



wwPDB EM Validation Summary Report ⓘ

Nov 27, 2022 – 12:14 PM EST

PDB ID : 6OWG
EMDB ID : EMD-20207
Title : Structure of a synthetic beta-carboxysome shell, T=4
Authors : Sutter, M.; Laughlin, T.G.; Davies, K.M.; Kerfeld, C.A.
Deposited on : 2019-05-09
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

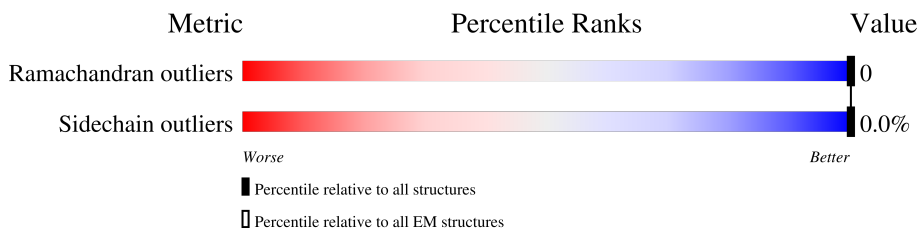
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 Å.

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





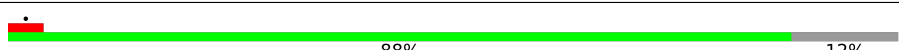
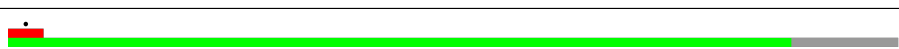

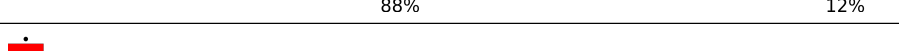
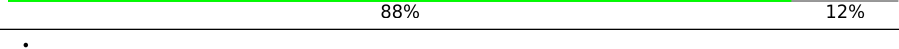





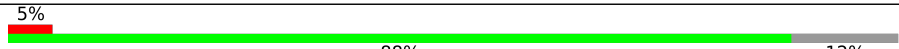


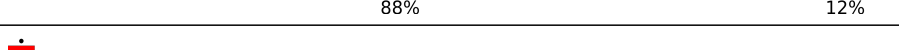








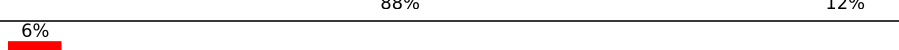
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	0	113	
1	2	113	
1	3	113	
1	4	113	
1	6	113	
1	7	113	
1	8	113	
1	A	113	
1	A0	113	


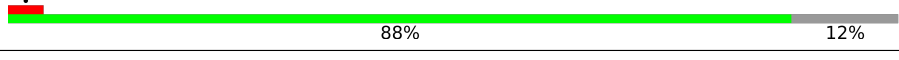
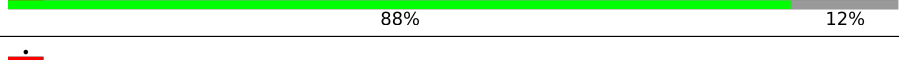
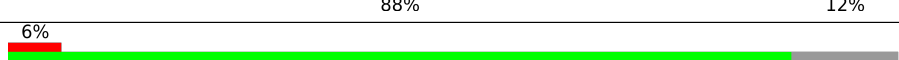
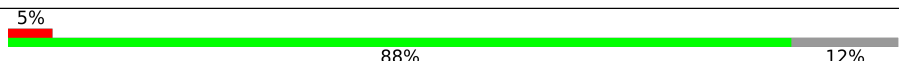


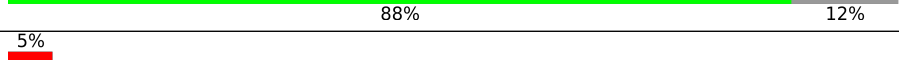
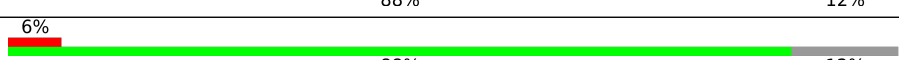
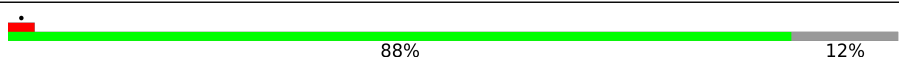



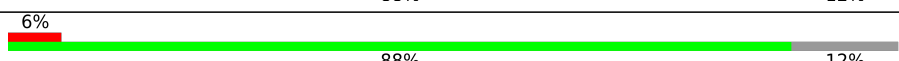






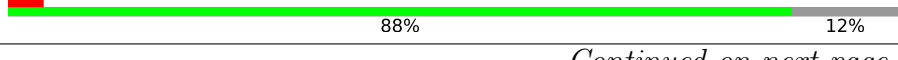



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Mol	Chain	Length	Quality of chain
1	A1	113	 88% 12%
1	A2	113	 88% 12%
1	A4	113	 88% 12%
1	A5	113	 88% 12%
1	A6	113	 88% 12%
1	A8	113	 88% 12%
1	A9	113	 88% 12%
1	AA	113	 88% 12%
1	AC	113	 88% 12%
1	AD	113	 88% 12%
1	AE	113	 88% 12%
1	AG	113	 88% 12%
1	AH	113	 88% 12%
1	AI	113	 88% 12%
1	AK	113	 88% 12%
1	AL	113	 88% 12%
1	AM	113	 88% 12%
1	AO	113	 88% 12%
1	AP	113	 88% 12%
1	AQ	113	 88% 12%
1	AS	113	 88% 12%
1	AT	113	 88% 12%
1	AU	113	 88% 12%
1	AW	113	 88% 12%
1	AX	113	 88% 12%

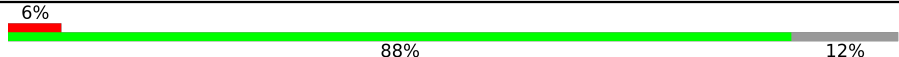
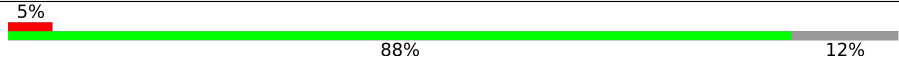







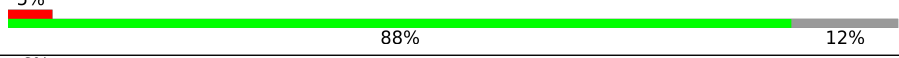

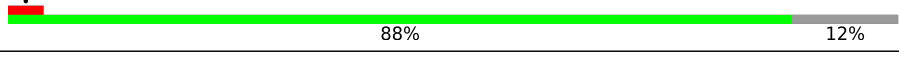
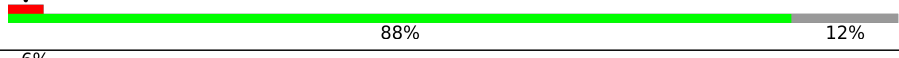
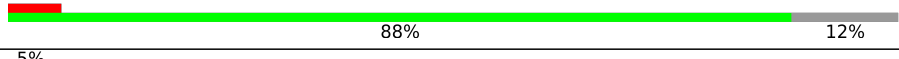
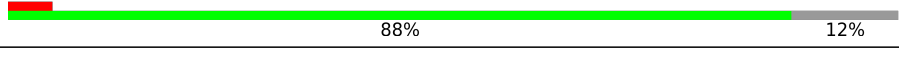
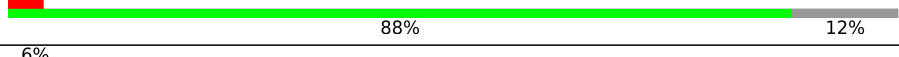









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Mol	Chain	Length	Quality of chain
1	AY	113	 6% 88% 12%
1	B	113	 6% 88% 12%
1	B0	113	 6% 88% 12%
1	B1	113	 6% 88% 12%
1	B2	113	 5% 88% 12%
1	B4	113	 5% 88% 12%
1	B5	113	 6% 88% 12%
1	B6	113	 7% 88% 12%
1	B8	113	 6% 88% 12%
1	B9	113	 5% 88% 12%
1	BA	113	 6% 88% 12%
1	BC	113	 6% 88% 12%
1	BD	113	 5% 88% 12%
1	BE	113	 6% 88% 12%
1	BG	113	 6% 88% 12%
1	BH	113	 6% 88% 12%
1	BI	113	 6% 88% 12%
1	BK	113	 6% 88% 12%
1	BL	113	 6% 88% 12%
1	BM	113	 6% 88% 12%
1	BO	113	 6% 88% 12%
1	BP	113	 5% 88% 12%
1	BQ	113	 6% 88% 12%
1	BS	113	 6% 88% 12%
1	BT	113	6% 88% 12%

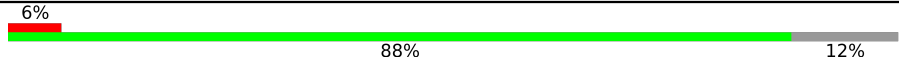
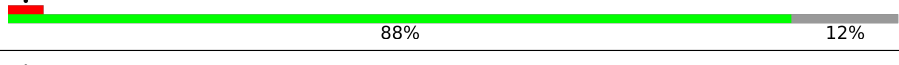
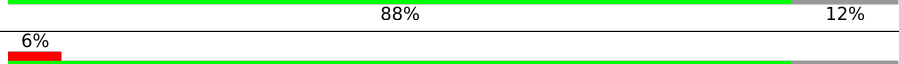
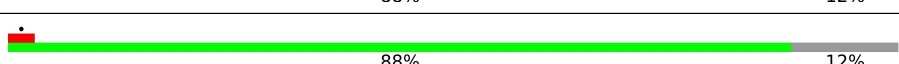

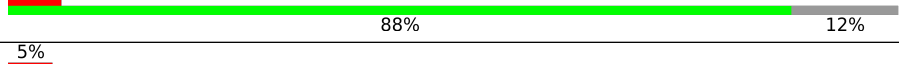
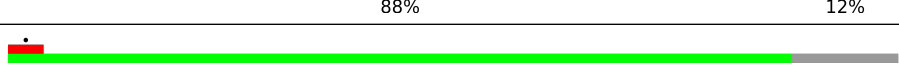

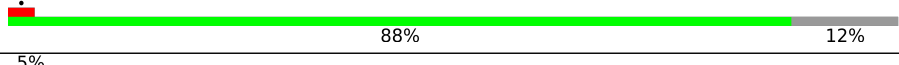

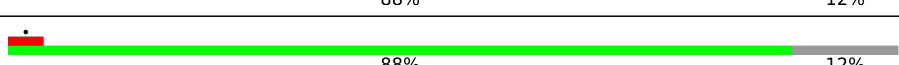

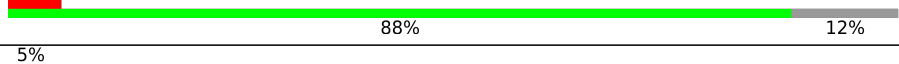


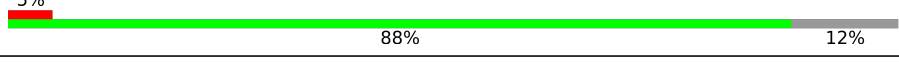



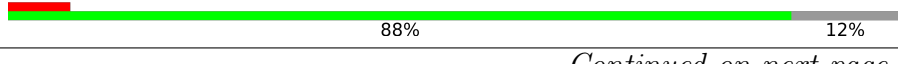



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Mol	Chain	Length	Quality of chain
1	BU	113	 6% 88% 12%
1	BW	113	 5% 88% 12%
1	BX	113	 6% 88% 12%
1	BY	113	 6% 88% 12%
1	C	113	 6% 88% 12%
1	C0	113	 6% 88% 12%
1	C1	113	 6% 88% 12%
1	C2	113	 6% 88% 12%
1	C4	113	 6% 88% 12%
1	C5	113	 5% 88% 12%
1	C6	113	 6% 88% 12%
1	C8	113	 6% 88% 12%
1	C9	113	 6% 88% 12%
1	CA	113	 6% 88% 12%
1	CC	113	 5% 88% 12%
1	CD	113	 6% 88% 12%
1	CE	113	 6% 88% 12%
1	CG	113	 5% 88% 12%
1	CH	113	 6% 88% 12%
1	CI	113	 6% 88% 12%
1	CK	113	 5% 88% 12%
1	CL	113	 6% 88% 12%
1	CM	113	 6% 88% 12%
1	CO	113	 6% 88% 12%
1	CP	113	 6% 88% 12%







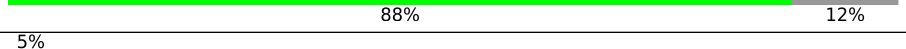
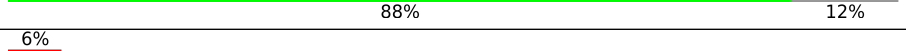
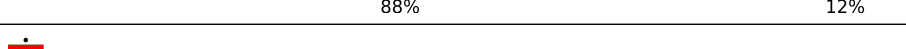
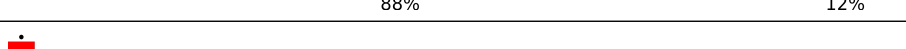
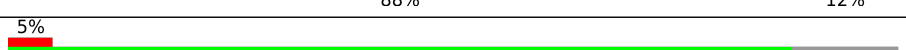

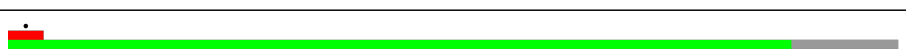

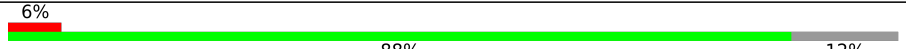





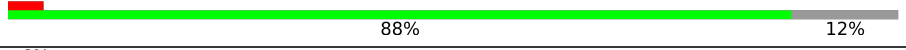
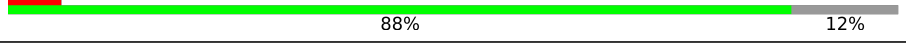



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Mol	Chain	Length	Quality of chain
1	CQ	113	 6% 88% 12%
1	CS	113	 6% 88% 12%
1	CT	113	 6% 88% 12%
1	CU	113	 6% 88% 12%
1	CW	113	 6% 88% 12%
1	CX	113	 6% 88% 12%
1	CY	113	 6% 88% 12%
1	D0	113	 5% 88% 12%
1	D1	113	 6% 88% 12%
1	D2	113	 7% 88% 12%
1	D4	113	 6% 88% 12%
1	D5	113	 5% 88% 12%
1	D6	113	 6% 88% 12%
1	D8	113	 6% 88% 12%
1	D9	113	 6% 88% 12%
1	DA	113	 6% 88% 12%
1	DC	113	 5% 88% 12%
1	DD	113	 6% 88% 12%
1	DE	113	 7% 88% 12%
1	DG	113	 5% 88% 12%
1	DH	113	 6% 88% 12%
1	DI	113	 6% 88% 12%
1	DK	113	 5% 88% 12%
1	DL	113	6% 88% 12%
1	DM	113	7% 88% 12%

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Mol	Chain	Length	Quality of chain
1	DO	113	 88% 12%
1	DP	113	 88% 12%
1	DQ	113	 88% 12%
1	DS	113	 88% 12%
1	DT	113	 88% 12%
1	DU	113	 88% 12%
1	DW	113	 88% 12%
1	DX	113	 88% 12%
1	DY	113	 88% 12%
1	E	113	 88% 12%
1	E0	113	 88% 12%
1	E1	113	 88% 12%
1	E2	113	 88% 12%
1	E4	113	 88% 12%
1	E5	113	 88% 12%
1	E6	113	 88% 12%
1	EA	113	 88% 12%
1	EC	113	 88% 12%
1	ED	113	 88% 12%
1	EE	113	 88% 12%
1	EG	113	 88% 12%
1	EH	113	 88% 12%
1	EI	113	 88% 12%
1	EK	113	 88% 12%
1	EL	113	 88% 12%













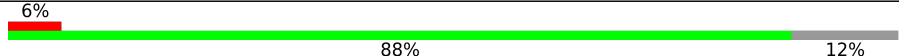
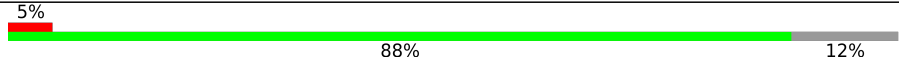
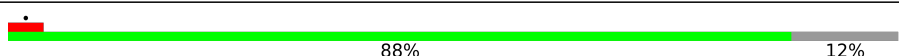

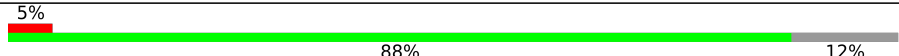
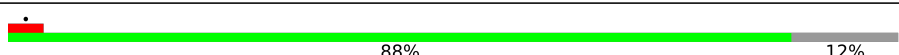
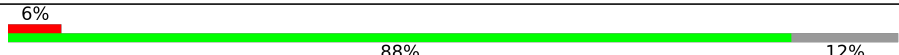
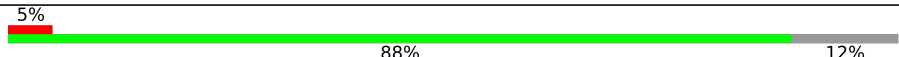
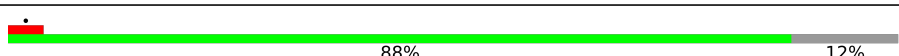
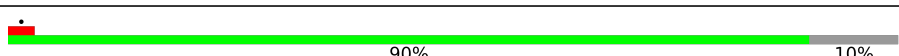
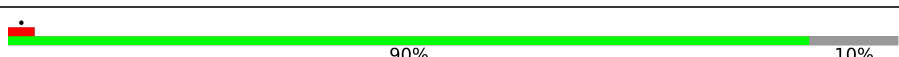
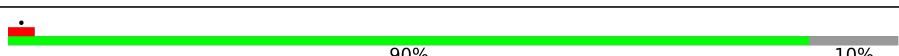
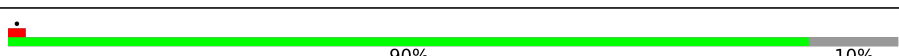
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Mol	Chain	Length	Quality of chain
1	EM	113	6% 88% 12%
1	EO	113	6% 88% 12%
1	EP	113	5% 88% 12%
1	EQ	113	6% 88% 12%
1	ES	113	6% 88% 12%
1	ET	113	6% 88% 12%
1	EU	113	6% 88% 12%
1	EW	113	5% 88% 12%
1	EX	113	6% 88% 12%
1	EY	113	7% 88% 12%
1	F	113	6% 88% 12%
1	G	113	6% 88% 12%
1	I	113	5% 88% 12%
1	J	113	6% 88% 12%
1	K	113	7% 88% 12%
1	M	113	6% 88% 12%
1	N	113	5% 88% 12%
1	O	113	6% 88% 12%
1	Q	113	5% 88% 12%
1	R	113	6% 88% 12%
1	S	113	7% 88% 12%
1	U	113	5% 88% 12%
1	V	113	6% 88% 12%
1	W	113	6% 88% 12%
1	Y	113	6% 88% 12%

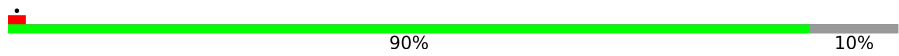
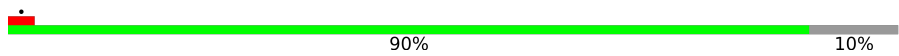
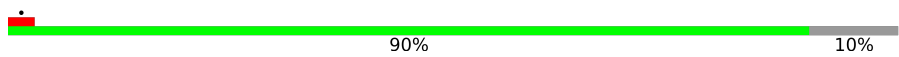
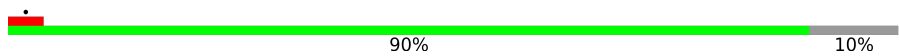
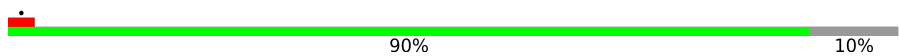
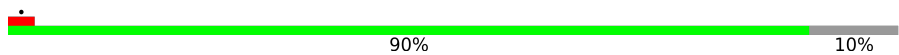
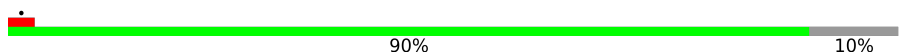
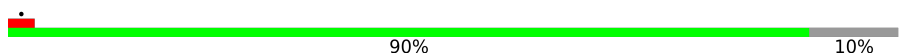


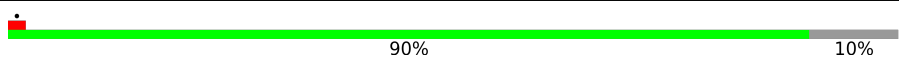

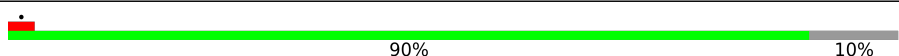
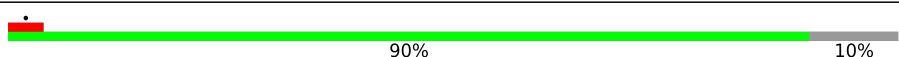
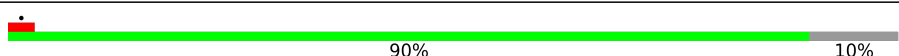
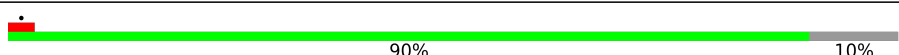
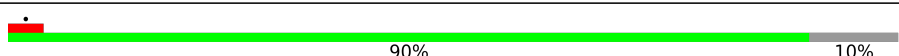
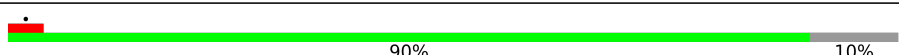
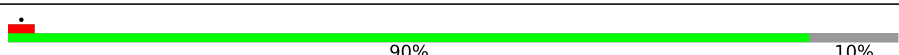
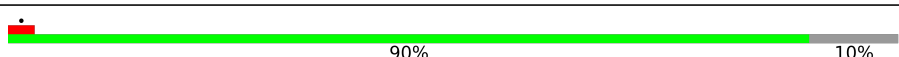
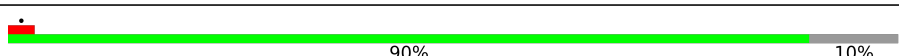
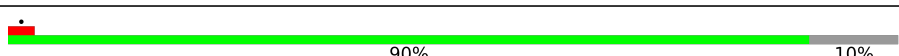
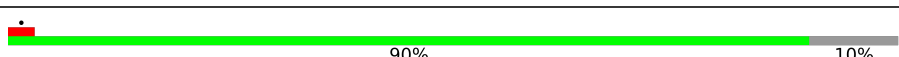
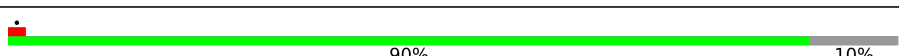
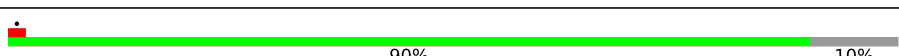
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Mol	Chain	Length	Quality of chain
1	Z	113	 88% 12%
1	a	113	 88% 12%
1	b	113	 88% 12%
1	c	113	 88% 12%
1	e	113	 88% 12%
1	f	113	 88% 12%
1	g	113	 88% 12%
1	i	113	 88% 12%
1	j	113	 88% 12%
1	k	113	 88% 12%
1	m	113	 88% 12%
1	n	113	 88% 12%
1	o	113	 88% 12%
1	q	113	 88% 12%
1	r	113	 88% 12%
1	s	113	 88% 12%
1	u	113	 88% 12%
1	v	113	 88% 12%
1	w	113	 88% 12%
1	y	113	 88% 12%
1	z	113	 88% 12%
2	1	105	 90% 10%
2	5	105	 90% 10%
2	9	105	 90% 10%
2	A3	105	 90% 10%

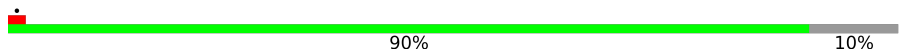
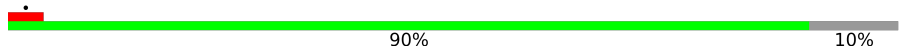
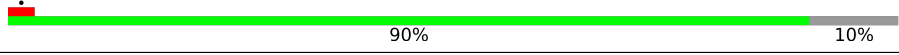
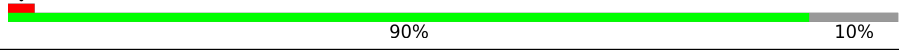
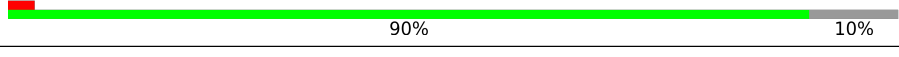
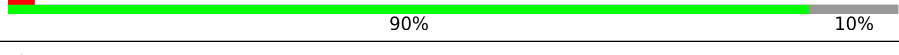
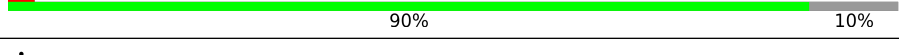
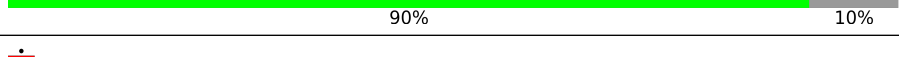
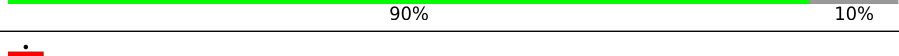
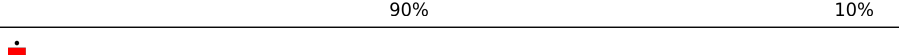
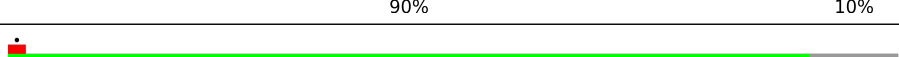
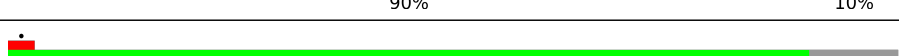
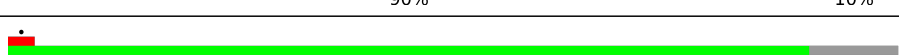
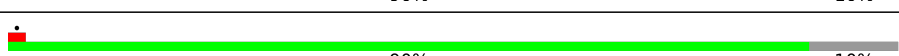
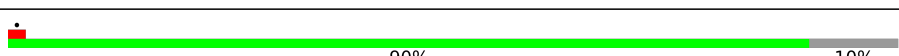
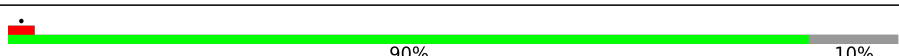
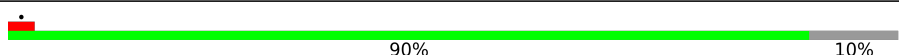

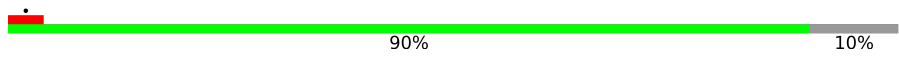
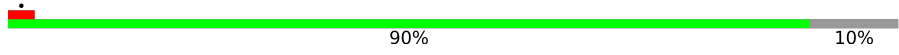
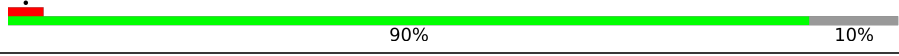
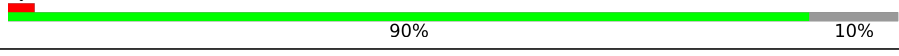
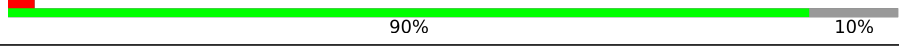
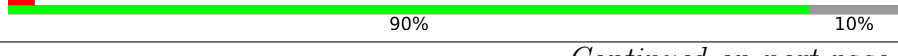

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Mol	Chain	Length	Quality of chain
2	A7	105	 90% 10%
2	AB	105	 90% 10%
2	AF	105	 90% 10%
2	AJ	105	 90% 10%
2	AN	105	 90% 10%
2	AR	105	 90% 10%
2	AV	105	 90% 10%
2	AZ	105	 90% 10%
2	B3	105	 90% 10%
2	B7	105	 90% 10%
2	BB	105	 90% 10%
2	BF	105	 90% 10%
2	BJ	105	 90% 10%
2	BN	105	 90% 10%
2	BR	105	 90% 10%
2	BV	105	 90% 10%
2	BZ	105	 90% 10%
2	C3	105	 90% 10%
2	C7	105	 90% 10%
2	CB	105	 90% 10%
2	CF	105	 90% 10%
2	CJ	105	 90% 10%
2	CN	105	 90% 10%
2	CR	105	 90% 10%
2	CV	105	 90% 10%

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Mol	Chain	Length	Quality of chain
2	CZ	105	 90% 10%
2	D	105	 90% 10%
2	D3	105	 90% 10%
2	D7	105	 90% 10%
2	DB	105	 90% 10%
2	DF	105	 90% 10%
2	DJ	105	 90% 10%
2	DN	105	 90% 10%
2	DR	105	 90% 10%
2	DV	105	 90% 10%
2	DZ	105	 90% 10%
2	E3	105	 90% 10%
2	E7	105	 90% 10%
2	EB	105	 90% 10%
2	EF	105	 90% 10%
2	EJ	105	 90% 10%
2	EN	105	 90% 10%
2	ER	105	 90% 10%
2	EV	105	 90% 10%
2	EZ	105	 90% 10%
2	H	105	 90% 10%
2	L	105	 90% 10%
2	P	105	 90% 10%
2	T	105	 90% 10%
2	X	105	 90% 10%

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Mol	Chain	Length	Quality of chain
2	d	105	 90% 10%
2	h	105	 90% 10%
2	l	105	 90% 10%
2	p	105	 90% 10%
2	t	105	 90% 10%
2	x	105	 90% 10%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 178080 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 Microcompartments protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	100	752	473	133	144	2	0	0
1	B	100	752	473	133	144	2	0	0
1	C	100	752	473	133	144	2	0	0
1	E	100	752	473	133	144	2	0	0
1	F	100	752	473	133	144	2	0	0
1	G	100	752	473	133	144	2	0	0
1	I	100	752	473	133	144	2	0	0
1	J	100	752	473	133	144	2	0	0
1	K	100	752	473	133	144	2	0	0
1	M	100	752	473	133	144	2	0	0
1	N	100	752	473	133	144	2	0	0
1	O	100	752	473	133	144	2	0	0
1	Q	100	752	473	133	144	2	0	0
1	R	100	752	473	133	144	2	0	0
1	S	100	752	473	133	144	2	0	0
1	U	100	752	473	133	144	2	0	0
1	V	100	752	473	133	144	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	W	100	752	473	133	144	2	0	0
1	Y	100	752	473	133	144	2	0	0
1	Z	100	752	473	133	144	2	0	0
1	0	100	752	473	133	144	2	0	0
1	2	100	752	473	133	144	2	0	0
1	3	100	752	473	133	144	2	0	0
1	4	100	752	473	133	144	2	0	0
1	6	100	752	473	133	144	2	0	0
1	7	100	752	473	133	144	2	0	0
1	8	100	752	473	133	144	2	0	0
1	a	100	752	473	133	144	2	0	0
1	b	100	752	473	133	144	2	0	0
1	c	100	752	473	133	144	2	0	0
1	e	100	752	473	133	144	2	0	0
1	f	100	752	473	133	144	2	0	0
1	g	100	752	473	133	144	2	0	0
1	i	100	752	473	133	144	2	0	0
1	j	100	752	473	133	144	2	0	0
1	k	100	752	473	133	144	2	0	0
1	m	100	752	473	133	144	2	0	0
1	n	100	752	473	133	144	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	o	100	752	473	133	144	2	0	0
1	q	100	752	473	133	144	2	0	0
1	r	100	752	473	133	144	2	0	0
1	s	100	752	473	133	144	2	0	0
1	u	100	752	473	133	144	2	0	0
1	v	100	752	473	133	144	2	0	0
1	w	100	752	473	133	144	2	0	0
1	y	100	752	473	133	144	2	0	0
1	z	100	752	473	133	144	2	0	0
1	AA	100	752	473	133	144	2	0	0
1	AC	100	752	473	133	144	2	0	0
1	AD	100	752	473	133	144	2	0	0
1	AE	100	752	473	133	144	2	0	0
1	AG	100	752	473	133	144	2	0	0
1	AH	100	752	473	133	144	2	0	0
1	AI	100	752	473	133	144	2	0	0
1	AK	100	752	473	133	144	2	0	0
1	AL	100	752	473	133	144	2	0	0
1	AM	100	752	473	133	144	2	0	0
1	AO	100	752	473	133	144	2	0	0
1	AP	100	752	473	133	144	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AQ	100	752	473	133	144	2	0	0
1	AS	100	752	473	133	144	2	0	0
1	AT	100	752	473	133	144	2	0	0
1	AU	100	752	473	133	144	2	0	0
1	AW	100	752	473	133	144	2	0	0
1	AX	100	752	473	133	144	2	0	0
1	AY	100	752	473	133	144	2	0	0
1	A0	100	752	473	133	144	2	0	0
1	A1	100	752	473	133	144	2	0	0
1	A2	100	752	473	133	144	2	0	0
1	A4	100	752	473	133	144	2	0	0
1	A5	100	752	473	133	144	2	0	0
1	A6	100	752	473	133	144	2	0	0
1	A8	100	752	473	133	144	2	0	0
1	A9	100	752	473	133	144	2	0	0
1	BA	100	752	473	133	144	2	0	0
1	BC	100	752	473	133	144	2	0	0
1	BD	100	752	473	133	144	2	0	0
1	BE	100	752	473	133	144	2	0	0
1	BG	100	752	473	133	144	2	0	0
1	BH	100	752	473	133	144	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	BI	100	752	473	133	144	2	0	0
1	BK	100	752	473	133	144	2	0	0
1	BL	100	752	473	133	144	2	0	0
1	BM	100	752	473	133	144	2	0	0
1	BO	100	752	473	133	144	2	0	0
1	BP	100	752	473	133	144	2	0	0
1	BQ	100	752	473	133	144	2	0	0
1	BS	100	752	473	133	144	2	0	0
1	BT	100	752	473	133	144	2	0	0
1	BU	100	752	473	133	144	2	0	0
1	BW	100	752	473	133	144	2	0	0
1	BX	100	752	473	133	144	2	0	0
1	BY	100	752	473	133	144	2	0	0
1	B0	100	752	473	133	144	2	0	0
1	B1	100	752	473	133	144	2	0	0
1	B2	100	752	473	133	144	2	0	0
1	B4	100	752	473	133	144	2	0	0
1	B5	100	752	473	133	144	2	0	0
1	B6	100	752	473	133	144	2	0	0
1	B8	100	752	473	133	144	2	0	0
1	B9	100	752	473	133	144	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	CA	100	752	473	133	144	2	0	0
1	CC	100	752	473	133	144	2	0	0
1	CD	100	752	473	133	144	2	0	0
1	CE	100	752	473	133	144	2	0	0
1	CG	100	752	473	133	144	2	0	0
1	CH	100	752	473	133	144	2	0	0
1	CI	100	752	473	133	144	2	0	0
1	CK	100	752	473	133	144	2	0	0
1	CL	100	752	473	133	144	2	0	0
1	CM	100	752	473	133	144	2	0	0
1	CO	100	752	473	133	144	2	0	0
1	CP	100	752	473	133	144	2	0	0
1	CQ	100	752	473	133	144	2	0	0
1	CS	100	752	473	133	144	2	0	0
1	CT	100	752	473	133	144	2	0	0
1	CU	100	752	473	133	144	2	0	0
1	CW	100	752	473	133	144	2	0	0
1	CX	100	752	473	133	144	2	0	0
1	CY	100	752	473	133	144	2	0	0
1	C0	100	752	473	133	144	2	0	0
1	C1	100	752	473	133	144	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C2	100	752	473	133	144	2	0	0
1	C4	100	752	473	133	144	2	0	0
1	C5	100	752	473	133	144	2	0	0
1	C6	100	752	473	133	144	2	0	0
1	C8	100	752	473	133	144	2	0	0
1	C9	100	752	473	133	144	2	0	0
1	DA	100	752	473	133	144	2	0	0
1	DC	100	752	473	133	144	2	0	0
1	DD	100	752	473	133	144	2	0	0
1	DE	100	752	473	133	144	2	0	0
1	DG	100	752	473	133	144	2	0	0
1	DH	100	752	473	133	144	2	0	0
1	DI	100	752	473	133	144	2	0	0
1	DK	100	752	473	133	144	2	0	0
1	DL	100	752	473	133	144	2	0	0
1	DM	100	752	473	133	144	2	0	0
1	DO	100	752	473	133	144	2	0	0
1	DP	100	752	473	133	144	2	0	0
1	DQ	100	752	473	133	144	2	0	0
1	DS	100	752	473	133	144	2	0	0
1	DT	100	752	473	133	144	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	DU	100	752	473	133	144	2	0	0
1	DW	100	752	473	133	144	2	0	0
1	DX	100	752	473	133	144	2	0	0
1	DY	100	752	473	133	144	2	0	0
1	D0	100	752	473	133	144	2	0	0
1	D1	100	752	473	133	144	2	0	0
1	D2	100	752	473	133	144	2	0	0
1	D4	100	752	473	133	144	2	0	0
1	D5	100	752	473	133	144	2	0	0
1	D6	100	752	473	133	144	2	0	0
1	D8	100	752	473	133	144	2	0	0
1	D9	100	752	473	133	144	2	0	0
1	EA	100	752	473	133	144	2	0	0
1	EC	100	752	473	133	144	2	0	0
1	ED	100	752	473	133	144	2	0	0
1	EE	100	752	473	133	144	2	0	0
1	EG	100	752	473	133	144	2	0	0
1	EH	100	752	473	133	144	2	0	0
1	EI	100	752	473	133	144	2	0	0
1	EK	100	752	473	133	144	2	0	0
1	EL	100	752	473	133	144	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	EM	100	Total	C	N	O	S	0	0
			752	473	133	144	2		
1	EO	100	Total	C	N	O	S	0	0
			752	473	133	144	2		
1	EP	100	Total	C	N	O	S	0	0
			752	473	133	144	2		
1	EQ	100	Total	C	N	O	S	0	0
			752	473	133	144	2		
1	ES	100	Total	C	N	O	S	0	0
			752	473	133	144	2		
1	ET	100	Total	C	N	O	S	0	0
			752	473	133	144	2		
1	EU	100	Total	C	N	O	S	0	0
			752	473	133	144	2		
1	EW	100	Total	C	N	O	S	0	0
			752	473	133	144	2		
1	EX	100	Total	C	N	O	S	0	0
			752	473	133	144	2		
1	EY	100	Total	C	N	O	S	0	0
			752	473	133	144	2		
1	E0	100	Total	C	N	O	S	0	0
			752	473	133	144	2		
1	E1	100	Total	C	N	O	S	0	0
			752	473	133	144	2		
1	E2	100	Total	C	N	O	S	0	0
			752	473	133	144	2		
1	E4	100	Total	C	N	O	S	0	0
			752	473	133	144	2		
1	E5	100	Total	C	N	O	S	0	0
			752	473	133	144	2		
1	E6	100	Total	C	N	O	S	0	0
			752	473	133	144	2		

- Molecule 2 is a protein called Ethanolamine utilization protein EutN/carboxysome structural protein Ccml.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	94	Total	C	N	O	S	0	0
			712	450	126	131	5		
2	H	94	Total	C	N	O	S	0	0
			712	450	126	131	5		
2	L	94	Total	C	N	O	S	0	0
			712	450	126	131	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	94	712	450	126	131	5	0	0
2	T	94	712	450	126	131	5	0	0
2	X	94	712	450	126	131	5	0	0
2	1	94	712	450	126	131	5	0	0
2	5	94	712	450	126	131	5	0	0
2	9	94	712	450	126	131	5	0	0
2	d	94	712	450	126	131	5	0	0
2	h	94	712	450	126	131	5	0	0
2	l	94	712	450	126	131	5	0	0
2	p	94	712	450	126	131	5	0	0
2	t	94	712	450	126	131	5	0	0
2	x	94	712	450	126	131	5	0	0
2	AB	94	712	450	126	131	5	0	0
2	AF	94	712	450	126	131	5	0	0
2	AJ	94	712	450	126	131	5	0	0
2	AN	94	712	450	126	131	5	0	0
2	AR	94	712	450	126	131	5	0	0
2	AV	94	712	450	126	131	5	0	0
2	AZ	94	712	450	126	131	5	0	0
2	A3	94	712	450	126	131	5	0	0
2	A7	94	712	450	126	131	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BB	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	BF	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	BJ	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	BN	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	BR	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	BV	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	BZ	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	B3	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	B7	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	CB	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	CF	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	CJ	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	CN	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	CR	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	CV	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	CZ	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	C3	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	C7	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	DB	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	DF	94	Total 712	C 450	N 126	O 131	S 5	0	0
2	DJ	94	Total 712	C 450	N 126	O 131	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	DN	94	712	450	126	131	5	0	0
2	DR	94	712	450	126	131	5	0	0
2	DV	94	712	450	126	131	5	0	0
2	DZ	94	712	450	126	131	5	0	0
2	D3	94	712	450	126	131	5	0	0
2	D7	94	712	450	126	131	5	0	0
2	EB	94	712	450	126	131	5	0	0
2	EF	94	712	450	126	131	5	0	0
2	EJ	94	712	450	126	131	5	0	0
2	EN	94	712	450	126	131	5	0	0
2	ER	94	712	450	126	131	5	0	0
2	EV	94	712	450	126	131	5	0	0
2	EZ	94	712	450	126	131	5	0	0
2	E3	94	712	450	126	131	5	0	0
2	E7	94	712	450	126	131	5	0	0

There are 600 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	96	GLY	-	expression tag	UNP K9YFK1
D	97	SER	-	expression tag	UNP K9YFK1
D	98	TRP	-	expression tag	UNP K9YFK1
D	99	SER	-	expression tag	UNP K9YFK1
D	100	HIS	-	expression tag	UNP K9YFK1
D	101	PRO	-	expression tag	UNP K9YFK1
D	102	GLN	-	expression tag	UNP K9YFK1
D	103	PHE	-	expression tag	UNP K9YFK1
D	104	GLU	-	expression tag	UNP K9YFK1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	105	LYS	-	expression tag	UNP K9YFK1
H	96	GLY	-	expression tag	UNP K9YFK1
H	97	SER	-	expression tag	UNP K9YFK1
H	98	TRP	-	expression tag	UNP K9YFK1
H	99	SER	-	expression tag	UNP K9YFK1
H	100	HIS	-	expression tag	UNP K9YFK1
H	101	PRO	-	expression tag	UNP K9YFK1
H	102	GLN	-	expression tag	UNP K9YFK1
H	103	PHE	-	expression tag	UNP K9YFK1
H	104	GLU	-	expression tag	UNP K9YFK1
H	105	LYS	-	expression tag	UNP K9YFK1
L	96	GLY	-	expression tag	UNP K9YFK1
L	97	SER	-	expression tag	UNP K9YFK1
L	98	TRP	-	expression tag	UNP K9YFK1
L	99	SER	-	expression tag	UNP K9YFK1
L	100	HIS	-	expression tag	UNP K9YFK1
L	101	PRO	-	expression tag	UNP K9YFK1
L	102	GLN	-	expression tag	UNP K9YFK1
L	103	PHE	-	expression tag	UNP K9YFK1
L	104	GLU	-	expression tag	UNP K9YFK1
L	105	LYS	-	expression tag	UNP K9YFK1
P	96	GLY	-	expression tag	UNP K9YFK1
P	97	SER	-	expression tag	UNP K9YFK1
P	98	TRP	-	expression tag	UNP K9YFK1
P	99	SER	-	expression tag	UNP K9YFK1
P	100	HIS	-	expression tag	UNP K9YFK1
P	101	PRO	-	expression tag	UNP K9YFK1
P	102	GLN	-	expression tag	UNP K9YFK1
P	103	PHE	-	expression tag	UNP K9YFK1
P	104	GLU	-	expression tag	UNP K9YFK1
P	105	LYS	-	expression tag	UNP K9YFK1
T	96	GLY	-	expression tag	UNP K9YFK1
T	97	SER	-	expression tag	UNP K9YFK1
T	98	TRP	-	expression tag	UNP K9YFK1
T	99	SER	-	expression tag	UNP K9YFK1
T	100	HIS	-	expression tag	UNP K9YFK1
T	101	PRO	-	expression tag	UNP K9YFK1
T	102	GLN	-	expression tag	UNP K9YFK1
T	103	PHE	-	expression tag	UNP K9YFK1
T	104	GLU	-	expression tag	UNP K9YFK1
T	105	LYS	-	expression tag	UNP K9YFK1
X	96	GLY	-	expression tag	UNP K9YFK1

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Chain	Residue	Modelled	Actual	Comment	Reference
X	97	SER	-	expression tag	UNP K9YFK1
X	98	TRP	-	expression tag	UNP K9YFK1
X	99	SER	-	expression tag	UNP K9YFK1
X	100	HIS	-	expression tag	UNP K9YFK1
X	101	PRO	-	expression tag	UNP K9YFK1
X	102	GLN	-	expression tag	UNP K9YFK1
X	103	PHE	-	expression tag	UNP K9YFK1
X	104	GLU	-	expression tag	UNP K9YFK1
X	105	LYS	-	expression tag	UNP K9YFK1
1	96	GLY	-	expression tag	UNP K9YFK1
1	97	SER	-	expression tag	UNP K9YFK1
1	98	TRP	-	expression tag	UNP K9YFK1
1	99	SER	-	expression tag	UNP K9YFK1
1	100	HIS	-	expression tag	UNP K9YFK1
1	101	PRO	-	expression tag	UNP K9YFK1
1	102	GLN	-	expression tag	UNP K9YFK1
1	103	PHE	-	expression tag	UNP K9YFK1
1	104	GLU	-	expression tag	UNP K9YFK1
1	105	LYS	-	expression tag	UNP K9YFK1
5	96	GLY	-	expression tag	UNP K9YFK1
5	97	SER	-	expression tag	UNP K9YFK1
5	98	TRP	-	expression tag	UNP K9YFK1
5	99	SER	-	expression tag	UNP K9YFK1
5	100	HIS	-	expression tag	UNP K9YFK1
5	101	PRO	-	expression tag	UNP K9YFK1
5	102	GLN	-	expression tag	UNP K9YFK1
5	103	PHE	-	expression tag	UNP K9YFK1
5	104	GLU	-	expression tag	UNP K9YFK1
5	105	LYS	-	expression tag	UNP K9YFK1
9	96	GLY	-	expression tag	UNP K9YFK1
9	97	SER	-	expression tag	UNP K9YFK1
9	98	TRP	-	expression tag	UNP K9YFK1
9	99	SER	-	expression tag	UNP K9YFK1
9	100	HIS	-	expression tag	UNP K9YFK1
9	101	PRO	-	expression tag	UNP K9YFK1
9	102	GLN	-	expression tag	UNP K9YFK1
9	103	PHE	-	expression tag	UNP K9YFK1
9	104	GLU	-	expression tag	UNP K9YFK1
9	105	LYS	-	expression tag	UNP K9YFK1
d	96	GLY	-	expression tag	UNP K9YFK1
d	97	SER	-	expression tag	UNP K9YFK1
d	98	TRP	-	expression tag	UNP K9YFK1

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Chain	Residue	Modelled	Actual	Comment	Reference
d	99	SER	-	expression tag	UNP K9YFK1
d	100	HIS	-	expression tag	UNP K9YFK1
d	101	PRO	-	expression tag	UNP K9YFK1
d	102	GLN	-	expression tag	UNP K9YFK1
d	103	PHE	-	expression tag	UNP K9YFK1
d	104	GLU	-	expression tag	UNP K9YFK1
d	105	LYS	-	expression tag	UNP K9YFK1
h	96	GLY	-	expression tag	UNP K9YFK1
h	97	SER	-	expression tag	UNP K9YFK1
h	98	TRP	-	expression tag	UNP K9YFK1
h	99	SER	-	expression tag	UNP K9YFK1
h	100	HIS	-	expression tag	UNP K9YFK1
h	101	PRO	-	expression tag	UNP K9YFK1
h	102	GLN	-	expression tag	UNP K9YFK1
h	103	PHE	-	expression tag	UNP K9YFK1
h	104	GLU	-	expression tag	UNP K9YFK1
h	105	LYS	-	expression tag	UNP K9YFK1
l	96	GLY	-	expression tag	UNP K9YFK1
l	97	SER	-	expression tag	UNP K9YFK1
l	98	TRP	-	expression tag	UNP K9YFK1
l	99	SER	-	expression tag	UNP K9YFK1
l	100	HIS	-	expression tag	UNP K9YFK1
l	101	PRO	-	expression tag	UNP K9YFK1
l	102	GLN	-	expression tag	UNP K9YFK1
l	103	PHE	-	expression tag	UNP K9YFK1
l	104	GLU	-	expression tag	UNP K9YFK1
l	105	LYS	-	expression tag	UNP K9YFK1
p	96	GLY	-	expression tag	UNP K9YFK1
p	97	SER	-	expression tag	UNP K9YFK1
p	98	TRP	-	expression tag	UNP K9YFK1
p	99	SER	-	expression tag	UNP K9YFK1
p	100	HIS	-	expression tag	UNP K9YFK1
p	101	PRO	-	expression tag	UNP K9YFK1
p	102	GLN	-	expression tag	UNP K9YFK1
p	103	PHE	-	expression tag	UNP K9YFK1
p	104	GLU	-	expression tag	UNP K9YFK1
p	105	LYS	-	expression tag	UNP K9YFK1
t	96	GLY	-	expression tag	UNP K9YFK1
t	97	SER	-	expression tag	UNP K9YFK1
t	98	TRP	-	expression tag	UNP K9YFK1
t	99	SER	-	expression tag	UNP K9YFK1
t	100	HIS	-	expression tag	UNP K9YFK1

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Chain	Residue	Modelled	Actual	Comment	Reference
t	101	PRO	-	expression tag	UNP K9YFK1
t	102	GLN	-	expression tag	UNP K9YFK1
t	103	PHE	-	expression tag	UNP K9YFK1
t	104	GLU	-	expression tag	UNP K9YFK1
t	105	LYS	-	expression tag	UNP K9YFK1
x	96	GLY	-	expression tag	UNP K9YFK1
x	97	SER	-	expression tag	UNP K9YFK1
x	98	TRP	-	expression tag	UNP K9YFK1
x	99	SER	-	expression tag	UNP K9YFK1
x	100	HIS	-	expression tag	UNP K9YFK1
x	101	PRO	-	expression tag	UNP K9YFK1
x	102	GLN	-	expression tag	UNP K9YFK1
x	103	PHE	-	expression tag	UNP K9YFK1
x	104	GLU	-	expression tag	UNP K9YFK1
x	105	LYS	-	expression tag	UNP K9YFK1
AB	96	GLY	-	expression tag	UNP K9YFK1
AB	97	SER	-	expression tag	UNP K9YFK1
AB	98	TRP	-	expression tag	UNP K9YFK1
AB	99	SER	-	expression tag	UNP K9YFK1
AB	100	HIS	-	expression tag	UNP K9YFK1
AB	101	PRO	-	expression tag	UNP K9YFK1
AB	102	GLN	-	expression tag	UNP K9YFK1
AB	103	PHE	-	expression tag	UNP K9YFK1
AB	104	GLU	-	expression tag	UNP K9YFK1
AB	105	LYS	-	expression tag	UNP K9YFK1
AF	96	GLY	-	expression tag	UNP K9YFK1
AF	97	SER	-	expression tag	UNP K9YFK1
AF	98	TRP	-	expression tag	UNP K9YFK1
AF	99	SER	-	expression tag	UNP K9YFK1
AF	100	HIS	-	expression tag	UNP K9YFK1
AF	101	PRO	-	expression tag	UNP K9YFK1
AF	102	GLN	-	expression tag	UNP K9YFK1
AF	103	PHE	-	expression tag	UNP K9YFK1
AF	104	GLU	-	expression tag	UNP K9YFK1
AF	105	LYS	-	expression tag	UNP K9YFK1
AJ	96	GLY	-	expression tag	UNP K9YFK1
AJ	97	SER	-	expression tag	UNP K9YFK1
AJ	98	TRP	-	expression tag	UNP K9YFK1
AJ	99	SER	-	expression tag	UNP K9YFK1
AJ	100	HIS	-	expression tag	UNP K9YFK1
AJ	101	PRO	-	expression tag	UNP K9YFK1
AJ	102	GLN	-	expression tag	UNP K9YFK1

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Chain	Residue	Modelled	Actual	Comment	Reference
AJ	103	PHE	-	expression tag	UNP K9YFK1
AJ	104	GLU	-	expression tag	UNP K9YFK1
AJ	105	LYS	-	expression tag	UNP K9YFK1
AN	96	GLY	-	expression tag	UNP K9YFK1
AN	97	SER	-	expression tag	UNP K9YFK1
AN	98	TRP	-	expression tag	UNP K9YFK1
AN	99	SER	-	expression tag	UNP K9YFK1
AN	100	HIS	-	expression tag	UNP K9YFK1
AN	101	PRO	-	expression tag	UNP K9YFK1
AN	102	GLN	-	expression tag	UNP K9YFK1
AN	103	PHE	-	expression tag	UNP K9YFK1
AN	104	GLU	-	expression tag	UNP K9YFK1
AN	105	LYS	-	expression tag	UNP K9YFK1
AR	96	GLY	-	expression tag	UNP K9YFK1
AR	97	SER	-	expression tag	UNP K9YFK1
AR	98	TRP	-	expression tag	UNP K9YFK1
AR	99	SER	-	expression tag	UNP K9YFK1
AR	100	HIS	-	expression tag	UNP K9YFK1
AR	101	PRO	-	expression tag	UNP K9YFK1
AR	102	GLN	-	expression tag	UNP K9YFK1
AR	103	PHE	-	expression tag	UNP K9YFK1
AR	104	GLU	-	expression tag	UNP K9YFK1
AR	105	LYS	-	expression tag	UNP K9YFK1
AV	96	GLY	-	expression tag	UNP K9YFK1
AV	97	SER	-	expression tag	UNP K9YFK1
AV	98	TRP	-	expression tag	UNP K9YFK1
AV	99	SER	-	expression tag	UNP K9YFK1
AV	100	HIS	-	expression tag	UNP K9YFK1
AV	101	PRO	-	expression tag	UNP K9YFK1
AV	102	GLN	-	expression tag	UNP K9YFK1
AV	103	PHE	-	expression tag	UNP K9YFK1
AV	104	GLU	-	expression tag	UNP K9YFK1
AV	105	LYS	-	expression tag	UNP K9YFK1
AZ	96	GLY	-	expression tag	UNP K9YFK1
AZ	97	SER	-	expression tag	UNP K9YFK1
AZ	98	TRP	-	expression tag	UNP K9YFK1
AZ	99	SER	-	expression tag	UNP K9YFK1
AZ	100	HIS	-	expression tag	UNP K9YFK1
AZ	101	PRO	-	expression tag	UNP K9YFK1
AZ	102	GLN	-	expression tag	UNP K9YFK1
AZ	103	PHE	-	expression tag	UNP K9YFK1
AZ	104	GLU	-	expression tag	UNP K9YFK1

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Chain	Residue	Modelled	Actual	Comment	Reference
AZ	105	LYS	-	expression tag	UNP K9YFK1
A3	96	GLY	-	expression tag	UNP K9YFK1
A3	97	SER	-	expression tag	UNP K9YFK1
A3	98	TRP	-	expression tag	UNP K9YFK1
A3	99	SER	-	expression tag	UNP K9YFK1
A3	100	HIS	-	expression tag	UNP K9YFK1
A3	101	PRO	-	expression tag	UNP K9YFK1
A3	102	GLN	-	expression tag	UNP K9YFK1
A3	103	PHE	-	expression tag	UNP K9YFK1
A3	104	GLU	-	expression tag	UNP K9YFK1
A3	105	LYS	-	expression tag	UNP K9YFK1
A7	96	GLY	-	expression tag	UNP K9YFK1
A7	97	SER	-	expression tag	UNP K9YFK1
A7	98	TRP	-	expression tag	UNP K9YFK1
A7	99	SER	-	expression tag	UNP K9YFK1
A7	100	HIS	-	expression tag	UNP K9YFK1
A7	101	PRO	-	expression tag	UNP K9YFK1
A7	102	GLN	-	expression tag	UNP K9YFK1
A7	103	PHE	-	expression tag	UNP K9YFK1
A7	104	GLU	-	expression tag	UNP K9YFK1
A7	105	LYS	-	expression tag	UNP K9YFK1
BB	96	GLY	-	expression tag	UNP K9YFK1
BB	97	SER	-	expression tag	UNP K9YFK1
BB	98	TRP	-	expression tag	UNP K9YFK1
BB	99	SER	-	expression tag	UNP K9YFK1
BB	100	HIS	-	expression tag	UNP K9YFK1
BB	101	PRO	-	expression tag	UNP K9YFK1
BB	102	GLN	-	expression tag	UNP K9YFK1
BB	103	PHE	-	expression tag	UNP K9YFK1
BB	104	GLU	-	expression tag	UNP K9YFK1
BB	105	LYS	-	expression tag	UNP K9YFK1
BF	96	GLY	-	expression tag	UNP K9YFK1
BF	97	SER	-	expression tag	UNP K9YFK1
BF	98	TRP	-	expression tag	UNP K9YFK1
BF	99	SER	-	expression tag	UNP K9YFK1
BF	100	HIS	-	expression tag	UNP K9YFK1
BF	101	PRO	-	expression tag	UNP K9YFK1
BF	102	GLN	-	expression tag	UNP K9YFK1
BF	103	PHE	-	expression tag	UNP K9YFK1
BF	104	GLU	-	expression tag	UNP K9YFK1
BF	105	LYS	-	expression tag	UNP K9YFK1
BJ	96	GLY	-	expression tag	UNP K9YFK1

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Chain	Residue	Modelled	Actual	Comment	Reference
BJ	97	SER	-	expression tag	UNP K9YFK1
BJ	98	TRP	-	expression tag	UNP K9YFK1
BJ	99	SER	-	expression tag	UNP K9YFK1
BJ	100	HIS	-	expression tag	UNP K9YFK1
BJ	101	PRO	-	expression tag	UNP K9YFK1
BJ	102	GLN	-	expression tag	UNP K9YFK1
BJ	103	PHE	-	expression tag	UNP K9YFK1
BJ	104	GLU	-	expression tag	UNP K9YFK1
BJ	105	LYS	-	expression tag	UNP K9YFK1
BN	96	GLY	-	expression tag	UNP K9YFK1
BN	97	SER	-	expression tag	UNP K9YFK1
BN	98	TRP	-	expression tag	UNP K9YFK1
BN	99	SER	-	expression tag	UNP K9YFK1
BN	100	HIS	-	expression tag	UNP K9YFK1
BN	101	PRO	-	expression tag	UNP K9YFK1
BN	102	GLN	-	expression tag	UNP K9YFK1
BN	103	PHE	-	expression tag	UNP K9YFK1
BN	104	GLU	-	expression tag	UNP K9YFK1
BN	105	LYS	-	expression tag	UNP K9YFK1
BR	96	GLY	-	expression tag	UNP K9YFK1
BR	97	SER	-	expression tag	UNP K9YFK1
BR	98	TRP	-	expression tag	UNP K9YFK1
BR	99	SER	-	expression tag	UNP K9YFK1
BR	100	HIS	-	expression tag	UNP K9YFK1
BR	101	PRO	-	expression tag	UNP K9YFK1
BR	102	GLN	-	expression tag	UNP K9YFK1
BR	103	PHE	-	expression tag	UNP K9YFK1
BR	104	GLU	-	expression tag	UNP K9YFK1
BR	105	LYS	-	expression tag	UNP K9YFK1
BV	96	GLY	-	expression tag	UNP K9YFK1
BV	97	SER	-	expression tag	UNP K9YFK1
BV	98	TRP	-	expression tag	UNP K9YFK1
BV	99	SER	-	expression tag	UNP K9YFK1
BV	100	HIS	-	expression tag	UNP K9YFK1
BV	101	PRO	-	expression tag	UNP K9YFK1
BV	102	GLN	-	expression tag	UNP K9YFK1
BV	103	PHE	-	expression tag	UNP K9YFK1
BV	104	GLU	-	expression tag	UNP K9YFK1
BV	105	LYS	-	expression tag	UNP K9YFK1
BZ	96	GLY	-	expression tag	UNP K9YFK1
BZ	97	SER	-	expression tag	UNP K9YFK1
BZ	98	TRP	-	expression tag	UNP K9YFK1

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Chain	Residue	Modelled	Actual	Comment	Reference
BZ	99	SER	-	expression tag	UNP K9YFK1
BZ	100	HIS	-	expression tag	UNP K9YFK1
BZ	101	PRO	-	expression tag	UNP K9YFK1
BZ	102	GLN	-	expression tag	UNP K9YFK1
BZ	103	PHE	-	expression tag	UNP K9YFK1
BZ	104	GLU	-	expression tag	UNP K9YFK1
BZ	105	LYS	-	expression tag	UNP K9YFK1
B3	96	GLY	-	expression tag	UNP K9YFK1
B3	97	SER	-	expression tag	UNP K9YFK1
B3	98	TRP	-	expression tag	UNP K9YFK1
B3	99	SER	-	expression tag	UNP K9YFK1
B3	100	HIS	-	expression tag	UNP K9YFK1
B3	101	PRO	-	expression tag	UNP K9YFK1
B3	102	GLN	-	expression tag	UNP K9YFK1
B3	103	PHE	-	expression tag	UNP K9YFK1
B3	104	GLU	-	expression tag	UNP K9YFK1
B3	105	LYS	-	expression tag	UNP K9YFK1
B7	96	GLY	-	expression tag	UNP K9YFK1
B7	97	SER	-	expression tag	UNP K9YFK1
B7	98	TRP	-	expression tag	UNP K9YFK1
B7	99	SER	-	expression tag	UNP K9YFK1
B7	100	HIS	-	expression tag	UNP K9YFK1
B7	101	PRO	-	expression tag	UNP K9YFK1
B7	102	GLN	-	expression tag	UNP K9YFK1
B7	103	PHE	-	expression tag	UNP K9YFK1
B7	104	GLU	-	expression tag	UNP K9YFK1
B7	105	LYS	-	expression tag	UNP K9YFK1
CB	96	GLY	-	expression tag	UNP K9YFK1
CB	97	SER	-	expression tag	UNP K9YFK1
CB	98	TRP	-	expression tag	UNP K9YFK1
CB	99	SER	-	expression tag	UNP K9YFK1
CB	100	HIS	-	expression tag	UNP K9YFK1
CB	101	PRO	-	expression tag	UNP K9YFK1
CB	102	GLN	-	expression tag	UNP K9YFK1
CB	103	PHE	-	expression tag	UNP K9YFK1
CB	104	GLU	-	expression tag	UNP K9YFK1
CB	105	LYS	-	expression tag	UNP K9YFK1
CF	96	GLY	-	expression tag	UNP K9YFK1
CF	97	SER	-	expression tag	UNP K9YFK1
CF	98	TRP	-	expression tag	UNP K9YFK1
CF	99	SER	-	expression tag	UNP K9YFK1
CF	100	HIS	-	expression tag	UNP K9YFK1

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Chain	Residue	Modelled	Actual	Comment	Reference
CF	101	PRO	-	expression tag	UNP K9YFK1
CF	102	GLN	-	expression tag	UNP K9YFK1
CF	103	PHE	-	expression tag	UNP K9YFK1
CF	104	GLU	-	expression tag	UNP K9YFK1
CF	105	LYS	-	expression tag	UNP K9YFK1
CJ	96	GLY	-	expression tag	UNP K9YFK1
CJ	97	SER	-	expression tag	UNP K9YFK1
CJ	98	TRP	-	expression tag	UNP K9YFK1
CJ	99	SER	-	expression tag	UNP K9YFK1
CJ	100	HIS	-	expression tag	UNP K9YFK1
CJ	101	PRO	-	expression tag	UNP K9YFK1
CJ	102	GLN	-	expression tag	UNP K9YFK1
CJ	103	PHE	-	expression tag	UNP K9YFK1
CJ	104	GLU	-	expression tag	UNP K9YFK1
CJ	105	LYS	-	expression tag	UNP K9YFK1
CN	96	GLY	-	expression tag	UNP K9YFK1
CN	97	SER	-	expression tag	UNP K9YFK1
CN	98	TRP	-	expression tag	UNP K9YFK1
CN	99	SER	-	expression tag	UNP K9YFK1
CN	100	HIS	-	expression tag	UNP K9YFK1
CN	101	PRO	-	expression tag	UNP K9YFK1
CN	102	GLN	-	expression tag	UNP K9YFK1
CN	103	PHE	-	expression tag	UNP K9YFK1
CN	104	GLU	-	expression tag	UNP K9YFK1
CN	105	LYS	-	expression tag	UNP K9YFK1
CR	96	GLY	-	expression tag	UNP K9YFK1
CR	97	SER	-	expression tag	UNP K9YFK1
CR	98	TRP	-	expression tag	UNP K9YFK1
CR	99	SER	-	expression tag	UNP K9YFK1
CR	100	HIS	-	expression tag	UNP K9YFK1
CR	101	PRO	-	expression tag	UNP K9YFK1
CR	102	GLN	-	expression tag	UNP K9YFK1
CR	103	PHE	-	expression tag	UNP K9YFK1
CR	104	GLU	-	expression tag	UNP K9YFK1
CR	105	LYS	-	expression tag	UNP K9YFK1
CV	96	GLY	-	expression tag	UNP K9YFK1
CV	97	SER	-	expression tag	UNP K9YFK1
CV	98	TRP	-	expression tag	UNP K9YFK1
CV	99	SER	-	expression tag	UNP K9YFK1
CV	100	HIS	-	expression tag	UNP K9YFK1
CV	101	PRO	-	expression tag	UNP K9YFK1
CV	102	GLN	-	expression tag	UNP K9YFK1

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Chain	Residue	Modelled	Actual	Comment	Reference
CV	103	PHE	-	expression tag	UNP K9YFK1
CV	104	GLU	-	expression tag	UNP K9YFK1
CV	105	LYS	-	expression tag	UNP K9YFK1
CZ	96	GLY	-	expression tag	UNP K9YFK1
CZ	97	SER	-	expression tag	UNP K9YFK1
CZ	98	TRP	-	expression tag	UNP K9YFK1
CZ	99	SER	-	expression tag	UNP K9YFK1
CZ	100	HIS	-	expression tag	UNP K9YFK1
CZ	101	PRO	-	expression tag	UNP K9YFK1
CZ	102	GLN	-	expression tag	UNP K9YFK1
CZ	103	PHE	-	expression tag	UNP K9YFK1
CZ	104	GLU	-	expression tag	UNP K9YFK1
CZ	105	LYS	-	expression tag	UNP K9YFK1
C3	96	GLY	-	expression tag	UNP K9YFK1
C3	97	SER	-	expression tag	UNP K9YFK1
C3	98	TRP	-	expression tag	UNP K9YFK1
C3	99	SER	-	expression tag	UNP K9YFK1
C3	100	HIS	-	expression tag	UNP K9YFK1
C3	101	PRO	-	expression tag	UNP K9YFK1
C3	102	GLN	-	expression tag	UNP K9YFK1
C3	103	PHE	-	expression tag	UNP K9YFK1
C3	104	GLU	-	expression tag	UNP K9YFK1
C3	105	LYS	-	expression tag	UNP K9YFK1
C7	96	GLY	-	expression tag	UNP K9YFK1
C7	97	SER	-	expression tag	UNP K9YFK1
C7	98	TRP	-	expression tag	UNP K9YFK1
C7	99	SER	-	expression tag	UNP K9YFK1
C7	100	HIS	-	expression tag	UNP K9YFK1
C7	101	PRO	-	expression tag	UNP K9YFK1
C7	102	GLN	-	expression tag	UNP K9YFK1
C7	103	PHE	-	expression tag	UNP K9YFK1
C7	104	GLU	-	expression tag	UNP K9YFK1
C7	105	LYS	-	expression tag	UNP K9YFK1
DB	96	GLY	-	expression tag	UNP K9YFK1
DB	97	SER	-	expression tag	UNP K9YFK1
DB	98	TRP	-	expression tag	UNP K9YFK1
DB	99	SER	-	expression tag	UNP K9YFK1
DB	100	HIS	-	expression tag	UNP K9YFK1
DB	101	PRO	-	expression tag	UNP K9YFK1
DB	102	GLN	-	expression tag	UNP K9YFK1
DB	103	PHE	-	expression tag	UNP K9YFK1
DB	104	GLU	-	expression tag	UNP K9YFK1

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Chain	Residue	Modelled	Actual	Comment	Reference
DB	105	LYS	-	expression tag	UNP K9YFK1
DF	96	GLY	-	expression tag	UNP K9YFK1
DF	97	SER	-	expression tag	UNP K9YFK1
DF	98	TRP	-	expression tag	UNP K9YFK1
DF	99	SER	-	expression tag	UNP K9YFK1
DF	100	HIS	-	expression tag	UNP K9YFK1
DF	101	PRO	-	expression tag	UNP K9YFK1
DF	102	GLN	-	expression tag	UNP K9YFK1
DF	103	PHE	-	expression tag	UNP K9YFK1
DF	104	GLU	-	expression tag	UNP K9YFK1
DF	105	LYS	-	expression tag	UNP K9YFK1
DJ	96	GLY	-	expression tag	UNP K9YFK1
DJ	97	SER	-	expression tag	UNP K9YFK1
DJ	98	TRP	-	expression tag	UNP K9YFK1
DJ	99	SER	-	expression tag	UNP K9YFK1
DJ	100	HIS	-	expression tag	UNP K9YFK1
DJ	101	PRO	-	expression tag	UNP K9YFK1
DJ	102	GLN	-	expression tag	UNP K9YFK1
DJ	103	PHE	-	expression tag	UNP K9YFK1
DJ	104	GLU	-	expression tag	UNP K9YFK1
DJ	105	LYS	-	expression tag	UNP K9YFK1
DN	96	GLY	-	expression tag	UNP K9YFK1
DN	97	SER	-	expression tag	UNP K9YFK1
DN	98	TRP	-	expression tag	UNP K9YFK1
DN	99	SER	-	expression tag	UNP K9YFK1
DN	100	HIS	-	expression tag	UNP K9YFK1
DN	101	PRO	-	expression tag	UNP K9YFK1
DN	102	GLN	-	expression tag	UNP K9YFK1
DN	103	PHE	-	expression tag	UNP K9YFK1
DN	104	GLU	-	expression tag	UNP K9YFK1
DN	105	LYS	-	expression tag	UNP K9YFK1
DR	96	GLY	-	expression tag	UNP K9YFK1
DR	97	SER	-	expression tag	UNP K9YFK1
DR	98	TRP	-	expression tag	UNP K9YFK1
DR	99	SER	-	expression tag	UNP K9YFK1
DR	100	HIS	-	expression tag	UNP K9YFK1
DR	101	PRO	-	expression tag	UNP K9YFK1
DR	102	GLN	-	expression tag	UNP K9YFK1
DR	103	PHE	-	expression tag	UNP K9YFK1
DR	104	GLU	-	expression tag	UNP K9YFK1
DR	105	LYS	-	expression tag	UNP K9YFK1
DV	96	GLY	-	expression tag	UNP K9YFK1

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Chain	Residue	Modelled	Actual	Comment	Reference
DV	97	SER	-	expression tag	UNP K9YFK1
DV	98	TRP	-	expression tag	UNP K9YFK1
DV	99	SER	-	expression tag	UNP K9YFK1
DV	100	HIS	-	expression tag	UNP K9YFK1
DV	101	PRO	-	expression tag	UNP K9YFK1
DV	102	GLN	-	expression tag	UNP K9YFK1
DV	103	PHE	-	expression tag	UNP K9YFK1
DV	104	GLU	-	expression tag	UNP K9YFK1
DV	105	LYS	-	expression tag	UNP K9YFK1
DZ	96	GLY	-	expression tag	UNP K9YFK1
DZ	97	SER	-	expression tag	UNP K9YFK1
DZ	98	TRP	-	expression tag	UNP K9YFK1
DZ	99	SER	-	expression tag	UNP K9YFK1
DZ	100	HIS	-	expression tag	UNP K9YFK1
DZ	101	PRO	-	expression tag	UNP K9YFK1
DZ	102	GLN	-	expression tag	UNP K9YFK1
DZ	103	PHE	-	expression tag	UNP K9YFK1
DZ	104	GLU	-	expression tag	UNP K9YFK1
DZ	105	LYS	-	expression tag	UNP K9YFK1
D3	96	GLY	-	expression tag	UNP K9YFK1
D3	97	SER	-	expression tag	UNP K9YFK1
D3	98	TRP	-	expression tag	UNP K9YFK1
D3	99	SER	-	expression tag	UNP K9YFK1
D3	100	HIS	-	expression tag	UNP K9YFK1
D3	101	PRO	-	expression tag	UNP K9YFK1
D3	102	GLN	-	expression tag	UNP K9YFK1
D3	103	PHE	-	expression tag	UNP K9YFK1
D3	104	GLU	-	expression tag	UNP K9YFK1
D3	105	LYS	-	expression tag	UNP K9YFK1
D7	96	GLY	-	expression tag	UNP K9YFK1
D7	97	SER	-	expression tag	UNP K9YFK1
D7	98	TRP	-	expression tag	UNP K9YFK1
D7	99	SER	-	expression tag	UNP K9YFK1
D7	100	HIS	-	expression tag	UNP K9YFK1
D7	101	PRO	-	expression tag	UNP K9YFK1
D7	102	GLN	-	expression tag	UNP K9YFK1
D7	103	PHE	-	expression tag	UNP K9YFK1
D7	104	GLU	-	expression tag	UNP K9YFK1
D7	105	LYS	-	expression tag	UNP K9YFK1
EB	96	GLY	-	expression tag	UNP K9YFK1
EB	97	SER	-	expression tag	UNP K9YFK1
EB	98	TRP	-	expression tag	UNP K9YFK1

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Chain	Residue	Modelled	Actual	Comment	Reference
EB	99	SER	-	expression tag	UNP K9YFK1
EB	100	HIS	-	expression tag	UNP K9YFK1
EB	101	PRO	-	expression tag	UNP K9YFK1
EB	102	GLN	-	expression tag	UNP K9YFK1
EB	103	PHE	-	expression tag	UNP K9YFK1
EB	104	GLU	-	expression tag	UNP K9YFK1
EB	105	LYS	-	expression tag	UNP K9YFK1
EF	96	GLY	-	expression tag	UNP K9YFK1
EF	97	SER	-	expression tag	UNP K9YFK1
EF	98	TRP	-	expression tag	UNP K9YFK1
EF	99	SER	-	expression tag	UNP K9YFK1
EF	100	HIS	-	expression tag	UNP K9YFK1
EF	101	PRO	-	expression tag	UNP K9YFK1
EF	102	GLN	-	expression tag	UNP K9YFK1
EF	103	PHE	-	expression tag	UNP K9YFK1
EF	104	GLU	-	expression tag	UNP K9YFK1
EF	105	LYS	-	expression tag	UNP K9YFK1
EJ	96	GLY	-	expression tag	UNP K9YFK1
EJ	97	SER	-	expression tag	UNP K9YFK1
EJ	98	TRP	-	expression tag	UNP K9YFK1
EJ	99	SER	-	expression tag	UNP K9YFK1
EJ	100	HIS	-	expression tag	UNP K9YFK1
EJ	101	PRO	-	expression tag	UNP K9YFK1
EJ	102	GLN	-	expression tag	UNP K9YFK1
EJ	103	PHE	-	expression tag	UNP K9YFK1
EJ	104	GLU	-	expression tag	UNP K9YFK1
EJ	105	LYS	-	expression tag	UNP K9YFK1
EN	96	GLY	-	expression tag	UNP K9YFK1
EN	97	SER	-	expression tag	UNP K9YFK1
EN	98	TRP	-	expression tag	UNP K9YFK1
EN	99	SER	-	expression tag	UNP K9YFK1
EN	100	HIS	-	expression tag	UNP K9YFK1
EN	101	PRO	-	expression tag	UNP K9YFK1
EN	102	GLN	-	expression tag	UNP K9YFK1
EN	103	PHE	-	expression tag	UNP K9YFK1
EN	104	GLU	-	expression tag	UNP K9YFK1
EN	105	LYS	-	expression tag	UNP K9YFK1
ER	96	GLY	-	expression tag	UNP K9YFK1
ER	97	SER	-	expression tag	UNP K9YFK1
ER	98	TRP	-	expression tag	UNP K9YFK1
ER	99	SER	-	expression tag	UNP K9YFK1
ER	100	HIS	-	expression tag	UNP K9YFK1

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Chain	Residue	Modelled	Actual	Comment	Reference
ER	101	PRO	-	expression tag	UNP K9YFK1
ER	102	GLN	-	expression tag	UNP K9YFK1
ER	103	PHE	-	expression tag	UNP K9YFK1
ER	104	GLU	-	expression tag	UNP K9YFK1
ER	105	LYS	-	expression tag	UNP K9YFK1
EV	96	GLY	-	expression tag	UNP K9YFK1
EV	97	SER	-	expression tag	UNP K9YFK1
EV	98	TRP	-	expression tag	UNP K9YFK1
EV	99	SER	-	expression tag	UNP K9YFK1
EV	100	HIS	-	expression tag	UNP K9YFK1
EV	101	PRO	-	expression tag	UNP K9YFK1
EV	102	GLN	-	expression tag	UNP K9YFK1
EV	103	PHE	-	expression tag	UNP K9YFK1
EV	104	GLU	-	expression tag	UNP K9YFK1
EV	105	LYS	-	expression tag	UNP K9YFK1
EZ	96	GLY	-	expression tag	UNP K9YFK1
EZ	97	SER	-	expression tag	UNP K9YFK1
EZ	98	TRP	-	expression tag	UNP K9YFK1
EZ	99	SER	-	expression tag	UNP K9YFK1
EZ	100	HIS	-	expression tag	UNP K9YFK1
EZ	101	PRO	-	expression tag	UNP K9YFK1
EZ	102	GLN	-	expression tag	UNP K9YFK1
EZ	103	PHE	-	expression tag	UNP K9YFK1
EZ	104	GLU	-	expression tag	UNP K9YFK1
EZ	105	LYS	-	expression tag	UNP K9YFK1
E3	96	GLY	-	expression tag	UNP K9YFK1
E3	97	SER	-	expression tag	UNP K9YFK1
E3	98	TRP	-	expression tag	UNP K9YFK1
E3	99	SER	-	expression tag	UNP K9YFK1
E3	100	HIS	-	expression tag	UNP K9YFK1
E3	101	PRO	-	expression tag	UNP K9YFK1
E3	102	GLN	-	expression tag	UNP K9YFK1
E3	103	PHE	-	expression tag	UNP K9YFK1
E3	104	GLU	-	expression tag	UNP K9YFK1
E3	105	LYS	-	expression tag	UNP K9YFK1
E7	96	GLY	-	expression tag	UNP K9YFK1
E7	97	SER	-	expression tag	UNP K9YFK1
E7	98	TRP	-	expression tag	UNP K9YFK1
E7	99	SER	-	expression tag	UNP K9YFK1
E7	100	HIS	-	expression tag	UNP K9YFK1
E7	101	PRO	-	expression tag	UNP K9YFK1
E7	102	GLN	-	expression tag	UNP K9YFK1

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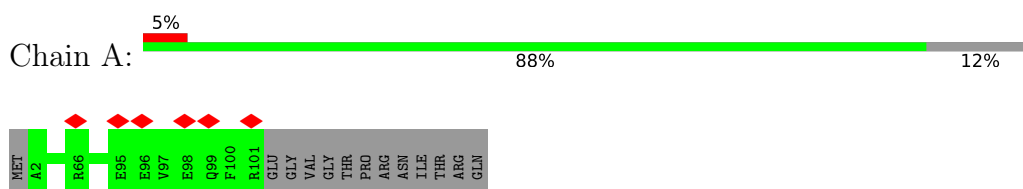
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Chain	Residue	Modelled	Actual	Comment	Reference
E7	103	PHE	-	expression tag	UNP K9YFK1
E7	104	GLU	-	expression tag	UNP K9YFK1
E7	105	LYS	-	expression tag	UNP K9YFK1

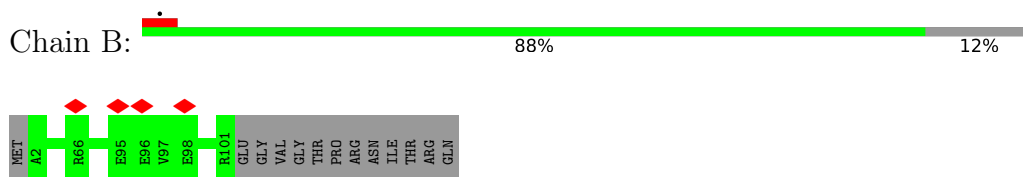
3 Residue-property plots [i](#)

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.

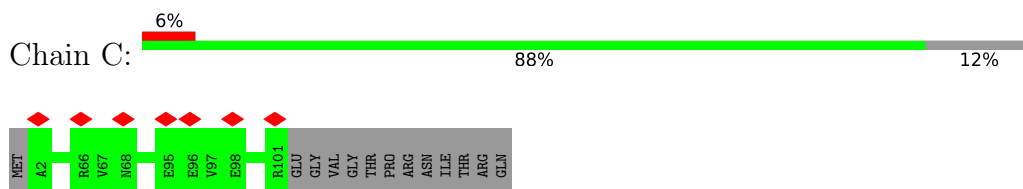
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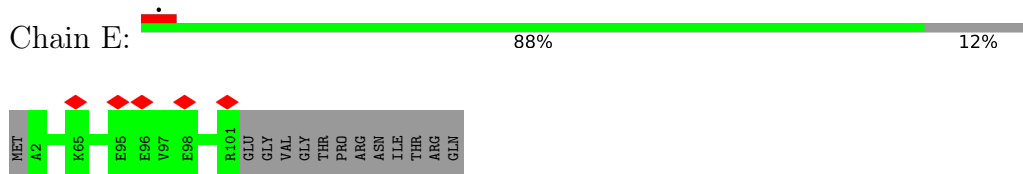
- Molecule 1: Microcompartments protein



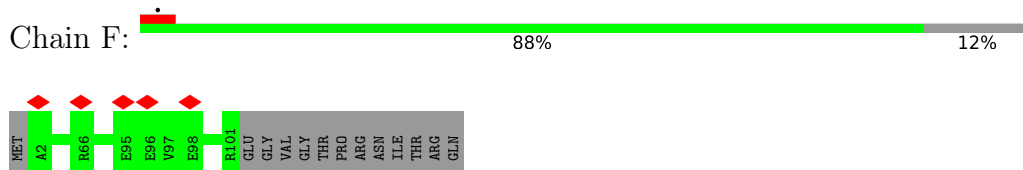
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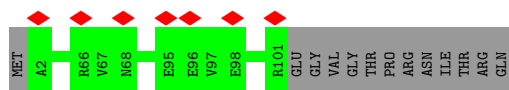
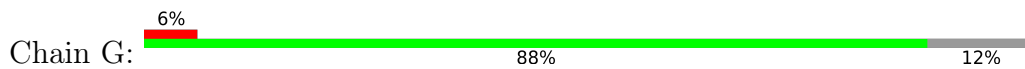
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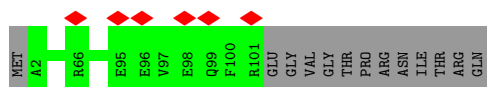
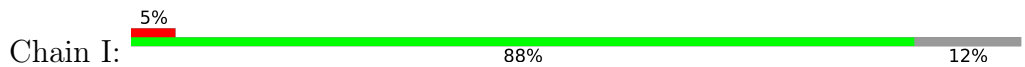
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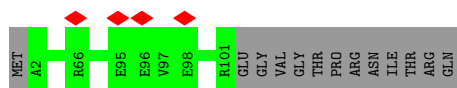
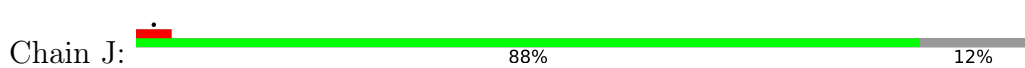
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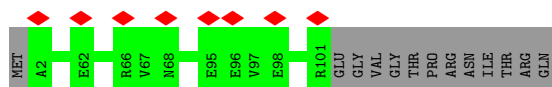
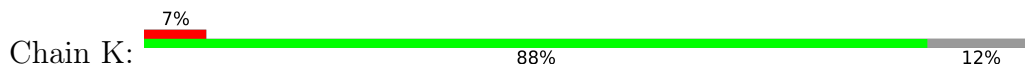
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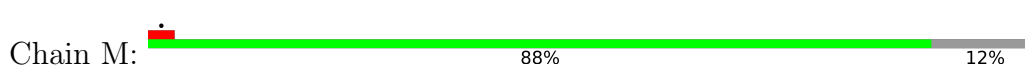
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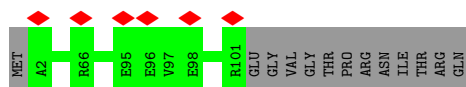
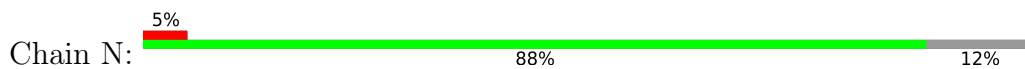
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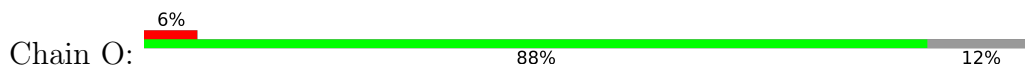
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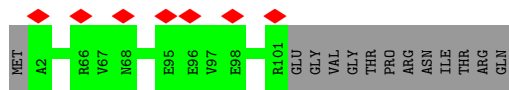


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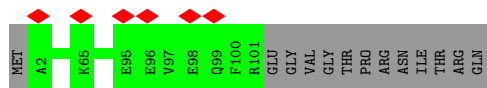
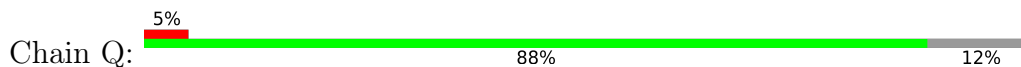


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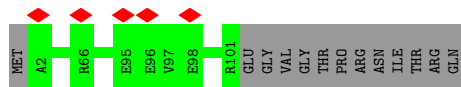
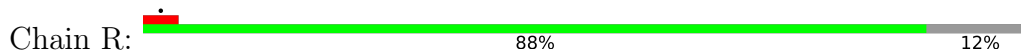




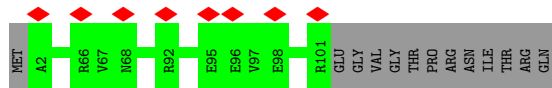
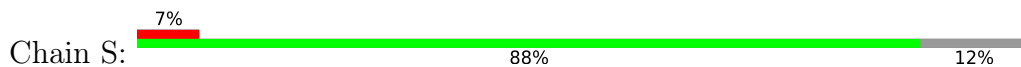
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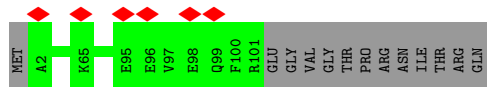
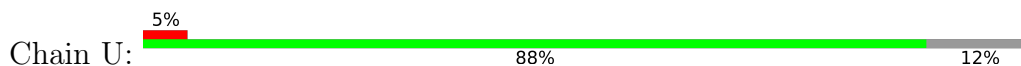
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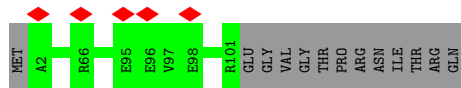
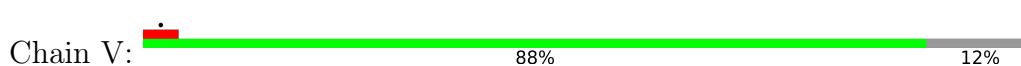
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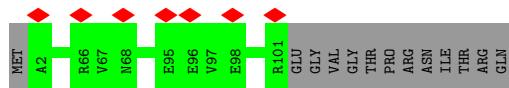
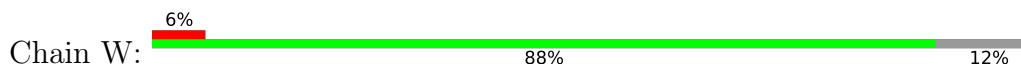
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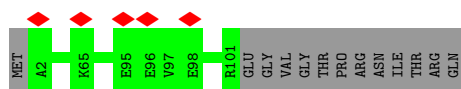
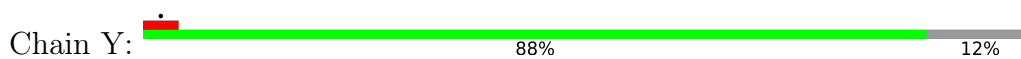
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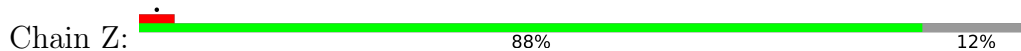
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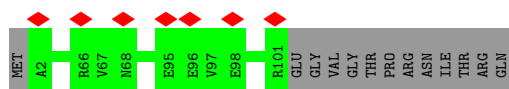
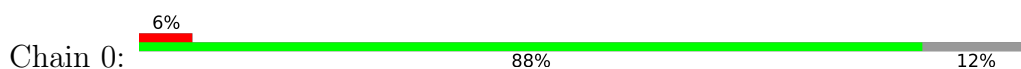
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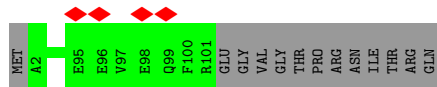
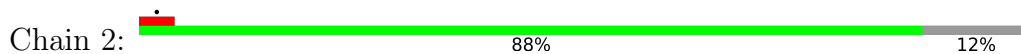
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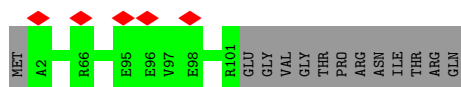
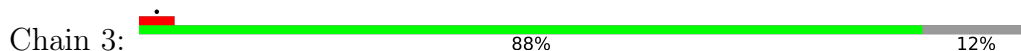
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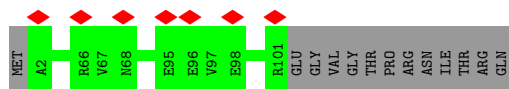
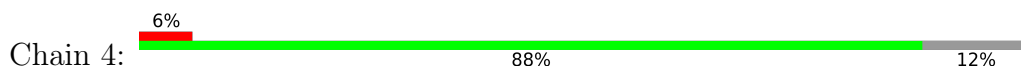
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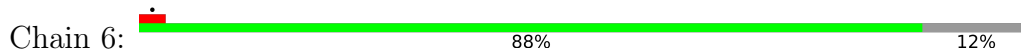
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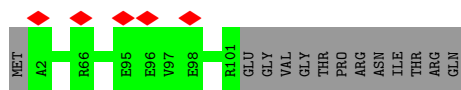
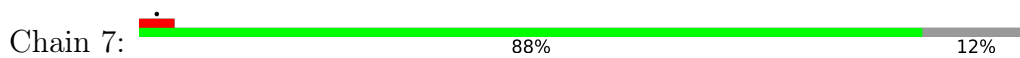
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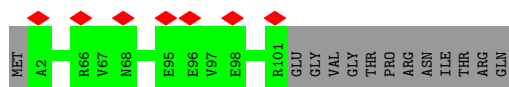
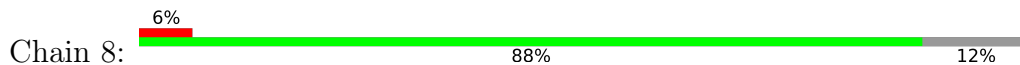
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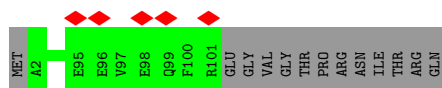
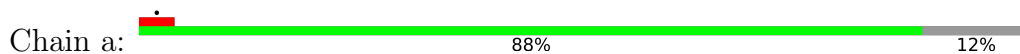
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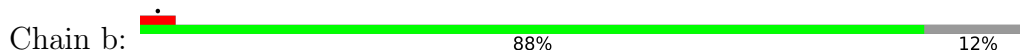
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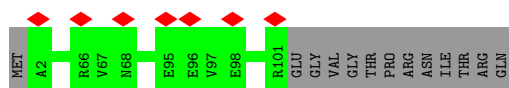
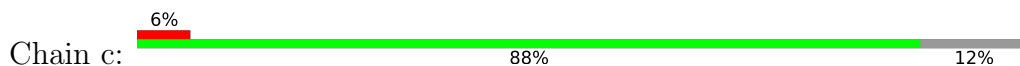
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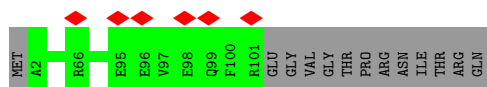
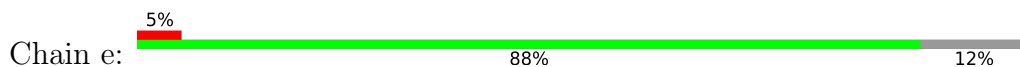
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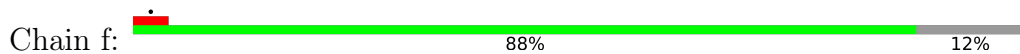
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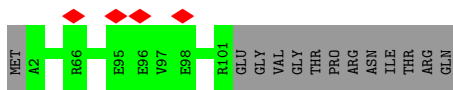


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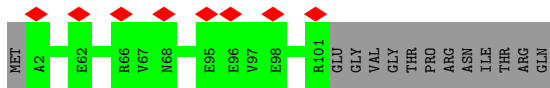
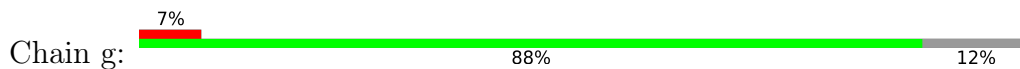


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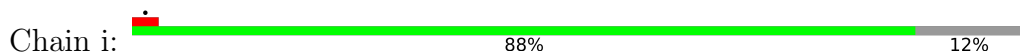




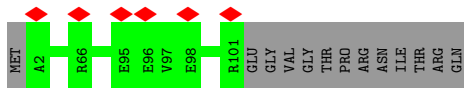
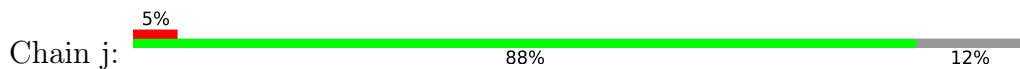
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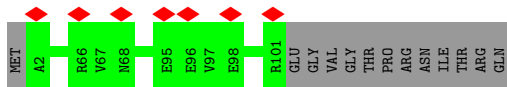
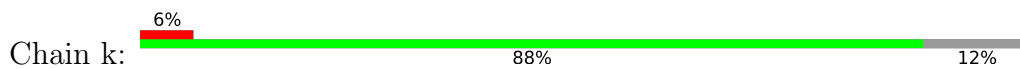
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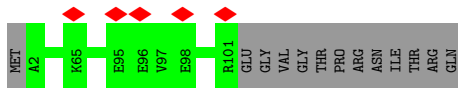
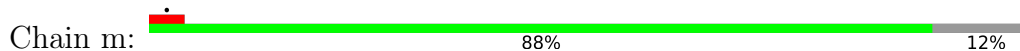
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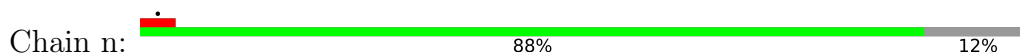
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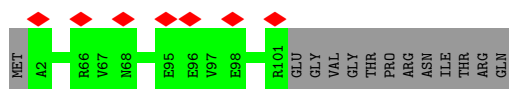
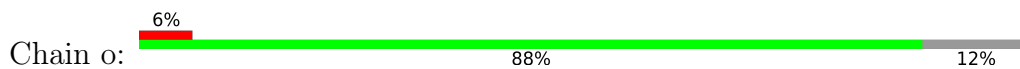
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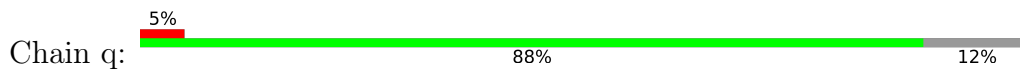
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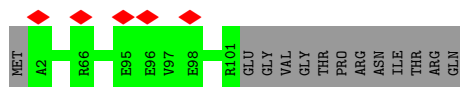
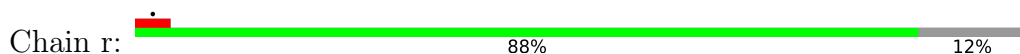
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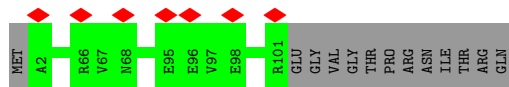
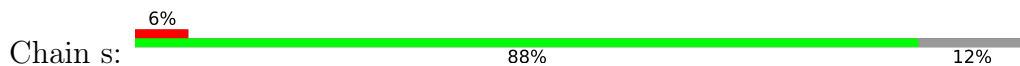
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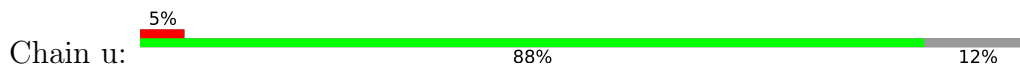
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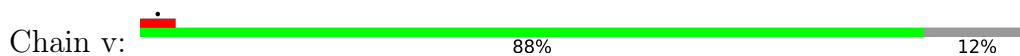
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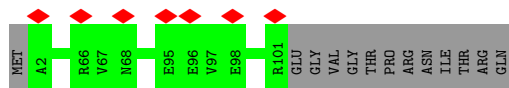
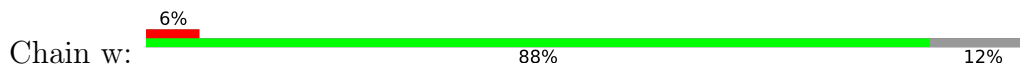
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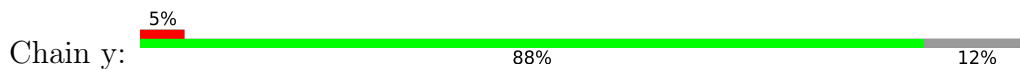
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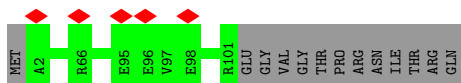
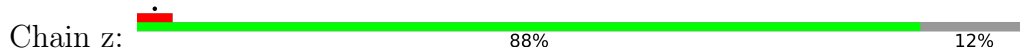
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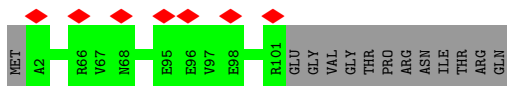
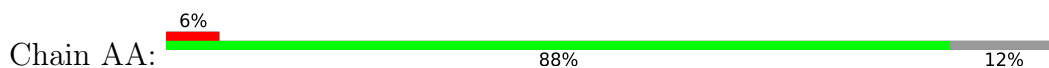
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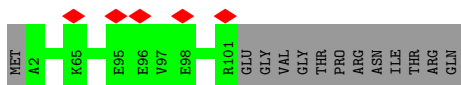
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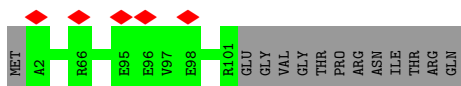
- Molecule 1: Microcompartments protein



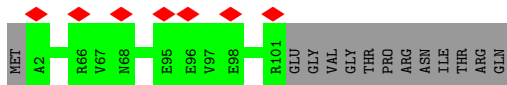
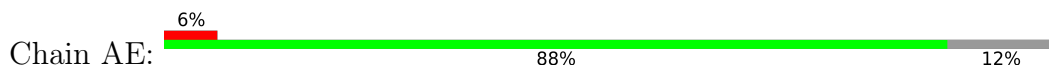
- Molecule 1: Microcompartments protein



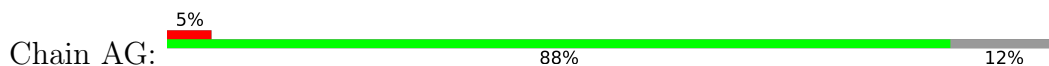
- Molecule 1: Microcompartments protein

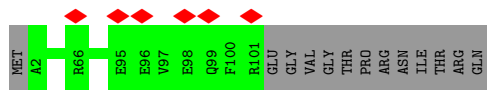


- Molecule 1: Microcompartments protein

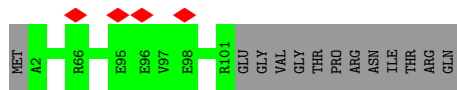
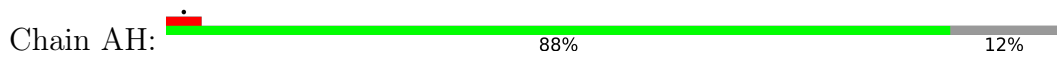


- Molecule 1: Microcompartments protein

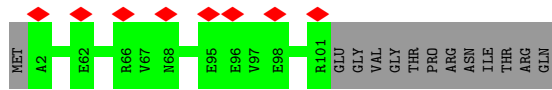
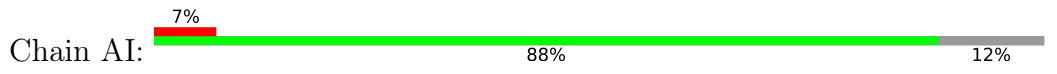




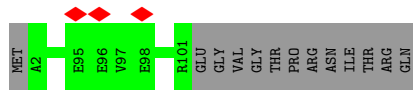
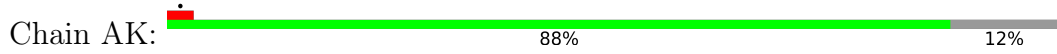
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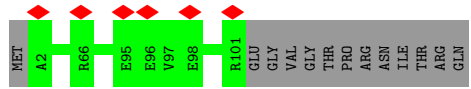
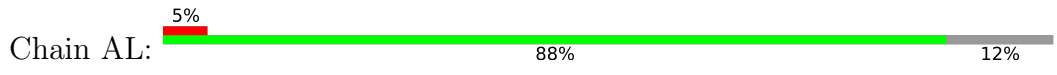
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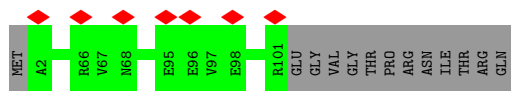
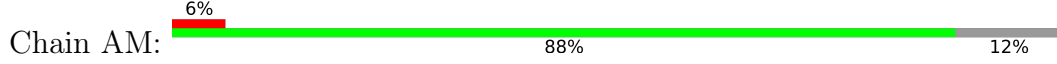
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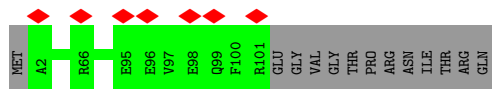
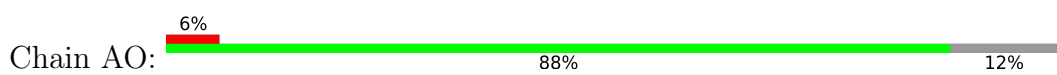
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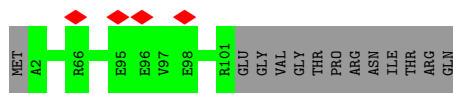
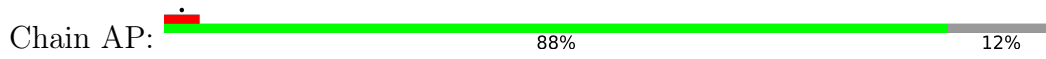
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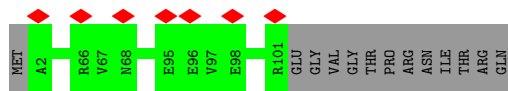
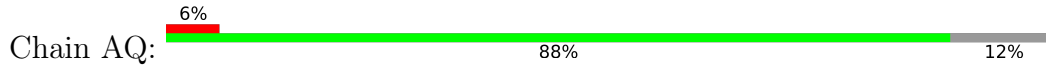
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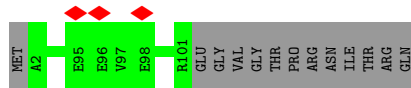
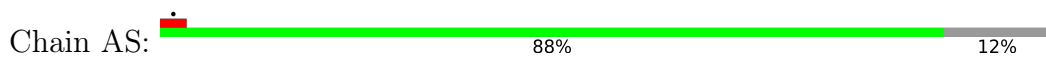
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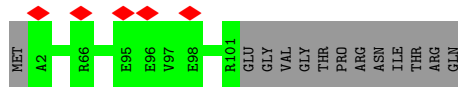
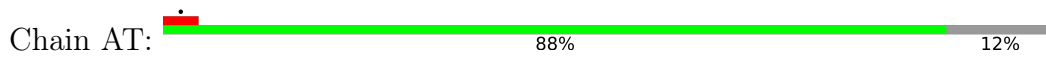
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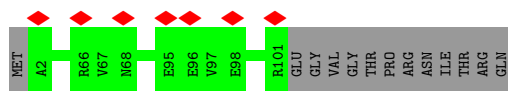
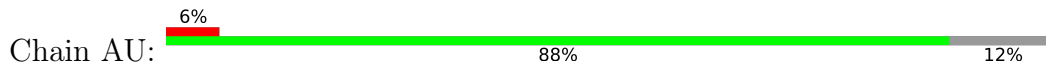
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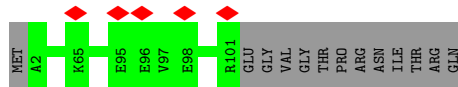
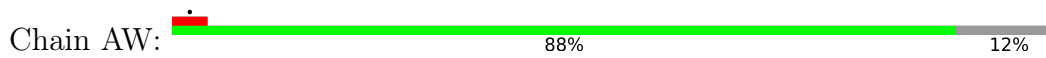
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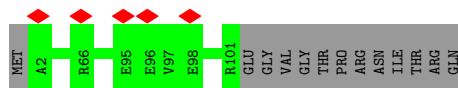
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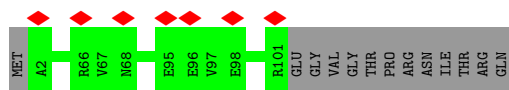
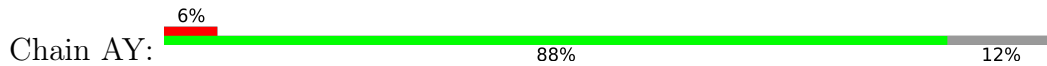
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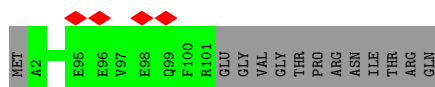
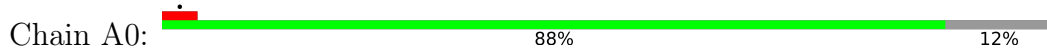
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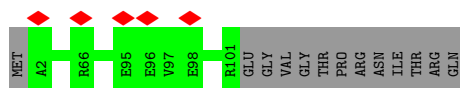
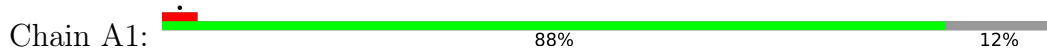
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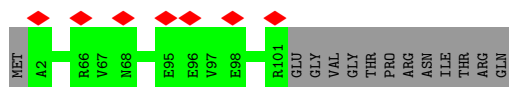
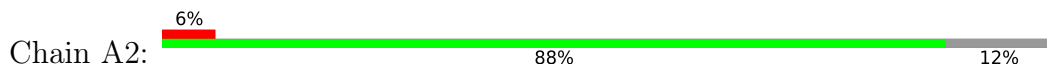
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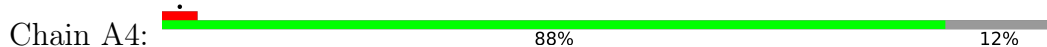
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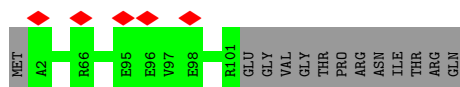
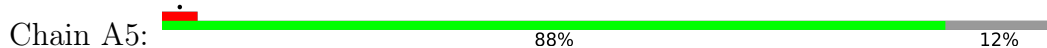
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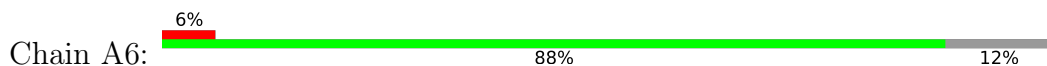
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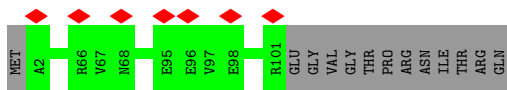


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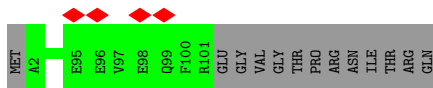
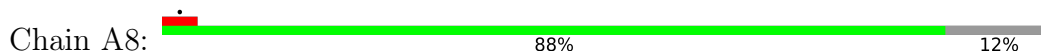


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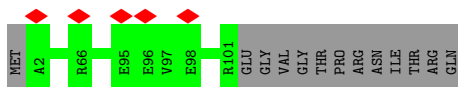




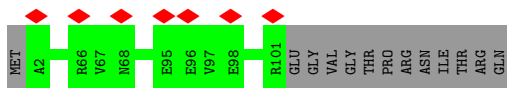
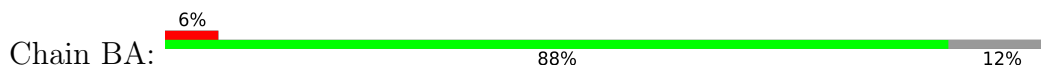
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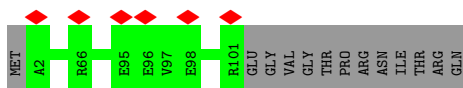
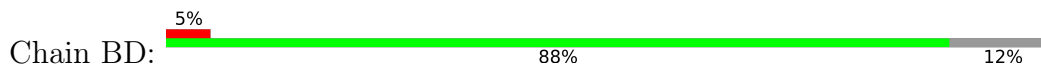
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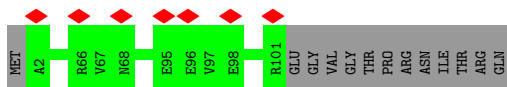
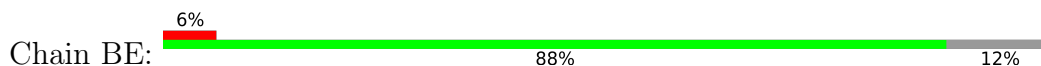
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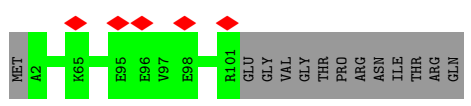
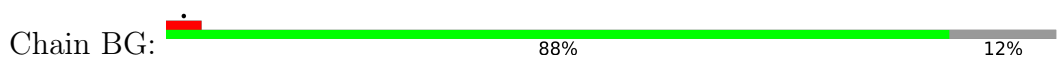
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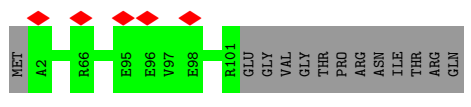
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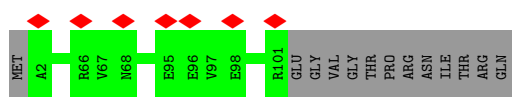
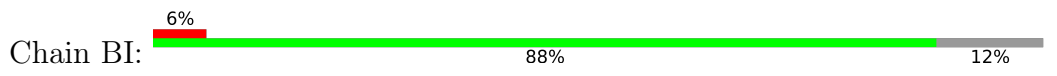
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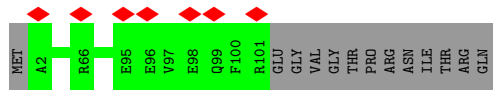
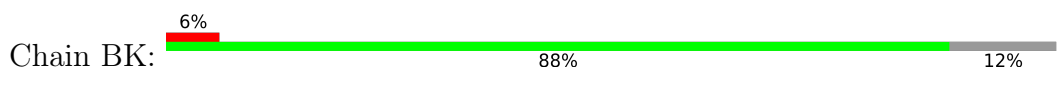
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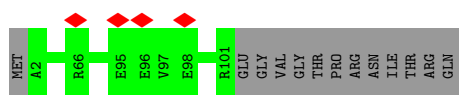
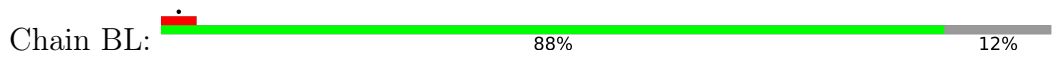
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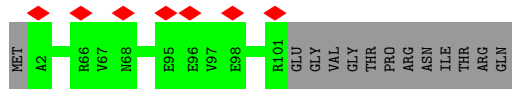
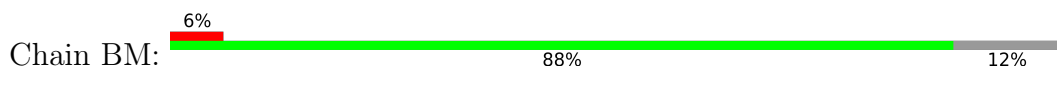
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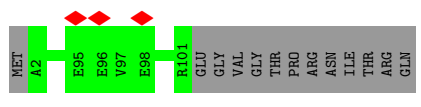
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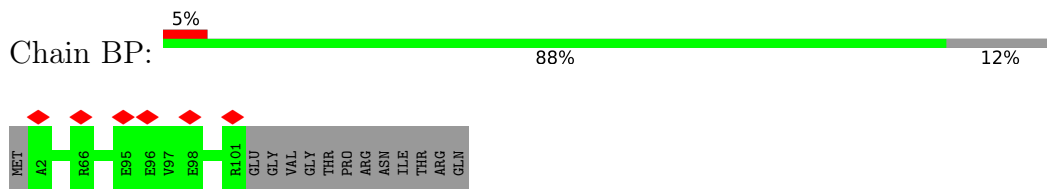
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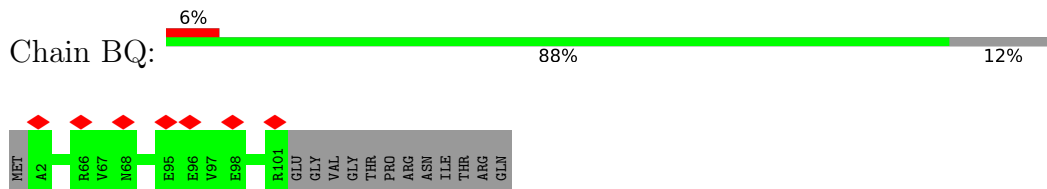
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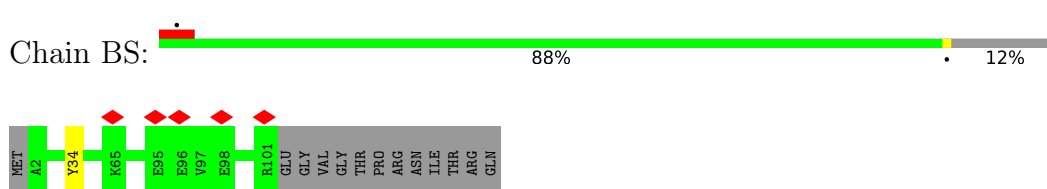
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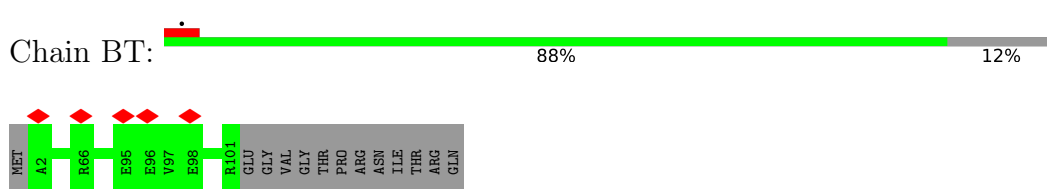
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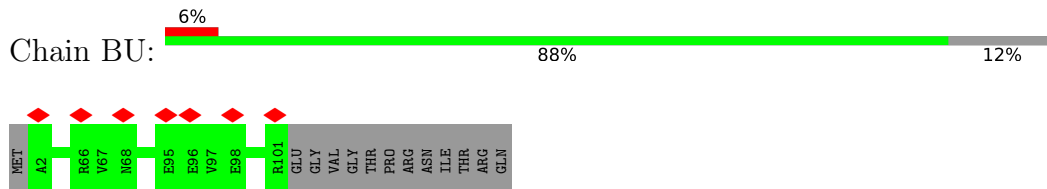
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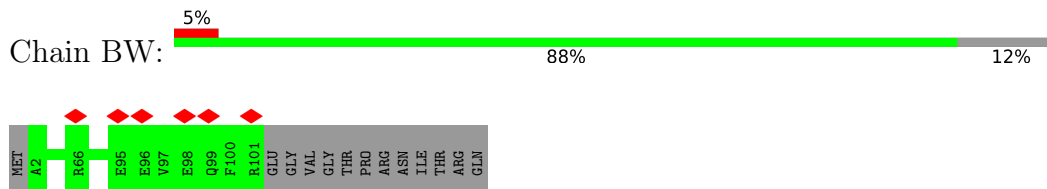
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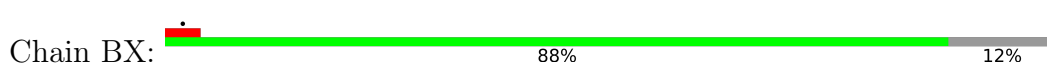
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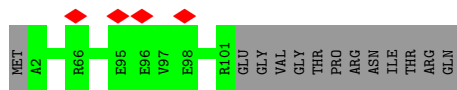


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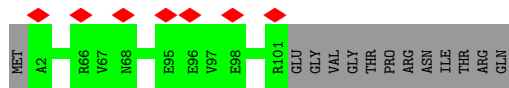
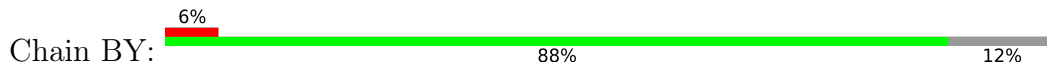


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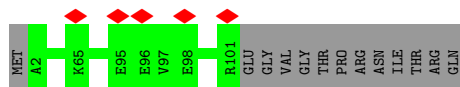
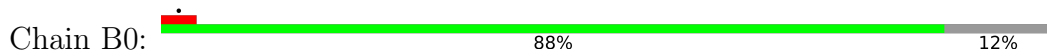




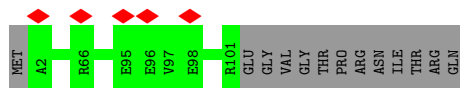
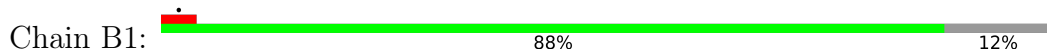
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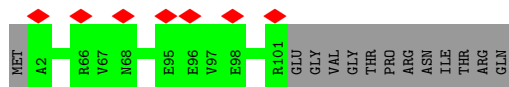
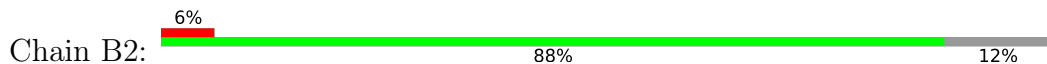
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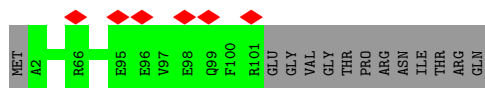
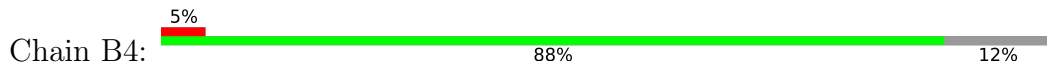
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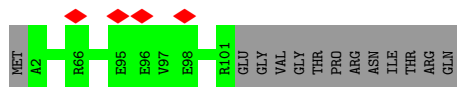
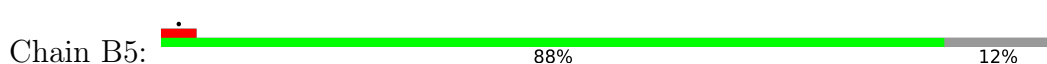
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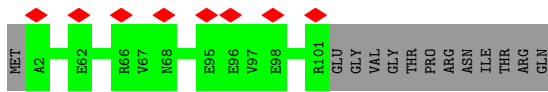
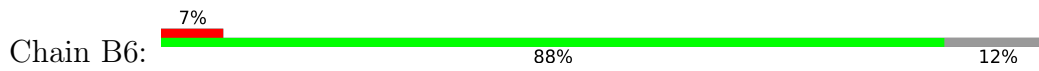
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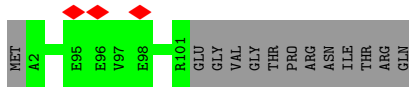
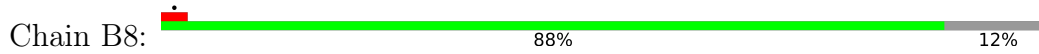
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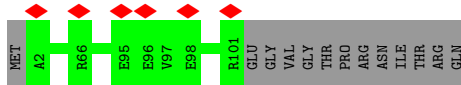
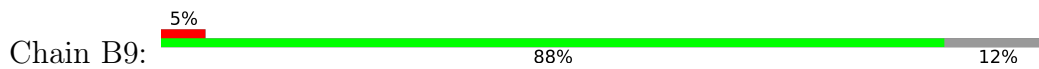
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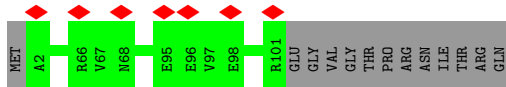
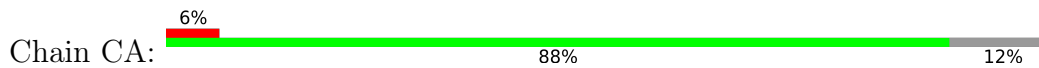
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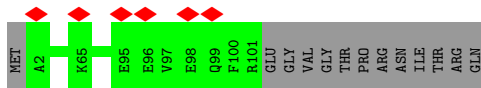
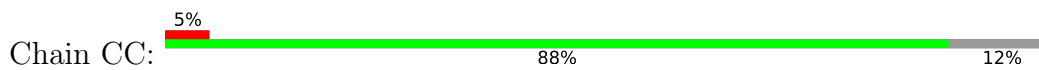
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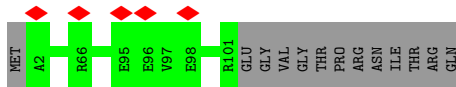
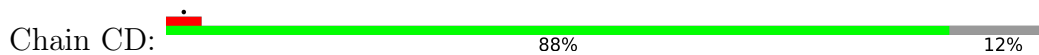
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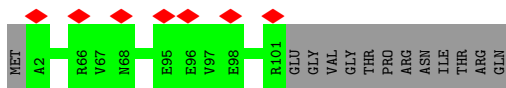
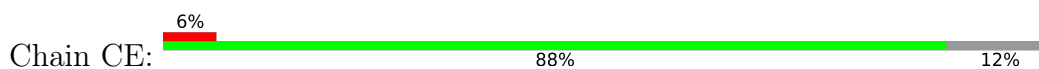
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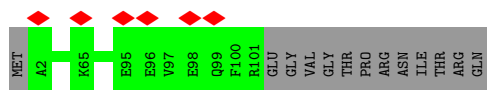
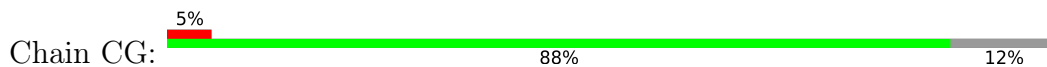
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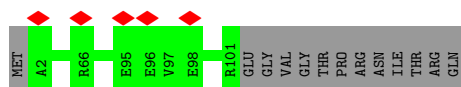
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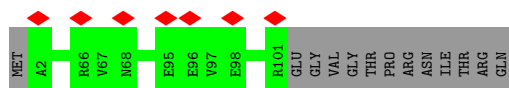
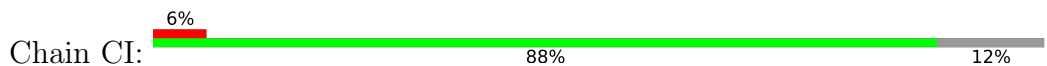
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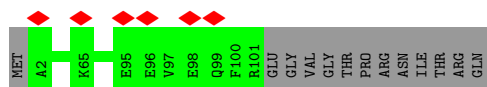
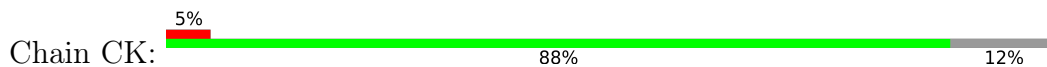
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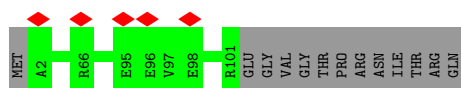
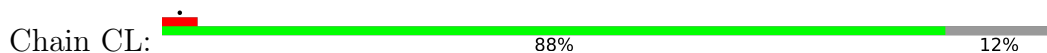
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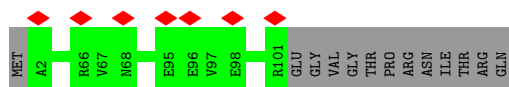
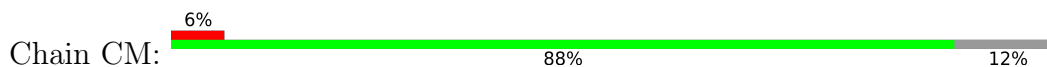
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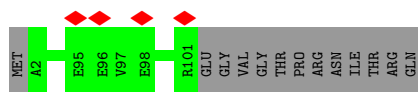


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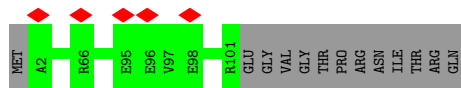
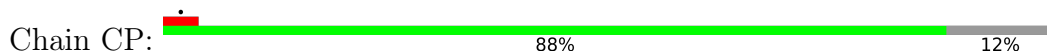


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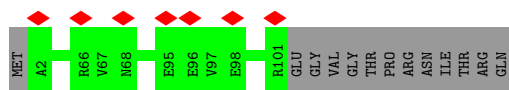
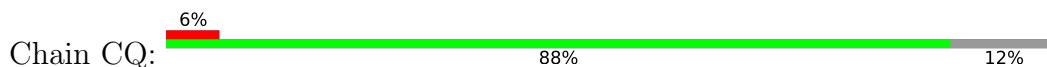




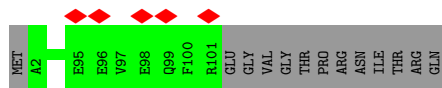
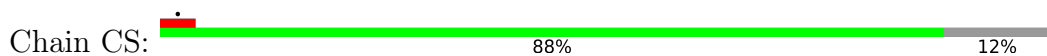
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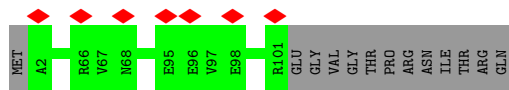
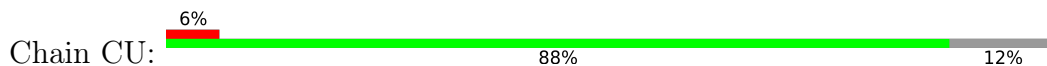
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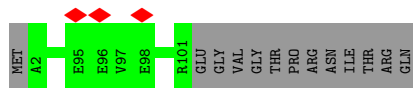
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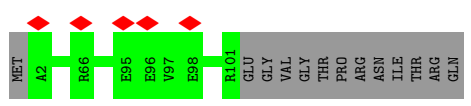
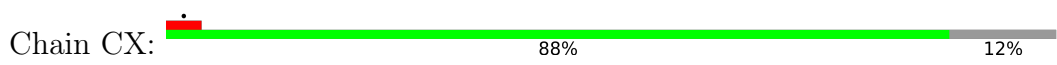
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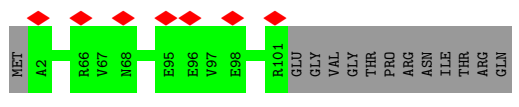
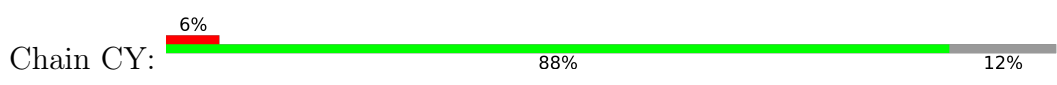
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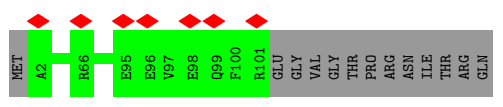
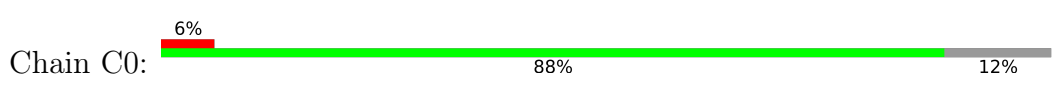
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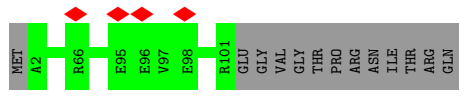
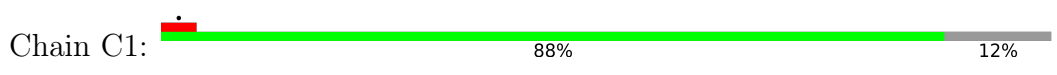
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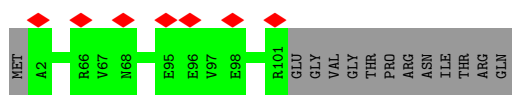
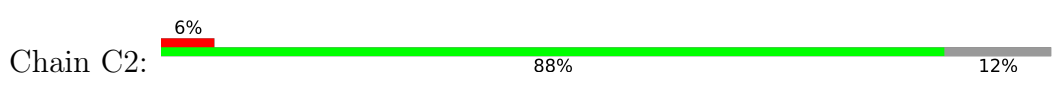
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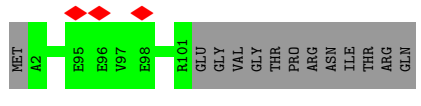
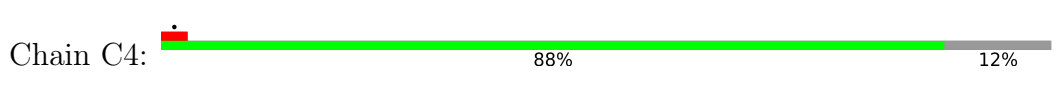
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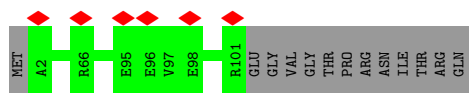
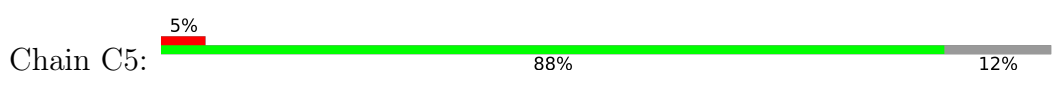
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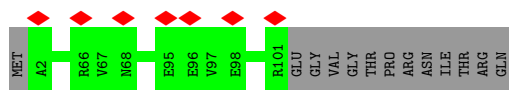
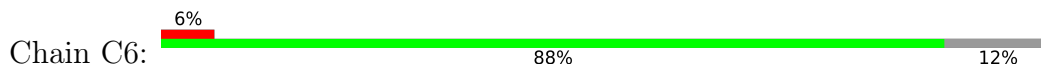
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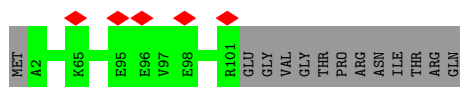
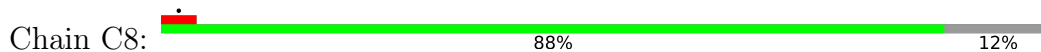
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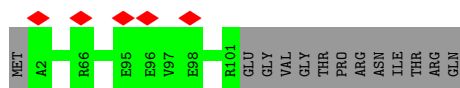
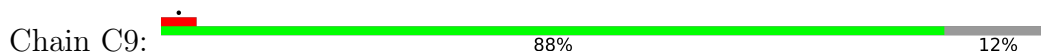
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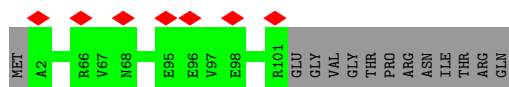
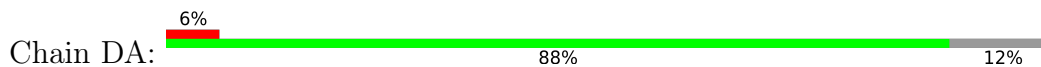
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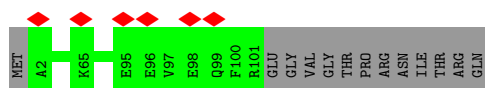
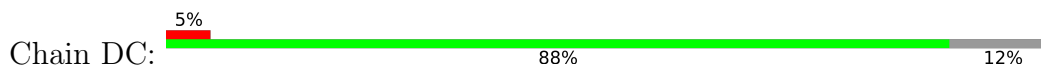
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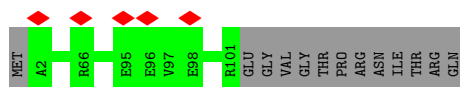
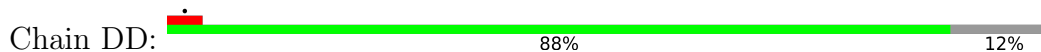
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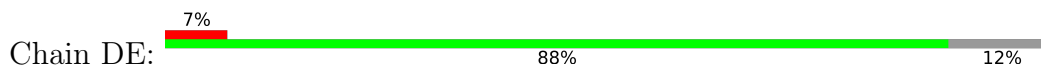
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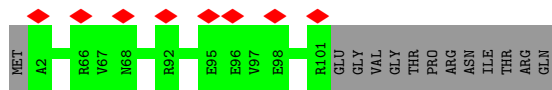


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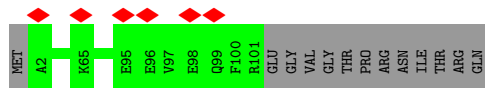
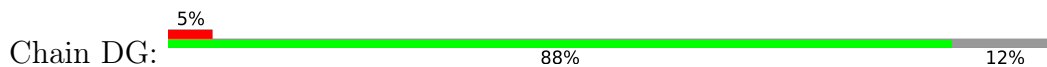


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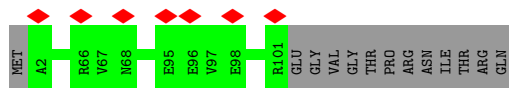
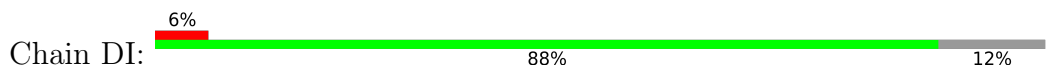
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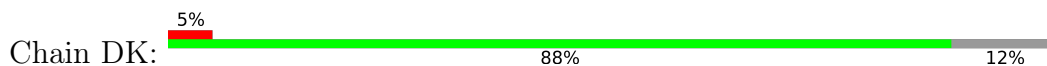
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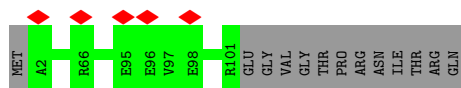
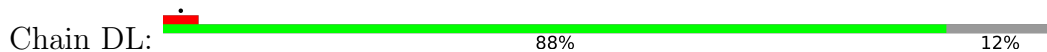
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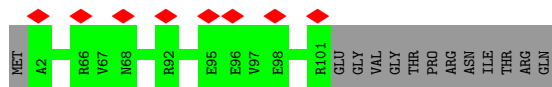
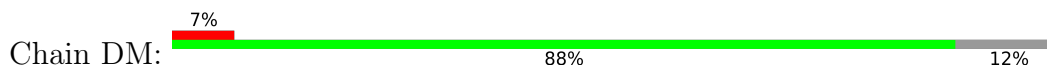
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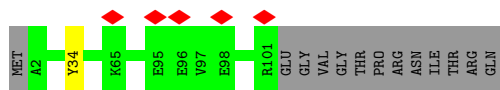
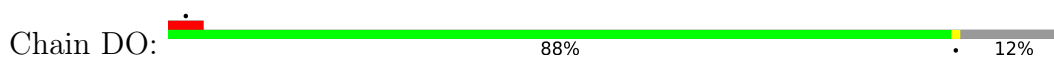
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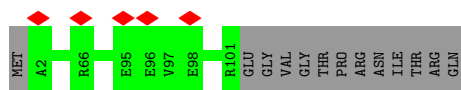
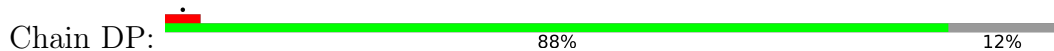
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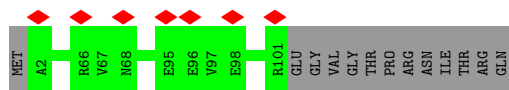
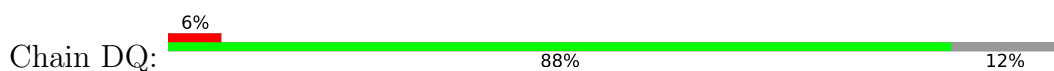
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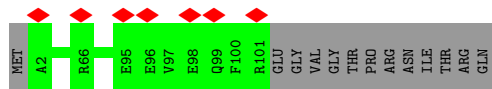
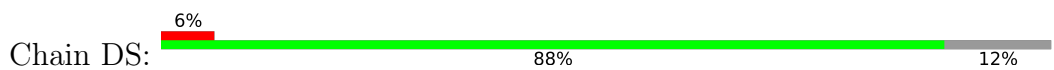
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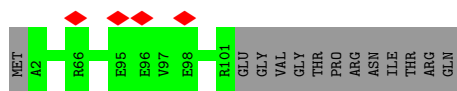
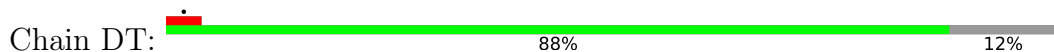
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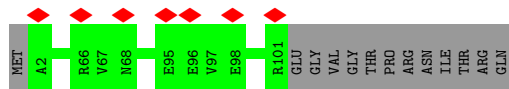
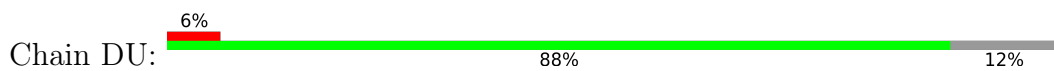
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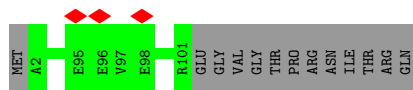
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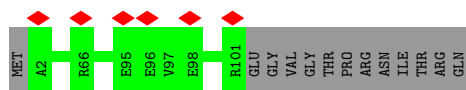
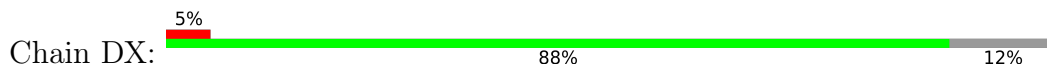
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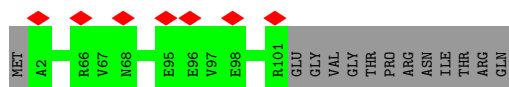
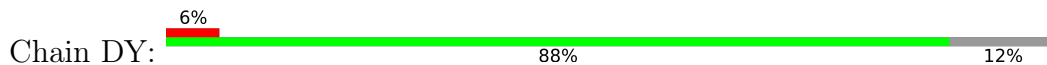
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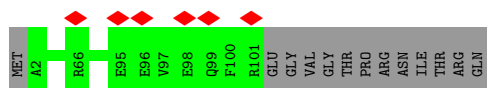
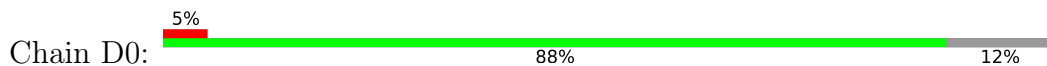
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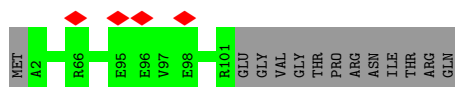
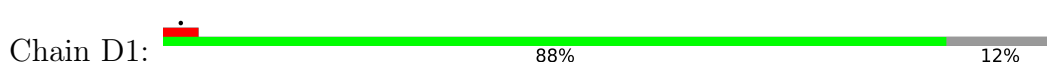
• Molecule 1: Microcompartments protein



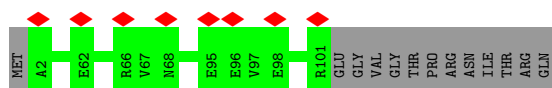
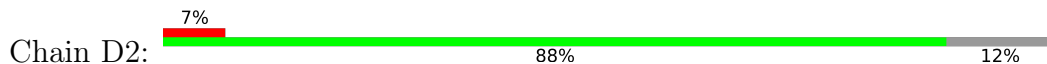
• Molecule 1: Microcompartments protein



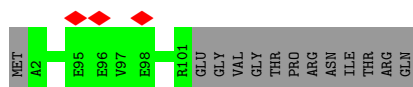
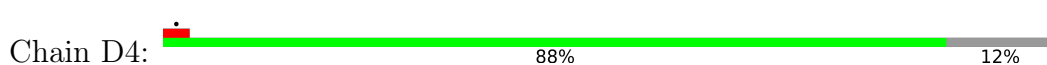
• Molecule 1: Microcompartments protein



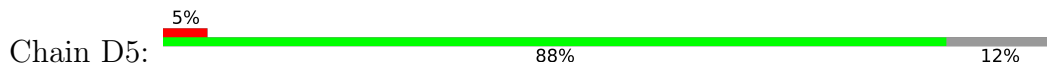
• Molecule 1: Microcompartments protein

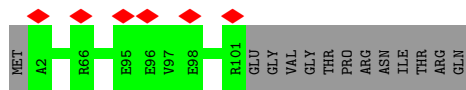


• Molecule 1: Microcompartments protein

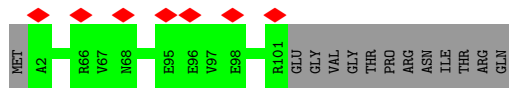
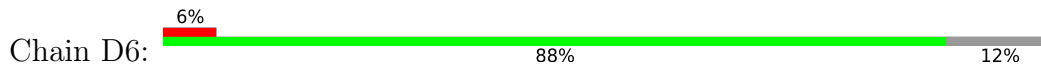


• Molecule 1: Microcompartments protein

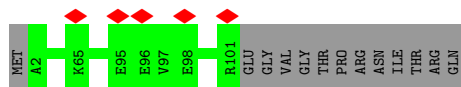




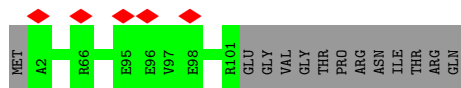
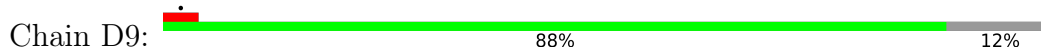
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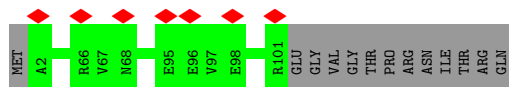
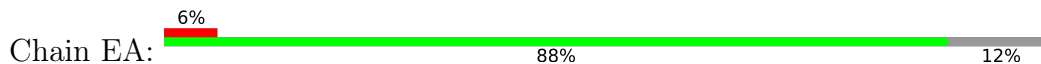
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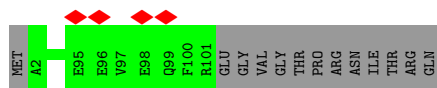
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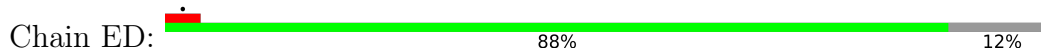
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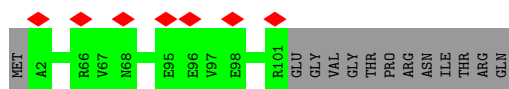
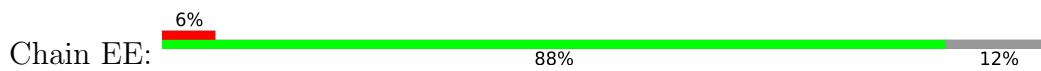
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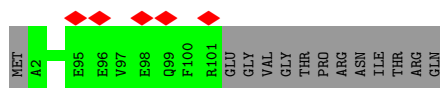
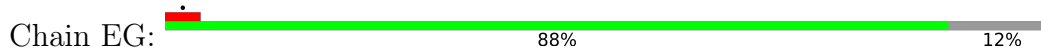
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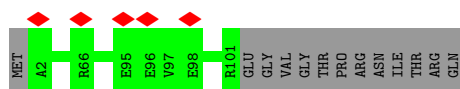
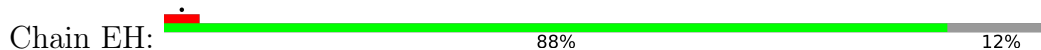
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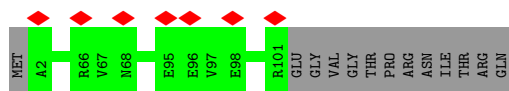
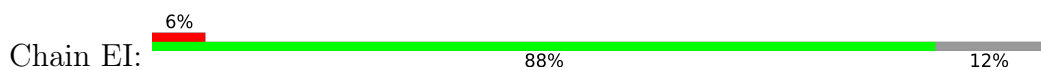
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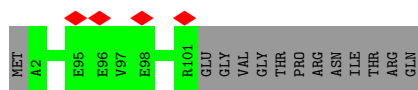
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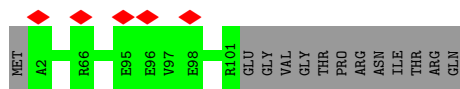
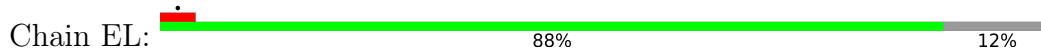
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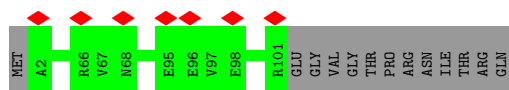
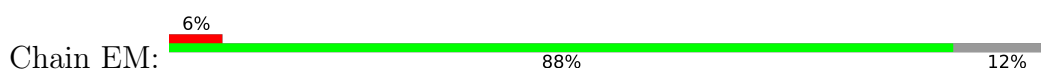
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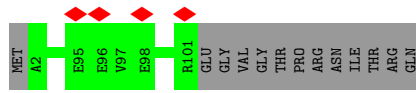
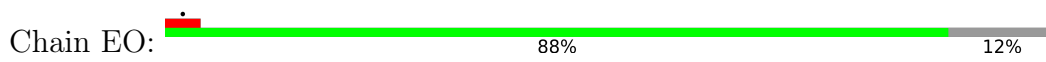
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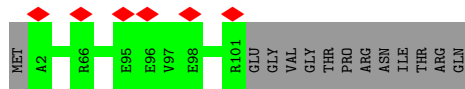
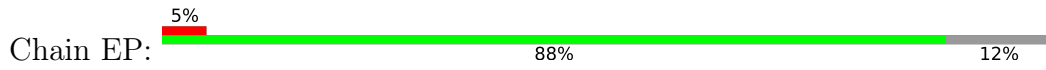
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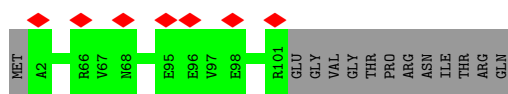
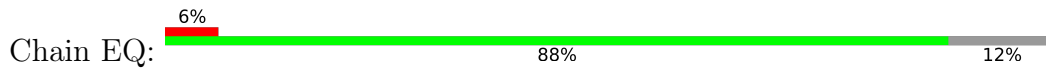
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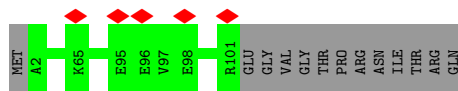
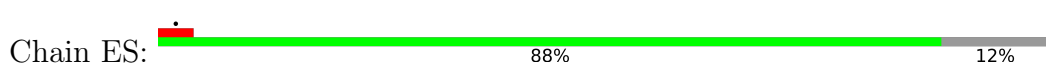
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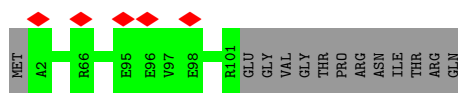
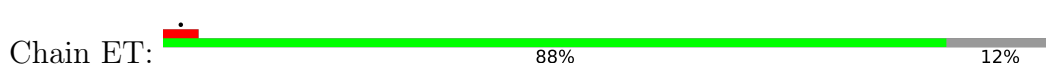
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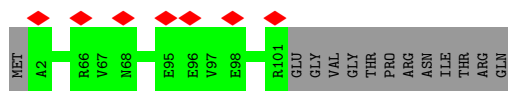
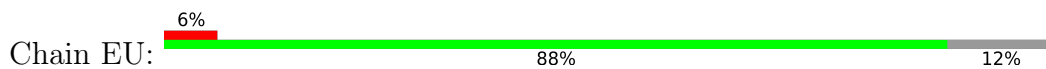
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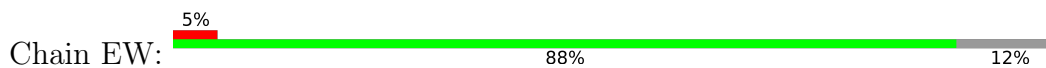
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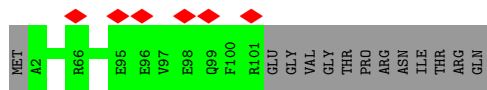


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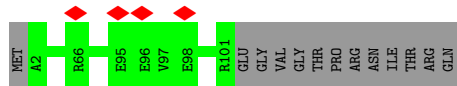
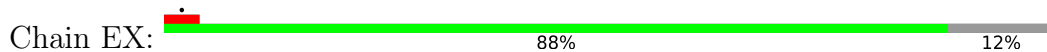


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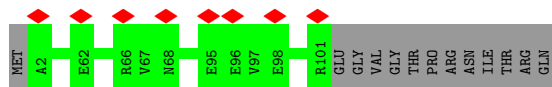
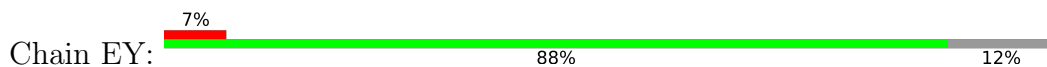




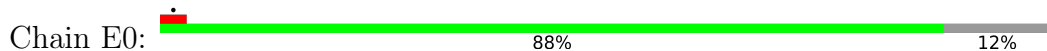
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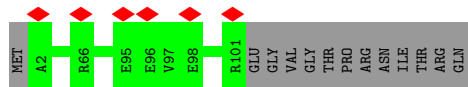
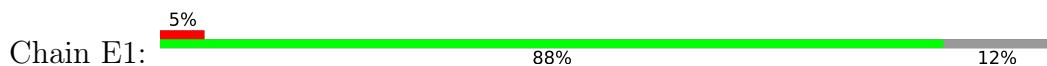
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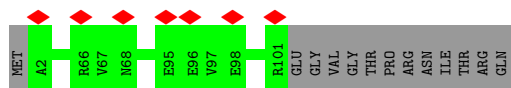
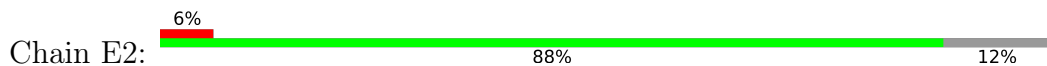
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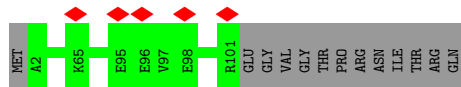
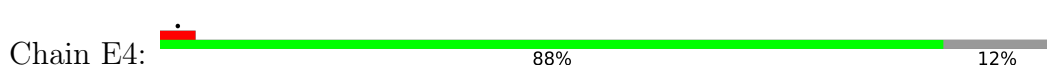
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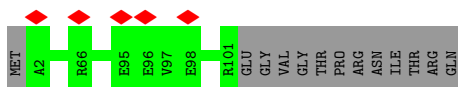
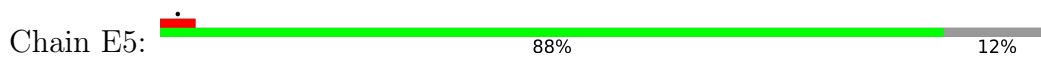
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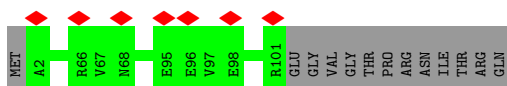
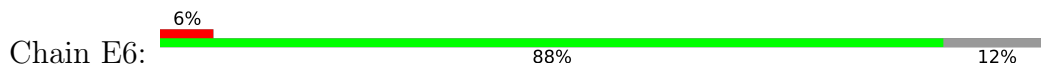
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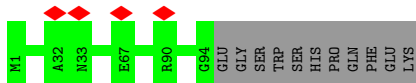
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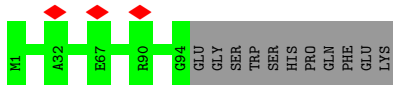
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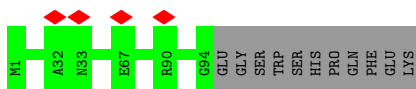
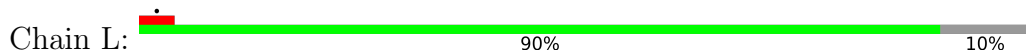
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



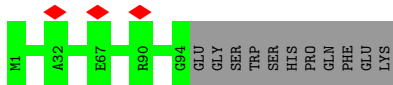
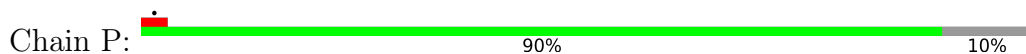
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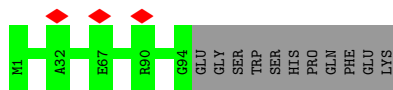


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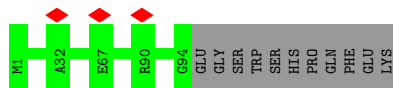
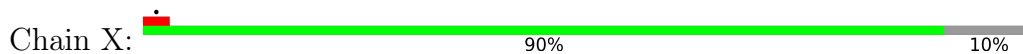


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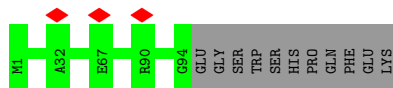
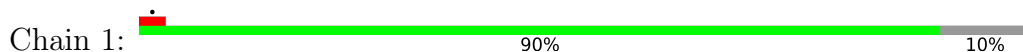




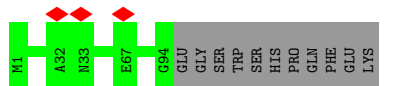
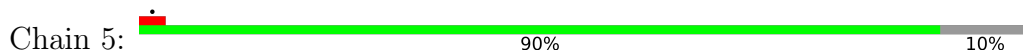
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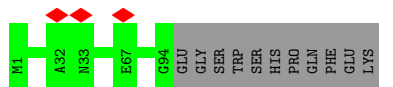
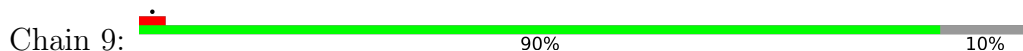
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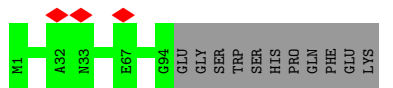
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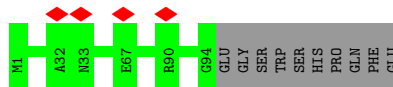
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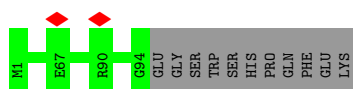
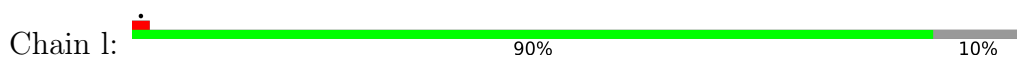
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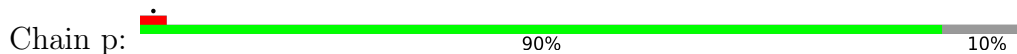
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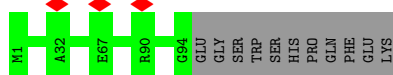
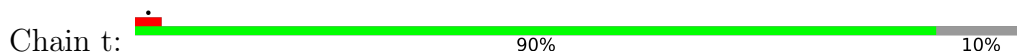
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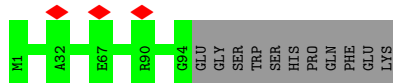
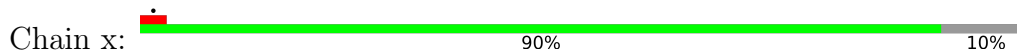
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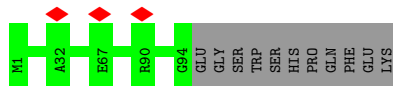
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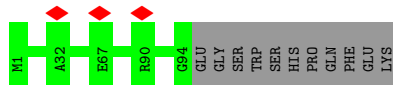
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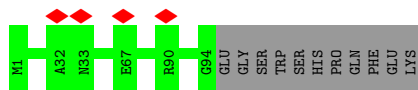


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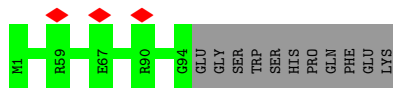
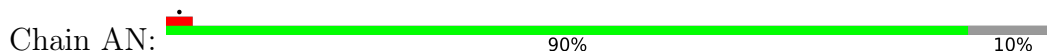


- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

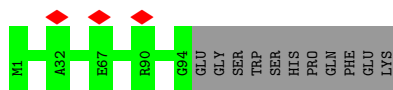




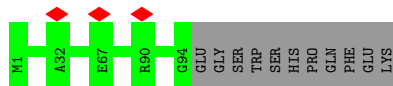
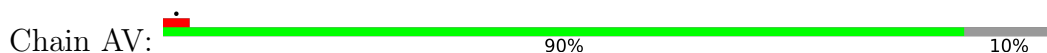
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



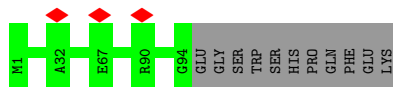
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



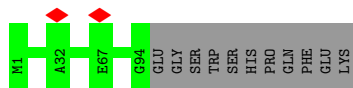
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



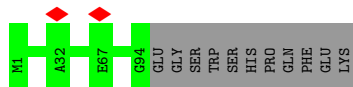
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



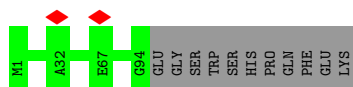
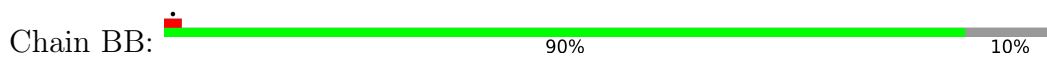
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



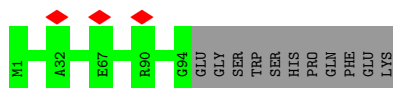
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



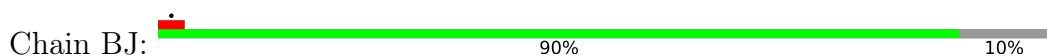
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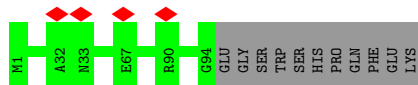
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



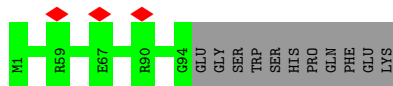
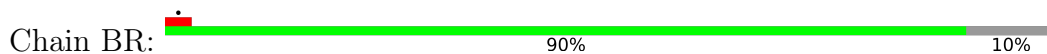
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



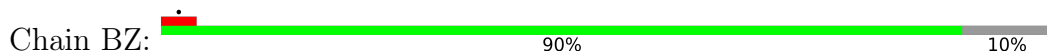
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

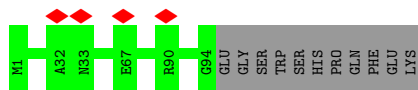


- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

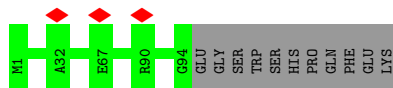
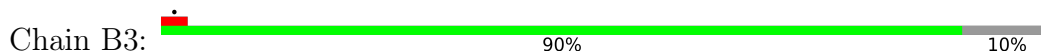


- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

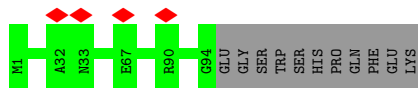
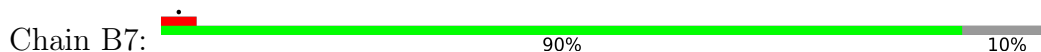




- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml



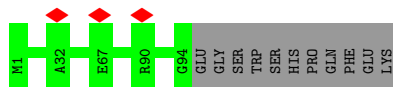
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml



- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml



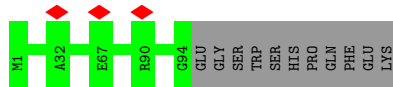
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml



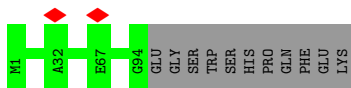
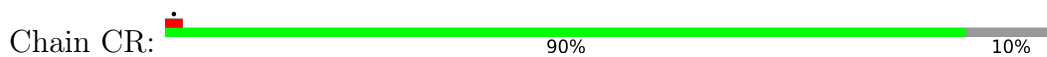
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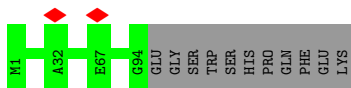
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml



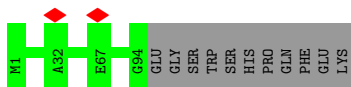
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml



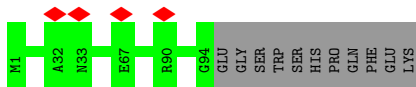
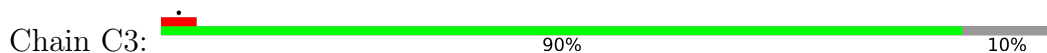
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



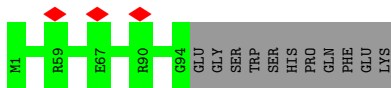
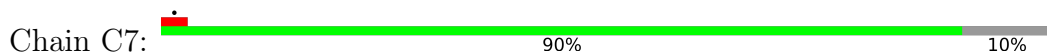
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



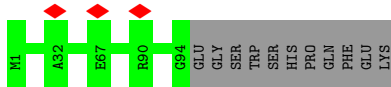
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



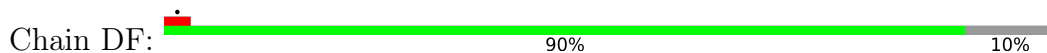
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

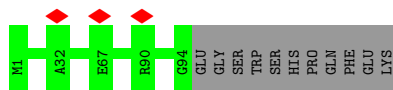


- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

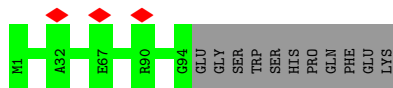
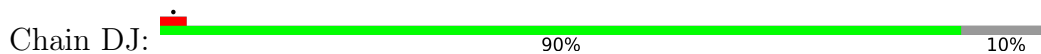


- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

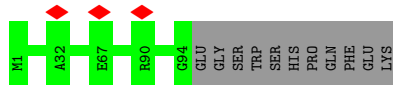




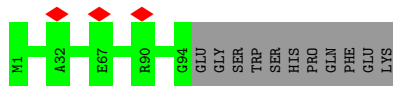
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml



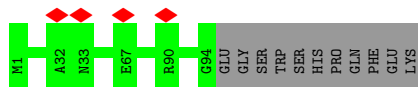
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml



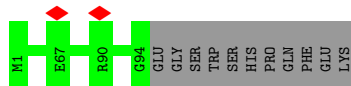
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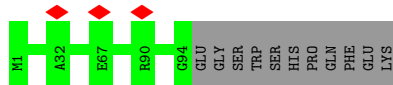
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml



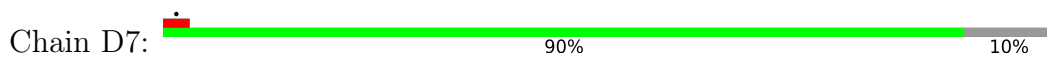
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml



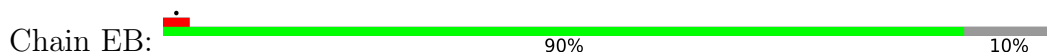
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml



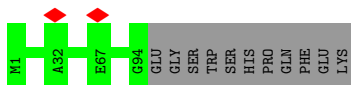
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml



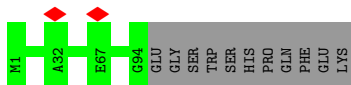
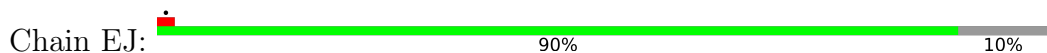
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



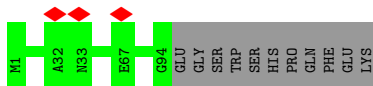
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



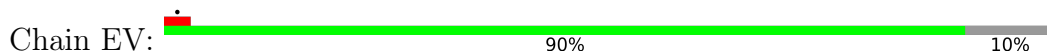
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

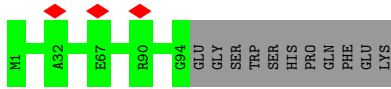


- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

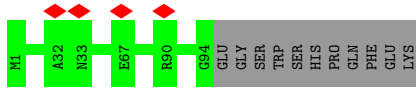
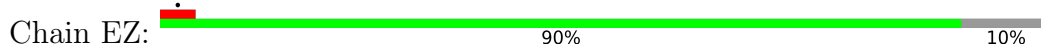


- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

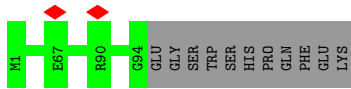




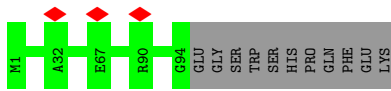
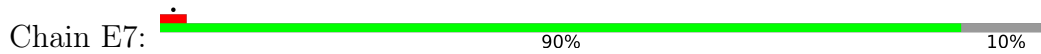
- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



- Molecule 2: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	35384	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)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	56000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	9.441	Depositor
Minimum map value	-5.735	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.8	Depositor
Map size (\AA)	245.8608, 245.8608, 245.8608	wwPDB
Map dimensions	276, 276, 276	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8908, 0.8908, 0.8908	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	0	0.33	0/761	0.51	0/1033
1	2	0.33	0/761	0.51	0/1033
1	3	0.33	0/761	0.49	0/1033
1	4	0.32	0/761	0.49	0/1033
1	6	0.32	0/761	0.51	0/1033
1	7	0.33	0/761	0.50	0/1033
1	8	0.33	0/761	0.50	0/1033
1	A	0.33	0/761	0.51	0/1033
1	A0	0.33	0/761	0.51	0/1033
1	A1	0.32	0/761	0.49	0/1033
1	A2	0.32	0/761	0.49	0/1033
1	A4	0.33	0/761	0.51	0/1033
1	A5	0.33	0/761	0.49	0/1033
1	A6	0.33	0/761	0.50	0/1033
1	A8	0.33	0/761	0.51	0/1033
1	A9	0.33	0/761	0.49	0/1033
1	AA	0.33	0/761	0.51	0/1033
1	AC	0.32	0/761	0.50	0/1033
1	AD	0.33	0/761	0.50	0/1033
1	AE	0.34	0/761	0.50	0/1033
1	AG	0.33	0/761	0.51	0/1033
1	AH	0.32	0/761	0.49	0/1033
1	AI	0.34	0/761	0.51	0/1033
1	AK	0.32	0/761	0.52	0/1033
1	AL	0.32	0/761	0.50	0/1033
1	AM	0.33	0/761	0.49	0/1033
1	AO	0.33	0/761	0.50	0/1033
1	AP	0.32	0/761	0.50	0/1033
1	AQ	0.34	0/761	0.51	0/1033
1	AS	0.33	0/761	0.52	0/1033
1	AT	0.33	0/761	0.50	0/1033
1	AU	0.32	0/761	0.49	0/1033
1	AW	0.32	0/761	0.50	0/1033
1	AX	0.33	0/761	0.50	0/1033

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AY	0.34	0/761	0.50	0/1033
1	B	0.32	0/761	0.50	0/1033
1	B0	0.32	0/761	0.50	0/1033
1	B1	0.33	0/761	0.51	0/1033
1	B2	0.34	0/761	0.51	0/1033
1	B4	0.33	0/761	0.51	0/1033
1	B5	0.32	0/761	0.50	0/1033
1	B6	0.34	0/761	0.51	0/1033
1	B8	0.33	0/761	0.51	0/1033
1	B9	0.32	0/761	0.50	0/1033
1	BA	0.32	0/761	0.49	0/1033
1	BC	0.33	0/761	0.52	0/1033
1	BD	0.33	0/761	0.50	0/1033
1	BE	0.33	0/761	0.49	0/1033
1	BG	0.32	0/761	0.50	0/1033
1	BH	0.33	0/761	0.50	0/1033
1	BI	0.34	0/761	0.51	0/1033
1	BK	0.32	0/761	0.51	0/1033
1	BL	0.32	0/761	0.50	0/1033
1	BM	0.34	0/761	0.51	0/1033
1	BO	0.33	0/761	0.52	0/1033
1	BP	0.33	0/761	0.50	0/1033
1	BQ	0.33	0/761	0.50	0/1033
1	BS	0.32	0/761	0.50	0/1033
1	BT	0.33	0/761	0.50	0/1033
1	BU	0.34	0/761	0.51	0/1033
1	BW	0.32	0/761	0.50	0/1033
1	BX	0.32	0/761	0.50	0/1033
1	BY	0.34	0/761	0.51	0/1033
1	C	0.34	0/761	0.50	0/1033
1	C0	0.33	0/761	0.51	0/1033
1	C1	0.32	0/761	0.50	0/1033
1	C2	0.33	0/761	0.50	0/1033
1	C4	0.33	0/761	0.52	0/1033
1	C5	0.33	0/761	0.50	0/1033
1	C6	0.33	0/761	0.50	0/1033
1	C8	0.32	0/761	0.50	0/1033
1	C9	0.33	0/761	0.51	0/1033
1	CA	0.33	0/761	0.50	0/1033
1	CC	0.32	0/761	0.51	0/1033
1	CD	0.32	0/761	0.49	0/1033
1	CE	0.33	0/761	0.51	0/1033
1	CG	0.33	0/761	0.51	0/1033

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CH	0.32	0/761	0.49	0/1033
1	CI	0.33	0/761	0.51	0/1033
1	CK	0.32	0/761	0.50	0/1033
1	CL	0.32	0/761	0.49	0/1033
1	CM	0.33	0/761	0.51	0/1033
1	CO	0.32	0/761	0.51	0/1033
1	CP	0.33	0/761	0.49	0/1033
1	CQ	0.33	0/761	0.50	0/1033
1	CS	0.32	0/761	0.51	0/1033
1	CT	0.33	0/761	0.49	0/1033
1	CU	0.32	0/761	0.49	0/1033
1	CW	0.33	0/761	0.52	0/1033
1	CX	0.33	0/761	0.49	0/1033
1	CY	0.32	0/761	0.50	0/1033
1	D0	0.33	0/761	0.51	0/1033
1	D1	0.32	0/761	0.50	0/1033
1	D2	0.33	0/761	0.51	0/1033
1	D4	0.33	0/761	0.52	0/1033
1	D5	0.32	0/761	0.50	0/1033
1	D6	0.32	0/761	0.49	0/1033
1	D8	0.32	0/761	0.50	0/1033
1	D9	0.33	0/761	0.50	0/1033
1	DA	0.33	0/761	0.51	0/1033
1	DC	0.32	0/761	0.50	0/1033
1	DD	0.32	0/761	0.49	0/1033
1	DE	0.34	0/761	0.51	0/1033
1	DG	0.32	0/761	0.51	0/1033
1	DH	0.32	0/761	0.49	0/1033
1	DI	0.33	0/761	0.50	0/1033
1	DK	0.33	0/761	0.51	0/1033
1	DL	0.32	0/761	0.49	0/1033
1	DM	0.34	0/761	0.50	0/1033
1	DO	0.32	0/761	0.50	0/1033
1	DP	0.33	0/761	0.50	0/1033
1	DQ	0.34	0/761	0.51	0/1033
1	DS	0.32	0/761	0.51	0/1033
1	DT	0.32	0/761	0.50	0/1033
1	DU	0.34	0/761	0.51	0/1033
1	DW	0.33	0/761	0.51	0/1033
1	DX	0.32	0/761	0.50	0/1033
1	DY	0.32	0/761	0.50	0/1033
1	E	0.32	0/761	0.50	0/1033
1	E0	0.33	0/761	0.52	0/1033

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E1	0.33	0/761	0.50	0/1033
1	E2	0.32	0/761	0.49	0/1033
1	E4	0.32	0/761	0.50	0/1033
1	E5	0.33	0/761	0.51	0/1033
1	E6	0.34	0/761	0.51	0/1033
1	EA	0.34	0/761	0.51	0/1033
1	EC	0.33	0/761	0.52	0/1033
1	ED	0.33	0/761	0.49	0/1033
1	EE	0.33	0/761	0.50	0/1033
1	EG	0.33	0/761	0.51	0/1033
1	EH	0.33	0/761	0.49	0/1033
1	EI	0.33	0/761	0.50	0/1033
1	EK	0.32	0/761	0.51	0/1033
1	EL	0.33	0/761	0.49	0/1033
1	EM	0.33	0/761	0.49	0/1033
1	EO	0.33	0/761	0.52	0/1033
1	EP	0.32	0/761	0.50	0/1033
1	EQ	0.33	0/761	0.50	0/1033
1	ES	0.32	0/761	0.50	0/1033
1	ET	0.33	0/761	0.50	0/1033
1	EU	0.34	0/761	0.51	0/1033
1	EW	0.33	0/761	0.51	0/1033
1	EX	0.32	0/761	0.50	0/1033
1	EY	0.33	0/761	0.50	0/1033
1	F	0.33	0/761	0.51	0/1033
1	G	0.34	0/761	0.50	0/1033
1	I	0.33	0/761	0.51	0/1033
1	J	0.32	0/761	0.50	0/1033
1	K	0.34	0/761	0.51	0/1033
1	M	0.33	0/761	0.51	0/1033
1	N	0.33	0/761	0.50	0/1033
1	O	0.33	0/761	0.50	0/1033
1	Q	0.32	0/761	0.50	0/1033
1	R	0.32	0/761	0.49	0/1033
1	S	0.33	0/761	0.51	0/1033
1	U	0.33	0/761	0.51	0/1033
1	V	0.32	0/761	0.50	0/1033
1	W	0.33	0/761	0.51	0/1033
1	Y	0.33	0/761	0.51	0/1033
1	Z	0.32	0/761	0.49	0/1033
1	a	0.32	0/761	0.51	0/1033
1	b	0.33	0/761	0.50	0/1033
1	c	0.33	0/761	0.50	0/1033

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	e	0.33	0/761	0.51	0/1033
1	f	0.32	0/761	0.50	0/1033
1	g	0.34	0/761	0.51	0/1033
1	i	0.33	0/761	0.52	0/1033
1	j	0.32	0/761	0.50	0/1033
1	k	0.33	0/761	0.50	0/1033
1	m	0.32	0/761	0.50	0/1033
1	n	0.33	0/761	0.50	0/1033
1	o	0.34	0/761	0.51	0/1033
1	q	0.32	0/761	0.50	0/1033
1	r	0.32	0/761	0.49	0/1033
1	s	0.33	0/761	0.51	0/1033
1	u	0.32	0/761	0.50	0/1033
1	v	0.32	0/761	0.50	0/1033
1	w	0.33	0/761	0.51	0/1033
1	y	0.32	0/761	0.50	0/1033
1	z	0.32	0/761	0.49	0/1033
2	1	0.33	0/722	0.52	0/980
2	5	0.32	0/722	0.51	0/980
2	9	0.32	0/722	0.51	0/980
2	A3	0.33	0/722	0.51	0/980
2	A7	0.32	0/722	0.51	0/980
2	AB	0.33	0/722	0.51	0/980
2	AF	0.32	0/722	0.52	0/980
2	AJ	0.32	0/722	0.51	0/980
2	AN	0.33	0/722	0.50	0/980
2	AR	0.32	0/722	0.52	0/980
2	AV	0.32	0/722	0.50	0/980
2	AZ	0.32	0/722	0.52	0/980
2	B3	0.32	0/722	0.52	0/980
2	B7	0.32	0/722	0.52	0/980
2	BB	0.32	0/722	0.51	0/980
2	BF	0.33	0/722	0.51	0/980
2	BJ	0.32	0/722	0.52	0/980
2	BN	0.32	0/722	0.52	0/980
2	BR	0.33	0/722	0.51	0/980
2	BV	0.32	0/722	0.51	0/980
2	BZ	0.33	0/722	0.52	0/980
2	C3	0.32	0/722	0.52	0/980
2	C7	0.32	0/722	0.51	0/980
2	CB	0.33	0/722	0.50	0/980
2	CF	0.32	0/722	0.52	0/980
2	CJ	0.33	0/722	0.52	0/980

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	CN	0.33	0/722	0.52	0/980
2	CR	0.32	0/722	0.51	0/980
2	CV	0.32	0/722	0.51	0/980
2	CZ	0.32	0/722	0.51	0/980
2	D	0.32	0/722	0.52	0/980
2	D3	0.32	0/722	0.52	0/980
2	D7	0.33	0/722	0.51	0/980
2	DB	0.32	0/722	0.52	0/980
2	DF	0.33	0/722	0.52	0/980
2	DJ	0.33	0/722	0.52	0/980
2	DN	0.33	0/722	0.52	0/980
2	DR	0.32	0/722	0.52	0/980
2	DV	0.32	0/722	0.52	0/980
2	DZ	0.33	0/722	0.51	0/980
2	E3	0.33	0/722	0.51	0/980
2	E7	0.32	0/722	0.52	0/980
2	EB	0.32	0/722	0.52	0/980
2	EF	0.32	0/722	0.52	0/980
2	EJ	0.33	0/722	0.51	0/980
2	EN	0.32	0/722	0.51	0/980
2	ER	0.33	0/722	0.50	0/980
2	EV	0.32	0/722	0.52	0/980
2	EZ	0.33	0/722	0.52	0/980
2	H	0.32	0/722	0.52	0/980
2	L	0.32	0/722	0.52	0/980
2	P	0.33	0/722	0.51	0/980
2	T	0.33	0/722	0.52	0/980
2	X	0.33	0/722	0.52	0/980
2	d	0.33	0/722	0.51	0/980
2	h	0.32	0/722	0.52	0/980
2	l	0.33	0/722	0.51	0/980
2	p	0.32	0/722	0.52	0/980
2	t	0.33	0/722	0.52	0/980
2	x	0.33	0/722	0.52	0/980
All	All	0.33	0/180300	0.51	0/244740

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	0	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	2	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	3	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	4	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	6	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	7	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	8	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	A	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	A0	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	A1	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	A2	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	A4	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	A5	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	A6	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	A8	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	A9	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	AA	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	AC	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	AD	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	AE	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	AG	98/113 (87%)	95 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AH	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	AI	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	AK	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	AL	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	AM	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	AO	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	AP	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	AQ	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	AS	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	AT	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	AU	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	AW	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	AX	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	AY	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	B	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	B0	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	B1	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	B2	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	B4	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	B5	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	B6	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	B8	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	B9	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	BA	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	BC	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	BD	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	BE	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	BG	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	BH	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	BI	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	BK	98/113 (87%)	95 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BL	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	BM	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	BO	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	BP	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	BQ	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	BS	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	BT	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	BU	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	BW	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	BX	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	BY	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	C	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	C0	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	C1	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	C2	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	C4	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	C5	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	C6	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	C8	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	C9	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	CA	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	CC	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	CD	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	CE	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	CG	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	CH	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	CI	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	CK	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	CL	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	CM	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	CO	98/113 (87%)	95 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CP	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	CQ	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	CS	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	CT	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	CU	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	CW	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	CX	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	CY	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	D0	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	D1	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	D2	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	D4	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	D5	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	D6	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	D8	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	D9	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	DA	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	DC	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	DD	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	DE	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	DG	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	DH	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	DI	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	DK	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	DL	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	DM	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	DO	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	DP	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	DQ	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	DS	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	DT	98/113 (87%)	97 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DU	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	DW	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	DX	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	DY	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	E	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	E0	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	E1	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	E2	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	E4	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	E5	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	E6	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	EA	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	EC	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	ED	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	EE	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	EG	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	EH	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	EI	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	EK	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	EL	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	EM	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	EO	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	EP	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	EQ	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	ES	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	ET	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	EU	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	EW	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	EX	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	EY	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	F	98/113 (87%)	97 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	I	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	J	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	K	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	M	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	N	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	O	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	Q	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	R	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	S	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	U	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	V	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	W	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	Y	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	Z	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	a	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	b	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	c	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	e	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	f	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	g	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	i	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	j	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	k	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	m	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	n	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	o	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	q	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	r	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	s	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	u	98/113 (87%)	95 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	v	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
1	w	98/113 (87%)	96 (98%)	2 (2%)	0	100	100
1	y	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
1	z	98/113 (87%)	97 (99%)	1 (1%)	0	100	100
2	1	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	5	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	9	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	A3	92/105 (88%)	90 (98%)	2 (2%)	0	100	100
2	A7	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	AB	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	AF	92/105 (88%)	90 (98%)	2 (2%)	0	100	100
2	AJ	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	AN	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	AR	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	AV	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	AZ	92/105 (88%)	90 (98%)	2 (2%)	0	100	100
2	B3	92/105 (88%)	90 (98%)	2 (2%)	0	100	100
2	B7	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	BB	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	BF	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	BJ	92/105 (88%)	90 (98%)	2 (2%)	0	100	100
2	BN	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	BR	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	BV	92/105 (88%)	90 (98%)	2 (2%)	0	100	100
2	BZ	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	C3	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	C7	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	CB	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	CF	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	CJ	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	CN	92/105 (88%)	89 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CR	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	CV	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	CZ	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	D	92/105 (88%)	90 (98%)	2 (2%)	0	100	100
2	D3	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	D7	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	DB	92/105 (88%)	90 (98%)	2 (2%)	0	100	100
2	DF	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	DJ	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	DN	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	DR	92/105 (88%)	90 (98%)	2 (2%)	0	100	100
2	DV	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	DZ	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	E3	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	E7	92/105 (88%)	90 (98%)	2 (2%)	0	100	100
2	EB	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	EF	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	EJ	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	EN	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	ER	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	EV	92/105 (88%)	90 (98%)	2 (2%)	0	100	100
2	EZ	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	H	92/105 (88%)	90 (98%)	2 (2%)	0	100	100
2	L	92/105 (88%)	90 (98%)	2 (2%)	0	100	100
2	P	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	T	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	X	92/105 (88%)	90 (98%)	2 (2%)	0	100	100
2	d	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	h	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	l	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	p	92/105 (88%)	90 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	t	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
2	x	92/105 (88%)	89 (97%)	3 (3%)	0	100	100
All	All	23160/26640 (87%)	22623 (98%)	537 (2%)	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	0	80/91 (88%)	80 (100%)	0	100	100
1	2	80/91 (88%)	80 (100%)	0	100	100
1	3	80/91 (88%)	80 (100%)	0	100	100
1	4	80/91 (88%)	80 (100%)	0	100	100
1	6	80/91 (88%)	80 (100%)	0	100	100
1	7	80/91 (88%)	80 (100%)	0	100	100
1	8	80/91 (88%)	80 (100%)	0	100	100
1	A	80/91 (88%)	80 (100%)	0	100	100
1	A0	80/91 (88%)	80 (100%)	0	100	100
1	A1	80/91 (88%)	80 (100%)	0	100	100
1	A2	80/91 (88%)	80 (100%)	0	100	100
1	A4	80/91 (88%)	80 (100%)	0	100	100
1	A5	80/91 (88%)	80 (100%)	0	100	100
1	A6	80/91 (88%)	80 (100%)	0	100	100
1	A8	80/91 (88%)	80 (100%)	0	100	100
1	A9	80/91 (88%)	80 (100%)	0	100	100
1	AA	80/91 (88%)	80 (100%)	0	100	100
1	AC	80/91 (88%)	80 (100%)	0	100	100
1	AD	80/91 (88%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AE	80/91 (88%)	80 (100%)	0	100	100
1	AG	80/91 (88%)	80 (100%)	0	100	100
1	AH	80/91 (88%)	80 (100%)	0	100	100
1	AI	80/91 (88%)	80 (100%)	0	100	100
1	AK	80/91 (88%)	80 (100%)	0	100	100
1	AL	80/91 (88%)	80 (100%)	0	100	100
1	AM	80/91 (88%)	80 (100%)	0	100	100
1	AO	80/91 (88%)	80 (100%)	0	100	100
1	AP	80/91 (88%)	80 (100%)	0	100	100
1	AQ	80/91 (88%)	80 (100%)	0	100	100
1	AS	80/91 (88%)	80 (100%)	0	100	100
1	AT	80/91 (88%)	80 (100%)	0	100	100
1	AU	80/91 (88%)	80 (100%)	0	100	100
1	AW	80/91 (88%)	80 (100%)	0	100	100
1	AX	80/91 (88%)	80 (100%)	0	100	100
1	AY	80/91 (88%)	80 (100%)	0	100	100
1	B	80/91 (88%)	80 (100%)	0	100	100
1	B0	80/91 (88%)	80 (100%)	0	100	100
1	B1	80/91 (88%)	80 (100%)	0	100	100
1	B2	80/91 (88%)	80 (100%)	0	100	100
1	B4	80/91 (88%)	80 (100%)	0	100	100
1	B5	80/91 (88%)	80 (100%)	0	100	100
1	B6	80/91 (88%)	80 (100%)	0	100	100
1	B8	80/91 (88%)	80 (100%)	0	100	100
1	B9	80/91 (88%)	80 (100%)	0	100	100
1	BA	80/91 (88%)	80 (100%)	0	100	100
1	BC	80/91 (88%)	80 (100%)	0	100	100
1	BD	80/91 (88%)	80 (100%)	0	100	100
1	BE	80/91 (88%)	80 (100%)	0	100	100
1	BG	80/91 (88%)	80 (100%)	0	100	100
1	BH	80/91 (88%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BI	80/91 (88%)	80 (100%)	0	100	100
1	BK	80/91 (88%)	80 (100%)	0	100	100
1	BL	80/91 (88%)	80 (100%)	0	100	100
1	BM	80/91 (88%)	80 (100%)	0	100	100
1	BO	80/91 (88%)	80 (100%)	0	100	100
1	BP	80/91 (88%)	80 (100%)	0	100	100
1	BQ	80/91 (88%)	80 (100%)	0	100	100
1	BS	80/91 (88%)	79 (99%)	1 (1%)	69	86
1	BT	80/91 (88%)	80 (100%)	0	100	100
1	BU	80/91 (88%)	80 (100%)	0	100	100
1	BW	80/91 (88%)	80 (100%)	0	100	100
1	BX	80/91 (88%)	80 (100%)	0	100	100
1	BY	80/91 (88%)	80 (100%)	0	100	100
1	C	80/91 (88%)	80 (100%)	0	100	100
1	C0	80/91 (88%)	80 (100%)	0	100	100
1	C1	80/91 (88%)	80 (100%)	0	100	100
1	C2	80/91 (88%)	80 (100%)	0	100	100
1	C4	80/91 (88%)	80 (100%)	0	100	100
1	C5	80/91 (88%)	80 (100%)	0	100	100
1	C6	80/91 (88%)	80 (100%)	0	100	100
1	C8	80/91 (88%)	80 (100%)	0	100	100
1	C9	80/91 (88%)	80 (100%)	0	100	100
1	CA	80/91 (88%)	80 (100%)	0	100	100
1	CC	80/91 (88%)	80 (100%)	0	100	100
1	CD	80/91 (88%)	80 (100%)	0	100	100
1	CE	80/91 (88%)	80 (100%)	0	100	100
1	CG	80/91 (88%)	80 (100%)	0	100	100
1	CH	80/91 (88%)	80 (100%)	0	100	100
1	CI	80/91 (88%)	80 (100%)	0	100	100
1	CK	80/91 (88%)	80 (100%)	0	100	100
1	CL	80/91 (88%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CM	80/91 (88%)	80 (100%)	0	100	100
1	CO	80/91 (88%)	80 (100%)	0	100	100
1	CP	80/91 (88%)	80 (100%)	0	100	100
1	CQ	80/91 (88%)	80 (100%)	0	100	100
1	CS	80/91 (88%)	80 (100%)	0	100	100
1	CT	80/91 (88%)	80 (100%)	0	100	100
1	CU	80/91 (88%)	80 (100%)	0	100	100
1	CW	80/91 (88%)	80 (100%)	0	100	100
1	CX	80/91 (88%)	80 (100%)	0	100	100
1	CY	80/91 (88%)	80 (100%)	0	100	100
1	D0	80/91 (88%)	80 (100%)	0	100	100
1	D1	80/91 (88%)	80 (100%)	0	100	100
1	D2	80/91 (88%)	80 (100%)	0	100	100
1	D4	80/91 (88%)	80 (100%)	0	100	100
1	D5	80/91 (88%)	80 (100%)	0	100	100
1	D6	80/91 (88%)	80 (100%)	0	100	100
1	D8	80/91 (88%)	80 (100%)	0	100	100
1	D9	80/91 (88%)	80 (100%)	0	100	100
1	DA	80/91 (88%)	80 (100%)	0	100	100
1	DC	80/91 (88%)	80 (100%)	0	100	100
1	DD	80/91 (88%)	80 (100%)	0	100	100
1	DE	80/91 (88%)	80 (100%)	0	100	100
1	DG	80/91 (88%)	80 (100%)	0	100	100
1	DH	80/91 (88%)	80 (100%)	0	100	100
1	DI	80/91 (88%)	80 (100%)	0	100	100
1	DK	80/91 (88%)	80 (100%)	0	100	100
1	DL	80/91 (88%)	80 (100%)	0	100	100
1	DM	80/91 (88%)	80 (100%)	0	100	100
1	DO	80/91 (88%)	79 (99%)	1 (1%)	69	86
1	DP	80/91 (88%)	80 (100%)	0	100	100
1	DQ	80/91 (88%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DS	80/91 (88%)	80 (100%)	0	100	100
1	DT	80/91 (88%)	80 (100%)	0	100	100
1	DU	80/91 (88%)	80 (100%)	0	100	100
1	DW	80/91 (88%)	80 (100%)	0	100	100
1	DX	80/91 (88%)	80 (100%)	0	100	100
1	DY	80/91 (88%)	80 (100%)	0	100	100
1	E	80/91 (88%)	80 (100%)	0	100	100
1	E0	80/91 (88%)	80 (100%)	0	100	100
1	E1	80/91 (88%)	80 (100%)	0	100	100
1	E2	80/91 (88%)	80 (100%)	0	100	100
1	E4	80/91 (88%)	80 (100%)	0	100	100
1	E5	80/91 (88%)	80 (100%)	0	100	100
1	E6	80/91 (88%)	80 (100%)	0	100	100
1	EA	80/91 (88%)	80 (100%)	0	100	100
1	EC	80/91 (88%)	80 (100%)	0	100	100
1	ED	80/91 (88%)	80 (100%)	0	100	100
1	EE	80/91 (88%)	80 (100%)	0	100	100
1	EG	80/91 (88%)	80 (100%)	0	100	100
1	EH	80/91 (88%)	80 (100%)	0	100	100
1	EI	80/91 (88%)	80 (100%)	0	100	100
1	EK	80/91 (88%)	80 (100%)	0	100	100
1	EL	80/91 (88%)	80 (100%)	0	100	100
1	EM	80/91 (88%)	80 (100%)	0	100	100
1	EO	80/91 (88%)	80 (100%)	0	100	100
1	EP	80/91 (88%)	80 (100%)	0	100	100
1	EQ	80/91 (88%)	80 (100%)	0	100	100
1	ES	80/91 (88%)	80 (100%)	0	100	100
1	ET	80/91 (88%)	80 (100%)	0	100	100
1	EU	80/91 (88%)	80 (100%)	0	100	100
1	EW	80/91 (88%)	80 (100%)	0	100	100
1	EX	80/91 (88%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EY	80/91 (88%)	80 (100%)	0	100	100
1	F	80/91 (88%)	80 (100%)	0	100	100
1	G	80/91 (88%)	80 (100%)	0	100	100
1	I	80/91 (88%)	80 (100%)	0	100	100
1	J	80/91 (88%)	80 (100%)	0	100	100
1	K	80/91 (88%)	80 (100%)	0	100	100
1	M	80/91 (88%)	80 (100%)	0	100	100
1	N	80/91 (88%)	80 (100%)	0	100	100
1	O	80/91 (88%)	80 (100%)	0	100	100
1	Q	80/91 (88%)	80 (100%)	0	100	100
1	R	80/91 (88%)	80 (100%)	0	100	100
1	S	80/91 (88%)	80 (100%)	0	100	100
1	U	80/91 (88%)	80 (100%)	0	100	100
1	V	80/91 (88%)	80 (100%)	0	100	100
1	W	80/91 (88%)	80 (100%)	0	100	100
1	Y	80/91 (88%)	80 (100%)	0	100	100
1	Z	80/91 (88%)	80 (100%)	0	100	100
1	a	80/91 (88%)	80 (100%)	0	100	100
1	b	80/91 (88%)	80 (100%)	0	100	100
1	c	80/91 (88%)	80 (100%)	0	100	100
1	e	80/91 (88%)	80 (100%)	0	100	100
1	f	80/91 (88%)	80 (100%)	0	100	100
1	g	80/91 (88%)	80 (100%)	0	100	100
1	i	80/91 (88%)	80 (100%)	0	100	100
1	j	80/91 (88%)	80 (100%)	0	100	100
1	k	80/91 (88%)	80 (100%)	0	100	100
1	m	80/91 (88%)	80 (100%)	0	100	100
1	n	80/91 (88%)	80 (100%)	0	100	100
1	o	80/91 (88%)	80 (100%)	0	100	100
1	q	80/91 (88%)	80 (100%)	0	100	100
1	r	80/91 (88%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	s	80/91 (88%)	80 (100%)	0	100	100
1	u	80/91 (88%)	80 (100%)	0	100	100
1	v	80/91 (88%)	80 (100%)	0	100	100
1	w	80/91 (88%)	80 (100%)	0	100	100
1	y	80/91 (88%)	80 (100%)	0	100	100
1	z	80/91 (88%)	80 (100%)	0	100	100
2	1	76/86 (88%)	76 (100%)	0	100	100
2	5	76/86 (88%)	76 (100%)	0	100	100
2	9	76/86 (88%)	76 (100%)	0	100	100
2	A3	76/86 (88%)	76 (100%)	0	100	100
2	A7	76/86 (88%)	76 (100%)	0	100	100
2	AB	76/86 (88%)	76 (100%)	0	100	100
2	AF	76/86 (88%)	76 (100%)	0	100	100
2	AJ	76/86 (88%)	76 (100%)	0	100	100
2	AN	76/86 (88%)	76 (100%)	0	100	100
2	AR	76/86 (88%)	76 (100%)	0	100	100
2	AV	76/86 (88%)	76 (100%)	0	100	100
2	AZ	76/86 (88%)	76 (100%)	0	100	100
2	B3	76/86 (88%)	76 (100%)	0	100	100
2	B7	76/86 (88%)	76 (100%)	0	100	100
2	BB	76/86 (88%)	76 (100%)	0	100	100
2	BF	76/86 (88%)	76 (100%)	0	100	100
2	BJ	76/86 (88%)	76 (100%)	0	100	100
2	BN	76/86 (88%)	76 (100%)	0	100	100
2	BR	76/86 (88%)	76 (100%)	0	100	100
2	BV	76/86 (88%)	76 (100%)	0	100	100
2	BZ	76/86 (88%)	76 (100%)	0	100	100
2	C3	76/86 (88%)	76 (100%)	0	100	100
2	C7	76/86 (88%)	76 (100%)	0	100	100
2	CB	76/86 (88%)	76 (100%)	0	100	100
2	CF	76/86 (88%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	CJ	76/86 (88%)	76 (100%)	0	100	100
2	CN	76/86 (88%)	76 (100%)	0	100	100
2	CR	76/86 (88%)	76 (100%)	0	100	100
2	CV	76/86 (88%)	76 (100%)	0	100	100
2	CZ	76/86 (88%)	76 (100%)	0	100	100
2	D	76/86 (88%)	76 (100%)	0	100	100
2	D3	76/86 (88%)	76 (100%)	0	100	100
2	D7	76/86 (88%)	76 (100%)	0	100	100
2	DB	76/86 (88%)	76 (100%)	0	100	100
2	DF	76/86 (88%)	76 (100%)	0	100	100
2	DJ	76/86 (88%)	76 (100%)	0	100	100
2	DN	76/86 (88%)	76 (100%)	0	100	100
2	DR	76/86 (88%)	76 (100%)	0	100	100
2	DV	76/86 (88%)	76 (100%)	0	100	100
2	DZ	76/86 (88%)	76 (100%)	0	100	100
2	E3	76/86 (88%)	76 (100%)	0	100	100
2	E7	76/86 (88%)	76 (100%)	0	100	100
2	EB	76/86 (88%)	76 (100%)	0	100	100
2	EF	76/86 (88%)	76 (100%)	0	100	100
2	EJ	76/86 (88%)	76 (100%)	0	100	100
2	EN	76/86 (88%)	76 (100%)	0	100	100
2	ER	76/86 (88%)	76 (100%)	0	100	100
2	EV	76/86 (88%)	76 (100%)	0	100	100
2	EZ	76/86 (88%)	76 (100%)	0	100	100
2	H	76/86 (88%)	76 (100%)	0	100	100
2	L	76/86 (88%)	76 (100%)	0	100	100
2	P	76/86 (88%)	76 (100%)	0	100	100
2	T	76/86 (88%)	76 (100%)	0	100	100
2	X	76/86 (88%)	76 (100%)	0	100	100
2	d	76/86 (88%)	76 (100%)	0	100	100
2	h	76/86 (88%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	l	76/86 (88%)	76 (100%)	0	100	100
2	p	76/86 (88%)	76 (100%)	0	100	100
2	t	76/86 (88%)	76 (100%)	0	100	100
2	x	76/86 (88%)	76 (100%)	0	100	100
All	All	18960/21540 (88%)	18958 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BS	34	TYR
1	DO	34	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 194 such sidechains are listed below:

Mol	Chain	Res	Type
1	CL	71	GLN
1	DH	71	GLN
1	CP	84	ASN
1	C1	71	GLN
1	DP	71	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 [i](#)

There are no chain breaks in this entry.

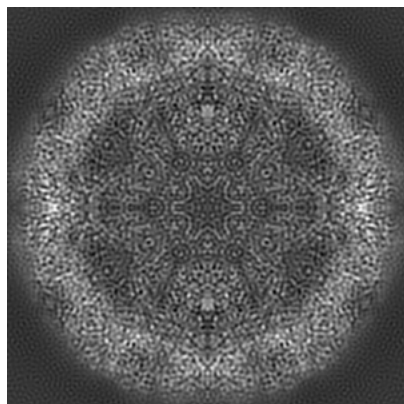
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20207. These allow visual inspection of the internal detail of the map and identification of artifacts.

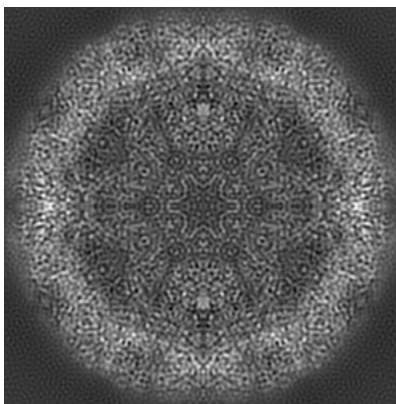
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

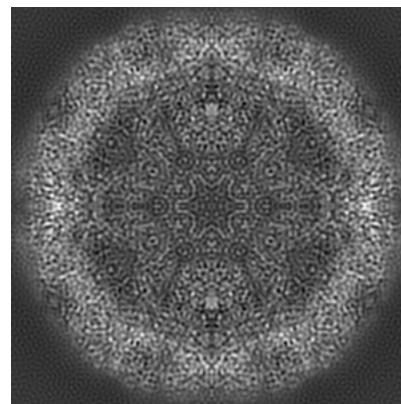
6.1.1 Primary map



X

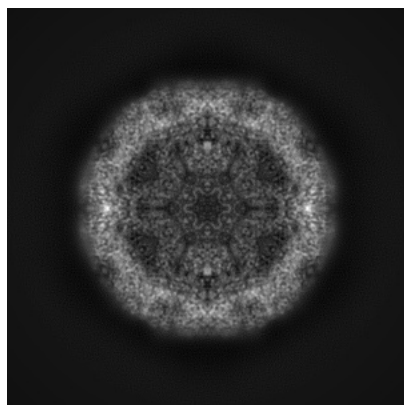


Y

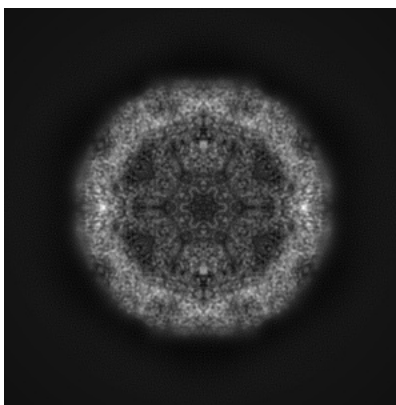


Z

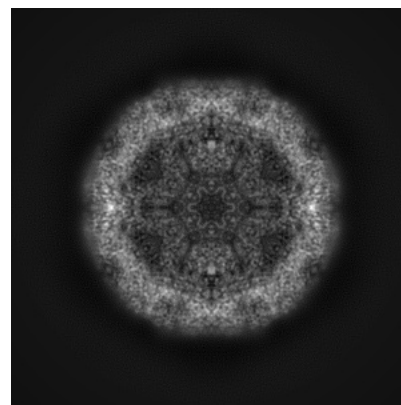
6.1.2 Raw map



X



Y

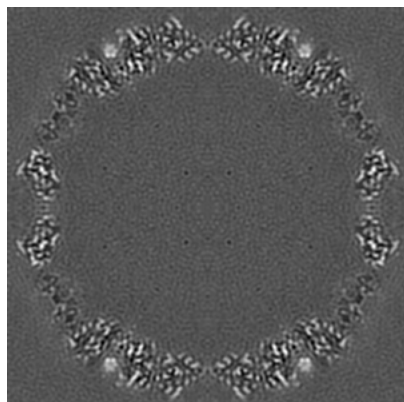


Z

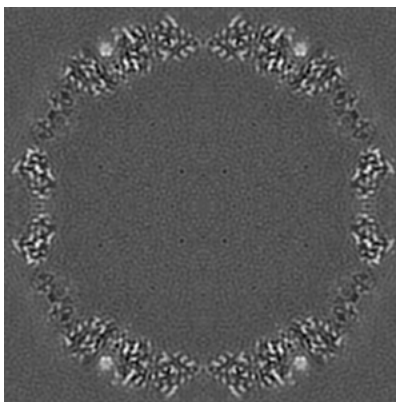
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

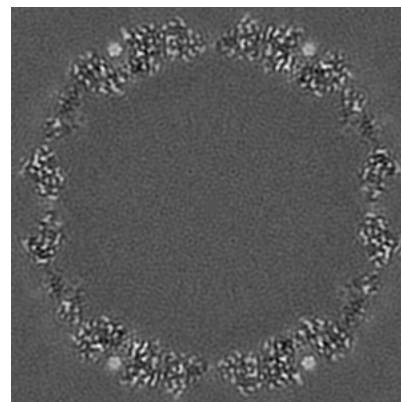
6.2.1 Primary map



X Index: 138

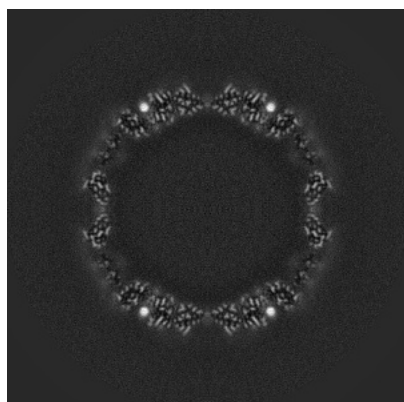


Y Index: 138

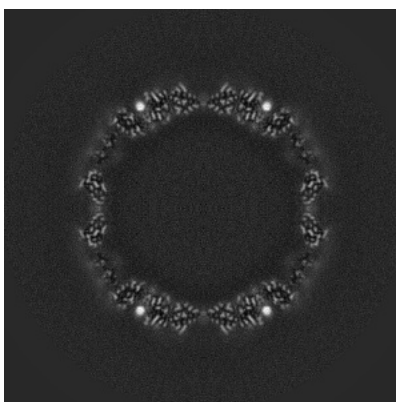


Z Index: 138

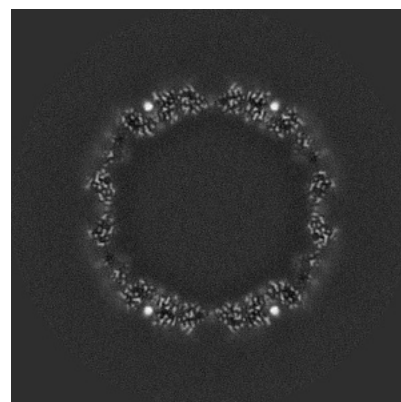
6.2.2 Raw map



X Index: 212



Y Index: 212

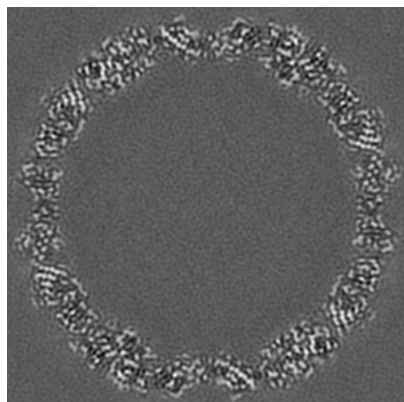


Z Index: 212

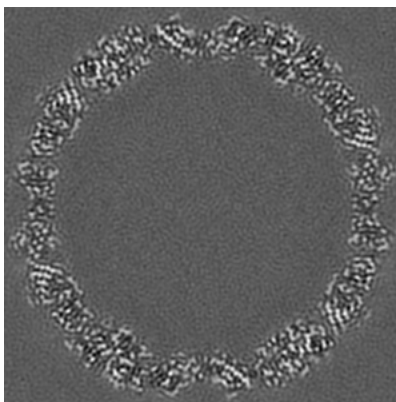
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

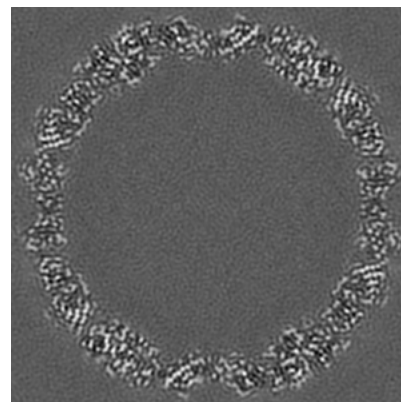
6.3.1 Primary map



X Index: 125

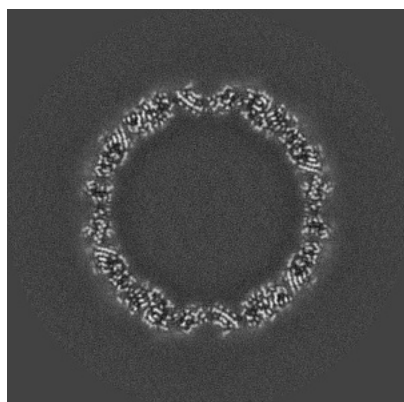


Y Index: 125

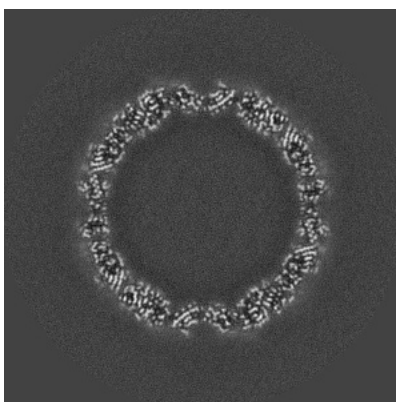


Z Index: 150

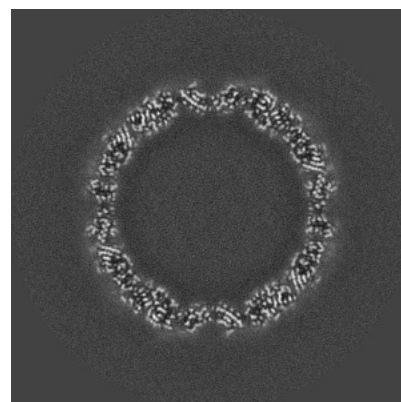
6.3.2 Raw map



X Index: 199



Y Index: 225

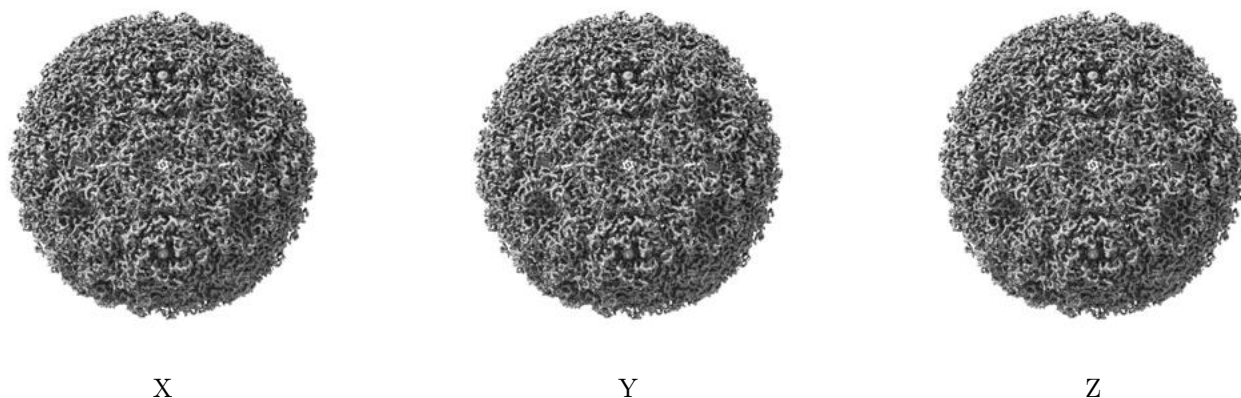


Z Index: 198

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

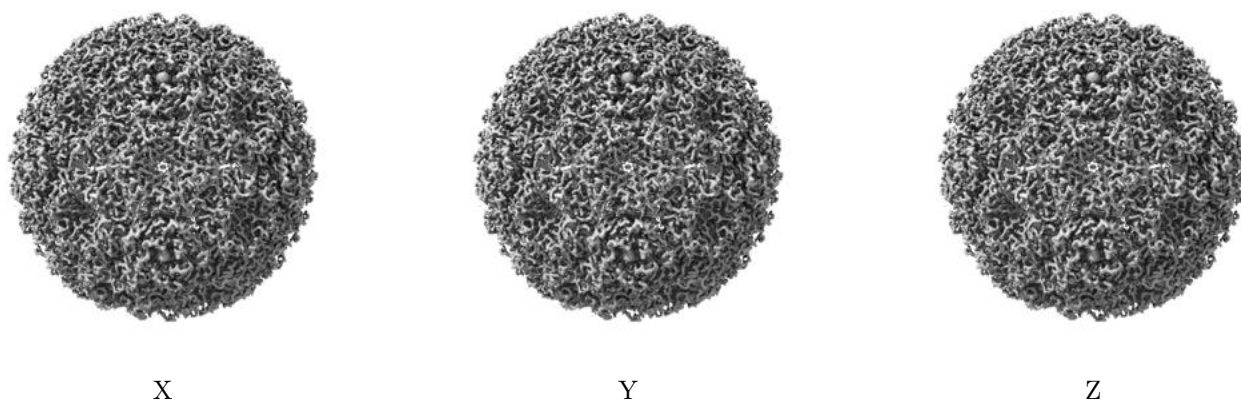
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

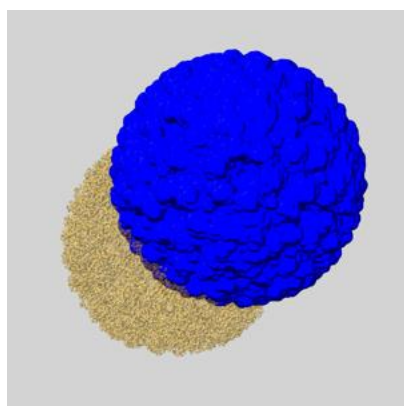
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

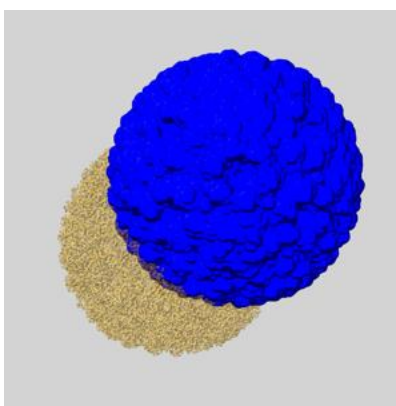
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

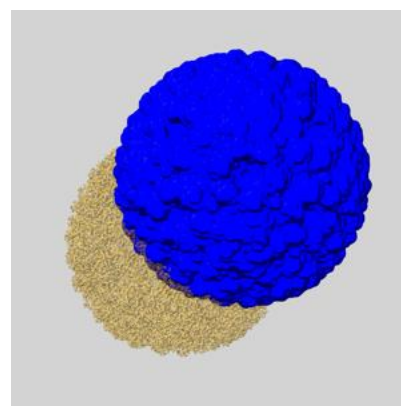
6.5.1 emd_20207_msk_1.map [i](#)



X



Y

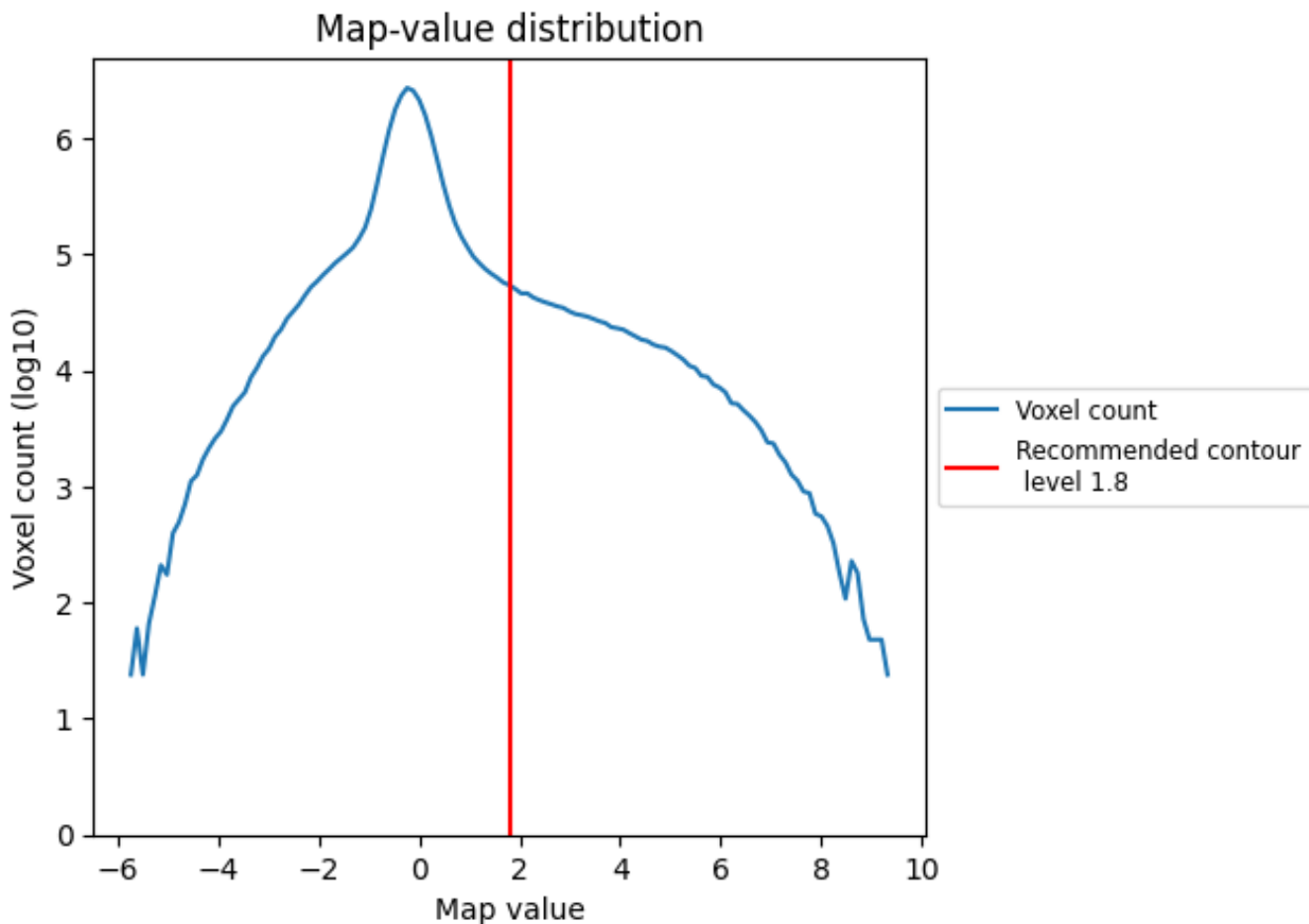


Z

7 Map analysis [i](#)

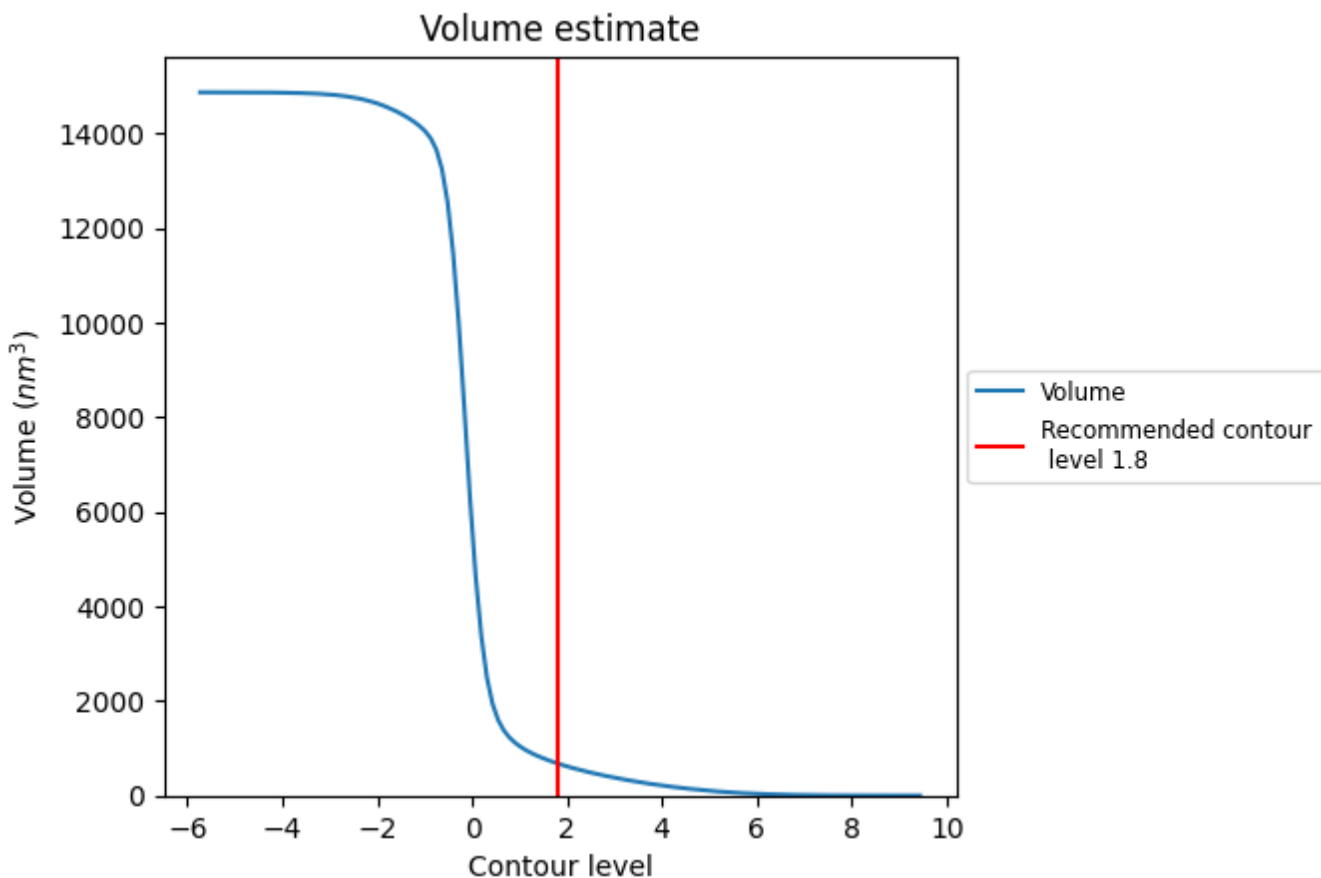
This section contains the results of statistical analysis of the map.

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.

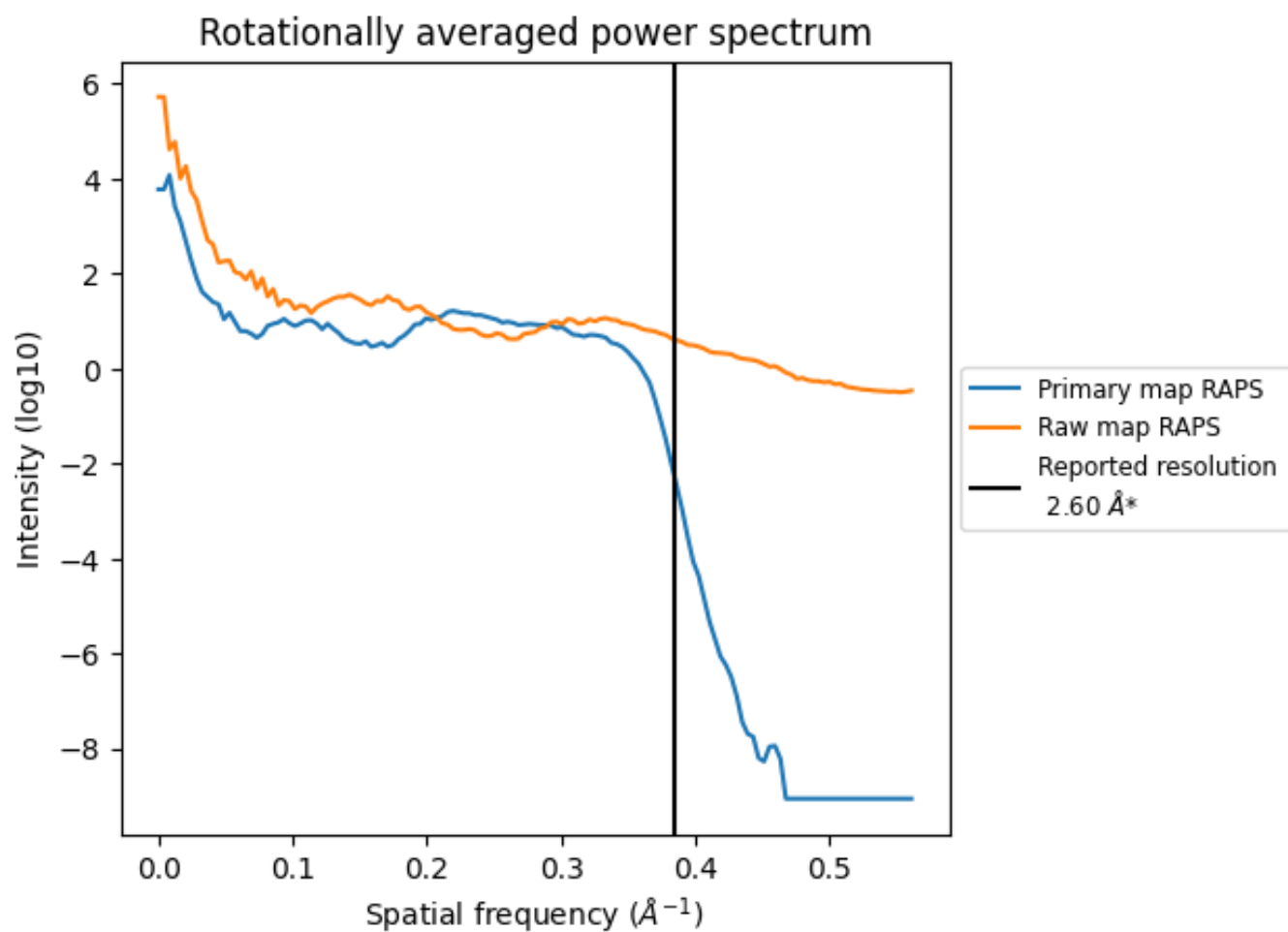
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 678 nm³; this corresponds to an approximate mass of 613 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

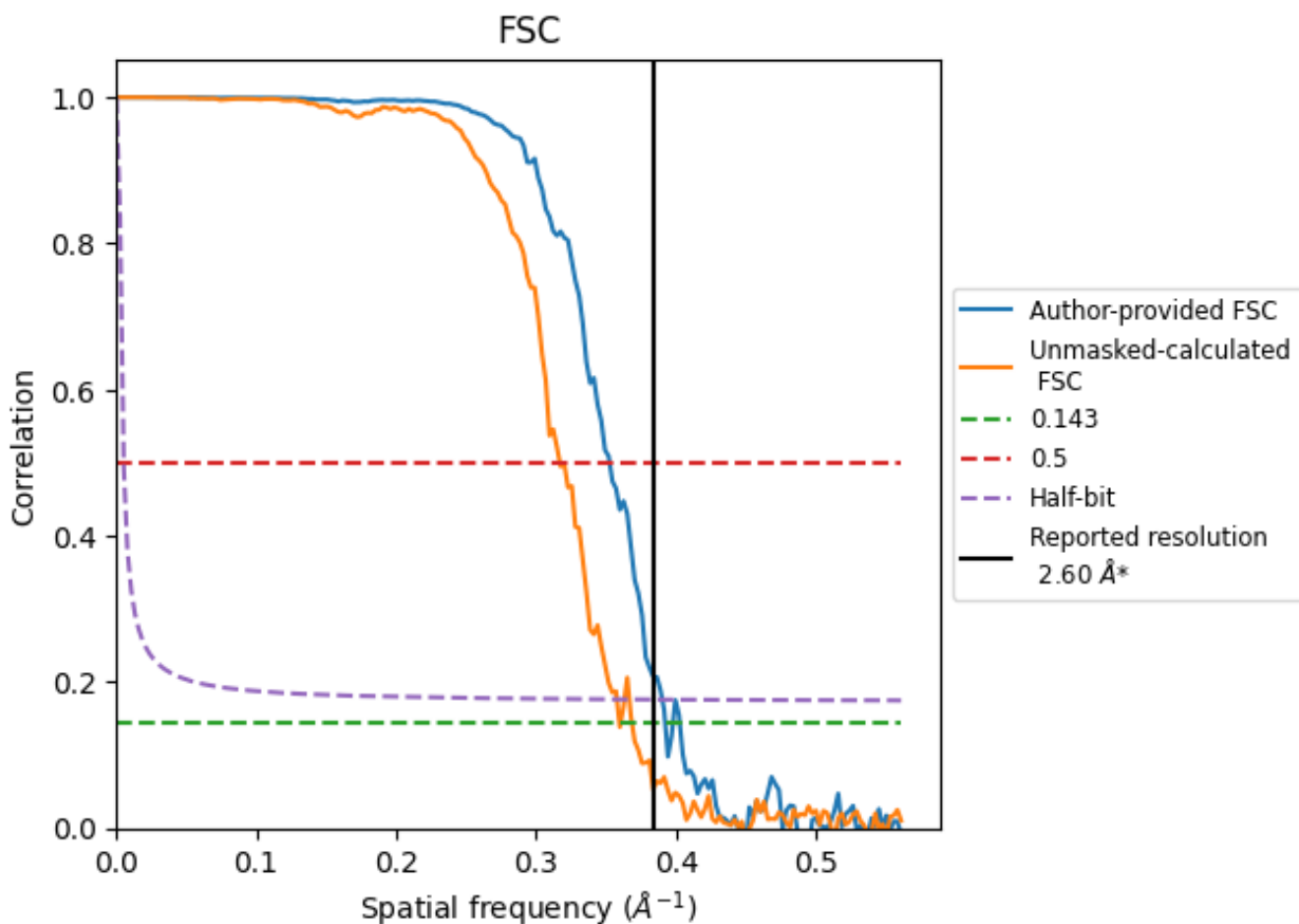


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

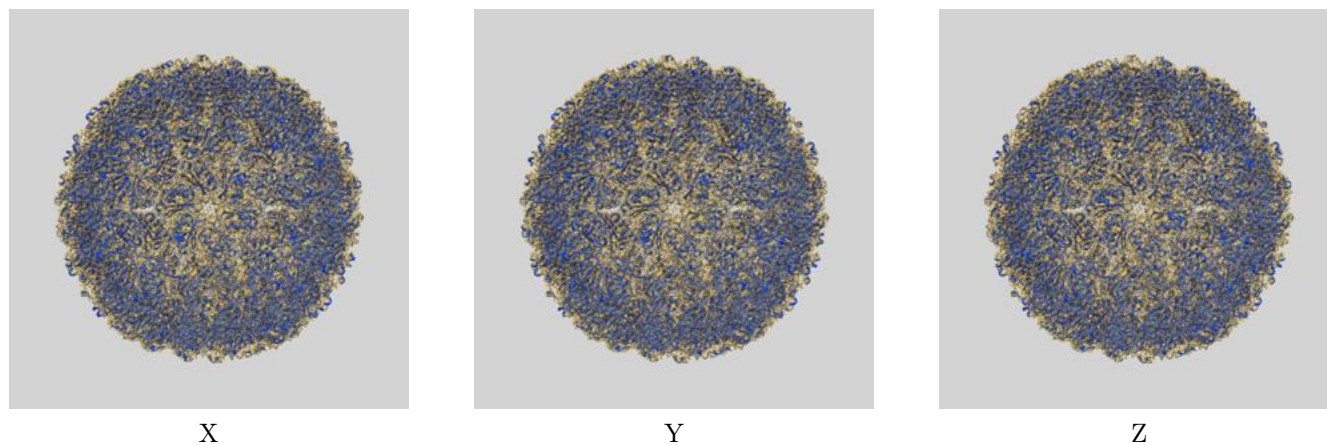
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.55	2.83	2.56
Unmasked-calculated*	2.78	3.15	2.79

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20207 and PDB model 6OWG. Per-residue inclusion information can be found in section 3 on page 40.

9.1 Map-model overlay [i](#)

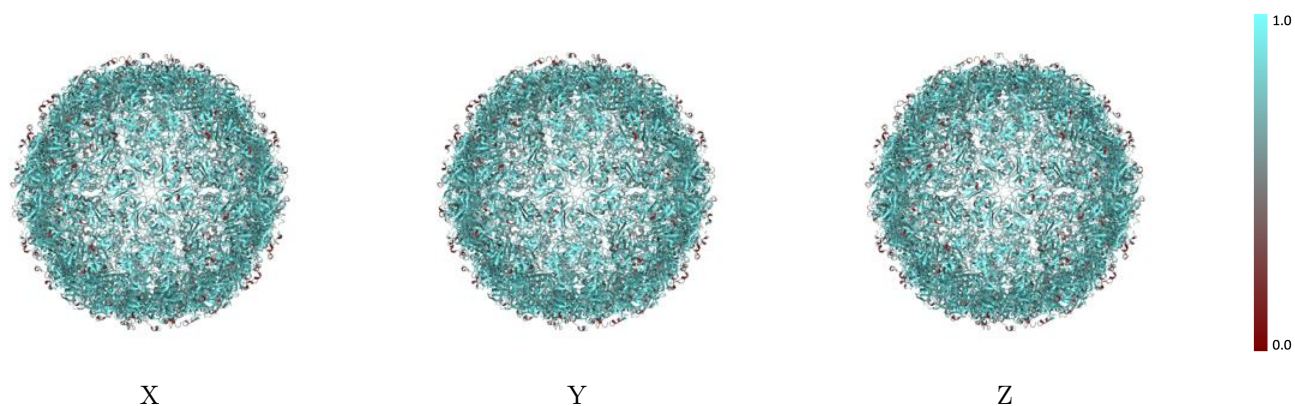


The images above show the 3D surface view of the map at the recommended contour level 1.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

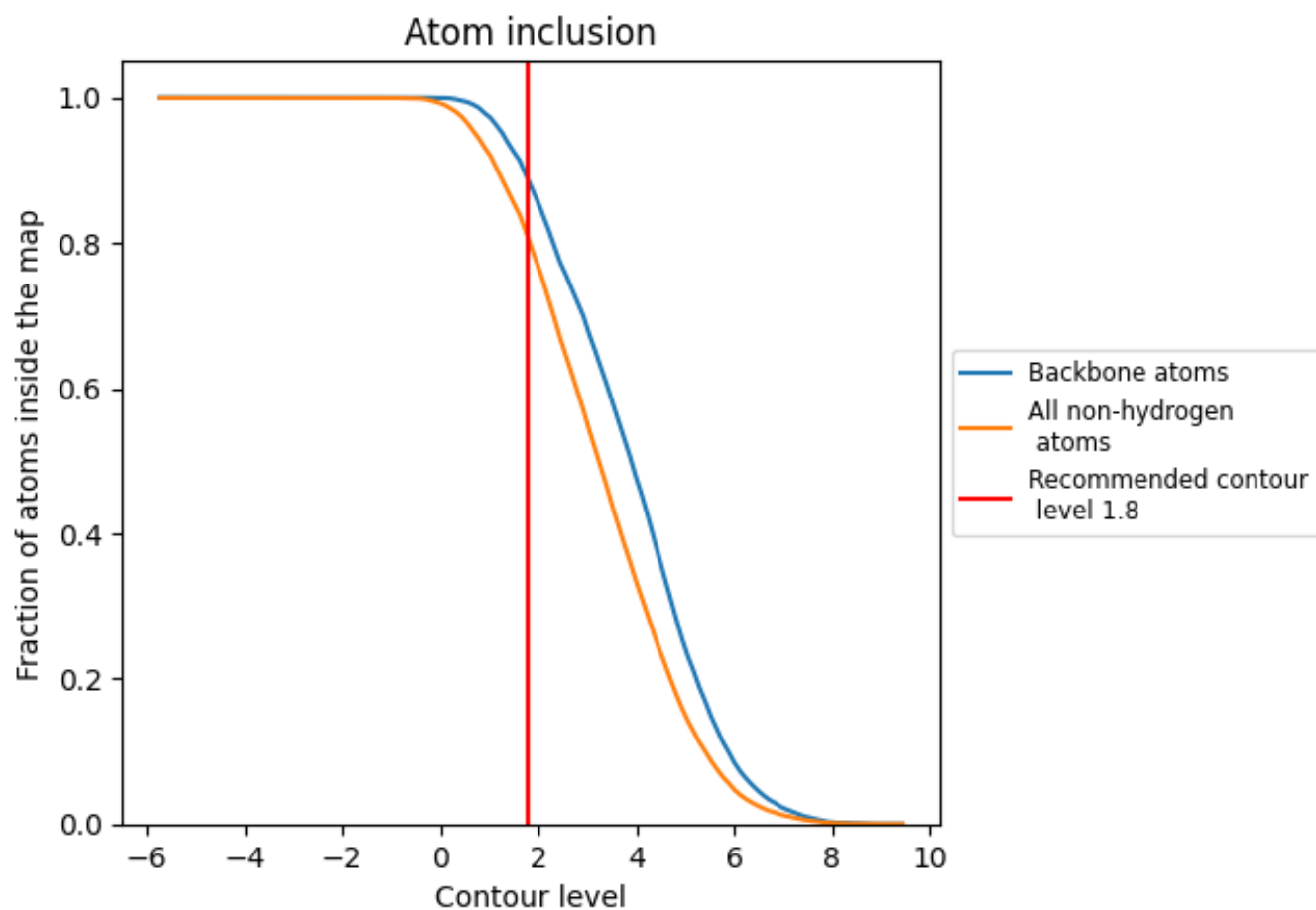
This section was not generated.

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 (1.8).




































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary











































The table lists the average atom inclusion at the recommended contour level (1.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	 0.8054
0	 0.7810
1	 0.8381
2	 0.8054
3	 0.8082
4	 0.7837
5	 0.8338
6	 0.8082
7	 0.8095
8	 0.7864
9	 0.8324
A	 0.7986
A0	 0.8054
A1	 0.8082
A2	 0.7837
A3	 0.8367
A4	 0.8068
A5	 0.8095
A6	 0.7850
A7	 0.8381
A8	 0.8068
A9	 0.8082
AA	 0.7782
AB	 0.8352
AC	 0.8014
AD	 0.8136
AE	 0.7728
AF	 0.8338
AG	 0.7986
AH	 0.8109
AI	 0.7810
AJ	 0.8338
AK	 0.7959
AL	 0.8041
AM	 0.7782













































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Chain	Atom inclusion
AN	 0.8324
AO	 0.7973
AP	 0.8095
AQ	 0.7796
AR	 0.8352
AS	 0.8014
AT	 0.8068
AU	 0.7769
AV	 0.8338
AW	 0.8014
AX	 0.8109
AY	 0.7714
AZ	 0.8367
B	 0.8095
B0	 0.7973
B1	 0.8095
B2	 0.7741
B3	 0.8352
B4	 0.8000
B5	 0.8122
B6	 0.7782
B7	 0.8338
B8	 0.7986
B9	 0.8054
BA	 0.7837
BB	 0.8410
BC	 0.8014
BD	 0.8082
BE	 0.7782
BF	 0.8352
BG	 0.8041
BH	 0.8095
BI	 0.7741
BJ	 0.8295
BK	 0.7973
BL	 0.8109
BM	 0.7769
BN	 0.8338
BO	 0.8027
BP	 0.8082
BQ	 0.7796
BR	 0.8309











































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Chain	Atom inclusion
BS	 0.8014
BT	 0.8122
BU	 0.7755
BV	 0.8324
BW	 0.7986
BX	 0.8122
BY	 0.7782
BZ	 0.8324
C	 0.7810
C0	 0.8014
C1	 0.8082
C2	 0.7782
C3	 0.8324
C4	 0.7986
C5	 0.8082
C6	 0.7796
C7	 0.8324
C8	 0.8000
C9	 0.8122
CA	 0.7796
CB	 0.8309
CC	 0.7973
CD	 0.8054
CE	 0.7810
CF	 0.8367
CG	 0.7959
CH	 0.8027
CI	 0.7810
CJ	 0.8381
CK	 0.7973
CL	 0.8027
CM	 0.7837
CN	 0.8381
CO	 0.8068
CP	 0.8095
CQ	 0.7837
CR	 0.8367
CS	 0.8041
CT	 0.8082
CU	 0.7864
CV	 0.8395
CW	 0.8082











































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Chain	Atom inclusion
CX	 0.8082
CY	 0.7850
CZ	 0.8352
D	 0.8324
D0	 0.8000
D1	 0.8136
D2	 0.7769
D3	 0.8367
D4	 0.8000
D5	 0.8054
D6	 0.7796
D7	 0.8324
D8	 0.7986
D9	 0.8122
DA	 0.7755
DB	 0.8338
DC	 0.8000
DD	 0.8014
DE	 0.7782
DF	 0.8352
DG	 0.7986
DH	 0.8041
DI	 0.7823
DJ	 0.8381
DK	 0.8000
DL	 0.8014
DM	 0.7810
DN	 0.8352
DO	 0.8041
DP	 0.8109
DQ	 0.7728
DR	 0.8338
DS	 0.7986
DT	 0.8109
DU	 0.7810
DV	 0.8338
DW	 0.8000
DX	 0.8068
DY	 0.7796
DZ	 0.8352
E	 0.8014
E0	 0.7946

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Chain	Atom inclusion
E1	 0.8054
E2	 0.7796
E3	 0.8367
E4	 0.8000
E5	 0.8136
E6	 0.7769
E7	 0.8367
EA	 0.7769
EB	 0.8338
EC	 0.8054
ED	 0.8095
EE	 0.7850
EF	 0.8410
EG	 0.8054
EH	 0.8068
EI	 0.7823
EJ	 0.8352
EK	 0.8068
EL	 0.8082
EM	 0.7864
EN	 0.8338
EO	 0.7959
EP	 0.8054
EQ	 0.7810
ER	 0.8309
ES	 0.7973
ET	 0.8109
EU	 0.7728
EV	 0.8367
EW	 0.7986
EX	 0.8109
EY	 0.7782
EZ	 0.8324
F	 0.8109
G	 0.7728
H	 0.8352
I	 0.7973
J	 0.8122
K	 0.7796
L	 0.8338
M	 0.7959
N	 0.8041

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Chain	Atom inclusion
O	0.7782
P	0.8338
Q	0.7973
R	0.8027
S	0.7810
T	0.8381
U	0.7986
V	0.8027
W	0.7823
X	0.8381
Y	0.7986
Z	0.8041
a	0.8068
b	0.8068
c	0.7823
d	0.8338
e	0.7986
f	0.8122
g	0.7782
h	0.8324
i	0.7986
j	0.8068
k	0.7796
l	0.8367
m	0.8027
n	0.8095
o	0.7714
p	0.8338
q	0.7959
r	0.8014
s	0.7823
t	0.8381
u	0.7986
v	0.8041
w	0.7810
x	0.8367
y	0.7973
z	0.8041