



## Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 06:02 AM EST

PDB ID : 7MUC  
EMDB ID : EMD-24004  
Title : Legionella pneumophila Dot/Icm T4SS C1 Reconstruction  
Authors : Sheedlo, M.J.; Durie, C.L.; Swanson, M.; Lacy, D.B.; Ohi, M.D.  
Deposited on : 2021-05-14  
Resolution : 3.80 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:

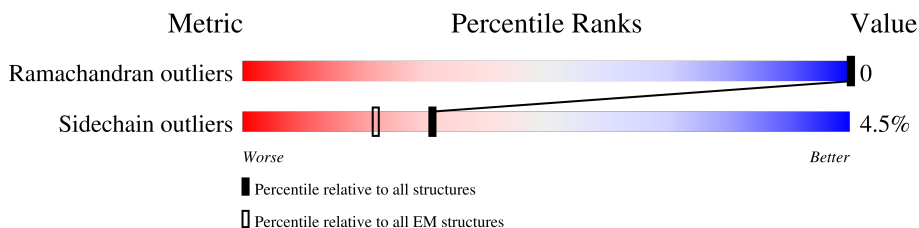
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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















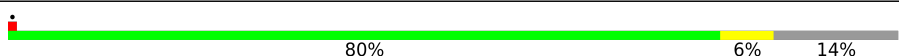
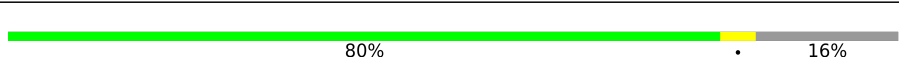
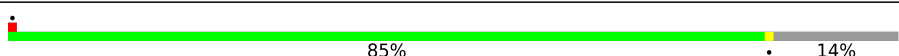

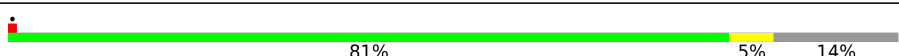
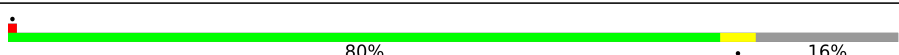
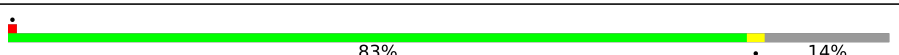
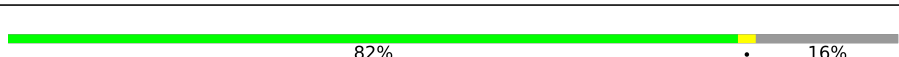
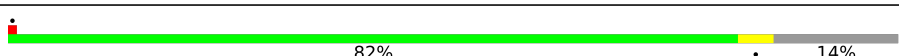



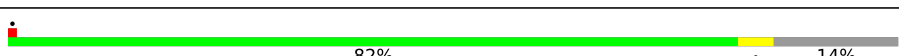
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AC	303	66%    30%
1	BC	303	66%    30%
1	CC	303	67%    30%
1	DC	303	67%    30%
1	EC	303	67%    30%
1	FC	303	66%    30%
1	GC	303	66%    30%
1	HC	303	67%    30%
1	IC	303	66%    30%

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Mol	Chain	Length	Quality of chain
1	JC	303	 67% 30%
1	KC	303	 66% 30%
1	LC	303	 67% 30%
1	MC	303	 66% 30%
2	AD	163	 82% 14%
2	Ad	163	 79% 5% 16%
2	BD	163	 81% 5% 14%
2	Bd	163	 79% 5% 16%
2	CD	163	 82% 14%
2	Cd	163	 77% 7% 16%
2	DD	163	 82% 14%
2	Dd	163	 80% 16%
2	ED	163	 80% 6% 14%
2	Ed	163	 80% 16%
2	FD	163	 85% 14%
2	Fd	163	 79% 5% 16%
2	GD	163	 81% 5% 14%
2	Gd	163	 80% 16%
2	HD	163	 83% 14%
2	Hd	163	 82% 16%
2	ID	163	 82% 14%
2	Id	163	 80% 16%
2	JD	163	 82% 14%
2	Jd	163	 82% 16%
2	KD	163	 82% 14%



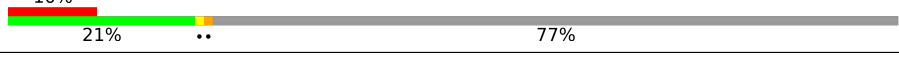




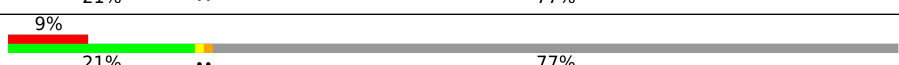


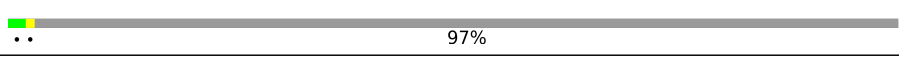
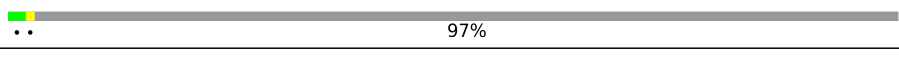
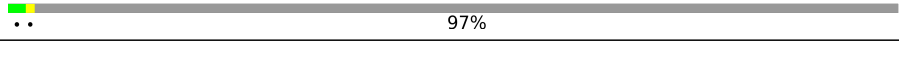
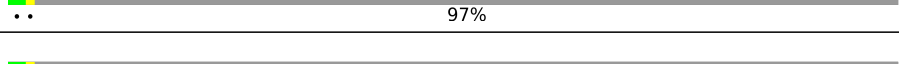
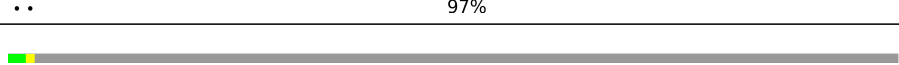
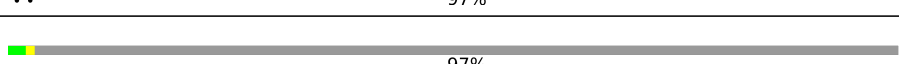
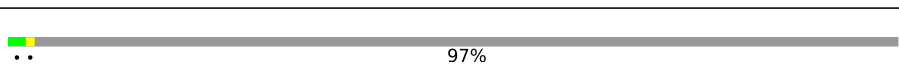
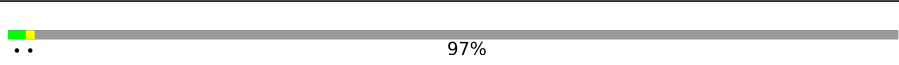
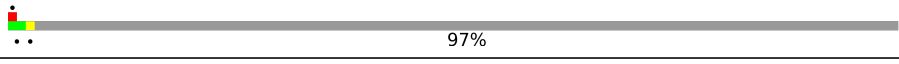
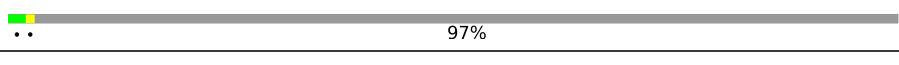
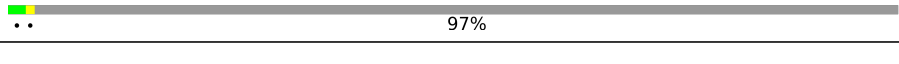
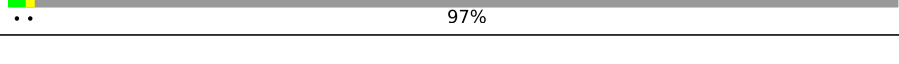
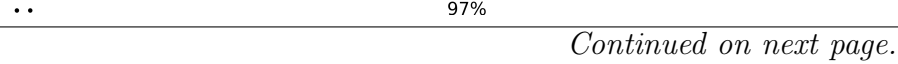


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Mol	Chain	Length	Quality of chain
2	Kd	163	79% 5% 16%
2	LD	163	82% 14%
2	Ld	163	80% 16%
2	MD	163	82% 14%
2	Md	163	80% 16%
3	AF	269	9% 21% 77%
3	Af	269	22% 78%
3	BF	269	10% 21% 77%
3	Bf	269	22% 78%
3	CF	269	11% 21% 77%
3	Cf	269	22% 78%
3	DF	269	10% 21% 77%
3	Df	269	22% 78%
3	EF	269	12% 21% 77%
3	Ef	269	22% 78%
3	FF	269	11% 21% 77%
3	Ff	269	22% 78%
3	GF	269	10% 21% 77%
3	Gf	269	22% 78%
3	HF	269	11% 21% 77%
3	Hf	269	22% 78%
3	IF	269	10% 21% 77%
3	If	269	22% 78%
3	JF	269	9% 21% 77%
3	Jf	269	22% 78%

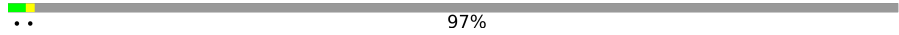
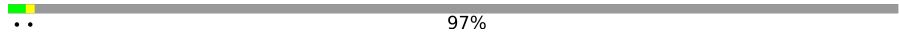
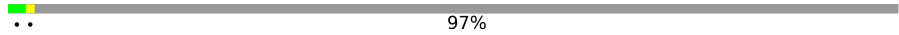
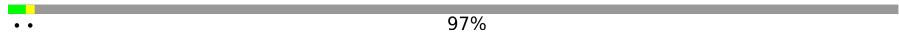





















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Mol	Chain	Length	Quality of chain
3	KF	269	 6% 21% .. 77%
3	Kf	269	 22% .. 78%
3	LF	269	 10% 21% .. 77%
3	Lf	269	 22% .. 78%
3	MF	269	 10% 21% .. 77%
3	Mf	269	 22% .. 78%
3	VF	269	 7% 21% .. 77%
3	WF	269	 10% 21% .. 77%
3	XF	269	 9% 21% .. 77%
3	YF	269	 9% 21% .. 77%
3	ZF	269	 10% 21% .. 77%
4	AG	1048	 .. 97%
4	BG	1048	 .. 97%
4	CG	1048	 .. 97%
4	DG	1048	 .. 97%
4	EG	1048	 .. 97%
4	FG	1048	 .. 97%
4	GG	1048	 .. 97%
4	HG	1048	 .. 97%
4	IG	1048	 .. 97%
4	JG	1048	 .. 97%
4	KG	1048	 .. 97%
4	LG	1048	 .. 97%
4	MG	1048	 .. 97%
4	VG	1048	 .. 97%

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Mol	Chain	Length	Quality of chain
4	WG	1048	 97%
4	XG	1048	 97%
4	YG	1048	 97%
4	ZG	1048	 97%
5	AH	361	 68%
5	BH	361	 68%
5	CH	361	 69%
5	DH	361	 69%
5	EH	361	 68%
5	FH	361	 69%
5	GH	361	 67%
5	HH	361	 68%
5	IH	361	 69%
5	JH	361	 68%
5	KH	361	 68%
5	LH	361	 68%
5	MH	361	 69%
5	VH	361	 65%
5	WH	361	 64%
5	XH	361	 66%
5	YH	361	 65%
5	ZH	361	 63%
6	AK	189	 75%
6	BK	189	 75%
6	CK	189	 75%

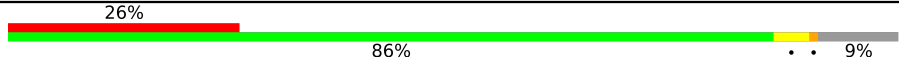
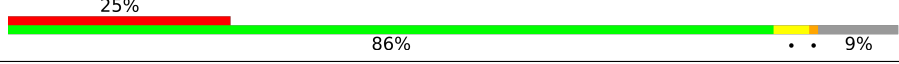
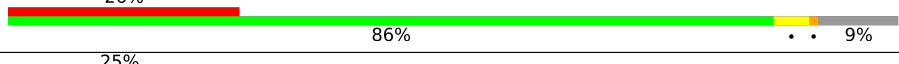


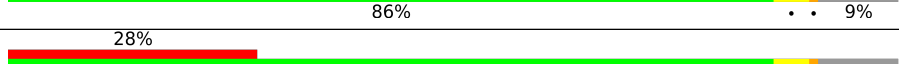
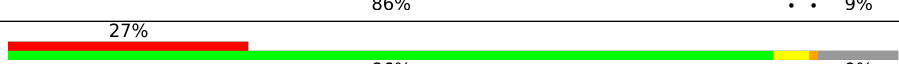
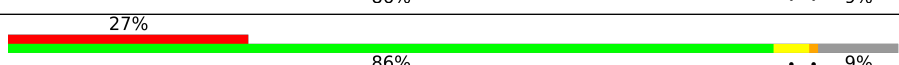
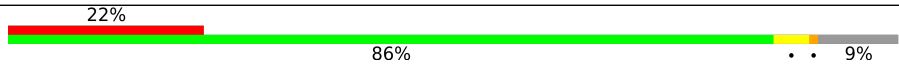


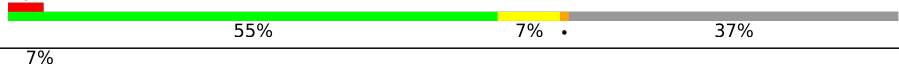
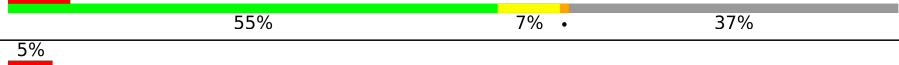

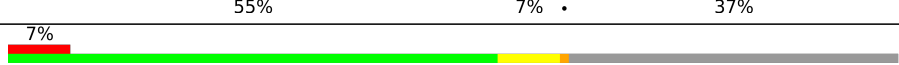







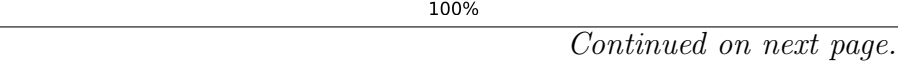


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Mol	Chain	Length	Quality of chain
6	DK	189	74% 5% 20%
6	EK	189	75% 5% 20%
6	FK	189	75% 5% 20%
6	GK	189	75% 5% 20%
6	HK	189	75% 5% 20%
6	IK	189	74% 5% 20%
6	JK	189	75% 5% 20%
6	KK	189	75% 5% 20%
6	LK	189	75% 5% 20%
6	MK	189	75% 5% 20%
7	AL	249	65% 5% 31%
7	BL	249	65% 5% 31%
7	CL	249	65% 5% 31%
7	DL	249	65% 5% 31%
7	EL	249	65% 5% 31%
7	FL	249	65% 5% 31%
7	GL	249	65% 5% 31%
7	HL	249	65% 5% 31%
7	IL	249	65% 5% 31%
7	JL	249	65% 5% 31%
7	KL	249	65% 5% 31%
7	LL	249	65% 5% 31%
7	ML	249	65% 5% 31%
8	AM	320	25% 86% 5% 9%
8	BM	320	24% 86% 5% 9%

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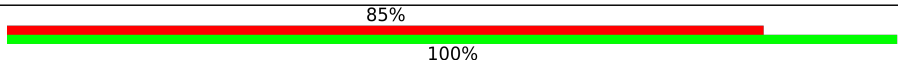
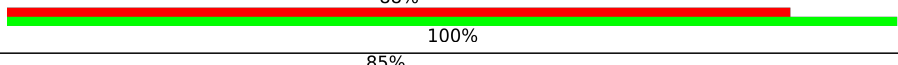

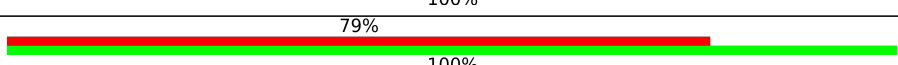
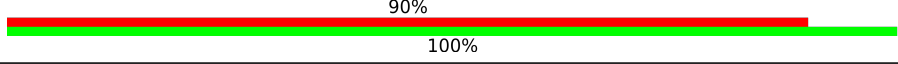
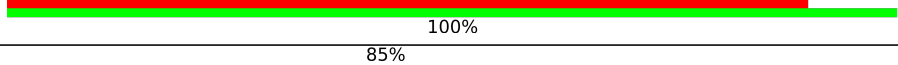
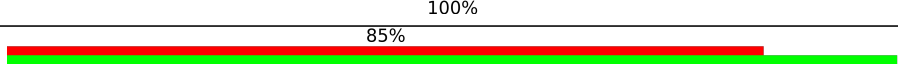
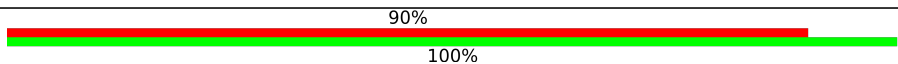
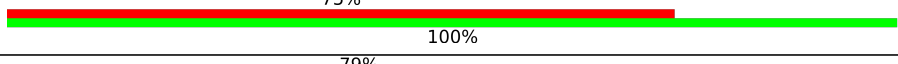
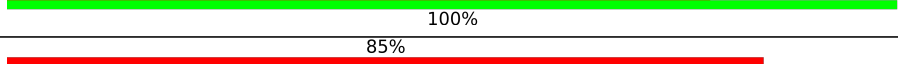
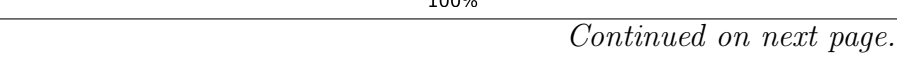


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Mol	Chain	Length	Quality of chain
8	CM	320	
8	DM	320	
8	EM	320	
8	FM	320	
8	GM	320	
8	HM	320	
8	IM	320	
8	JM	320	
8	KM	320	
8	LM	320	
8	MM	320	
9	AN	124	
9	BN	124	
9	CN	124	
9	DN	124	
9	EN	124	
9	FN	124	
9	GN	124	
9	HN	124	
9	IN	124	
9	JN	124	
9	KN	124	
9	LN	124	
9	MN	124	
10	AU	9	

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Mol	Chain	Length	Quality of chain
10	BU	9	 100%
10	CU	9	 100%
10	DU	9	 100%
10	EU	9	 100%
10	FU	9	 100%
10	GU	9	 100%
10	HU	9	 100%
10	IU	9	 100%
10	JU	9	 100%
10	KU	9	 100%
10	LU	9	 100%
10	MU	9	 100%
11	AX	48	 85% 100%
11	BX	48	 88% 100%
11	CX	48	 85% 100%
11	DX	48	 81% 100%
11	EX	48	 79% 100%
11	FX	48	 90% 100%
11	GX	48	 90% 100%
11	HX	48	 85% 100%
11	IX	48	 85% 100%
11	JX	48	 90% 100%
11	KX	48	 75% 100%
11	LX	48	 79% 100%
11	MX	48	 85% 100%

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Mol	Chain	Length	Quality of chain
11	VX	48	81%  100%
11	WX	48	88%  100%
11	XX	48	83%  100%
11	YX	48	83%  100%
11	ZX	48	83%  100%

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 180380 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DotC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AC	213	1685	1068	295	316	6	0	0
1	BC	213	1685	1068	295	316	6	0	0
1	CC	213	1685	1068	295	316	6	0	0
1	DC	213	1685	1068	295	316	6	0	0
1	EC	213	1685	1068	295	316	6	0	0
1	FC	213	1685	1068	295	316	6	0	0
1	GC	213	1685	1068	295	316	6	0	0
1	HC	213	1685	1068	295	316	6	0	0
1	IC	213	1685	1068	295	316	6	0	0
1	JC	213	1685	1068	295	316	6	0	0
1	KC	213	1685	1068	295	316	6	0	0
1	LC	213	1685	1068	295	316	6	0	0
1	MC	213	1685	1068	295	316	6	0	0

- Molecule 2 is a protein called DotD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AD	140	1086	692	185	206	3	0	0
2	Ad	137	1058	672	182	202	2	0	0

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ld	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		
2	MD	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		
2	Md	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		

- Molecule 3 is a protein called DotF.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
3	Af	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
3	BF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
3	Bf	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
3	CF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
3	Cf	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
3	DF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
3	Df	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
3	EF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
3	Ef	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
3	FF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
3	Ff	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
3	GF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
3	Gf	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
3	HF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
3	Hf	59	Total	C	N	O	S	0	0
			449	290	77	81	1		

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

- Molecule 4 is a protein called IcmE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	BG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	CG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	DG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	EG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	FG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	GG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	HG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	IG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	JG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	KG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	LG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	MG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	VG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	WG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	XG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	YG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	ZG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		

- Molecule 5 is a protein called Type IV secretion protein IcmK.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
5	BH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
5	CH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
5	DH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
5	EH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		

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

- Molecule 6 is a protein called Inner membrane lipoprotein YiaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AK	151	Total	C	N	O	S	0	0
			1175	747	209	215	4		
6	BK	151	Total	C	N	O	S	0	0
			1175	747	209	215	4		
6	CK	151	Total	C	N	O	S	0	0
			1175	747	209	215	4		
6	DK	151	Total	C	N	O	S	0	0
			1175	747	209	215	4		
6	EK	151	Total	C	N	O	S	0	0
			1175	747	209	215	4		
6	FK	151	Total	C	N	O	S	0	0
			1175	747	209	215	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	GK	151	Total	C	N	O	S	0	0
			1175	747	209	215	4		
6	HK	151	Total	C	N	O	S	0	0
			1175	747	209	215	4		
6	IK	151	Total	C	N	O	S	0	0
			1175	747	209	215	4		
6	JK	151	Total	C	N	O	S	0	0
			1175	747	209	215	4		
6	KK	151	Total	C	N	O	S	0	0
			1175	747	209	215	4		
6	LK	151	Total	C	N	O	S	0	0
			1175	747	209	215	4		
6	MK	151	Total	C	N	O	S	0	0
			1175	747	209	215	4		

- Molecule 7 is a protein called Outer membrane protein, OmpA family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		
7	BL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		
7	CL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		
7	DL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		
7	EL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		
7	FL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		
7	GL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		
7	HL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		
7	IL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		
7	JL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		
7	KL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		
7	LL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	ML	173	1388	877	253	253	5	0	0

- Molecule 8 is a protein called DUF2807 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AM	292	2320	1467	416	433	4	0	0
8	BM	292	2320	1467	416	433	4	0	0
8	CM	292	2320	1467	416	433	4	0	0
8	DM	292	2320	1467	416	433	4	0	0
8	EM	292	2320	1467	416	433	4	0	0
8	FM	292	2320	1467	416	433	4	0	0
8	GM	292	2320	1467	416	433	4	0	0
8	HM	292	2320	1467	416	433	4	0	0
8	IM	292	2320	1467	416	433	4	0	0
8	JM	292	2320	1467	416	433	4	0	0
8	KM	292	2320	1467	416	433	4	0	0
8	LM	292	2320	1467	416	433	4	0	0
8	MM	292	2320	1467	416	433	4	0	0

- Molecule 9 is a protein called Neurogenic locus notch.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	AN	78	582	357	99	113	13	0	0
9	BN	78	582	357	99	113	13	0	0
9	CN	78	582	357	99	113	13	0	0

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

- Molecule 10 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	AU	9	Total 45	C 27	N 9	O 9	0	0
10	BU	9	Total 45	C 27	N 9	O 9	0	0
10	CU	9	Total 45	C 27	N 9	O 9	0	0
10	DU	9	Total 45	C 27	N 9	O 9	0	0
10	EU	9	Total 45	C 27	N 9	O 9	0	0
10	FU	9	Total 45	C 27	N 9	O 9	0	0
10	GU	9	Total 45	C 27	N 9	O 9	0	0
10	HU	9	Total 45	C 27	N 9	O 9	0	0
10	IU	9	Total 45	C 27	N 9	O 9	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	JU	9	Total	C	N	O	0	0
			45	27	9	9		
10	KU	9	Total	C	N	O	0	0
			45	27	9	9		
10	LU	9	Total	C	N	O	0	0
			45	27	9	9		
10	MU	9	Total	C	N	O	0	0
			45	27	9	9		

- Molecule 11 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	AX	48	Total	C	N	O	0	0
			240	144	48	48		
11	BX	48	Total	C	N	O	0	0
			240	144	48	48		
11	CX	48	Total	C	N	O	0	0
			240	144	48	48		
11	DX	48	Total	C	N	O	0	0
			240	144	48	48		
11	EX	48	Total	C	N	O	0	0
			240	144	48	48		
11	FX	48	Total	C	N	O	0	0
			240	144	48	48		
11	GX	48	Total	C	N	O	0	0
			240	144	48	48		
11	HX	48	Total	C	N	O	0	0
			240	144	48	48		
11	IX	48	Total	C	N	O	0	0
			240	144	48	48		
11	JX	48	Total	C	N	O	0	0
			240	144	48	48		
11	KX	48	Total	C	N	O	0	0
			240	144	48	48		
11	LX	48	Total	C	N	O	0	0
			240	144	48	48		
11	MX	48	Total	C	N	O	0	0
			240	144	48	48		
11	VX	48	Total	C	N	O	0	0
			240	144	48	48		
11	WX	48	Total	C	N	O	0	0
			240	144	48	48		

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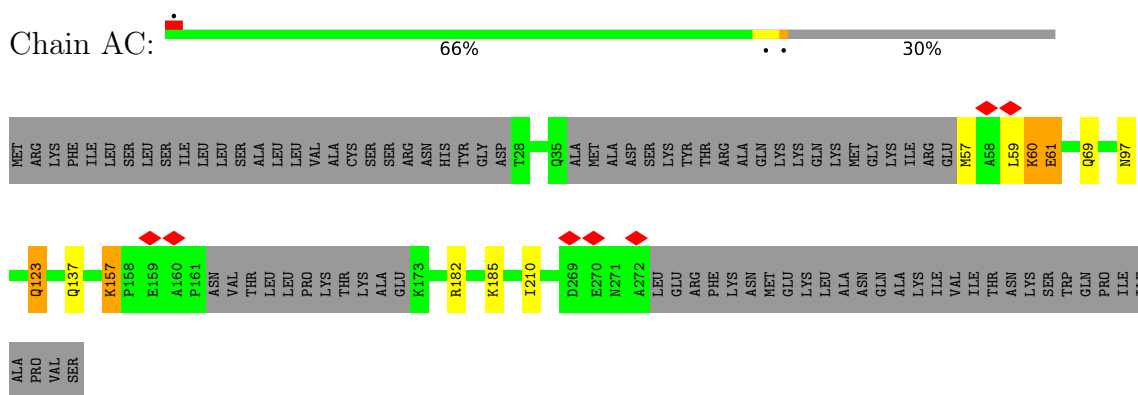
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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	XX	48	Total 240	C 144	N 48	O 48	0	0
11	YX	48	Total 240	C 144	N 48	O 48	0	0
11	ZX	48	Total 240	C 144	N 48	O 48	0	0

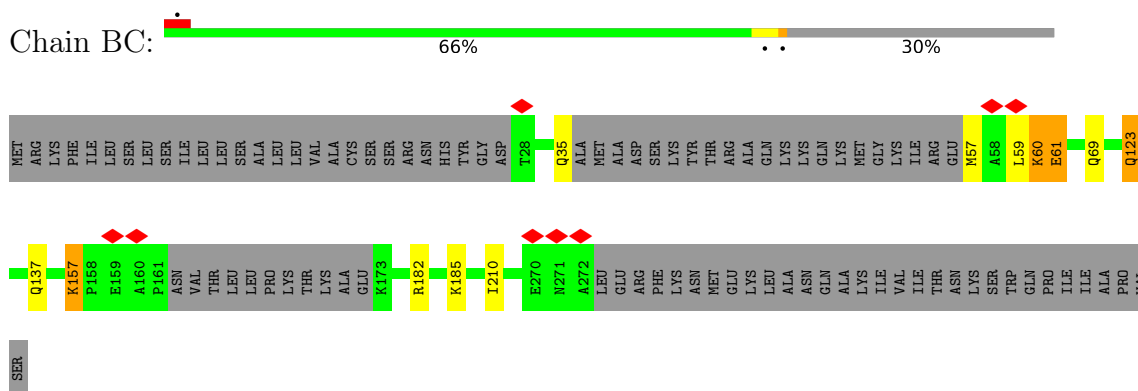
### 3 Residue-property plots [i](#)

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

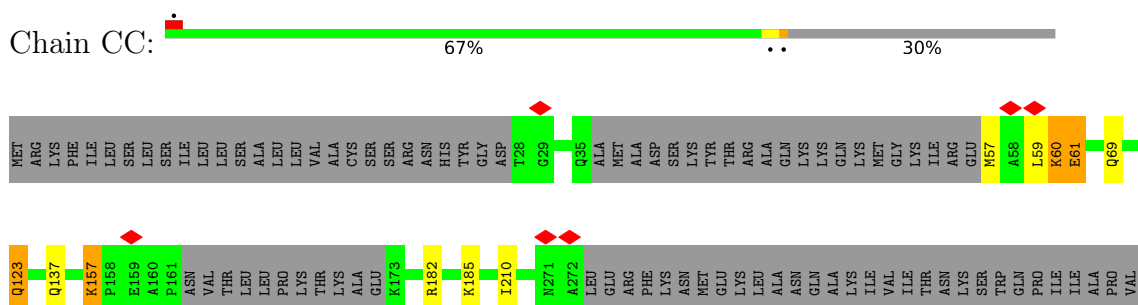
- Molecule 1: DotC



- Molecule 1: DotC

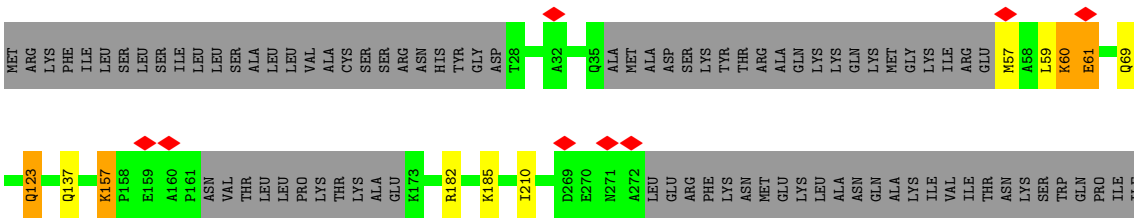


- Molecule 1: DotC



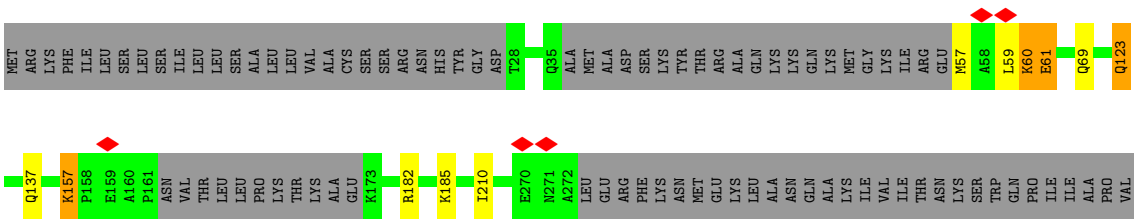
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• Molecule 1: DotC



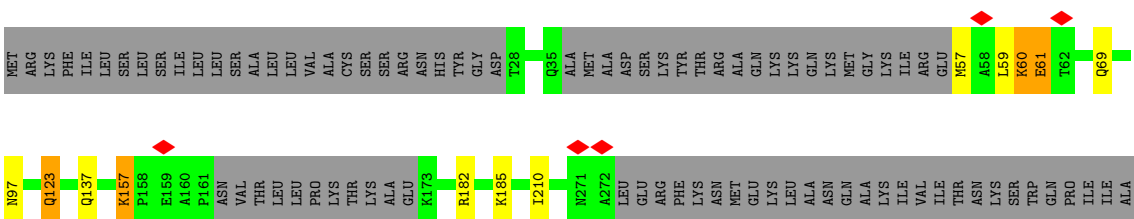
ALA PRO VAL SER

• Molecule 1: DotC



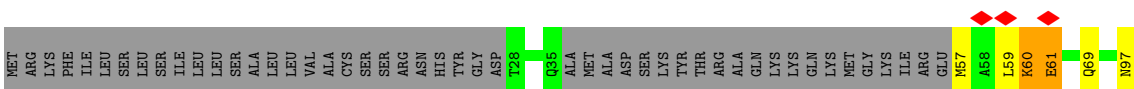
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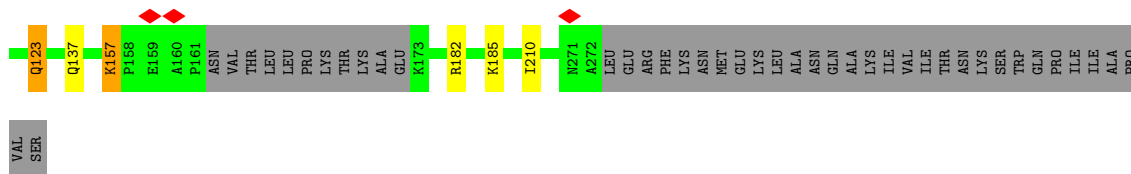
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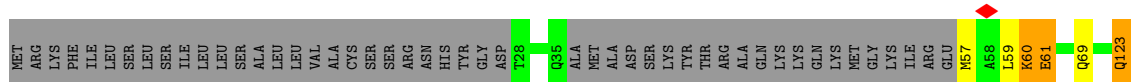
PRO VAL SER

• Molecule 1: DotC

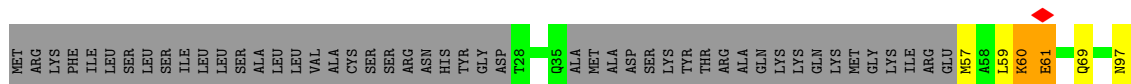




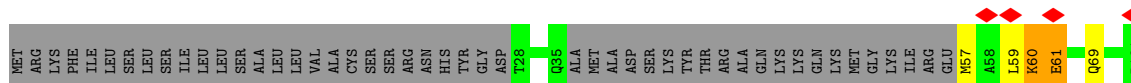
• Molecule 1: DotC



• Molecule 1: DotC



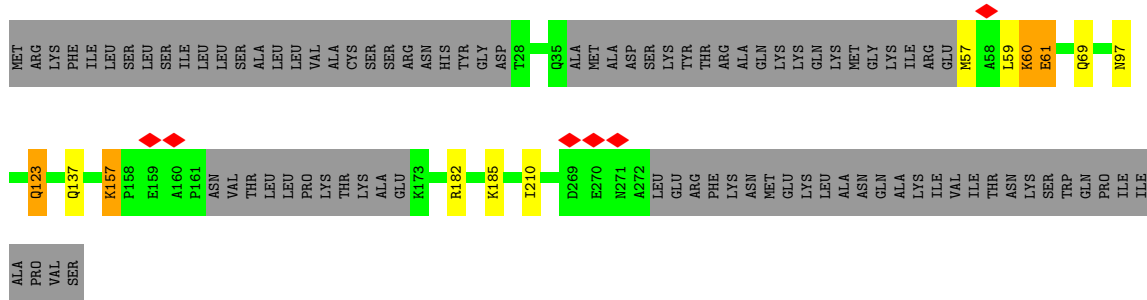
• Molecule 1: DotC



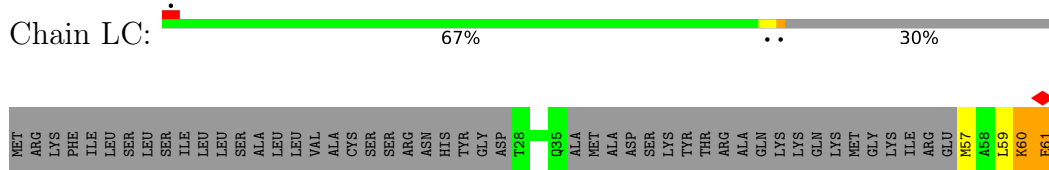
• Molecule 1: DotC







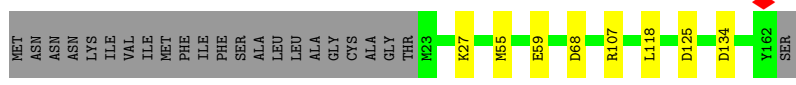
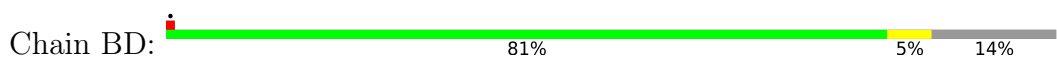
• Molecule 1: DotC



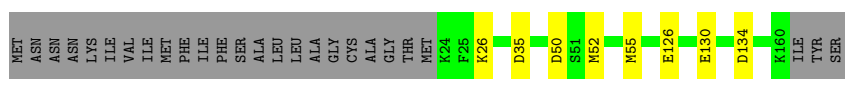
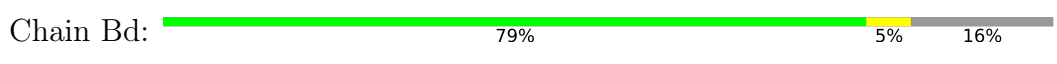
• Molecule 2: DotD



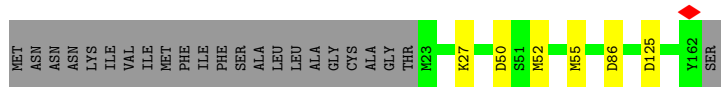
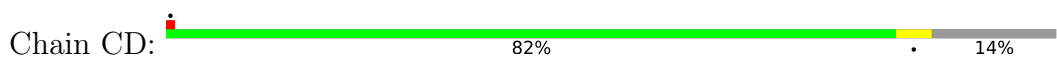
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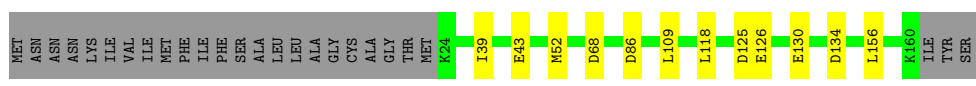
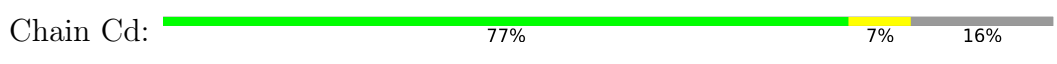
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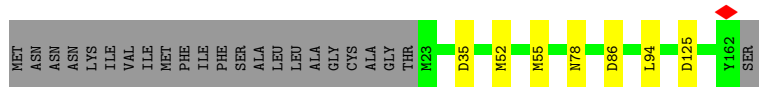
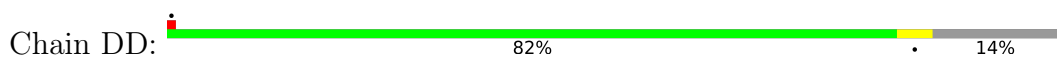
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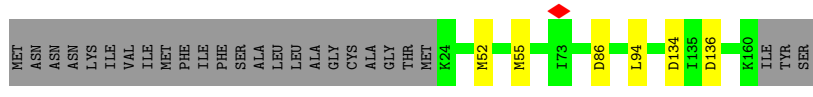
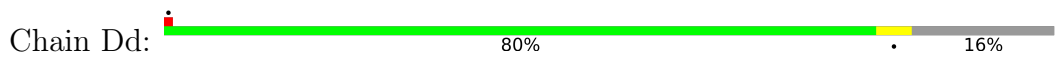
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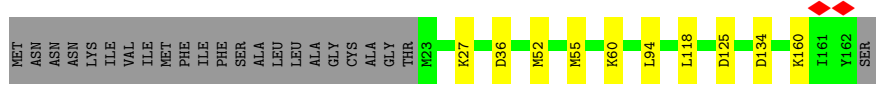
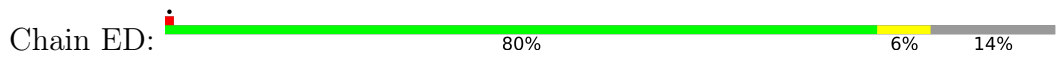
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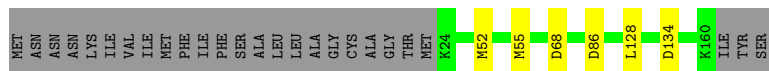
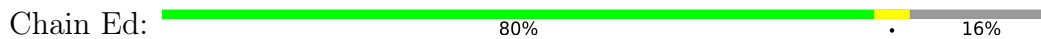
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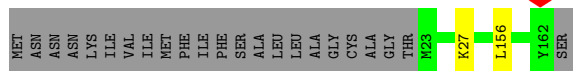
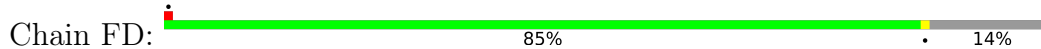
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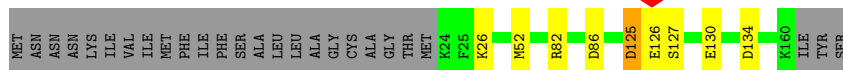
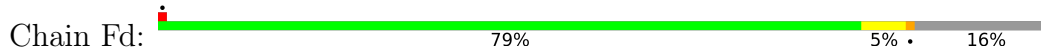
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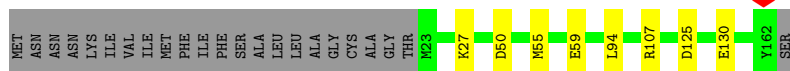
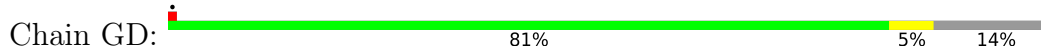
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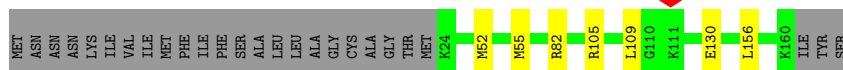
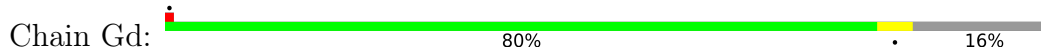
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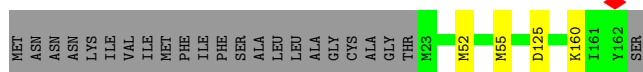
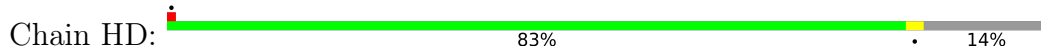
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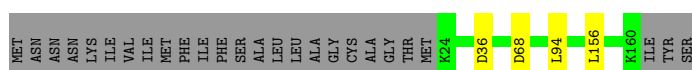
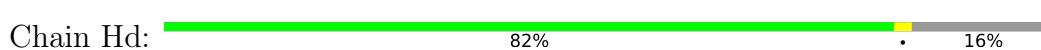
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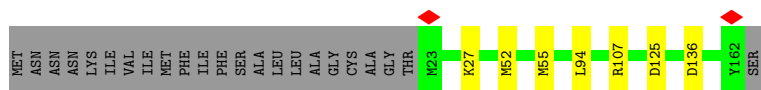
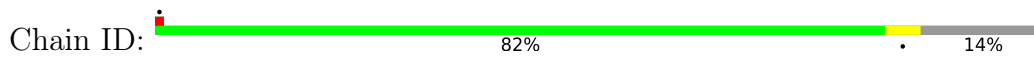
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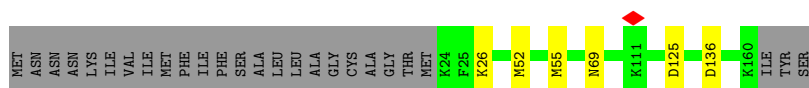
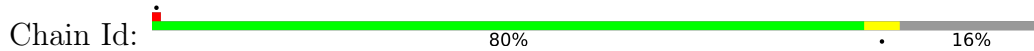
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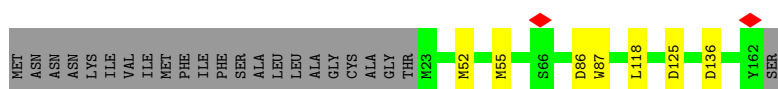
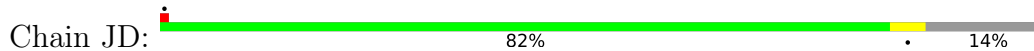
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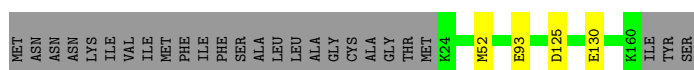
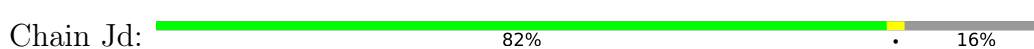
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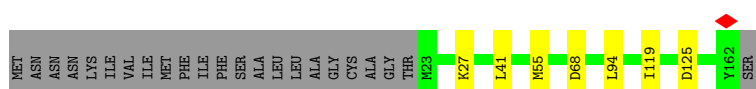
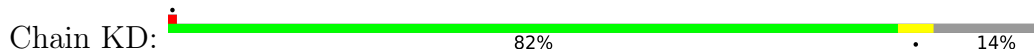
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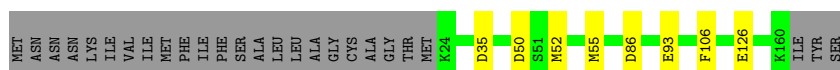
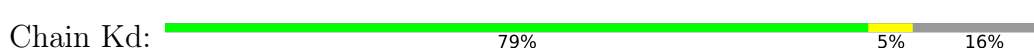
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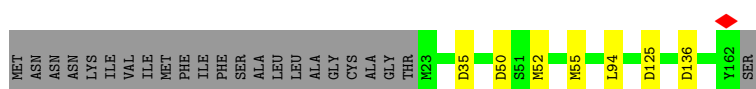
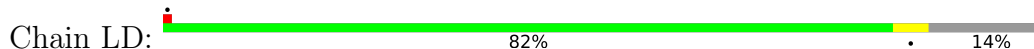
• Molecule 2: DotD



• Molecule 2: DotD

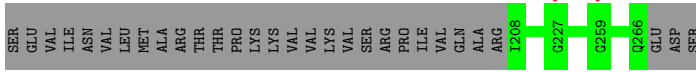


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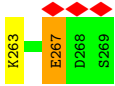
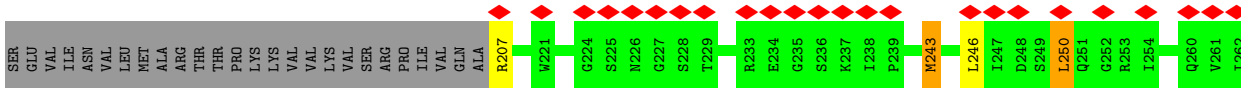
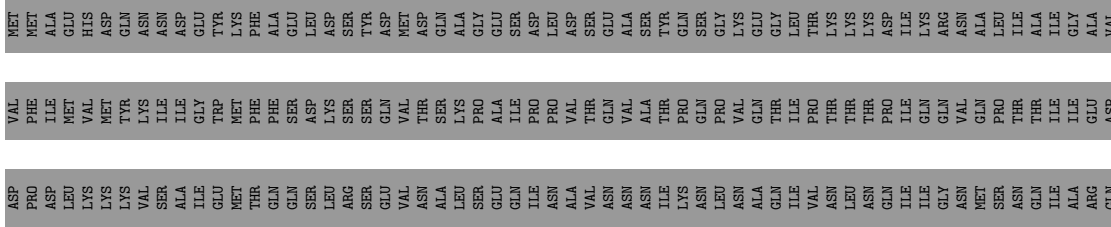


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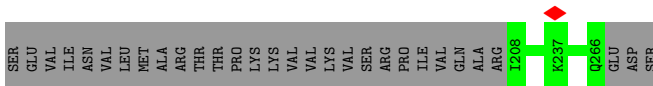
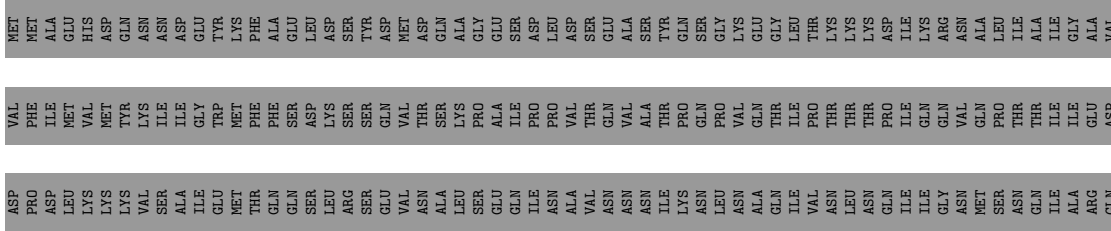




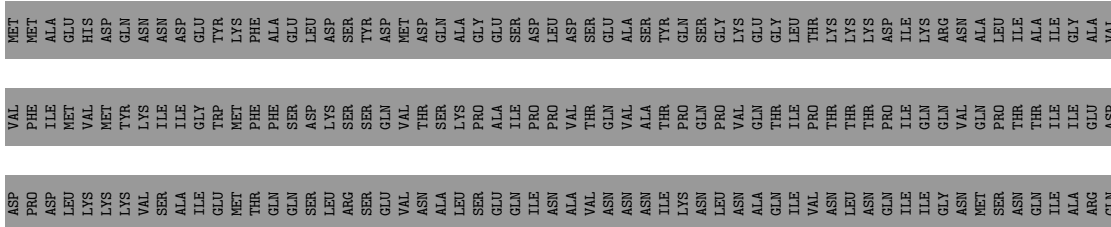
• Molecule 3: DotF



• Molecule 3: DotF



• Molecule 3: DotF











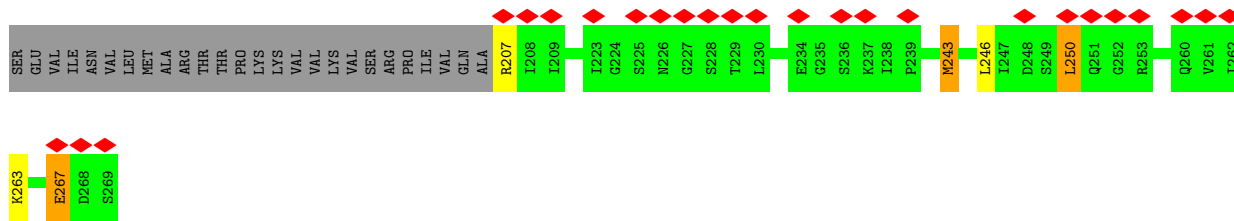




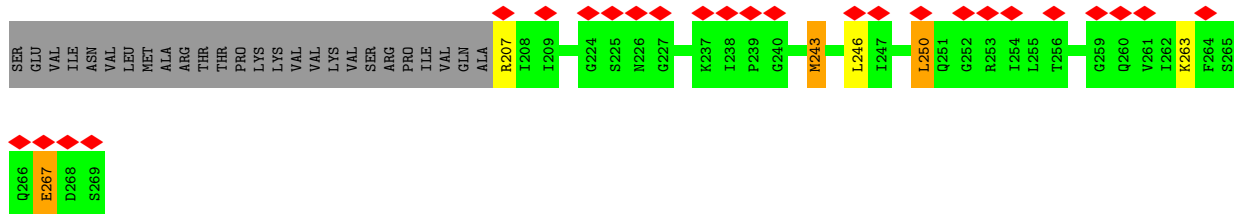
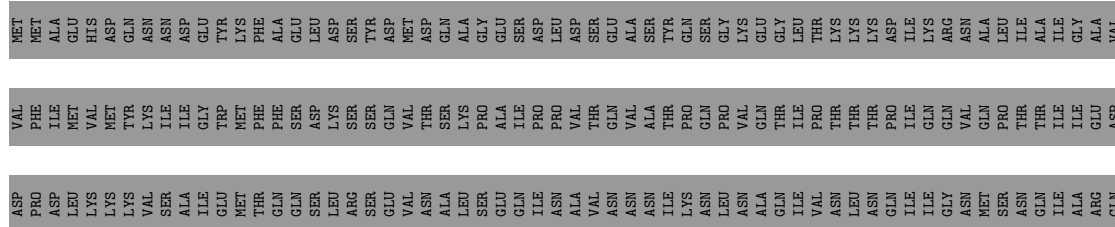




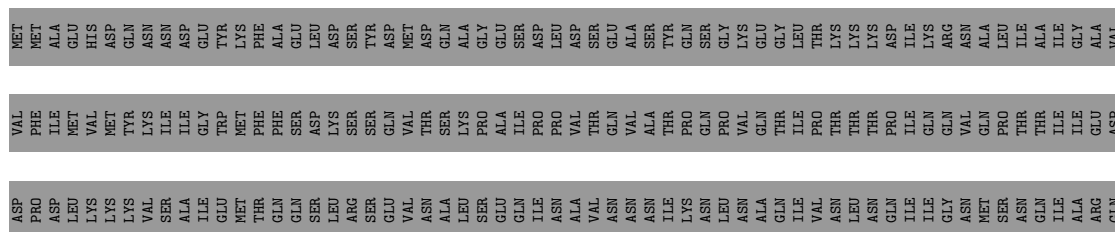




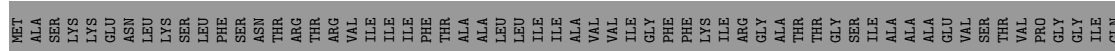
• Molecule 3: DotF



• Molecule 3: DotF



• Molecule 4: IcmE protein























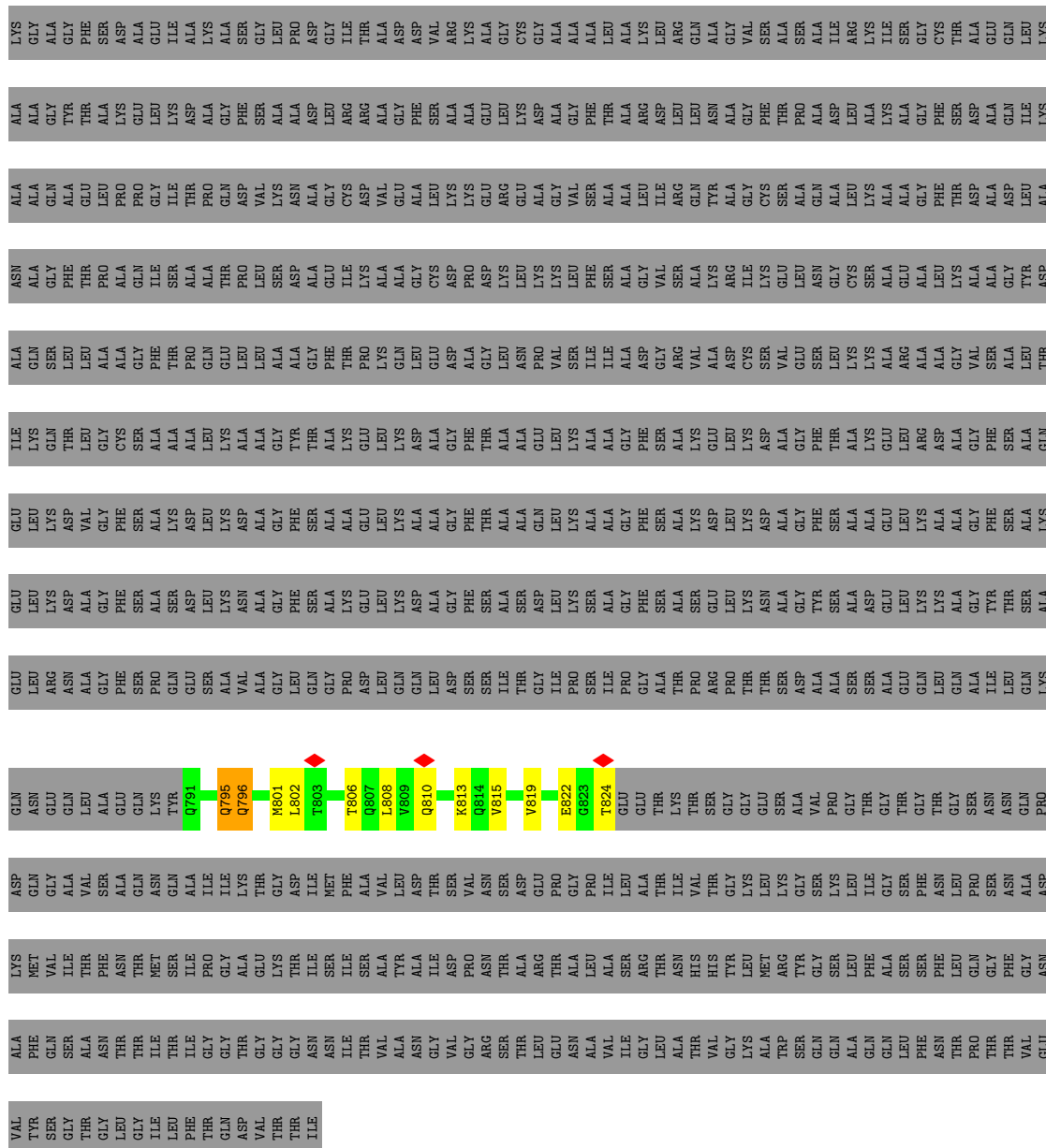






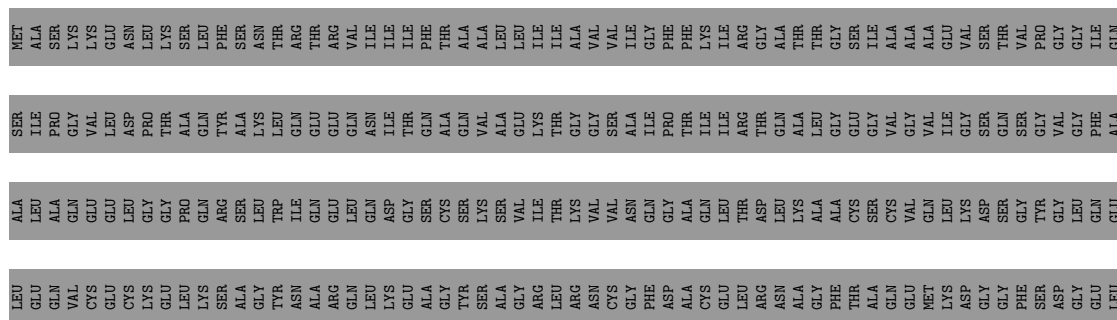






• Molecule 4: IcmE protein

Chain WG:  97%

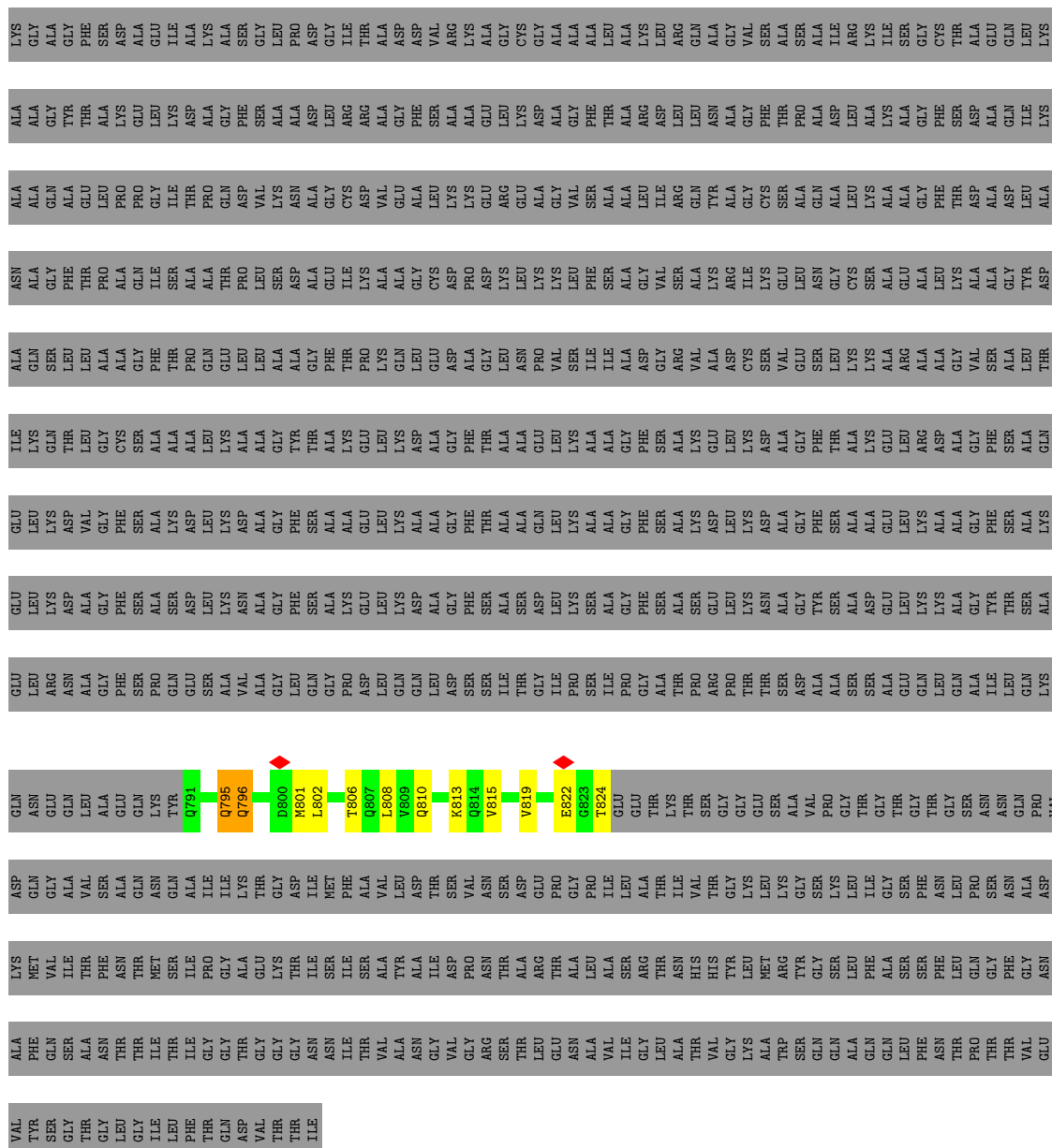




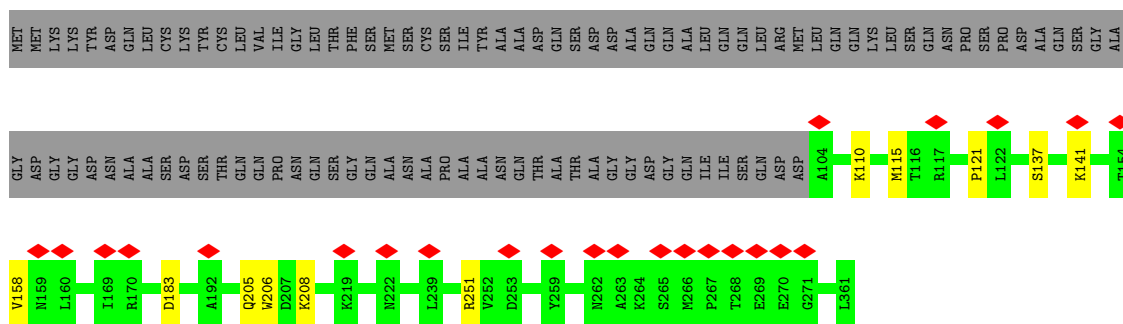






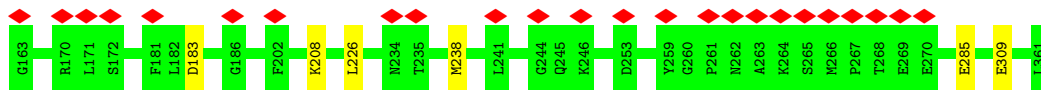


● Molecule 5: Type IV secretion protein IcmK

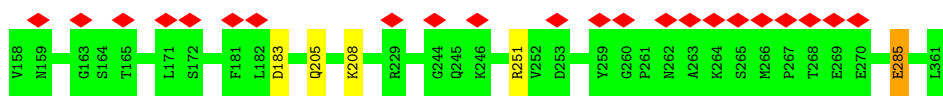
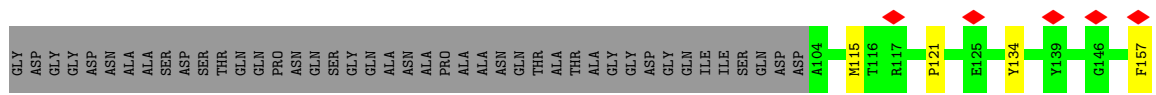
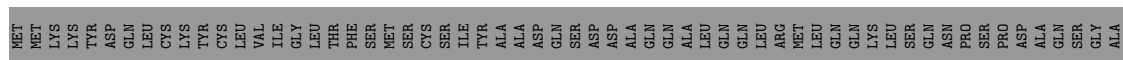


● Molecule 5: Type IV secretion protein IcmK

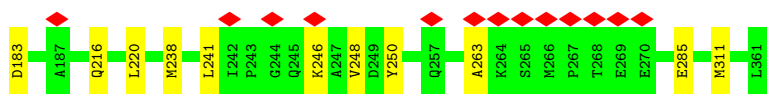
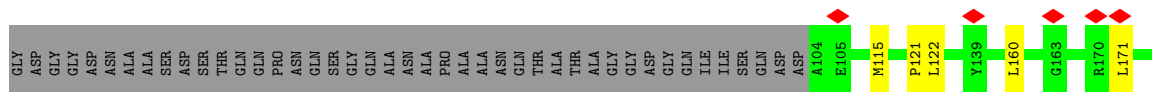
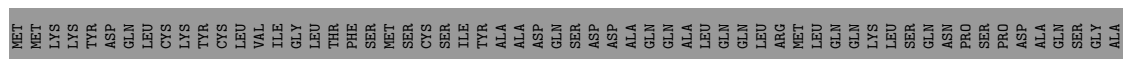




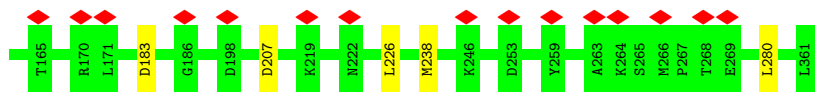
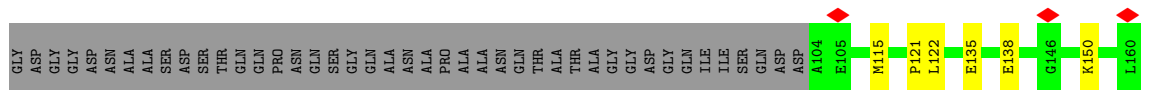
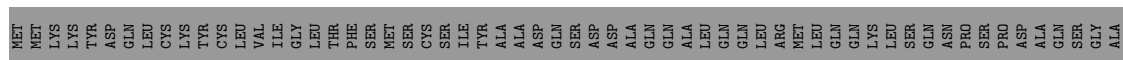
• Molecule 5: Type IV secretion protein IcmK



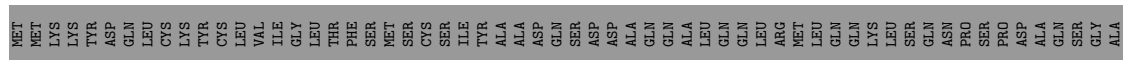
• Molecule 5: Type IV secretion protein IcmK



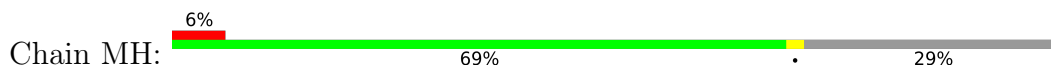
• Molecule 5: Type IV secretion protein IcmK



• Molecule 5: Type IV secretion protein IcmK







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GLY ASP GLY ASP ASN ALA ALA ASP THR GLN PRO ASN GLN THR GLN ALA ALA ILE ILE GLN LEU ASP A104 I107 D108 A111 R117 P121 L122 Y134 L160 L171

G174 L179 D183 G186 A187 D207 G244 L254 Y259 M262 A263 K264 S265 M266 E269 E270 L280 M311 L361

• Molecule 5: Type IV secretion protein IcmK



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

GLY ASP GLY ASP ASN ALA ALA SER ASP THR GLN PRO ASN GLN THR GLN ALA ALA ILE ILE GLN LEU ASP A104 A111 M115 L122 Y134 G146 M159 R170 L171 S172

L179 D183 A187 M222 L226 R229 Q257 G258 Y259 G260 A263 LYS SER MET THR ALA ASN GLU GLY THR PRO PRO ASN D278 L281 H282 E285 G286 P290 G291 S292 R293 R294 L295 V296 V297 G299 G300 D301 A302 R303 S307 R308 E309 R310

R314 K328 T329 S330 A331 G333 Q340 K341 W349 H350 G351 K352 E359 G360 LEU

• Molecule 5: Type IV secretion protein IcmK



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

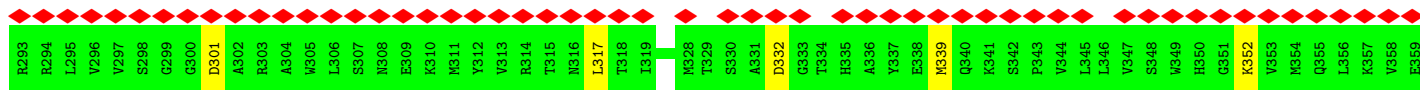
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G163 D183 G186 Q205 W206 D207 T212 K219 M238 G244 D253 L254 R255 V256 Y259 N262 A263 LYS SER MET PRO THR GLU GLY ILE ILE PRO PRO SER ASP ALA D278 L279 L280 L281 H282 V283 L284 E285 G286 V287 P288 P289 P290 S292 R293 R294 L295 V296

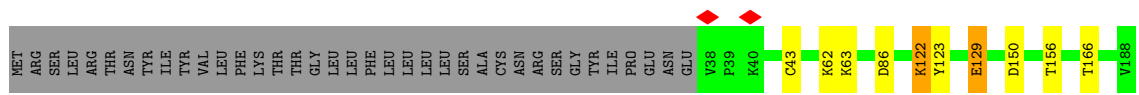
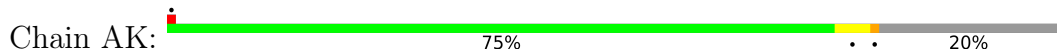
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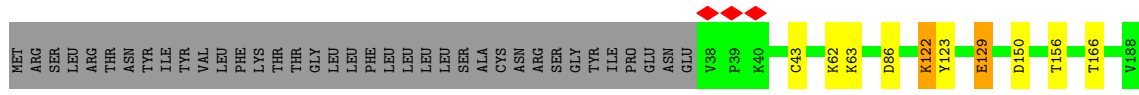
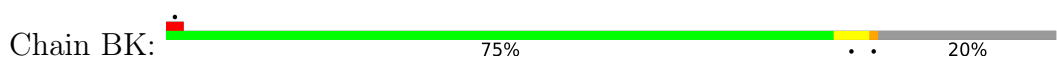




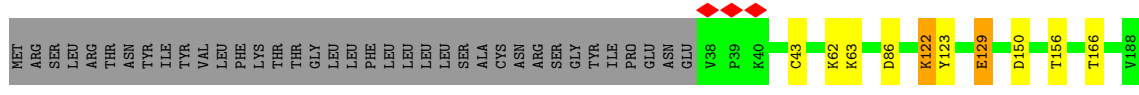
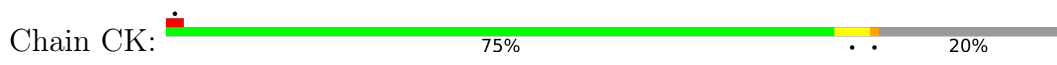
• Molecule 6: Inner membrane lipoprotein YiaD



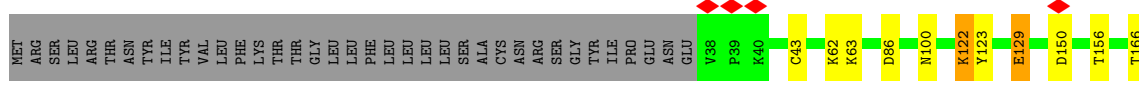
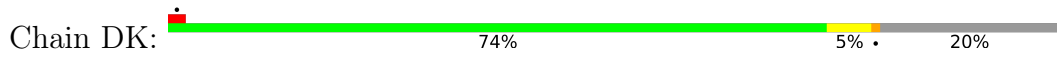
• Molecule 6: Inner membrane lipoprotein YiaD



• Molecule 6: Inner membrane lipoprotein YiaD



• Molecule 6: Inner membrane lipoprotein YiaD



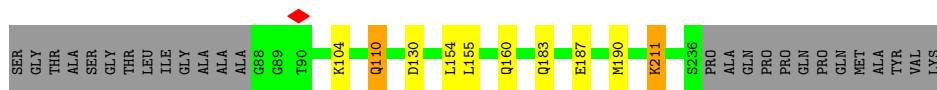
• Molecule 6: Inner membrane lipoprotein YiaD



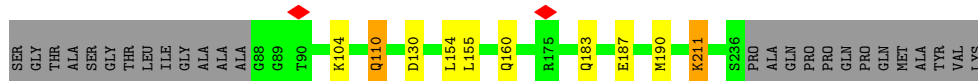
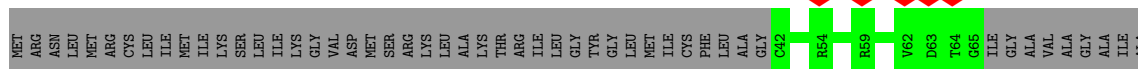




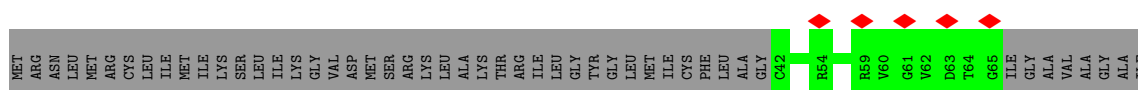




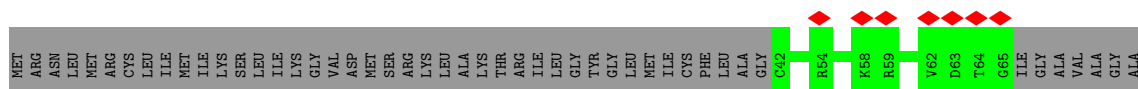
• Molecule 7: Outer membrane protein, OmpA family protein



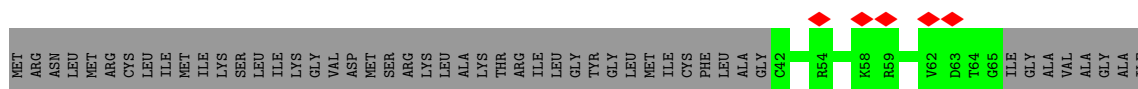
• Molecule 7: Outer membrane protein, OmpA family protein



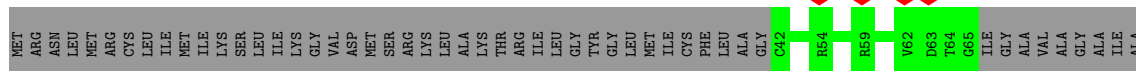
• Molecule 7: Outer membrane protein, OmpA family protein



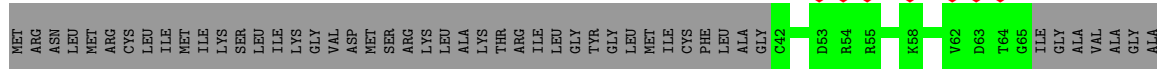
• Molecule 7: Outer membrane protein, OmpA family protein



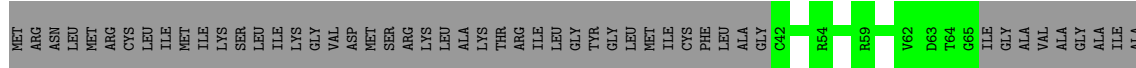
• Molecule 7: Outer membrane protein, OmpA family protein



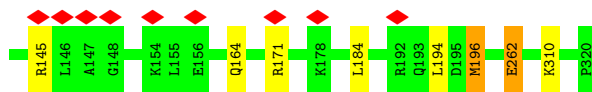
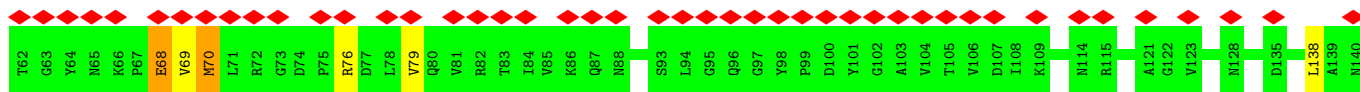
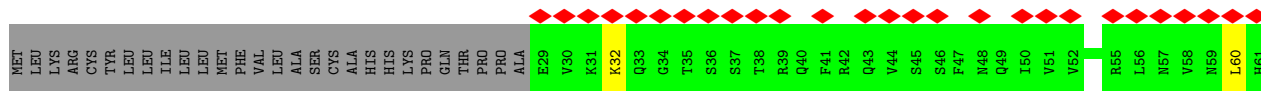
• Molecule 7: Outer membrane protein, OmpA family protein



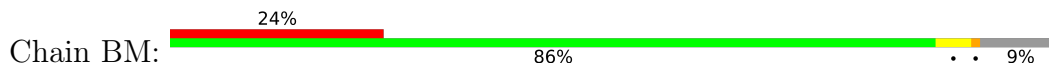
• Molecule 7: Outer membrane protein, OmpA family protein

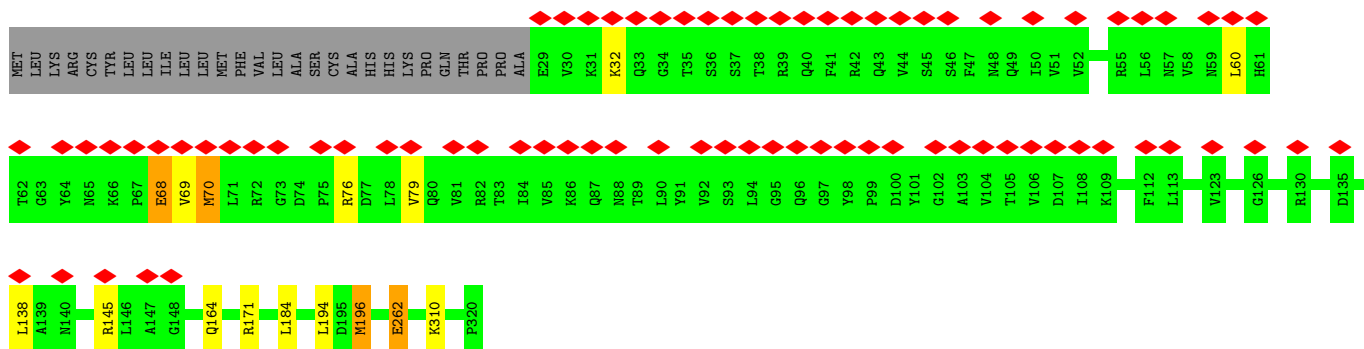


• Molecule 8: DUF2807 domain-containing protein

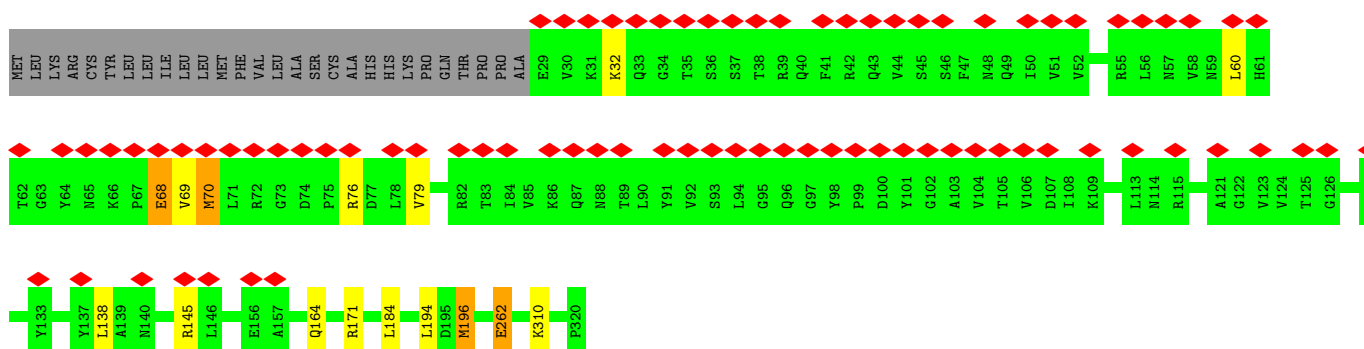
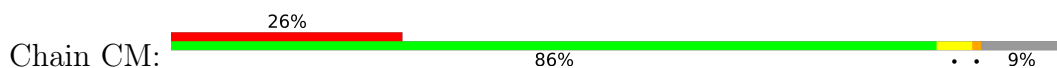


• Molecule 8: DUF2807 domain-containing protein





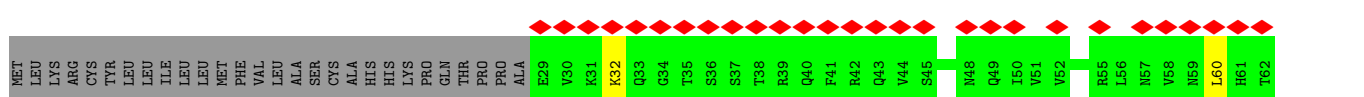
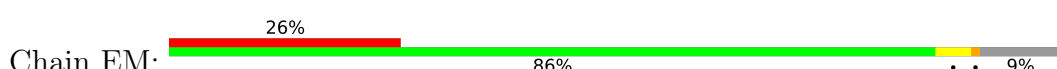
• Molecule 8: DUF2807 domain-containing protein

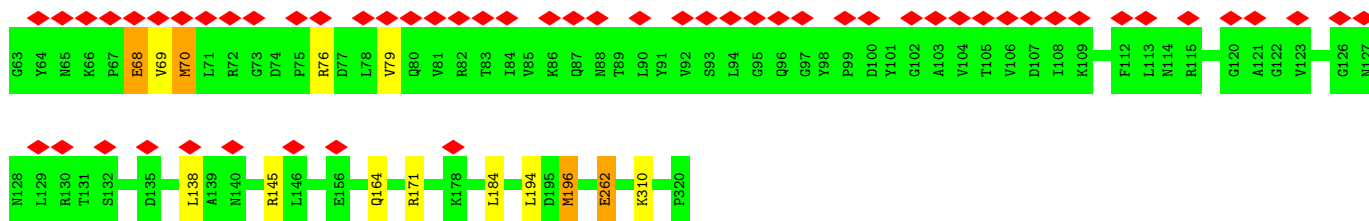


• Molecule 8: DUF2807 domain-containing protein

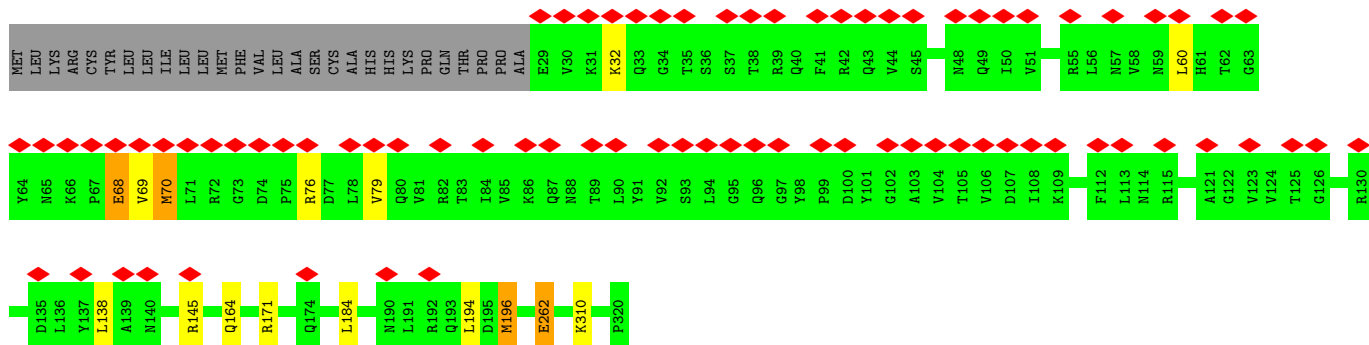
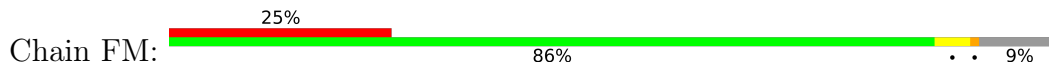


• Molecule 8: DUF2807 domain-containing protein

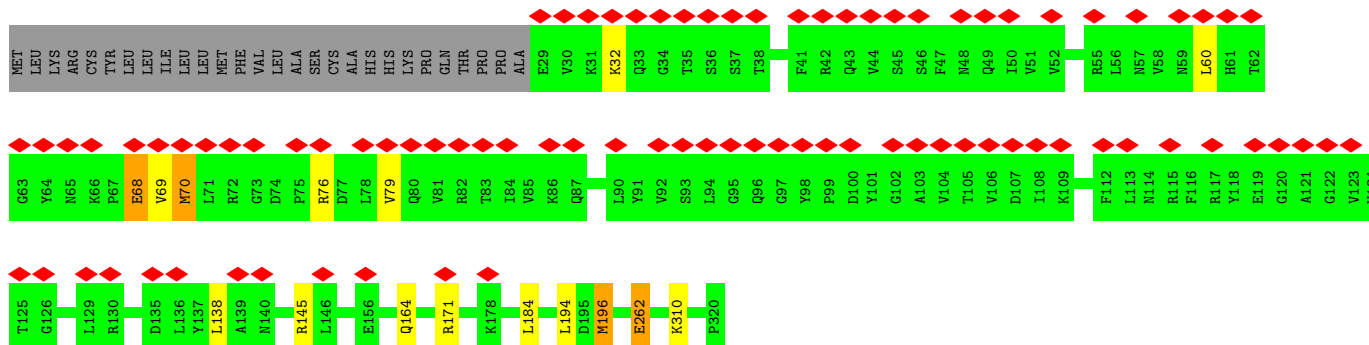
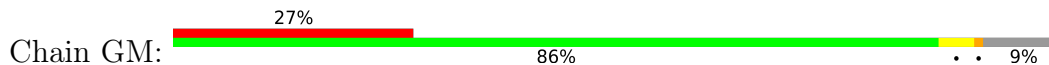




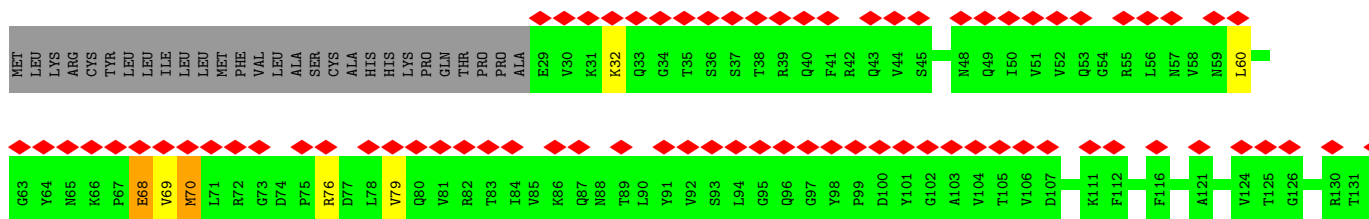
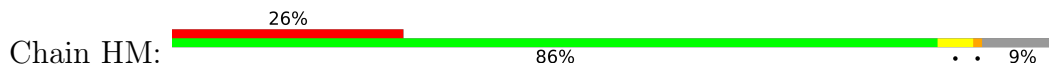
• Molecule 8: DUF2807 domain-containing protein



• Molecule 8: DUF2807 domain-containing protein

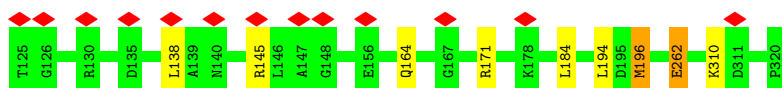
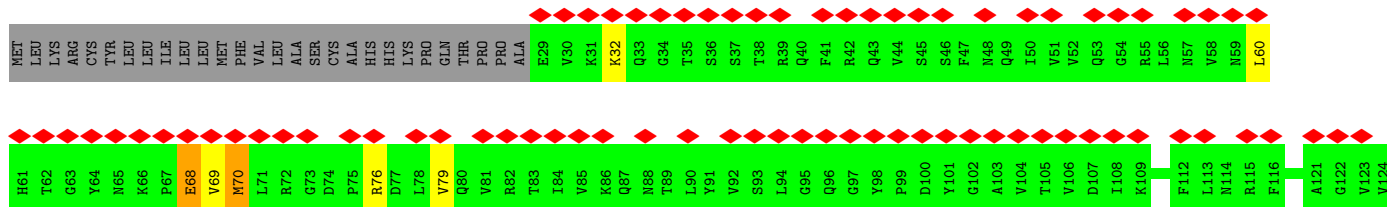
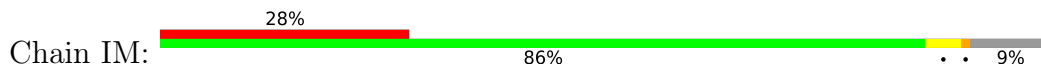


• Molecule 8: DUF2807 domain-containing protein

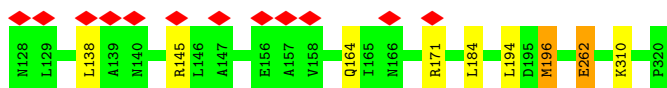
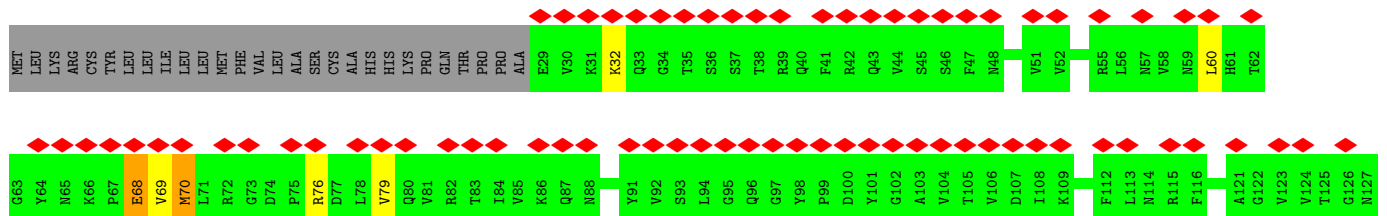
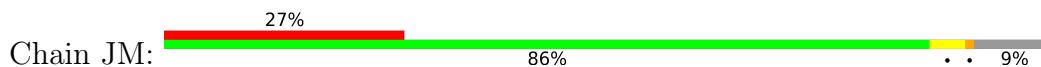




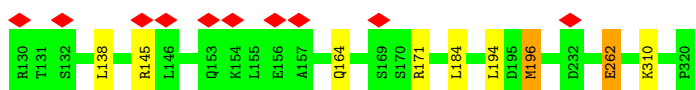
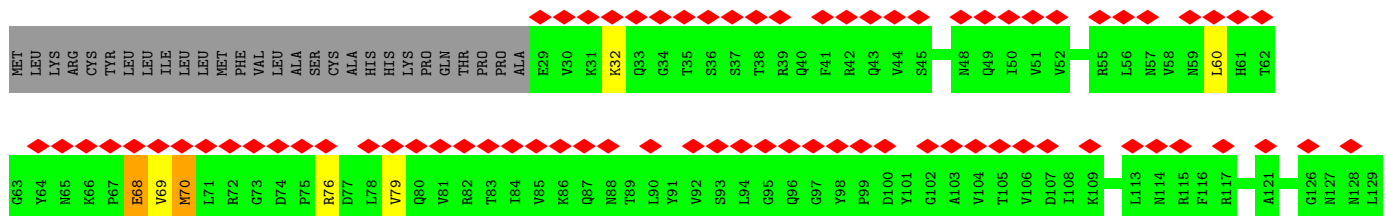
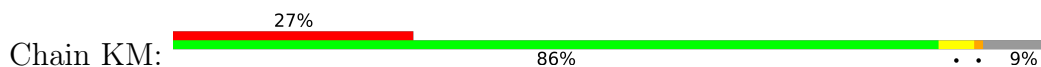
- Molecule 8: DUF2807 domain-containing protein



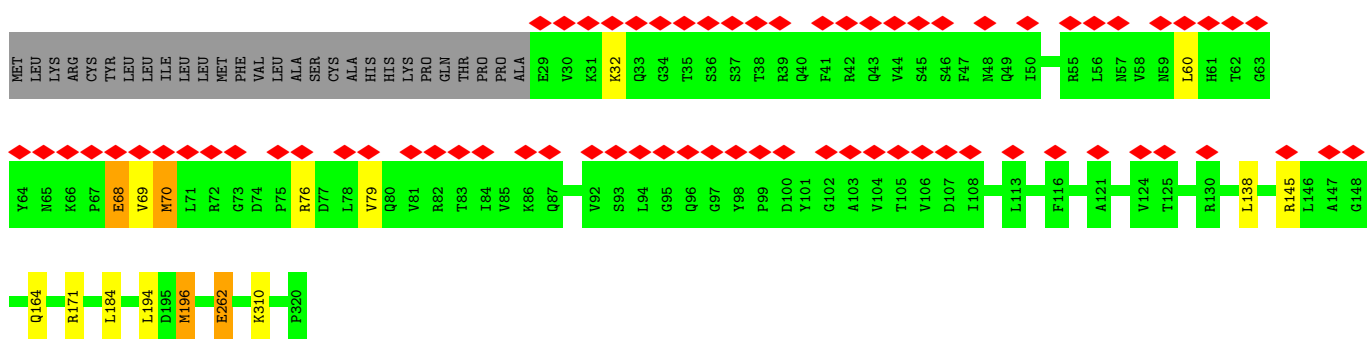
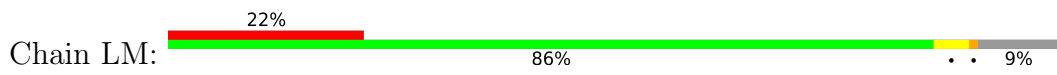
- Molecule 8: DUF2807 domain-containing protein



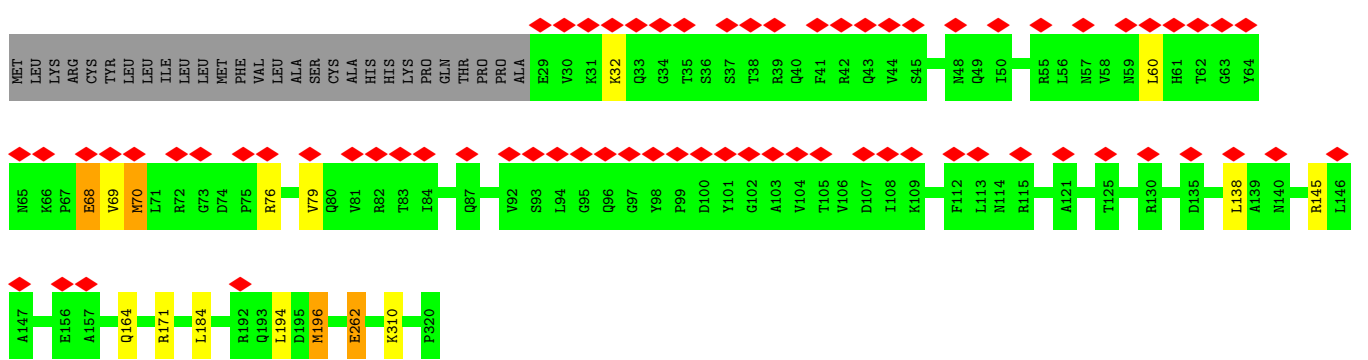
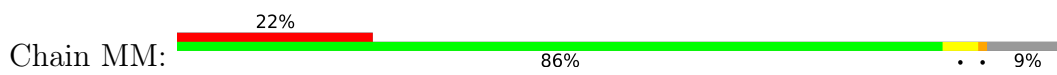
- Molecule 8: DUF2807 domain-containing protein



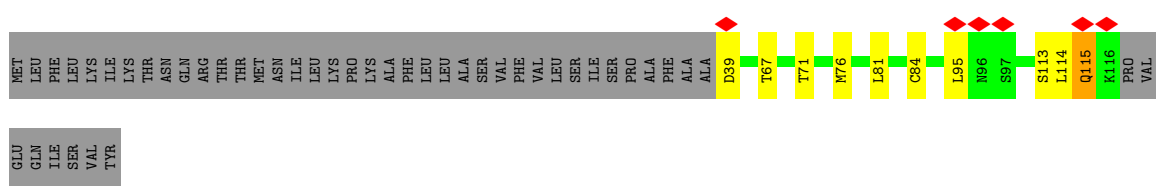
- Molecule 8: DUF2807 domain-containing protein



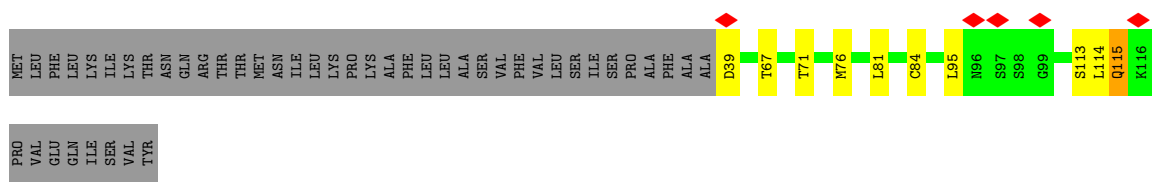
• Molecule 8: DUF2807 domain-containing protein



• Molecule 9: Neurogenic locus notch

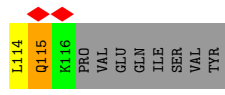
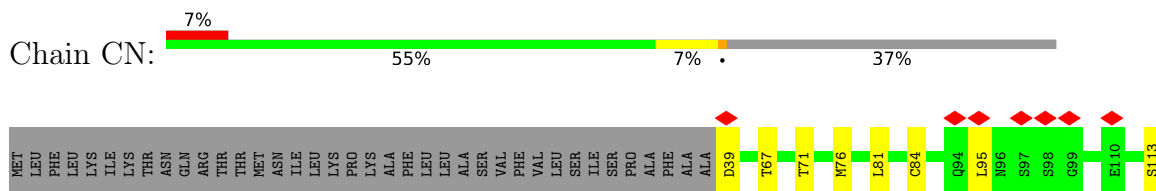


• Molecule 9: Neurogenic locus notch

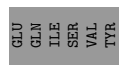
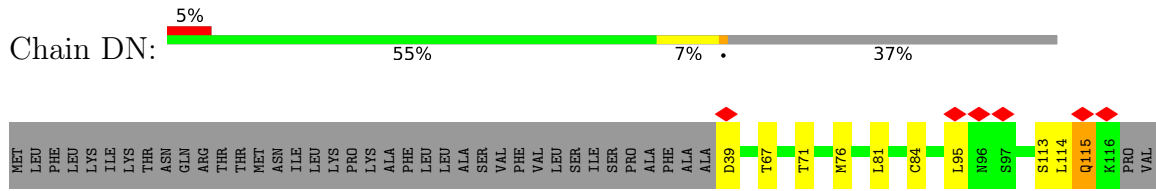


• Molecule 9: Neurogenic locus notch

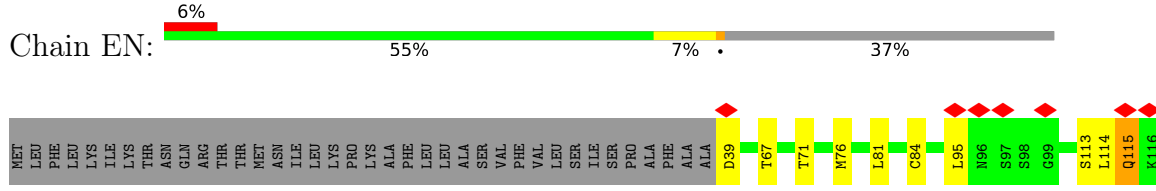




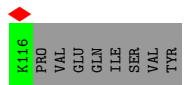
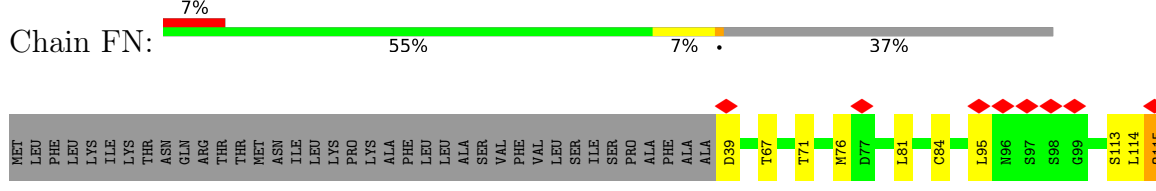
• Molecule 9: Neurogenic locus notch



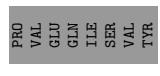
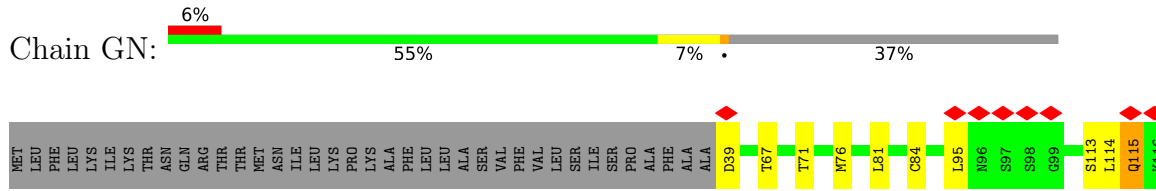
• Molecule 9: Neurogenic locus notch



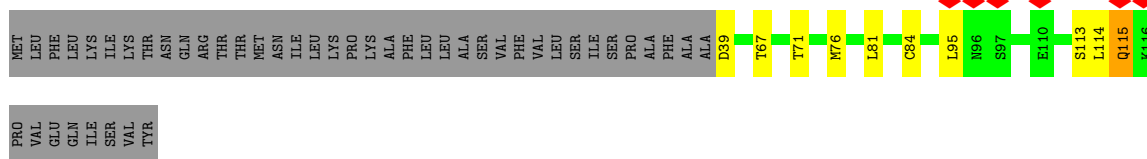
• Molecule 9: Neurogenic locus notch



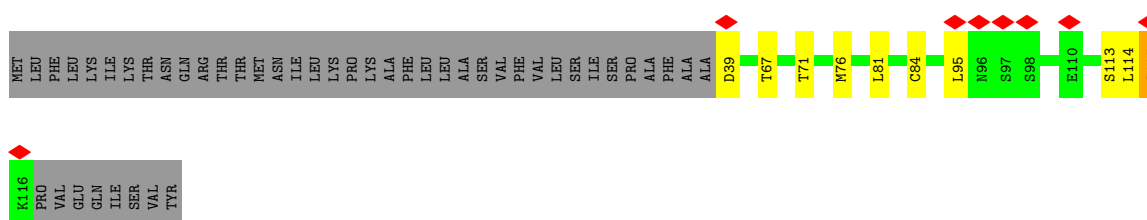
• Molecule 9: Neurogenic locus notch



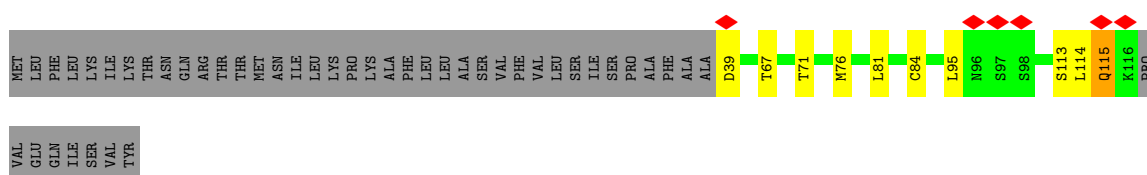
• Molecule 9: Neurogenic locus notch



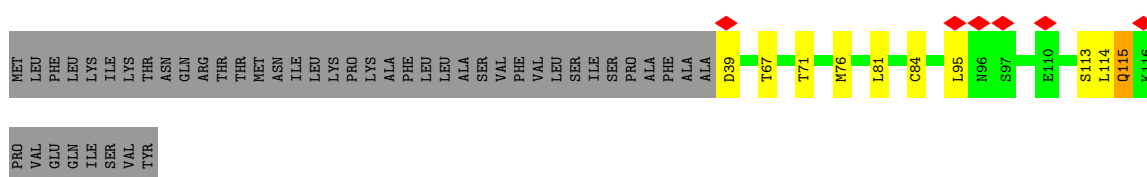
• Molecule 9: Neurogenic locus notch



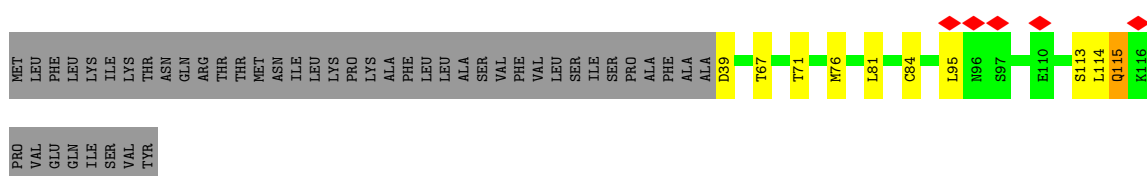
• Molecule 9: Neurogenic locus notch



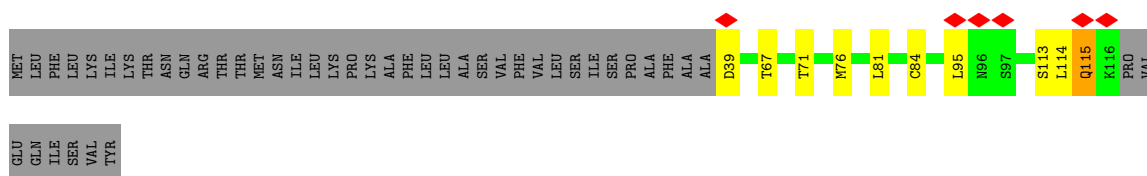
• Molecule 9: Neurogenic locus notch



• Molecule 9: Neurogenic locus notch



- Molecule 9: Neurogenic locus notch



- Molecule 10: Unknown protein fragment



There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment



There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment



There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment



There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment



There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment



There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment



There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment

Chain HU:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment

Chain IU:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment

Chain JU:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment

Chain KU:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment

Chain LU:  100%


There are no outlier residues recorded for this chain.

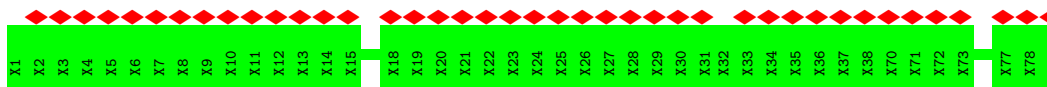
- Molecule 10: Unknown protein fragment

Chain MU:  100%


There are no outlier residues recorded for this chain.

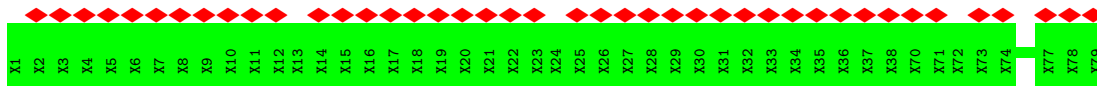
- Molecule 11: Unknown protein fragment

Chain AX:  85%  
100%




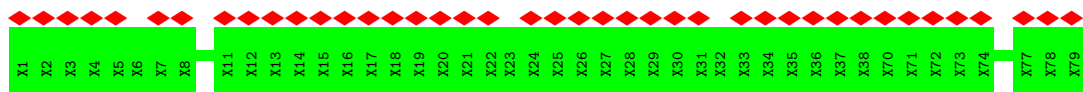
- Molecule 11: Unknown protein fragment

Chain BX:  88%  
100%

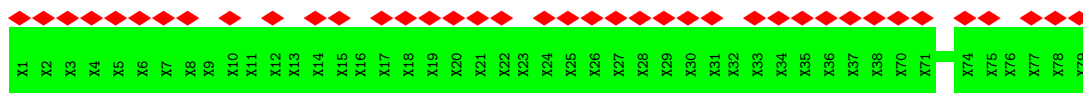
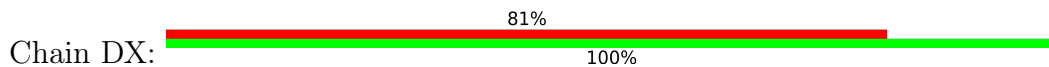


- Molecule 11: Unknown protein fragment

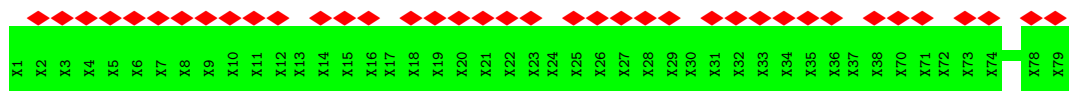
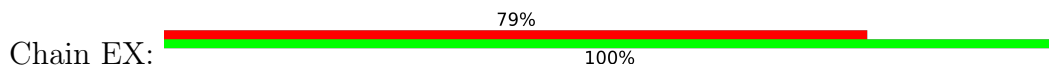
Chain CX:  85%  
100%



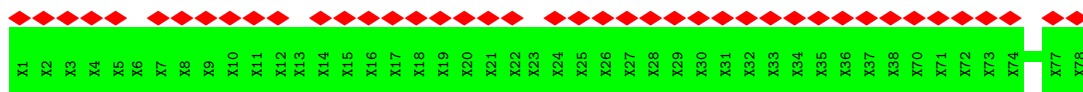
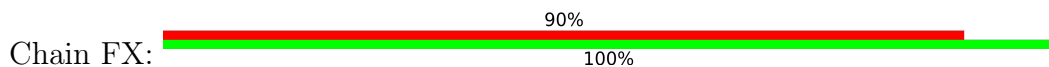
• Molecule 11: Unknown protein fragment



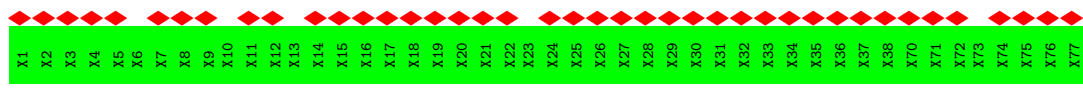
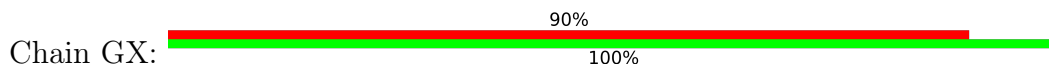
• Molecule 11: Unknown protein fragment



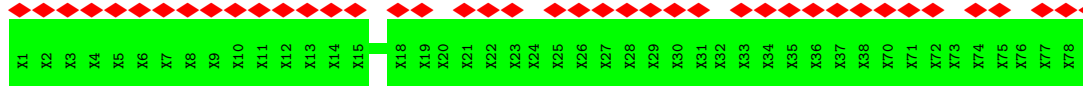
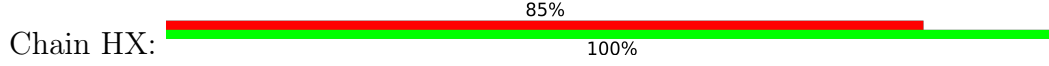
• Molecule 11: Unknown protein fragment



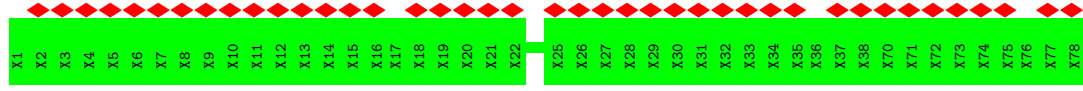
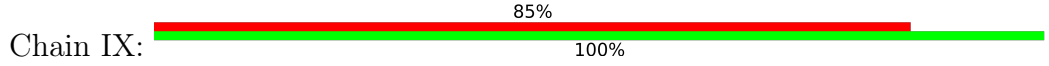
• Molecule 11: Unknown protein fragment



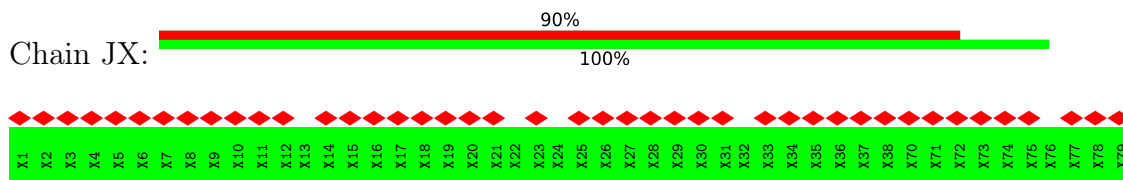
• Molecule 11: Unknown protein fragment



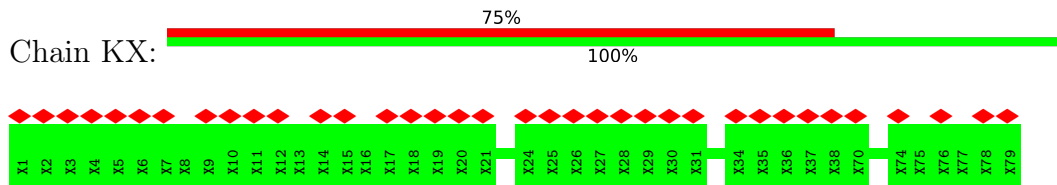
• Molecule 11: Unknown protein fragment



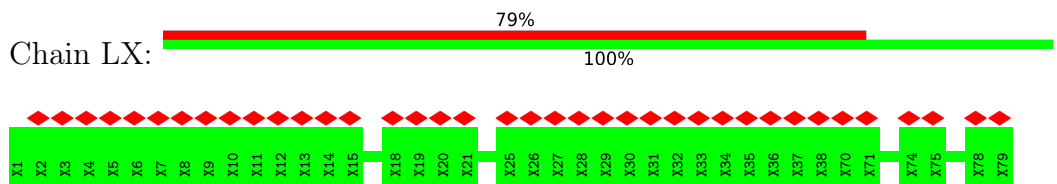
• Molecule 11: Unknown protein fragment



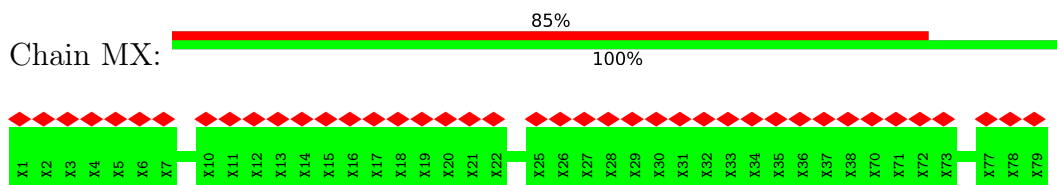
• Molecule 11: Unknown protein fragment



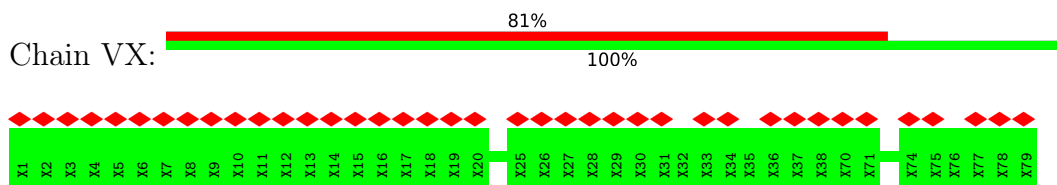
• Molecule 11: Unknown protein fragment



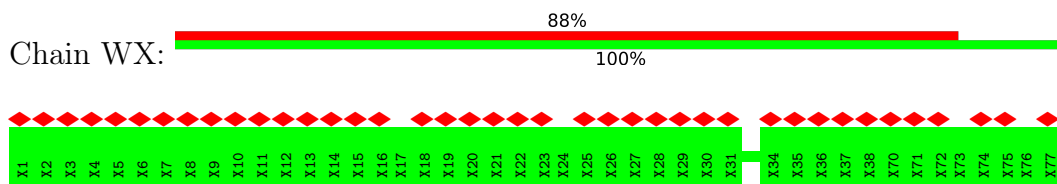
• Molecule 11: Unknown protein fragment



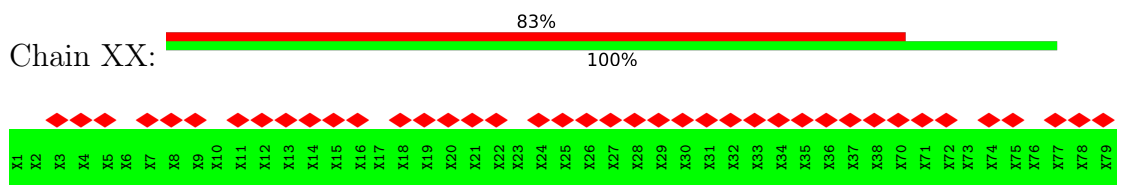
• Molecule 11: Unknown protein fragment




• Molecule 11: Unknown protein fragment

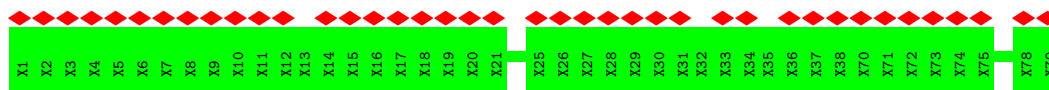


• Molecule 11: Unknown protein fragment




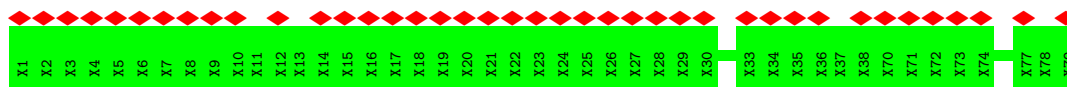
- Molecule 11: Unknown protein fragment

Chain YX:  83%  
100%



- Molecule 11: Unknown protein fragment

Chain ZX:  83%  
100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136818	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	2.337	Depositor
Minimum map value	-1.017	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.106	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	561.0, 561.0, 561.0	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor



## 5 Model quality i

### 5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AC	0.50	0/1717	0.83	6/2331 (0.3%)
1	BC	0.50	0/1717	0.83	6/2331 (0.3%)
1	CC	0.50	0/1717	0.83	6/2331 (0.3%)
1	DC	0.50	0/1717	0.84	6/2331 (0.3%)
1	EC	0.50	0/1717	0.83	6/2331 (0.3%)
1	FC	0.50	0/1717	0.83	6/2331 (0.3%)
1	GC	0.50	0/1717	0.83	6/2331 (0.3%)
1	HC	0.50	0/1717	0.84	6/2331 (0.3%)
1	IC	0.50	0/1717	0.84	6/2331 (0.3%)
1	JC	0.50	0/1717	0.83	6/2331 (0.3%)
1	KC	0.50	0/1717	0.83	6/2331 (0.3%)
1	LC	0.50	0/1717	0.84	6/2331 (0.3%)
1	MC	0.50	0/1717	0.84	6/2331 (0.3%)
2	AD	0.64	2/1107 (0.2%)	0.94	7/1502 (0.5%)
2	Ad	0.56	0/1078	0.97	8/1463 (0.5%)
2	BD	0.66	1/1107 (0.1%)	0.94	7/1502 (0.5%)
2	Bd	0.67	4/1078 (0.4%)	0.91	5/1463 (0.3%)
2	CD	0.58	0/1107	0.91	7/1502 (0.5%)
2	Cd	0.73	3/1078 (0.3%)	1.03	11/1463 (0.8%)
2	DD	0.61	0/1107	0.93	7/1502 (0.5%)
2	Dd	0.57	0/1078	0.94	6/1463 (0.4%)
2	ED	0.66	0/1107	1.09	11/1502 (0.7%)
2	Ed	0.57	0/1078	0.86	6/1463 (0.4%)
2	FD	0.57	0/1107	0.78	1/1502 (0.1%)
2	Fd	1.09	8/1078 (0.7%)	1.10	11/1463 (0.8%)
2	GD	0.64	1/1107 (0.1%)	0.89	7/1502 (0.5%)
2	Gd	0.64	3/1078 (0.3%)	0.97	8/1463 (0.5%)
2	HD	0.64	0/1107	0.90	6/1502 (0.4%)
2	Hd	0.62	1/1078 (0.1%)	0.84	4/1463 (0.3%)
2	ID	0.56	0/1107	0.92	7/1502 (0.5%)
2	Id	0.58	0/1078	0.93	6/1463 (0.4%)
2	JD	0.58	1/1107 (0.1%)	0.87	6/1502 (0.4%)
2	Jd	0.63	2/1078 (0.2%)	0.86	3/1463 (0.2%)
2	KD	0.60	0/1107	0.88	6/1502 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	Kd	0.62	2/1078 (0.2%)	0.94	10/1463 (0.7%)
2	LD	0.63	1/1107 (0.1%)	0.96	10/1502 (0.7%)
2	Ld	0.57	1/1078 (0.1%)	0.96	6/1463 (0.4%)
2	MD	0.60	1/1107 (0.1%)	0.82	4/1502 (0.3%)
2	Md	0.63	2/1078 (0.2%)	0.88	3/1463 (0.2%)
3	AF	0.35	0/490	1.02	4/660 (0.6%)
3	Af	0.28	0/456	0.62	0/615
3	BF	0.35	0/490	1.02	4/660 (0.6%)
3	Bf	0.29	0/456	0.67	0/615
3	CF	0.35	0/490	1.02	4/660 (0.6%)
3	Cf	0.27	0/456	0.62	0/615
3	DF	0.35	0/490	1.02	4/660 (0.6%)
3	Df	0.27	0/456	0.66	0/615
3	EF	0.35	0/490	1.02	4/660 (0.6%)
3	Ef	0.28	0/456	0.64	0/615
3	FF	0.35	0/490	1.02	4/660 (0.6%)
3	Ff	0.29	0/456	0.65	0/615
3	GF	0.35	0/490	1.02	4/660 (0.6%)
3	Gf	0.27	0/456	0.57	0/615
3	HF	0.35	0/490	1.02	4/660 (0.6%)
3	Hf	0.27	0/456	0.64	0/615
3	IF	0.35	0/490	1.02	4/660 (0.6%)
3	If	0.27	0/456	0.65	0/615
3	JF	0.35	0/490	1.02	4/660 (0.6%)
3	Jf	0.27	0/456	0.62	0/615
3	KF	0.35	0/490	1.02	4/660 (0.6%)
3	Kf	0.28	0/456	0.64	0/615
3	LF	0.35	0/490	1.02	4/660 (0.6%)
3	Lf	0.26	0/456	0.59	0/615
3	MF	0.35	0/490	1.02	4/660 (0.6%)
3	Mf	0.27	0/456	0.67	0/615
3	VF	0.35	0/490	1.02	4/660 (0.6%)
3	WF	0.35	0/490	1.02	4/660 (0.6%)
3	XF	0.35	0/490	1.02	4/660 (0.6%)
3	YF	0.35	0/490	1.02	4/660 (0.6%)
3	ZF	0.35	0/490	1.02	4/660 (0.6%)
4	AG	0.76	0/278	1.63	7/377 (1.9%)
4	BG	0.75	0/278	1.63	7/377 (1.9%)
4	CG	0.76	0/278	1.63	7/377 (1.9%)
4	DG	0.76	0/278	1.63	7/377 (1.9%)
4	EG	0.75	0/278	1.63	7/377 (1.9%)
4	FG	0.76	0/278	1.63	7/377 (1.9%)
4	GG	0.76	0/278	1.63	7/377 (1.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	HG	0.76	0/278	1.63	7/377 (1.9%)
4	IG	0.76	0/278	1.63	7/377 (1.9%)
4	JG	0.75	0/278	1.63	7/377 (1.9%)
4	KG	0.75	0/278	1.63	7/377 (1.9%)
4	LG	0.76	0/278	1.63	7/377 (1.9%)
4	MG	0.76	0/278	1.63	7/377 (1.9%)
4	VG	0.76	0/278	1.63	7/377 (1.9%)
4	WG	0.75	0/278	1.63	7/377 (1.9%)
4	XG	0.75	0/278	1.63	7/377 (1.9%)
4	YG	0.75	0/278	1.63	7/377 (1.9%)
4	ZG	0.76	0/278	1.63	7/377 (1.9%)
5	AH	0.80	4/2033 (0.2%)	0.92	11/2775 (0.4%)
5	BH	0.56	3/2033 (0.1%)	0.95	11/2775 (0.4%)
5	CH	0.73	5/2033 (0.2%)	1.03	7/2775 (0.3%)
5	DH	0.72	4/2033 (0.2%)	0.97	10/2775 (0.4%)
5	EH	0.82	5/2033 (0.2%)	1.08	21/2775 (0.8%)
5	FH	0.79	6/2033 (0.3%)	0.98	12/2775 (0.4%)
5	GH	0.67	5/2033 (0.2%)	1.01	16/2775 (0.6%)
5	HH	0.70	3/2033 (0.1%)	1.04	11/2775 (0.4%)
5	IH	0.63	2/2033 (0.1%)	1.05	14/2775 (0.5%)
5	JH	0.61	1/2033 (0.0%)	1.01	10/2775 (0.4%)
5	KH	0.55	1/2033 (0.0%)	0.96	11/2775 (0.4%)
5	LH	0.69	5/2033 (0.2%)	0.98	11/2775 (0.4%)
5	MH	0.63	0/2033	0.99	10/2775 (0.4%)
5	VH	0.47	1/1921 (0.1%)	0.87	7/2620 (0.3%)
5	WH	0.53	3/1921 (0.2%)	0.94	12/2620 (0.5%)
5	XH	0.54	2/1921 (0.1%)	0.99	6/2620 (0.2%)
5	YH	0.64	5/1921 (0.3%)	1.00	7/2620 (0.3%)
5	ZH	0.61	4/1921 (0.2%)	1.09	17/2620 (0.6%)
6	AK	0.54	0/1195	0.86	3/1616 (0.2%)
6	BK	0.55	0/1195	0.86	3/1616 (0.2%)
6	CK	0.54	0/1195	0.86	3/1616 (0.2%)
6	DK	0.55	0/1195	0.86	3/1616 (0.2%)
6	EK	0.55	0/1195	0.86	3/1616 (0.2%)
6	FK	0.54	0/1195	0.86	3/1616 (0.2%)
6	GK	0.54	0/1195	0.86	3/1616 (0.2%)
6	HK	0.54	0/1195	0.86	3/1616 (0.2%)
6	IK	0.54	0/1195	0.86	3/1616 (0.2%)
6	JK	0.54	0/1195	0.86	3/1616 (0.2%)
6	KK	0.54	0/1195	0.86	3/1616 (0.2%)
6	LK	0.54	0/1195	0.86	3/1616 (0.2%)
6	MK	0.54	0/1195	0.86	3/1616 (0.2%)
7	AL	0.53	1/1417 (0.1%)	1.30	7/1912 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
7	BL	0.53	1/1417 (0.1%)	1.30	7/1912 (0.4%)
7	CL	0.53	1/1417 (0.1%)	1.30	7/1912 (0.4%)
7	DL	0.53	1/1417 (0.1%)	1.30	7/1912 (0.4%)
7	EL	0.53	1/1417 (0.1%)	1.30	7/1912 (0.4%)
7	FL	0.53	1/1417 (0.1%)	1.30	7/1912 (0.4%)
7	GL	0.53	1/1417 (0.1%)	1.30	7/1912 (0.4%)
7	HL	0.53	1/1417 (0.1%)	1.30	7/1912 (0.4%)
7	IL	0.53	1/1417 (0.1%)	1.30	7/1912 (0.4%)
7	JL	0.53	1/1417 (0.1%)	1.30	7/1912 (0.4%)
7	KL	0.53	1/1417 (0.1%)	1.30	7/1912 (0.4%)
7	LL	0.53	1/1417 (0.1%)	1.30	7/1912 (0.4%)
7	ML	0.53	1/1417 (0.1%)	1.30	7/1912 (0.4%)
8	AM	0.48	2/2359 (0.1%)	0.89	12/3183 (0.4%)
8	BM	0.48	2/2359 (0.1%)	0.89	12/3183 (0.4%)
8	CM	0.48	2/2359 (0.1%)	0.89	12/3183 (0.4%)
8	DM	0.48	2/2359 (0.1%)	0.89	12/3183 (0.4%)
8	EM	0.48	2/2359 (0.1%)	0.89	12/3183 (0.4%)
8	FM	0.48	2/2359 (0.1%)	0.89	12/3183 (0.4%)
8	GM	0.48	2/2359 (0.1%)	0.89	12/3183 (0.4%)
8	HM	0.48	2/2359 (0.1%)	0.89	12/3183 (0.4%)
8	IM	0.48	2/2359 (0.1%)	0.89	12/3183 (0.4%)
8	JM	0.48	2/2359 (0.1%)	0.89	12/3183 (0.4%)
8	KM	0.48	2/2359 (0.1%)	0.89	12/3183 (0.4%)
8	LM	0.48	2/2359 (0.1%)	0.89	12/3183 (0.4%)
8	MM	0.48	2/2359 (0.1%)	0.89	12/3183 (0.4%)
9	AN	0.55	0/593	0.96	3/799 (0.4%)
9	BN	0.55	0/593	0.96	3/799 (0.4%)
9	CN	0.54	0/593	0.96	3/799 (0.4%)
9	DN	0.55	0/593	0.96	3/799 (0.4%)
9	EN	0.54	0/593	0.96	3/799 (0.4%)
9	FN	0.55	0/593	0.96	3/799 (0.4%)
9	GN	0.55	0/593	0.96	3/799 (0.4%)
9	HN	0.55	0/593	0.96	3/799 (0.4%)
9	IN	0.55	0/593	0.96	3/799 (0.4%)
9	JN	0.54	0/593	0.96	3/799 (0.4%)
9	KN	0.55	0/593	0.96	3/799 (0.4%)
9	LN	0.55	0/593	0.96	3/799 (0.4%)
9	MN	0.55	0/593	0.96	3/799 (0.4%)
All	All	0.56	131/178844 (0.1%)	0.99	978/242314 (0.4%)

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	AD	0	1
2	BD	0	1
2	Bd	0	1
2	CD	0	1
2	Cd	0	1
2	DD	0	1
2	ED	0	1
2	FD	0	1
2	Fd	0	1
2	GD	0	1
2	ID	0	1
2	KD	0	1
2	MD	0	1
5	AH	0	2
5	BH	0	1
5	DH	0	1
5	EH	0	1
5	FH	0	2
5	GH	0	2
5	HH	0	1
5	IH	0	1
5	JH	0	3
5	KH	0	2
5	LH	0	1
5	MH	0	1
5	VH	0	1
5	WH	0	1
5	XH	0	1
5	YH	0	2
5	ZH	0	1
8	AM	0	1
8	BM	0	1
8	CM	0	1
8	DM	0	1
8	EM	0	1
8	FM	0	1
8	GM	0	1
8	HM	0	1
8	IM	0	1
8	JM	0	1
8	KM	0	1
8	LM	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	MM	0	1
9	AN	0	1
9	BN	0	1
9	CN	0	1
9	DN	0	1
9	EN	0	1
9	FN	0	1
9	GN	0	1
9	HN	0	1
9	IN	0	1
9	JN	0	1
9	KN	0	1
9	LN	0	1
9	MN	0	1
All	All	0	63

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	EH	285	GLU	CG-CD	-18.04	1.24	1.51
5	AH	205	GLN	CG-CD	-17.70	1.10	1.51
5	FH	285	GLU	CG-CD	-16.69	1.26	1.51
2	Fd	126	GLU	CB-CG	-16.40	1.21	1.52
5	EH	285	GLU	CB-CG	-15.16	1.23	1.52
2	Fd	82	ARG	CB-CG	14.53	1.91	1.52
5	DH	285	GLU	CG-CD	-13.69	1.31	1.51
5	FH	285	GLU	CB-CG	-13.28	1.26	1.52
5	IH	115	MET	CB-CG	-11.28	1.15	1.51
5	CH	250	TYR	CD2-CE2	-11.25	1.22	1.39
5	HH	115	MET	CG-SD	-11.13	1.52	1.81
5	HH	115	MET	CB-CG	-10.72	1.17	1.51
5	AH	205	GLN	CB-CG	-10.60	1.24	1.52
5	DH	115	MET	CB-CG	-10.55	1.17	1.51
2	Fd	82	ARG	CG-CD	-10.51	1.25	1.51
5	YH	115	MET	CB-CG	-10.29	1.18	1.51
5	DH	115	MET	CG-SD	-10.21	1.54	1.81
5	AH	206	TRP	CB-CG	-9.79	1.32	1.50
5	GH	248	VAL	CB-CG1	-9.70	1.32	1.52
5	YH	115	MET	CG-SD	-9.37	1.56	1.81
5	LH	115	MET	CG-SD	-9.06	1.57	1.81
5	ZH	115	MET	CB-CG	-9.04	1.22	1.51
5	XH	115	MET	CG-SD	-8.68	1.58	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	GH	250	TYR	CD2-CE2	-8.63	1.26	1.39
2	Cd	43	GLU	CB-CG	-8.61	1.35	1.52
5	WH	115	MET	CG-SD	-8.52	1.58	1.81
5	DH	285	GLU	CB-CG	-8.52	1.35	1.52
2	Cd	130	GLU	CD-OE2	-8.51	1.16	1.25
5	XH	115	MET	CB-CG	-7.98	1.25	1.51
2	Fd	82	ARG	CD-NE	-7.71	1.33	1.46
8	HM	68	GLU	CD-OE2	-7.59	1.17	1.25
8	EM	68	GLU	CD-OE2	-7.59	1.17	1.25
8	IM	68	GLU	CD-OE2	-7.58	1.17	1.25
5	JH	238	MET	CB-CG	-7.55	1.27	1.51
8	JM	68	GLU	CD-OE2	-7.53	1.17	1.25
8	AM	68	GLU	CD-OE2	-7.52	1.17	1.25
8	DM	68	GLU	CD-OE2	-7.51	1.17	1.25
5	EH	117	ARG	CB-CG	-7.51	1.32	1.52
8	CM	68	GLU	CD-OE2	-7.51	1.17	1.25
8	FM	68	GLU	CD-OE2	-7.50	1.17	1.25
8	MM	68	GLU	CD-OE2	-7.49	1.17	1.25
8	BM	68	GLU	CD-OE2	-7.48	1.17	1.25
8	GM	68	GLU	CD-OE2	-7.48	1.17	1.25
8	LM	68	GLU	CD-OE2	-7.47	1.17	1.25
8	KM	68	GLU	CD-OE2	-7.46	1.17	1.25
5	WH	115	MET	CB-CG	-7.41	1.27	1.51
5	LH	115	MET	CB-CG	-7.26	1.28	1.51
2	Fd	82	ARG	NE-CZ	-7.03	1.24	1.33
5	EH	115	MET	CB-CG	-7.02	1.28	1.51
2	Cd	130	GLU	CB-CG	-7.00	1.38	1.52
2	Md	130	GLU	CB-CG	-6.96	1.39	1.52
5	FH	115	MET	CB-CG	-6.92	1.29	1.51
2	Fd	125	ASP	CB-CG	6.91	1.66	1.51
2	BD	59	GLU	CD-OE1	-6.90	1.18	1.25
2	Bd	130	GLU	CG-CD	-6.83	1.41	1.51
2	Jd	130	GLU	CB-CG	-6.67	1.39	1.52
5	FH	134	TYR	CB-CG	-6.60	1.41	1.51
5	ZH	115	MET	CG-SD	-6.57	1.64	1.81
2	Bd	126	GLU	CG-CD	-6.55	1.42	1.51
5	YH	285	GLU	CG-CD	-6.52	1.42	1.51
2	Gd	130	GLU	CB-CG	-6.48	1.39	1.52
5	LH	252	VAL	CB-CG1	-6.38	1.39	1.52
5	CH	115	MET	CB-CG	-6.38	1.30	1.51
5	LH	158	VAL	CB-CG2	-6.35	1.39	1.52
8	GM	68	GLU	CG-CD	-6.33	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	EH	117	ARG	CZ-NH1	6.33	1.41	1.33
2	Kd	93	GLU	CG-CD	-6.33	1.42	1.51
8	HM	68	GLU	CG-CD	-6.32	1.42	1.51
8	FM	68	GLU	CG-CD	-6.31	1.42	1.51
8	KM	68	GLU	CG-CD	-6.31	1.42	1.51
8	CM	68	GLU	CG-CD	-6.30	1.42	1.51
8	DM	68	GLU	CG-CD	-6.30	1.42	1.51
8	LM	68	GLU	CG-CD	-6.29	1.42	1.51
8	BM	68	GLU	CG-CD	-6.28	1.42	1.51
8	EM	68	GLU	CG-CD	-6.27	1.42	1.51
8	MM	68	GLU	CG-CD	-6.26	1.42	1.51
2	AD	59	GLU	CB-CG	-6.25	1.40	1.52
8	IM	68	GLU	CG-CD	-6.25	1.42	1.51
8	AM	68	GLU	CG-CD	-6.24	1.42	1.51
8	JM	68	GLU	CG-CD	-6.22	1.42	1.51
5	LH	132	GLN	CB-CG	-6.17	1.35	1.52
2	AD	59	GLU	CG-CD	-6.12	1.42	1.51
2	Fd	126	GLU	CG-CD	6.04	1.61	1.51
2	Hd	36	ASP	CB-CG	-6.01	1.39	1.51
2	Ld	93	GLU	CG-CD	6.01	1.60	1.51
5	HH	207	ASP	CB-CG	-5.93	1.39	1.51
5	CH	151	PRO	CB-CG	-5.92	1.20	1.50
5	AH	115	MET	CB-CG	-5.80	1.32	1.51
5	ZH	208	LYS	CB-CG	-5.75	1.37	1.52
5	VH	115	MET	CG-SD	-5.74	1.66	1.81
5	FH	285	GLU	CD-OE2	-5.70	1.19	1.25
2	JD	87	TRP	CB-CG	-5.69	1.40	1.50
7	KL	187	GLU	CG-CD	-5.67	1.43	1.51
7	LL	187	GLU	CG-CD	-5.65	1.43	1.51
5	CH	250	TYR	CG-CD2	-5.65	1.31	1.39
7	AL	187	GLU	CG-CD	-5.63	1.43	1.51
7	EL	187	GLU	CG-CD	-5.62	1.43	1.51
5	YH	250	TYR	CD2-CE2	-5.62	1.30	1.39
5	BH	139	TYR	CD1-CE1	-5.62	1.30	1.39
7	HL	187	GLU	CG-CD	-5.62	1.43	1.51
7	IL	187	GLU	CG-CD	-5.60	1.43	1.51
5	GH	285	GLU	CG-CD	-5.60	1.43	1.51
2	Gd	82	ARG	CB-CG	5.60	1.67	1.52
7	CL	187	GLU	CG-CD	-5.60	1.43	1.51
7	GL	187	GLU	CG-CD	-5.59	1.43	1.51
7	DL	187	GLU	CG-CD	-5.59	1.43	1.51
7	JL	187	GLU	CG-CD	-5.59	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	FL	187	GLU	CG-CD	-5.58	1.43	1.51
2	Fd	127	SER	CA-CB	5.55	1.61	1.52
7	BL	187	GLU	CG-CD	-5.54	1.43	1.51
7	ML	187	GLU	CG-CD	-5.54	1.43	1.51
2	Md	148	TYR	CD2-CE2	-5.52	1.31	1.39
2	LD	52	MET	CB-CG	-5.49	1.33	1.51
5	BH	115	MET	CB-CG	-5.43	1.33	1.51
2	GD	59	GLU	CB-CG	-5.41	1.41	1.52
2	Bd	126	GLU	CD-OE2	-5.40	1.19	1.25
2	Kd	126	GLU	CD-OE2	-5.36	1.19	1.25
2	Bd	130	GLU	CB-CG	-5.35	1.42	1.52
2	Gd	130	GLU	CD-OE2	-5.34	1.19	1.25
5	CH	250	TYR	CD1-CE1	-5.33	1.31	1.39
5	BH	110	LYS	CB-CG	-5.33	1.38	1.52
2	Jd	93	GLU	CB-CG	-5.25	1.42	1.52
5	KH	158	VAL	CB-CG2	-5.22	1.41	1.52
5	IH	115	MET	CA-CB	-5.17	1.42	1.53
2	MD	126	GLU	CB-CG	-5.16	1.42	1.52
5	GH	285	GLU	CB-CG	-5.15	1.42	1.52
5	YH	285	GLU	CB-CG	-5.10	1.42	1.52
5	ZH	208	LYS	CD-CE	-5.09	1.38	1.51
5	FH	134	TYR	CD1-CE1	-5.09	1.31	1.39
5	GH	115	MET	CG-SD	-5.08	1.68	1.81
5	WH	120	TYR	CD1-CE1	-5.04	1.31	1.39

All (978) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	KL	187	GLU	OE1-CD-OE2	-32.00	84.90	123.30
7	DL	187	GLU	OE1-CD-OE2	-31.97	84.94	123.30
7	FL	187	GLU	OE1-CD-OE2	-31.96	84.95	123.30
7	IL	187	GLU	OE1-CD-OE2	-31.96	84.95	123.30
7	AL	187	GLU	OE1-CD-OE2	-31.95	84.96	123.30
7	CL	187	GLU	OE1-CD-OE2	-31.95	84.96	123.30
7	JL	187	GLU	OE1-CD-OE2	-31.94	84.97	123.30
7	LL	187	GLU	OE1-CD-OE2	-31.93	84.99	123.30
7	GL	187	GLU	OE1-CD-OE2	-31.91	85.00	123.30
7	EL	187	GLU	OE1-CD-OE2	-31.90	85.02	123.30
7	HL	187	GLU	OE1-CD-OE2	-31.90	85.02	123.30
7	ML	187	GLU	OE1-CD-OE2	-31.90	85.02	123.30
7	BL	187	GLU	OE1-CD-OE2	-31.87	85.06	123.30
7	EL	187	GLU	CG-CD-OE2	23.83	165.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	BL	187	GLU	CG-CD-OE2	23.83	165.95	118.30
7	HL	187	GLU	CG-CD-OE2	23.82	165.94	118.30
7	AL	187	GLU	CG-CD-OE2	23.81	165.92	118.30
7	GL	187	GLU	CG-CD-OE2	23.79	165.89	118.30
7	ML	187	GLU	CG-CD-OE2	23.79	165.87	118.30
7	CL	187	GLU	CG-CD-OE2	23.78	165.87	118.30
7	LL	187	GLU	CG-CD-OE2	23.78	165.87	118.30
7	JL	187	GLU	CG-CD-OE2	23.78	165.86	118.30
7	IL	187	GLU	CG-CD-OE2	23.78	165.85	118.30
7	DL	187	GLU	CG-CD-OE2	23.77	165.84	118.30
7	FL	187	GLU	CG-CD-OE2	23.77	165.84	118.30
7	KL	187	GLU	CG-CD-OE2	23.76	165.82	118.30
5	YH	115	MET	CG-SD-CE	-22.06	64.91	100.20
5	HH	115	MET	CG-SD-CE	-21.02	66.56	100.20
5	IH	115	MET	CG-SD-CE	-20.95	66.67	100.20
5	JH	238	MET	CG-SD-CE	-20.94	66.69	100.20
5	ZH	115	MET	CG-SD-CE	-20.46	67.47	100.20
2	ED	160	LYS	CD-CE-NZ	-20.39	64.80	111.70
5	XH	115	MET	CG-SD-CE	-20.19	67.90	100.20
5	DH	115	MET	CG-SD-CE	-20.09	68.05	100.20
5	FH	115	MET	CB-CG-SD	-18.46	57.03	112.40
5	KH	238	MET	CG-SD-CE	-18.22	71.05	100.20
5	CH	115	MET	CG-SD-CE	-18.15	71.17	100.20
5	LH	115	MET	CG-SD-CE	-17.86	71.62	100.20
5	EH	115	MET	CG-SD-CE	-16.65	73.55	100.20
7	IL	187	GLU	CG-CD-OE1	-15.94	86.42	118.30
7	ML	187	GLU	CG-CD-OE1	-15.94	86.42	118.30
7	BL	187	GLU	CG-CD-OE1	-15.94	86.43	118.30
7	FL	187	GLU	CG-CD-OE1	-15.93	86.45	118.30
7	LL	187	GLU	CG-CD-OE1	-15.92	86.46	118.30
7	CL	187	GLU	CG-CD-OE1	-15.92	86.46	118.30
7	GL	187	GLU	CG-CD-OE1	-15.91	86.47	118.30
7	JL	187	GLU	CG-CD-OE1	-15.91	86.47	118.30
7	AL	187	GLU	CG-CD-OE1	-15.91	86.48	118.30
7	DL	187	GLU	CG-CD-OE1	-15.91	86.48	118.30
7	HL	187	GLU	CG-CD-OE1	-15.90	86.49	118.30
7	KL	187	GLU	CG-CD-OE1	-15.90	86.51	118.30
7	EL	187	GLU	CG-CD-OE1	-15.89	86.52	118.30
5	CH	115	MET	CA-CB-CG	-15.59	86.80	113.30
5	WH	115	MET	CG-SD-CE	-15.52	75.37	100.20
5	XH	238	MET	CG-SD-CE	-15.47	75.44	100.20
5	HH	115	MET	CA-CB-CG	-14.77	88.19	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BG	801	MET	CA-CB-CG	14.39	137.76	113.30
4	GG	801	MET	CA-CB-CG	14.35	137.70	113.30
4	AG	801	MET	CA-CB-CG	14.35	137.70	113.30
4	HG	801	MET	CA-CB-CG	14.35	137.69	113.30
4	CG	801	MET	CA-CB-CG	14.35	137.69	113.30
4	IG	801	MET	CA-CB-CG	14.35	137.69	113.30
4	DG	801	MET	CA-CB-CG	14.34	137.68	113.30
4	VG	801	MET	CA-CB-CG	14.34	137.68	113.30
4	LG	801	MET	CA-CB-CG	14.34	137.67	113.30
4	EG	801	MET	CA-CB-CG	14.33	137.66	113.30
4	XG	801	MET	CA-CB-CG	14.33	137.66	113.30
4	JG	801	MET	CA-CB-CG	14.33	137.66	113.30
4	YG	801	MET	CA-CB-CG	14.33	137.65	113.30
4	FG	801	MET	CA-CB-CG	14.32	137.65	113.30
4	WG	801	MET	CA-CB-CG	14.32	137.65	113.30
5	GH	238	MET	CG-SD-CE	-14.32	77.29	100.20
4	ZG	801	MET	CA-CB-CG	14.31	137.63	113.30
4	MG	801	MET	CA-CB-CG	14.31	137.63	113.30
4	KG	801	MET	CA-CB-CG	14.31	137.62	113.30
2	Ld	55	MET	CG-SD-CE	-14.29	77.33	100.20
5	IH	115	MET	CB-CG-SD	-13.77	71.11	112.40
5	DH	115	MET	CA-CB-CG	-13.29	90.71	113.30
2	Fd	26	LYS	CD-CE-NZ	-13.21	81.33	111.70
2	Ad	55	MET	CG-SD-CE	-13.11	79.22	100.20
5	BH	115	MET	CG-SD-CE	-13.05	79.33	100.20
5	JH	115	MET	CG-SD-CE	-12.91	79.53	100.20
2	CD	50	ASP	CB-CG-OD1	12.77	129.79	118.30
5	HH	238	MET	CG-SD-CE	-12.32	80.49	100.20
5	EH	285	GLU	OE1-CD-OE2	12.01	137.72	123.30
5	VH	115	MET	CB-CG-SD	-11.83	76.90	112.40
2	Id	136	ASP	CB-CG-OD1	11.64	128.78	118.30
2	Dd	136	ASP	CB-CG-OD1	11.34	128.51	118.30
5	MH	207	ASP	CB-CG-OD1	11.27	128.44	118.30
5	EH	285	GLU	CG-CD-OE2	-11.04	96.23	118.30
5	KH	130	LEU	CA-CB-CG	10.99	140.58	115.30
5	GH	115	MET	CB-CG-SD	-10.93	79.61	112.40
5	XH	115	MET	CB-CG-SD	-10.91	79.68	112.40
5	FH	285	GLU	CG-CD-OE2	-10.62	97.06	118.30
6	LK	150	ASP	CB-CG-OD1	10.58	127.82	118.30
6	EK	150	ASP	CB-CG-OD1	10.56	127.81	118.30
6	CK	150	ASP	CB-CG-OD1	10.52	127.77	118.30
5	EH	208	LYS	CA-CB-CG	10.52	136.54	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	JK	150	ASP	CB-CG-OD1	10.52	127.77	118.30
6	KK	150	ASP	CB-CG-OD1	10.51	127.76	118.30
6	MK	150	ASP	CB-CG-OD1	10.51	127.76	118.30
6	BK	150	ASP	CB-CG-OD1	10.51	127.76	118.30
6	GK	150	ASP	CB-CG-OD1	10.51	127.76	118.30
6	DK	150	ASP	CB-CG-OD1	10.51	127.76	118.30
6	AK	150	ASP	CB-CG-OD1	10.49	127.74	118.30
6	IK	150	ASP	CB-CG-OD1	10.49	127.74	118.30
6	FK	150	ASP	CB-CG-OD1	10.49	127.74	118.30
6	HK	150	ASP	CB-CG-OD1	10.45	127.71	118.30
5	AH	115	MET	CG-SD-CE	-10.42	83.52	100.20
5	ZH	114	ASP	CB-CG-OD2	-9.94	109.36	118.30
5	CH	122	LEU	CB-CG-CD2	-9.89	94.18	111.00
4	FG	796	GLN	CA-CB-CG	9.82	135.01	113.40
4	XG	796	GLN	CA-CB-CG	9.81	134.99	113.40
4	YG	796	GLN	CA-CB-CG	9.81	134.99	113.40
4	VG	796	GLN	CA-CB-CG	9.81	134.98	113.40
4	ZG	796	GLN	CA-CB-CG	9.81	134.97	113.40
4	CG	796	GLN	CA-CB-CG	9.81	134.97	113.40
4	HG	796	GLN	CA-CB-CG	9.80	134.97	113.40
4	AG	796	GLN	CA-CB-CG	9.80	134.96	113.40
4	EG	796	GLN	CA-CB-CG	9.79	134.94	113.40
4	JG	796	GLN	CA-CB-CG	9.79	134.93	113.40
4	LG	796	GLN	CA-CB-CG	9.79	134.93	113.40
4	MG	796	GLN	CA-CB-CG	9.78	134.92	113.40
4	KG	796	GLN	CA-CB-CG	9.78	134.92	113.40
4	DG	796	GLN	CA-CB-CG	9.78	134.91	113.40
4	IG	796	GLN	CA-CB-CG	9.78	134.91	113.40
2	LD	50	ASP	CB-CG-OD1	9.77	127.10	118.30
2	Md	134	ASP	CB-CG-OD1	9.77	127.10	118.30
4	GG	796	GLN	CA-CB-CG	9.77	134.89	113.40
4	WG	796	GLN	CA-CB-CG	9.77	134.88	113.40
4	BG	796	GLN	CA-CB-CG	9.76	134.88	113.40
2	DD	35	ASP	CB-CG-OD1	9.68	127.01	118.30
2	Kd	106	PHE	CB-CG-CD1	-9.62	114.06	120.80
5	JH	208	LYS	CD-CE-NZ	-9.61	89.59	111.70
5	DH	285	GLU	OE1-CD-OE2	9.60	134.82	123.30
8	DM	196	MET	CA-CB-CG	9.60	129.62	113.30
8	FM	196	MET	CA-CB-CG	9.59	129.60	113.30
8	BM	196	MET	CA-CB-CG	9.59	129.60	113.30
2	Cd	52	MET	CA-CB-CG	9.58	129.59	113.30
8	GM	196	MET	CA-CB-CG	9.58	129.59	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	CM	196	MET	CA-CB-CG	9.58	129.59	113.30
8	IM	196	MET	CA-CB-CG	9.58	129.59	113.30
8	LM	196	MET	CA-CB-CG	9.57	129.57	113.30
8	MM	196	MET	CA-CB-CG	9.57	129.56	113.30
8	AM	196	MET	CA-CB-CG	9.56	129.56	113.30
8	HM	196	MET	CA-CB-CG	9.55	129.54	113.30
8	EM	196	MET	CA-CB-CG	9.54	129.52	113.30
8	JM	196	MET	CA-CB-CG	9.54	129.52	113.30
2	BD	55	MET	CG-SD-CE	-9.53	84.96	100.20
8	KM	196	MET	CA-CB-CG	9.52	129.49	113.30
5	GH	160	LEU	CB-CG-CD2	-9.47	94.89	111.00
2	Fd	82	ARG	CA-CB-CG	9.39	134.06	113.40
2	ID	136	ASP	CB-CG-OD1	9.36	126.73	118.30
8	DM	68	GLU	OE1-CD-OE2	-9.28	112.16	123.30
8	CM	68	GLU	OE1-CD-OE2	-9.27	112.17	123.30
8	KM	68	GLU	OE1-CD-OE2	-9.27	112.18	123.30
8	LM	68	GLU	OE1-CD-OE2	-9.27	112.18	123.30
8	MM	68	GLU	OE1-CD-OE2	-9.26	112.19	123.30
8	BM	68	GLU	OE1-CD-OE2	-9.25	112.20	123.30
8	HM	68	GLU	OE1-CD-OE2	-9.25	112.20	123.30
8	GM	68	GLU	OE1-CD-OE2	-9.25	112.20	123.30
8	FM	68	GLU	OE1-CD-OE2	-9.24	112.21	123.30
8	IM	68	GLU	OE1-CD-OE2	-9.23	112.23	123.30
2	AD	134	ASP	CB-CG-OD1	9.22	126.60	118.30
5	ZH	317	LEU	CB-CG-CD1	-9.22	95.32	111.00
2	Fd	82	ARG	CB-CG-CD	-9.21	87.66	111.60
8	JM	68	GLU	OE1-CD-OE2	-9.21	112.25	123.30
8	EM	68	GLU	OE1-CD-OE2	-9.19	112.27	123.30
2	ED	134	ASP	CB-CG-OD1	9.17	126.55	118.30
8	AM	68	GLU	OE1-CD-OE2	-9.17	112.30	123.30
5	EH	115	MET	CA-CB-CG	-9.15	97.75	113.30
2	Jd	125	ASP	CB-CG-OD1	9.07	126.47	118.30
2	Fd	126	GLU	OE1-CD-OE2	-9.06	112.43	123.30
2	Fd	82	ARG	CG-CD-NE	-9.06	92.78	111.80
5	WH	238	MET	CG-SD-CE	-9.05	85.72	100.20
2	Cd	134	ASP	CB-CG-OD1	9.04	126.44	118.30
5	BH	130	LEU	CA-CB-CG	9.03	136.06	115.30
2	DD	125	ASP	CB-CG-OD1	8.94	126.34	118.30
5	YH	115	MET	CA-CB-CG	-8.86	98.23	113.30
5	GH	115	MET	CG-SD-CE	-8.84	86.05	100.20
5	EH	130	LEU	CA-CB-CG	8.80	135.55	115.30
2	DD	52	MET	CG-SD-CE	-8.75	86.20	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	MC	123	GLN	CA-CB-CG	8.63	132.39	113.40
1	HC	123	GLN	CA-CB-CG	8.63	132.38	113.40
1	LC	123	GLN	CA-CB-CG	8.62	132.38	113.40
1	FC	123	GLN	CA-CB-CG	8.62	132.37	113.40
1	DC	123	GLN	CA-CB-CG	8.62	132.36	113.40
1	IC	123	GLN	CA-CB-CG	8.61	132.34	113.40
1	CC	123	GLN	CA-CB-CG	8.61	132.34	113.40
1	EC	123	GLN	CA-CB-CG	8.61	132.34	113.40
1	GC	123	GLN	CA-CB-CG	8.61	132.34	113.40
1	AC	123	GLN	CA-CB-CG	8.60	132.32	113.40
1	JC	123	GLN	CA-CB-CG	8.60	132.31	113.40
1	KC	123	GLN	CA-CB-CG	8.60	132.32	113.40
1	BC	123	GLN	CA-CB-CG	8.60	132.31	113.40
2	Ld	52	MET	CA-CB-CG	8.52	127.79	113.30
2	ID	52	MET	CG-SD-CE	-8.51	86.58	100.20
5	KH	115	MET	CG-SD-CE	-8.51	86.58	100.20
1	MC	60	LYS	CA-CB-CG	8.48	132.06	113.40
2	AD	50	ASP	CB-CG-OD1	8.48	125.93	118.30
1	LC	60	LYS	CA-CB-CG	8.48	132.06	113.40
1	AC	60	LYS	CA-CB-CG	8.48	132.05	113.40
1	GC	60	LYS	CA-CB-CG	8.47	132.04	113.40
1	HC	60	LYS	CA-CB-CG	8.47	132.03	113.40
1	CC	60	LYS	CA-CB-CG	8.46	132.02	113.40
1	IC	60	LYS	CA-CB-CG	8.46	132.02	113.40
1	KC	60	LYS	CA-CB-CG	8.46	132.01	113.40
5	MH	280	LEU	CA-CB-CG	8.46	134.75	115.30
1	JC	60	LYS	CA-CB-CG	8.45	132.00	113.40
1	BC	60	LYS	CA-CB-CG	8.45	131.99	113.40
1	EC	60	LYS	CA-CB-CG	8.45	131.98	113.40
1	FC	60	LYS	CA-CB-CG	8.43	131.95	113.40
1	DC	60	LYS	CA-CB-CG	8.43	131.94	113.40
5	EH	117	ARG	N-CA-CB	-8.43	95.43	110.60
5	VH	328	MET	CA-CB-CG	8.38	127.55	113.30
5	GH	183	ASP	CB-CG-OD1	8.37	125.83	118.30
5	ZH	339	MET	CG-SD-CE	-8.34	86.85	100.20
5	HH	115	MET	CB-CG-SD	-8.26	87.64	112.40
5	EH	117	ARG	CD-NE-CZ	-8.25	112.05	123.60
2	Dd	52	MET	CG-SD-CE	8.22	113.36	100.20
5	BH	354	MET	CG-SD-CE	-8.22	87.05	100.20
2	ED	52	MET	CG-SD-CE	-8.22	87.05	100.20
2	Fd	126	GLU	CG-CD-OE1	8.21	134.71	118.30
5	MH	179	LEU	CA-CB-CG	8.18	134.11	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Id	55	MET	CG-SD-CE	-8.14	87.17	100.20
9	EN	84	CYS	CA-CB-SG	8.13	128.63	114.00
9	JN	84	CYS	CA-CB-SG	8.13	128.63	114.00
5	BH	220	LEU	CA-CB-CG	8.12	133.99	115.30
9	KN	84	CYS	CA-CB-SG	8.13	128.63	114.00
9	AN	84	CYS	CA-CB-SG	8.12	128.61	114.00
9	CN	84	CYS	CA-CB-SG	8.12	128.61	114.00
9	FN	84	CYS	CA-CB-SG	8.12	128.61	114.00
9	LN	84	CYS	CA-CB-SG	8.12	128.61	114.00
9	DN	84	CYS	CA-CB-SG	8.11	128.60	114.00
9	HN	84	CYS	CA-CB-SG	8.11	128.60	114.00
9	GN	84	CYS	CA-CB-SG	8.11	128.59	114.00
9	BN	84	CYS	CA-CB-SG	8.10	128.59	114.00
9	MN	84	CYS	CA-CB-SG	8.10	128.58	114.00
9	IN	84	CYS	CA-CB-SG	8.10	128.57	114.00
5	IH	214	MET	CA-CB-CG	8.05	126.99	113.30
7	CL	110	GLN	CA-CB-CG	7.99	130.98	113.40
5	MH	122	LEU	CA-CB-CG	7.98	133.65	115.30
7	FL	110	GLN	CA-CB-CG	7.97	130.94	113.40
7	IL	110	GLN	CA-CB-CG	7.97	130.93	113.40
7	GL	110	GLN	CA-CB-CG	7.97	130.93	113.40
7	EL	110	GLN	CA-CB-CG	7.96	130.92	113.40
7	BL	110	GLN	CA-CB-CG	7.95	130.89	113.40
7	LL	110	GLN	CA-CB-CG	7.95	130.88	113.40
7	HL	110	GLN	CA-CB-CG	7.94	130.87	113.40
7	JL	110	GLN	CA-CB-CG	7.94	130.87	113.40
7	ML	110	GLN	CA-CB-CG	7.94	130.87	113.40
7	AL	110	GLN	CA-CB-CG	7.94	130.86	113.40
7	KL	110	GLN	CA-CB-CG	7.94	130.86	113.40
7	DL	110	GLN	CA-CB-CG	7.93	130.86	113.40
8	CM	70	MET	CA-CB-CG	7.93	126.78	113.30
8	HM	70	MET	CA-CB-CG	7.92	126.77	113.30
8	DM	70	MET	CA-CB-CG	7.91	126.75	113.30
8	FM	70	MET	CA-CB-CG	7.91	126.74	113.30
8	KM	70	MET	CA-CB-CG	7.91	126.74	113.30
8	MM	70	MET	CA-CB-CG	7.90	126.74	113.30
8	GM	70	MET	CA-CB-CG	7.88	126.69	113.30
2	Kd	106	PHE	CB-CG-CD2	7.87	126.31	120.80
5	LH	157	PHE	CB-CG-CD1	-7.87	115.29	120.80
8	BM	70	MET	CA-CB-CG	7.87	126.67	113.30
8	JM	70	MET	CA-CB-CG	7.86	126.67	113.30
8	EM	70	MET	CA-CB-CG	7.86	126.66	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	IM	70	MET	CA-CB-CG	7.85	126.65	113.30
8	LM	70	MET	CA-CB-CG	7.85	126.65	113.30
8	AM	70	MET	CA-CB-CG	7.85	126.65	113.30
2	GD	125	ASP	CB-CG-OD1	7.85	125.36	118.30
7	AL	211	LYS	CB-CG-CD	7.82	131.92	111.60
7	FL	211	LYS	CB-CG-CD	7.82	131.93	111.60
7	EL	211	LYS	CB-CG-CD	7.82	131.92	111.60
7	CL	211	LYS	CB-CG-CD	7.81	131.91	111.60
4	XG	813	LYS	CA-CB-CG	7.81	130.59	113.40
4	BG	813	LYS	CA-CB-CG	7.81	130.59	113.40
7	HL	211	LYS	CB-CG-CD	7.81	131.90	111.60
4	MG	813	LYS	CA-CB-CG	7.81	130.58	113.40
4	GG	813	LYS	CA-CB-CG	7.80	130.57	113.40
7	KL	211	LYS	CB-CG-CD	7.80	131.89	111.60
4	EG	813	LYS	CA-CB-CG	7.80	130.56	113.40
4	FG	813	LYS	CA-CB-CG	7.80	130.56	113.40
7	BL	211	LYS	CB-CG-CD	7.80	131.88	111.60
7	DL	211	LYS	CB-CG-CD	7.80	131.88	111.60
4	LG	813	LYS	CA-CB-CG	7.80	130.56	113.40
7	IL	211	LYS	CB-CG-CD	7.80	131.87	111.60
4	AG	813	LYS	CA-CB-CG	7.79	130.55	113.40
4	WG	813	LYS	CA-CB-CG	7.79	130.55	113.40
4	YG	813	LYS	CA-CB-CG	7.79	130.55	113.40
4	HG	813	LYS	CA-CB-CG	7.79	130.55	113.40
7	ML	211	LYS	CB-CG-CD	7.79	131.86	111.60
7	LL	211	LYS	CB-CG-CD	7.79	131.85	111.60
4	VG	813	LYS	CA-CB-CG	7.79	130.54	113.40
7	GL	211	LYS	CB-CG-CD	7.79	131.85	111.60
4	JG	813	LYS	CA-CB-CG	7.79	130.53	113.40
4	ZG	813	LYS	CA-CB-CG	7.78	130.51	113.40
7	JL	211	LYS	CB-CG-CD	7.78	131.82	111.60
4	CG	813	LYS	CA-CB-CG	7.78	130.51	113.40
4	KG	813	LYS	CA-CB-CG	7.78	130.51	113.40
4	DG	813	LYS	CA-CB-CG	7.78	130.50	113.40
4	IG	813	LYS	CA-CB-CG	7.77	130.49	113.40
2	BD	134	ASP	CB-CG-OD1	7.76	125.28	118.30
2	Cd	86	ASP	CB-CG-OD1	7.69	125.22	118.30
5	EH	238	MET	CG-SD-CE	-7.69	87.89	100.20
5	MH	207	ASP	OD1-CG-OD2	-7.66	108.74	123.30
5	BH	214	MET	CA-CB-CG	7.65	126.31	113.30
2	HD	55	MET	CG-SD-CE	-7.64	87.98	100.20
3	ZF	243	MET	CA-CB-CG	7.63	126.27	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	FF	243	MET	CA-CB-CG	7.63	126.27	113.30
3	VF	243	MET	CA-CB-CG	7.62	126.25	113.30
3	YF	243	MET	CA-CB-CG	7.62	126.25	113.30
3	JF	243	MET	CA-CB-CG	7.62	126.25	113.30
3	DF	243	MET	CA-CB-CG	7.61	126.24	113.30
3	EF	243	MET	CA-CB-CG	7.61	126.24	113.30
3	CF	243	MET	CA-CB-CG	7.61	126.24	113.30
3	AF	243	MET	CA-CB-CG	7.61	126.23	113.30
3	GF	243	MET	CA-CB-CG	7.60	126.22	113.30
3	IF	243	MET	CA-CB-CG	7.60	126.22	113.30
3	HF	243	MET	CA-CB-CG	7.60	126.22	113.30
3	MF	243	MET	CA-CB-CG	7.60	126.22	113.30
5	XH	328	MET	CG-SD-CE	-7.60	88.05	100.20
3	KF	243	MET	CA-CB-CG	7.59	126.21	113.30
3	XF	243	MET	CA-CB-CG	7.59	126.20	113.30
3	BF	243	MET	CA-CB-CG	7.59	126.20	113.30
2	Kd	52	MET	CA-CB-CG	7.58	126.19	113.30
3	LF	243	MET	CA-CB-CG	7.58	126.18	113.30
2	Gd	82	ARG	CG-CD-NE	-7.57	95.91	111.80
5	IH	150	LYS	CA-CB-CG	7.57	130.04	113.40
3	WF	243	MET	CA-CB-CG	7.56	126.16	113.30
2	DD	55	MET	CG-SD-CE	-7.53	88.16	100.20
5	BH	279	LEU	CB-CG-CD1	-7.50	98.26	111.00
5	DH	285	GLU	CA-CB-CG	-7.48	96.95	113.40
2	Bd	134	ASP	CB-CG-OD1	7.45	125.00	118.30
2	ED	125	ASP	CB-CG-OD1	7.42	124.98	118.30
2	CD	125	ASP	CB-CG-OD1	7.42	124.97	118.30
2	Bd	52	MET	CA-CB-CG	7.41	125.89	113.30
5	JH	354	MET	CG-SD-CE	-7.37	88.41	100.20
2	Dd	55	MET	CG-SD-CE	-7.37	88.42	100.20
5	XH	354	MET	CG-SD-CE	-7.36	88.42	100.20
5	KH	241	LEU	CA-CB-CG	7.33	132.17	115.30
3	HF	267	GLU	CA-CB-CG	7.33	129.53	113.40
2	Fd	52	MET	CG-SD-CE	-7.32	88.48	100.20
5	LH	157	PHE	CB-CG-CD2	7.32	125.92	120.80
3	XF	267	GLU	CA-CB-CG	7.32	129.50	113.40
2	DD	94	LEU	CB-CG-CD2	7.32	123.44	111.00
3	JF	267	GLU	CA-CB-CG	7.31	129.49	113.40
3	EF	267	GLU	CA-CB-CG	7.31	129.48	113.40
3	GF	267	GLU	CA-CB-CG	7.31	129.47	113.40
3	ZF	267	GLU	CA-CB-CG	7.31	129.47	113.40
3	VF	267	GLU	CA-CB-CG	7.30	129.47	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	YF	267	GLU	CA-CB-CG	7.30	129.46	113.40
3	AF	267	GLU	CA-CB-CG	7.30	129.45	113.40
3	DF	267	GLU	CA-CB-CG	7.29	129.45	113.40
3	LF	267	GLU	CA-CB-CG	7.29	129.45	113.40
3	BF	267	GLU	CA-CB-CG	7.29	129.44	113.40
2	Gd	52	MET	CA-CB-CG	7.29	125.70	113.30
3	WF	267	GLU	CA-CB-CG	7.29	129.44	113.40
3	CF	267	GLU	CA-CB-CG	7.29	129.43	113.40
3	FF	267	GLU	CA-CB-CG	7.29	129.43	113.40
5	KH	157	PHE	CB-CG-CD1	-7.28	115.70	120.80
3	IF	267	GLU	CA-CB-CG	7.28	129.42	113.40
3	KF	267	GLU	CA-CB-CG	7.28	129.41	113.40
3	MF	267	GLU	CA-CB-CG	7.28	129.41	113.40
2	BD	107	ARG	NE-CZ-NH2	-7.26	116.67	120.30
5	FH	208	LYS	CD-CE-NZ	-7.26	95.00	111.70
5	GH	122	LEU	CB-CG-CD2	-7.25	98.68	111.00
2	Jd	52	MET	CG-SD-CE	-7.25	88.61	100.20
5	LH	158	VAL	CG1-CB-CG2	-7.23	99.33	110.90
2	MD	125	ASP	CB-CG-OD1	7.21	124.79	118.30
5	IH	150	LYS	CB-CG-CD	7.21	130.35	111.60
5	AH	205	GLN	CA-CB-CG	-7.21	97.54	113.40
2	LD	52	MET	CG-SD-CE	-7.19	88.69	100.20
5	WH	207	ASP	CB-CG-OD2	-7.19	111.83	118.30
5	IH	208	LYS	N-CA-CB	-7.16	97.72	110.60
5	WH	356	LEU	CA-CB-CG	7.15	131.74	115.30
2	Id	52	MET	CA-CB-CG	7.15	125.45	113.30
5	ZH	214	MET	CA-CB-CG	7.11	125.38	113.30
8	IM	60	LEU	CA-CB-CG	7.10	131.63	115.30
8	EM	60	LEU	CA-CB-CG	7.10	131.62	115.30
8	CM	60	LEU	CA-CB-CG	7.09	131.62	115.30
8	KM	60	LEU	CA-CB-CG	7.09	131.61	115.30
8	MM	60	LEU	CA-CB-CG	7.09	131.60	115.30
8	JM	60	LEU	CA-CB-CG	7.08	131.59	115.30
8	BM	60	LEU	CA-CB-CG	7.08	131.59	115.30
8	DM	60	LEU	CA-CB-CG	7.08	131.59	115.30
2	Fd	134	ASP	CB-CG-OD1	7.08	124.67	118.30
8	GM	60	LEU	CA-CB-CG	7.08	131.58	115.30
8	FM	60	LEU	CA-CB-CG	7.08	131.57	115.30
8	HM	60	LEU	CA-CB-CG	7.07	131.57	115.30
8	LM	60	LEU	CA-CB-CG	7.07	131.57	115.30
8	AM	60	LEU	CA-CB-CG	7.06	131.54	115.30
5	ZH	114	ASP	CB-CG-OD1	7.05	124.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BD	107	ARG	NE-CZ-NH1	7.05	123.83	120.30
5	EH	157	PHE	CB-CG-CD1	-7.04	115.87	120.80
2	GD	107	ARG	CG-CD-NE	7.03	126.57	111.80
5	HH	122	LEU	CB-CG-CD2	-7.02	99.06	111.00
5	IH	208	LYS	CA-CB-CG	7.01	128.83	113.40
2	LD	52	MET	CB-CG-SD	-7.01	91.36	112.40
2	AD	125	ASP	CB-CG-OD1	6.99	124.59	118.30
5	EH	285	GLU	CA-CB-CG	-6.98	98.04	113.40
2	LD	55	MET	CA-CB-CG	6.98	125.16	113.30
5	CH	238	MET	CB-CG-SD	-6.97	91.48	112.40
8	EM	262	GLU	CA-CB-CG	6.95	128.69	113.40
8	IM	262	GLU	CA-CB-CG	6.95	128.69	113.40
8	GM	262	GLU	CA-CB-CG	6.94	128.67	113.40
8	CM	262	GLU	CA-CB-CG	6.94	128.67	113.40
8	JM	262	GLU	CA-CB-CG	6.94	128.66	113.40
8	KM	262	GLU	CA-CB-CG	6.94	128.67	113.40
2	ID	55	MET	CG-SD-CE	-6.94	89.10	100.20
8	DM	262	GLU	CA-CB-CG	6.93	128.65	113.40
8	FM	262	GLU	CA-CB-CG	6.93	128.65	113.40
8	HM	262	GLU	CA-CB-CG	6.93	128.65	113.40
8	LM	262	GLU	CA-CB-CG	6.93	128.64	113.40
8	AM	262	GLU	CA-CB-CG	6.92	128.63	113.40
8	MM	262	GLU	CA-CB-CG	6.92	128.63	113.40
5	MH	311	MET	CB-CG-SD	-6.91	91.67	112.40
8	BM	262	GLU	CA-CB-CG	6.91	128.59	113.40
5	GH	311	MET	CB-CG-SD	-6.90	91.69	112.40
5	GH	248	VAL	CG1-CB-CG2	-6.90	99.86	110.90
5	JH	157	PHE	CB-CG-CD1	-6.90	115.97	120.80
2	CD	50	ASP	CB-CG-OD2	-6.90	112.09	118.30
5	KH	226	LEU	CA-CB-CG	6.89	131.14	115.30
2	BD	68	ASP	CB-CG-OD1	6.88	124.50	118.30
5	BH	115	MET	CA-CB-CG	-6.88	101.60	113.30
5	ZH	284	LEU	CA-CB-CG	6.88	131.11	115.30
2	KD	125	ASP	CB-CG-OD1	6.84	124.46	118.30
2	HD	52	MET	CB-CG-SD	-6.82	91.93	112.40
2	Bd	55	MET	CG-SD-CE	-6.82	89.30	100.20
2	Cd	126	GLU	CG-CD-OE2	6.82	131.93	118.30
2	LD	94	LEU	CB-CG-CD2	6.76	122.50	111.00
2	MD	94	LEU	CB-CG-CD2	6.76	122.50	111.00
2	Ad	94	LEU	CB-CG-CD2	6.74	122.46	111.00
2	AD	128	LEU	CB-CG-CD1	-6.73	99.56	111.00
7	IL	211	LYS	CA-CB-CG	6.73	128.20	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	KL	211	LYS	CA-CB-CG	6.73	128.20	113.40
7	LL	211	LYS	CA-CB-CG	6.72	128.18	113.40
7	JL	211	LYS	CA-CB-CG	6.72	128.17	113.40
7	GL	211	LYS	CA-CB-CG	6.71	128.17	113.40
7	EL	211	LYS	CA-CB-CG	6.71	128.17	113.40
7	ML	211	LYS	CA-CB-CG	6.71	128.17	113.40
1	EC	60	LYS	CB-CG-CD	6.71	129.05	111.60
1	FC	60	LYS	CB-CG-CD	6.70	129.03	111.60
7	FL	211	LYS	CA-CB-CG	6.70	128.15	113.40
7	HL	211	LYS	CA-CB-CG	6.70	128.15	113.40
7	BL	211	LYS	CA-CB-CG	6.70	128.15	113.40
1	CC	60	LYS	CB-CG-CD	6.70	129.01	111.60
7	AL	211	LYS	CA-CB-CG	6.70	128.13	113.40
7	DL	211	LYS	CA-CB-CG	6.70	128.13	113.40
2	Gd	105	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	KC	60	LYS	CB-CG-CD	6.69	129.00	111.60
1	JC	60	LYS	CB-CG-CD	6.69	128.99	111.60
1	DC	60	LYS	CB-CG-CD	6.68	128.98	111.60
1	AC	60	LYS	CB-CG-CD	6.68	128.97	111.60
1	BC	60	LYS	CB-CG-CD	6.68	128.98	111.60
1	HC	60	LYS	CB-CG-CD	6.68	128.97	111.60
1	IC	60	LYS	CB-CG-CD	6.68	128.96	111.60
1	LC	60	LYS	CB-CG-CD	6.68	128.96	111.60
7	CL	211	LYS	CA-CB-CG	6.68	128.09	113.40
1	GC	60	LYS	CB-CG-CD	6.66	128.93	111.60
5	LH	216	GLN	N-CA-CB	6.66	122.59	110.60
1	MC	60	LYS	CB-CG-CD	6.66	128.91	111.60
2	BD	118	LEU	CB-CG-CD2	-6.66	99.68	111.00
2	Bd	35	ASP	CB-CG-OD1	6.65	124.29	118.30
4	IG	795	GLN	CA-CB-CG	6.65	128.02	113.40
2	Gd	82	ARG	CA-CB-CG	6.63	127.99	113.40
4	DG	795	GLN	CA-CB-CG	6.63	127.99	113.40
4	AG	795	GLN	CA-CB-CG	6.63	127.99	113.40
4	WG	795	GLN	CA-CB-CG	6.63	127.98	113.40
4	ZG	795	GLN	CA-CB-CG	6.63	127.98	113.40
4	CG	795	GLN	CA-CB-CG	6.63	127.98	113.40
4	MG	795	GLN	CA-CB-CG	6.62	127.97	113.40
4	FG	795	GLN	CA-CB-CG	6.62	127.97	113.40
4	KG	795	GLN	CA-CB-CG	6.62	127.97	113.40
4	JG	795	GLN	CA-CB-CG	6.62	127.96	113.40
4	BG	795	GLN	CA-CB-CG	6.62	127.96	113.40
4	VG	795	GLN	CA-CB-CG	6.62	127.96	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	YG	795	GLN	CA-CB-CG	6.62	127.96	113.40
4	HG	795	GLN	CA-CB-CG	6.61	127.95	113.40
4	XG	795	GLN	CA-CB-CG	6.61	127.95	113.40
4	GG	795	GLN	CA-CB-CG	6.61	127.94	113.40
4	EG	795	GLN	CA-CB-CG	6.60	127.92	113.40
4	LG	795	GLN	CA-CB-CG	6.60	127.91	113.40
8	AM	76	ARG	CB-CG-CD	-6.58	94.49	111.60
8	BM	76	ARG	CB-CG-CD	-6.58	94.49	111.60
8	CM	76	ARG	CB-CG-CD	-6.58	94.49	111.60
8	EM	76	ARG	CB-CG-CD	-6.58	94.49	111.60
8	KM	76	ARG	CB-CG-CD	-6.57	94.51	111.60
8	MM	76	ARG	CB-CG-CD	-6.57	94.51	111.60
8	DM	76	ARG	CB-CG-CD	-6.56	94.54	111.60
8	JM	76	ARG	CB-CG-CD	-6.56	94.54	111.60
8	GM	76	ARG	CB-CG-CD	-6.56	94.55	111.60
8	LM	76	ARG	CB-CG-CD	-6.56	94.55	111.60
8	IM	76	ARG	CB-CG-CD	-6.55	94.56	111.60
2	ED	52	MET	CA-CB-CG	-6.55	102.16	113.30
8	FM	76	ARG	CB-CG-CD	-6.55	94.56	111.60
2	CD	52	MET	CA-CB-CG	-6.54	102.17	113.30
8	HM	76	ARG	CB-CG-CD	-6.54	94.59	111.60
2	Ed	134	ASP	CB-CG-OD1	6.54	124.18	118.30
5	ZH	301	ASP	CB-CG-OD1	6.54	124.18	118.30
2	Fd	130	GLU	OE1-CD-OE2	-6.53	115.47	123.30
6	MK	122	LYS	CD-CE-NZ	6.53	126.71	111.70
6	AK	122	LYS	CD-CE-NZ	6.52	126.69	111.70
6	HK	129	GLU	CA-CB-CG	6.52	127.74	113.40
5	WH	328	MET	CA-CB-CG	6.51	124.37	113.30
5	EH	157	PHE	CB-CG-CD2	6.51	125.36	120.80
6	IK	122	LYS	CD-CE-NZ	6.51	126.67	111.70
6	BK	122	LYS	CD-CE-NZ	6.51	126.67	111.70
6	FK	122	LYS	CD-CE-NZ	6.50	126.65	111.70
6	JK	122	LYS	CD-CE-NZ	6.50	126.65	111.70
6	IK	129	GLU	CA-CB-CG	6.50	127.69	113.40
6	MK	129	GLU	CA-CB-CG	6.50	127.69	113.40
6	CK	129	GLU	CA-CB-CG	6.49	127.68	113.40
6	FK	129	GLU	CA-CB-CG	6.49	127.68	113.40
6	EK	122	LYS	CD-CE-NZ	6.49	126.62	111.70
2	ID	125	ASP	CB-CG-OD1	6.49	124.14	118.30
2	KD	55	MET	CA-CB-CG	6.49	124.33	113.30
6	JK	129	GLU	CA-CB-CG	6.49	127.67	113.40
6	LK	129	GLU	CA-CB-CG	6.49	127.67	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	GK	122	LYS	CD-CE-NZ	6.48	126.61	111.70
6	EK	129	GLU	CA-CB-CG	6.48	127.65	113.40
6	AK	129	GLU	CA-CB-CG	6.47	127.64	113.40
6	GK	129	GLU	CA-CB-CG	6.47	127.64	113.40
6	CK	122	LYS	CD-CE-NZ	6.47	126.59	111.70
6	LK	122	LYS	CD-CE-NZ	6.47	126.59	111.70
6	DK	129	GLU	CA-CB-CG	6.47	127.64	113.40
6	DK	122	LYS	CD-CE-NZ	6.47	126.58	111.70
6	HK	122	LYS	CD-CE-NZ	6.47	126.58	111.70
6	KK	122	LYS	CD-CE-NZ	6.46	126.57	111.70
6	KK	129	GLU	CA-CB-CG	6.46	127.61	113.40
2	Jd	52	MET	CA-CB-CG	6.45	124.26	113.30
5	DH	130	LEU	CA-CB-CG	6.44	130.12	115.30
6	BK	129	GLU	CA-CB-CG	6.44	127.58	113.40
5	IH	196	LEU	CB-CG-CD2	-6.44	100.05	111.00
2	ED	55	MET	CG-SD-CE	-6.43	89.91	100.20
8	HM	196	MET	CB-CG-SD	6.43	131.69	112.40
8	KM	196	MET	CB-CG-SD	6.43	131.69	112.40
8	IM	196	MET	CB-CG-SD	6.43	131.68	112.40
8	JM	196	MET	CB-CG-SD	6.43	131.68	112.40
8	CM	196	MET	CB-CG-SD	6.41	131.64	112.40
8	EM	196	MET	CB-CG-SD	6.41	131.64	112.40
8	GM	196	MET	CB-CG-SD	6.41	131.64	112.40
8	AM	196	MET	CB-CG-SD	6.41	131.63	112.40
8	MM	196	MET	CB-CG-SD	6.41	131.63	112.40
8	LM	196	MET	CB-CG-SD	6.41	131.62	112.40
2	KD	68	ASP	CB-CG-OD1	6.40	124.06	118.30
8	DM	196	MET	CB-CG-SD	6.40	131.61	112.40
2	Dd	86	ASP	CB-CG-OD1	6.40	124.06	118.30
8	FM	196	MET	CB-CG-SD	6.40	131.59	112.40
8	BM	196	MET	CB-CG-SD	6.39	131.58	112.40
2	GD	94	LEU	CB-CG-CD2	6.38	121.85	111.00
5	ZH	208	LYS	N-CA-CB	-6.38	99.11	110.60
5	EH	138	GLU	CA-CB-CG	6.36	127.39	113.40
4	EG	801	MET	CG-SD-CE	-6.36	90.03	100.20
4	KG	801	MET	CG-SD-CE	-6.35	90.03	100.20
5	JH	157	PHE	CB-CG-CD2	6.35	125.25	120.80
4	XG	801	MET	CG-SD-CE	-6.35	90.04	100.20
5	VH	115	MET	CG-SD-CE	-6.35	90.04	100.20
4	FG	801	MET	CG-SD-CE	-6.35	90.05	100.20
4	MG	801	MET	CG-SD-CE	-6.34	90.05	100.20
2	Cd	156	LEU	CB-CG-CD2	6.34	121.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	GG	801	MET	CG-SD-CE	-6.34	90.05	100.20
4	JG	801	MET	CG-SD-CE	-6.34	90.05	100.20
4	AG	801	MET	CG-SD-CE	-6.34	90.06	100.20
4	YG	801	MET	CG-SD-CE	-6.34	90.06	100.20
5	LH	189	TRP	CA-CB-CG	6.33	125.74	113.70
4	ZG	801	MET	CG-SD-CE	-6.33	90.06	100.20
4	DG	801	MET	CG-SD-CE	-6.33	90.07	100.20
4	VG	801	MET	CG-SD-CE	-6.33	90.07	100.20
2	Ed	86	ASP	CB-CG-OD1	6.33	124.00	118.30
2	DD	52	MET	CA-CB-CG	-6.33	102.54	113.30
4	CG	801	MET	CG-SD-CE	-6.32	90.09	100.20
2	ED	94	LEU	CB-CG-CD2	6.32	121.74	111.00
4	HG	801	MET	CG-SD-CE	-6.32	90.09	100.20
4	IG	801	MET	CG-SD-CE	-6.32	90.09	100.20
4	BG	801	MET	CG-SD-CE	-6.31	90.10	100.20
2	DD	86	ASP	CB-CG-OD1	6.31	123.98	118.30
4	WG	801	MET	CG-SD-CE	-6.31	90.11	100.20
4	LG	801	MET	CG-SD-CE	-6.30	90.11	100.20
2	Gd	109	LEU	CB-CG-CD1	6.30	121.70	111.00
5	KH	214	MET	CG-SD-CE	-6.29	90.13	100.20
2	Kd	86	ASP	CB-CG-OD1	6.29	123.96	118.30
2	KD	41	LEU	CB-CG-CD1	6.28	121.68	111.00
5	FH	157	PHE	CB-CG-CD1	-6.28	116.40	120.80
2	Hd	36	ASP	CB-CG-OD2	-6.27	112.66	118.30
2	LD	52	MET	CA-CB-CG	-6.27	102.64	113.30
5	FH	134	TYR	CB-CG-CD1	-6.25	117.25	121.00
2	HD	125	ASP	CB-CG-OD1	6.24	123.91	118.30
2	Md	94	LEU	CB-CG-CD2	6.24	121.60	111.00
2	Id	125	ASP	CB-CG-OD1	6.24	123.91	118.30
8	DM	145	ARG	CA-CB-CG	6.21	127.06	113.40
5	YH	183	ASP	CB-CG-OD1	6.21	123.89	118.30
8	KM	145	ARG	CA-CB-CG	6.20	127.04	113.40
8	BM	145	ARG	CA-CB-CG	6.20	127.04	113.40
2	HD	52	MET	CG-SD-CE	-6.20	90.28	100.20
8	LM	145	ARG	CA-CB-CG	6.20	127.04	113.40
5	ZH	317	LEU	CB-CG-CD2	6.20	121.54	111.00
8	EM	145	ARG	CA-CB-CG	6.20	127.03	113.40
8	AM	145	ARG	CA-CB-CG	6.19	127.02	113.40
8	CM	145	ARG	CA-CB-CG	6.19	127.01	113.40
8	GM	145	ARG	CA-CB-CG	6.18	127.00	113.40
8	FM	145	ARG	CA-CB-CG	6.18	127.00	113.40
8	HM	145	ARG	CA-CB-CG	6.18	126.99	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	MM	145	ARG	CA-CB-CG	6.17	126.99	113.40
8	IM	145	ARG	CA-CB-CG	6.17	126.98	113.40
8	JM	145	ARG	CA-CB-CG	6.17	126.97	113.40
2	GD	55	MET	CG-SD-CE	-6.16	90.34	100.20
5	DH	354	MET	CG-SD-CE	-6.16	90.34	100.20
2	Dd	94	LEU	CB-CG-CD2	6.15	121.45	111.00
5	EH	183	ASP	CB-CG-OD1	6.13	123.82	118.30
5	YH	238	MET	CG-SD-CE	-6.13	90.39	100.20
2	ID	94	LEU	CB-CG-CD2	6.13	121.42	111.00
2	CD	55	MET	CG-SD-CE	-6.11	90.43	100.20
5	KH	157	PHE	CB-CG-CD2	6.10	125.07	120.80
8	JM	68	GLU	CG-CD-OE1	6.09	130.48	118.30
8	BM	68	GLU	CG-CD-OE1	6.09	130.47	118.30
5	IH	231	ARG	NE-CZ-NH1	-6.08	117.26	120.30
8	HM	68	GLU	CG-CD-OE1	6.08	130.46	118.30
8	LM	68	GLU	CG-CD-OE1	6.08	130.45	118.30
8	CM	68	GLU	CG-CD-OE1	6.08	130.45	118.30
8	GM	68	GLU	CG-CD-OE1	6.07	130.45	118.30
8	FM	68	GLU	CG-CD-OE1	6.07	130.44	118.30
8	KM	68	GLU	CG-CD-OE1	6.07	130.43	118.30
8	DM	68	GLU	CG-CD-OE1	6.06	130.43	118.30
5	WH	115	MET	CA-CB-CG	-6.06	102.99	113.30
8	IM	68	GLU	CG-CD-OE1	6.06	130.41	118.30
8	AM	68	GLU	CG-CD-OE1	6.05	130.40	118.30
8	EM	68	GLU	CG-CD-OE1	6.05	130.40	118.30
8	MM	68	GLU	CG-CD-OE1	6.05	130.40	118.30
2	ED	118	LEU	CB-CG-CD2	-6.05	100.72	111.00
7	CL	160	GLN	CA-CB-CG	6.03	126.67	113.40
5	HH	226	LEU	CA-CB-CG	6.03	129.18	115.30
7	LL	160	GLN	CA-CB-CG	6.03	126.67	113.40
7	DL	160	GLN	CA-CB-CG	6.01	126.63	113.40
2	LD	136	ASP	CB-CG-OD1	6.01	123.71	118.30
7	GL	160	GLN	CA-CB-CG	6.01	126.61	113.40
7	HL	160	GLN	CA-CB-CG	6.01	126.61	113.40
2	MD	71	LEU	CB-CG-CD2	-6.01	100.79	111.00
7	AL	160	GLN	CA-CB-CG	6.00	126.61	113.40
7	IL	160	GLN	CA-CB-CG	6.00	126.61	113.40
7	KL	160	GLN	CA-CB-CG	6.00	126.61	113.40
7	BL	160	GLN	CA-CB-CG	6.00	126.60	113.40
7	ML	160	GLN	CA-CB-CG	6.00	126.60	113.40
7	EL	160	GLN	CA-CB-CG	6.00	126.59	113.40
7	FL	160	GLN	CA-CB-CG	6.00	126.59	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	JL	160	GLN	CA-CB-CG	5.98	126.56	113.40
5	YH	326	ALA	N-CA-CB	5.96	118.44	110.10
5	YH	214	MET	CA-CB-CG	5.96	123.43	113.30
2	Ad	156	LEU	CB-CG-CD2	5.96	121.13	111.00
2	ED	52	MET	CB-CG-SD	-5.95	94.56	112.40
2	Kd	55	MET	CG-SD-CE	-5.93	90.72	100.20
2	AD	117	VAL	CG1-CB-CG2	-5.92	101.43	110.90
2	Ad	86	ASP	CB-CG-OD1	5.91	123.62	118.30
5	KH	246	LYS	CD-CE-NZ	-5.91	98.11	111.70
9	IN	115	GLN	CA-CB-CG	5.89	126.36	113.40
4	WG	796	GLN	N-CA-CB	5.89	121.20	110.60
9	AN	115	GLN	CA-CB-CG	5.88	126.34	113.40
5	GH	250	TYR	CB-CG-CD2	-5.88	117.47	121.00
9	KN	115	GLN	CA-CB-CG	5.88	126.33	113.40
9	MN	115	GLN	CA-CB-CG	5.88	126.33	113.40
9	BN	115	GLN	CA-CB-CG	5.87	126.32	113.40
8	CM	184	LEU	CA-CB-CG	5.87	128.81	115.30
9	DN	115	GLN	CA-CB-CG	5.87	126.32	113.40
9	FN	115	GLN	CA-CB-CG	5.87	126.32	113.40
2	KD	94	LEU	CB-CG-CD2	5.87	120.98	111.00
9	JN	115	GLN	CA-CB-CG	5.87	126.31	113.40
8	AM	184	LEU	CA-CB-CG	5.87	128.79	115.30
4	KG	796	GLN	N-CA-CB	5.87	121.16	110.60
3	GF	246	LEU	CB-CG-CD2	-5.87	101.03	111.00
4	BG	796	GLN	N-CA-CB	5.86	121.15	110.60
9	EN	115	GLN	CA-CB-CG	5.86	126.30	113.40
9	CN	115	GLN	CA-CB-CG	5.86	126.29	113.40
9	LN	115	GLN	CA-CB-CG	5.86	126.29	113.40
3	VF	246	LEU	CB-CG-CD2	-5.86	101.04	111.00
4	AG	796	GLN	N-CA-CB	5.86	121.14	110.60
8	KM	184	LEU	CA-CB-CG	5.86	128.76	115.30
4	IG	796	GLN	N-CA-CB	5.85	121.14	110.60
8	DM	184	LEU	CA-CB-CG	5.85	128.76	115.30
3	HF	246	LEU	CB-CG-CD2	-5.85	101.05	111.00
4	GG	796	GLN	N-CA-CB	5.85	121.13	110.60
9	HN	115	GLN	CA-CB-CG	5.85	126.27	113.40
2	Ld	68	ASP	CB-CG-OD1	5.85	123.56	118.30
4	XG	796	GLN	N-CA-CB	5.85	121.13	110.60
8	HM	184	LEU	CA-CB-CG	5.85	128.75	115.30
4	DG	796	GLN	N-CA-CB	5.85	121.12	110.60
8	EM	184	LEU	CA-CB-CG	5.85	128.75	115.30
8	IM	184	LEU	CA-CB-CG	5.85	128.75	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	JG	796	GLN	N-CA-CB	5.85	121.12	110.60
4	CG	796	GLN	N-CA-CB	5.84	121.12	110.60
4	EG	796	GLN	N-CA-CB	5.84	121.11	110.60
8	FM	184	LEU	CA-CB-CG	5.84	128.73	115.30
4	MG	796	GLN	N-CA-CB	5.84	121.11	110.60
8	MM	184	LEU	CA-CB-CG	5.84	128.73	115.30
4	HG	796	GLN	N-CA-CB	5.84	121.11	110.60
8	LM	184	LEU	CA-CB-CG	5.84	128.73	115.30
3	MF	246	LEU	CB-CG-CD2	-5.84	101.07	111.00
4	ZG	796	GLN	N-CA-CB	5.84	121.11	110.60
4	LG	796	GLN	N-CA-CB	5.84	121.11	110.60
8	BM	184	LEU	CA-CB-CG	5.84	128.73	115.30
3	CF	246	LEU	CB-CG-CD2	-5.84	101.08	111.00
8	GM	184	LEU	CA-CB-CG	5.84	128.73	115.30
3	KF	246	LEU	CB-CG-CD2	-5.84	101.08	111.00
3	YF	246	LEU	CB-CG-CD2	-5.84	101.08	111.00
2	ID	107	ARG	NE-CZ-NH1	-5.83	117.38	120.30
2	BD	125	ASP	CB-CG-OD1	5.83	123.55	118.30
3	JF	246	LEU	CB-CG-CD2	-5.83	101.08	111.00
8	JM	184	LEU	CA-CB-CG	5.83	128.72	115.30
2	CD	52	MET	CB-CG-SD	-5.83	94.90	112.40
3	EF	246	LEU	CB-CG-CD2	-5.83	101.09	111.00
2	Hd	156	LEU	CB-CG-CD2	5.83	120.92	111.00
5	ZH	183	ASP	CB-CG-OD1	5.83	123.55	118.30
4	FG	796	GLN	N-CA-CB	5.83	121.09	110.60
3	LF	246	LEU	CB-CG-CD2	-5.83	101.09	111.00
4	VG	796	GLN	N-CA-CB	5.83	121.08	110.60
3	WF	246	LEU	CB-CG-CD2	-5.83	101.09	111.00
3	XF	246	LEU	CB-CG-CD2	-5.83	101.09	111.00
4	YG	796	GLN	N-CA-CB	5.83	121.09	110.60
2	ID	52	MET	CA-CB-CG	-5.82	103.40	113.30
3	ZF	246	LEU	CB-CG-CD2	-5.82	101.10	111.00
5	IH	311	MET	CG-SD-CE	5.82	109.51	100.20
9	GN	115	GLN	CA-CB-CG	5.82	126.20	113.40
3	DF	246	LEU	CB-CG-CD2	-5.82	101.11	111.00
3	FF	246	LEU	CB-CG-CD2	-5.81	101.12	111.00
5	MH	179	LEU	CB-CG-CD2	-5.81	101.12	111.00
3	AF	246	LEU	CB-CG-CD2	-5.81	101.12	111.00
3	BF	246	LEU	CB-CG-CD2	-5.81	101.12	111.00
5	GH	250	TYR	CZ-CE2-CD2	5.80	125.02	119.80
3	IF	246	LEU	CB-CG-CD2	-5.80	101.15	111.00
5	CH	250	TYR	CB-CG-CD2	-5.78	117.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Ad	68	ASP	CB-CG-OD1	5.77	123.50	118.30
2	JD	55	MET	CG-SD-CE	-5.77	90.97	100.20
5	HH	183	ASP	CB-CG-OD1	5.77	123.49	118.30
2	Ed	68	ASP	CB-CG-OD1	5.75	123.48	118.30
5	JH	183	ASP	CB-CG-OD1	5.75	123.47	118.30
2	Ad	105	ARG	NE-CZ-NH1	5.74	123.17	120.30
5	ZH	115	MET	N-CA-CB	-5.73	100.28	110.60
2	MD	55	MET	CG-SD-CE	-5.72	91.04	100.20
5	CH	280	LEU	CA-CB-CG	5.72	128.45	115.30
2	JD	86	ASP	CB-CG-OD1	5.71	123.44	118.30
4	ZG	813	LYS	CB-CA-C	-5.70	99.00	110.40
5	HH	150	LYS	CA-CB-CG	5.69	125.93	113.40
4	CG	813	LYS	CB-CA-C	-5.69	99.02	110.40
4	AG	813	LYS	CB-CA-C	-5.69	99.03	110.40
5	FH	157	PHE	CB-CG-CD2	5.69	124.78	120.80
2	Gd	156	LEU	CB-CG-CD2	5.69	120.67	111.00
4	VG	813	LYS	CB-CA-C	-5.69	99.03	110.40
5	AH	158	VAL	CG1-CB-CG2	-5.69	101.80	110.90
4	DG	813	LYS	CB-CA-C	-5.68	99.03	110.40
4	LG	813	LYS	CB-CA-C	-5.68	99.03	110.40
4	JG	813	LYS	CB-CA-C	-5.68	99.04	110.40
4	WG	813	LYS	CB-CA-C	-5.68	99.04	110.40
4	EG	813	LYS	CB-CA-C	-5.68	99.04	110.40
4	HG	813	LYS	CB-CA-C	-5.68	99.04	110.40
5	FH	285	GLU	CA-CB-CG	-5.68	100.91	113.40
2	JD	125	ASP	CB-CG-OD1	5.67	123.41	118.30
5	AH	205	GLN	N-CA-CB	-5.67	100.39	110.60
5	HH	135	GLU	N-CA-CB	5.67	120.81	110.60
4	KG	813	LYS	CB-CA-C	-5.67	99.05	110.40
4	YG	813	LYS	CB-CA-C	-5.67	99.05	110.40
4	MG	813	LYS	CB-CA-C	-5.67	99.06	110.40
5	IH	115	MET	CB-CA-C	-5.67	99.06	110.40
4	GG	813	LYS	CB-CA-C	-5.67	99.07	110.40
1	IC	210	ILE	CG1-CB-CG2	-5.67	98.94	111.40
2	Md	55	MET	CG-SD-CE	-5.67	91.14	100.20
4	IG	813	LYS	CB-CA-C	-5.66	99.07	110.40
1	DC	210	ILE	CG1-CB-CG2	-5.66	98.95	111.40
1	HC	210	ILE	CG1-CB-CG2	-5.66	98.95	111.40
4	FG	813	LYS	CB-CA-C	-5.66	99.09	110.40
1	FC	210	ILE	CG1-CB-CG2	-5.65	98.96	111.40
5	IH	183	ASP	CB-CG-OD1	5.65	123.39	118.30
1	KC	210	ILE	CG1-CB-CG2	-5.65	98.97	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	XG	813	LYS	CB-CA-C	-5.65	99.10	110.40
5	XH	183	ASP	CB-CG-OD1	5.65	123.39	118.30
1	BC	210	ILE	CG1-CB-CG2	-5.65	98.97	111.40
4	BG	813	LYS	CB-CA-C	-5.65	99.10	110.40
1	CC	210	ILE	CG1-CB-CG2	-5.65	98.98	111.40
1	JC	210	ILE	CG1-CB-CG2	-5.65	98.98	111.40
1	EC	210	ILE	CG1-CB-CG2	-5.64	98.98	111.40
1	LC	210	ILE	CG1-CB-CG2	-5.64	98.98	111.40
1	MC	210	ILE	CG1-CB-CG2	-5.64	98.98	111.40
1	GC	210	ILE	CG1-CB-CG2	-5.64	98.99	111.40
5	HH	138	GLU	N-CA-CB	5.64	120.75	110.60
2	Kd	126	GLU	CG-CD-OE2	-5.64	107.03	118.30
1	AC	210	ILE	CG1-CB-CG2	-5.63	99.01	111.40
2	FD	156	LEU	CB-CG-CD2	5.62	120.55	111.00
2	HD	160	LYS	CD-CE-NZ	-5.60	98.82	111.70
3	CF	250	LEU	CA-CB-CG	5.59	128.16	115.30
5	EH	117	ARG	NE-CZ-NH1	-5.59	117.50	120.30
5	GH	171	LEU	CB-CG-CD1	-5.59	101.50	111.00
3	LF	250	LEU	CA-CB-CG	5.59	128.15	115.30
3	ZF	250	LEU	CA-CB-CG	5.59	128.15	115.30
2	Cd	68	ASP	CB-CG-OD1	5.58	123.33	118.30
3	WF	250	LEU	CA-CB-CG	5.58	128.15	115.30
5	IH	214	MET	CB-CG-SD	5.58	129.15	112.40
3	JF	250	LEU	CA-CB-CG	5.58	128.14	115.30
3	YF	250	LEU	CA-CB-CG	5.58	128.14	115.30
3	BF	250	LEU	CA-CB-CG	5.58	128.12	115.30
5	MH	183	ASP	CB-CG-OD1	5.58	123.32	118.30
3	XF	250	LEU	CA-CB-CG	5.58	128.12	115.30
3	DF	250	LEU	CA-CB-CG	5.57	128.12	115.30
3	EF	250	LEU	CA-CB-CG	5.57	128.11	115.30
3	FF	250	LEU	CA-CB-CG	5.57	128.11	115.30
3	KF	250	LEU	CA-CB-CG	5.57	128.11	115.30
2	Cd	109	LEU	CB-CG-CD1	5.57	120.46	111.00
3	GF	250	LEU	CA-CB-CG	5.56	128.09	115.30
2	Gd	55	MET	CG-SD-CE	-5.56	91.30	100.20
3	HF	250	LEU	CA-CB-CG	5.56	128.08	115.30
3	MF	250	LEU	CA-CB-CG	5.56	128.08	115.30
2	LD	35	ASP	CB-CG-OD1	5.55	123.30	118.30
3	VF	250	LEU	CA-CB-CG	5.55	128.08	115.30
5	EH	138	GLU	N-CA-CB	5.55	120.60	110.60
3	IF	250	LEU	CA-CB-CG	5.54	128.05	115.30
3	AF	250	LEU	CA-CB-CG	5.54	128.04	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AD	59	GLU	CB-CA-C	-5.52	99.36	110.40
5	ZH	281	LEU	CB-CG-CD1	-5.52	101.62	111.00
5	DH	135	GLU	N-CA-CB	5.52	120.53	110.60
5	GH	246	LYS	CD-CE-NZ	-5.51	99.03	111.70
5	BH	214	MET	CB-CG-SD	5.50	128.90	112.40
2	Cd	109	LEU	CB-CG-CD2	-5.50	101.66	111.00
5	LH	183	ASP	CB-CG-OD1	5.49	123.25	118.30
5	FH	115	MET	CB-CA-C	-5.48	99.44	110.40
5	FH	183	ASP	CB-CG-OD1	5.48	123.23	118.30
2	GD	130	GLU	OE1-CD-OE2	-5.47	116.73	123.30
5	JH	311	MET	CB-CG-SD	-5.47	96.00	112.40
5	VH	183	ASP	CB-CG-OD1	5.46	123.21	118.30
2	Hd	94	LEU	CB-CG-CD2	5.43	120.23	111.00
2	Ld	53	LEU	CB-CG-CD2	5.43	120.23	111.00
2	Id	136	ASP	CB-CG-OD2	-5.43	113.41	118.30
5	BH	115	MET	CB-CG-SD	-5.42	96.14	112.40
2	Fd	127	SER	N-CA-CB	5.42	118.63	110.50
5	FH	251	ARG	N-CA-CB	5.41	120.33	110.60
5	LH	230	LEU	CB-CG-CD2	5.41	120.19	111.00
5	EH	226	LEU	CA-CB-CG	5.38	127.69	115.30
9	LN	81	LEU	CB-CG-CD2	-5.38	101.85	111.00
2	Bd	50	ASP	CB-CG-OD1	5.37	123.13	118.30
9	AN	81	LEU	CB-CG-CD2	-5.36	101.89	111.00
5	AH	208	LYS	N-CA-CB	-5.36	100.96	110.60
2	GD	50	ASP	CB-CG-OD1	5.35	123.12	118.30
9	KN	81	LEU	CB-CG-CD2	-5.35	101.91	111.00
9	HN	81	LEU	CB-CG-CD2	-5.35	101.91	111.00
5	AH	251	ARG	NE-CZ-NH1	-5.34	117.63	120.30
5	DH	285	GLU	CG-CD-OE2	-5.34	107.61	118.30
5	ZH	208	LYS	CA-CB-CG	5.34	125.16	113.40
9	BN	81	LEU	CB-CG-CD2	-5.34	101.92	111.00
9	DN	81	LEU	CB-CG-CD2	-5.34	101.92	111.00
9	GN	81	LEU	CB-CG-CD2	-5.34	101.92	111.00
2	Cd	118	LEU	CA-CB-CG	5.34	127.58	115.30
5	GH	250	TYR	CB-CG-CD1	5.34	124.20	121.00
9	JN	81	LEU	CB-CG-CD2	-5.34	101.93	111.00
9	CN	81	LEU	CB-CG-CD2	-5.33	101.93	111.00
2	Ld	52	MET	CB-CG-SD	-5.33	96.41	112.40
9	MN	81	LEU	CB-CG-CD2	-5.33	101.94	111.00
2	Kd	50	ASP	CB-CG-OD1	5.33	123.10	118.30
2	Kd	93	GLU	OE1-CD-OE2	5.33	129.69	123.30
5	ZH	150	LYS	CG-CD-CE	-5.33	95.92	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	HD	55	MET	CA-CB-CG	5.32	122.35	113.30
9	IN	81	LEU	CB-CG-CD2	-5.32	101.95	111.00
1	DC	61	GLU	CA-CB-CG	5.32	125.10	113.40
9	EN	81	LEU	CB-CG-CD2	-5.32	101.96	111.00
5	IH	115	MET	N-CA-CB	5.32	120.17	110.60
1	GC	61	GLU	CA-CB-CG	5.31	125.09	113.40
1	BC	61	GLU	CA-CB-CG	5.31	125.08	113.40
1	CC	61	GLU	CA-CB-CG	5.31	125.08	113.40
1	EC	61	GLU	CA-CB-CG	5.31	125.08	113.40
5	EH	208	LYS	N-CA-CB	-5.30	101.05	110.60
1	FC	61	GLU	CA-CB-CG	5.30	125.06	113.40
9	FN	81	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	JC	61	GLU	CA-CB-CG	5.30	125.06	113.40
5	JH	285	GLU	OE1-CD-OE2	-5.30	116.94	123.30
2	Ad	52	MET	CB-CG-SD	-5.30	96.51	112.40
2	ED	36	ASP	CB-CG-OD1	5.30	123.07	118.30
2	Hd	68	ASP	CB-CG-OD1	5.29	123.06	118.30
5	EH	122	LEU	CB-CG-CD2	-5.29	102.00	111.00
1	IC	61	GLU	CA-CB-CG	5.29	125.04	113.40
5	FH	205	GLN	N-CA-CB	5.29	120.11	110.60
8	IM	138	LEU	CA-CB-CG	5.29	127.45	115.30
8	JM	138	LEU	CA-CB-CG	5.29	127.46	115.30
1	MC	61	GLU	CA-CB-CG	5.29	125.03	113.40
1	KC	61	GLU	CA-CB-CG	5.28	125.03	113.40
2	GD	55	MET	CA-CB-CG	5.28	122.28	113.30
1	LC	61	GLU	CA-CB-CG	5.28	125.01	113.40
8	MM	138	LEU	CA-CB-CG	5.28	127.44	115.30
2	Ad	125	ASP	CB-CG-OD1	5.28	123.05	118.30
2	ED	160	LYS	CA-CB-CG	5.27	125.00	113.40
5	KH	183	ASP	CB-CG-OD1	5.27	123.05	118.30
8	EM	138	LEU	CA-CB-CG	5.27	127.43	115.30
1	HC	157	LYS	CA-CB-CG	5.27	125.00	113.40
5	WH	354	MET	CG-SD-CE	-5.27	91.76	100.20
1	AC	157	LYS	CA-CB-CG	5.27	124.99	113.40
8	BM	138	LEU	CA-CB-CG	5.27	127.42	115.30
1	HC	61	GLU	CA-CB-CG	5.27	124.99	113.40
5	ZH	130	LEU	CA-CB-CG	5.27	127.42	115.30
8	AM	138	LEU	CA-CB-CG	5.27	127.41	115.30
1	AC	61	GLU	CA-CB-CG	5.26	124.98	113.40
8	DM	138	LEU	CA-CB-CG	5.26	127.41	115.30
8	GM	138	LEU	CA-CB-CG	5.26	127.41	115.30
2	Ed	52	MET	CA-CB-CG	5.26	122.24	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	KM	138	LEU	CA-CB-CG	5.26	127.40	115.30
5	FH	285	GLU	N-CA-CB	-5.25	101.14	110.60
2	Cd	130	GLU	CG-CD-OE2	-5.25	107.79	118.30
8	LM	138	LEU	CA-CB-CG	5.25	127.38	115.30
1	MC	157	LYS	CA-CB-CG	5.25	124.95	113.40
1	KC	157	LYS	CA-CB-CG	5.25	124.94	113.40
1	IC	157	LYS	CA-CB-CG	5.25	124.94	113.40
2	JD	52	MET	CB-CG-SD	-5.25	96.66	112.40
1	LC	157	LYS	CA-CB-CG	5.25	124.94	113.40
2	LD	125	ASP	CB-CG-OD1	5.25	123.02	118.30
1	BC	157	LYS	CA-CB-CG	5.24	124.94	113.40
8	CM	138	LEU	CA-CB-CG	5.24	127.36	115.30
5	JH	138	GLU	N-CA-CB	5.24	120.04	110.60
1	DC	157	LYS	CA-CB-CG	5.24	124.93	113.40
8	FM	138	LEU	CA-CB-CG	5.24	127.35	115.30
8	HM	138	LEU	CA-CB-CG	5.24	127.35	115.30
5	MH	134	TYR	CB-CG-CD1	-5.24	117.86	121.00
8	IM	70	MET	CB-CG-SD	5.24	128.12	112.40
5	CH	183	ASP	CB-CG-OD1	5.24	123.01	118.30
1	GC	157	LYS	CA-CB-CG	5.23	124.91	113.40
5	HH	280	LEU	CA-CB-CG	5.23	127.33	115.30
1	JC	157	LYS	CA-CB-CG	5.23	124.91	113.40
8	LM	70	MET	CB-CG-SD	5.23	128.09	112.40
1	CC	157	LYS	CA-CB-CG	5.23	124.90	113.40
1	EC	157	LYS	CA-CB-CG	5.23	124.90	113.40
1	FC	157	LYS	CA-CB-CG	5.22	124.89	113.40
8	GM	70	MET	CB-CG-SD	5.22	128.07	112.40
8	EM	70	MET	CB-CG-SD	5.22	128.07	112.40
8	AM	70	MET	CB-CG-SD	5.22	128.06	112.40
5	WH	122	LEU	CB-CG-CD2	-5.22	102.12	111.00
8	JM	70	MET	CB-CG-SD	5.22	128.06	112.40
2	Fd	86	ASP	CB-CG-OD1	5.22	123.00	118.30
5	DH	183	ASP	CB-CG-OD1	5.21	122.99	118.30
8	DM	70	MET	CB-CG-SD	5.21	128.03	112.40
5	BH	259	TYR	CB-CG-CD1	-5.21	117.87	121.00
8	BM	70	MET	CB-CG-SD	5.21	128.03	112.40
8	MM	70	MET	CB-CG-SD	5.21	128.03	112.40
5	KH	285	GLU	OE1-CD-OE2	-5.21	117.05	123.30
2	KD	119	ILE	CA-CB-CG2	5.20	121.31	110.90
8	CM	70	MET	CB-CG-SD	5.20	128.01	112.40
2	Id	26	LYS	CD-CE-NZ	-5.20	99.74	111.70
8	FM	70	MET	CB-CG-SD	5.20	128.00	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	KM	70	MET	CB-CG-SD	5.20	128.00	112.40
5	AH	110	LYS	CA-CB-CG	5.19	124.82	113.40
8	HM	70	MET	CB-CG-SD	5.19	127.97	112.40
5	GH	216	GLN	N-CA-CB	5.18	119.93	110.60
2	Kd	35	ASP	CB-CG-OD1	5.18	122.96	118.30
2	Ld	130	GLU	CB-CA-C	5.17	120.74	110.40
5	MH	179	LEU	CB-CA-C	5.17	120.02	110.20
5	LH	226	LEU	CA-CB-CG	5.16	127.18	115.30
5	GH	241	LEU	CA-CB-CG	5.16	127.17	115.30
2	JD	136	ASP	CB-CG-OD1	5.16	122.94	118.30
5	VH	281	LEU	CB-CG-CD2	5.16	119.77	111.00
5	DH	309	GLU	CA-CB-CG	5.15	124.72	113.40
5	LH	266	MET	CB-CA-C	-5.15	100.11	110.40
5	WH	183	ASP	CB-CG-OD1	5.14	122.93	118.30
2	CD	86	ASP	CB-CG-OD1	5.14	122.92	118.30
5	YH	338	GLU	N-CA-CB	5.14	119.85	110.60
2	Ed	128	LEU	CB-CG-CD1	-5.13	102.28	111.00
2	Dd	134	ASP	CB-CG-OD1	5.13	122.91	118.30
5	BH	183	ASP	CB-CG-OD1	5.12	122.91	118.30
5	AH	183	ASP	CB-CG-OD1	5.12	122.91	118.30
5	EH	309	GLU	CA-CB-CG	5.12	124.66	113.40
2	Cd	125	ASP	C-N-CA	-5.10	108.94	121.70
5	WH	120	TYR	CB-CG-CD1	-5.10	117.94	121.00
2	Gd	105	ARG	NE-CZ-NH2	-5.09	117.75	120.30
2	JD	118	LEU	CB-CG-CD2	-5.09	102.35	111.00
5	EH	135	GLU	N-CA-CB	5.08	119.75	110.60
5	AH	110	LYS	CD-CE-NZ	5.08	123.38	111.70
2	AD	128	LEU	CB-CG-CD2	5.08	119.63	111.00
5	AH	110	LYS	CB-CA-C	5.08	120.55	110.40
5	WH	320	LEU	CB-CG-CD2	-5.07	102.39	111.00
5	AH	141	LYS	CG-CD-CE	-5.06	96.72	111.90
2	Kd	126	GLU	CG-CD-OE1	5.05	128.40	118.30
5	ZH	332	ASP	CB-CG-OD1	5.04	122.84	118.30
2	LD	50	ASP	CB-CG-OD2	-5.04	113.77	118.30
5	LH	285	GLU	OE1-CD-OE2	-5.03	117.27	123.30
5	GH	220	LEU	CA-CB-CG	-5.02	103.75	115.30
5	VH	226	LEU	CA-CB-CG	5.01	126.83	115.30
2	Ed	55	MET	CG-SD-CE	-5.01	92.18	100.20
5	WH	326	ALA	N-CA-CB	5.01	117.11	110.10
5	VH	309	GLU	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.



All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AD	27	LYS	Peptide
5	AH	121	PRO	Mainchain
5	AH	137	SER	Mainchain
8	AM	68	GLU	Sidechain
9	AN	115	GLN	Peptide
2	BD	27	LYS	Peptide
5	BH	121	PRO	Mainchain
8	BM	68	GLU	Sidechain
9	BN	115	GLN	Peptide
2	Bd	26	LYS	Mainchain
2	CD	27	LYS	Peptide
8	CM	68	GLU	Sidechain
9	CN	115	GLN	Peptide
2	Cd	39	ILE	Mainchain
2	DD	78	ASN	Peptide
5	DH	131	LYS	Mainchain
8	DM	68	GLU	Sidechain
9	DN	115	GLN	Peptide
2	ED	27	LYS	Peptide
5	EH	131	LYS	Mainchain
8	EM	68	GLU	Sidechain
9	EN	115	GLN	Peptide
2	FD	27	LYS	Peptide
5	FH	121	PRO	Mainchain
5	FH	285	GLU	Sidechain
8	FM	68	GLU	Sidechain
9	FN	115	GLN	Peptide
2	Fd	125	ASP	Mainchain
2	GD	27	LYS	Peptide
5	GH	121	PRO	Mainchain
5	GH	263	ALA	Peptide
8	GM	68	GLU	Sidechain
9	GN	115	GLN	Peptide
5	HH	121	PRO	Mainchain
8	HM	68	GLU	Sidechain
9	HN	115	GLN	Peptide
2	ID	27	LYS	Peptide
5	IH	121	PRO	Mainchain
8	IM	68	GLU	Sidechain
9	IN	115	GLN	Peptide
5	JH	121	PRO	Mainchain
5	JH	125	GLU	Sidechain

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Mol	Chain	Res	Type	Group
5	JH	267	PRO	Peptide
8	JM	68	GLU	Sidechain
9	JN	115	GLN	Peptide
2	KD	27	LYS	Peptide
5	KH	121	PRO	Mainchain
5	KH	263	ALA	Peptide
8	KM	68	GLU	Sidechain
9	KN	115	GLN	Peptide
5	LH	121	PRO	Mainchain
8	LM	68	GLU	Sidechain
9	LN	115	GLN	Peptide
2	MD	27	LYS	Peptide
5	MH	121	PRO	Mainchain
8	MM	68	GLU	Sidechain
9	MN	115	GLN	Peptide
5	VH	134	TYR	Mainchain
5	WH	121	PRO	Mainchain
5	XH	121	PRO	Mainchain
5	YH	121	PRO	Mainchain
5	YH	350	HIS	Sidechain
5	ZH	121	PRO	Mainchain

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AC	207/303 (68%)	202 (98%)	5 (2%)	0	100   100
1	BC	207/303 (68%)	202 (98%)	5 (2%)	0	100   100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	DC	207/303 (68%)	201 (97%)	6 (3%)	0	100	100
1	EC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	FC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	GC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	HC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	IC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	JC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	KC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	LC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	MC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
2	AD	138/163 (85%)	133 (96%)	5 (4%)	0	100	100
2	Ad	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
2	BD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Bd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
2	CD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Cd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
2	DD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Dd	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
2	ED	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Ed	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
2	FD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Fd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
2	GD	138/163 (85%)	133 (96%)	5 (4%)	0	100	100
2	Gd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
2	HD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Hd	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
2	ID	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Id	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
2	JD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Jd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	KD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Kd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
2	LD	138/163 (85%)	133 (96%)	5 (4%)	0	100	100
2	Ld	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
2	MD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Md	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
3	AF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Af	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
3	BF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Bf	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	CF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Cf	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
3	DF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Df	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	EF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Ef	57/269 (21%)	52 (91%)	5 (9%)	0	100	100
3	FF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Ff	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	GF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Gf	57/269 (21%)	56 (98%)	1 (2%)	0	100	100
3	HF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Hf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	IF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	If	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	JF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Jf	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	KF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Kf	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
3	LF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Lf	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	MF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Mf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	VF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	WF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	XF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	YF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	ZF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
4	AG	32/1048 (3%)	32 (100%)	0	0	100	100
4	BG	32/1048 (3%)	32 (100%)	0	0	100	100
4	CG	32/1048 (3%)	32 (100%)	0	0	100	100
4	DG	32/1048 (3%)	32 (100%)	0	0	100	100
4	EG	32/1048 (3%)	32 (100%)	0	0	100	100
4	FG	32/1048 (3%)	32 (100%)	0	0	100	100
4	GG	32/1048 (3%)	32 (100%)	0	0	100	100
4	HG	32/1048 (3%)	32 (100%)	0	0	100	100
4	IG	32/1048 (3%)	32 (100%)	0	0	100	100
4	JG	32/1048 (3%)	32 (100%)	0	0	100	100
4	KG	32/1048 (3%)	32 (100%)	0	0	100	100
4	LG	32/1048 (3%)	32 (100%)	0	0	100	100
4	MG	32/1048 (3%)	32 (100%)	0	0	100	100
4	VG	32/1048 (3%)	32 (100%)	0	0	100	100
4	WG	32/1048 (3%)	32 (100%)	0	0	100	100
4	XG	32/1048 (3%)	32 (100%)	0	0	100	100
4	YG	32/1048 (3%)	32 (100%)	0	0	100	100
4	ZG	32/1048 (3%)	32 (100%)	0	0	100	100
5	AH	256/361 (71%)	243 (95%)	13 (5%)	0	100	100
5	BH	256/361 (71%)	243 (95%)	13 (5%)	0	100	100
5	CH	256/361 (71%)	245 (96%)	11 (4%)	0	100	100
5	DH	256/361 (71%)	243 (95%)	13 (5%)	0	100	100
5	EH	256/361 (71%)	245 (96%)	11 (4%)	0	100	100
5	FH	256/361 (71%)	242 (94%)	14 (6%)	0	100	100
5	GH	256/361 (71%)	241 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	HH	256/361 (71%)	245 (96%)	11 (4%)	0	100	100
5	IH	256/361 (71%)	240 (94%)	16 (6%)	0	100	100
5	JH	256/361 (71%)	242 (94%)	14 (6%)	0	100	100
5	KH	256/361 (71%)	242 (94%)	14 (6%)	0	100	100
5	LH	256/361 (71%)	241 (94%)	15 (6%)	0	100	100
5	MH	256/361 (71%)	243 (95%)	13 (5%)	0	100	100
5	VH	239/361 (66%)	231 (97%)	8 (3%)	0	100	100
5	WH	239/361 (66%)	231 (97%)	8 (3%)	0	100	100
5	XH	239/361 (66%)	230 (96%)	9 (4%)	0	100	100
5	YH	239/361 (66%)	232 (97%)	7 (3%)	0	100	100
5	ZH	239/361 (66%)	232 (97%)	7 (3%)	0	100	100
6	AK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	BK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	CK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	DK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	EK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	FK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	GK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	HK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	IK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	JK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	KK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	LK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	MK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
7	AL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	BL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	CL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	DL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	EL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	FL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	GL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	HL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	IL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	JL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	KL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	LL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	ML	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
8	AM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	BM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	CM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	DM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	EM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	FM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	GM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	HM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	IM	290/320 (91%)	266 (92%)	24 (8%)	0	100	100
8	JM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	KM	290/320 (91%)	266 (92%)	24 (8%)	0	100	100
8	LM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	MM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
9	AN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	BN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	CN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	DN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	EN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	FN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	GN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	HN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	IN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	JN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	KN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	LN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	MN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
All	All	22070/53344 (41%)	20933 (95%)	1137 (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	AC	178/257 (69%)	167 (94%)	11 (6%)	18	49
1	BC	178/257 (69%)	167 (94%)	11 (6%)	18	49
1	CC	178/257 (69%)	168 (94%)	10 (6%)	21	52
1	DC	178/257 (69%)	168 (94%)	10 (6%)	21	52
1	EC	178/257 (69%)	168 (94%)	10 (6%)	21	52
1	FC	178/257 (69%)	167 (94%)	11 (6%)	18	49
1	GC	178/257 (69%)	167 (94%)	11 (6%)	18	49
1	HC	178/257 (69%)	168 (94%)	10 (6%)	21	52
1	IC	178/257 (69%)	167 (94%)	11 (6%)	18	49
1	JC	178/257 (69%)	168 (94%)	10 (6%)	21	52
1	KC	178/257 (69%)	167 (94%)	11 (6%)	18	49
1	LC	178/257 (69%)	168 (94%)	10 (6%)	21	52
1	MC	178/257 (69%)	167 (94%)	11 (6%)	18	49
2	AD	121/139 (87%)	121 (100%)	0	100	100
2	Ad	118/139 (85%)	118 (100%)	0	100	100
2	BD	121/139 (87%)	121 (100%)	0	100	100
2	Bd	118/139 (85%)	118 (100%)	0	100	100
2	CD	121/139 (87%)	121 (100%)	0	100	100
2	Cd	118/139 (85%)	118 (100%)	0	100	100
2	DD	121/139 (87%)	121 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Dd	118/139 (85%)	118 (100%)	0	100	100
2	ED	121/139 (87%)	120 (99%)	1 (1%)	81	89
2	Ed	118/139 (85%)	118 (100%)	0	100	100
2	FD	121/139 (87%)	121 (100%)	0	100	100
2	Fd	118/139 (85%)	118 (100%)	0	100	100
2	GD	121/139 (87%)	121 (100%)	0	100	100
2	Gd	118/139 (85%)	118 (100%)	0	100	100
2	HD	121/139 (87%)	121 (100%)	0	100	100
2	Hd	118/139 (85%)	118 (100%)	0	100	100
2	ID	121/139 (87%)	121 (100%)	0	100	100
2	Id	118/139 (85%)	117 (99%)	1 (1%)	81	89
2	JD	121/139 (87%)	121 (100%)	0	100	100
2	Jd	118/139 (85%)	118 (100%)	0	100	100
2	KD	121/139 (87%)	121 (100%)	0	100	100
2	Kd	118/139 (85%)	118 (100%)	0	100	100
2	LD	121/139 (87%)	121 (100%)	0	100	100
2	Ld	118/139 (85%)	118 (100%)	0	100	100
2	MD	121/139 (87%)	121 (100%)	0	100	100
2	Md	118/139 (85%)	117 (99%)	1 (1%)	81	89
3	AF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	Af	49/237 (21%)	49 (100%)	0	100	100
3	BF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	Bf	49/237 (21%)	49 (100%)	0	100	100
3	CF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	Cf	49/237 (21%)	49 (100%)	0	100	100
3	DF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	Df	49/237 (21%)	49 (100%)	0	100	100
3	EF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	Ef	49/237 (21%)	49 (100%)	0	100	100
3	FF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	Ff	49/237 (21%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	GF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	Gf	49/237 (21%)	49 (100%)	0	100	100
3	HF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	Hf	49/237 (21%)	49 (100%)	0	100	100
3	IF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	If	49/237 (21%)	49 (100%)	0	100	100
3	JF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	Jf	49/237 (21%)	49 (100%)	0	100	100
3	KF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	Kf	49/237 (21%)	49 (100%)	0	100	100
3	LF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	Lf	49/237 (21%)	49 (100%)	0	100	100
3	MF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	Mf	49/237 (21%)	48 (98%)	1 (2%)	55	75
3	VF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	WF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	XF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	YF	53/237 (22%)	48 (91%)	5 (9%)	8	35
3	ZF	53/237 (22%)	48 (91%)	5 (9%)	8	35
4	AG	31/765 (4%)	21 (68%)	10 (32%)	0	2
4	BG	31/765 (4%)	21 (68%)	10 (32%)	0	2
4	CG	31/765 (4%)	21 (68%)	10 (32%)	0	2
4	DG	31/765 (4%)	21 (68%)	10 (32%)	0	2
4	EG	31/765 (4%)	21 (68%)	10 (32%)	0	2
4	FG	31/765 (4%)	21 (68%)	10 (32%)	0	2
4	GG	31/765 (4%)	21 (68%)	10 (32%)	0	2
4	HG	31/765 (4%)	21 (68%)	10 (32%)	0	2
4	IG	31/765 (4%)	21 (68%)	10 (32%)	0	2
4	JG	31/765 (4%)	21 (68%)	10 (32%)	0	2
4	KG	31/765 (4%)	21 (68%)	10 (32%)	0	2
4	LG	31/765 (4%)	21 (68%)	10 (32%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	MG	31/765 (4%)	21 (68%)	10 (32%)	0	2
4	VG	31/765 (4%)	21 (68%)	10 (32%)	0	2
4	WG	31/765 (4%)	21 (68%)	10 (32%)	0	2
4	XG	31/765 (4%)	21 (68%)	10 (32%)	0	2
4	YG	31/765 (4%)	21 (68%)	10 (32%)	0	2
4	ZG	31/765 (4%)	21 (68%)	10 (32%)	0	2
5	AH	220/300 (73%)	220 (100%)	0	100	100
5	BH	220/300 (73%)	220 (100%)	0	100	100
5	CH	220/300 (73%)	219 (100%)	1 (0%)	88	94
5	DH	220/300 (73%)	219 (100%)	1 (0%)	88	94
5	EH	220/300 (73%)	219 (100%)	1 (0%)	88	94
5	FH	220/300 (73%)	220 (100%)	0	100	100
5	GH	220/300 (73%)	220 (100%)	0	100	100
5	HH	220/300 (73%)	220 (100%)	0	100	100
5	IH	220/300 (73%)	219 (100%)	1 (0%)	88	94
5	JH	220/300 (73%)	220 (100%)	0	100	100
5	KH	220/300 (73%)	220 (100%)	0	100	100
5	LH	220/300 (73%)	220 (100%)	0	100	100
5	MH	220/300 (73%)	219 (100%)	1 (0%)	88	94
5	VH	207/300 (69%)	207 (100%)	0	100	100
5	WH	207/300 (69%)	207 (100%)	0	100	100
5	XH	207/300 (69%)	207 (100%)	0	100	100
5	YH	207/300 (69%)	207 (100%)	0	100	100
5	ZH	207/300 (69%)	206 (100%)	1 (0%)	88	94
6	AK	129/163 (79%)	120 (93%)	9 (7%)	15	46
6	BK	129/163 (79%)	120 (93%)	9 (7%)	15	46
6	CK	129/163 (79%)	120 (93%)	9 (7%)	15	46
6	DK	129/163 (79%)	119 (92%)	10 (8%)	12	42
6	EK	129/163 (79%)	120 (93%)	9 (7%)	15	46
6	FK	129/163 (79%)	120 (93%)	9 (7%)	15	46
6	GK	129/163 (79%)	120 (93%)	9 (7%)	15	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	HK	129/163 (79%)	120 (93%)	9 (7%)	15	46
6	IK	129/163 (79%)	119 (92%)	10 (8%)	12	42
6	JK	129/163 (79%)	120 (93%)	9 (7%)	15	46
6	KK	129/163 (79%)	120 (93%)	9 (7%)	15	46
6	LK	129/163 (79%)	120 (93%)	9 (7%)	15	46
6	MK	129/163 (79%)	120 (93%)	9 (7%)	15	46
7	AL	148/203 (73%)	140 (95%)	8 (5%)	22	53
7	BL	148/203 (73%)	140 (95%)	8 (5%)	22	53
7	CL	148/203 (73%)	140 (95%)	8 (5%)	22	53
7	DL	148/203 (73%)	140 (95%)	8 (5%)	22	53
7	EL	148/203 (73%)	140 (95%)	8 (5%)	22	53
7	FL	148/203 (73%)	140 (95%)	8 (5%)	22	53
7	GL	148/203 (73%)	140 (95%)	8 (5%)	22	53
7	HL	148/203 (73%)	140 (95%)	8 (5%)	22	53
7	IL	148/203 (73%)	140 (95%)	8 (5%)	22	53
7	JL	148/203 (73%)	140 (95%)	8 (5%)	22	53
7	KL	148/203 (73%)	140 (95%)	8 (5%)	22	53
7	LL	148/203 (73%)	140 (95%)	8 (5%)	22	53
7	ML	148/203 (73%)	140 (95%)	8 (5%)	22	53
8	AM	251/276 (91%)	241 (96%)	10 (4%)	31	59
8	BM	251/276 (91%)	241 (96%)	10 (4%)	31	59
8	CM	251/276 (91%)	241 (96%)	10 (4%)	31	59
8	DM	251/276 (91%)	241 (96%)	10 (4%)	31	59
8	EM	251/276 (91%)	241 (96%)	10 (4%)	31	59
8	FM	251/276 (91%)	241 (96%)	10 (4%)	31	59
8	GM	251/276 (91%)	241 (96%)	10 (4%)	31	59
8	HM	251/276 (91%)	241 (96%)	10 (4%)	31	59
8	IM	251/276 (91%)	241 (96%)	10 (4%)	31	59
8	JM	251/276 (91%)	241 (96%)	10 (4%)	31	59
8	KM	251/276 (91%)	241 (96%)	10 (4%)	31	59
8	LM	251/276 (91%)	241 (96%)	10 (4%)	31	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	MM	251/276 (91%)	241 (96%)	10 (4%)	31	59
9	AN	66/107 (62%)	59 (89%)	7 (11%)	6	30
9	BN	66/107 (62%)	59 (89%)	7 (11%)	6	30
9	CN	66/107 (62%)	59 (89%)	7 (11%)	6	30
9	DN	66/107 (62%)	59 (89%)	7 (11%)	6	30
9	EN	66/107 (62%)	59 (89%)	7 (11%)	6	30
9	FN	66/107 (62%)	59 (89%)	7 (11%)	6	30
9	GN	66/107 (62%)	59 (89%)	7 (11%)	6	30
9	HN	66/107 (62%)	59 (89%)	7 (11%)	6	30
9	IN	66/107 (62%)	59 (89%)	7 (11%)	6	30
9	JN	66/107 (62%)	59 (89%)	7 (11%)	6	30
9	KN	66/107 (62%)	59 (89%)	7 (11%)	6	30
9	LN	66/107 (62%)	59 (89%)	7 (11%)	6	30
9	MN	66/107 (62%)	59 (89%)	7 (11%)	6	30
All	All	19187/43209 (44%)	18326 (96%)	861 (4%)	31	57

All (861) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AC	57	MET
1	AC	59	LEU
1	AC	60	LYS
1	AC	61	GLU
1	AC	69	GLN
1	AC	97	ASN
1	AC	123	GLN
1	AC	137	GLN
1	AC	157	LYS
1	AC	182	ARG
1	AC	185	LYS
3	AF	207	ARG
3	AF	243	MET
3	AF	250	LEU
3	AF	263	LYS
3	AF	267	GLU
4	AG	795	GLN
4	AG	796	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	AG	802	LEU
4	AG	806	THR
4	AG	808	LEU
4	AG	810	GLN
4	AG	815	VAL
4	AG	819	VAL
4	AG	822	GLU
4	AG	824	THR
6	AK	43	CYS
6	AK	62	LYS
6	AK	63	LYS
6	AK	86	ASP
6	AK	122	LYS
6	AK	123	TYR
6	AK	129	GLU
6	AK	156	THR
6	AK	166	THR
7	AL	104	LYS
7	AL	110	GLN
7	AL	130	ASP
7	AL	154	LEU
7	AL	155	LEU
7	AL	183	GLN
7	AL	190	MET
7	AL	211	LYS
8	AM	32	LYS
8	AM	69	VAL
8	AM	70	MET
8	AM	79	VAL
8	AM	164	GLN
8	AM	171	ARG
8	AM	194	LEU
8	AM	196	MET
8	AM	262	GLU
8	AM	310	LYS
9	AN	39	ASP
9	AN	67	THR
9	AN	71	THR
9	AN	76	MET
9	AN	95	LEU
9	AN	113	SER
9	AN	114	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	BC	35	GLN
1	BC	57	MET
1	BC	59	LEU
1	BC	60	LYS
1	BC	61	GLU
1	BC	69	GLN
1	BC	123	GLN
1	BC	137	GLN
1	BC	157	LYS
1	BC	182	ARG
1	BC	185	LYS
3	BF	207	ARG
3	BF	243	MET
3	BF	250	LEU
3	BF	263	LYS
3	BF	267	GLU
4	BG	795	GLN
4	BG	796	GLN
4	BG	802	LEU
4	BG	806	THR
4	BG	808	LEU
4	BG	810	GLN
4	BG	815	VAL
4	BG	819	VAL
4	BG	822	GLU
4	BG	824	THR
6	BK	43	CYS
6	BK	62	LYS
6	BK	63	LYS
6	BK	86	ASP
6	BK	122	LYS
6	BK	123	TYR
6	BK	129	GLU
6	BK	156	THR
6	BK	166	THR
7	BL	104	LYS
7	BL	110	GLN
7	BL	130	ASP
7	BL	154	LEU
7	BL	155	LEU
7	BL	183	GLN
7	BL	190	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	BL	211	LYS
8	BM	32	LYS
8	BM	69	VAL
8	BM	70	MET
8	BM	79	VAL
8	BM	164	GLN
8	BM	171	ARG
8	BM	194	LEU
8	BM	196	MET
8	BM	262	GLU
8	BM	310	LYS
9	BN	39	ASP
9	BN	67	THR
9	BN	71	THR
9	BN	76	MET
9	BN	95	LEU
9	BN	113	SER
9	BN	114	LEU
1	CC	57	MET
1	CC	59	LEU
1	CC	60	LYS
1	CC	61	GLU
1	CC	69	GLN
1	CC	123	GLN
1	CC	137	GLN
1	CC	157	LYS
1	CC	182	ARG
1	CC	185	LYS
3	CF	207	ARG
3	CF	243	MET
3	CF	250	LEU
3	CF	263	LYS
3	CF	267	GLU
4	CG	795	GLN
4	CG	796	GLN
4	CG	802	LEU
4	CG	806	THR
4	CG	808	LEU
4	CG	810	GLN
4	CG	815	VAL
4	CG	819	VAL
4	CG	822	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	CG	824	THR
5	CH	245	GLN
6	CK	43	CYS
6	CK	62	LYS
6	CK	63	LYS
6	CK	86	ASP
6	CK	122	LYS
6	CK	123	TYR
6	CK	129	GLU
6	CK	156	THR
6	CK	166	THR
7	CL	104	LYS
7	CL	110	GLN
7	CL	130	ASP
7	CL	154	LEU
7	CL	155	LEU
7	CL	183	GLN
7	CL	190	MET
7	CL	211	LYS
8	CM	32	LYS
8	CM	69	VAL
8	CM	70	MET
8	CM	79	VAL
8	CM	164	GLN
8	CM	171	ARG
8	CM	194	LEU
8	CM	196	MET
8	CM	262	GLU
8	CM	310	LYS
9	CN	39	ASP
9	CN	67	THR
9	CN	71	THR
9	CN	76	MET
9	CN	95	LEU
9	CN	113	SER
9	CN	114	LEU
1	DC	57	MET
1	DC	59	LEU
1	DC	60	LYS
1	DC	61	GLU
1	DC	69	GLN
1	DC	123	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	DC	137	GLN
1	DC	157	LYS
1	DC	182	ARG
1	DC	185	LYS
3	DF	207	ARG
3	DF	243	MET
3	DF	250	LEU
3	DF	263	LYS
3	DF	267	GLU
4	DG	795	GLN
4	DG	796	GLN
4	DG	802	LEU
4	DG	806	THR
4	DG	808	LEU
4	DG	810	GLN
4	DG	815	VAL
4	DG	819	VAL
4	DG	822	GLU
4	DG	824	THR
5	DH	225	ASN
6	DK	43	CYS
6	DK	62	LYS
6	DK	63	LYS
6	DK	86	ASP
6	DK	100	ASN
6	DK	122	LYS
6	DK	123	TYR
6	DK	129	GLU
6	DK	156	THR
6	DK	166	THR
7	DL	104	LYS
7	DL	110	GLN
7	DL	130	ASP
7	DL	154	LEU
7	DL	155	LEU
7	DL	183	GLN
7	DL	190	MET
7	DL	211	LYS
8	DM	32	LYS
8	DM	69	VAL
8	DM	70	MET
8	DM	79	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	DM	164	GLN
8	DM	171	ARG
8	DM	194	LEU
8	DM	196	MET
8	DM	262	GLU
8	DM	310	LYS
9	DN	39	ASP
9	DN	67	THR
9	DN	71	THR
9	DN	76	MET
9	DN	95	LEU
9	DN	113	SER
9	DN	114	LEU
1	EC	57	MET
1	EC	59	LEU
1	EC	60	LYS
1	EC	61	GLU
1	EC	69	GLN
1	EC	123	GLN
1	EC	137	GLN
1	EC	157	LYS
1	EC	182	ARG
1	EC	185	LYS
2	ED	60	LYS
3	EF	207	ARG
3	EF	243	MET
3	EF	250	LEU
3	EF	263	LYS
3	EF	267	GLU
4	EG	795	GLN
4	EG	796	GLN
4	EG	802	LEU
4	EG	806	THR
4	EG	808	LEU
4	EG	810	GLN
4	EG	815	VAL
4	EG	819	VAL
4	EG	822	GLU
4	EG	824	THR
5	EH	117	ARG
6	EK	43	CYS
6	EK	62	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	EK	63	LYS
6	EK	86	ASP
6	EK	122	LYS
6	EK	123	TYR
6	EK	129	GLU
6	EK	156	THR
6	EK	166	THR
7	EL	104	LYS
7	EL	110	GLN
7	EL	130	ASP
7	EL	154	LEU
7	EL	155	LEU
7	EL	183	GLN
7	EL	190	MET
7	EL	211	LYS
8	EM	32	LYS
8	EM	69	VAL
8	EM	70	MET
8	EM	79	VAL
8	EM	164	GLN
8	EM	171	ARG
8	EM	194	LEU
8	EM	196	MET
8	EM	262	GLU
8	EM	310	LYS
9	EN	39	ASP
9	EN	67	THR
9	EN	71	THR
9	EN	76	MET
9	EN	95	LEU
9	EN	113	SER
9	EN	114	LEU
1	FC	57	MET
1	FC	59	LEU
1	FC	60	LYS
1	FC	61	GLU
1	FC	69	GLN
1	FC	97	ASN
1	FC	123	GLN
1	FC	137	GLN
1	FC	157	LYS
1	FC	182	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	FC	185	LYS
3	FF	207	ARG
3	FF	243	MET
3	FF	250	LEU
3	FF	263	LYS
3	FF	267	GLU
4	FG	795	GLN
4	FG	796	GLN
4	FG	802	LEU
4	FG	806	THR
4	FG	808	LEU
4	FG	810	GLN
4	FG	815	VAL
4	FG	819	VAL
4	FG	822	GLU
4	FG	824	THR
6	FK	43	CYS
6	FK	62	LYS
6	FK	63	LYS
6	FK	86	ASP
6	FK	122	LYS
6	FK	123	TYR
6	FK	129	GLU
6	FK	156	THR
6	FK	166	THR
7	FL	104	LYS
7	FL	110	GLN
7	FL	130	ASP
7	FL	154	LEU
7	FL	155	LEU
7	FL	183	GLN
7	FL	190	MET
7	FL	211	LYS
8	FM	32	LYS
8	FM	69	VAL
8	FM	70	MET
8	FM	79	VAL
8	FM	164	GLN
8	FM	171	ARG
8	FM	194	LEU
8	FM	196	MET
8	FM	262	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	FM	310	LYS
9	FN	39	ASP
9	FN	67	THR
9	FN	71	THR
9	FN	76	MET
9	FN	95	LEU
9	FN	113	SER
9	FN	114	LEU
1	GC	57	MET
1	GC	59	LEU
1	GC	60	LYS
1	GC	61	GLU
1	GC	69	GLN
1	GC	97	ASN
1	GC	123	GLN
1	GC	137	GLN
1	GC	157	LYS
1	GC	182	ARG
1	GC	185	LYS
3	GF	207	ARG
3	GF	243	MET
3	GF	250	LEU
3	GF	263	LYS
3	GF	267	GLU
4	GG	795	GLN
4	GG	796	GLN
4	GG	802	LEU
4	GG	806	THR
4	GG	808	LEU
4	GG	810	GLN
4	GG	815	VAL
4	GG	819	VAL
4	GG	822	GLU
4	GG	824	THR
6	GK	43	CYS
6	GK	62	LYS
6	GK	63	LYS
6	GK	86	ASP
6	GK	122	LYS
6	GK	123	TYR
6	GK	129	GLU
6	GK	156	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	GK	166	THR
7	GL	104	LYS
7	GL	110	GLN
7	GL	130	ASP
7	GL	154	LEU
7	GL	155	LEU
7	GL	183	GLN
7	GL	190	MET
7	GL	211	LYS
8	GM	32	LYS
8	GM	69	VAL
8	GM	70	MET
8	GM	79	VAL
8	GM	164	GLN
8	GM	171	ARG
8	GM	194	LEU
8	GM	196	MET
8	GM	262	GLU
8	GM	310	LYS
9	GN	39	ASP
9	GN	67	THR
9	GN	71	THR
9	GN	76	MET
9	GN	95	LEU
9	GN	113	SER
9	GN	114	LEU
1	HC	57	MET
1	HC	59	LEU
1	HC	60	LYS
1	HC	61	GLU
1	HC	69	GLN
1	HC	123	GLN
1	HC	137	GLN
1	HC	157	LYS
1	HC	182	ARG
1	HC	185	LYS
3	HF	207	ARG
3	HF	243	MET
3	HF	250	LEU
3	HF	263	LYS
3	HF	267	GLU
4	HG	795	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	HG	796	GLN
4	HG	802	LEU
4	HG	806	THR
4	HG	808	LEU
4	HG	810	GLN
4	HG	815	VAL
4	HG	819	VAL
4	HG	822	GLU
4	HG	824	THR
6	HK	43	CYS
6	HK	62	LYS
6	HK	63	LYS
6	HK	86	ASP
6	HK	122	LYS
6	HK	123	TYR
6	HK	129	GLU
6	HK	156	THR
6	HK	166	THR
7	HL	104	LYS
7	HL	110	GLN
7	HL	130	ASP
7	HL	154	LEU
7	HL	155	LEU
7	HL	183	GLN
7	HL	190	MET
7	HL	211	LYS
8	HM	32	LYS
8	HM	69	VAL
8	HM	70	MET
8	HM	79	VAL
8	HM	164	GLN
8	HM	171	ARG
8	HM	194	LEU
8	HM	196	MET
8	HM	262	GLU
8	HM	310	LYS
9	HN	39	ASP
9	HN	67	THR
9	HN	71	THR
9	HN	76	MET
9	HN	95	LEU
9	HN	113	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	HN	114	LEU
1	IC	57	MET
1	IC	59	LEU
1	IC	60	LYS
1	IC	61	GLU
1	IC	69	GLN
1	IC	97	ASN
1	IC	123	GLN
1	IC	137	GLN
1	IC	157	LYS
1	IC	182	ARG
1	IC	185	LYS
3	IF	207	ARG
3	IF	243	MET
3	IF	250	LEU
3	IF	263	LYS
3	IF	267	GLU
4	IG	795	GLN
4	IG	796	GLN
4	IG	802	LEU
4	IG	806	THR
4	IG	808	LEU
4	IG	810	GLN
4	IG	815	VAL
4	IG	819	VAL
4	IG	822	GLU
4	IG	824	THR
5	IH	225	ASN
6	IK	43	CYS
6	IK	62	LYS
6	IK	63	LYS
6	IK	86	ASP
6	IK	100	ASN
6	IK	122	LYS
6	IK	123	TYR
6	IK	129	GLU
6	IK	156	THR
6	IK	166	THR
7	IL	104	LYS
7	IL	110	GLN
7	IL	130	ASP
7	IL	154	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	IL	155	LEU
7	IL	183	GLN
7	IL	190	MET
7	IL	211	LYS
8	IM	32	LYS
8	IM	69	VAL
8	IM	70	MET
8	IM	79	VAL
8	IM	164	GLN
8	IM	171	ARG
8	IM	194	LEU
8	IM	196	MET
8	IM	262	GLU
8	IM	310	LYS
9	IN	39	ASP
9	IN	67	THR
9	IN	71	THR
9	IN	76	MET
9	IN	95	LEU
9	IN	113	SER
9	IN	114	LEU
2	Id	69	ASN
1	JC	57	MET
1	JC	59	LEU
1	JC	60	LYS
1	JC	61	GLU
1	JC	69	GLN
1	JC	123	GLN
1	JC	137	GLN
1	JC	157	LYS
1	JC	182	ARG
1	JC	185	LYS
3	JF	207	ARG
3	JF	243	MET
3	JF	250	LEU
3	JF	263	LYS
3	JF	267	GLU
4	JG	795	GLN
4	JG	796	GLN
4	JG	802	LEU
4	JG	806	THR
4	JG	808	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	JG	810	GLN
4	JG	815	VAL
4	JG	819	VAL
4	JG	822	GLU
4	JG	824	THR
6	JK	43	CYS
6	JK	62	LYS
6	JK	63	LYS
6	JK	86	ASP
6	JK	122	LYS
6	JK	123	TYR
6	JK	129	GLU
6	JK	156	THR
6	JK	166	THR
7	JL	104	LYS
7	JL	110	GLN
7	JL	130	ASP
7	JL	154	LEU
7	JL	155	LEU
7	JL	183	GLN
7	JL	190	MET
7	JL	211	LYS
8	JM	32	LYS
8	JM	69	VAL
8	JM	70	MET
8	JM	79	VAL
8	JM	164	GLN
8	JM	171	ARG
8	JM	194	LEU
8	JM	196	MET
8	JM	262	GLU
8	JM	310	LYS
9	JN	39	ASP
9	JN	67	THR
9	JN	71	THR
9	JN	76	MET
9	JN	95	LEU
9	JN	113	SER
9	JN	114	LEU
1	KC	57	MET
1	KC	59	LEU
1	KC	60	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	KC	61	GLU
1	KC	69	GLN
1	KC	97	ASN
1	KC	123	GLN
1	KC	137	GLN
1	KC	157	LYS
1	KC	182	ARG
1	KC	185	LYS
3	KF	207	ARG
3	KF	243	MET
3	KF	250	LEU
3	KF	263	LYS
3	KF	267	GLU
4	KG	795	GLN
4	KG	796	GLN
4	KG	802	LEU
4	KG	806	THR
4	KG	808	LEU
4	KG	810	GLN
4	KG	815	VAL
4	KG	819	VAL
4	KG	822	GLU
4	KG	824	THR
6	KK	43	CYS
6	KK	62	LYS
6	KK	63	LYS
6	KK	86	ASP
6	KK	122	LYS
6	KK	123	TYR
6	KK	129	GLU
6	KK	156	THR
6	KK	166	THR
7	KL	104	LYS
7	KL	110	GLN
7	KL	130	ASP
7	KL	154	LEU
7	KL	155	LEU
7	KL	183	GLN
7	KL	190	MET
7	KL	211	LYS
8	KM	32	LYS
8	KM	69	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	KM	70	MET
8	KM	79	VAL
8	KM	164	GLN
8	KM	171	ARG
8	KM	194	LEU
8	KM	196	MET
8	KM	262	GLU
8	KM	310	LYS
9	KN	39	ASP
9	KN	67	THR
9	KN	71	THR
9	KN	76	MET
9	KN	95	LEU
9	KN	113	SER
9	KN	114	LEU
1	LC	57	MET
1	LC	59	LEU
1	LC	60	LYS
1	LC	61	GLU
1	LC	69	GLN
1	LC	123	GLN
1	LC	137	GLN
1	LC	157	LYS
1	LC	182	ARG
1	LC	185	LYS
3	LF	207	ARG
3	LF	243	MET
3	LF	250	LEU
3	LF	263	LYS
3	LF	267	GLU
4	LG	795	GLN
4	LG	796	GLN
4	LG	802	LEU
4	LG	806	THR
4	LG	808	LEU
4	LG	810	GLN
4	LG	815	VAL
4	LG	819	VAL
4	LG	822	GLU
4	LG	824	THR
6	LK	43	CYS
6	LK	62	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	LK	63	LYS
6	LK	86	ASP
6	LK	122	LYS
6	LK	123	TYR
6	LK	129	GLU
6	LK	156	THR
6	LK	166	THR
7	LL	104	LYS
7	LL	110	GLN
7	LL	130	ASP
7	LL	154	LEU
7	LL	155	LEU
7	LL	183	GLN
7	LL	190	MET
7	LL	211	LYS
8	LM	32	LYS
8	LM	69	VAL
8	LM	70	MET
8	LM	79	VAL
8	LM	164	GLN
8	LM	171	ARG
8	LM	194	LEU
8	LM	196	MET
8	LM	262	GLU
8	LM	310	LYS
9	LN	39	ASP
9	LN	67	THR
9	LN	71	THR
9	LN	76	MET
9	LN	95	LEU
9	LN	113	SER
9	LN	114	LEU
1	MC	35	GLN
1	MC	57	MET
1	MC	59	LEU
1	MC	60	LYS
1	MC	61	GLU
1	MC	69	GLN
1	MC	123	GLN
1	MC	137	GLN
1	MC	157	LYS
1	MC	182	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	MC	185	LYS
3	MF	207	ARG
3	MF	243	MET
3	MF	250	LEU
3	MF	263	LYS
3	MF	267	GLU
4	MG	795	GLN
4	MG	796	GLN
4	MG	802	LEU
4	MG	806	THR
4	MG	808	LEU
4	MG	810	GLN
4	MG	815	VAL
4	MG	819	VAL
4	MG	822	GLU
4	MG	824	THR
5	MH	264	LYS
6	MK	43	CYS
6	MK	62	LYS
6	MK	63	LYS
6	MK	86	ASP
6	MK	122	LYS
6	MK	123	TYR
6	MK	129	GLU
6	MK	156	THR
6	MK	166	THR
7	ML	104	LYS
7	ML	110	GLN
7	ML	130	ASP
7	ML	154	LEU
7	ML	155	LEU
7	ML	183	GLN
7	ML	190	MET
7	ML	211	LYS
8	MM	32	LYS
8	MM	69	VAL
8	MM	70	MET
8	MM	79	VAL
8	MM	164	GLN
8	MM	171	ARG
8	MM	194	LEU
8	MM	196	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	MM	262	GLU
8	MM	310	LYS
9	MN	39	ASP
9	MN	67	THR
9	MN	71	THR
9	MN	76	MET
9	MN	95	LEU
9	MN	113	SER
9	MN	114	LEU
2	Md	67	LYS
3	Mf	219	ARG
3	VF	207	ARG
3	VF	243	MET
3	VF	250	LEU
3	VF	263	LYS
3	VF	267	GLU
4	VG	795	GLN
4	VG	796	GLN
4	VG	802	LEU
4	VG	806	THR
4	VG	808	LEU
4	VG	810	GLN
4	VG	815	VAL
4	VG	819	VAL
4	VG	822	GLU
4	VG	824	THR
3	WF	207	ARG
3	WF	243	MET
3	WF	250	LEU
3	WF	263	LYS
3	WF	267	GLU
4	WG	795	GLN
4	WG	796	GLN
4	WG	802	LEU
4	WG	806	THR
4	WG	808	LEU
4	WG	810	GLN
4	WG	815	VAL
4	WG	819	VAL
4	WG	822	GLU
4	WG	824	THR
3	XF	207	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	XF	243	MET
3	XF	250	LEU
3	XF	263	LYS
3	XF	267	GLU
4	XG	795	GLN
4	XG	796	GLN
4	XG	802	LEU
4	XG	806	THR
4	XG	808	LEU
4	XG	810	GLN
4	XG	815	VAL
4	XG	819	VAL
4	XG	822	GLU
4	XG	824	THR
3	YF	207	ARG
3	YF	243	MET
3	YF	250	LEU
3	YF	263	LYS
3	YF	267	GLU
4	YG	795	GLN
4	YG	796	GLN
4	YG	802	LEU
4	YG	806	THR
4	YG	808	LEU
4	YG	810	GLN
4	YG	815	VAL
4	YG	819	VAL
4	YG	822	GLU
4	YG	824	THR
3	ZF	207	ARG
3	ZF	243	MET
3	ZF	250	LEU
3	ZF	263	LYS
3	ZF	267	GLU
4	ZG	795	GLN
4	ZG	796	GLN
4	ZG	802	LEU
4	ZG	806	THR
4	ZG	808	LEU
4	ZG	810	GLN
4	ZG	815	VAL
4	ZG	819	VAL

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Mol	Chain	Res	Type
4	ZG	822	GLU
4	ZG	824	THR
5	ZH	352	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	AC	35	GLN
1	AC	97	ASN
1	AC	137	GLN
5	AH	132	GLN
8	AM	40	GLN
1	BC	137	GLN
8	BM	40	GLN
1	CC	35	GLN
1	CC	137	GLN
4	CG	818	GLN
5	CH	203	ASN
5	CH	205	GLN
6	CK	100	ASN
8	CM	40	GLN
1	DC	35	GLN
4	DG	818	GLN
5	DH	203	ASN
5	DH	205	GLN
8	DM	40	GLN
9	DN	115	GLN
1	EC	137	GLN
8	EM	40	GLN
9	EN	115	GLN
1	FC	69	GLN
1	FC	97	ASN
1	FC	137	GLN
4	FG	818	GLN
8	FM	40	GLN
1	GC	35	GLN
1	GC	97	ASN
8	GM	40	GLN
8	GM	306	GLN
1	HC	35	GLN
5	HH	216	GLN
5	HH	257	GLN

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Mol	Chain	Res	Type
8	HM	40	GLN
1	IC	97	ASN
1	IC	137	GLN
8	IM	40	GLN
1	JC	35	GLN
1	JC	137	GLN
5	JH	173	GLN
5	JH	245	GLN
8	JM	40	GLN
1	KC	97	ASN
1	KC	137	GLN
8	KM	40	GLN
1	LC	137	GLN
5	LH	216	GLN
8	LM	40	GLN
1	MC	137	GLN
8	MM	40	GLN
3	YF	251	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AX	38:UNK	C	70:UNK	N	24.20
1	BX	38:UNK	C	70:UNK	N	24.20
1	CX	38:UNK	C	70:UNK	N	24.20
1	DX	38:UNK	C	70:UNK	N	24.20
1	EX	38:UNK	C	70:UNK	N	24.20
1	FX	38:UNK	C	70:UNK	N	24.20
1	GX	38:UNK	C	70:UNK	N	24.20
1	HX	38:UNK	C	70:UNK	N	24.20
1	IX	38:UNK	C	70:UNK	N	24.20
1	JX	38:UNK	C	70:UNK	N	24.20
1	KX	38:UNK	C	70:UNK	N	24.20
1	LX	38:UNK	C	70:UNK	N	24.20
1	MX	38:UNK	C	70:UNK	N	24.20
1	VX	38:UNK	C	70:UNK	N	24.20
1	WX	38:UNK	C	70:UNK	N	24.20
1	XX	38:UNK	C	70:UNK	N	24.20
1	YX	38:UNK	C	70:UNK	N	24.20
1	ZX	38:UNK	C	70:UNK	N	24.20

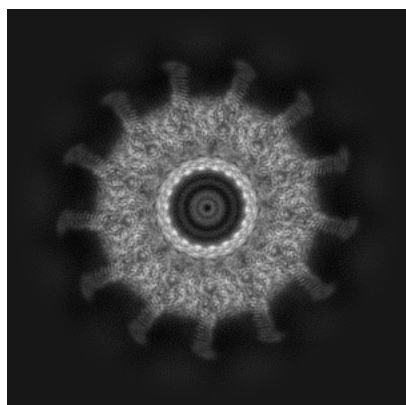
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24004. These allow visual inspection of the internal detail of the map and identification of artifacts.

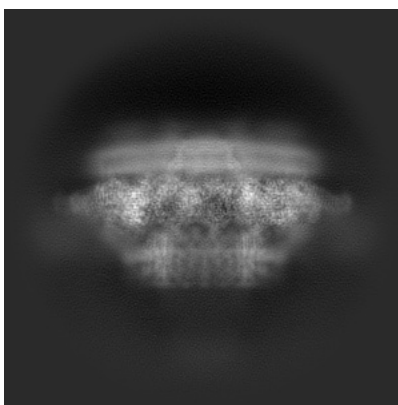
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

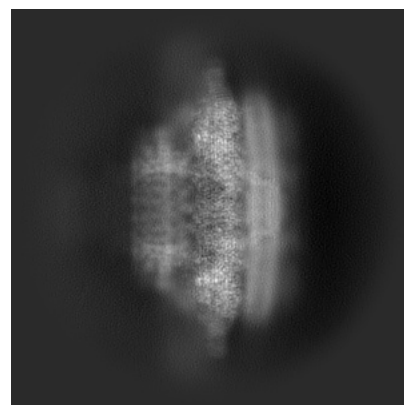
#### 6.1.1 Primary map



X



Y

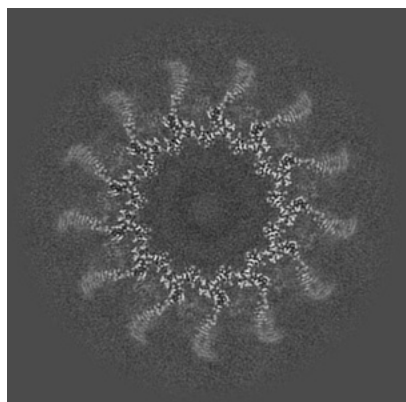


Z

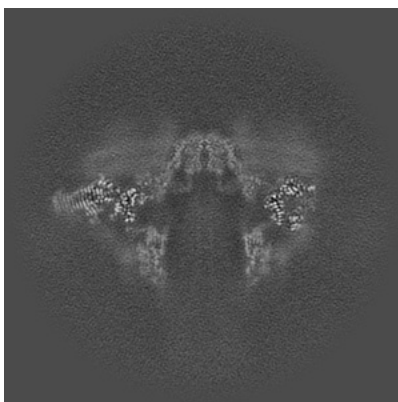
The images above show the map projected in three orthogonal directions.

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

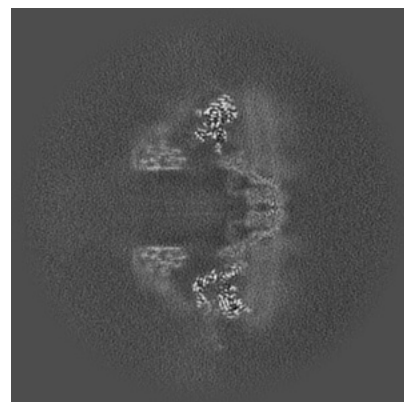
#### 6.2.1 Primary map



X Index: 255



Y Index: 255

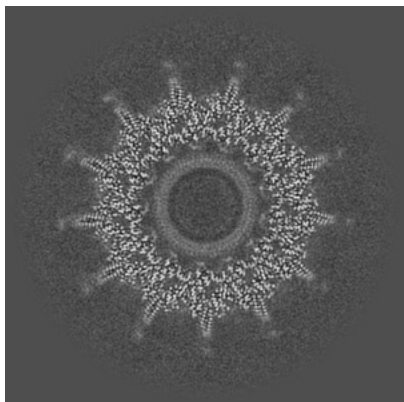


Z Index: 255

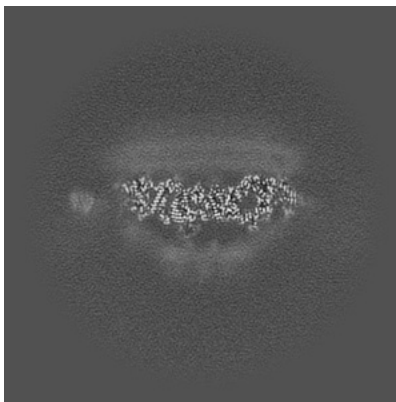
The images above show central slices of the map in three orthogonal directions.

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

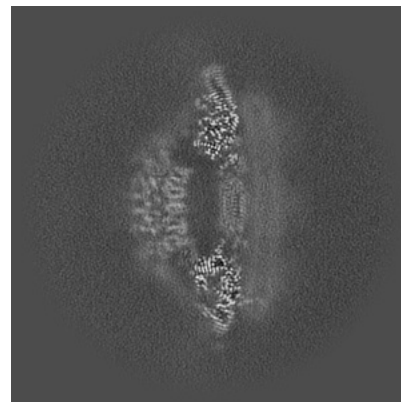
### 6.3.1 Primary map



X Index: 274



Y Index: 164



Z Index: 309

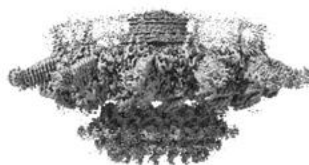
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

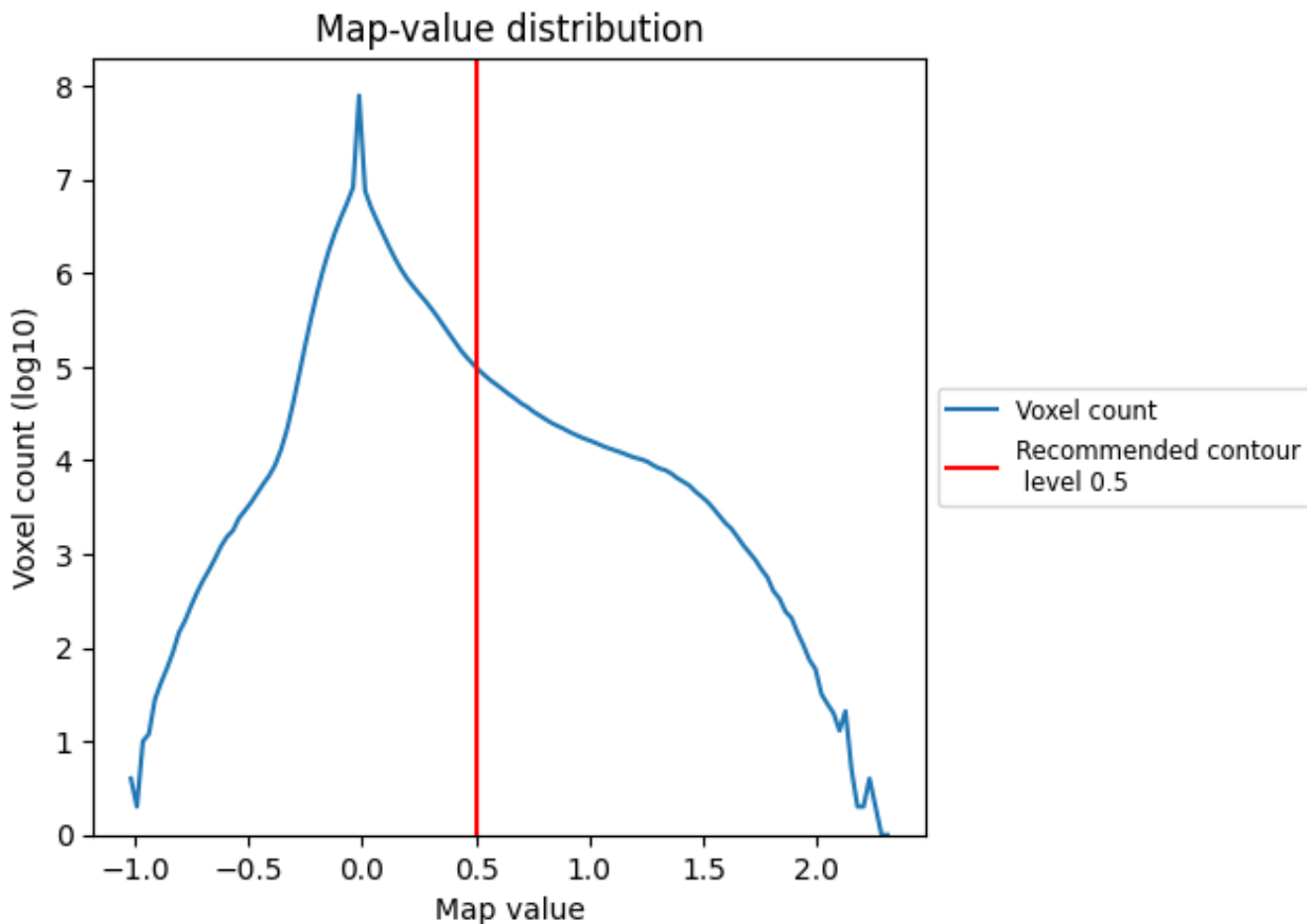
## 6.5 Mask visualisation

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.

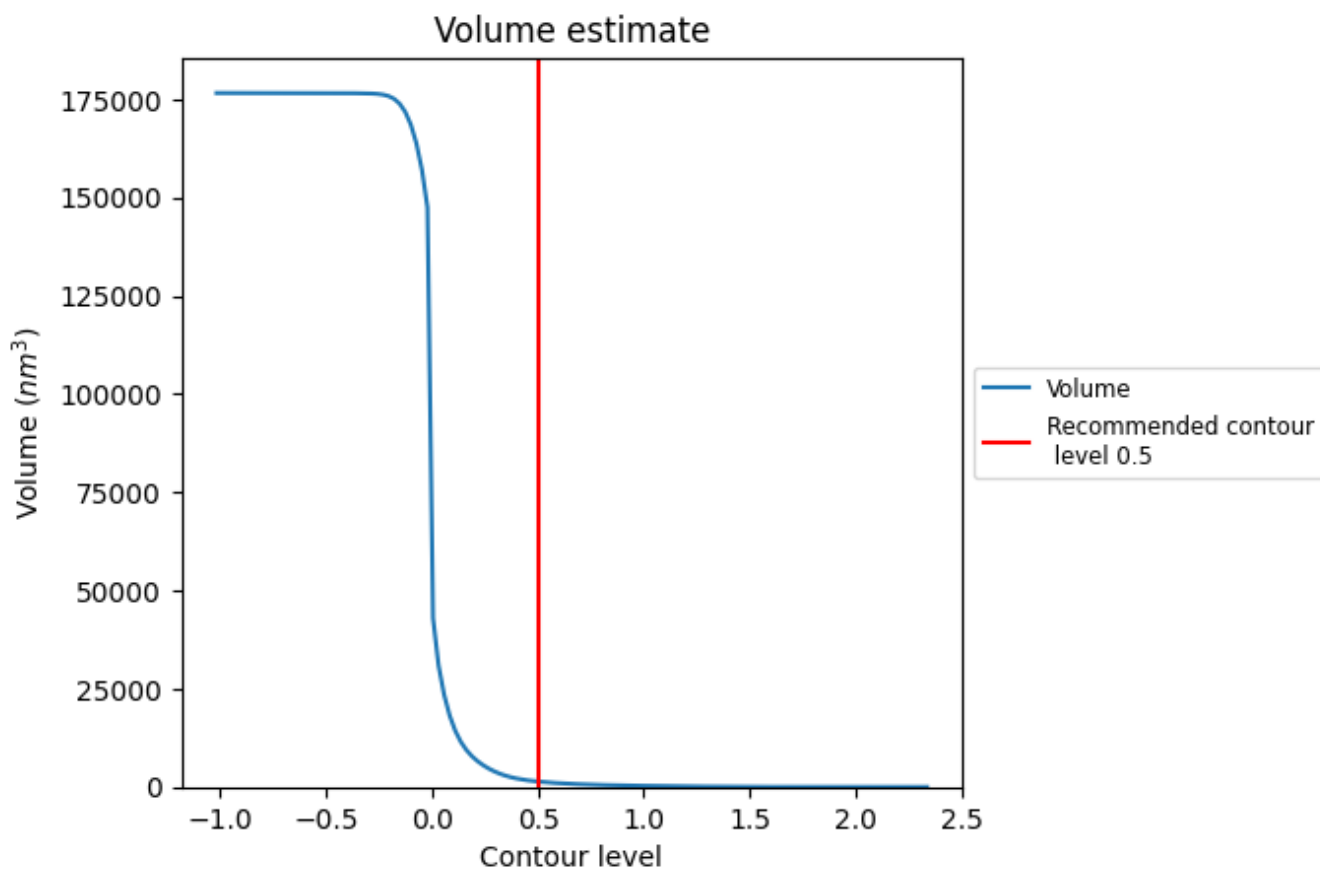
### 7.1 Map-value distribution [i](#)



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.



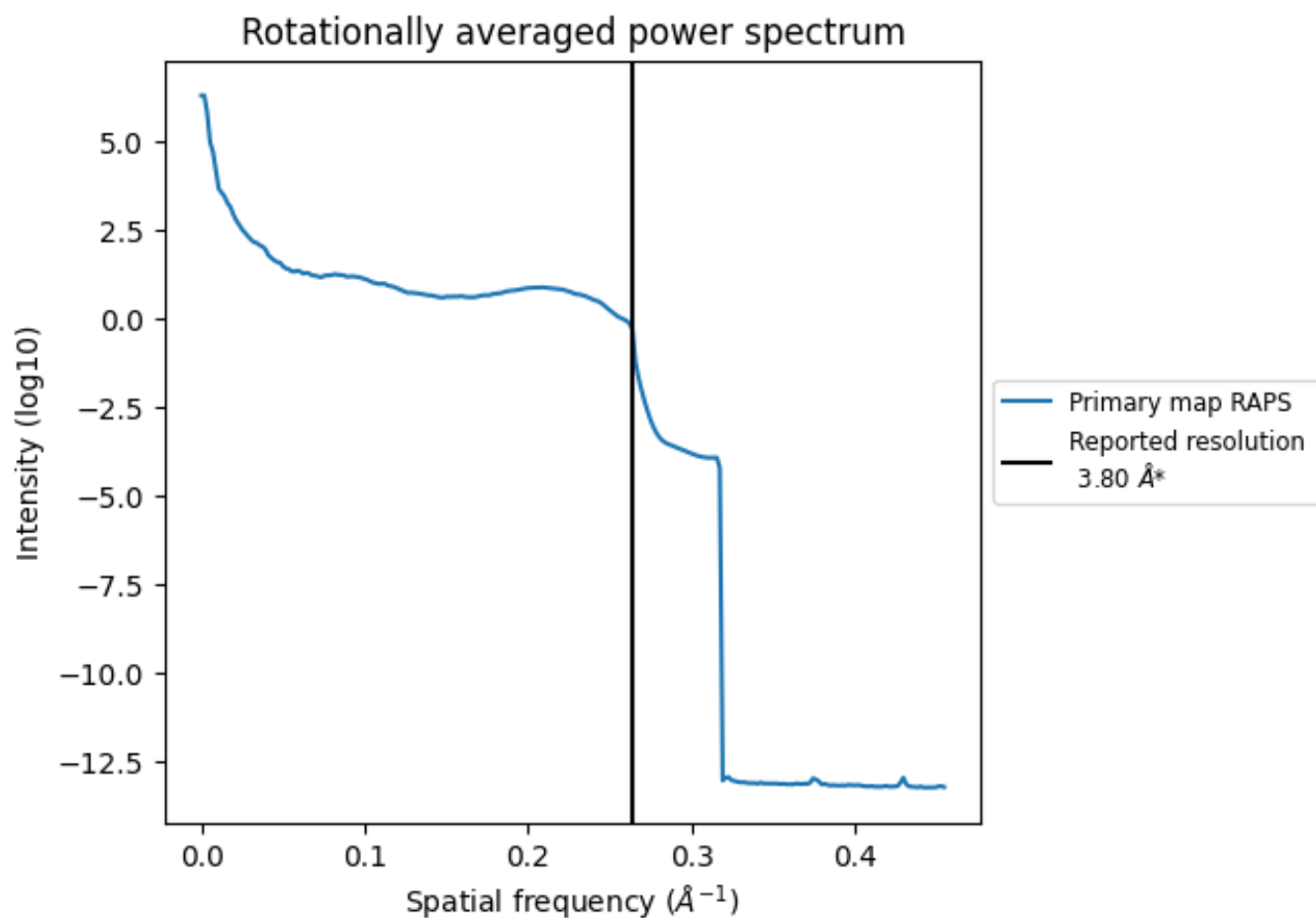
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1376 nm<sup>3</sup>; this corresponds to an approximate mass of 1243 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 0.263 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](#)

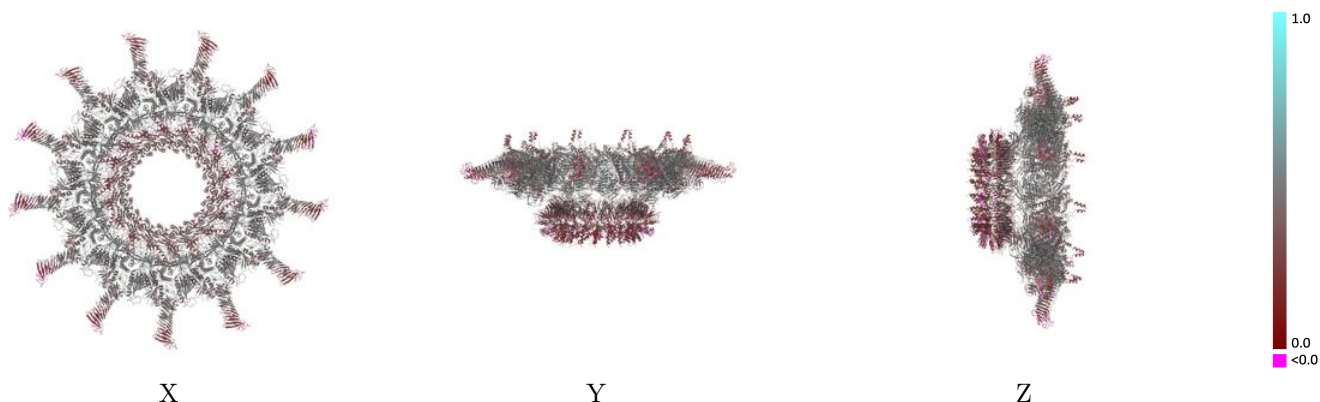
This section contains information regarding the fit between EMDB map EMD-24004 and PDB model 7MUC. Per-residue inclusion information can be found in section [3](#) on page [22](#).

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



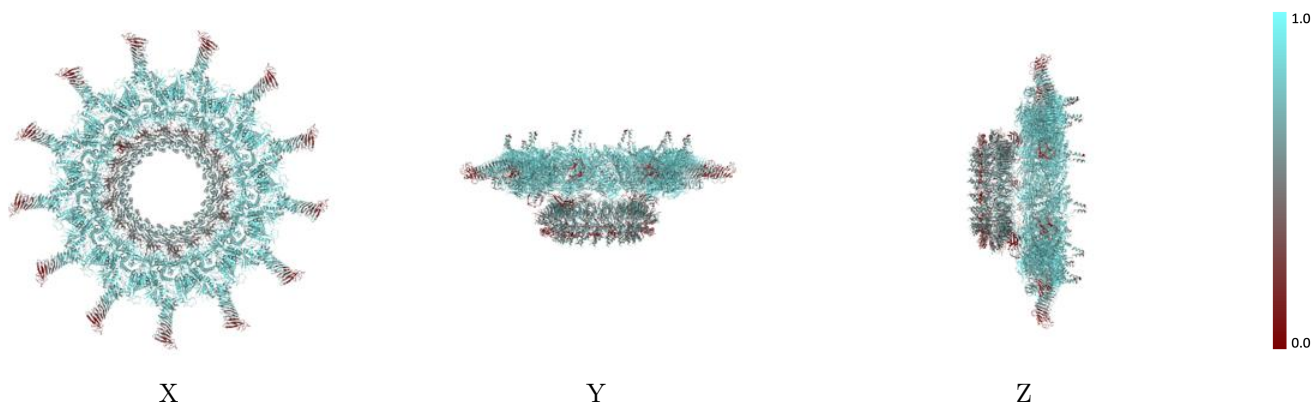
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



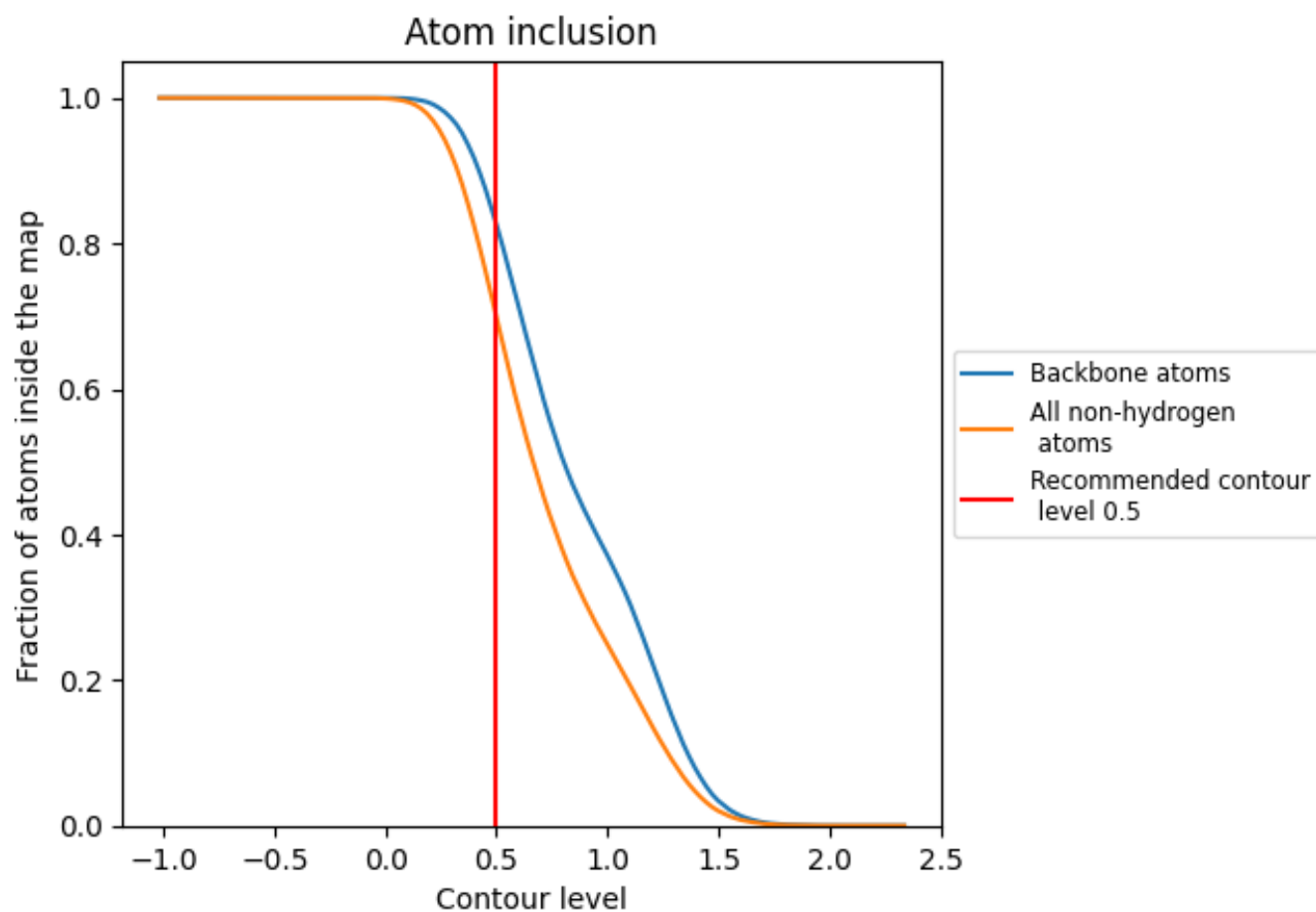
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6984	0.3930
AC	0.8192	0.4550
AD	0.8240	0.4650
AF	0.4501	0.1820
AG	0.6250	0.2810
AH	0.7012	0.3920
AK	0.8416	0.4630
AL	0.8058	0.4360
AM	0.5885	0.3380
AN	0.7552	0.4370
AU	0.9778	0.5100
AX	0.2000	0.1820
Ad	0.8213	0.4560
Af	0.6811	0.3970
BC	0.8204	0.4520
BD	0.8258	0.4700
BF	0.4501	0.2010
BG	0.5956	0.2570
BH	0.7033	0.3960
BK	0.8311	0.4620
BL	0.8021	0.4370
BM	0.5837	0.3440
BN	0.7745	0.4500
BU	0.9778	0.4820
BX	0.2458	0.1950
Bd	0.8184	0.4450
Bf	0.6948	0.4160
CC	0.8131	0.4560
CD	0.8071	0.4570
CF	0.4628	0.2440
CG	0.6140	0.2620
CH	0.7136	0.3900
CK	0.8268	0.4540
CL	0.7961	0.4250
CM	0.5762	0.3460



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Chain	Atom inclusion	Q-score
CN	 0.7762	 0.4520
CU	 0.9556	 0.4740
CX	 0.2292	 0.2120
Cd	 0.8117	 0.4340
Cf	 0.6993	 0.4220
DC	 0.8192	 0.4540
DD	 0.8099	 0.4530
DF	 0.4501	 0.2320
DG	 0.6213	 0.2840
DH	 0.6940	 0.3890
DK	 0.8180	 0.4550
DL	 0.7784	 0.4060
DM	 0.5815	 0.3490
DN	 0.7657	 0.4460
DU	 0.9778	 0.4920
DX	 0.1875	 0.1930
Dd	 0.7944	 0.4430
Df	 0.6401	 0.3980
EC	 0.8052	 0.4460
ED	 0.8071	 0.4580
EF	 0.4246	 0.2200
EG	 0.6360	 0.2780
EH	 0.6894	 0.3750
EK	 0.8259	 0.4550
EL	 0.7924	 0.4160
EM	 0.5726	 0.3520
EN	 0.7640	 0.4370
EU	 0.9333	 0.4800
EX	 0.2417	 0.2010
Ed	 0.8127	 0.4420
Ef	 0.6697	 0.4050
FC	 0.8137	 0.4510
FD	 0.8165	 0.4560
FF	 0.4225	 0.2120
FG	 0.6213	 0.2620
FH	 0.6858	 0.3820
FK	 0.8233	 0.4560
FL	 0.7872	 0.4180
FM	 0.5757	 0.3380
FN	 0.7517	 0.4420
FU	 0.9778	 0.4960
FX	 0.1750	 0.1330

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









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Chain	Atom inclusion	Q-score
Fd	 0.8021	 0.4400
Ff	 0.6674	 0.4050
GC	 0.8216	 0.4500
GD	 0.8071	 0.4550
GF	 0.4289	 0.2140
GG	 0.6029	 0.2800
GH	 0.6920	 0.3900
GK	 0.8215	 0.4580
GL	 0.8028	 0.4330
GM	 0.5740	 0.3360
GN	 0.7657	 0.4420
GU	 1.0000	 0.4930
GX	 0.1375	 0.1290
Gd	 0.8117	 0.4500
Gf	 0.6720	 0.4280
HC	 0.8155	 0.4510
HD	 0.8137	 0.4590
HF	 0.4459	 0.2430
HG	 0.6029	 0.2610
HH	 0.7012	 0.3910
HK	 0.8268	 0.4580
HL	 0.8199	 0.4290
HM	 0.5775	 0.3400
HN	 0.7727	 0.4470
HU	 0.9778	 0.4870
HX	 0.2458	 0.1990
Hd	 0.7992	 0.4530
Hf	 0.6538	 0.4050
IC	 0.8058	 0.4400
ID	 0.8006	 0.4520
IF	 0.4692	 0.2400
IG	 0.5882	 0.2820
IH	 0.6966	 0.3920
IK	 0.8154	 0.4440
IL	 0.8021	 0.4310
IM	 0.5607	 0.3410
IN	 0.7605	 0.4540
IU	 0.9333	 0.4920
IX	 0.2083	 0.1450
Id	 0.7896	 0.4370
If	 0.6902	 0.4050
JC	 0.8016	 0.4300



























































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Chain	Atom inclusion	Q-score
JD	 0.8081	 0.4530
JF	 0.4607	 0.2370
JG	 0.5441	 0.2460
JH	 0.7094	 0.3910
JK	 0.8154	 0.4500
JL	 0.8013	 0.4270
JM	 0.5792	 0.3450
JN	 0.7657	 0.4470
JU	 0.9778	 0.5140
JX	 0.1958	 0.2150
Jd	 0.8136	 0.4430
Jf	 0.6720	 0.4180
KC	 0.8101	 0.4390
KD	 0.8155	 0.4540
KF	 0.5011	 0.2500
KG	 0.5809	 0.2350
KH	 0.6992	 0.3820
KK	 0.8206	 0.4490
KL	 0.8073	 0.4250
KM	 0.5823	 0.3400
KN	 0.7710	 0.4510
KU	 0.9333	 0.5000
KX	 0.2708	 0.2290
Kd	 0.8031	 0.4480
Kf	 0.6925	 0.4170
LC	 0.8155	 0.4490
LD	 0.8174	 0.4600
LF	 0.4777	 0.2500
LG	 0.5919	 0.2450
LH	 0.6940	 0.3830
LK	 0.8320	 0.4530
LL	 0.8080	 0.4230
LM	 0.6000	 0.3570
LN	 0.7815	 0.4580
LU	 0.8889	 0.4570
LX	 0.2125	 0.2290
Ld	 0.8213	 0.4480
Lf	 0.6970	 0.4160
MC	 0.8252	 0.4520
MD	 0.8137	 0.4600
MF	 0.4671	 0.2240
MG	 0.6029	 0.2910

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Chain	Atom inclusion	Q-score
MH	 0.7228	 0.4020
MK	 0.8303	 0.4590
ML	 0.8117	 0.4330
MM	 0.6079	 0.3410
MN	 0.7727	 0.4500
MU	 0.9556	 0.4940
MX	 0.2250	 0.2070
Md	 0.8127	 0.4450
Mf	 0.6811	 0.4110
VF	 0.4713	 0.2340
VG	 0.5919	 0.2670
VH	 0.5598	 0.3600
VX	 0.2625	 0.2330
WF	 0.4119	 0.1920
WG	 0.6103	 0.2230
WH	 0.4277	 0.3360
WX	 0.1750	 0.1610
XF	 0.4522	 0.2420
XG	 0.6103	 0.2740
XH	 0.5636	 0.3700
XX	 0.1958	 0.1580
YF	 0.4798	 0.2430
YG	 0.6176	 0.2900
YH	 0.5065	 0.3500
YX	 0.2292	 0.2210
ZF	 0.4310	 0.2010
ZG	 0.5882	 0.2450
ZH	 0.4766	 0.3490
ZX	 0.2167	 0.2010