	0/1502
9	Dd	0.28	0/1078	0.51	0/1463
9	ED	0.29	0/1107	0.52	0/1502
9	Ed	0.28	0/1078	0.49	0/1463
9	FD	0.30	0/1107	0.53	0/1502
9	Fd	0.28	0/1078	0.51	0/1463
9	GD	0.29	0/1107	0.54	0/1502
9	Gd	0.28	0/1078	0.50	0/1463
9	HD	0.29	0/1107	0.54	0/1502
9	Hd	0.27	0/1078	0.50	0/1463

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
9	ID	0.29	0/1107	0.54	0/1502
9	Id	0.29	0/1078	0.48	0/1463
9	JD	0.30	0/1107	0.50	0/1502
9	Jd	0.29	0/1078	0.49	0/1463
9	KD	0.30	0/1107	0.52	0/1502
9	Kd	0.28	0/1078	0.48	0/1463
9	LD	0.29	0/1107	0.51	0/1502
9	Ld	0.28	0/1078	0.50	0/1463
9	MD	0.30	0/1107	0.53	0/1502
9	Md	0.29	0/1078	0.49	0/1463
10	AF	0.26	0/490	0.55	0/660
10	Af	0.28	0/456	0.57	0/615
10	BF	0.27	0/490	0.53	0/660
10	Bf	0.27	0/456	0.51	0/615
10	CF	0.27	0/490	0.53	0/660
10	Cf	0.27	0/456	0.52	0/615
10	DF	0.27	0/490	0.57	0/660
10	Df	0.27	0/456	0.53	0/615
10	EF	0.26	0/490	0.53	0/660
10	Ef	0.27	0/456	0.51	0/615
10	FF	0.27	0/490	0.55	0/660
10	Ff	0.27	0/456	0.53	0/615
10	GF	0.26	0/490	0.53	0/660
10	Gf	0.26	0/456	0.54	0/615
10	HF	0.27	0/490	0.56	0/660
10	Hf	0.28	0/456	0.54	0/615
10	IF	0.27	0/490	0.55	0/660
10	If	0.27	0/456	0.53	0/615
10	JF	0.26	0/490	0.54	0/660
10	Jf	0.26	0/456	0.52	0/615
10	KF	0.26	0/490	0.55	0/660
10	Kf	0.27	0/456	0.51	0/615
10	LF	0.26	0/490	0.54	0/660
10	Lf	0.28	0/456	0.52	0/615
10	MF	0.27	0/490	0.53	0/660
10	Mf	0.27	0/456	0.53	0/615
10	VF	0.26	0/490	0.53	0/660
10	WF	0.26	0/490	0.55	0/660
10	XF	0.26	0/490	0.53	0/660
10	YF	0.27	0/490	0.53	0/660
10	ZF	0.27	0/490	0.55	0/660
11	AC	0.29	0/1957	0.51	0/2651
11	BC	0.28	0/1957	0.51	0/2651



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
11	CC	0.29	0/1702	0.52	0/2315
11	DC	0.30	0/1702	0.51	0/2315
11	EC	0.30	0/1702	0.52	0/2315
11	FC	0.29	0/1957	0.51	0/2651
11	GC	0.29	0/1702	0.52	0/2315
11	HC	0.29	0/1702	0.51	0/2315
11	IC	0.30	0/1702	0.50	0/2315
11	JC	0.28	0/1957	0.51	0/2651
11	KC	0.29	0/1702	0.51	0/2315
11	LC	0.29	0/1702	0.52	0/2315
11	MC	0.29	0/1702	0.51	0/2315
All	All	0.29	0/190816	0.53	2/258661 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	BH	0	1
2	JH	0	1
2	MH	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	NG	965	LEU	CA-CB-CG	5.15	127.15	115.30
1	OG	965	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	BH	321	SER	Peptide
2	JH	321	SER	Peptide
2	MH	321	SER	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AG	161/1048 (15%)	153 (95%)	8 (5%)	0	100	100
1	Ag	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	BG	161/1048 (15%)	153 (95%)	8 (5%)	0	100	100
1	Bg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	CG	161/1048 (15%)	156 (97%)	5 (3%)	0	100	100
1	Cg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	DG	161/1048 (15%)	157 (98%)	4 (2%)	0	100	100
1	Dg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	EG	161/1048 (15%)	158 (98%)	3 (2%)	0	100	100
1	Eg	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	FG	161/1048 (15%)	153 (95%)	8 (5%)	0	100	100
1	Fg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	GG	161/1048 (15%)	155 (96%)	6 (4%)	0	100	100
1	Gg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	HG	161/1048 (15%)	151 (94%)	10 (6%)	0	100	100
1	Hg	32/1048 (3%)	32 (100%)	0	0	100	100
1	IG	161/1048 (15%)	153 (95%)	8 (5%)	0	100	100
1	Ig	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	JG	161/1048 (15%)	154 (96%)	7 (4%)	0	100	100
1	Jg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	KG	161/1048 (15%)	157 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Kg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	LG	161/1048 (15%)	154 (96%)	7 (4%)	0	100	100
1	Lg	32/1048 (3%)	32 (100%)	0	0	100	100
1	MG	161/1048 (15%)	152 (94%)	9 (6%)	0	100	100
1	Mg	32/1048 (3%)	29 (91%)	3 (9%)	0	100	100
1	NG	161/1048 (15%)	154 (96%)	7 (4%)	0	100	100
1	OG	161/1048 (15%)	158 (98%)	3 (2%)	0	100	100
1	PG	161/1048 (15%)	155 (96%)	6 (4%)	0	100	100
1	VG	32/1048 (3%)	32 (100%)	0	0	100	100
1	WG	32/1048 (3%)	32 (100%)	0	0	100	100
1	XG	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	YG	32/1048 (3%)	32 (100%)	0	0	100	100
1	ZG	32/1048 (3%)	32 (100%)	0	0	100	100
2	AH	256/361 (71%)	240 (94%)	16 (6%)	0	100	100
2	BH	256/361 (71%)	239 (93%)	17 (7%)	0	100	100
2	CH	256/361 (71%)	247 (96%)	9 (4%)	0	100	100
2	DH	256/361 (71%)	244 (95%)	12 (5%)	0	100	100
2	EH	256/361 (71%)	245 (96%)	11 (4%)	0	100	100
2	FH	256/361 (71%)	246 (96%)	10 (4%)	0	100	100
2	GH	256/361 (71%)	246 (96%)	10 (4%)	0	100	100
2	HH	256/361 (71%)	247 (96%)	9 (4%)	0	100	100
2	IH	256/361 (71%)	240 (94%)	16 (6%)	0	100	100
2	JH	256/361 (71%)	242 (94%)	14 (6%)	0	100	100
2	KH	256/361 (71%)	242 (94%)	14 (6%)	0	100	100
2	LH	256/361 (71%)	243 (95%)	13 (5%)	0	100	100
2	MH	256/361 (71%)	240 (94%)	16 (6%)	0	100	100
2	VH	239/361 (66%)	229 (96%)	10 (4%)	0	100	100
2	WH	239/361 (66%)	232 (97%)	7 (3%)	0	100	100
2	XH	239/361 (66%)	232 (97%)	7 (3%)	0	100	100
2	YH	239/361 (66%)	231 (97%)	8 (3%)	0	100	100
2	ZH	239/361 (66%)	231 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AK	149/189 (79%)	140 (94%)	9 (6%)	0	100	100
3	BK	149/189 (79%)	145 (97%)	4 (3%)	0	100	100
3	CK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
3	DK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
3	EK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
3	FK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
3	GK	149/189 (79%)	143 (96%)	6 (4%)	0	100	100
3	HK	149/189 (79%)	143 (96%)	6 (4%)	0	100	100
3	IK	149/189 (79%)	143 (96%)	6 (4%)	0	100	100
3	JK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
3	KK	149/189 (79%)	142 (95%)	7 (5%)	0	100	100
3	LK	149/189 (79%)	143 (96%)	6 (4%)	0	100	100
3	MK	149/189 (79%)	142 (95%)	7 (5%)	0	100	100
4	AL	169/249 (68%)	160 (95%)	9 (5%)	0	100	100
4	BL	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
4	CL	169/249 (68%)	163 (96%)	6 (4%)	0	100	100
4	DL	169/249 (68%)	163 (96%)	6 (4%)	0	100	100
4	EL	169/249 (68%)	160 (95%)	9 (5%)	0	100	100
4	FL	169/249 (68%)	162 (96%)	7 (4%)	0	100	100
4	GL	169/249 (68%)	164 (97%)	5 (3%)	0	100	100
4	HL	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
4	IL	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
4	JL	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
4	KL	169/249 (68%)	165 (98%)	4 (2%)	0	100	100
4	LL	169/249 (68%)	162 (96%)	7 (4%)	0	100	100
4	ML	169/249 (68%)	164 (97%)	5 (3%)	0	100	100
5	AM	206/320 (64%)	189 (92%)	17 (8%)	0	100	100
5	BM	206/320 (64%)	193 (94%)	13 (6%)	0	100	100
5	CM	206/320 (64%)	191 (93%)	15 (7%)	0	100	100
5	DM	206/320 (64%)	194 (94%)	12 (6%)	0	100	100
5	EM	206/320 (64%)	189 (92%)	17 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	FM	206/320 (64%)	193 (94%)	13 (6%)	0	100	100
5	GM	206/320 (64%)	194 (94%)	12 (6%)	0	100	100
5	HM	206/320 (64%)	191 (93%)	15 (7%)	0	100	100
5	IM	206/320 (64%)	192 (93%)	14 (7%)	0	100	100
5	JM	206/320 (64%)	191 (93%)	15 (7%)	0	100	100
5	KM	206/320 (64%)	191 (93%)	15 (7%)	0	100	100
5	LM	206/320 (64%)	197 (96%)	9 (4%)	0	100	100
5	MM	206/320 (64%)	195 (95%)	11 (5%)	0	100	100
6	AN	76/124 (61%)	71 (93%)	5 (7%)	0	100	100
6	BN	76/124 (61%)	69 (91%)	7 (9%)	0	100	100
6	CN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
6	DN	76/124 (61%)	70 (92%)	6 (8%)	0	100	100
6	EN	76/124 (61%)	72 (95%)	4 (5%)	0	100	100
6	FN	76/124 (61%)	69 (91%)	7 (9%)	0	100	100
6	GN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
6	HN	76/124 (61%)	70 (92%)	6 (8%)	0	100	100
6	IN	76/124 (61%)	72 (95%)	4 (5%)	0	100	100
6	JN	76/124 (61%)	73 (96%)	3 (4%)	0	100	100
6	KN	76/124 (61%)	69 (91%)	7 (9%)	0	100	100
6	LN	76/124 (61%)	67 (88%)	9 (12%)	0	100	100
6	MN	76/124 (61%)	73 (96%)	3 (4%)	0	100	100
9	AD	138/163 (85%)	131 (95%)	7 (5%)	0	100	100
9	Ad	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
9	BD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
9	Bd	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
9	CD	138/163 (85%)	132 (96%)	6 (4%)	0	100	100
9	Cd	135/163 (83%)	127 (94%)	8 (6%)	0	100	100
9	DD	138/163 (85%)	132 (96%)	6 (4%)	0	100	100
9	Dd	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
9	ED	138/163 (85%)	133 (96%)	5 (4%)	0	100	100
9	Ed	135/163 (83%)	130 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	FD	138/163 (85%)	132 (96%)	6 (4%)	0	100	100
9	Fd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
9	GD	138/163 (85%)	132 (96%)	6 (4%)	0	100	100
9	Gd	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
9	HD	138/163 (85%)	135 (98%)	3 (2%)	0	100	100
9	Hd	135/163 (83%)	127 (94%)	8 (6%)	0	100	100
9	ID	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
9	Id	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
9	JD	138/163 (85%)	130 (94%)	8 (6%)	0	100	100
9	Jd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
9	KD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
9	Kd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
9	LD	138/163 (85%)	130 (94%)	8 (6%)	0	100	100
9	Ld	135/163 (83%)	126 (93%)	9 (7%)	0	100	100
9	MD	138/163 (85%)	131 (95%)	7 (5%)	0	100	100
9	Md	135/163 (83%)	127 (94%)	8 (6%)	0	100	100
10	AF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
10	Af	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
10	BF	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
10	Bf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
10	CF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
10	Cf	57/269 (21%)	50 (88%)	7 (12%)	0	100	100
10	DF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
10	Df	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
10	EF	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
10	Ef	57/269 (21%)	51 (90%)	6 (10%)	0	100	100
10	FF	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
10	Ff	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
10	GF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
10	Gf	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
10	HF	61/269 (23%)	59 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	Hf	57/269 (21%)	52 (91%)	5 (9%)	0	100	100
10	IF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
10	If	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
10	JF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
10	Jf	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
10	KF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
10	Kf	57/269 (21%)	52 (91%)	5 (9%)	0	100	100
10	LF	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
10	Lf	57/269 (21%)	52 (91%)	5 (9%)	0	100	100
10	MF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
10	Mf	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
10	VF	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
10	WF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
10	XF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
10	YF	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
10	ZF	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
11	AC	241/303 (80%)	231 (96%)	10 (4%)	0	100	100
11	BC	241/303 (80%)	236 (98%)	5 (2%)	0	100	100
11	CC	207/303 (68%)	191 (92%)	16 (8%)	0	100	100
11	DC	207/303 (68%)	196 (95%)	11 (5%)	0	100	100
11	EC	207/303 (68%)	198 (96%)	9 (4%)	0	100	100
11	FC	241/303 (80%)	231 (96%)	10 (4%)	0	100	100
11	GC	207/303 (68%)	196 (95%)	11 (5%)	0	100	100
11	HC	207/303 (68%)	196 (95%)	11 (5%)	0	100	100
11	IC	207/303 (68%)	189 (91%)	18 (9%)	0	100	100
11	JC	241/303 (80%)	229 (95%)	12 (5%)	0	100	100
11	KC	207/303 (68%)	195 (94%)	12 (6%)	0	100	100
11	LC	207/303 (68%)	195 (94%)	12 (6%)	0	100	100
11	MC	207/303 (68%)	192 (93%)	15 (7%)	0	100	100
All	All	23690/70112 (34%)	22525 (95%)	1165 (5%)	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	AG	135/765 (18%)	113 (84%)	22 (16%)	2	14
1	Ag	31/765 (4%)	24 (77%)	7 (23%)	1	6
1	BG	135/765 (18%)	120 (89%)	15 (11%)	6	25
1	Bg	31/765 (4%)	24 (77%)	7 (23%)	1	6
1	CG	135/765 (18%)	120 (89%)	15 (11%)	6	25
1	Cg	31/765 (4%)	26 (84%)	5 (16%)	2	15
1	DG	135/765 (18%)	116 (86%)	19 (14%)	3	18
1	Dg	31/765 (4%)	27 (87%)	4 (13%)	4	20
1	EG	135/765 (18%)	121 (90%)	14 (10%)	7	27
1	Eg	31/765 (4%)	29 (94%)	2 (6%)	17	44
1	FG	135/765 (18%)	118 (87%)	17 (13%)	4	21
1	Fg	31/765 (4%)	30 (97%)	1 (3%)	39	62
1	GG	135/765 (18%)	120 (89%)	15 (11%)	6	25
1	Gg	31/765 (4%)	28 (90%)	3 (10%)	8	29
1	HG	135/765 (18%)	115 (85%)	20 (15%)	3	17
1	Hg	31/765 (4%)	25 (81%)	6 (19%)	1	9
1	IG	135/765 (18%)	121 (90%)	14 (10%)	7	27
1	Ig	31/765 (4%)	26 (84%)	5 (16%)	2	15
1	JG	135/765 (18%)	122 (90%)	13 (10%)	8	29
1	Jg	31/765 (4%)	25 (81%)	6 (19%)	1	9
1	KG	135/765 (18%)	123 (91%)	12 (9%)	9	33
1	Kg	31/765 (4%)	25 (81%)	6 (19%)	1	9
1	LG	135/765 (18%)	115 (85%)	20 (15%)	3	17
1	Lg	31/765 (4%)	27 (87%)	4 (13%)	4	20
1	MG	135/765 (18%)	114 (84%)	21 (16%)	2	16
1	Mg	31/765 (4%)	25 (81%)	6 (19%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	NG	135/765 (18%)	114 (84%)	21 (16%)	2	16
1	OG	135/765 (18%)	112 (83%)	23 (17%)	2	13
1	PG	135/765 (18%)	114 (84%)	21 (16%)	2	16
1	VG	31/765 (4%)	24 (77%)	7 (23%)	1	6
1	WG	31/765 (4%)	23 (74%)	8 (26%)	0	4
1	XG	31/765 (4%)	24 (77%)	7 (23%)	1	6
1	YG	31/765 (4%)	28 (90%)	3 (10%)	8	29
1	ZG	31/765 (4%)	30 (97%)	1 (3%)	39	62
2	AH	220/300 (73%)	192 (87%)	28 (13%)	4	21
2	BH	220/300 (73%)	194 (88%)	26 (12%)	5	23
2	CH	220/300 (73%)	198 (90%)	22 (10%)	7	28
2	DH	220/300 (73%)	196 (89%)	24 (11%)	6	25
2	EH	220/300 (73%)	190 (86%)	30 (14%)	3	19
2	FH	220/300 (73%)	193 (88%)	27 (12%)	4	22
2	GH	220/300 (73%)	199 (90%)	21 (10%)	8	29
2	HH	220/300 (73%)	203 (92%)	17 (8%)	13	39
2	IH	220/300 (73%)	198 (90%)	22 (10%)	7	28
2	JH	220/300 (73%)	192 (87%)	28 (13%)	4	21
2	KH	220/300 (73%)	200 (91%)	20 (9%)	9	31
2	LH	220/300 (73%)	196 (89%)	24 (11%)	6	25
2	MH	220/300 (73%)	193 (88%)	27 (12%)	4	22
2	VH	207/300 (69%)	182 (88%)	25 (12%)	5	22
2	WH	207/300 (69%)	182 (88%)	25 (12%)	5	22
2	XH	207/300 (69%)	183 (88%)	24 (12%)	5	23
2	YH	207/300 (69%)	181 (87%)	26 (13%)	4	21
2	ZH	207/300 (69%)	179 (86%)	28 (14%)	4	19
3	AK	129/163 (79%)	114 (88%)	15 (12%)	5	23
3	BK	129/163 (79%)	112 (87%)	17 (13%)	4	20
3	CK	129/163 (79%)	114 (88%)	15 (12%)	5	23
3	DK	129/163 (79%)	121 (94%)	8 (6%)	18	45
3	EK	129/163 (79%)	118 (92%)	11 (8%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	FK	129/163 (79%)	117 (91%)	12 (9%)	9	30
3	GK	129/163 (79%)	117 (91%)	12 (9%)	9	30
3	HK	129/163 (79%)	117 (91%)	12 (9%)	9	30
3	IK	129/163 (79%)	117 (91%)	12 (9%)	9	30
3	JK	129/163 (79%)	116 (90%)	13 (10%)	7	27
3	KK	129/163 (79%)	111 (86%)	18 (14%)	3	19
3	LK	129/163 (79%)	117 (91%)	12 (9%)	9	30
3	MK	129/163 (79%)	110 (85%)	19 (15%)	3	17
4	AL	148/203 (73%)	137 (93%)	11 (7%)	13	40
4	BL	148/203 (73%)	129 (87%)	19 (13%)	4	21
4	CL	148/203 (73%)	137 (93%)	11 (7%)	13	40
4	DL	148/203 (73%)	134 (90%)	14 (10%)	8	29
4	EL	148/203 (73%)	132 (89%)	16 (11%)	6	26
4	FL	148/203 (73%)	132 (89%)	16 (11%)	6	26
4	GL	148/203 (73%)	130 (88%)	18 (12%)	5	22
4	HL	148/203 (73%)	136 (92%)	12 (8%)	11	37
4	IL	148/203 (73%)	137 (93%)	11 (7%)	13	40
4	JL	148/203 (73%)	137 (93%)	11 (7%)	13	40
4	KL	148/203 (73%)	132 (89%)	16 (11%)	6	26
4	LL	148/203 (73%)	140 (95%)	8 (5%)	22	49
4	ML	148/203 (73%)	138 (93%)	10 (7%)	16	42
5	AM	175/276 (63%)	144 (82%)	31 (18%)	2	12
5	BM	175/276 (63%)	155 (89%)	20 (11%)	5	24
5	CM	175/276 (63%)	150 (86%)	25 (14%)	3	18
5	DM	175/276 (63%)	156 (89%)	19 (11%)	6	25
5	EM	175/276 (63%)	152 (87%)	23 (13%)	4	20
5	FM	175/276 (63%)	150 (86%)	25 (14%)	3	18
5	GM	175/276 (63%)	144 (82%)	31 (18%)	2	12
5	HM	175/276 (63%)	152 (87%)	23 (13%)	4	20
5	IM	175/276 (63%)	158 (90%)	17 (10%)	8	29
5	JM	175/276 (63%)	150 (86%)	25 (14%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	KM	175/276 (63%)	153 (87%)	22 (13%)	4	21
5	LM	175/276 (63%)	155 (89%)	20 (11%)	5	24
5	MM	175/276 (63%)	155 (89%)	20 (11%)	5	24
6	AN	66/107 (62%)	55 (83%)	11 (17%)	2	14
6	BN	66/107 (62%)	53 (80%)	13 (20%)	1	9
6	CN	66/107 (62%)	54 (82%)	12 (18%)	1	11
6	DN	66/107 (62%)	56 (85%)	10 (15%)	3	16
6	EN	66/107 (62%)	58 (88%)	8 (12%)	5	22
6	FN	66/107 (62%)	61 (92%)	5 (8%)	13	39
6	GN	66/107 (62%)	55 (83%)	11 (17%)	2	14
6	HN	66/107 (62%)	57 (86%)	9 (14%)	3	19
6	IN	66/107 (62%)	56 (85%)	10 (15%)	3	16
6	JN	66/107 (62%)	55 (83%)	11 (17%)	2	14
6	KN	66/107 (62%)	55 (83%)	11 (17%)	2	14
6	LN	66/107 (62%)	59 (89%)	7 (11%)	6	26
6	MN	66/107 (62%)	54 (82%)	12 (18%)	1	11
9	AD	121/139 (87%)	112 (93%)	9 (7%)	13	40
9	Ad	118/139 (85%)	106 (90%)	12 (10%)	7	27
9	BD	121/139 (87%)	111 (92%)	10 (8%)	11	36
9	Bd	118/139 (85%)	105 (89%)	13 (11%)	6	25
9	CD	121/139 (87%)	106 (88%)	15 (12%)	4	21
9	Cd	118/139 (85%)	103 (87%)	15 (13%)	4	21
9	DD	121/139 (87%)	110 (91%)	11 (9%)	9	31
9	Dd	118/139 (85%)	105 (89%)	13 (11%)	6	25
9	ED	121/139 (87%)	111 (92%)	10 (8%)	11	36
9	Ed	118/139 (85%)	107 (91%)	11 (9%)	9	30
9	FD	121/139 (87%)	110 (91%)	11 (9%)	9	31
9	Fd	118/139 (85%)	109 (92%)	9 (8%)	13	39
9	GD	121/139 (87%)	104 (86%)	17 (14%)	3	19
9	Gd	118/139 (85%)	106 (90%)	12 (10%)	7	27
9	HD	121/139 (87%)	110 (91%)	11 (9%)	9	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	Hd	118/139 (85%)	109 (92%)	9 (8%)	13	39
9	ID	121/139 (87%)	111 (92%)	10 (8%)	11	36
9	Id	118/139 (85%)	108 (92%)	10 (8%)	10	36
9	JD	121/139 (87%)	112 (93%)	9 (7%)	13	40
9	Jd	118/139 (85%)	110 (93%)	8 (7%)	16	42
9	KD	121/139 (87%)	110 (91%)	11 (9%)	9	31
9	Kd	118/139 (85%)	107 (91%)	11 (9%)	9	30
9	LD	121/139 (87%)	105 (87%)	16 (13%)	4	20
9	Ld	118/139 (85%)	105 (89%)	13 (11%)	6	25
9	MD	121/139 (87%)	114 (94%)	7 (6%)	20	47
9	Md	118/139 (85%)	102 (86%)	16 (14%)	3	19
10	AF	53/237 (22%)	46 (87%)	7 (13%)	4	20
10	Af	49/237 (21%)	44 (90%)	5 (10%)	7	27
10	BF	53/237 (22%)	47 (89%)	6 (11%)	6	24
10	Bf	49/237 (21%)	43 (88%)	6 (12%)	5	22
10	CF	53/237 (22%)	47 (89%)	6 (11%)	6	24
10	Cf	49/237 (21%)	42 (86%)	7 (14%)	3	18
10	DF	53/237 (22%)	46 (87%)	7 (13%)	4	20
10	Df	49/237 (21%)	41 (84%)	8 (16%)	2	14
10	EF	53/237 (22%)	45 (85%)	8 (15%)	3	16
10	Ef	49/237 (21%)	44 (90%)	5 (10%)	7	27
10	FF	53/237 (22%)	47 (89%)	6 (11%)	6	24
10	Ff	49/237 (21%)	42 (86%)	7 (14%)	3	18
10	GF	53/237 (22%)	48 (91%)	5 (9%)	8	30
10	Gf	49/237 (21%)	44 (90%)	5 (10%)	7	27
10	HF	53/237 (22%)	47 (89%)	6 (11%)	6	24
10	Hf	49/237 (21%)	46 (94%)	3 (6%)	18	46
10	IF	53/237 (22%)	48 (91%)	5 (9%)	8	30
10	If	49/237 (21%)	43 (88%)	6 (12%)	5	22
10	JF	53/237 (22%)	49 (92%)	4 (8%)	13	40
10	Jf	49/237 (21%)	44 (90%)	5 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	KF	53/237 (22%)	45 (85%)	8 (15%)	3	16
10	Kf	49/237 (21%)	43 (88%)	6 (12%)	5	22
10	LF	53/237 (22%)	46 (87%)	7 (13%)	4	20
10	Lf	49/237 (21%)	47 (96%)	2 (4%)	30	56
10	MF	53/237 (22%)	47 (89%)	6 (11%)	6	24
10	Mf	49/237 (21%)	42 (86%)	7 (14%)	3	18
10	VF	53/237 (22%)	49 (92%)	4 (8%)	13	40
10	WF	53/237 (22%)	47 (89%)	6 (11%)	6	24
10	XF	53/237 (22%)	47 (89%)	6 (11%)	6	24
10	YF	53/237 (22%)	47 (89%)	6 (11%)	6	24
10	ZF	53/237 (22%)	50 (94%)	3 (6%)	20	47
11	AC	203/257 (79%)	181 (89%)	22 (11%)	6	26
11	BC	203/257 (79%)	180 (89%)	23 (11%)	6	24
11	CC	178/257 (69%)	156 (88%)	22 (12%)	4	21
11	DC	178/257 (69%)	158 (89%)	20 (11%)	6	24
11	EC	178/257 (69%)	157 (88%)	21 (12%)	5	23
11	FC	203/257 (79%)	181 (89%)	22 (11%)	6	26
11	GC	178/257 (69%)	158 (89%)	20 (11%)	6	24
11	HC	178/257 (69%)	154 (86%)	24 (14%)	4	19
11	IC	178/257 (69%)	158 (89%)	20 (11%)	6	24
11	JC	203/257 (79%)	176 (87%)	27 (13%)	4	20
11	KC	178/257 (69%)	165 (93%)	13 (7%)	14	40
11	LC	178/257 (69%)	160 (90%)	18 (10%)	7	27
11	MC	178/257 (69%)	152 (85%)	26 (15%)	3	17
All	All	20459/55449 (37%)	18110 (88%)	2349 (12%)	9	23

All (2349) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AG	865	THR
1	AG	869	MET
1	AG	873	LEU
1	AG	886	LEU
1	AG	898	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AG	904	ASN
1	AG	911	LYS
1	AG	913	VAL
1	AG	916	PHE
1	AG	930	ILE
1	AG	935	ILE
1	AG	936	ASP
1	AG	939	THR
1	AG	944	LEU
1	AG	956	TYR
1	AG	962	SER
1	AG	965	LEU
1	AG	968	PHE
1	AG	972	PHE
1	AG	1010	THR
1	AG	1037	LEU
1	AG	1045	VAL
2	EH	107	ILE
2	EH	108	ASP
2	EH	109	LYS
2	EH	115	MET
2	EH	134	TYR
2	EH	147	THR
2	EH	154	THR
2	EH	170	ARG
2	EH	180	VAL
2	EH	183	ASP
2	EH	184	SER
2	EH	208	LYS
2	EH	219	LYS
2	EH	221	TYR
2	EH	233	LEU
2	EH	240	THR
2	EH	248	VAL
2	EH	253	ASP
2	EH	256	VAL
2	EH	266	MET
2	EH	278	ASP
2	EH	287	VAL
2	EH	294	ARG
2	EH	296	VAL
2	EH	306	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	EH	316	ASN
2	EH	332	ASP
2	EH	342	SER
2	EH	344	VAL
2	EH	352	LYS
3	EK	50	ASP
3	EK	60	LEU
3	EK	70	VAL
3	EK	88	SER
3	EK	92	ASN
3	EK	111	LYS
3	EK	152	ARG
3	EK	156	THR
3	EK	162	ASP
3	EK	163	LYS
3	EK	183	THR
4	EL	57	VAL
4	EL	103	ARG
4	EL	104	LYS
4	EL	108	ASP
4	EL	109	LEU
4	EL	125	LEU
4	EL	130	ASP
4	EL	142	GLU
4	EL	169	THR
4	EL	172	VAL
4	EL	177	HIS
4	EL	204	LYS
4	EL	210	ASP
4	EL	211	LYS
4	EL	212	ASN
4	EL	225	GLN
5	EM	127	ASN
5	EM	136	LEU
5	EM	146	LEU
5	EM	152	LEU
5	EM	162	VAL
5	EM	171	ARG
5	EM	173	LEU
5	EM	176	VAL
5	EM	178	LYS
5	EM	184	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	EM	185	ILE
5	EM	204	LEU
5	EM	212	LEU
5	EM	221	LYS
5	EM	222	ILE
5	EM	229	ASN
5	EM	231	LEU
5	EM	232	ASP
5	EM	242	LYS
5	EM	263	ILE
5	EM	271	SER
5	EM	292	MET
5	EM	310	LYS
6	EN	57	ARG
6	EN	69	TYR
6	EN	78	LEU
6	EN	81	LEU
6	EN	84	CYS
6	EN	108	VAL
6	EN	111	GLU
6	EN	116	LYS
9	Ed	41	LEU
9	Ed	61	VAL
9	Ed	63	THR
9	Ed	70	THR
9	Ed	105	ARG
9	Ed	115	VAL
9	Ed	121	ILE
9	Ed	126	GLU
9	Ed	128	LEU
9	Ed	145	ILE
9	Ed	147	VAL
10	Ef	213	GLN
10	Ef	215	VAL
10	Ef	232	VAL
10	Ef	245	LYS
10	Ef	255	LEU
9	FD	23	MET
9	FD	51	SER
9	FD	61	VAL
9	FD	71	LEU
9	FD	73	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	FD	92	GLU
9	FD	108	VAL
9	FD	128	LEU
9	FD	141	LYS
9	FD	150	ASN
9	FD	156	LEU
10	FF	215	VAL
10	FF	231	THR
10	FF	233	ARG
10	FF	238	ILE
10	FF	256	THR
10	FF	261	VAL
1	Fg	814	GLN
2	FH	108	ASP
2	FH	109	LYS
2	FH	147	THR
2	FH	152	THR
2	FH	180	VAL
2	FH	202	PHE
2	FH	208	LYS
2	FH	209	THR
2	FH	213	LEU
2	FH	218	THR
2	FH	225	ASN
2	FH	237	VAL
2	FH	238	MET
2	FH	239	LEU
2	FH	240	THR
2	FH	241	LEU
2	FH	249	ASP
2	FH	253	ASP
2	FH	256	VAL
2	FH	266	MET
2	FH	268	THR
2	FH	278	ASP
2	FH	287	VAL
2	FH	296	VAL
2	FH	313	VAL
2	FH	341	LYS
2	FH	344	VAL
3	FK	46	ASP
3	FK	70	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	FK	92	ASN
3	FK	111	LYS
3	FK	149	VAL
3	FK	156	THR
3	FK	162	ASP
3	FK	169	THR
3	FK	177	ASN
3	FK	180	VAL
3	FK	182	ILE
3	FK	183	THR
4	FL	53	ASP
4	FL	63	ASP
4	FL	93	LEU
4	FL	108	ASP
4	FL	109	LEU
4	FL	121	ASP
4	FL	130	ASP
4	FL	133	PHE
4	FL	155	LEU
4	FL	163	ILE
4	FL	165	VAL
4	FL	172	VAL
4	FL	174	SER
4	FL	190	MET
4	FL	212	ASN
4	FL	219	ILE
5	FM	115	ARG
5	FM	129	LEU
5	FM	130	ARG
5	FM	134	LEU
5	FM	146	LEU
5	FM	149	ASN
5	FM	152	LEU
5	FM	173	LEU
5	FM	174	GLN
5	FM	175	ILE
5	FM	176	VAL
5	FM	180	ASP
5	FM	182	LYS
5	FM	191	LEU
5	FM	192	ARG
5	FM	194	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	FM	202	LEU
5	FM	207	ILE
5	FM	212	LEU
5	FM	215	ARG
5	FM	228	VAL
5	FM	231	LEU
5	FM	245	TYR
5	FM	271	SER
5	FM	292	MET
6	FN	48	ILE
6	FN	81	LEU
6	FN	84	CYS
6	FN	94	GLN
6	FN	95	LEU
9	Fd	41	LEU
9	Fd	53	LEU
9	Fd	59	GLU
9	Fd	61	VAL
9	Fd	63	THR
9	Fd	82	ARG
9	Fd	115	VAL
9	Fd	150	ASN
9	Fd	153	VAL
10	Ff	213	GLN
10	Ff	215	VAL
10	Ff	219	ARG
10	Ff	232	VAL
10	Ff	243	MET
10	Ff	244	VAL
10	Ff	264	PHE
11	BC	28	THR
11	BC	35	GLN
11	BC	48	LYS
11	BC	49	GLN
11	BC	54	ILE
11	BC	56	GLU
11	BC	59	LEU
11	BC	83	LEU
11	BC	85	LYS
11	BC	89	ASN
11	BC	91	ASP
11	BC	99	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	BC	112	GLU
11	BC	165	LEU
11	BC	169	THR
11	BC	184	TRP
11	BC	195	LEU
11	BC	226	VAL
11	BC	230	ASP
11	BC	239	GLU
11	BC	249	ILE
11	BC	256	ASN
11	BC	266	VAL
10	AF	208	ILE
10	AF	211	TYR
10	AF	215	VAL
10	AF	238	ILE
10	AF	250	LEU
10	AF	256	THR
10	AF	263	LYS
9	GD	23	MET
9	GD	24	LYS
9	GD	35	ASP
9	GD	41	LEU
9	GD	51	SER
9	GD	53	LEU
9	GD	55	MET
9	GD	67	LYS
9	GD	73	ILE
9	GD	85	VAL
9	GD	108	VAL
9	GD	109	LEU
9	GD	124	LYS
9	GD	127	SER
9	GD	138	GLN
9	GD	154	VAL
9	GD	156	LEU
10	GF	208	ILE
10	GF	215	VAL
10	GF	245	LYS
10	GF	250	LEU
10	GF	256	THR
1	Gg	798	THR
1	Gg	801	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Gg	814	GLN
1	BG	865	THR
1	BG	867	ASP
1	BG	869	MET
1	BG	898	LYS
1	BG	913	VAL
1	BG	916	PHE
1	BG	930	ILE
1	BG	933	TYR
1	BG	936	ASP
1	BG	944	LEU
1	BG	962	SER
1	BG	965	LEU
1	BG	972	PHE
1	BG	1010	THR
1	BG	1040	LEU
2	GH	134	TYR
2	GH	147	THR
2	GH	184	SER
2	GH	185	THR
2	GH	207	ASP
2	GH	225	ASN
2	GH	233	LEU
2	GH	234	ASN
2	GH	237	VAL
2	GH	238	MET
2	GH	248	VAL
2	GH	250	TYR
2	GH	253	ASP
2	GH	265	SER
2	GH	278	ASP
2	GH	280	LEU
2	GH	313	VAL
2	GH	327	SER
2	GH	329	THR
2	GH	334	THR
2	GH	361	LEU
3	GK	50	ASP
3	GK	60	LEU
3	GK	67	VAL
3	GK	83	LEU
3	GK	92	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	GK	93	TRP
3	GK	99	LEU
3	GK	111	LYS
3	GK	129	GLU
3	GK	156	THR
3	GK	170	LEU
3	GK	183	THR
4	GL	49	ASN
4	GL	53	ASP
4	GL	57	VAL
4	GL	96	SER
4	GL	99	ARG
4	GL	109	LEU
4	GL	110	GLN
4	GL	115	GLN
4	GL	125	LEU
4	GL	129	THR
4	GL	130	ASP
4	GL	133	PHE
4	GL	140	LEU
4	GL	155	LEU
4	GL	163	ILE
4	GL	174	SER
4	GL	217	ASN
4	GL	227	ARG
5	GM	127	ASN
5	GM	130	ARG
5	GM	131	THR
5	GM	134	LEU
5	GM	145	ARG
5	GM	146	LEU
5	GM	149	ASN
5	GM	152	LEU
5	GM	154	LYS
5	GM	171	ARG
5	GM	173	LEU
5	GM	182	LYS
5	GM	183	VAL
5	GM	184	LEU
5	GM	190	ASN
5	GM	192	ARG
5	GM	202	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	GM	210	ASP
5	GM	215	ARG
5	GM	221	LYS
5	GM	228	VAL
5	GM	245	TYR
5	GM	263	ILE
5	GM	266	VAL
5	GM	275	ASP
5	GM	287	THR
5	GM	292	MET
5	GM	301	MET
5	GM	303	GLU
5	GM	312	PHE
5	GM	316	ASN
6	GN	48	ILE
6	GN	70	CYS
6	GN	75	VAL
6	GN	81	LEU
6	GN	91	VAL
6	GN	94	GLN
6	GN	95	LEU
6	GN	100	LEU
6	GN	101	VAL
6	GN	111	GLU
6	GN	112	CYS
9	Gd	31	ASN
9	Gd	50	ASP
9	Gd	53	LEU
9	Gd	61	VAL
9	Gd	63	THR
9	Gd	78	ASN
9	Gd	82	ARG
9	Gd	92	GLU
9	Gd	108	VAL
9	Gd	128	LEU
9	Gd	147	VAL
9	Gd	150	ASN
10	Gf	211	TYR
10	Gf	215	VAL
10	Gf	236	SER
10	Gf	244	VAL
10	Gf	264	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	HD	30	ILE
9	HD	50	ASP
9	HD	52	MET
9	HD	59	GLU
9	HD	108	VAL
9	HD	115	VAL
9	HD	126	GLU
9	HD	154	VAL
9	HD	156	LEU
9	HD	160	LYS
9	HD	162	TYR
10	HF	215	VAL
10	HF	230	LEU
10	HF	238	ILE
10	HF	246	LEU
10	HF	250	LEU
10	HF	256	THR
1	Hg	793	GLU
1	Hg	794	ILE
1	Hg	801	MET
1	Hg	803	THR
1	Hg	814	GLN
1	Hg	819	VAL
2	HH	108	ASP
2	HH	125	GLU
2	HH	138	GLU
2	HH	170	ARG
2	HH	180	VAL
2	HH	203	ASN
2	HH	204	ILE
2	HH	218	THR
2	HH	225	ASN
2	HH	226	LEU
2	HH	238	MET
2	HH	240	THR
2	HH	241	LEU
2	HH	248	VAL
2	HH	249	ASP
2	HH	253	ASP
2	HH	313	VAL
3	HK	40	LYS
3	HK	63	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	HK	67	VAL
3	HK	70	VAL
3	HK	92	ASN
3	HK	109	PHE
3	HK	111	LYS
3	HK	126	VAL
3	HK	129	GLU
3	HK	149	VAL
3	HK	156	THR
3	HK	173	ASP
4	HL	53	ASP
4	HL	101	SER
4	HL	113	ASP
4	HL	130	ASP
4	HL	154	LEU
4	HL	177	HIS
4	HL	182	SER
4	HL	193	LEU
4	HL	210	ASP
4	HL	212	ASN
4	HL	225	GLN
4	HL	227	ARG
5	HM	129	LEU
5	HM	134	LEU
5	HM	146	LEU
5	HM	149	ASN
5	HM	152	LEU
5	HM	176	VAL
5	HM	180	ASP
5	HM	181	PRO
5	HM	183	VAL
5	HM	184	LEU
5	HM	191	LEU
5	HM	192	ARG
5	HM	201	THR
5	HM	207	ILE
5	HM	215	ARG
5	HM	245	TYR
5	HM	267	ASN
5	HM	271	SER
5	HM	290	ASP
5	HM	292	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	HM	301	MET
5	HM	313	ASP
5	HM	316	ASN
6	HN	62	ASN
6	HN	84	CYS
6	HN	91	VAL
6	HN	95	LEU
6	HN	100	LEU
6	HN	101	VAL
6	HN	102	VAL
6	HN	114	LEU
6	HN	115	GLN
9	Hd	31	ASN
9	Hd	36	ASP
9	Hd	61	VAL
9	Hd	63	THR
9	Hd	91	ILE
9	Hd	115	VAL
9	Hd	147	VAL
9	Hd	150	ASN
9	Hd	154	VAL
10	Hf	215	VAL
10	Hf	244	VAL
10	Hf	262	ILE
1	Bg	797	ARG
1	Bg	802	LEU
1	Bg	808	LEU
1	Bg	815	VAL
1	Bg	816	GLU
1	Bg	817	THR
1	Bg	819	VAL
9	ID	26	LYS
9	ID	32	ASN
9	ID	35	ASP
9	ID	55	MET
9	ID	115	VAL
9	ID	118	LEU
9	ID	121	ILE
9	ID	125	ASP
9	ID	134	ASP
9	ID	147	VAL
10	IF	215	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	IF	232	VAL
10	IF	233	ARG
10	IF	238	ILE
10	IF	250	LEU
1	Ig	795	GLN
1	Ig	808	LEU
1	Ig	814	GLN
1	Ig	815	VAL
1	Ig	819	VAL
2	IH	115	MET
2	IH	123	ASN
2	IH	136	THR
2	IH	147	THR
2	IH	180	VAL
2	IH	185	THR
2	IH	203	ASN
2	IH	211	ASN
2	IH	221	TYR
2	IH	223	TYR
2	IH	234	ASN
2	IH	240	THR
2	IH	245	GLN
2	IH	248	VAL
2	IH	250	TYR
2	IH	253	ASP
2	IH	262	ASN
2	IH	278	ASP
2	IH	313	VAL
2	IH	344	VAL
2	IH	353	VAL
2	IH	361	LEU
1	CG	865	THR
1	CG	898	LYS
1	CG	900	ILE
1	CG	904	ASN
1	CG	905	LEU
1	CG	913	VAL
1	CG	916	PHE
1	CG	930	ILE
1	CG	944	LEU
1	CG	965	LEU
1	CG	972	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	CG	1010	THR
1	CG	1028	THR
1	CG	1037	LEU
1	CG	1045	VAL
3	IK	50	ASP
3	IK	70	VAL
3	IK	73	ASN
3	IK	75	LEU
3	IK	83	LEU
3	IK	92	ASN
3	IK	112	ILE
3	IK	126	VAL
3	IK	144	LEU
3	IK	156	THR
3	IK	162	ASP
3	IK	180	VAL
4	IL	54	ARG
4	IL	93	LEU
4	IL	100	ASP
4	IL	109	LEU
4	IL	130	ASP
4	IL	154	LEU
4	IL	163	ILE
4	IL	172	VAL
4	IL	174	SER
4	IL	177	HIS
4	IL	190	MET
5	IM	129	LEU
5	IM	146	LEU
5	IM	152	LEU
5	IM	160	ASN
5	IM	184	LEU
5	IM	188	PHE
5	IM	191	LEU
5	IM	192	ARG
5	IM	201	THR
5	IM	207	ILE
5	IM	229	ASN
5	IM	231	LEU
5	IM	255	THR
5	IM	274	THR
5	IM	292	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	IM	301	MET
5	IM	312	PHE
6	IN	45	MET
6	IN	48	ILE
6	IN	51	CYS
6	IN	81	LEU
6	IN	84	CYS
6	IN	91	VAL
6	IN	94	GLN
6	IN	101	VAL
6	IN	102	VAL
6	IN	114	LEU
9	Id	43	GLU
9	Id	59	GLU
9	Id	61	VAL
9	Id	73	ILE
9	Id	108	VAL
9	Id	115	VAL
9	Id	128	LEU
9	Id	141	LYS
9	Id	150	ASN
9	Id	153	VAL
10	If	215	VAL
10	If	238	ILE
10	If	244	VAL
10	If	255	LEU
10	If	257	SER
10	If	261	VAL
9	JD	50	ASP
9	JD	53	LEU
9	JD	71	LEU
9	JD	91	ILE
9	JD	92	GLU
9	JD	115	VAL
9	JD	138	GLN
9	JD	153	VAL
9	JD	156	LEU
10	JF	215	VAL
10	JF	216	ILE
10	JF	231	THR
10	JF	238	ILE
1	Jg	792	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Jg	793	GLU
1	Jg	802	LEU
1	Jg	808	LEU
1	Jg	814	GLN
1	Jg	819	VAL
2	JH	108	ASP
2	JH	115	MET
2	JH	134	TYR
2	JH	139	TYR
2	JH	147	THR
2	JH	168	VAL
2	JH	170	ARG
2	JH	179	LEU
2	JH	180	VAL
2	JH	223	TYR
2	JH	240	THR
2	JH	241	LEU
2	JH	246	LYS
2	JH	248	VAL
2	JH	249	ASP
2	JH	253	ASP
2	JH	255	ARG
2	JH	266	MET
2	JH	270	GLU
2	JH	278	ASP
2	JH	279	LEU
2	JH	287	VAL
2	JH	294	ARG
2	JH	314	ARG
2	JH	319	ILE
2	JH	339	MET
2	JH	344	VAL
2	JH	353	VAL
3	JK	60	LEU
3	JK	67	VAL
3	JK	70	VAL
3	JK	83	LEU
3	JK	98	LEU
3	JK	111	LYS
3	JK	126	VAL
3	JK	149	VAL
3	JK	152	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	JK	156	THR
3	JK	157	GLN
3	JK	170	LEU
3	JK	180	VAL
4	JL	47	TYR
4	JL	53	ASP
4	JL	93	LEU
4	JL	129	THR
4	JL	130	ASP
4	JL	131	LYS
4	JL	133	PHE
4	JL	163	ILE
4	JL	172	VAL
4	JL	174	SER
4	JL	223	SER
5	JM	134	LEU
5	JM	135	ASP
5	JM	144	THR
5	JM	152	LEU
5	JM	162	VAL
5	JM	176	VAL
5	JM	178	LYS
5	JM	182	LYS
5	JM	184	LEU
5	JM	191	LEU
5	JM	197	TYR
5	JM	215	ARG
5	JM	221	LYS
5	JM	229	ASN
5	JM	233	VAL
5	JM	240	GLN
5	JM	245	TYR
5	JM	259	SER
5	JM	263	ILE
5	JM	277	SER
5	JM	292	MET
5	JM	301	MET
5	JM	303	GLU
5	JM	316	ASN
5	JM	318	GLN
6	JN	51	CYS
6	JN	59	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	JN	67	THR
6	JN	69	TYR
6	JN	78	LEU
6	JN	81	LEU
6	JN	94	GLN
6	JN	101	VAL
6	JN	102	VAL
6	JN	111	GLU
6	JN	115	GLN
9	Jd	41	LEU
9	Jd	61	VAL
9	Jd	63	THR
9	Jd	72	THR
9	Jd	93	GLU
9	Jd	108	VAL
9	Jd	115	VAL
9	Jd	123	THR
10	Jf	230	LEU
10	Jf	232	VAL
10	Jf	236	SER
10	Jf	246	LEU
10	Jf	263	LYS
2	AH	109	LYS
2	AH	114	ASP
2	AH	115	MET
2	AH	117	ARG
2	AH	132	GLN
2	AH	134	TYR
2	AH	147	THR
2	AH	156	GLN
2	AH	160	LEU
2	AH	170	ARG
2	AH	213	LEU
2	AH	233	LEU
2	AH	237	VAL
2	AH	238	MET
2	AH	240	THR
2	AH	248	VAL
2	AH	250	TYR
2	AH	253	ASP
2	AH	256	VAL
2	AH	262	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	AH	264	LYS
2	AH	280	LEU
2	AH	287	VAL
2	AH	296	VAL
2	AH	313	VAL
2	AH	342	SER
2	AH	350	HIS
2	AH	353	VAL
9	KD	30	ILE
9	KD	47	SER
9	KD	50	ASP
9	KD	55	MET
9	KD	63	THR
9	KD	72	THR
9	KD	85	VAL
9	KD	86	ASP
9	KD	108	VAL
9	KD	123	THR
9	KD	156	LEU
11	CC	61	GLU
11	CC	62	THR
11	CC	75	ARG
11	CC	89	ASN
11	CC	97	ASN
11	CC	102	GLU
11	CC	105	ILE
11	CC	116	THR
11	CC	125	ILE
11	CC	127	ILE
11	CC	140	PHE
11	CC	143	THR
11	CC	146	THR
11	CC	156	VAL
11	CC	184	TRP
11	CC	195	LEU
11	CC	214	LYS
11	CC	226	VAL
11	CC	234	THR
11	CC	247	LEU
11	CC	263	ARG
11	CC	266	VAL
10	KF	211	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	KF	215	VAL
10	KF	223	ILE
10	KF	230	LEU
10	KF	238	ILE
10	KF	261	VAL
10	KF	264	PHE
10	KF	266	GLN
1	Kg	796	GLN
1	Kg	801	MET
1	Kg	802	LEU
1	Kg	815	VAL
1	Kg	816	GLU
1	Kg	819	VAL
2	KH	105	GLU
2	KH	147	THR
2	KH	170	ARG
2	KH	180	VAL
2	KH	183	ASP
2	KH	195	ASP
2	KH	210	SER
2	KH	218	THR
2	KH	238	MET
2	KH	241	LEU
2	KH	248	VAL
2	KH	249	ASP
2	KH	250	TYR
2	KH	270	GLU
2	KH	287	VAL
2	KH	313	VAL
2	KH	329	THR
2	KH	332	ASP
2	KH	344	VAL
2	KH	346	LEU
1	DG	869	MET
1	DG	873	LEU
1	DG	893	LYS
1	DG	898	LYS
1	DG	900	ILE
1	DG	913	VAL
1	DG	916	PHE
1	DG	919	MET
1	DG	930	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	DG	944	LEU
1	DG	946	SER
1	DG	947	ARG
1	DG	962	SER
1	DG	965	LEU
1	DG	972	PHE
1	DG	1010	THR
1	DG	1017	GLN
1	DG	1027	THR
1	DG	1037	LEU
3	KK	40	LYS
3	KK	46	ASP
3	KK	50	ASP
3	KK	65	ILE
3	KK	67	VAL
3	KK	70	VAL
3	KK	76	ILE
3	KK	83	LEU
3	KK	100	ASN
3	KK	107	LYS
3	KK	111	LYS
3	KK	116	VAL
3	KK	126	VAL
3	KK	149	VAL
3	KK	156	THR
3	KK	162	ASP
3	KK	180	VAL
3	KK	182	ILE
4	KL	48	ASN
4	KL	57	VAL
4	KL	58	LYS
4	KL	59	ARG
4	KL	93	LEU
4	KL	100	ASP
4	KL	116	TYR
4	KL	129	THR
4	KL	130	ASP
4	KL	154	LEU
4	KL	162	THR
4	KL	165	VAL
4	KL	172	VAL
4	KL	201	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	KL	217	ASN
4	KL	227	ARG
5	KM	114	ASN
5	KM	123	VAL
5	KM	127	ASN
5	KM	131	THR
5	KM	134	LEU
5	KM	146	LEU
5	KM	173	LEU
5	KM	176	VAL
5	KM	183	VAL
5	KM	190	ASN
5	KM	191	LEU
5	KM	192	ARG
5	KM	202	LEU
5	KM	207	ILE
5	KM	212	LEU
5	KM	221	LYS
5	KM	222	ILE
5	KM	233	VAL
5	KM	259	SER
5	KM	277	SER
5	KM	292	MET
5	KM	308	ASP
6	KN	48	ILE
6	KN	65	TYR
6	KN	69	TYR
6	KN	70	CYS
6	KN	71	THR
6	KN	81	LEU
6	KN	84	CYS
6	KN	91	VAL
6	KN	94	GLN
6	KN	100	LEU
6	KN	114	LEU
9	Kd	36	ASP
9	Kd	55	MET
9	Kd	61	VAL
9	Kd	63	THR
9	Kd	68	ASP
9	Kd	69	ASN
9	Kd	93	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	Kd	111	LYS
9	Kd	123	THR
9	Kd	150	ASN
9	Kd	153	VAL
10	Kf	215	VAL
10	Kf	222	LEU
10	Kf	232	VAL
10	Kf	244	VAL
10	Kf	260	GLN
10	Kf	261	VAL
9	CD	35	ASP
9	CD	50	ASP
9	CD	55	MET
9	CD	78	ASN
9	CD	82	ARG
9	CD	85	VAL
9	CD	86	ASP
9	CD	92	GLU
9	CD	94	LEU
9	CD	108	VAL
9	CD	126	GLU
9	CD	127	SER
9	CD	138	GLN
9	CD	156	LEU
9	CD	162	TYR
9	LD	30	ILE
9	LD	50	ASP
9	LD	51	SER
9	LD	53	LEU
9	LD	54	GLU
9	LD	67	LYS
9	LD	79	LEU
9	LD	85	VAL
9	LD	91	ILE
9	LD	95	THR
9	LD	115	VAL
9	LD	123	THR
9	LD	124	LYS
9	LD	127	SER
9	LD	147	VAL
9	LD	154	VAL
10	LF	211	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	LF	215	VAL
10	LF	230	LEU
10	LF	231	THR
10	LF	234	GLU
10	LF	238	ILE
10	LF	267	GLU
1	Lg	808	LEU
1	Lg	814	GLN
1	Lg	815	VAL
1	Lg	819	VAL
2	LH	105	GLU
2	LH	107	ILE
2	LH	108	ASP
2	LH	123	ASN
2	LH	147	THR
2	LH	152	THR
2	LH	160	LEU
2	LH	170	ARG
2	LH	176	VAL
2	LH	180	VAL
2	LH	207	ASP
2	LH	216	GLN
2	LH	218	THR
2	LH	240	THR
2	LH	248	VAL
2	LH	249	ASP
2	LH	262	ASN
2	LH	280	LEU
2	LH	281	LEU
2	LH	284	LEU
2	LH	294	ARG
2	LH	313	VAL
2	LH	329	THR
2	LH	344	VAL
3	LK	45	VAL
3	LK	70	VAL
3	LK	73	ASN
3	LK	83	LEU
3	LK	84	PHE
3	LK	92	ASN
3	LK	101	GLU
3	LK	111	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	LK	156	THR
3	LK	165	ILE
3	LK	180	VAL
3	LK	183	THR
4	LL	57	VAL
4	LL	100	ASP
4	LL	109	LEU
4	LL	130	ASP
4	LL	133	PHE
4	LL	172	VAL
4	LL	175	ARG
4	LL	181	LEU
5	LM	134	LEU
5	LM	146	LEU
5	LM	162	VAL
5	LM	173	LEU
5	LM	176	VAL
5	LM	183	VAL
5	LM	184	LEU
5	LM	188	PHE
5	LM	190	ASN
5	LM	203	SER
5	LM	205	TYR
5	LM	207	ILE
5	LM	221	LYS
5	LM	222	ILE
5	LM	231	LEU
5	LM	251	SER
5	LM	257	ASP
5	LM	259	SER
5	LM	284	LEU
5	LM	292	MET
6	LN	62	ASN
6	LN	70	CYS
6	LN	75	VAL
6	LN	81	LEU
6	LN	101	VAL
6	LN	102	VAL
6	LN	115	GLN
9	Ld	30	ILE
9	Ld	41	LEU
9	Ld	61	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	Ld	63	THR
9	Ld	70	THR
9	Ld	78	ASN
9	Ld	108	VAL
9	Ld	115	VAL
9	Ld	123	THR
9	Ld	128	LEU
9	Ld	145	ILE
9	Ld	147	VAL
9	Ld	150	ASN
10	Lf	232	VAL
10	Lf	253	ARG
3	AK	45	VAL
3	AK	65	ILE
3	AK	72	GLN
3	AK	73	ASN
3	AK	92	ASN
3	AK	105	PHE
3	AK	111	LYS
3	AK	112	ILE
3	AK	115	THR
3	AK	126	VAL
3	AK	156	THR
3	AK	162	ASP
3	AK	180	VAL
3	AK	182	ILE
3	AK	183	THR
9	MD	38	THR
9	MD	70	THR
9	MD	108	VAL
9	MD	115	VAL
9	MD	126	GLU
9	MD	147	VAL
9	MD	154	VAL
10	MF	211	TYR
10	MF	215	VAL
10	MF	223	ILE
10	MF	233	ARG
10	MF	256	THR
10	MF	264	PHE
1	Mg	793	GLU
1	Mg	813	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Mg	815	VAL
1	Mg	818	GLN
1	Mg	819	VAL
1	Mg	821	THR
2	MH	108	ASP
2	MH	109	LYS
2	MH	113	LYS
2	MH	125	GLU
2	MH	130	LEU
2	MH	134	TYR
2	MH	147	THR
2	MH	154	THR
2	MH	158	VAL
2	MH	181	PHE
2	MH	208	LYS
2	MH	216	GLN
2	MH	226	LEU
2	MH	231	ARG
2	MH	238	MET
2	MH	240	THR
2	MH	248	VAL
2	MH	252	VAL
2	MH	265	SER
2	MH	268	THR
2	MH	285	GLU
2	MH	287	VAL
2	MH	313	VAL
2	MH	328	MET
2	MH	332	ASP
2	MH	344	VAL
2	MH	353	VAL
1	EG	877	VAL
1	EG	898	LYS
1	EG	911	LYS
1	EG	916	PHE
1	EG	930	ILE
1	EG	944	LEU
1	EG	962	SER
1	EG	965	LEU
1	EG	968	PHE
1	EG	972	PHE
1	EG	1010	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	EG	1017	GLN
1	EG	1028	THR
1	EG	1037	LEU
3	MK	45	VAL
3	MK	50	ASP
3	MK	62	LYS
3	MK	67	VAL
3	MK	70	VAL
3	MK	75	LEU
3	MK	83	LEU
3	MK	88	SER
3	MK	111	LYS
3	MK	112	ILE
3	MK	114	ILE
3	MK	116	VAL
3	MK	117	THR
3	MK	125	SER
3	MK	126	VAL
3	MK	127	LYS
3	MK	150	ASP
3	MK	156	THR
3	MK	182	ILE
4	ML	93	LEU
4	ML	104	LYS
4	ML	109	LEU
4	ML	130	ASP
4	ML	140	LEU
4	ML	172	VAL
4	ML	174	SER
4	ML	177	HIS
4	ML	181	LEU
4	ML	189	MET
5	MM	127	ASN
5	MM	134	LEU
5	MM	146	LEU
5	MM	149	ASN
5	MM	155	LEU
5	MM	162	VAL
5	MM	176	VAL
5	MM	180	ASP
5	MM	182	LYS
5	MM	184	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	MM	215	ARG
5	MM	221	LYS
5	MM	222	ILE
5	MM	231	LEU
5	MM	271	SER
5	MM	275	ASP
5	MM	292	MET
5	MM	301	MET
5	MM	303	GLU
5	MM	308	ASP
6	MN	69	TYR
6	MN	70	CYS
6	MN	72	ARG
6	MN	86	LEU
6	MN	91	VAL
6	MN	95	LEU
6	MN	101	VAL
6	MN	108	VAL
6	MN	110	GLU
6	MN	112	CYS
6	MN	114	LEU
6	MN	115	GLN
9	Md	41	LEU
9	Md	53	LEU
9	Md	55	MET
9	Md	61	VAL
9	Md	63	THR
9	Md	67	LYS
9	Md	70	THR
9	Md	73	ILE
9	Md	91	ILE
9	Md	108	VAL
9	Md	115	VAL
9	Md	120	SER
9	Md	145	ILE
9	Md	147	VAL
9	Md	150	ASN
9	Md	154	VAL
10	CF	208	ILE
10	CF	215	VAL
10	CF	230	LEU
10	CF	231	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	CF	238	ILE
10	CF	253	ARG
10	Mf	213	GLN
10	Mf	219	ARG
10	Mf	232	VAL
10	Mf	233	ARG
10	Mf	236	SER
10	Mf	250	LEU
10	Mf	256	THR
10	VF	215	VAL
10	VF	230	LEU
10	VF	231	THR
10	VF	256	THR
1	VG	793	GLU
1	VG	800	ASP
1	VG	802	LEU
1	VG	808	LEU
1	VG	810	GLN
1	VG	814	GLN
1	VG	819	VAL
2	VH	108	ASP
2	VH	113	LYS
2	VH	125	GLU
2	VH	134	TYR
2	VH	147	THR
2	VH	160	LEU
2	VH	180	VAL
2	VH	205	GLN
2	VH	221	TYR
2	VH	226	LEU
2	VH	233	LEU
2	VH	238	MET
2	VH	239	LEU
2	VH	240	THR
2	VH	248	VAL
2	VH	253	ASP
2	VH	262	ASN
2	VH	296	VAL
2	VH	297	VAL
2	VH	313	VAL
2	VH	329	THR
2	VH	338	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	VH	347	VAL
2	VH	352	LYS
2	VH	358	VAL
10	WF	215	VAL
10	WF	231	THR
10	WF	238	ILE
10	WF	256	THR
10	WF	261	VAL
10	WF	264	PHE
1	WG	793	GLU
1	WG	796	GLN
1	WG	797	ARG
1	WG	800	ASP
1	WG	801	MET
1	WG	802	LEU
1	WG	817	THR
1	WG	819	VAL
2	WH	108	ASP
2	WH	113	LYS
2	WH	115	MET
2	WH	134	TYR
2	WH	141	LYS
2	WH	147	THR
2	WH	168	VAL
2	WH	170	ARG
2	WH	180	VAL
2	WH	215	ILE
2	WH	218	THR
2	WH	231	ARG
2	WH	240	THR
2	WH	248	VAL
2	WH	253	ASP
2	WH	254	LEU
2	WH	262	ASN
2	WH	279	LEU
2	WH	281	LEU
2	WH	313	VAL
2	WH	315	THR
2	WH	325	LEU
2	WH	329	THR
2	WH	349	TRP
2	WH	354	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	XF	208	ILE
10	XF	215	VAL
10	XF	230	LEU
10	XF	232	VAL
10	XF	233	ARG
10	XF	256	THR
1	XG	793	GLU
1	XG	795	GLN
1	XG	808	LEU
1	XG	814	GLN
1	XG	817	THR
1	XG	818	GLN
1	XG	819	VAL
2	XH	115	MET
2	XH	147	THR
2	XH	170	ARG
2	XH	176	VAL
2	XH	180	VAL
2	XH	185	THR
2	XH	203	ASN
2	XH	208	LYS
2	XH	223	TYR
2	XH	238	MET
2	XH	240	THR
2	XH	241	LEU
2	XH	248	VAL
2	XH	249	ASP
2	XH	250	TYR
2	XH	253	ASP
2	XH	256	VAL
2	XH	262	ASN
2	XH	297	VAL
2	XH	301	ASP
2	XH	313	VAL
2	XH	318	THR
2	XH	354	MET
2	XH	359	GLU
10	YF	215	VAL
10	YF	231	THR
10	YF	233	ARG
10	YF	246	LEU
10	YF	256	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	YF	263	LYS
4	AL	93	LEU
4	AL	100	ASP
4	AL	113	ASP
4	AL	121	ASP
4	AL	130	ASP
4	AL	154	LEU
4	AL	169	THR
4	AL	172	VAL
4	AL	174	SER
4	AL	212	ASN
4	AL	216	ASP
1	YG	793	GLU
1	YG	815	VAL
1	YG	817	THR
2	YH	109	LYS
2	YH	113	LYS
2	YH	115	MET
2	YH	134	TYR
2	YH	147	THR
2	YH	160	LEU
2	YH	170	ARG
2	YH	175	PHE
2	YH	176	VAL
2	YH	180	VAL
2	YH	185	THR
2	YH	204	ILE
2	YH	240	THR
2	YH	248	VAL
2	YH	250	TYR
2	YH	253	ASP
2	YH	278	ASP
2	YH	282	HIS
2	YH	295	LEU
2	YH	311	MET
2	YH	316	ASN
2	YH	318	THR
2	YH	339	MET
2	YH	353	VAL
2	YH	356	LEU
2	YH	358	VAL
11	DC	61	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	DC	69	GLN
11	DC	83	LEU
11	DC	89	ASN
11	DC	90	LEU
11	DC	96	PHE
11	DC	112	GLU
11	DC	116	THR
11	DC	119	LEU
11	DC	143	THR
11	DC	146	THR
11	DC	163	VAL
11	DC	166	LEU
11	DC	169	THR
11	DC	193	THR
11	DC	221	VAL
11	DC	226	VAL
11	DC	230	ASP
11	DC	241	HIS
11	DC	258	ASN
1	FG	869	MET
1	FG	873	LEU
1	FG	898	LYS
1	FG	900	ILE
1	FG	913	VAL
1	FG	916	PHE
1	FG	930	ILE
1	FG	935	ILE
1	FG	941	ARG
1	FG	944	LEU
1	FG	962	SER
1	FG	965	LEU
1	FG	972	PHE
1	FG	1010	THR
1	FG	1017	GLN
1	FG	1037	LEU
1	FG	1044	ASP
10	ZF	215	VAL
10	ZF	245	LYS
10	ZF	251	GLN
1	ZG	793	GLU
2	ZH	105	GLU
2	ZH	108	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	ZH	115	MET
2	ZH	130	LEU
2	ZH	136	THR
2	ZH	147	THR
2	ZH	180	VAL
2	ZH	183	ASP
2	ZH	213	LEU
2	ZH	221	TYR
2	ZH	233	LEU
2	ZH	238	MET
2	ZH	239	LEU
2	ZH	240	THR
2	ZH	248	VAL
2	ZH	253	ASP
2	ZH	281	LEU
2	ZH	285	GLU
2	ZH	297	VAL
2	ZH	305	TRP
2	ZH	320	LEU
2	ZH	321	SER
2	ZH	328	MET
2	ZH	329	THR
2	ZH	339	MET
2	ZH	340	GLN
2	ZH	350	HIS
2	ZH	352	LYS
5	AM	114	ASN
5	AM	134	LEU
5	AM	136	LEU
5	AM	146	LEU
5	AM	149	ASN
5	AM	152	LEU
5	AM	175	ILE
5	AM	176	VAL
5	AM	182	LYS
5	AM	184	LEU
5	AM	188	PHE
5	AM	191	LEU
5	AM	201	THR
5	AM	204	LEU
5	AM	205	TYR
5	AM	207	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	AM	212	LEU
5	AM	215	ARG
5	AM	222	ILE
5	AM	251	SER
5	AM	255	THR
5	AM	263	ILE
5	AM	269	GLN
5	AM	274	THR
5	AM	277	SER
5	AM	287	THR
5	AM	292	MET
5	AM	301	MET
5	AM	303	GLU
5	AM	308	ASP
5	AM	316	ASN
6	AN	39	ASP
6	AN	62	ASN
6	AN	70	CYS
6	AN	72	ARG
6	AN	77	ASP
6	AN	84	CYS
6	AN	91	VAL
6	AN	101	VAL
6	AN	102	VAL
6	AN	108	VAL
6	AN	114	LEU
1	Cg	801	MET
1	Cg	808	LEU
1	Cg	809	VAL
1	Cg	814	GLN
1	Cg	819	VAL
9	Ad	30	ILE
9	Ad	36	ASP
9	Ad	41	LEU
9	Ad	61	VAL
9	Ad	63	THR
9	Ad	73	ILE
9	Ad	94	LEU
9	Ad	108	VAL
9	Ad	115	VAL
9	Ad	119	ILE
9	Ad	133	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	Ad	150	ASN
10	Af	215	VAL
10	Af	232	VAL
10	Af	238	ILE
10	Af	247	ILE
10	Af	260	GLN
9	BD	23	MET
9	BD	38	THR
9	BD	50	ASP
9	BD	70	THR
9	BD	78	ASN
9	BD	85	VAL
9	BD	127	SER
9	BD	128	LEU
9	BD	137	TYR
9	BD	156	LEU
10	BF	207	ARG
10	BF	215	VAL
10	BF	216	ILE
10	BF	231	THR
10	BF	250	LEU
10	BF	256	THR
2	BH	107	ILE
2	BH	108	ASP
2	BH	109	LYS
2	BH	147	THR
2	BH	160	LEU
2	BH	170	ARG
2	BH	171	LEU
2	BH	175	PHE
2	BH	176	VAL
2	BH	180	VAL
2	BH	184	SER
2	BH	218	THR
2	BH	233	LEU
2	BH	234	ASN
2	BH	242	ILE
2	BH	248	VAL
2	BH	251	ARG
2	BH	257	GLN
2	BH	278	ASP
2	BH	287	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	BH	292	SER
2	BH	294	ARG
2	BH	296	VAL
2	BH	313	VAL
2	BH	356	LEU
2	BH	357	LYS
3	BK	45	VAL
3	BK	69	SER
3	BK	70	VAL
3	BK	73	ASN
3	BK	106	LEU
3	BK	111	LYS
3	BK	122	LYS
3	BK	126	VAL
3	BK	134	LEU
3	BK	137	SER
3	BK	150	ASP
3	BK	156	THR
3	BK	157	GLN
3	BK	159	LEU
3	BK	169	THR
3	BK	180	VAL
3	BK	183	THR
4	BL	48	ASN
4	BL	57	VAL
4	BL	93	LEU
4	BL	98	TYR
4	BL	109	LEU
4	BL	121	ASP
4	BL	129	THR
4	BL	130	ASP
4	BL	133	PHE
4	BL	154	LEU
4	BL	163	ILE
4	BL	165	VAL
4	BL	172	VAL
4	BL	175	ARG
4	BL	185	GLN
4	BL	206	GLU
4	BL	212	ASN
4	BL	225	GLN
4	BL	227	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	BM	115	ARG
5	BM	134	LEU
5	BM	152	LEU
5	BM	155	LEU
5	BM	162	VAL
5	BM	175	ILE
5	BM	176	VAL
5	BM	177	LEU
5	BM	182	LYS
5	BM	184	LEU
5	BM	191	LEU
5	BM	202	LEU
5	BM	204	LEU
5	BM	205	TYR
5	BM	222	ILE
5	BM	245	TYR
5	BM	259	SER
5	BM	269	GLN
5	BM	292	MET
5	BM	312	PHE
6	BN	51	CYS
6	BN	59	VAL
6	BN	67	THR
6	BN	78	LEU
6	BN	81	LEU
6	BN	94	GLN
6	BN	95	LEU
6	BN	100	LEU
6	BN	104	ASN
6	BN	105	ASP
6	BN	108	VAL
6	BN	112	CYS
6	BN	114	LEU
9	Bd	27	LYS
9	Bd	31	ASN
9	Bd	41	LEU
9	Bd	53	LEU
9	Bd	59	GLU
9	Bd	61	VAL
9	Bd	63	THR
9	Bd	78	ASN
9	Bd	115	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	Bd	119	ILE
9	Bd	126	GLU
9	Bd	130	GLU
9	Bd	150	ASN
10	Bf	222	LEU
10	Bf	233	ARG
10	Bf	245	LYS
10	Bf	247	ILE
10	Bf	260	GLN
10	Bf	261	VAL
11	EC	65	SER
11	EC	84	ASN
11	EC	89	ASN
11	EC	97	ASN
11	EC	119	LEU
11	EC	129	ASP
11	EC	143	THR
11	EC	146	THR
11	EC	148	ARG
11	EC	149	GLN
11	EC	156	VAL
11	EC	174	GLU
11	EC	181	GLU
11	EC	195	LEU
11	EC	206	PHE
11	EC	215	LEU
11	EC	221	VAL
11	EC	233	VAL
11	EC	241	HIS
11	EC	256	ASN
11	EC	266	VAL
11	FC	28	THR
11	FC	30	SER
11	FC	35	GLN
11	FC	48	LYS
11	FC	49	GLN
11	FC	56	GLU
11	FC	85	LYS
11	FC	89	ASN
11	FC	91	ASP
11	FC	97	ASN
11	FC	116	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	FC	127	ILE
11	FC	165	LEU
11	FC	170	LYS
11	FC	195	LEU
11	FC	203	LYS
11	FC	206	PHE
11	FC	221	VAL
11	FC	226	VAL
11	FC	228	HIS
11	FC	248	ARG
11	FC	256	ASN
11	GC	105	ILE
11	GC	116	THR
11	GC	119	LEU
11	GC	127	ILE
11	GC	143	THR
11	GC	146	THR
11	GC	153	MET
11	GC	166	LEU
11	GC	168	LYS
11	GC	181	GLU
11	GC	184	TRP
11	GC	193	THR
11	GC	195	LEU
11	GC	203	LYS
11	GC	206	PHE
11	GC	220	MET
11	GC	226	VAL
11	GC	229	THR
11	GC	233	VAL
11	GC	266	VAL
1	GG	865	THR
1	GG	886	LEU
1	GG	895	LYS
1	GG	898	LYS
1	GG	900	ILE
1	GG	912	MET
1	GG	913	VAL
1	GG	916	PHE
1	GG	930	ILE
1	GG	944	LEU
1	GG	962	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	GG	965	LEU
1	GG	972	PHE
1	GG	1010	THR
1	GG	1017	GLN
11	HC	64	LEU
11	HC	84	ASN
11	HC	97	ASN
11	HC	105	ILE
11	HC	112	GLU
11	HC	118	ASN
11	HC	143	THR
11	HC	148	ARG
11	HC	159	GLU
11	HC	165	LEU
11	HC	169	THR
11	HC	184	TRP
11	HC	189	ASP
11	HC	193	THR
11	HC	195	LEU
11	HC	206	PHE
11	HC	211	LEU
11	HC	221	VAL
11	HC	228	HIS
11	HC	233	VAL
11	HC	241	HIS
11	HC	258	ASN
11	HC	263	ARG
11	HC	266	VAL
11	IC	81	GLU
11	IC	86	GLN
11	IC	89	ASN
11	IC	90	LEU
11	IC	91	ASP
11	IC	111	LEU
11	IC	116	THR
11	IC	121	ASP
11	IC	125	ILE
11	IC	127	ILE
11	IC	146	THR
11	IC	153	MET
11	IC	156	VAL
11	IC	163	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	IC	181	GLU
11	IC	195	LEU
11	IC	204	GLU
11	IC	214	LYS
11	IC	226	VAL
11	IC	268	LYS
11	JC	28	THR
11	JC	30	SER
11	JC	35	GLN
11	JC	42	TYR
11	JC	44	ARG
11	JC	48	LYS
11	JC	49	GLN
11	JC	59	LEU
11	JC	60	LYS
11	JC	64	LEU
11	JC	91	ASP
11	JC	97	ASN
11	JC	104	ASN
11	JC	105	ILE
11	JC	117	LEU
11	JC	123	GLN
11	JC	125	ILE
11	JC	149	GLN
11	JC	162	ASN
11	JC	184	TRP
11	JC	195	LEU
11	JC	204	GLU
11	JC	225	TYR
11	JC	226	VAL
11	JC	234	THR
11	JC	249	ILE
11	JC	256	ASN
11	KC	89	ASN
11	KC	119	LEU
11	KC	125	ILE
11	KC	146	THR
11	KC	170	LYS
11	KC	182	ARG
11	KC	193	THR
11	KC	206	PHE
11	KC	214	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	KC	221	VAL
11	KC	226	VAL
11	KC	230	ASP
11	KC	249	ILE
11	LC	61	GLU
11	LC	91	ASP
11	LC	109	VAL
11	LC	116	THR
11	LC	119	LEU
11	LC	143	THR
11	LC	146	THR
11	LC	148	ARG
11	LC	172	GLU
11	LC	195	LEU
11	LC	214	LYS
11	LC	226	VAL
11	LC	234	THR
11	LC	243	ASP
11	LC	245	ARG
11	LC	255	LEU
11	LC	258	ASN
11	LC	263	ARG
11	MC	91	ASP
11	MC	105	ILE
11	MC	109	VAL
11	MC	116	THR
11	MC	119	LEU
11	MC	125	ILE
11	MC	127	ILE
11	MC	133	LYS
11	MC	143	THR
11	MC	146	THR
11	MC	148	ARG
11	MC	151	LEU
11	MC	156	VAL
11	MC	163	VAL
11	MC	165	LEU
11	MC	169	THR
11	MC	176	TRP
11	MC	181	GLU
11	MC	206	PHE
11	MC	211	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	MC	214	LYS
11	MC	226	VAL
11	MC	228	HIS
11	MC	233	VAL
11	MC	256	ASN
11	MC	266	VAL
2	CH	109	LYS
2	CH	130	LEU
2	CH	134	TYR
2	CH	139	TYR
2	CH	155	SER
2	CH	175	PHE
2	CH	180	VAL
2	CH	201	SER
2	CH	203	ASN
2	CH	204	ILE
2	CH	221	TYR
2	CH	240	THR
2	CH	248	VAL
2	CH	253	ASP
2	CH	287	VAL
2	CH	294	ARG
2	CH	306	LEU
2	CH	313	VAL
2	CH	329	THR
2	CH	334	THR
2	CH	335	HIS
2	CH	353	VAL
3	CK	44	ARG
3	CK	45	VAL
3	CK	50	ASP
3	CK	73	ASN
3	CK	75	LEU
3	CK	108	GLN
3	CK	111	LYS
3	CK	116	VAL
3	CK	144	LEU
3	CK	150	ASP
3	CK	153	ILE
3	CK	156	THR
3	CK	163	LYS
3	CK	180	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	CK	181	GLU
4	CL	49	ASN
4	CL	109	LEU
4	CL	121	ASP
4	CL	129	THR
4	CL	133	PHE
4	CL	140	LEU
4	CL	172	VAL
4	CL	174	SER
4	CL	190	MET
4	CL	212	ASN
4	CL	225	GLN
5	CM	134	LEU
5	CM	146	LEU
5	CM	149	ASN
5	CM	155	LEU
5	CM	160	ASN
5	CM	162	VAL
5	CM	164	GLN
5	CM	176	VAL
5	CM	178	LYS
5	CM	180	ASP
5	CM	182	LYS
5	CM	192	ARG
5	CM	205	TYR
5	CM	208	LYS
5	CM	222	ILE
5	CM	231	LEU
5	CM	242	LYS
5	CM	257	ASP
5	CM	263	ILE
5	CM	284	LEU
5	CM	292	MET
5	CM	301	MET
5	CM	308	ASP
5	CM	312	PHE
5	CM	313	ASP
6	CN	48	ILE
6	CN	62	ASN
6	CN	69	TYR
6	CN	70	CYS
6	CN	71	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	CN	78	LEU
6	CN	80	PHE
6	CN	91	VAL
6	CN	101	VAL
6	CN	102	VAL
6	CN	108	VAL
6	CN	112	CYS
9	Cd	27	LYS
9	Cd	30	ILE
9	Cd	41	LEU
9	Cd	53	LEU
9	Cd	55	MET
9	Cd	61	VAL
9	Cd	70	THR
9	Cd	93	GLU
9	Cd	105	ARG
9	Cd	108	VAL
9	Cd	115	VAL
9	Cd	128	LEU
9	Cd	145	ILE
9	Cd	147	VAL
9	Cd	150	ASN
10	Cf	215	VAL
10	Cf	223	ILE
10	Cf	232	VAL
10	Cf	243	MET
10	Cf	247	ILE
10	Cf	253	ARG
10	Cf	261	VAL
9	DD	41	LEU
9	DD	51	SER
9	DD	54	GLU
9	DD	70	THR
9	DD	85	VAL
9	DD	86	ASP
9	DD	108	VAL
9	DD	115	VAL
9	DD	123	THR
9	DD	131	ILE
9	DD	161	ILE
10	DF	208	ILE
10	DF	213	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	DF	215	VAL
10	DF	232	VAL
10	DF	233	ARG
10	DF	238	ILE
10	DF	244	VAL
1	Dg	798	THR
1	Dg	802	LEU
1	Dg	814	GLN
1	Dg	819	VAL
2	DH	109	LYS
2	DH	114	ASP
2	DH	115	MET
2	DH	138	GLU
2	DH	147	THR
2	DH	180	VAL
2	DH	185	THR
2	DH	205	GLN
2	DH	208	LYS
2	DH	218	THR
2	DH	225	ASN
2	DH	234	ASN
2	DH	238	MET
2	DH	248	VAL
2	DH	250	TYR
2	DH	252	VAL
2	DH	253	ASP
2	DH	256	VAL
2	DH	287	VAL
2	DH	313	VAL
2	DH	328	MET
2	DH	329	THR
2	DH	344	VAL
2	DH	353	VAL
3	DK	50	ASP
3	DK	116	VAL
3	DK	117	THR
3	DK	125	SER
3	DK	126	VAL
3	DK	149	VAL
3	DK	156	THR
3	DK	183	THR
4	DL	44	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	DL	47	TYR
4	DL	93	LEU
4	DL	109	LEU
4	DL	125	LEU
4	DL	130	ASP
4	DL	140	LEU
4	DL	160	GLN
4	DL	172	VAL
4	DL	175	ARG
4	DL	177	HIS
4	DL	216	ASP
4	DL	225	GLN
4	DL	227	ARG
5	DM	131	THR
5	DM	134	LEU
5	DM	146	LEU
5	DM	149	ASN
5	DM	152	LEU
5	DM	176	VAL
5	DM	178	LYS
5	DM	184	LEU
5	DM	191	LEU
5	DM	194	LEU
5	DM	201	THR
5	DM	204	LEU
5	DM	222	ILE
5	DM	257	ASP
5	DM	259	SER
5	DM	263	ILE
5	DM	275	ASP
5	DM	292	MET
5	DM	310	LYS
6	DN	67	THR
6	DN	77	ASP
6	DN	78	LEU
6	DN	84	CYS
6	DN	88	HIS
6	DN	94	GLN
6	DN	95	LEU
6	DN	101	VAL
6	DN	108	VAL
6	DN	114	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	HG	865	THR
1	HG	867	ASP
1	HG	869	MET
1	HG	873	LEU
1	HG	893	LYS
1	HG	898	LYS
1	HG	910	ASP
1	HG	912	MET
1	HG	913	VAL
1	HG	916	PHE
1	HG	930	ILE
1	HG	939	THR
1	HG	944	LEU
1	HG	956	TYR
1	HG	962	SER
1	HG	965	LEU
1	HG	972	PHE
1	HG	1010	THR
1	HG	1017	GLN
1	HG	1040	LEU
1	IG	865	THR
1	IG	895	LYS
1	IG	900	ILE
1	IG	912	MET
1	IG	913	VAL
1	IG	930	ILE
1	IG	944	LEU
1	IG	962	SER
1	IG	963	SER
1	IG	965	LEU
1	IG	968	PHE
1	IG	972	PHE
1	IG	1010	THR
1	IG	1045	VAL
1	JG	865	THR
1	JG	900	ILE
1	JG	912	MET
1	JG	913	VAL
1	JG	916	PHE
1	JG	930	ILE
1	JG	944	LEU
1	JG	962	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	JG	965	LEU
1	JG	972	PHE
1	JG	1010	THR
1	JG	1017	GLN
1	JG	1037	LEU
1	KG	890	VAL
1	KG	893	LYS
1	KG	900	ILE
1	KG	913	VAL
1	KG	916	PHE
1	KG	930	ILE
1	KG	944	LEU
1	KG	962	SER
1	KG	963	SER
1	KG	965	LEU
1	KG	972	PHE
1	KG	1017	GLN
1	LG	869	MET
1	LG	873	LEU
1	LG	874	ASP
1	LG	898	LYS
1	LG	910	ASP
1	LG	911	LYS
1	LG	913	VAL
1	LG	916	PHE
1	LG	930	ILE
1	LG	939	THR
1	LG	944	LEU
1	LG	956	TYR
1	LG	962	SER
1	LG	965	LEU
1	LG	972	PHE
1	LG	1010	THR
1	LG	1017	GLN
1	LG	1027	THR
1	LG	1028	THR
1	LG	1037	LEU
1	MG	864	LYS
1	MG	869	MET
1	MG	877	VAL
1	MG	886	LEU
1	MG	898	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	MG	911	LYS
1	MG	913	VAL
1	MG	916	PHE
1	MG	919	MET
1	MG	939	THR
1	MG	944	LEU
1	MG	956	TYR
1	MG	962	SER
1	MG	963	SER
1	MG	964	PHE
1	MG	965	LEU
1	MG	972	PHE
1	MG	1010	THR
1	MG	1017	GLN
1	MG	1030	GLU
1	MG	1037	LEU
1	NG	867	ASP
1	NG	873	LEU
1	NG	885	ILE
1	NG	898	LYS
1	NG	900	ILE
1	NG	904	ASN
1	NG	911	LYS
1	NG	913	VAL
1	NG	916	PHE
1	NG	930	ILE
1	NG	933	TYR
1	NG	944	LEU
1	NG	947	ARG
1	NG	962	SER
1	NG	963	SER
1	NG	965	LEU
1	NG	968	PHE
1	NG	972	PHE
1	NG	1010	THR
1	NG	1017	GLN
1	NG	1037	LEU
1	OG	867	ASP
1	OG	877	VAL
1	OG	880	ASP
1	OG	898	LYS
1	OG	900	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	OG	911	LYS
1	OG	913	VAL
1	OG	916	PHE
1	OG	917	ASN
1	OG	930	ILE
1	OG	944	LEU
1	OG	947	ARG
1	OG	962	SER
1	OG	963	SER
1	OG	965	LEU
1	OG	968	PHE
1	OG	972	PHE
1	OG	973	GLN
1	OG	1010	THR
1	OG	1028	THR
1	OG	1037	LEU
1	OG	1044	ASP
1	OG	1045	VAL
1	PG	865	THR
1	PG	869	MET
1	PG	898	LYS
1	PG	900	ILE
1	PG	910	ASP
1	PG	912	MET
1	PG	913	VAL
1	PG	916	PHE
1	PG	930	ILE
1	PG	944	LEU
1	PG	947	ARG
1	PG	956	TYR
1	PG	962	SER
1	PG	965	LEU
1	PG	966	GLN
1	PG	968	PHE
1	PG	972	PHE
1	PG	1010	THR
1	PG	1017	GLN
1	PG	1020	GLN
1	PG	1037	LEU
11	AC	28	THR
11	AC	35	GLN
11	AC	49	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	AC	57	MET
11	AC	60	LYS
11	AC	83	LEU
11	AC	86	GLN
11	AC	104	ASN
11	AC	105	ILE
11	AC	112	GLU
11	AC	125	ILE
11	AC	153	MET
11	AC	162	ASN
11	AC	165	LEU
11	AC	174	GLU
11	AC	195	LEU
11	AC	204	GLU
11	AC	206	PHE
11	AC	221	VAL
11	AC	233	VAL
11	AC	234	THR
11	AC	245	ARG
9	Dd	41	LEU
9	Dd	61	VAL
9	Dd	78	ASN
9	Dd	93	GLU
9	Dd	108	VAL
9	Dd	115	VAL
9	Dd	123	THR
9	Dd	126	GLU
9	Dd	128	LEU
9	Dd	147	VAL
9	Dd	150	ASN
9	Dd	155	GLU
9	Dd	156	LEU
1	Ag	794	ILE
1	Ag	795	GLN
1	Ag	798	THR
1	Ag	800	ASP
1	Ag	801	MET
1	Ag	815	VAL
1	Ag	818	GLN
10	Df	215	VAL
10	Df	222	LEU
10	Df	229	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	Df	230	LEU
10	Df	232	VAL
10	Df	245	LYS
10	Df	253	ARG
10	Df	262	ILE
9	AD	23	MET
9	AD	55	MET
9	AD	85	VAL
9	AD	93	GLU
9	AD	115	VAL
9	AD	117	VAL
9	AD	138	GLN
9	AD	145	ILE
9	AD	154	VAL
9	ED	35	ASP
9	ED	50	ASP
9	ED	55	MET
9	ED	63	THR
9	ED	70	THR
9	ED	91	ILE
9	ED	115	VAL
9	ED	127	SER
9	ED	154	VAL
9	ED	156	LEU
10	EF	207	ARG
10	EF	215	VAL
10	EF	230	LEU
10	EF	231	THR
10	EF	233	ARG
10	EF	238	ILE
10	EF	256	THR
10	EF	263	LYS
1	Eg	815	VAL
1	Eg	824	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	EL	225	GLN
5	EM	249	GLN
5	EM	267	ASN
9	Ed	32	ASN

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Mol	Chain	Res	Type
6	FN	79	GLN
1	Gg	807	GLN
1	Gg	810	GLN
1	BG	938	ASN
9	Gd	32	ASN
2	HH	257	GLN
4	IL	196	ASN
10	If	251	GLN
2	AH	132	GLN
2	KH	159	ASN
2	KH	257	GLN
1	Lg	818	GLN
2	LH	203	ASN
2	LH	205	GLN
10	MF	266	GLN
2	MH	216	GLN
1	EG	1020	GLN
10	XF	260	GLN
1	YG	818	GLN
1	FG	1017	GLN
6	AN	49	ASN
6	AN	61	ASN
1	Cg	807	GLN
9	Ad	32	ASN
10	BF	251	GLN
5	BM	249	GLN
5	BM	267	ASN
11	GC	162	ASN
1	GG	1020	GLN
11	JC	46	GLN
2	CH	257	GLN
5	CM	164	GLN
4	DL	160	GLN
5	DM	267	ASN
1	MG	1043	GLN

### 5.3.3 RNA

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	HX	1
8	JX	1
8	VX	1
8	ZX	1
8	BX	1
8	IX	1
8	YX	1
8	EX	1
8	CX	1
8	FX	1
8	KX	1
8	MX	1
8	WX	1
8	GX	1
8	DX	1
8	AX	1
8	LX	1
8	XX	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	HX	38:UNK	C	70:UNK	N	26.96
1	JX	38:UNK	C	70:UNK	N	26.39
1	VX	38:UNK	C	70:UNK	N	26.34
1	ZX	38:UNK	C	70:UNK	N	26.34
1	BX	38:UNK	C	70:UNK	N	25.84
1	IX	38:UNK	C	70:UNK	N	25.69
1	YX	38:UNK	C	70:UNK	N	25.34
1	EX	38:UNK	C	70:UNK	N	25.28
1	CX	38:UNK	C	70:UNK	N	25.22
1	FX	38:UNK	C	70:UNK	N	25.21
1	KX	38:UNK	C	70:UNK	N	25.16
1	MX	38:UNK	C	70:UNK	N	24.83
1	WX	38:UNK	C	70:UNK	N	24.82
1	GX	38:UNK	C	70:UNK	N	24.45
1	DX	38:UNK	C	70:UNK	N	24.25
1	AX	38:UNK	C	70:UNK	N	23.39
1	LX	38:UNK	C	70:UNK	N	23.11
1	XX	38:UNK	C	70:UNK	N	22.04



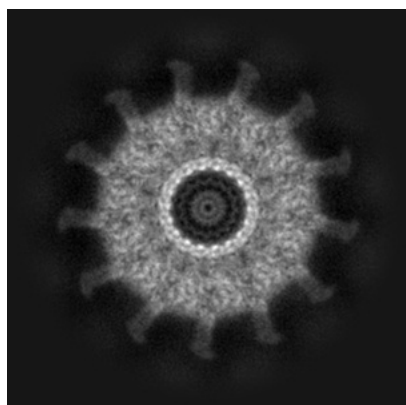
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24024. These allow visual inspection of the internal detail of the map and identification of artifacts.

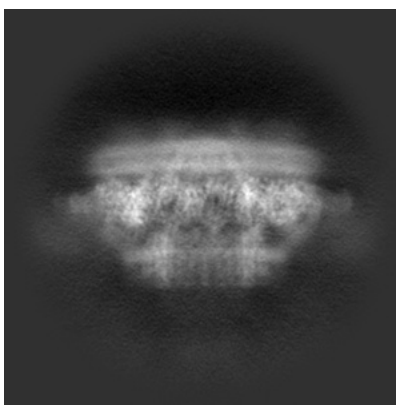
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

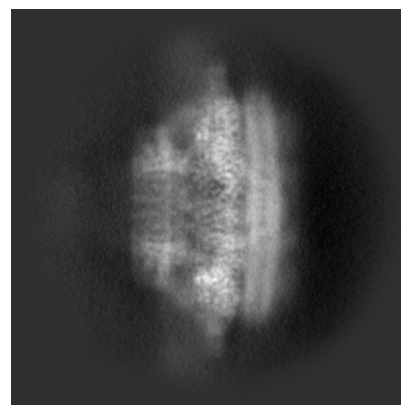
#### 6.1.1 Primary map



X



Y

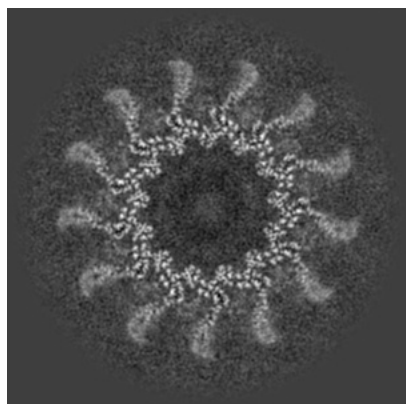


Z

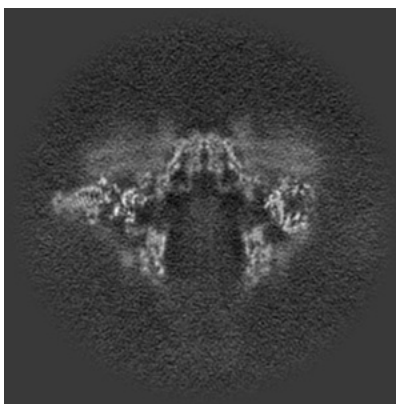
The images above show the map projected in three orthogonal directions.

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

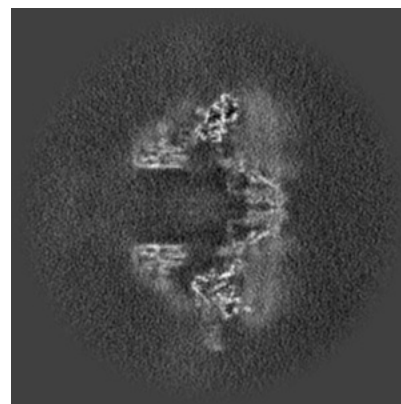
#### 6.2.1 Primary map



X Index: 125



Y Index: 125

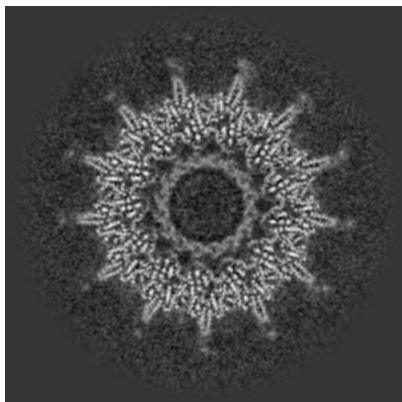


Z Index: 125

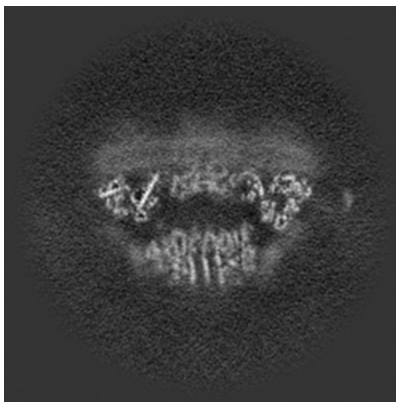
The images above show central slices of the map in three orthogonal directions.

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

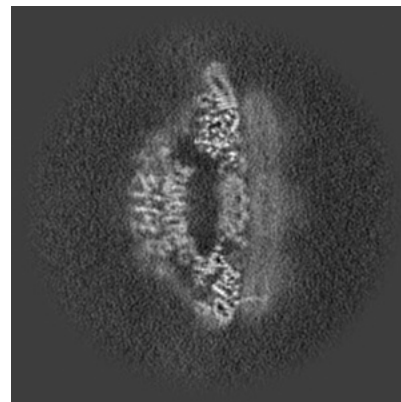
### 6.3.1 Primary map



X Index: 134



Y Index: 101

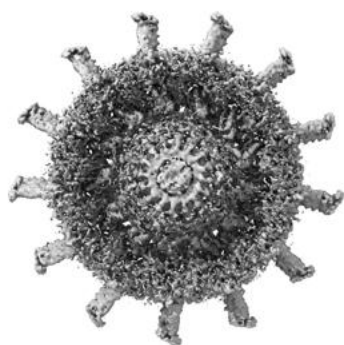


Z Index: 151

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

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

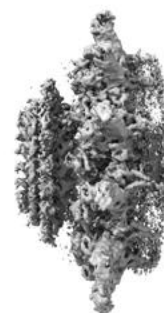
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

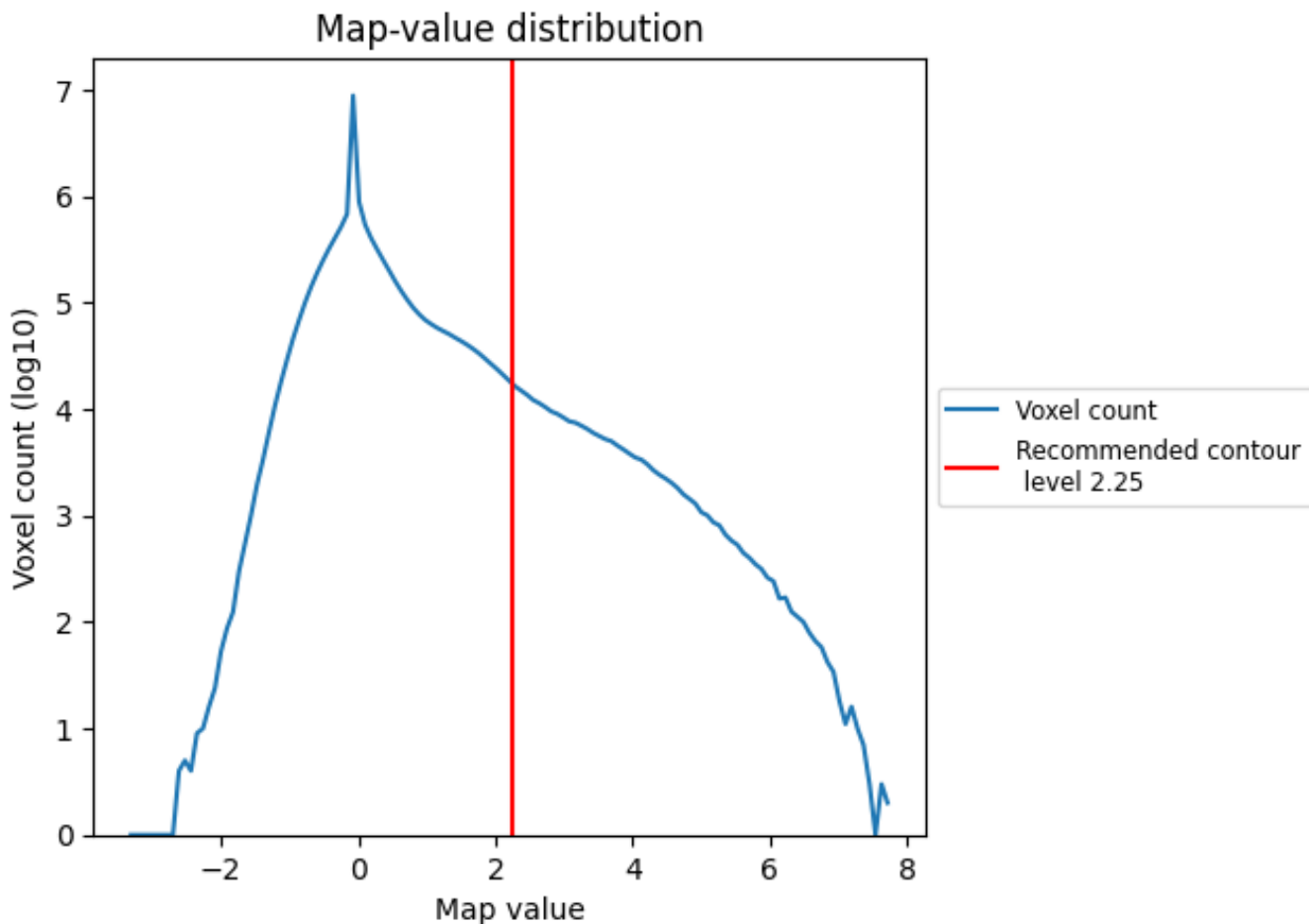
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

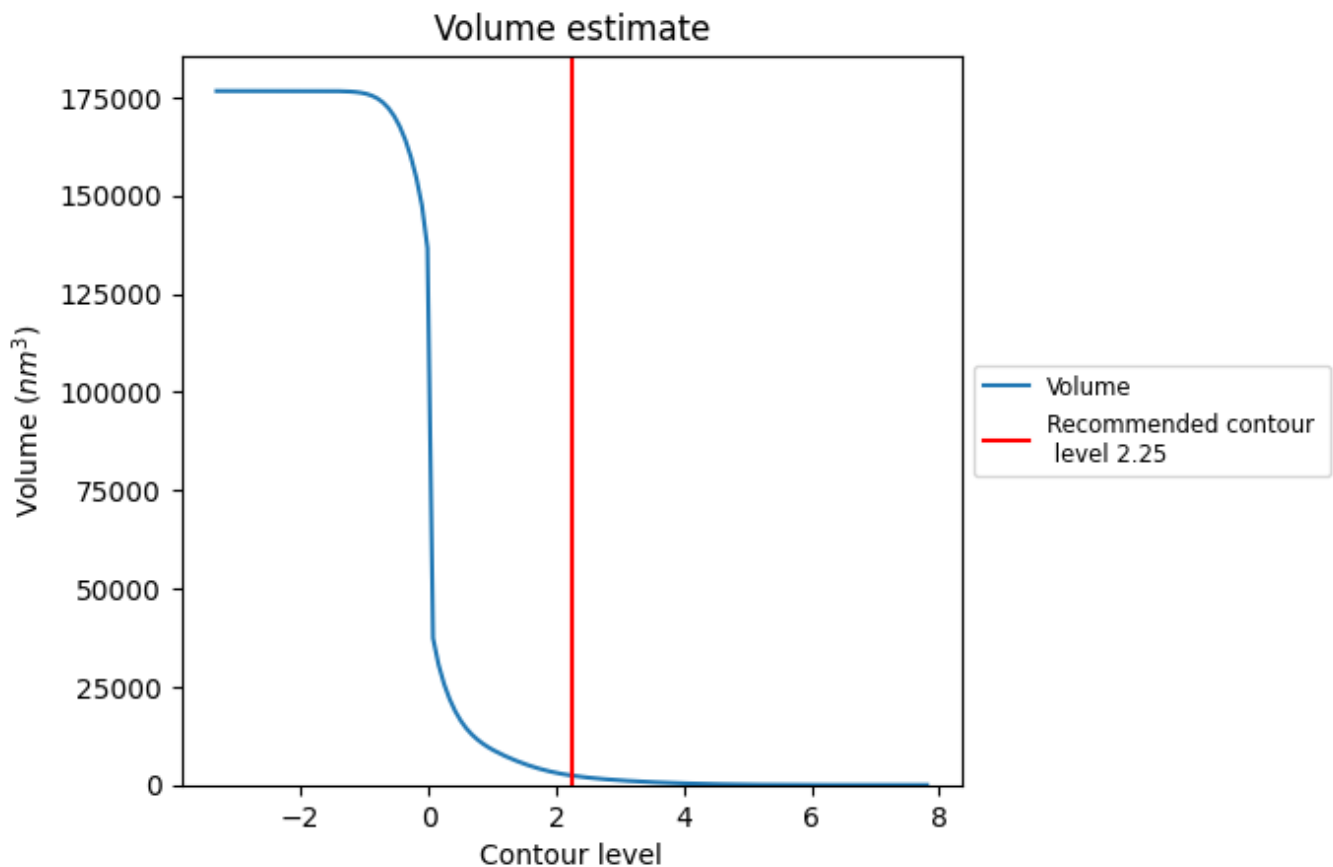
This section contains the results of statistical analysis of the map.

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



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

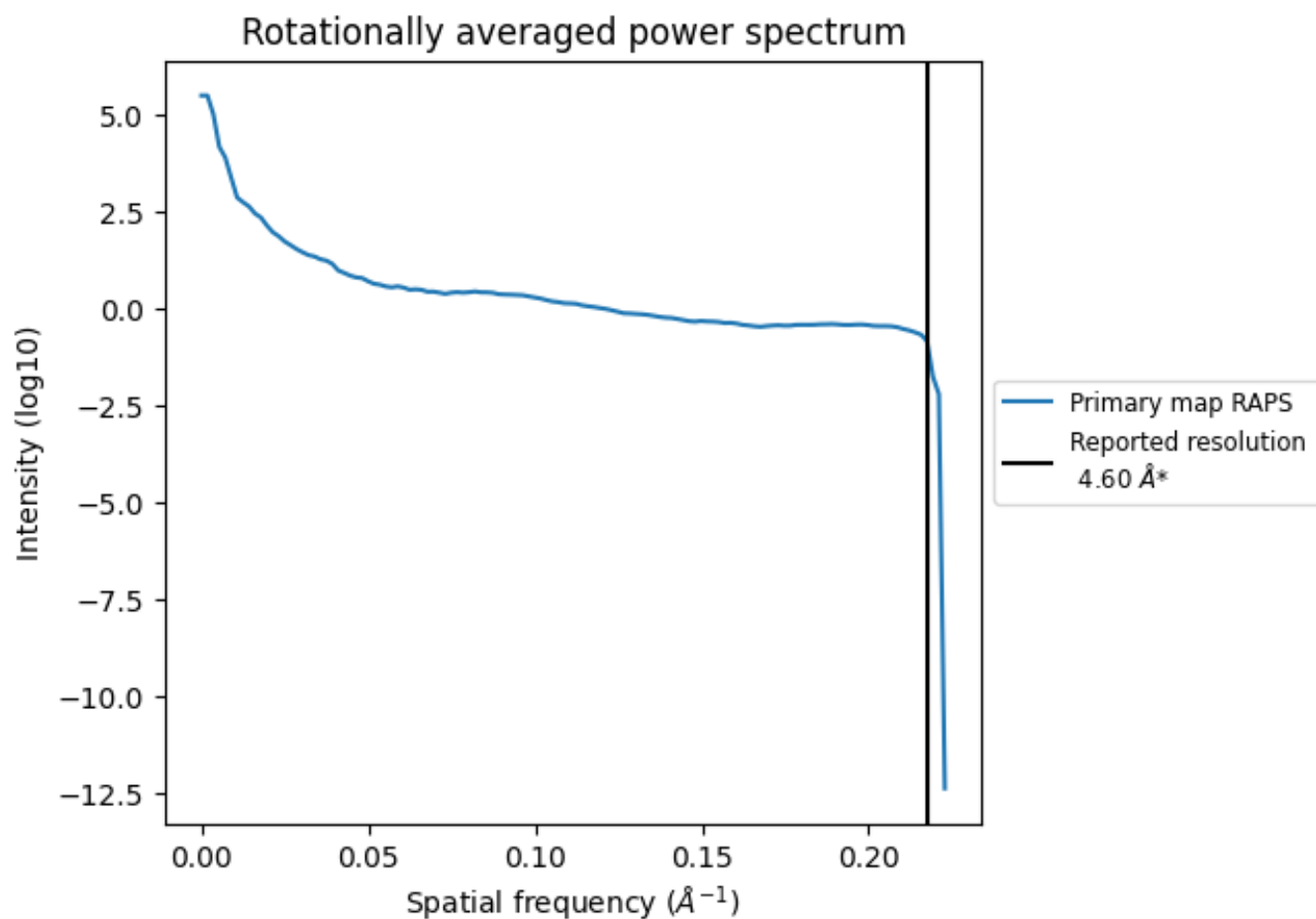
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2386  $\text{nm}^3$ ; this corresponds to an approximate mass of 2155 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 0.217 Å<sup>-1</sup>

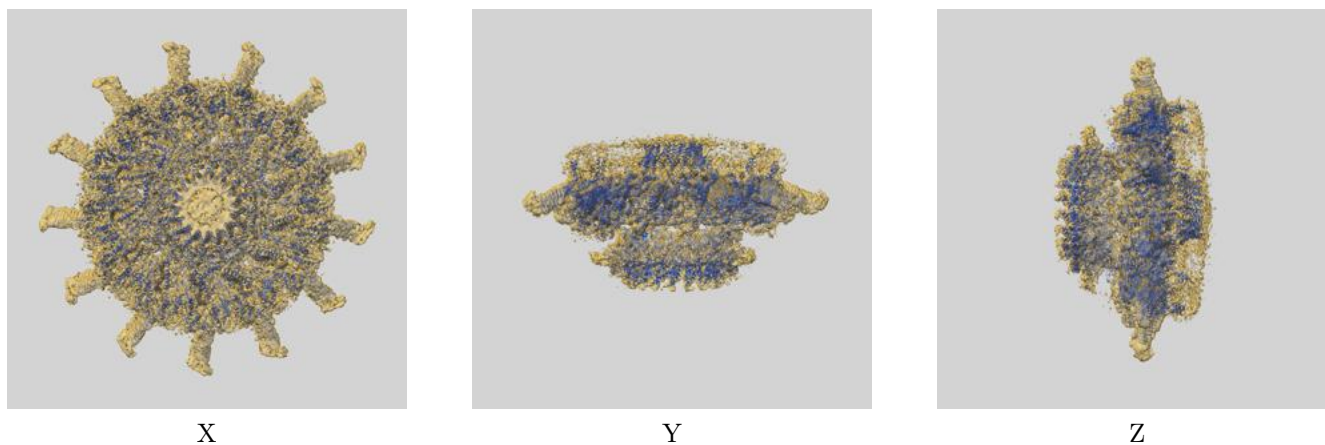
## 8 Fourier-Shell correlation

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

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

This section contains information regarding the fit between EMDB map EMD-24024 and PDB model 7MUW. Per-residue inclusion information can be found in section 3 on page 22.

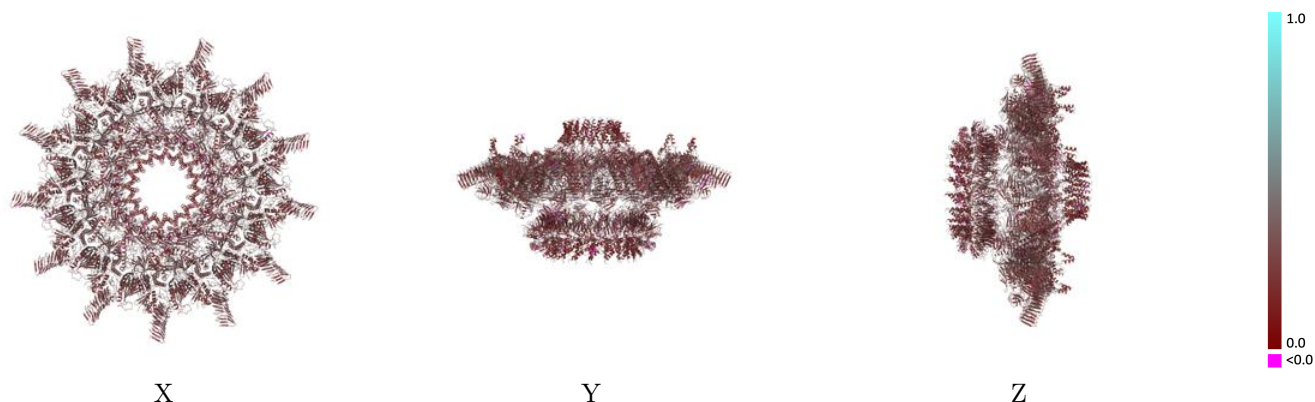
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 2.25 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.

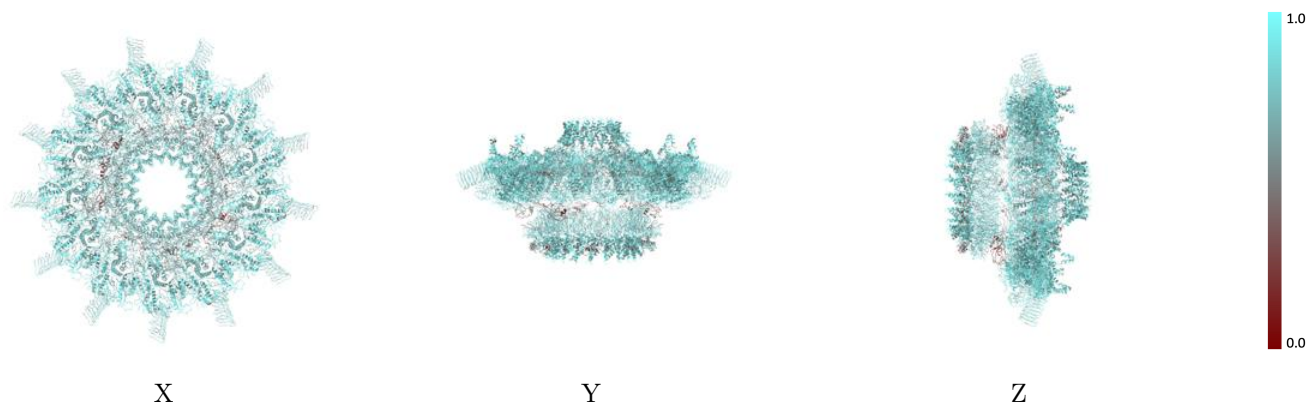


## 9.2 Q-score mapped to coordinate model [\(i\)](#)



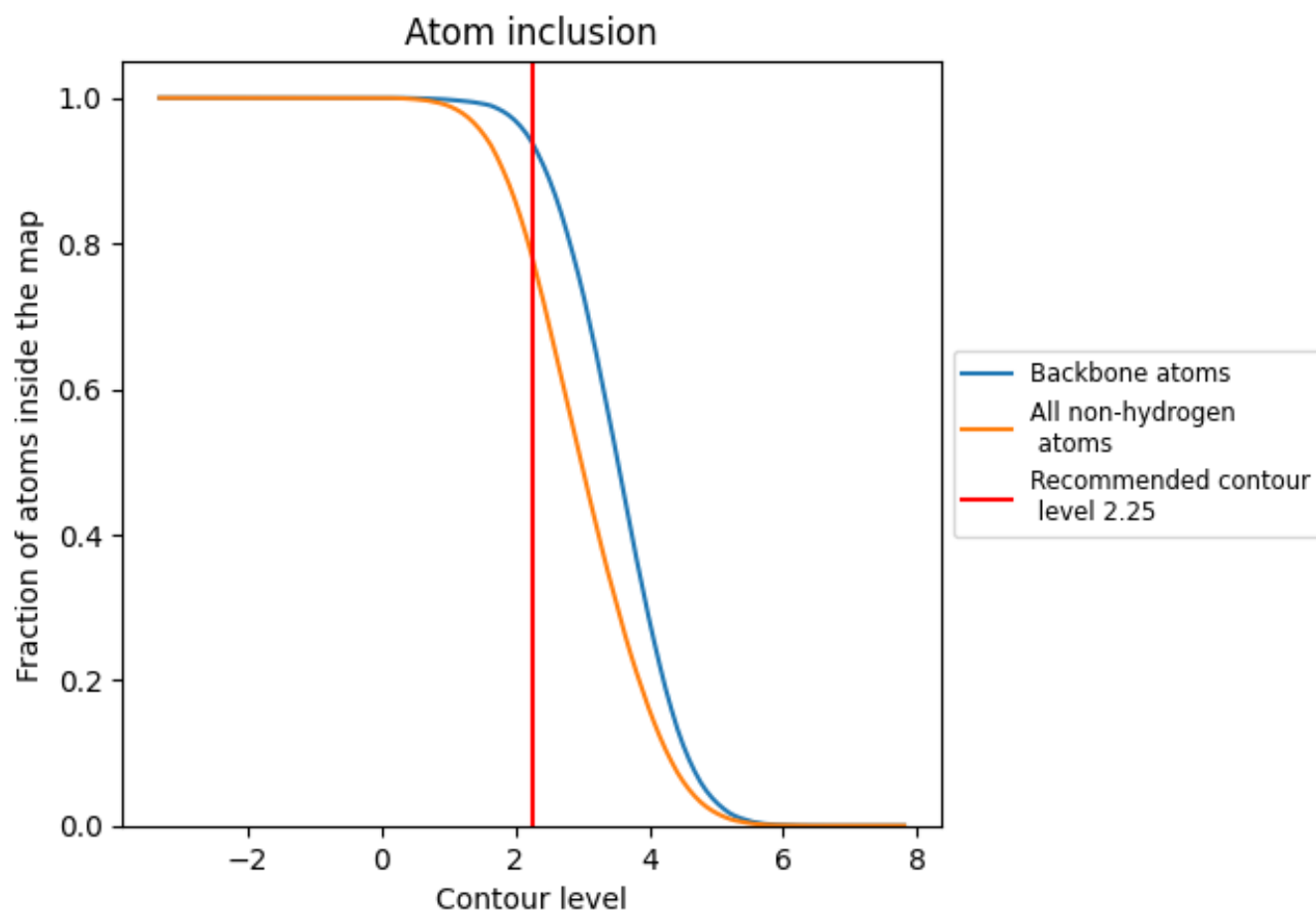
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.25).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 78% 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 (2.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7815	 0.2820
AC	 0.7717	 0.2930
AD	 0.8081	 0.3200
AF	 0.7983	 0.2290
AG	 0.6913	 0.2430
AH	 0.7818	 0.2740
AK	 0.8110	 0.3060
AL	 0.8199	 0.2840
AM	 0.7871	 0.2930
AN	 0.7605	 0.3330
AU	 0.9556	 0.4410
AX	 0.6542	 0.2400
Ad	 0.8242	 0.3120
Af	 0.7927	 0.2740
Ag	 0.8125	 0.2550
BC	 0.7589	 0.2830
BD	 0.8090	 0.3110
BF	 0.7792	 0.2220
BG	 0.6552	 0.2250
BH	 0.7931	 0.2730
BK	 0.8303	 0.3040
BL	 0.8302	 0.2900
BM	 0.7989	 0.2910
BN	 0.7325	 0.3180
BU	 0.9778	 0.4590
BX	 0.5667	 0.2260
Bd	 0.8136	 0.3090
Bf	 0.7790	 0.2820
Bg	 0.8640	 0.2740
CC	 0.8135	 0.2900
CD	 0.8109	 0.3160
CF	 0.7134	 0.2400
CG	 0.6568	 0.2330
CH	 0.8090	 0.2930
CK	 0.8241	 0.3160























































































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Chain	Atom inclusion	Q-score
CL	 0.8428	 0.2900
CM	 0.8107	 0.2840
CN	 0.7413	 0.3220
CU	 0.9778	 0.4900
CX	 0.5875	 0.2190
Cd	 0.8348	 0.2900
Cf	 0.7745	 0.2780
Cg	 0.8566	 0.2580
DC	 0.8252	 0.2920
DD	 0.8155	 0.3020
DF	 0.7728	 0.2310
DG	 0.7184	 0.2500
DH	 0.7957	 0.2850
DK	 0.8110	 0.3100
DL	 0.8488	 0.2920
DM	 0.7846	 0.2850
DN	 0.7727	 0.3330
DU	 1.0000	 0.4410
DX	 0.7333	 0.2560
Dd	 0.8136	 0.3120
Df	 0.7198	 0.2590
Dg	 0.8382	 0.2790
EC	 0.8172	 0.3040
ED	 0.8052	 0.3150
EF	 0.7983	 0.2260
EG	 0.6691	 0.2430
EH	 0.7890	 0.2790
EK	 0.8294	 0.3130
EL	 0.8451	 0.2940
EM	 0.8094	 0.2850
EN	 0.7815	 0.3230
EU	 0.9556	 0.4260
EX	 0.5417	 0.2110
Ed	 0.8213	 0.3000
Ef	 0.7882	 0.2840
Eg	 0.8529	 0.2540
FC	 0.7839	 0.2970
FD	 0.8127	 0.3080
FF	 0.7983	 0.2380
FG	 0.6897	 0.2290
FH	 0.8060	 0.2820
FK	 0.8031	 0.3050





















































































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Chain	Atom inclusion	Q-score
FL	 0.8317	 0.2990
FM	 0.8144	 0.3010
FN	 0.7552	 0.3230
FU	 1.0000	 0.4520
FX	 0.7417	 0.2780
Fd	 0.8290	 0.3060
Ff	 0.8178	 0.2950
Fg	 0.8493	 0.2650
GC	 0.8110	 0.3010
GD	 0.8099	 0.3150
GF	 0.7771	 0.2370
GG	 0.7044	 0.2260
GH	 0.7967	 0.2810
GK	 0.8058	 0.3080
GL	 0.8236	 0.2930
GM	 0.8218	 0.2920
GN	 0.7605	 0.3200
GU	 0.9556	 0.4710
GX	 0.4750	 0.2200
Gd	 0.8223	 0.3050
Gf	 0.7745	 0.2860
Gg	 0.8529	 0.2540
HC	 0.8221	 0.2950
HD	 0.8221	 0.3190
HF	 0.7707	 0.2330
HG	 0.7044	 0.2250
HH	 0.8080	 0.2820
HK	 0.8189	 0.3070
HL	 0.8340	 0.2900
HM	 0.8287	 0.2940
HN	 0.7920	 0.3310
HU	 0.9556	 0.4480
HX	 0.5583	 0.2450
Hd	 0.8473	 0.2990
Hf	 0.8109	 0.2690
Hg	 0.7978	 0.2550
IC	 0.8135	 0.3000
ID	 0.8109	 0.3060
IF	 0.7834	 0.2030
IG	 0.7102	 0.2390
IH	 0.7911	 0.2720
IK	 0.8364	 0.3120





















































































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Chain	Atom inclusion	Q-score
IL	 0.8347	 0.2950
IM	 0.8113	 0.2800
IN	 0.7850	 0.3260
IU	 0.9333	 0.4260
IX	 0.6542	 0.2380
Id	 0.8415	 0.3010
If	 0.8292	 0.2920
Ig	 0.8603	 0.2490
JC	 0.7807	 0.2900
JD	 0.8015	 0.3070
JF	 0.7792	 0.2370
JG	 0.6593	 0.2230
JH	 0.8044	 0.2750
JK	 0.8136	 0.3050
JL	 0.8406	 0.2920
JM	 0.8101	 0.2950
JN	 0.7413	 0.3150
JU	 0.9778	 0.4640
JX	 0.6458	 0.2330
Jd	 0.8002	 0.3030
Jf	 0.8064	 0.2840
Jg	 0.8566	 0.2550
KC	 0.7853	 0.2970
KD	 0.8071	 0.3070
KF	 0.7558	 0.2220
KG	 0.6732	 0.2060
KH	 0.8075	 0.2820
KK	 0.8250	 0.3130
KL	 0.8302	 0.2990
KM	 0.8299	 0.2920
KN	 0.7517	 0.3300
KU	 0.9778	 0.4760
KX	 0.5542	 0.2180
Kd	 0.8290	 0.3060
Kf	 0.8087	 0.2910
Kg	 0.8346	 0.2420
LC	 0.8178	 0.3000
LD	 0.8081	 0.3160
LF	 0.8025	 0.2350
LG	 0.6568	 0.1890
LH	 0.7972	 0.2680
LK	 0.8259	 0.3160




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Chain	Atom inclusion	Q-score
LL	 0.8265	 0.2960
LM	 0.8038	 0.2770
LN	 0.8112	 0.3390
LU	 0.9778	 0.4700
LX	 0.5500	 0.2410
Ld	 0.8290	 0.2960
Lf	 0.8132	 0.2690
Lg	 0.8529	 0.2520
MC	 0.8190	 0.3040
MD	 0.7856	 0.3160
MF	 0.8132	 0.2280
MG	 0.6765	 0.2120
MH	 0.8003	 0.2760
MK	 0.8040	 0.3160
ML	 0.8095	 0.2910
MM	 0.7939	 0.2850
MN	 0.7762	 0.3210
MU	 0.9111	 0.4900
MX	 0.6333	 0.2400
Md	 0.8165	 0.2970
Mf	 0.8109	 0.2730
Mg	 0.8603	 0.2570
NG	 0.6617	 0.2190
OG	 0.6831	 0.2440
PG	 0.7069	 0.2390
VF	 0.7410	 0.2360
VG	 0.8199	 0.2480
VH	 0.6663	 0.2670
VX	 0.6583	 0.2130
WF	 0.7813	 0.2360
WG	 0.8382	 0.2530
WH	 0.6179	 0.2580
WX	 0.6542	 0.2510
XF	 0.7707	 0.2190
XG	 0.7978	 0.2540
XH	 0.5891	 0.2530
XX	 0.6667	 0.2320
YF	 0.7941	 0.2290
YG	 0.8088	 0.2510
YH	 0.7005	 0.2540
YX	 0.6208	 0.2590
ZF	 0.8344	 0.2440

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Chain	Atom inclusion	Q-score
ZG	 0.7721	 0.2470
ZH	 0.5397	 0.2220
ZX	 0.5625	 0.2240