



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 01:37 AM UTC

PDB ID : 5V74 / pdb_00005v74
Title : Structure of the intact Haliangium ochraceum microcompartment shell
Authors : Sutter, M.; Kerfeld, C.A.
Deposited on : 2017-03-17
Resolution : 3.51 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

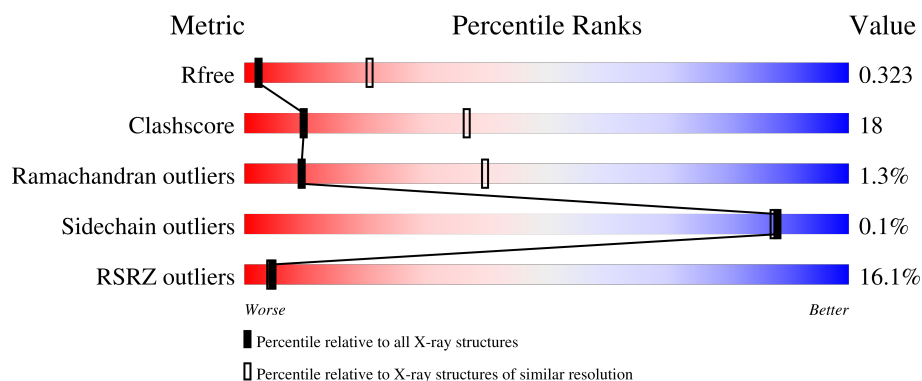
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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.



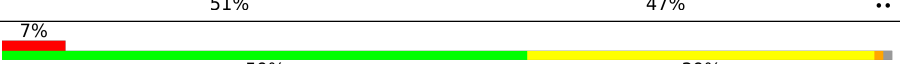
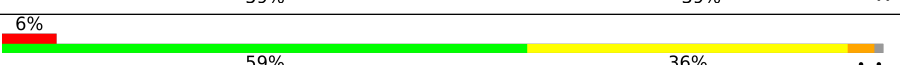
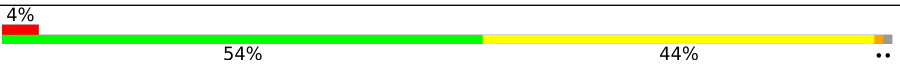
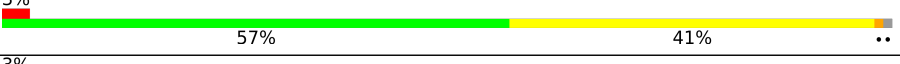
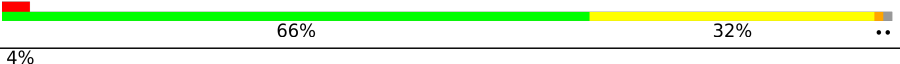
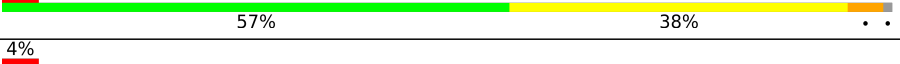
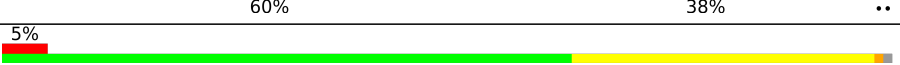
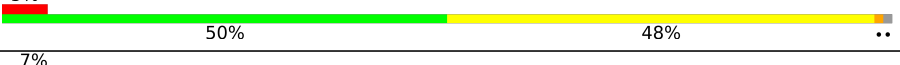
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	11	96	3% 59%36% ..
1	21	96	5% 63%35% ..
1	31	96	4% 48%46% ..
1	41	96	3% 65%32% ..
1	A1	96	5% 51%45% ..

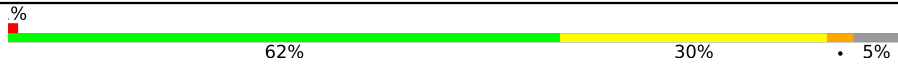
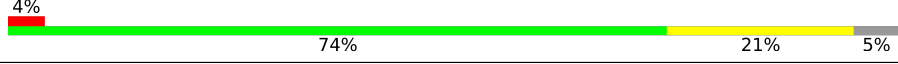
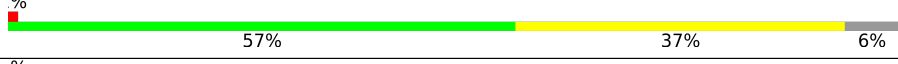
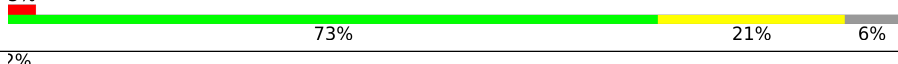
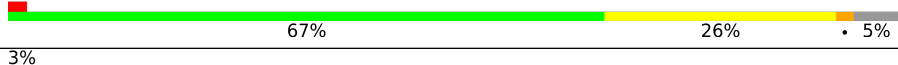
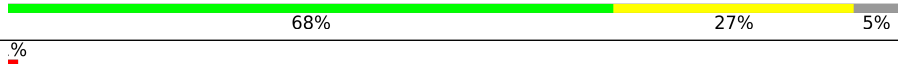
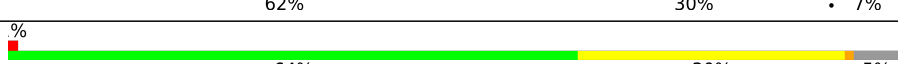
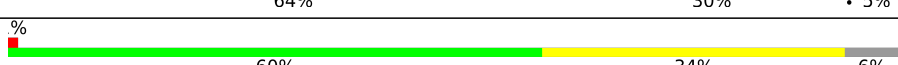
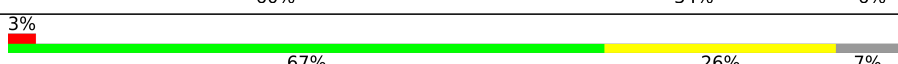
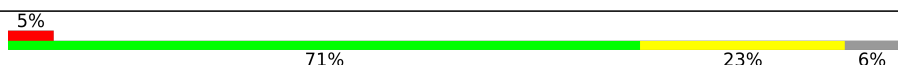
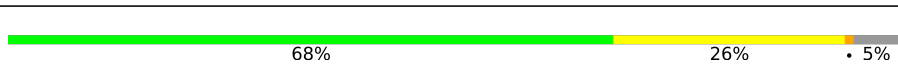
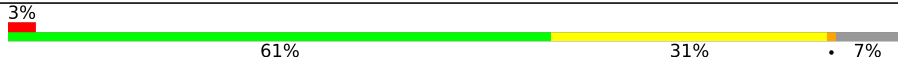
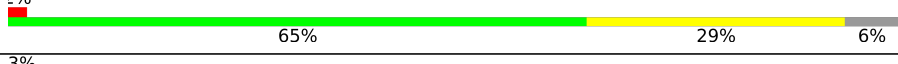
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Mol	Chain	Length	Quality of chain	
1	B1	96	5% 	..
1	C1	96	3% 	..
1	D1	96	5% 	..
1	E1	96	4% 	..
1	F1	96	3% 	..
1	G1	96	5% 	..
1	H1	96	7% 	..
1	I1	96	6% 	..
1	J1	96	4% 	..
1	K1	96	3% 	..
1	L1	96	3% 	..
1	M1	96	3% 	..
1	N1	96	4% 	..
1	O1	96	4% 	..
1	P1	96	5% 	..
1	Q1	96	5% 	..
1	R1	96	3% 	..
1	S1	96	6% 	..
1	T1	96	7% 	..
1	U1	96	4% 	..
1	V1	96	5% 	..
1	W1	96	7% 	..
1	X1	96	3% 	..
1	Y1	96	4% 	..
1	Z1	96	4% 	..

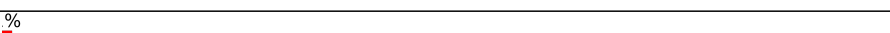
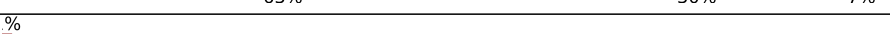
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Mol	Chain	Length	Quality of chain
2	12	99	
2	13	99	
2	14	99	
2	15	99	
2	16	99	
2	17	99	
2	22	99	
2	23	99	
2	24	99	
2	25	99	
2	26	99	
2	27	99	
2	32	99	
2	33	99	
2	34	99	
2	35	99	
2	36	99	
2	37	99	
2	42	99	
2	43	99	
2	44	99	
2	45	99	
2	46	99	
2	47	99	
2	A2	99	

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Mol	Chain	Length	Quality of chain
2	A3	99	
2	A4	99	
2	A5	99	
2	A6	99	
2	A7	99	
2	B2	99	
2	B3	99	
2	B4	99	
2	B5	99	
2	B6	99	
2	B7	99	
2	C2	99	
2	C3	99	
2	C4	99	
2	C5	99	
2	C6	99	
2	C7	99	
2	D2	99	
2	D3	99	
2	D4	99	
2	D5	99	
2	D6	99	
2	D7	99	
2	E2	99	
2	E3	99	

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Mol	Chain	Length	Quality of chain
2	E4	99	
2	E5	99	
2	E6	99	
2	E7	99	
2	F2	99	
2	F3	99	
2	F4	99	
2	F5	99	
2	F6	99	
2	F7	99	
2	G2	99	
2	G3	99	
2	G4	99	
2	G5	99	
2	G6	99	
2	G7	99	
2	H2	99	
2	H3	99	
2	H4	99	
2	H5	99	
2	H6	99	
2	H7	99	
2	I2	99	
2	I3	99	
2	I4	99	

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Mol	Chain	Length	Quality of chain
2	I5	99	
2	I6	99	
2	I7	99	
2	J2	99	
2	J3	99	
2	J4	99	
2	J5	99	
2	J6	99	
2	J7	99	
2	K2	99	
2	K3	99	
2	K4	99	
2	K5	99	
2	K6	99	
2	K7	99	
2	L2	99	
2	L3	99	
2	L4	99	
2	L5	99	
2	L6	99	
2	L7	99	
2	M2	99	
2	M3	99	
2	M4	99	
2	M5	99	

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Mol	Chain	Length	Quality of chain
2	M6	99	
2	M7	99	
2	N2	99	
2	N3	99	
2	N4	99	
2	N5	99	
2	N6	99	
2	N7	99	
2	O2	99	
2	O3	99	
2	O4	99	
2	O5	99	
2	O6	99	
2	O7	99	
2	P2	99	
2	P3	99	
2	P4	99	
2	P5	99	
2	P6	99	
2	P7	99	
2	Q2	99	
2	Q3	99	
2	Q4	99	
2	Q5	99	
2	Q6	99	

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Mol	Chain	Length	Quality of chain
2	Q7	99	
2	R2	99	
2	R3	99	
2	R4	99	
2	R5	99	
2	R6	99	
2	R7	99	
2	S2	99	
2	S3	99	
2	S4	99	
2	S5	99	
2	S6	99	
2	S7	99	
2	T2	99	
2	T3	99	
2	T4	99	
2	T5	99	
2	T6	99	
2	T7	99	
2	U2	99	
2	U3	99	
2	U4	99	
2	U5	99	
2	U6	99	
2	U7	99	

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Mol	Chain	Length	Quality of chain
2	V2	99	
2	V3	99	
2	V4	99	
2	V5	99	
2	V6	99	
2	V7	99	
2	W2	99	
2	W3	99	
2	W4	99	
2	W5	99	
2	W6	99	
2	W7	99	
2	X2	99	
2	X3	99	
2	X4	99	
2	X5	99	
2	X6	99	
2	X7	99	
2	Y2	99	
2	Y3	99	
2	Y4	99	
2	Y5	99	
2	Y6	99	
2	Y7	99	
2	Z2	99	

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Mol	Chain	Length	Quality of chain
2	Z3	99	
2	Z4	99	
2	Z5	99	
2	Z6	99	
2	Z7	99	
3	18	212	
3	19	212	
3	28	212	
3	29	212	
3	38	212	
3	39	212	
3	48	212	
3	49	212	
3	A8	212	
3	A9	212	
3	B8	212	
3	B9	212	
3	C8	212	
3	C9	212	
3	D8	212	
3	D9	212	
3	E8	212	
3	E9	212	
3	F8	212	
3	F9	212	

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Mol	Chain	Length	Quality of chain
3	G8	212	
3	G9	212	
3	H8	212	
3	H9	212	
3	I8	212	
3	I9	212	
3	J8	212	
3	J9	212	
3	K8	212	
3	K9	212	
3	L8	212	
3	L9	212	
3	M8	212	
3	M9	212	
3	N8	212	
3	N9	212	
3	O8	212	
3	O9	212	
3	P8	212	
3	P9	212	
3	Q8	212	
3	Q9	212	
3	R8	212	
3	R9	212	
3	S8	212	

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Mol	Chain	Length	Quality of chain
3	S9	212	
3	T8	212	
3	T9	212	
3	U8	212	
3	U9	212	
3	V8	212	
3	V9	212	
3	W8	212	
3	W9	212	
3	X8	212	
3	X9	212	
3	Y8	212	
3	Y9	212	
3	Z8	212	
3	Z9	212	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 215283 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Ethanolamine utilization protein EutN/carboxysome structural protein Ccml.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	B1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	C1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	D1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	E1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	F1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	G1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	H1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	I1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	J1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	K1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	L1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	M1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	N1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	O1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	P1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q1	95	Total 678	C 419	N 122	O 132	S 5	0	0	0
1	R1	95	Total 678	C 419	N 122	O 132	S 5	0	0	0
1	S1	95	Total 678	C 419	N 122	O 132	S 5	0	0	0
1	T1	95	Total 678	C 419	N 122	O 132	S 5	0	0	0
1	U1	95	Total 678	C 419	N 122	O 132	S 5	0	0	0
1	V1	95	Total 678	C 419	N 122	O 132	S 5	0	0	0
1	W1	95	Total 678	C 419	N 122	O 132	S 5	0	0	0
1	X1	95	Total 678	C 419	N 122	O 132	S 5	0	0	0
1	Y1	95	Total 678	C 419	N 122	O 132	S 5	0	0	0
1	Z1	95	Total 678	C 419	N 122	O 132	S 5	0	0	0
1	11	95	Total 678	C 419	N 122	O 132	S 5	0	0	0
1	21	95	Total 678	C 419	N 122	O 132	S 5	0	0	0
1	31	94	Total 669	C 413	N 120	O 131	S 5	0	0	0
1	41	95	Total 678	C 419	N 122	O 132	S 5	0	0	0

- Molecule 2 is a protein called Microcompartments protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A2	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	A3	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	A4	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	A5	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	A6	92	Total 658	C 413	N 120	O 122	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A7	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	B2	91	Total 651	C 408	N 119	O 121	S 3	0	0	0
2	B3	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	B4	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	B5	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	B6	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	B7	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	C2	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	C3	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	C4	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	C5	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	C6	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	C7	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	D2	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	D3	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	D4	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	D5	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	D6	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	D7	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	E2	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	E3	92	Total 658	C 413	N 120	O 122	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E4	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	E5	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	E6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	E7	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	F2	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	F3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	F4	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	F5	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	F6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	F7	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	G2	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	G3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	G4	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	G5	91	Total	C	N	O	S	0	0	0
			653	410	119	121	3			
2	G6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	G7	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	H2	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	H3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	H4	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	H5	91	Total	C	N	O	S	0	0	0
			653	410	119	121	3			
2	H6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H7	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	I2	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	I3	91	Total	C	N	O	S	0	0	0
			653	410	119	121	3			
2	I4	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	I5	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	I6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	I7	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	J2	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	J3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	J4	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	J5	91	Total	C	N	O	S	0	0	0
			653	410	119	121	3			
2	J6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	J7	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	K2	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	K3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	K4	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	K5	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	K6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	K7	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	L2	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	L3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L4	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	L5	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	L6	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	L7	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	M2	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	M3	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	M4	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	M5	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	M6	91	Total 653	C 410	N 119	O 121	S 3	0	0	0
2	M7	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	N2	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	N3	91	Total 653	C 410	N 119	O 121	S 3	0	0	0
2	N4	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	N5	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	N6	91	Total 653	C 410	N 119	O 121	S 3	0	0	0
2	N7	92	Total 657	C 412	N 120	O 122	S 3	0	0	0
2	O2	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	O3	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	O4	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	O5	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	O6	92	Total 658	C 413	N 120	O 122	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O7	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	P2	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	P3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	P4	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	P5	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	P6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	P7	91	Total	C	N	O	S	0	0	0
			649	408	119	119	3			
2	Q2	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	Q3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	Q4	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	Q5	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	Q6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	Q7	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	R2	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	R3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	R4	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	R5	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	R6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	R7	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	S2	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	S3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S4	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	S5	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	S6	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	S7	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	T2	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	T3	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	T4	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	T5	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	T6	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	T7	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	U2	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	U3	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	U4	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	U5	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	U6	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	U7	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	V2	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	V3	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	V4	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	V5	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	V6	92	Total 658	C 413	N 120	O 122	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V7	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	W2	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	W3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	W4	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	W5	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	W6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	W7	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	X2	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	X3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	X4	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	X5	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	X6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	X7	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	Y2	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	Y3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	Y4	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	Y5	92	Total	C	N	O	S	0	0	0
			657	412	120	122	3			
2	Y6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	Y7	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	Z2	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	Z3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z4	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	Z5	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	Z6	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	Z7	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	12	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	13	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	14	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	15	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	16	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	17	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	22	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	23	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	24	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	25	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	26	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	27	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	32	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	33	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	34	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	35	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	36	92	Total 658	C 413	N 120	O 122	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	37	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	42	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	43	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	44	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	45	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	46	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	47	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			

- Molecule 3 is a protein called Microcompartments protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	A9	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	B8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	B9	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	C8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	C9	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	D8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	D9	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	E8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	E9	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	F8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	F9	203	Total	C	N	O		0	0	0
			1000	594	203	203				

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	G9	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	H8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	H9	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	I8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	I9	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	J8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	J9	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	K8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	K9	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	L8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	L9	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	M8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	M9	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	N8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	N9	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	O8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	O9	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	P8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	P9	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	Q8	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q9	203	Total	C	N	O	0	0	0
			1000	594	203	203			
3	R8	203	Total	C	N	O	0	0	0
			1533	977	266	287			
3	R9	203	Total	C	N	O	0	0	0
			1000	594	203	203			
3	S8	203	Total	C	N	O	0	0	0
			1533	977	266	287			
3	S9	203	Total	C	N	O	0	0	0
			1000	594	203	203			
3	T8	203	Total	C	N	O	0	0	0
			1533	977	266	287			
3	T9	203	Total	C	N	O	0	0	0
			1000	594	203	203			
3	U8	203	Total	C	N	O	0	0	0
			1533	977	266	287			
3	U9	203	Total	C	N	O	0	0	0
			1000	594	203	203			
3	V8	203	Total	C	N	O	0	0	0
			1533	977	266	287			
3	V9	203	Total	C	N	O	0	0	0
			1000	594	203	203			
3	W8	203	Total	C	N	O	0	0	0
			1533	977	266	287			
3	W9	203	Total	C	N	O	0	0	0
			1000	594	203	203			
3	X8	203	Total	C	N	O	0	0	0
			1533	977	266	287			
3	X9	203	Total	C	N	O	0	0	0
			1000	594	203	203			
3	Y8	203	Total	C	N	O	0	0	0
			1533	977	266	287			
3	Y9	203	Total	C	N	O	0	0	0
			1000	594	203	203			
3	Z8	203	Total	C	N	O	0	0	0
			1533	977	266	287			
3	Z9	203	Total	C	N	O	0	0	0
			1000	594	203	203			
3	18	203	Total	C	N	O	0	0	0
			1533	977	266	287			
3	19	198	Total	C	N	O	0	0	0
			975	579	198	198			

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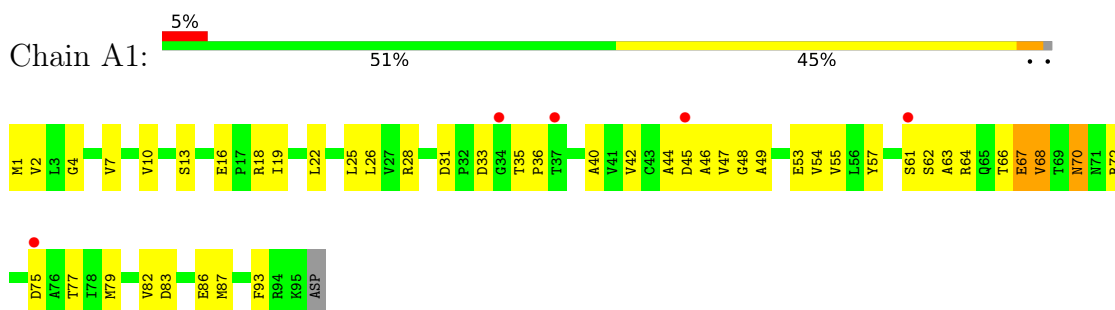
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	28	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	29	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	38	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	39	203	Total	C	N	O		0	0	0
			1000	594	203	203				
3	48	203	Total	C	N	O	S	0	0	0
			1533	977	266	287	3			
3	49	203	Total	C	N	O		0	0	0
			1000	594	203	203				

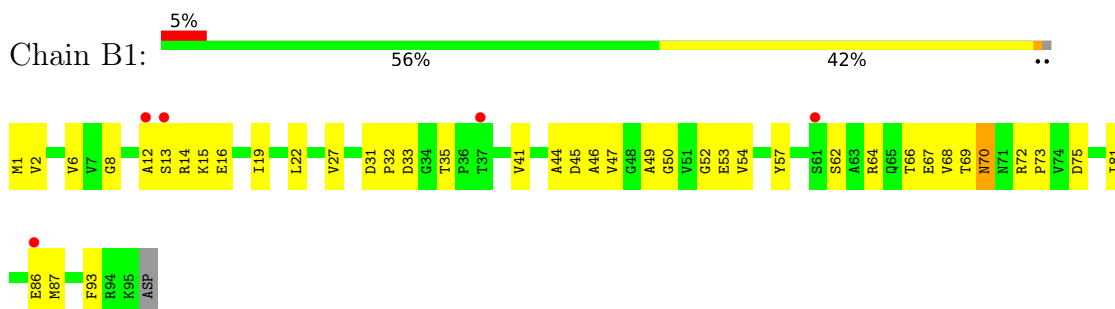
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

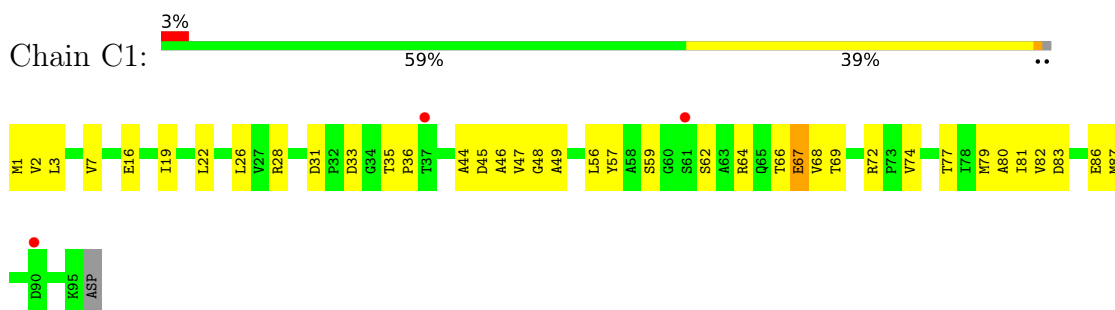
- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

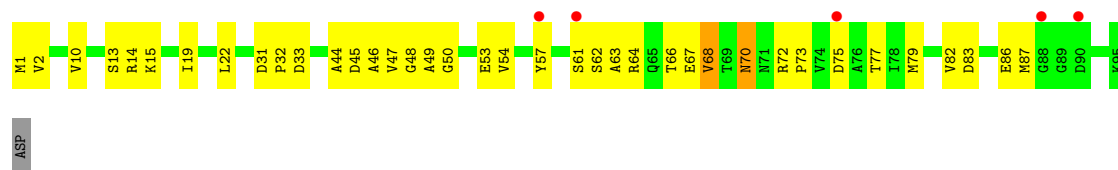


- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

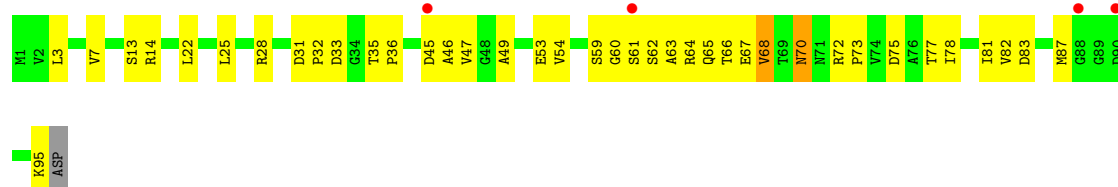


- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

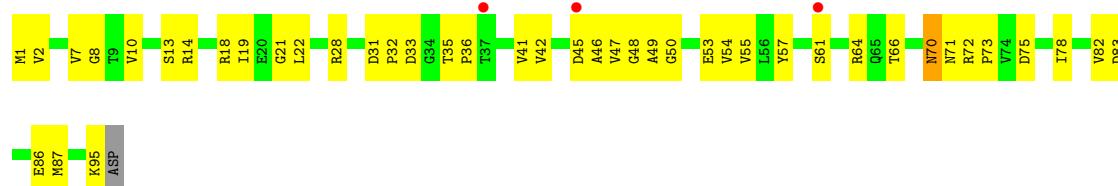




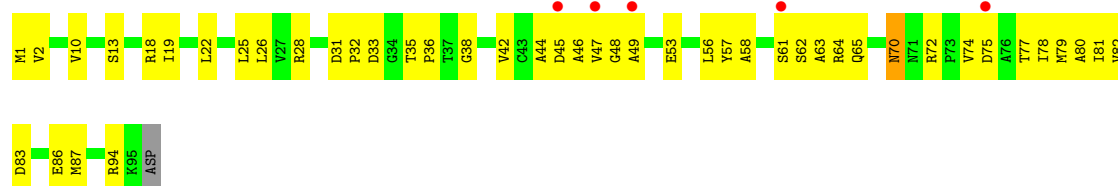
- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



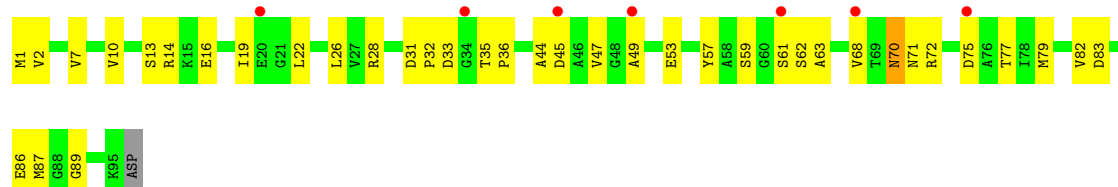
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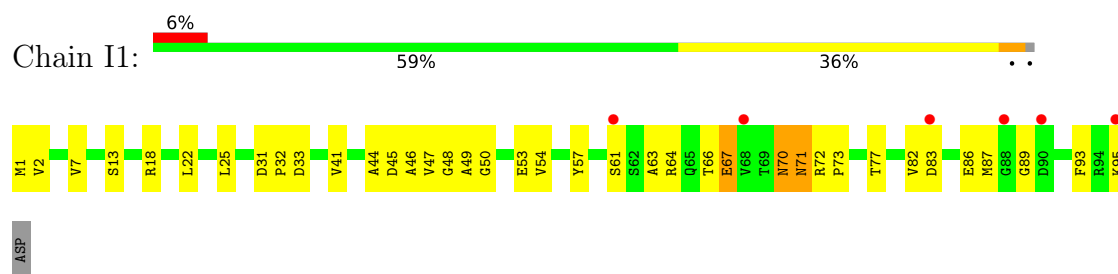
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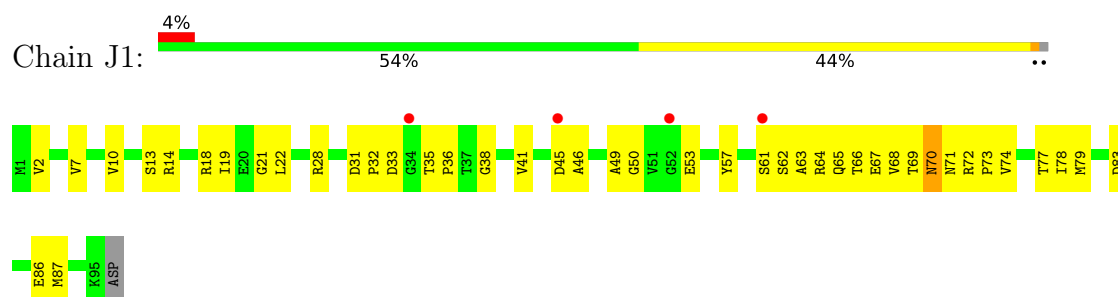
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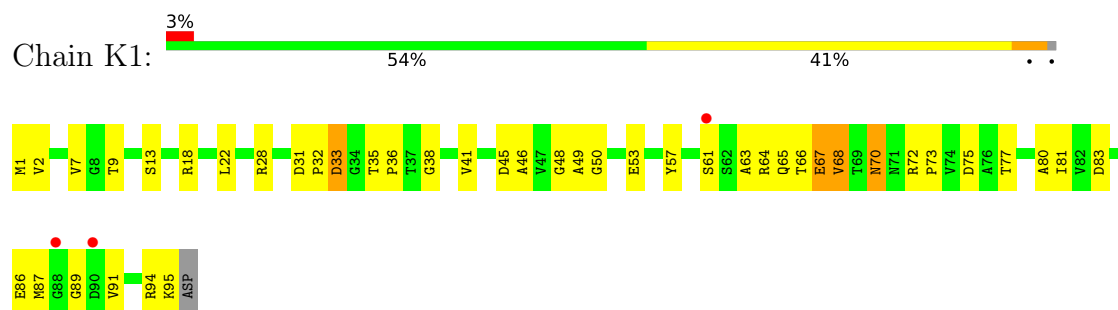
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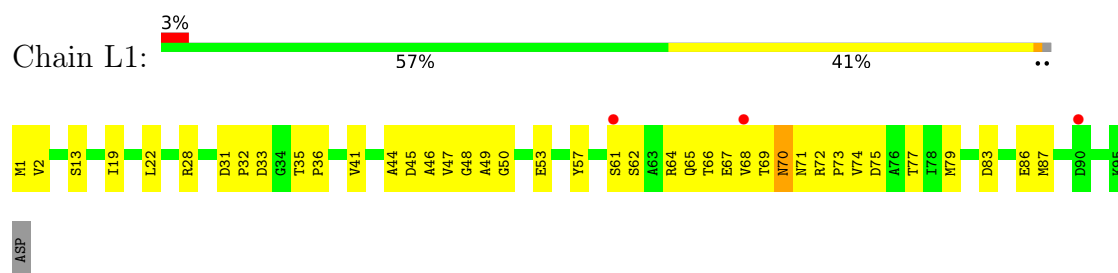
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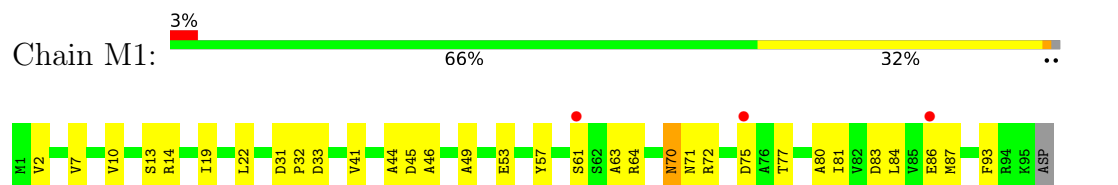
- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

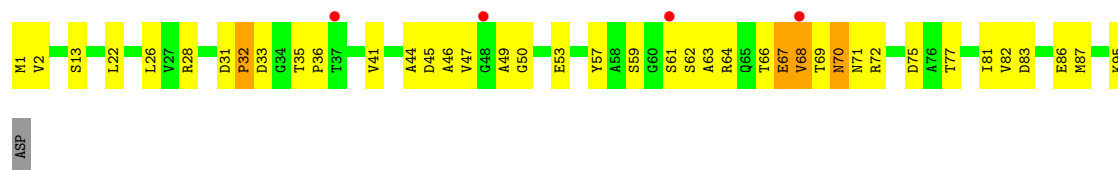


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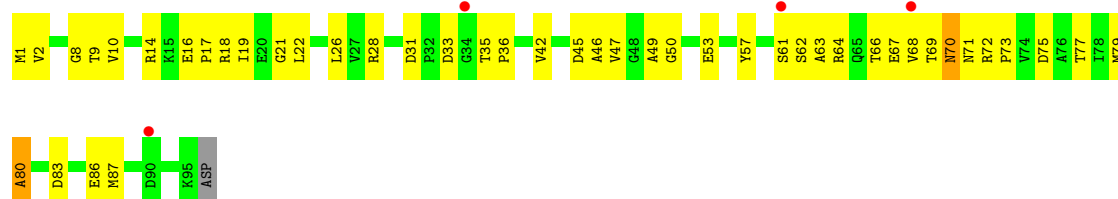


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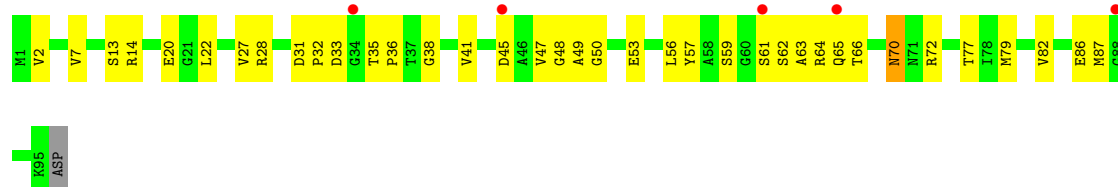




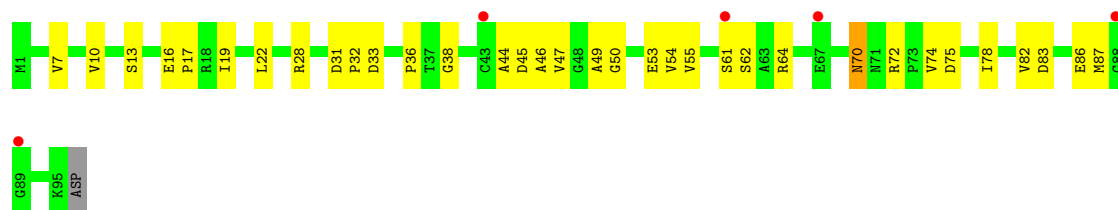
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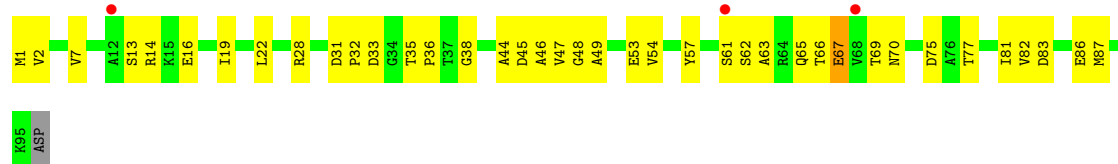
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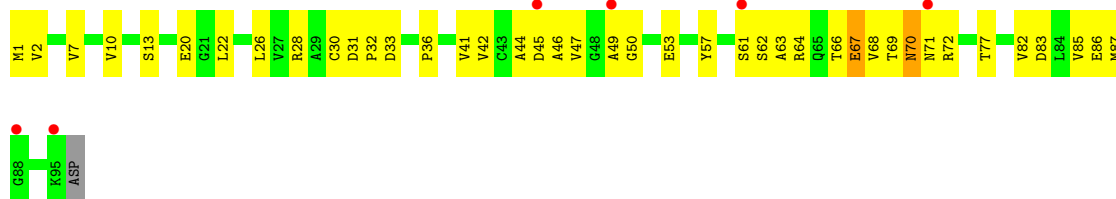


- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

Chain S1: 



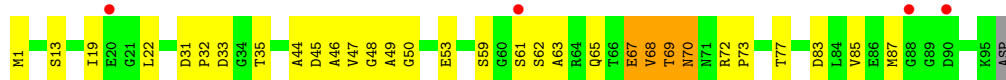
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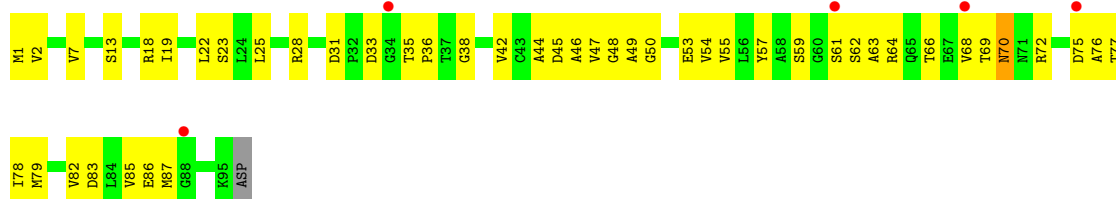
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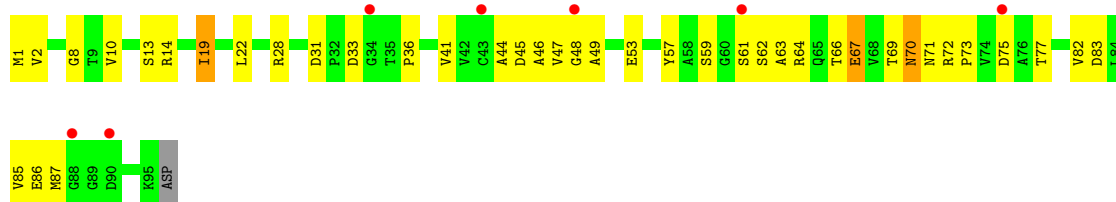
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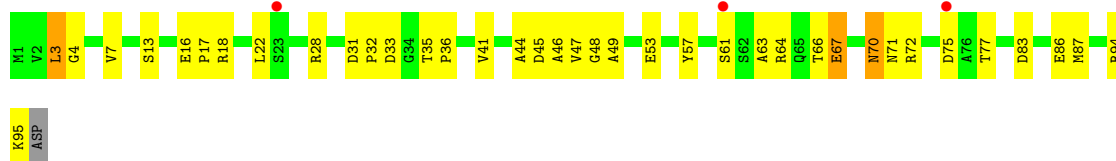
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Chain W1: 



- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

Chain X1: 



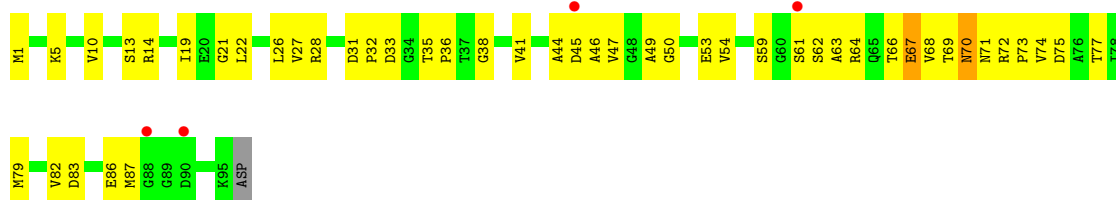
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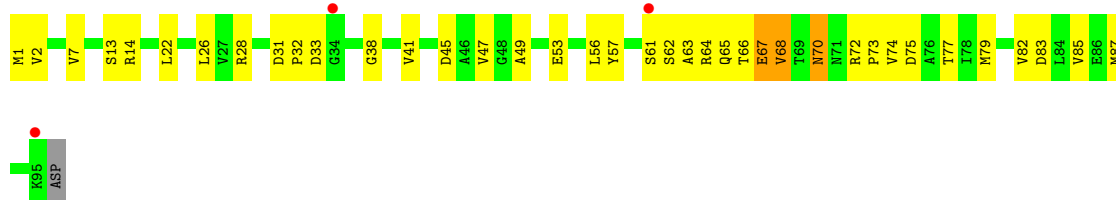
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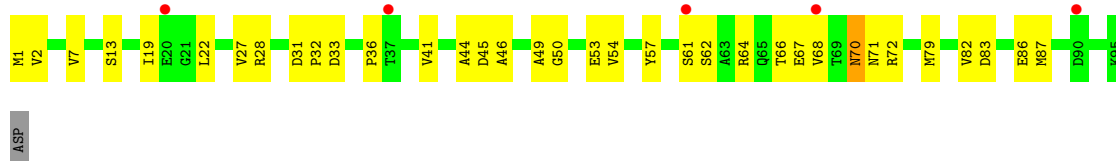
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Chain 11: 

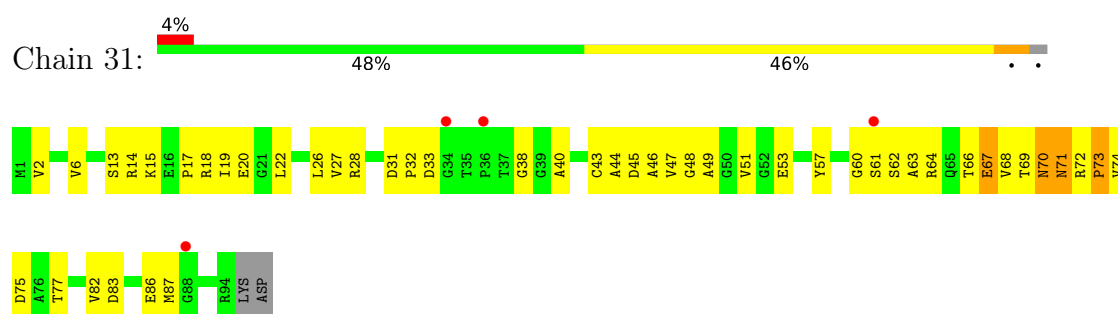


- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

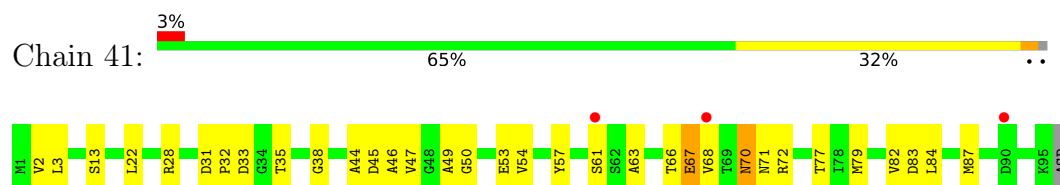
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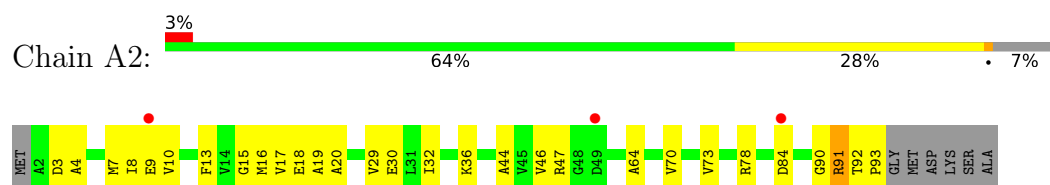
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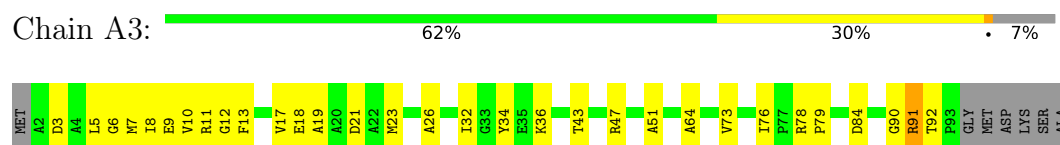
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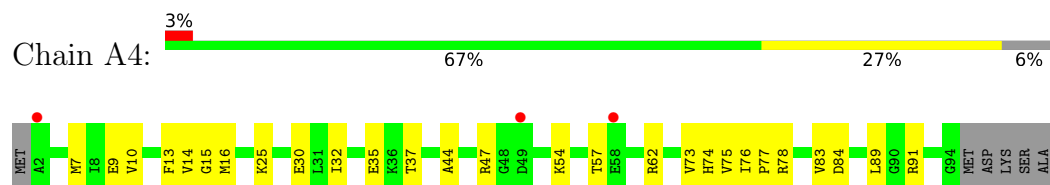
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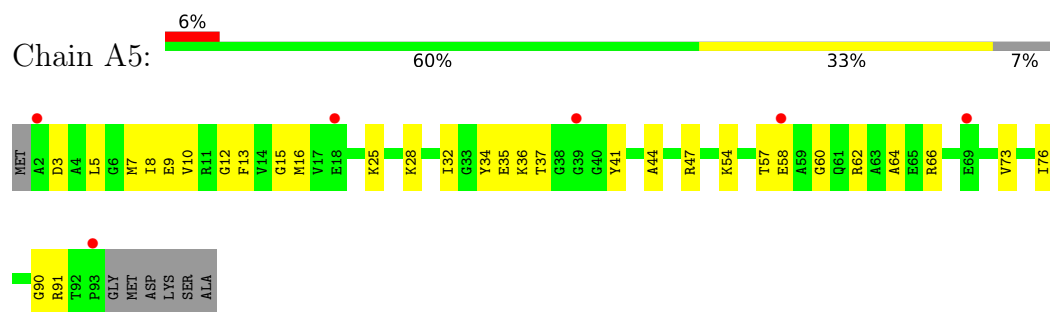
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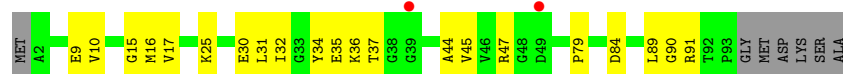
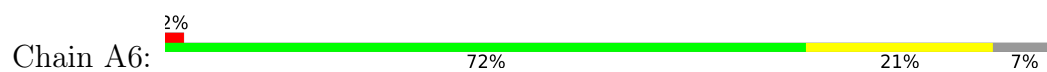
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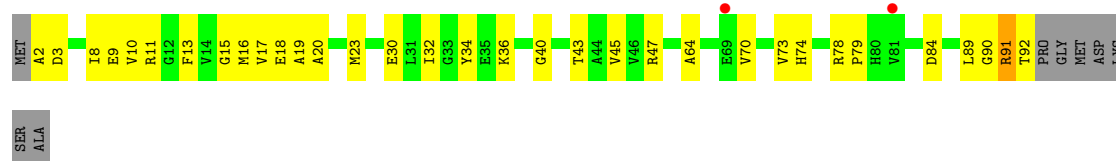
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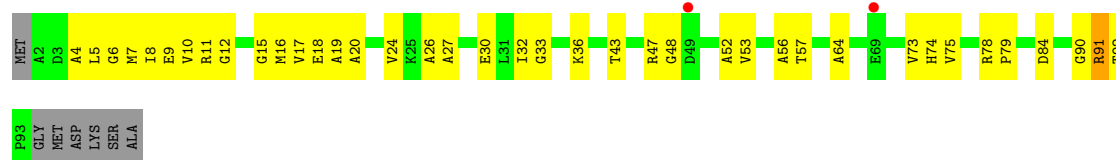
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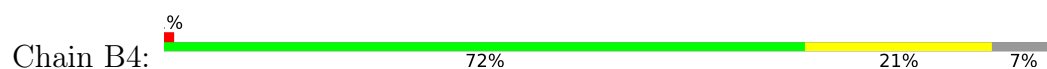
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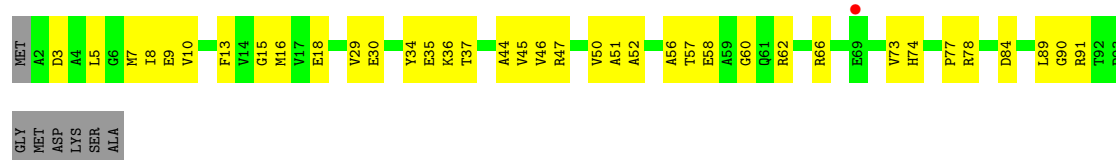
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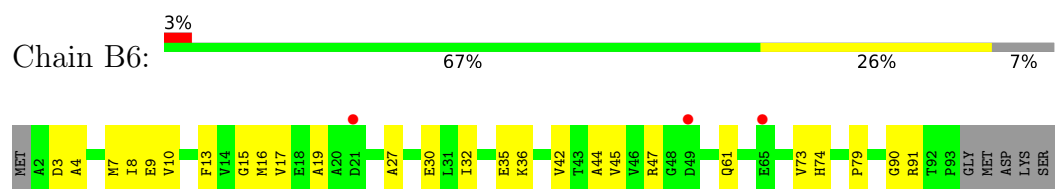
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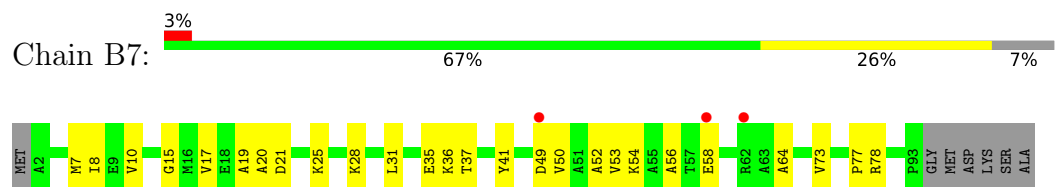
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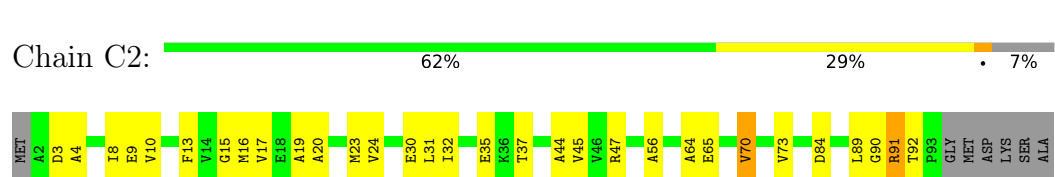
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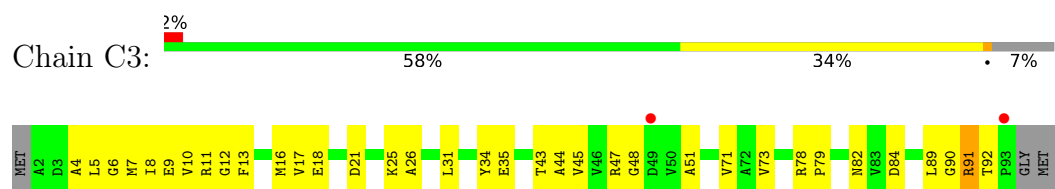
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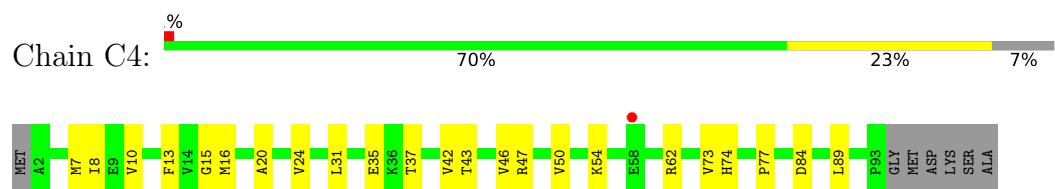
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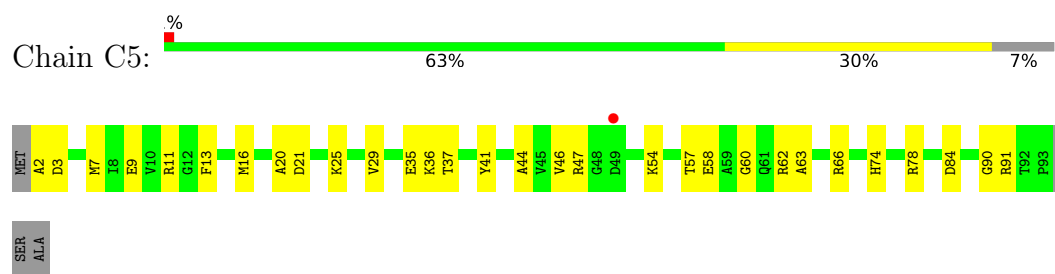
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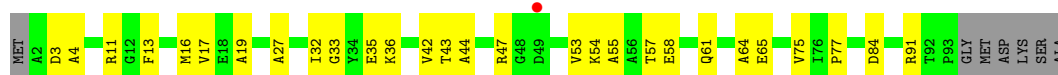


● Molecule 2: Microcompartments protein



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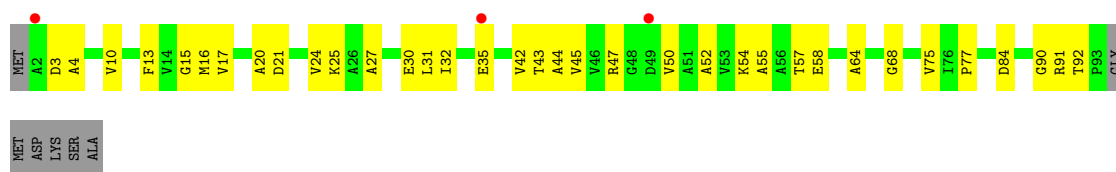


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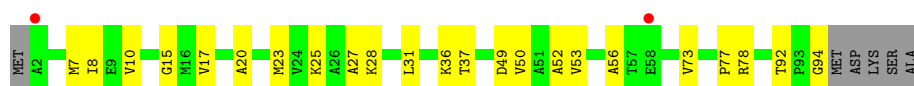
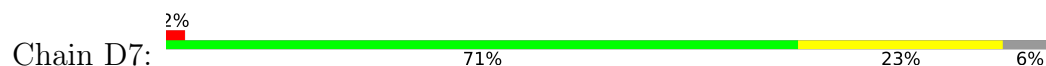


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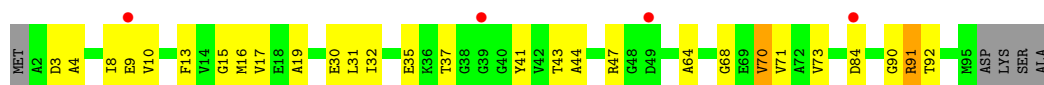




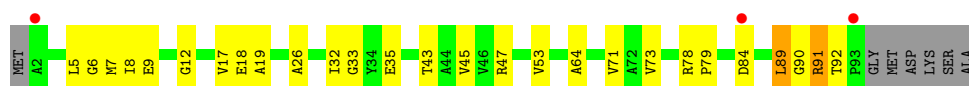
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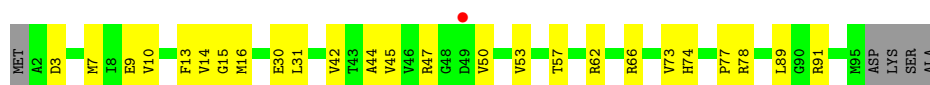
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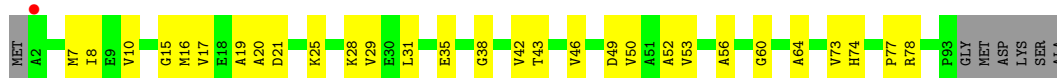


• Molecule 2: Microcompartments protein



MET
ASP
LYS
SER
ALA

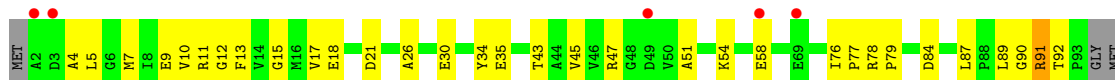
• Molecule 2: Microcompartments protein



• Molecule 2: Microcompartments protein



• Molecule 2: Microcompartments protein



ASP
LYS
SER
ALA

• Molecule 2: Microcompartments protein



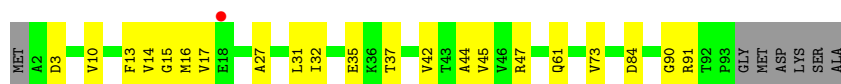
GLY
MET
ASP
LYS
SER
ALA

• Molecule 2: Microcompartments protein



• Molecule 2: Microcompartments protein

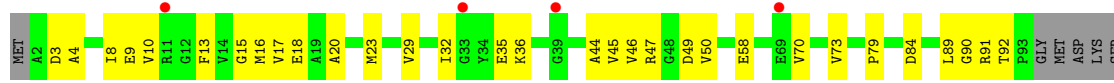




- Molecule 2: Microcompartments protein

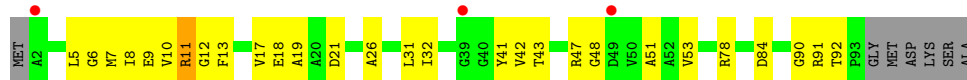


- Molecule 2: Microcompartments protein



ALA

- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



LYS
SER
ALA

- Molecule 2: Microcompartments protein



ASP
LYS
SER
ALA

- Molecule 2: Microcompartments protein



• Molecule 2: Microcompartments protein



• Molecule 2: Microcompartments protein



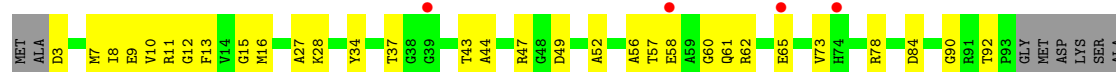
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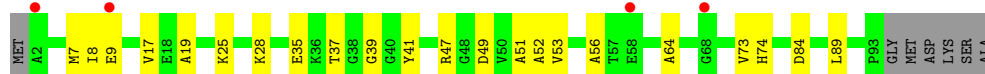
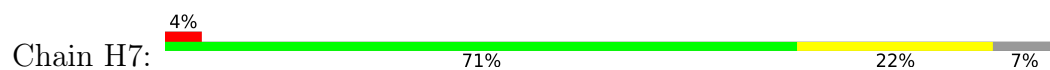
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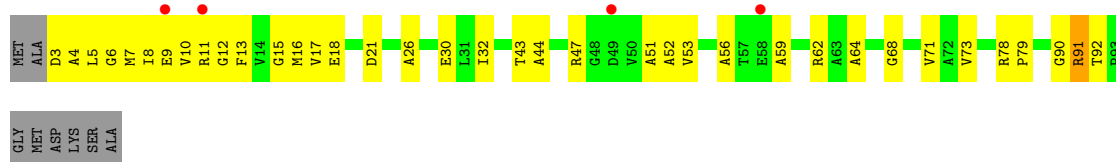
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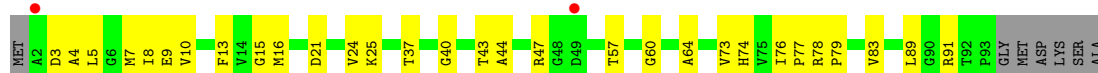
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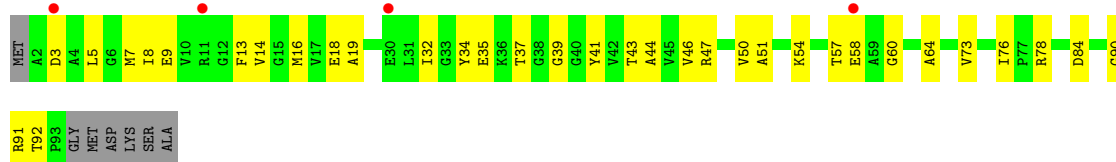
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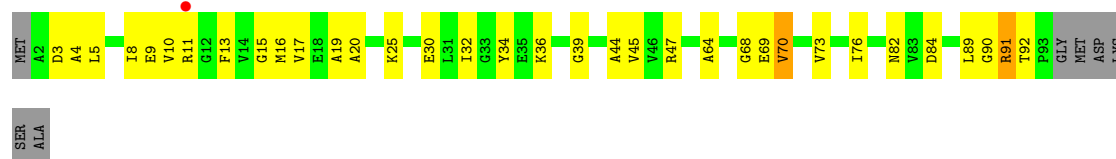
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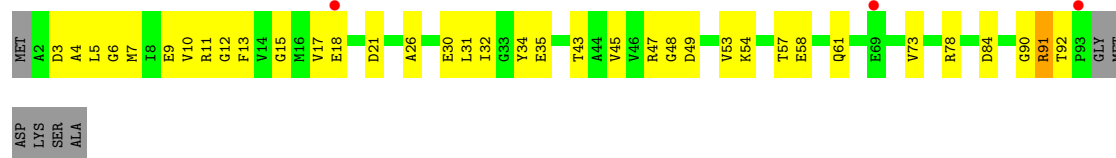
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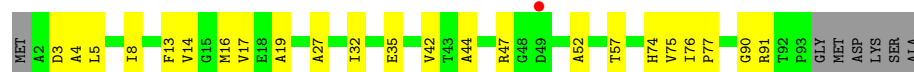
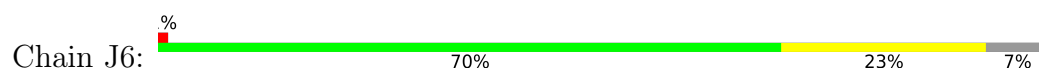
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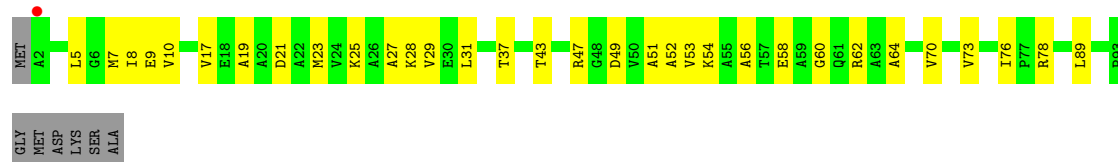
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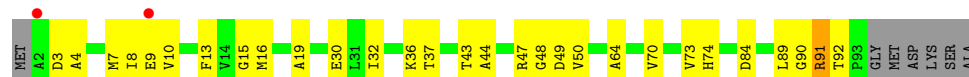
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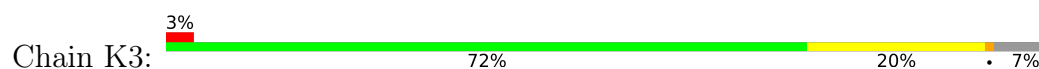
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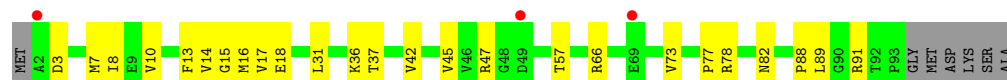
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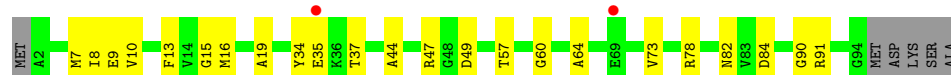
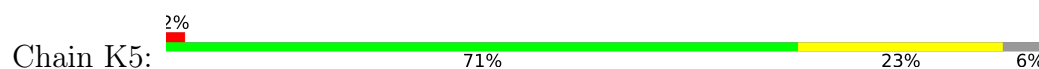
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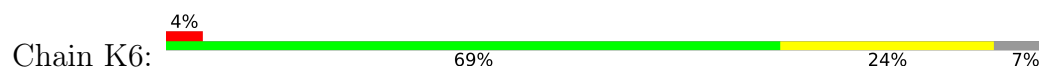
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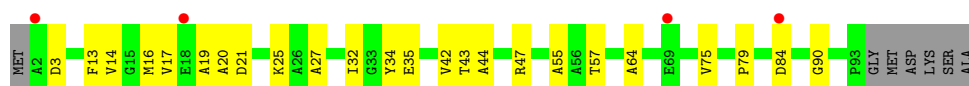


- Molecule 2: Microcompartments protein

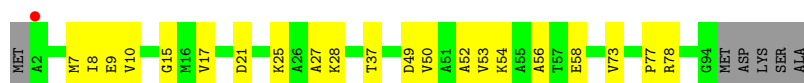
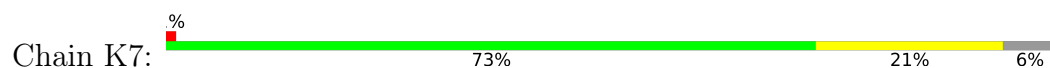


- Molecule 2: Microcompartments protein





- Molecule 2: Microcompartments protein



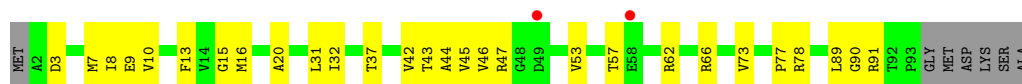
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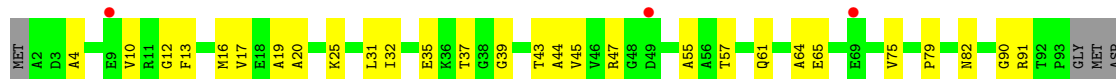
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- Molecule 2: Microcompartments protein



LYS
SER
ALA

• Molecule 2: Microcompartments protein



MET A2 M7 I8 E9 R11 G12 G15 M16 M17 E18 A19 V24 V29 V30 I32 K36 K37 V42 V46 D49 V50 A51 A52 V53 A56 T57 E58 A59 R62 A63 A64 V73 P77 R78 G90 R91 T92 P93 G94 MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein



MET A2 D3 A4 L5 G6 M7 I8 E9 R11 G12 G15 M16 A19 A20 E30 L31 I32 E35 K36 K37 R47 E54 E58 A64 E69 V70 V73 R78 P79 L89 G90 R91 T92 P93 G94 MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein



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• Molecule 2: Microcompartments protein



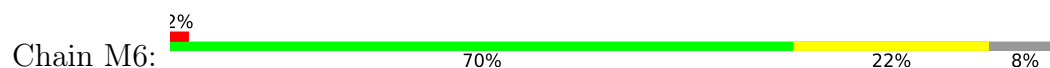
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• Molecule 2: Microcompartments protein



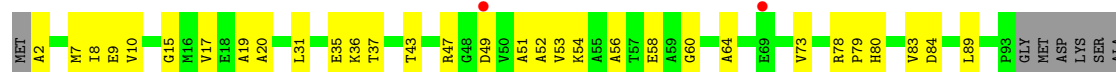
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• Molecule 2: Microcompartments protein



MET ALA D3 E9 F13 V14 G15 M16 E18 A19 E30 L31 I32 E35 K36 T43 A44 R47 G48 D49 A55 Q61 A64 E69 V73 I76 P77 G90 R91 T92 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein



• Molecule 2: Microcompartments protein



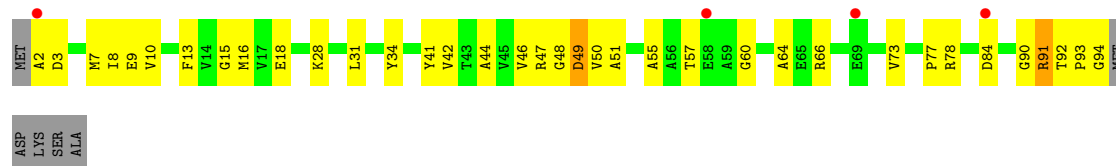
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• Molecule 2: Microcompartments protein



• Molecule 2: Microcompartments protein



• Molecule 2: Microcompartments protein





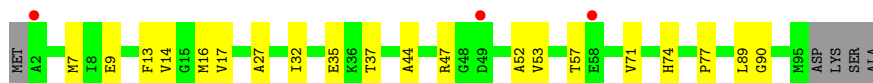
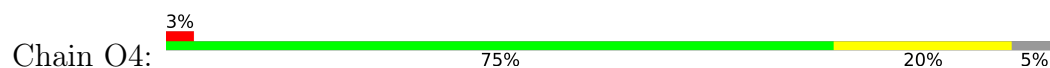
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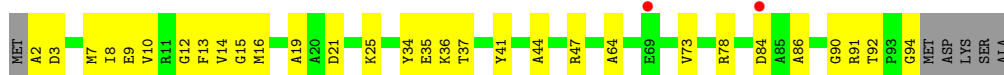
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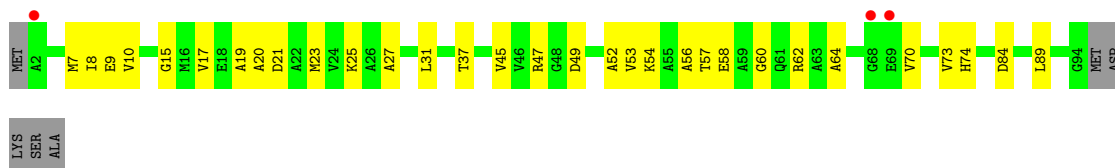
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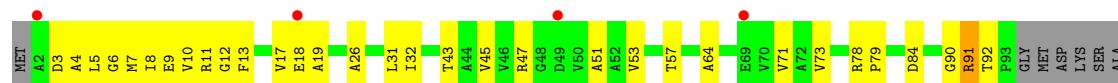
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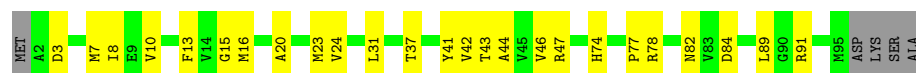
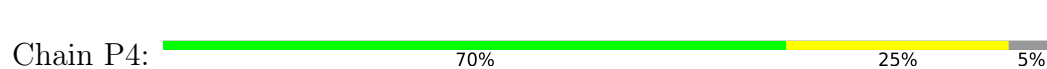
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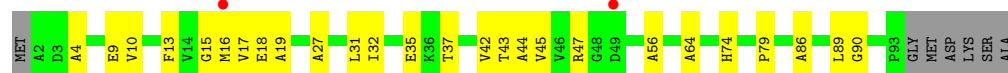
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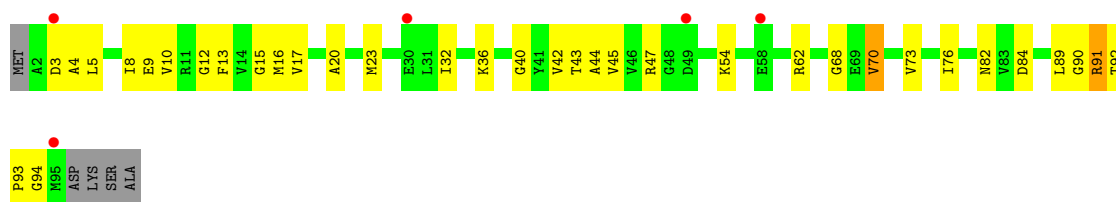


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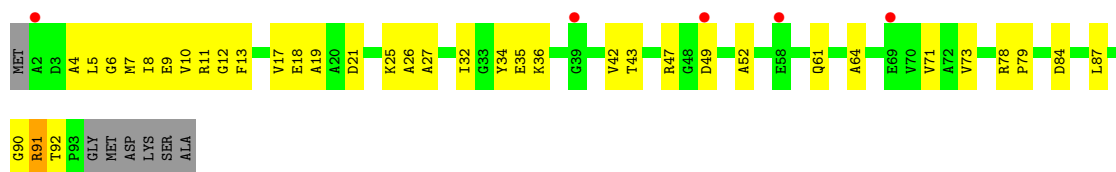


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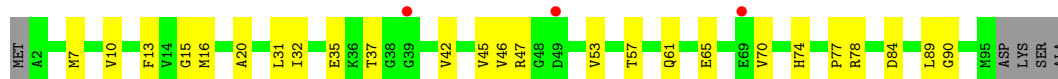
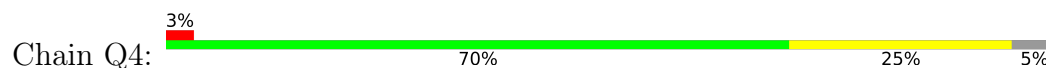




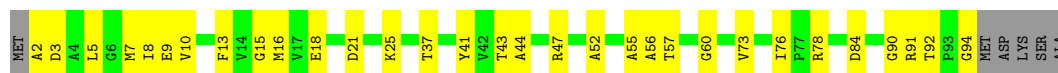
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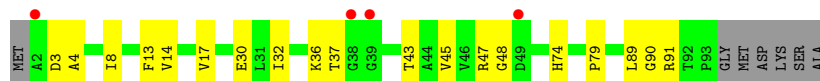
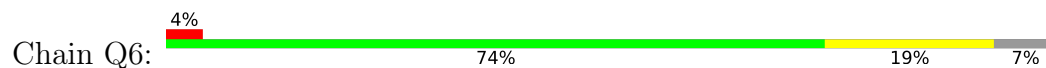
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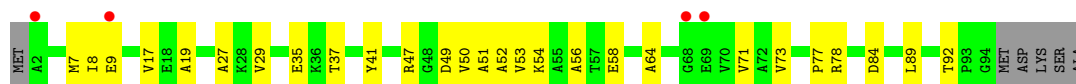
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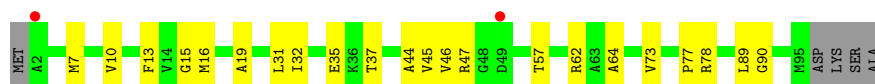
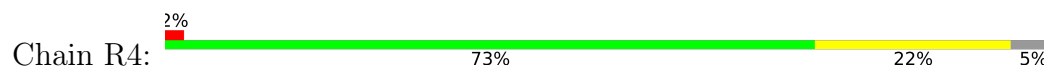




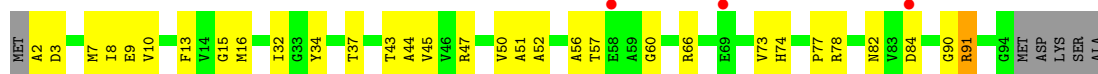
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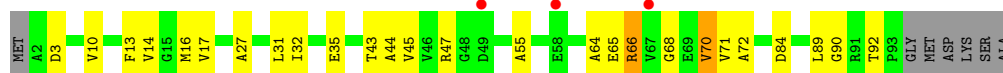
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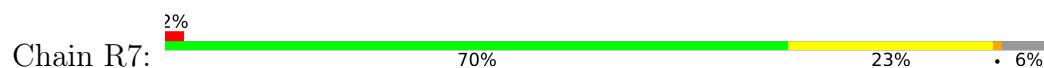
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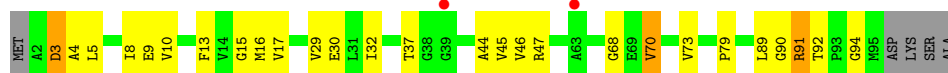
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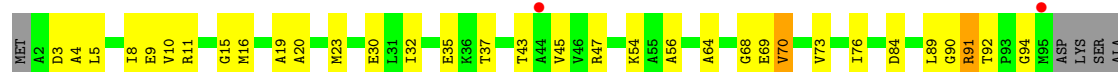
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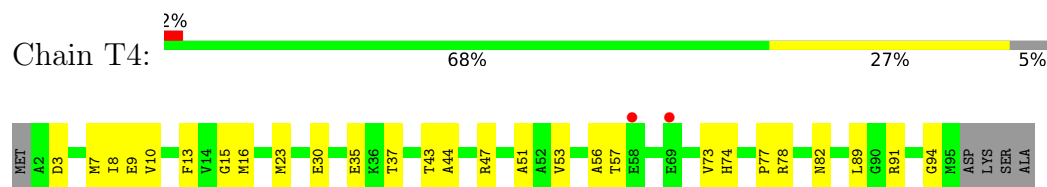
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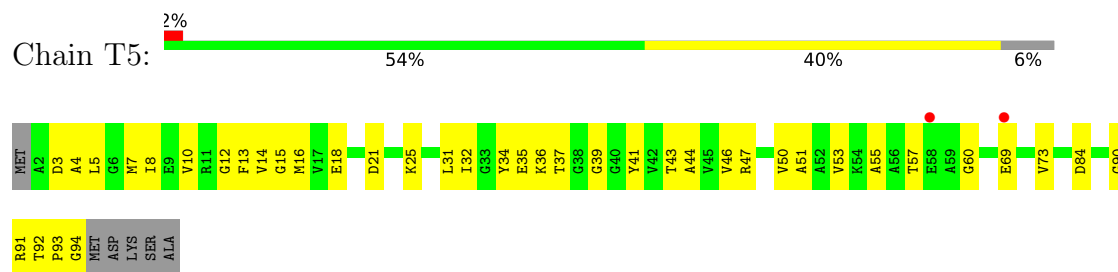
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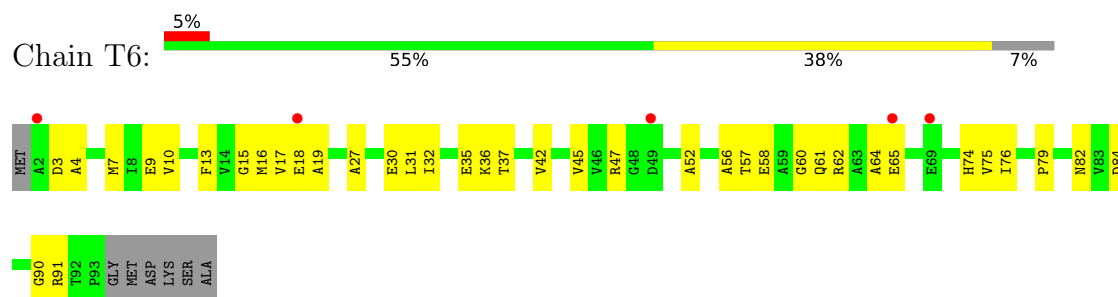
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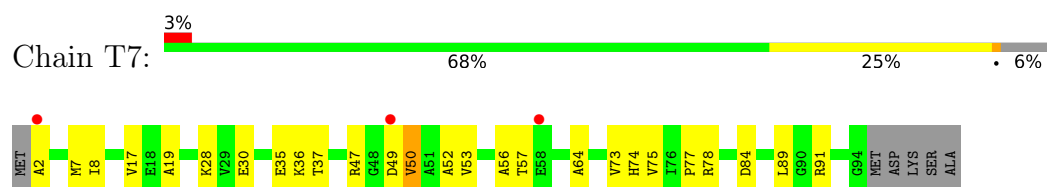
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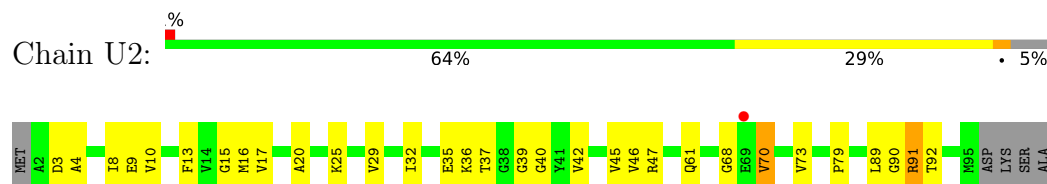
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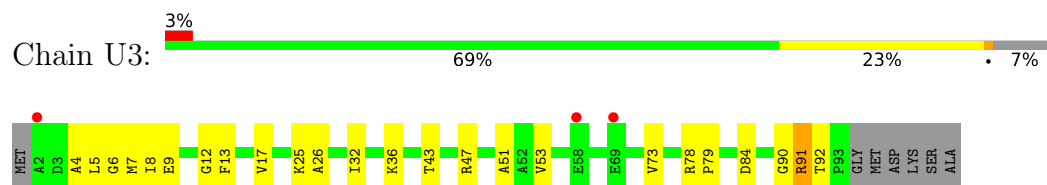
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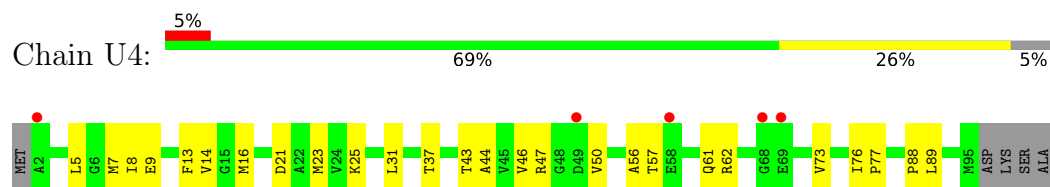
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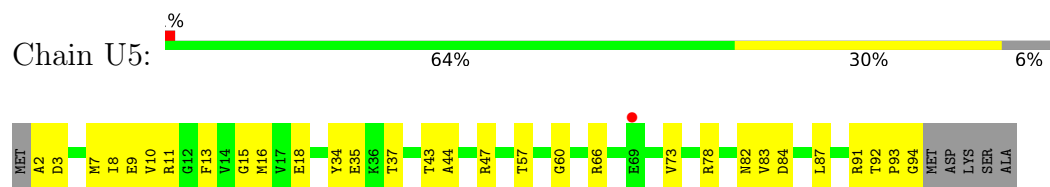
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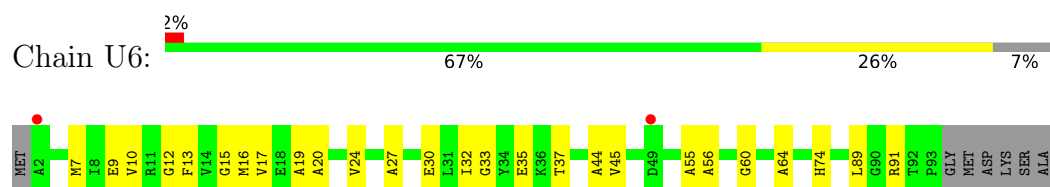
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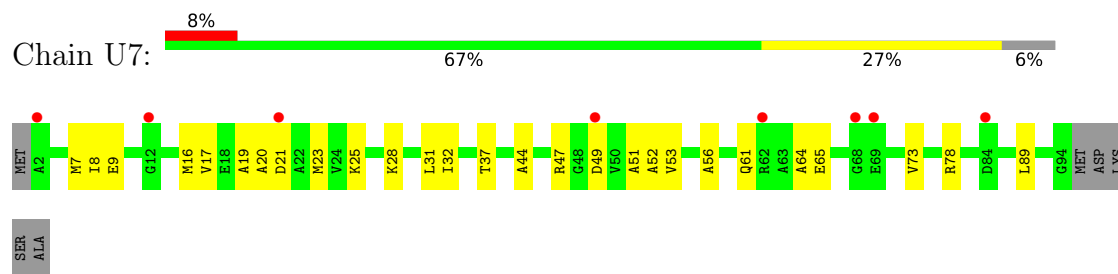
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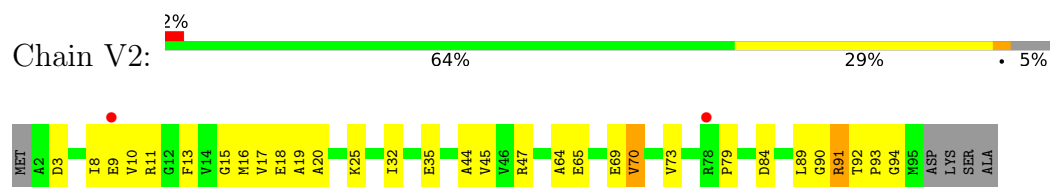
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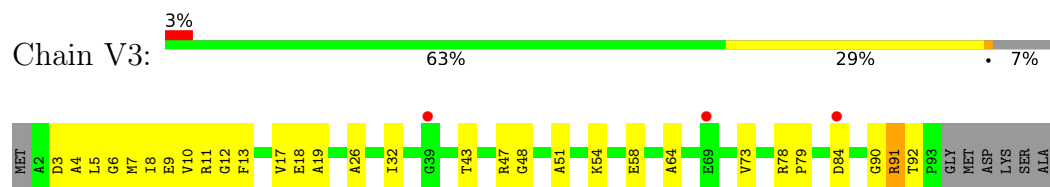
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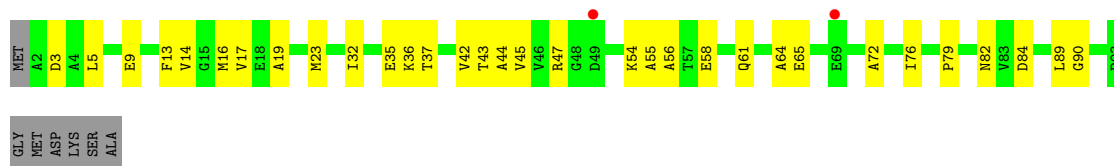




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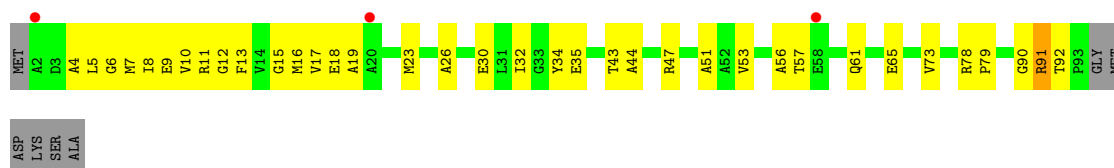
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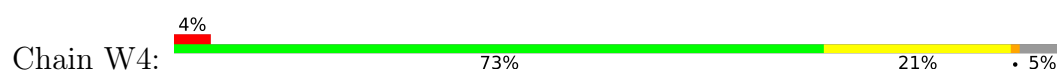
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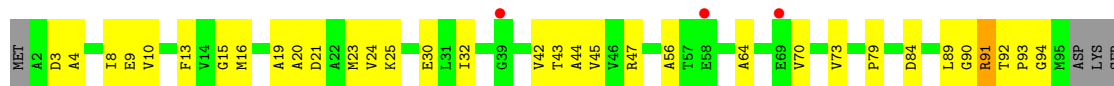
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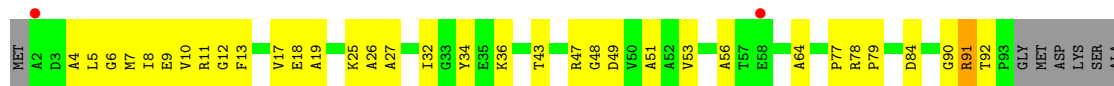
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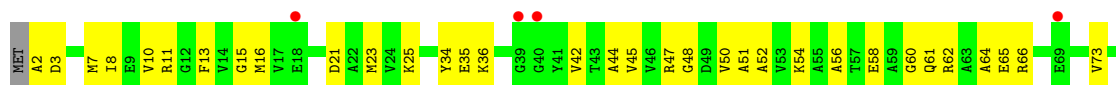


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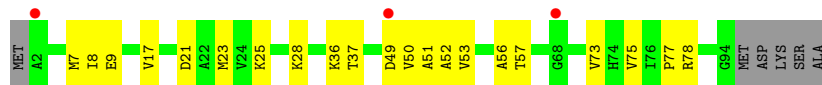
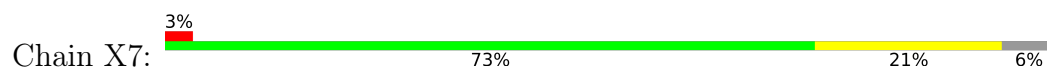
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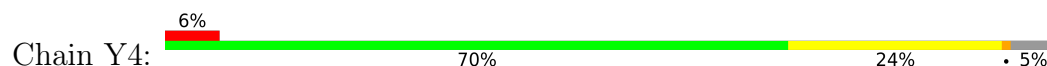
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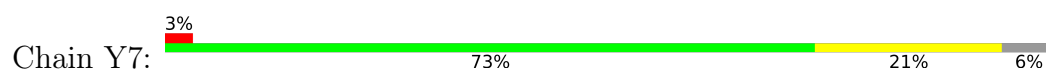
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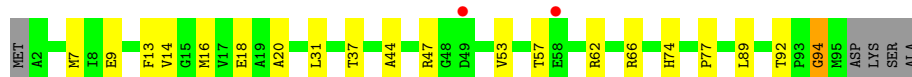
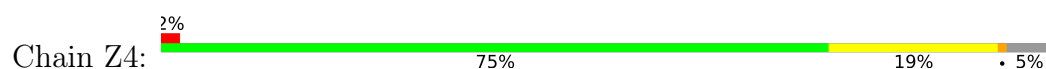
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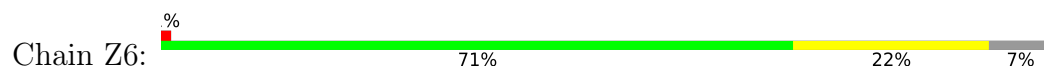
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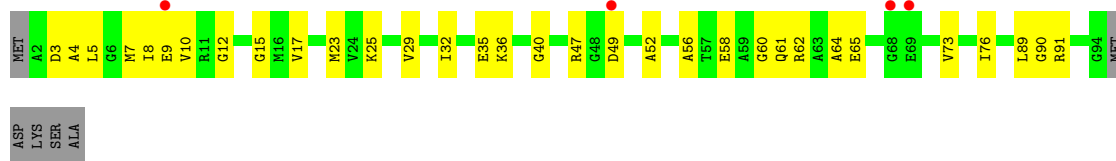
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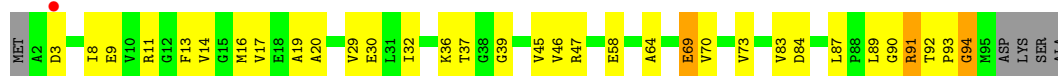
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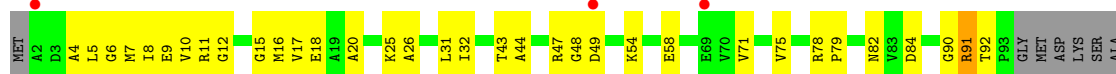
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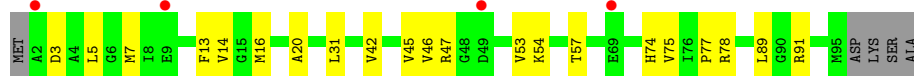
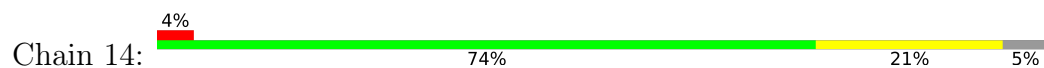
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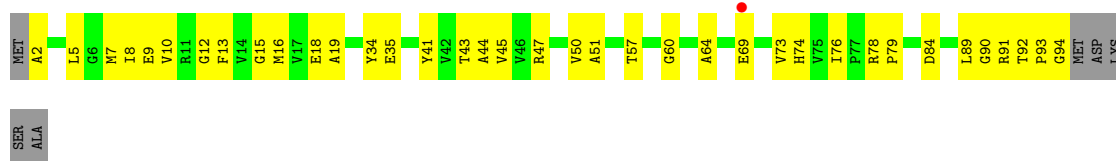


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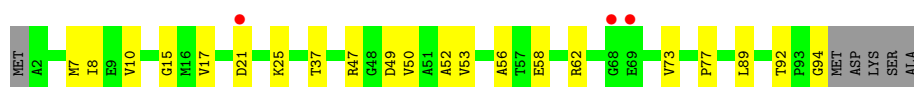
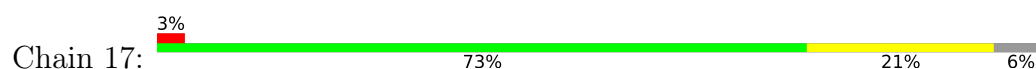




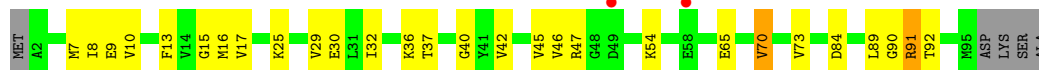
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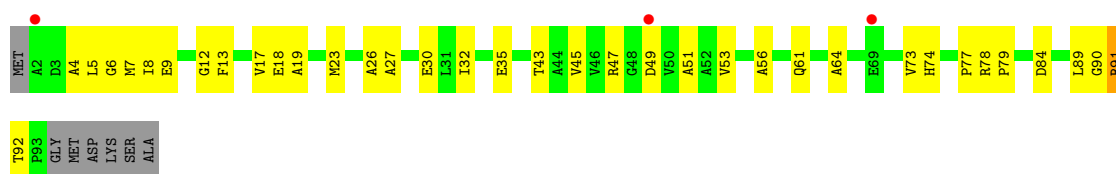
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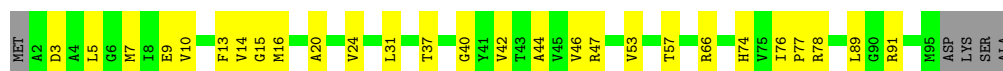
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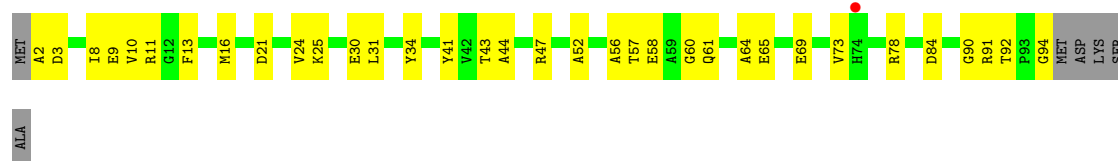


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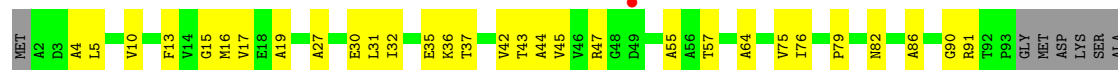


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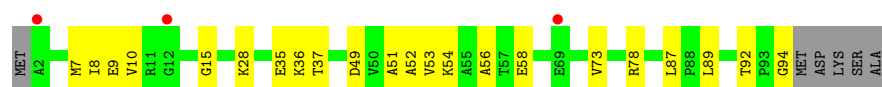
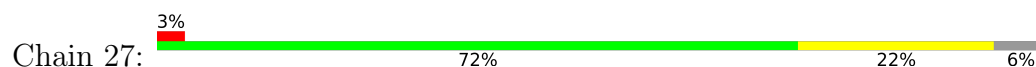




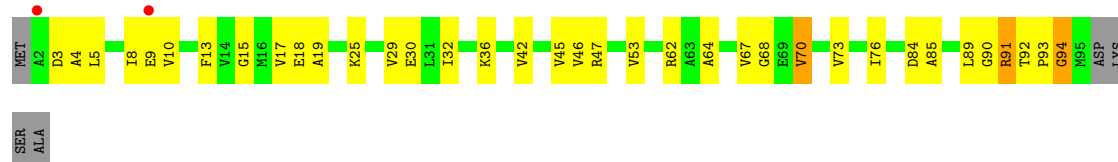
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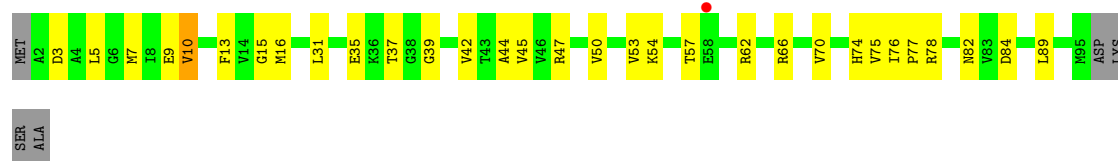
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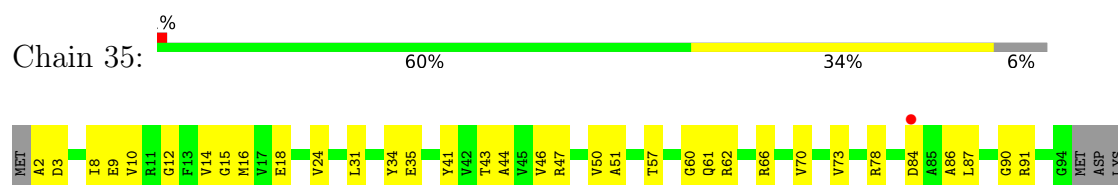
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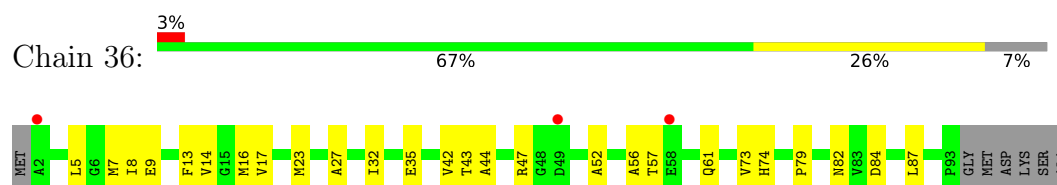
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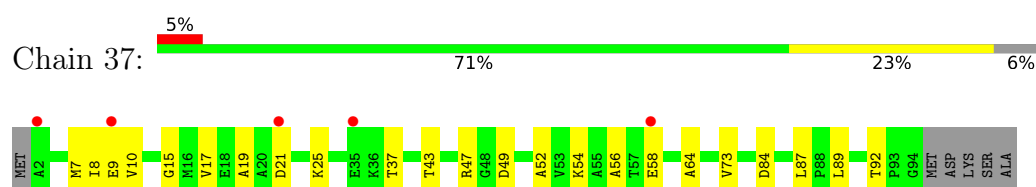
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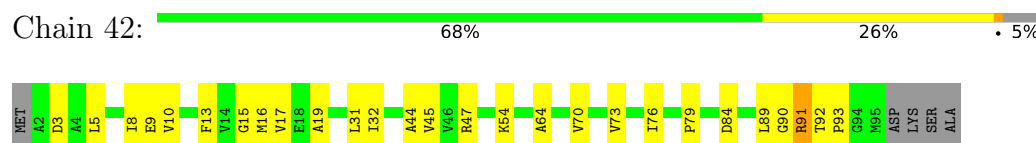
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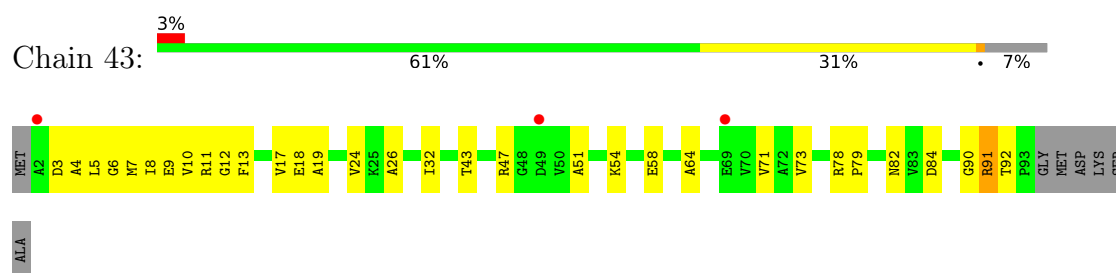
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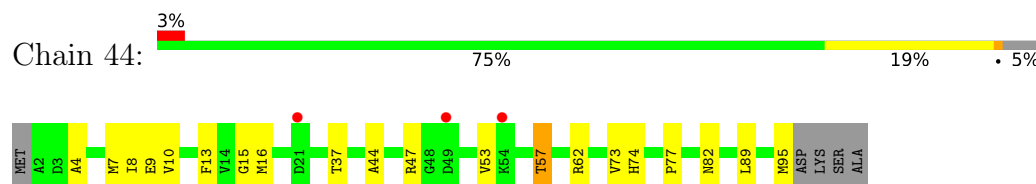
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- Molecule 2: Microcompartments protein





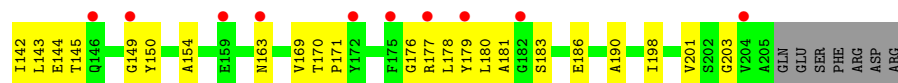
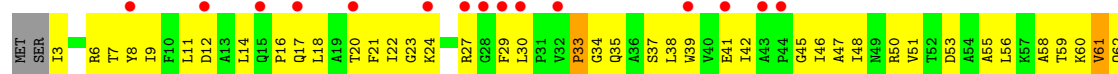
• Molecule 2: Microcompartments protein



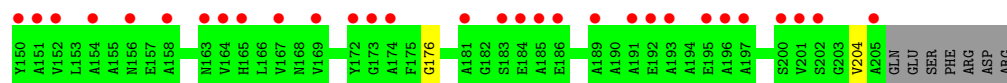
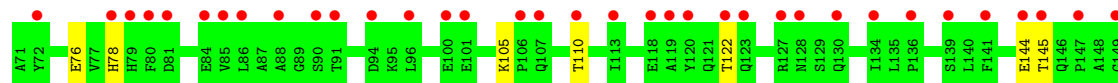
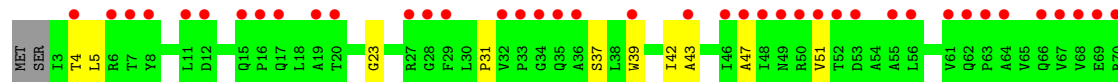
• Molecule 2: Microcompartments protein



• Molecule 3: Microcompartments protein

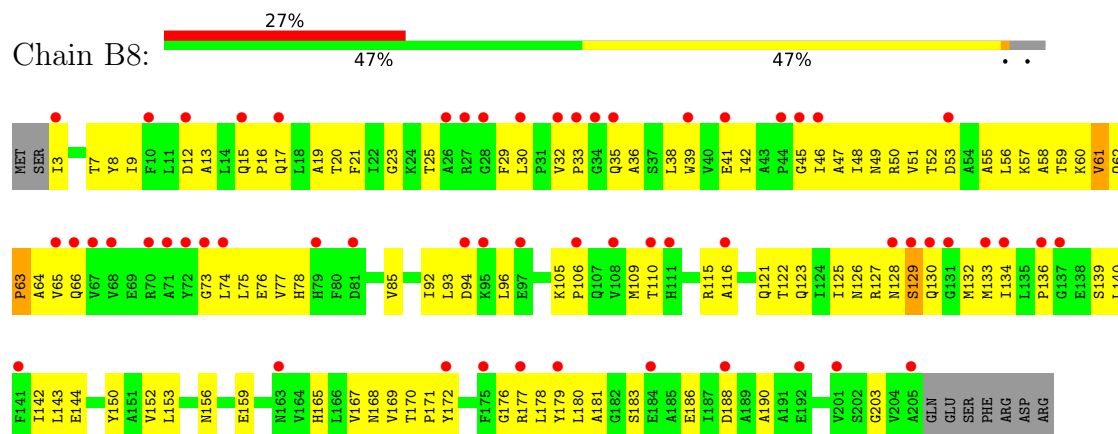


• Molecule 3: Microcompartments protein



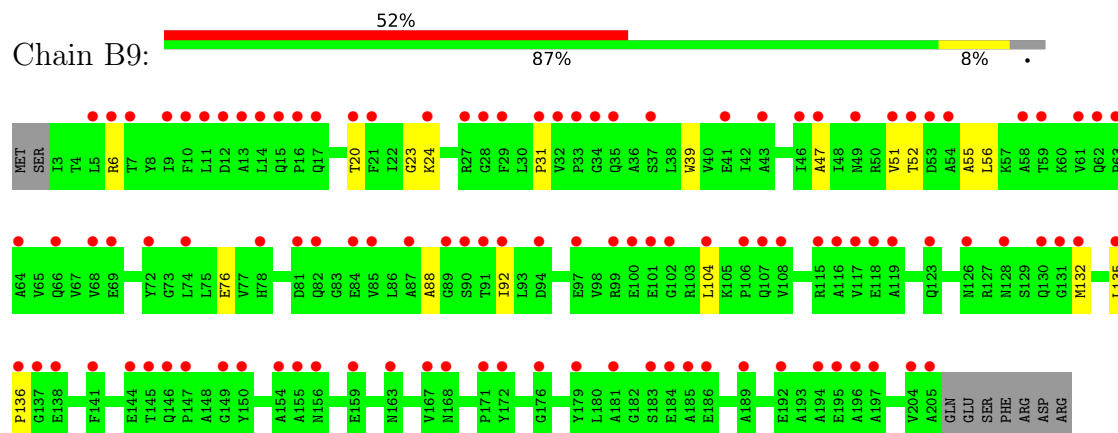
- Molecule 3: Microcompartments protein

Chain B8:



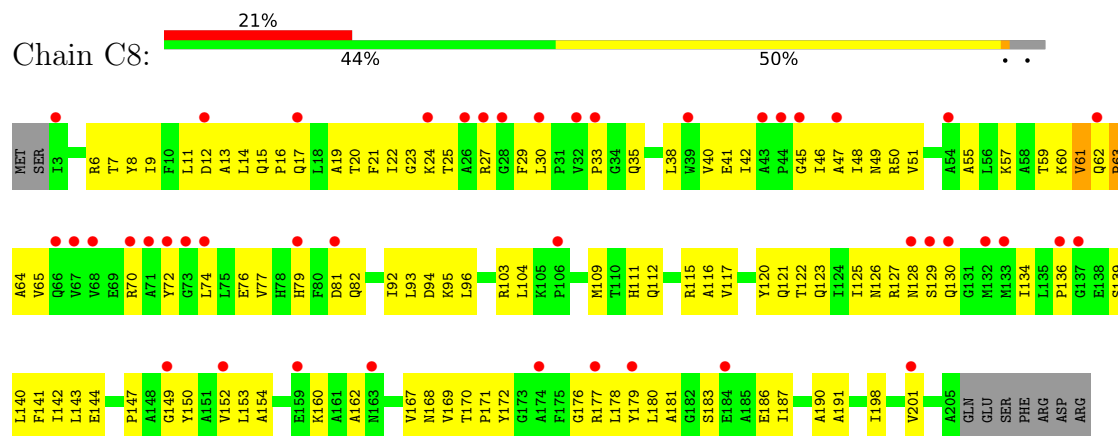
- Molecule 3: Microcompartments protein

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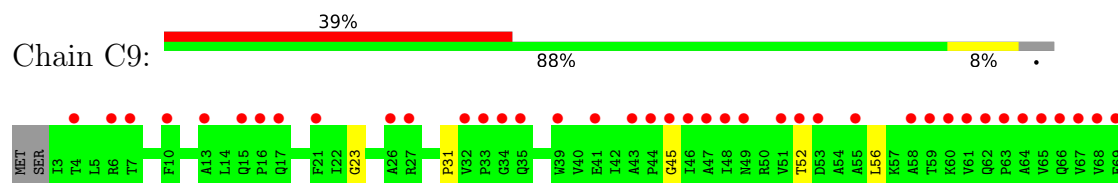
- Molecule 3: Microcompartments protein

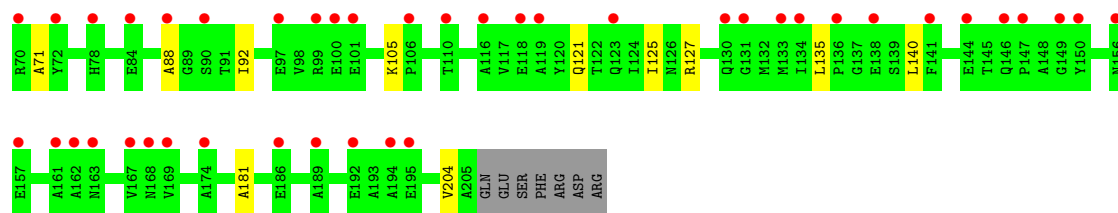
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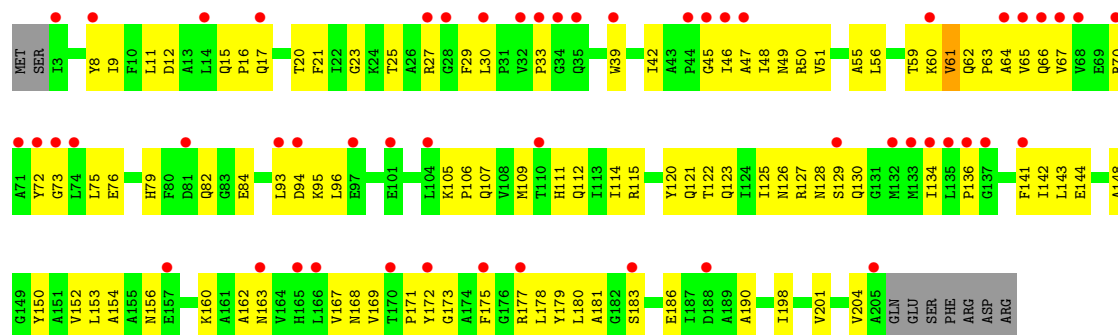
- Molecule 3: Microcompartments protein

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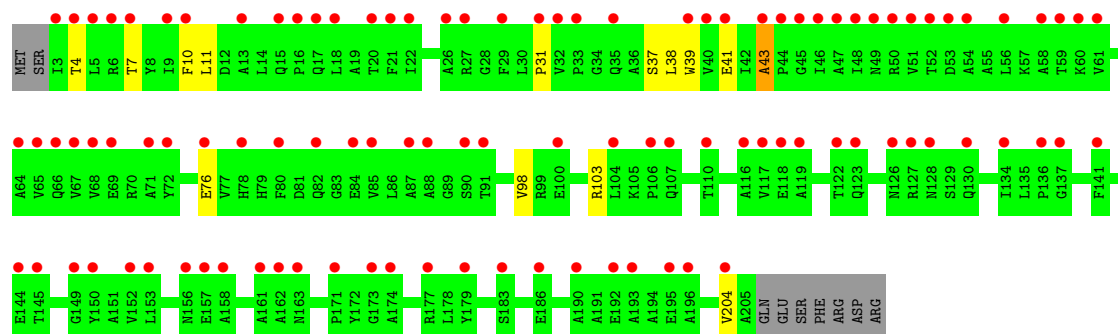
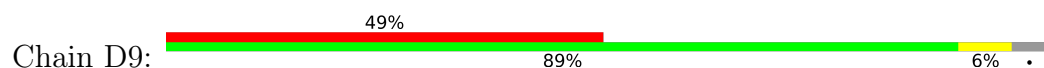




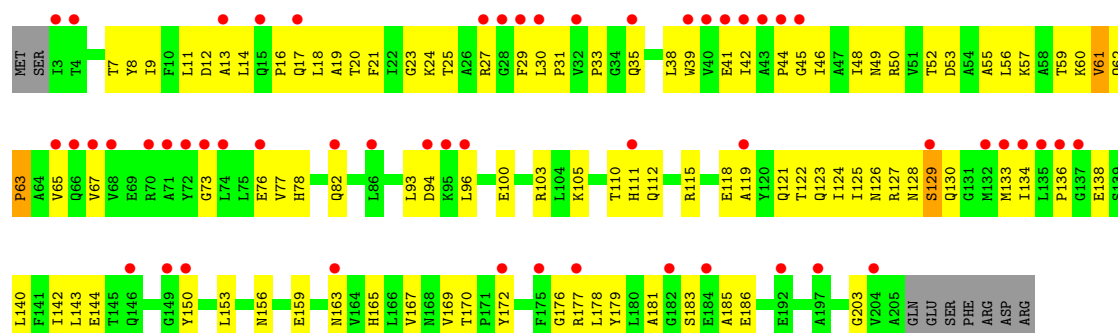
• Molecule 3: Microcompartments protein



• Molecule 3: Microcompartments protein

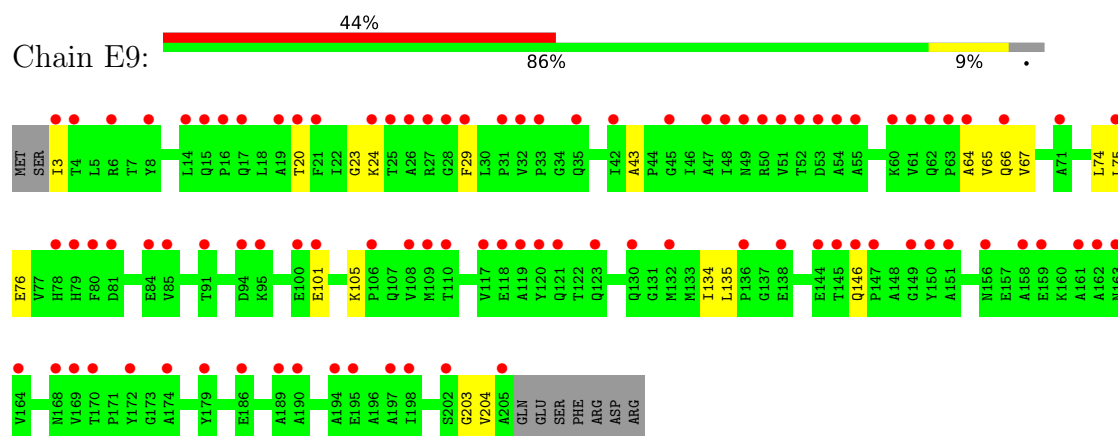


• Molecule 3: Microcompartments protein



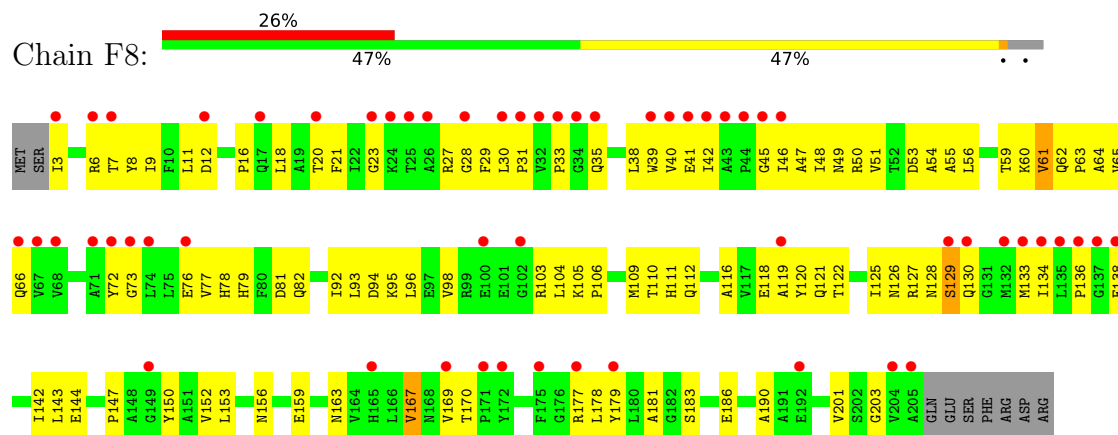
- Molecule 3: Microcompartments protein

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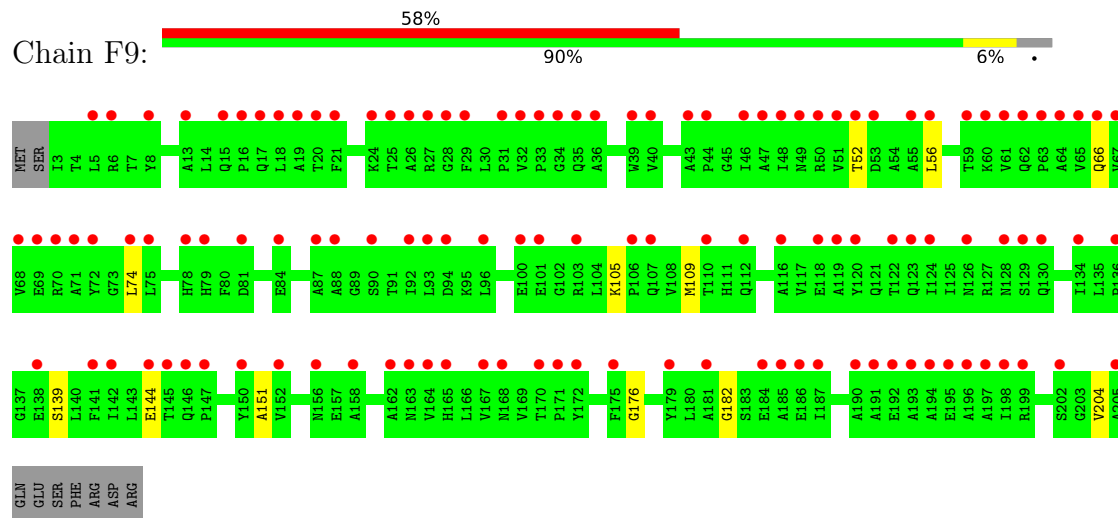
- Molecule 3: Microcompartments protein

Chain F8:



- Molecule 3: Microcompartments protein

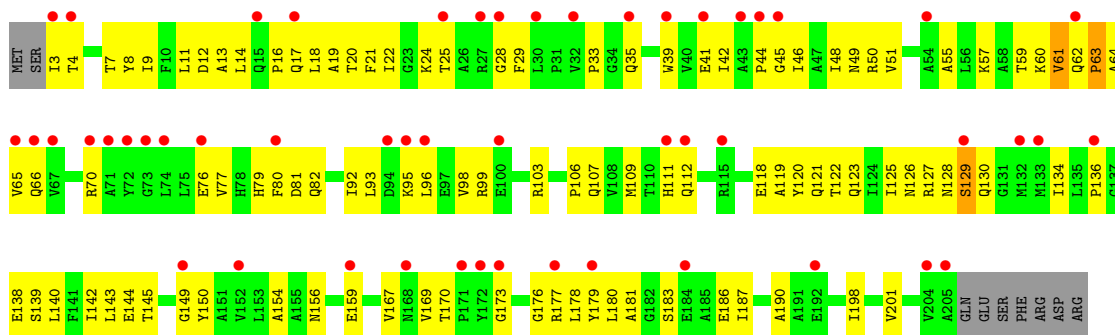
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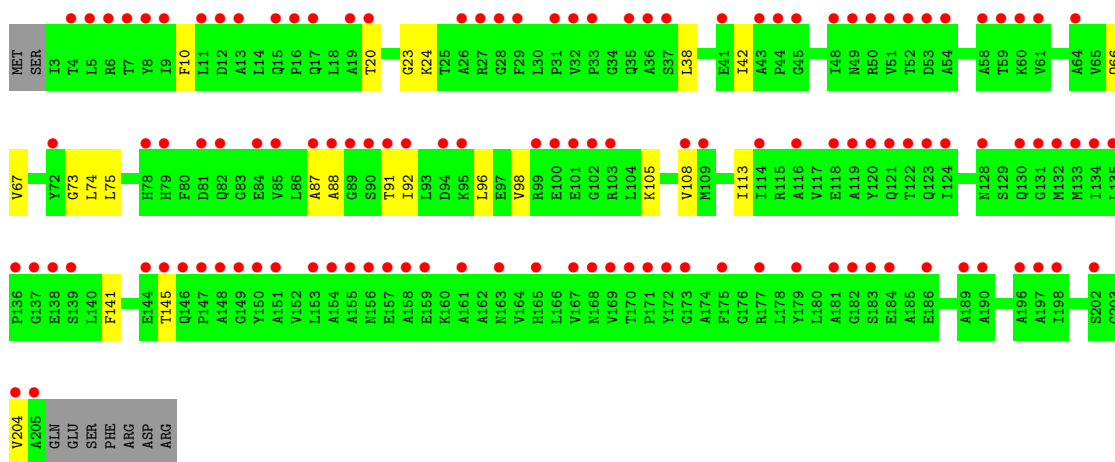
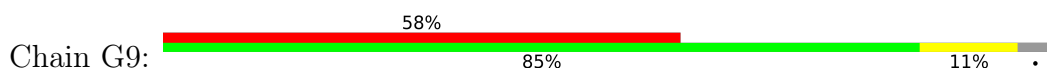
- Molecule 3: Microcompartments protein

Chain G8:

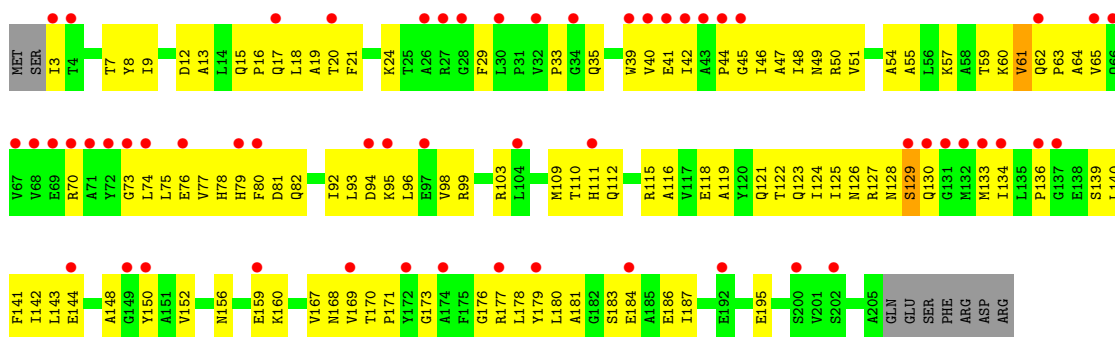




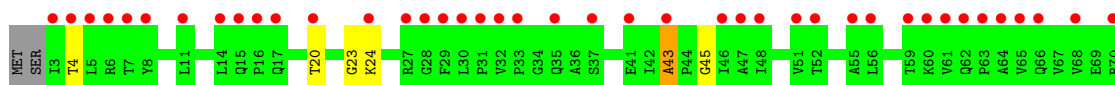
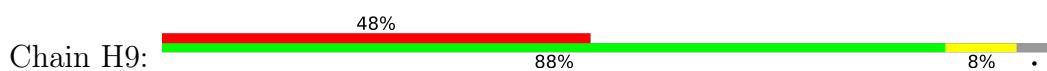
• Molecule 3: Microcompartments protein

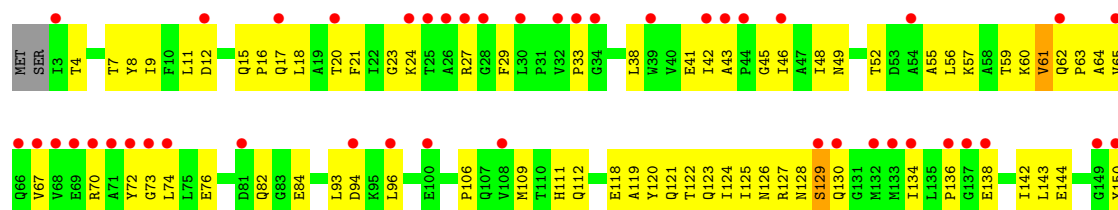


• Molecule 3: Microcompartments protein



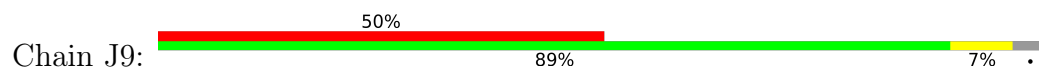
• Molecule 3: Microcompartments protein



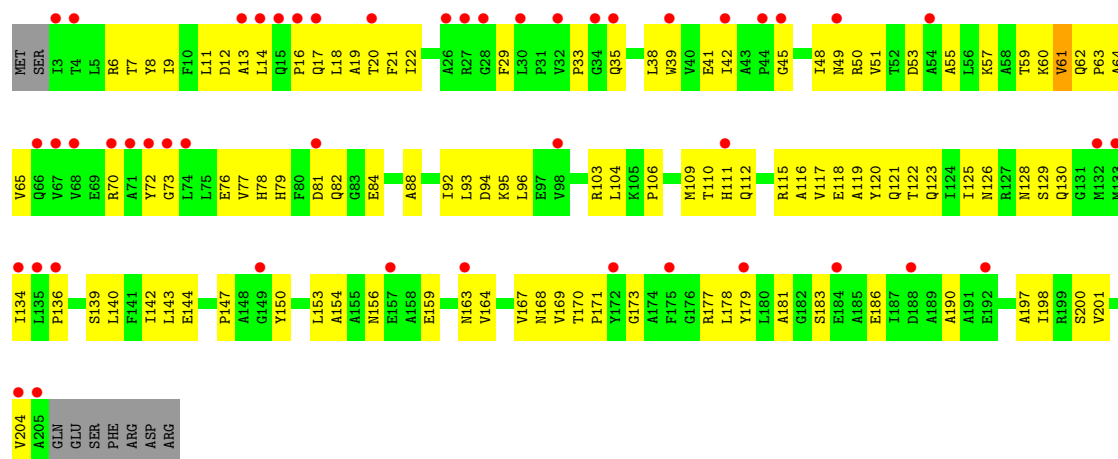




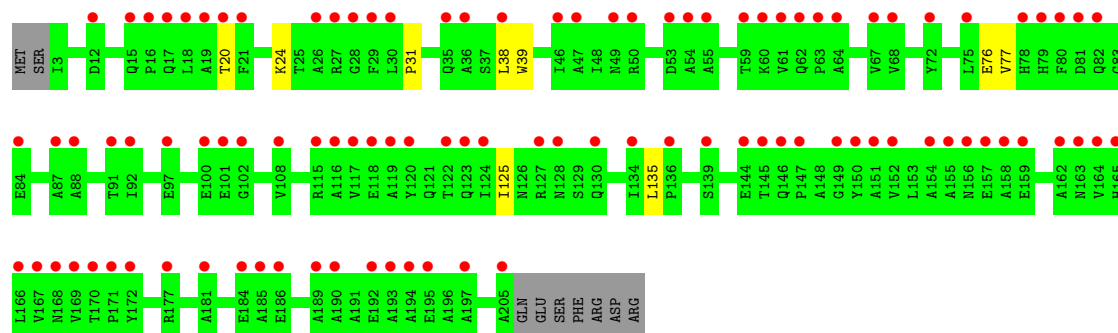
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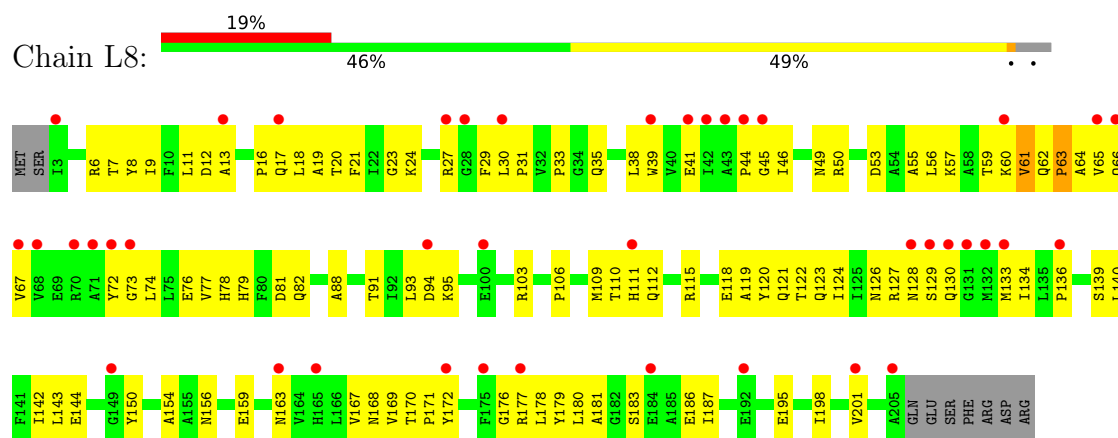
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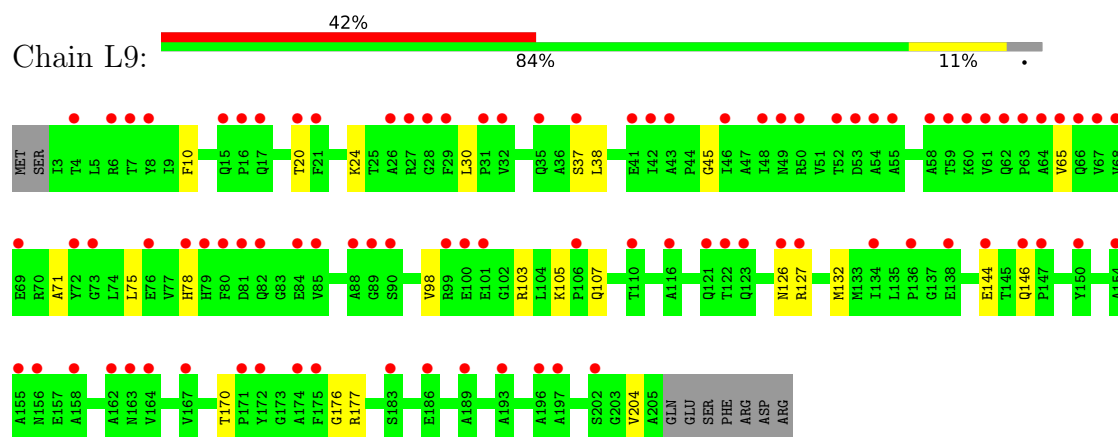
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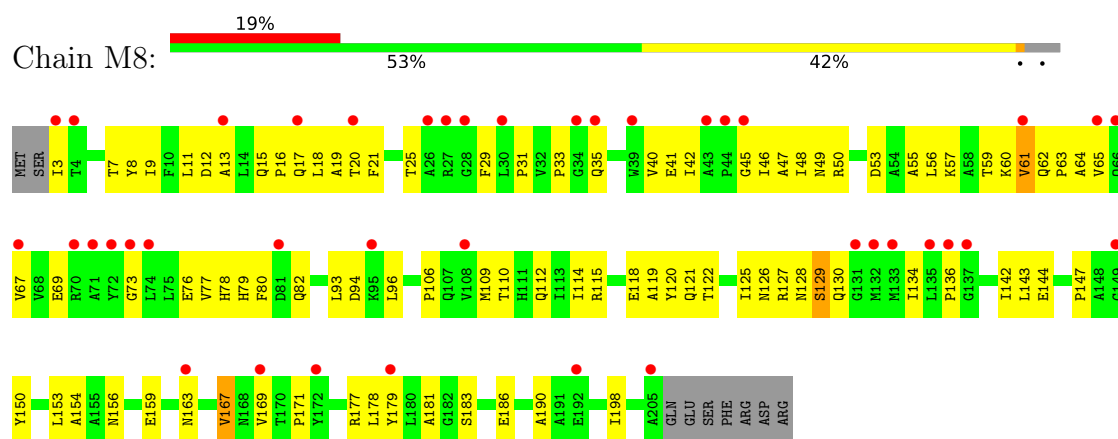
- Molecule 3: Microcompartments protein



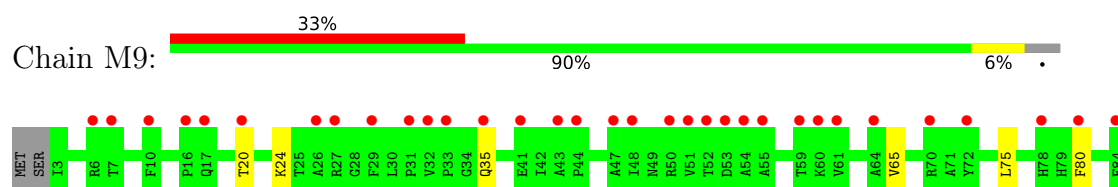
- Molecule 3: Microcompartments protein

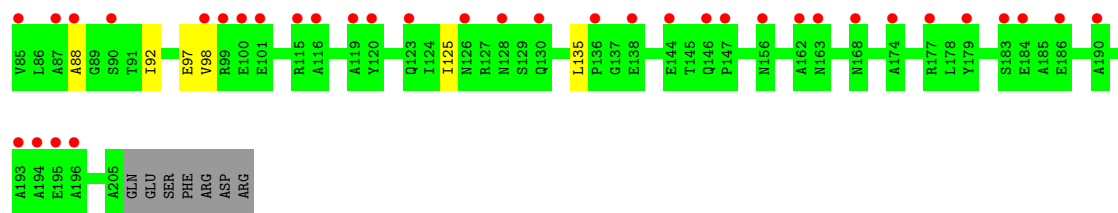


- Molecule 3: Microcompartments protein

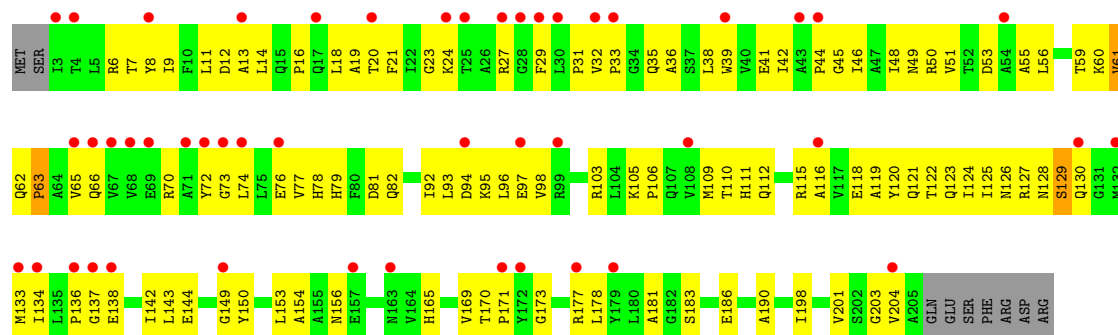


- Molecule 3: Microcompartments protein

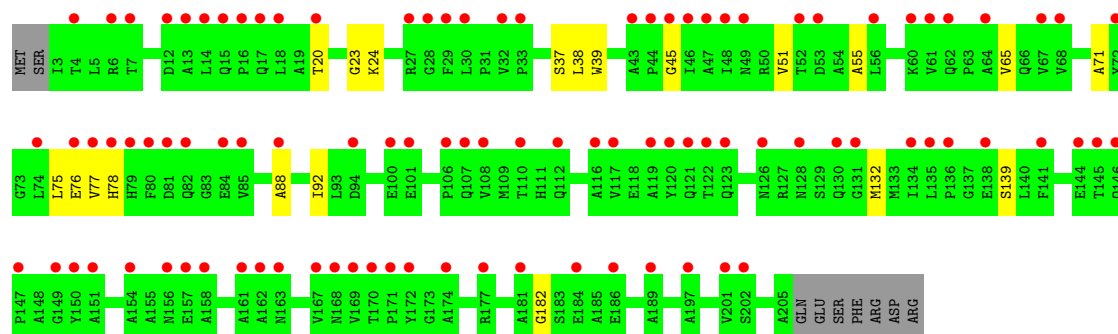
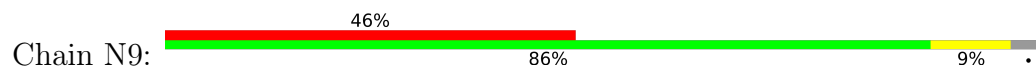




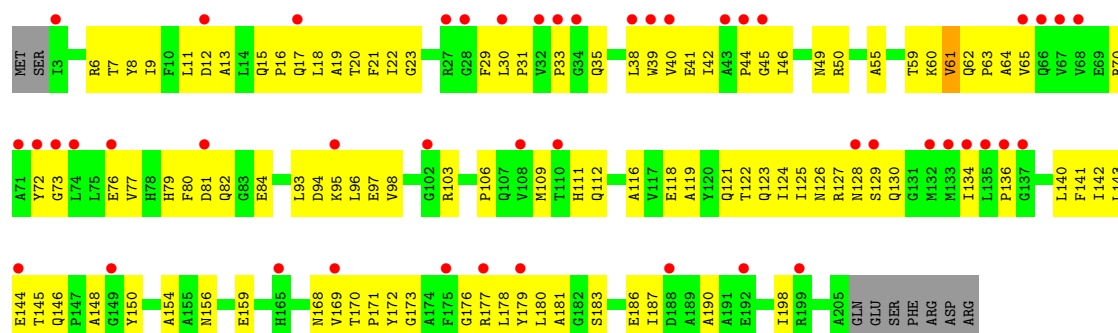
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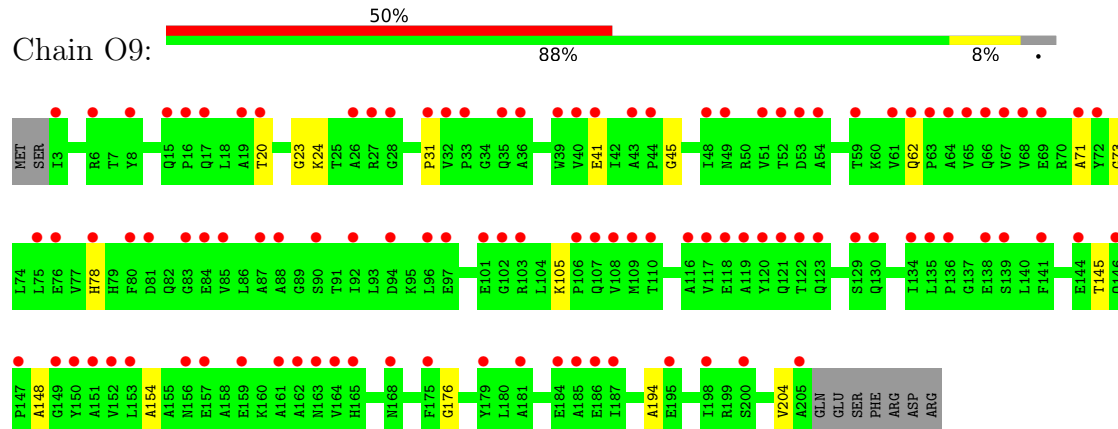
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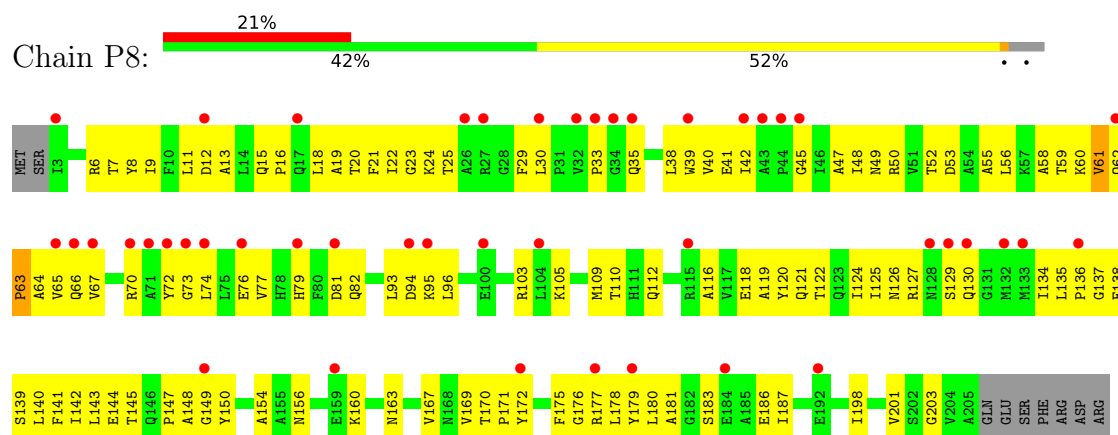
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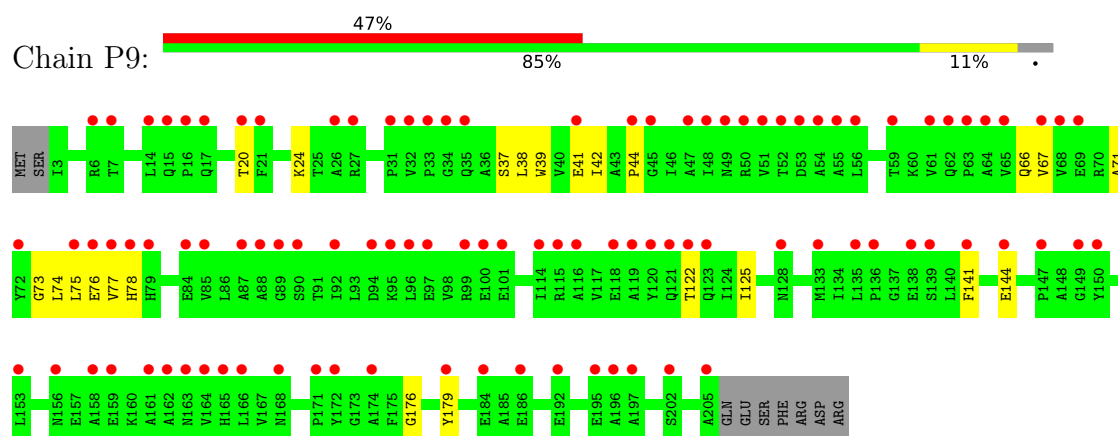
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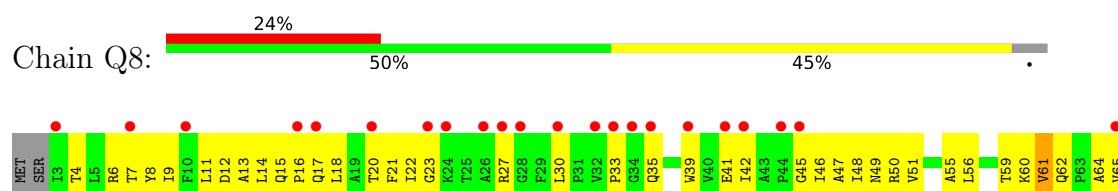
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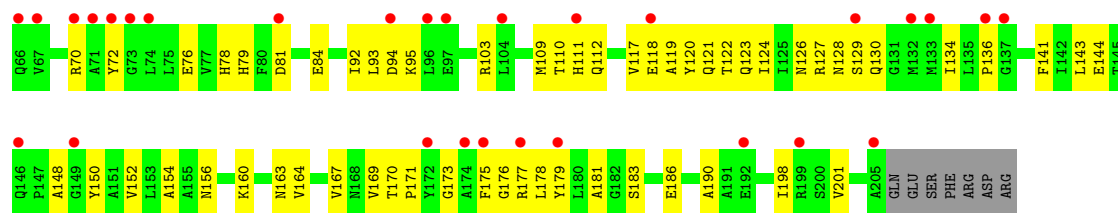


- Molecule 3: Microcompartments protein

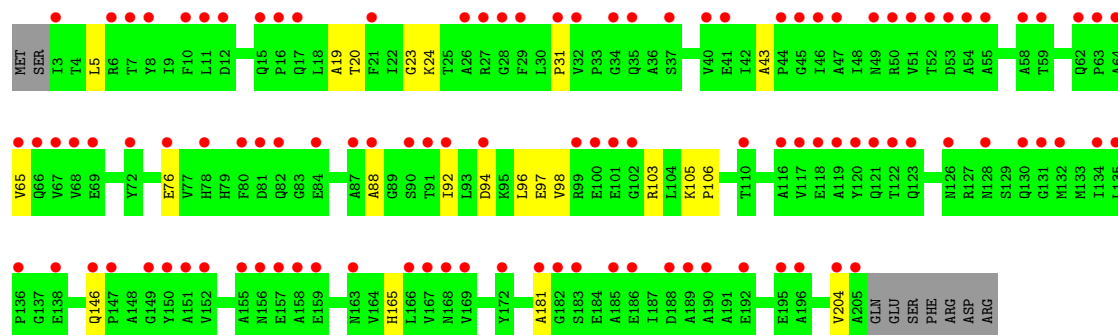
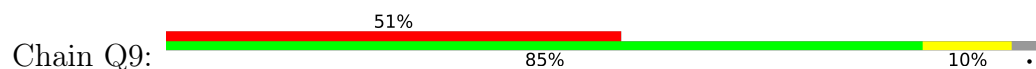


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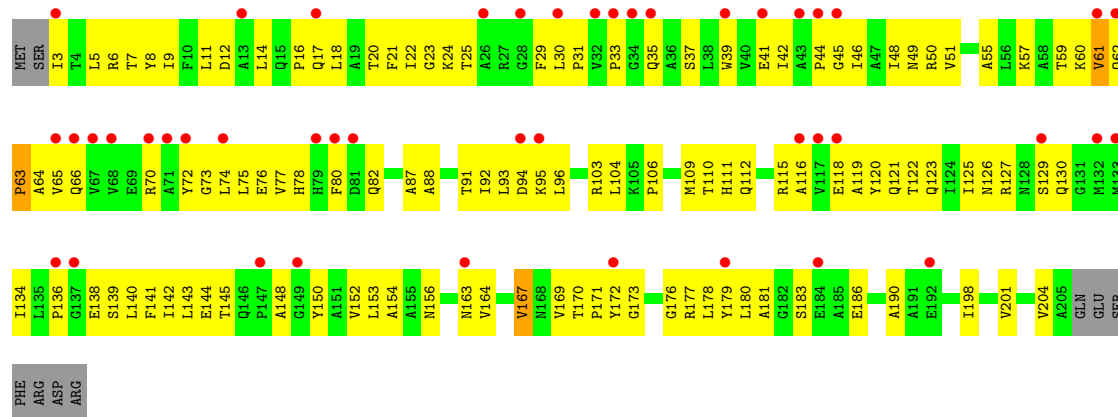




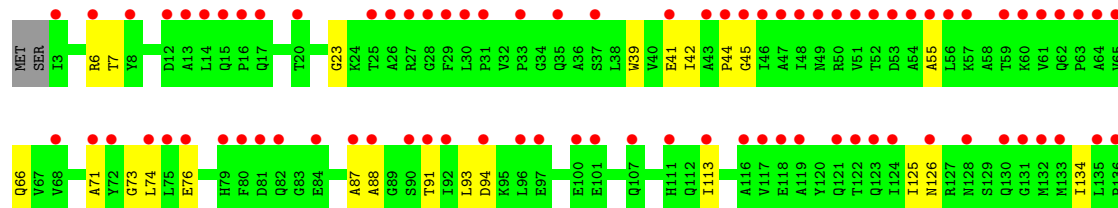
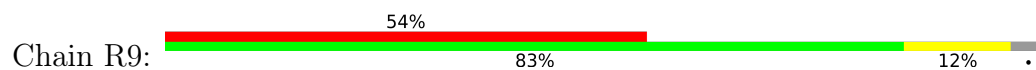
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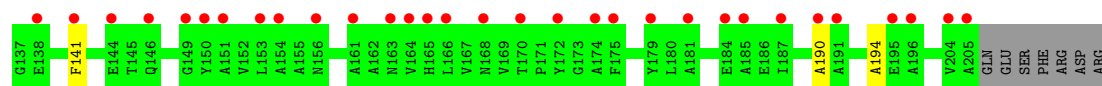


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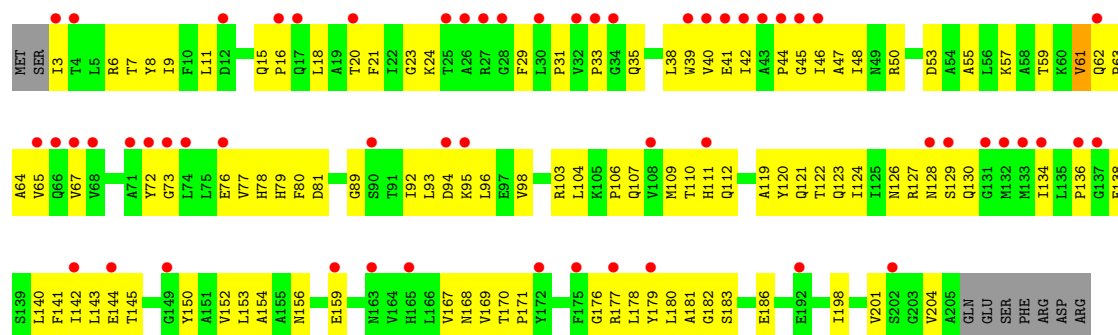


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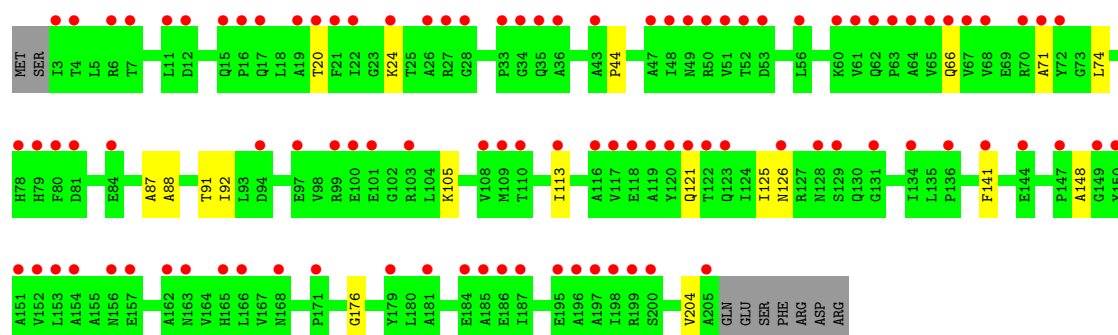




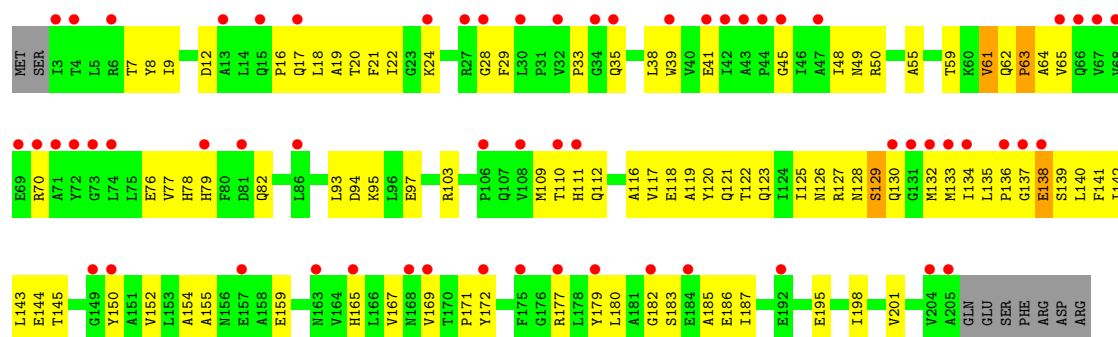
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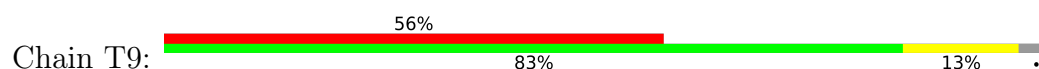
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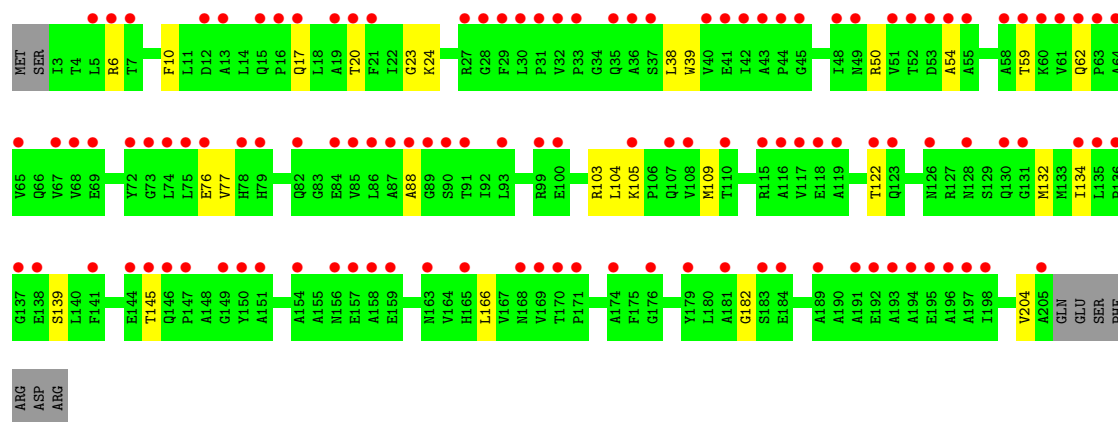


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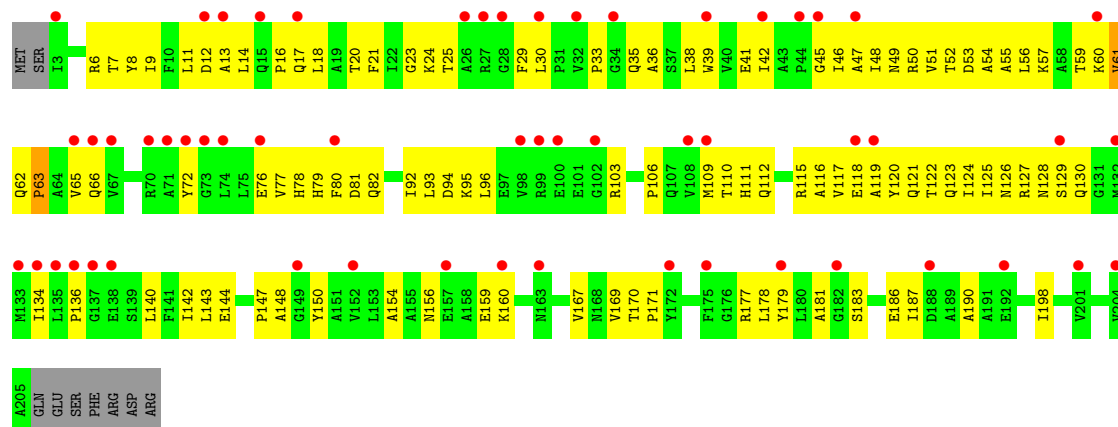


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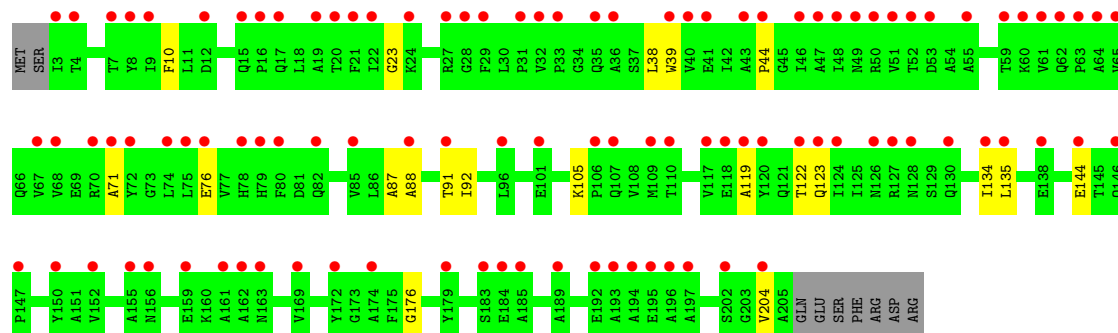
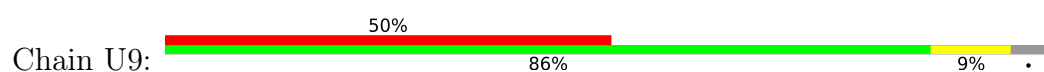




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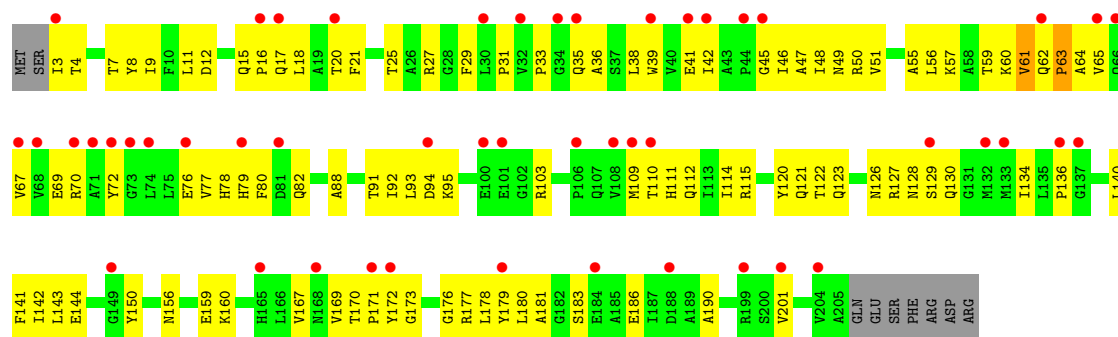


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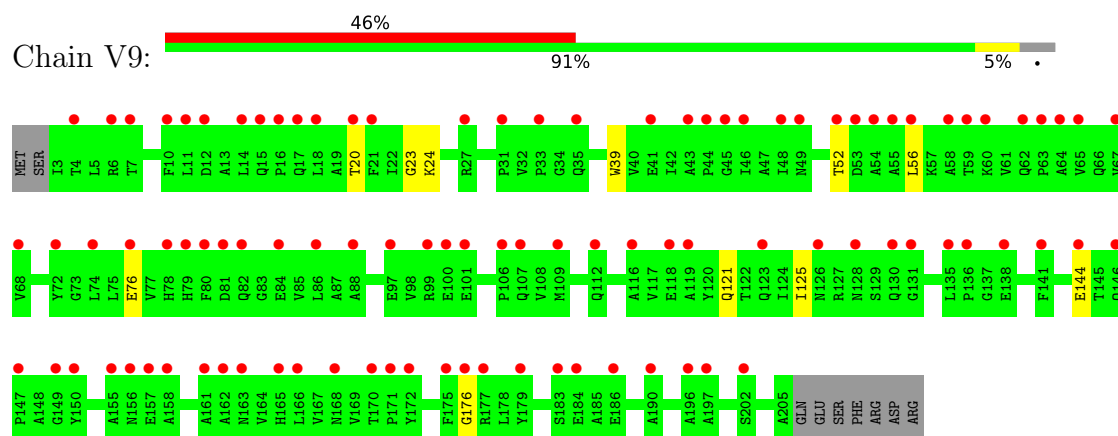


• Molecule 3: Microcompartments protein

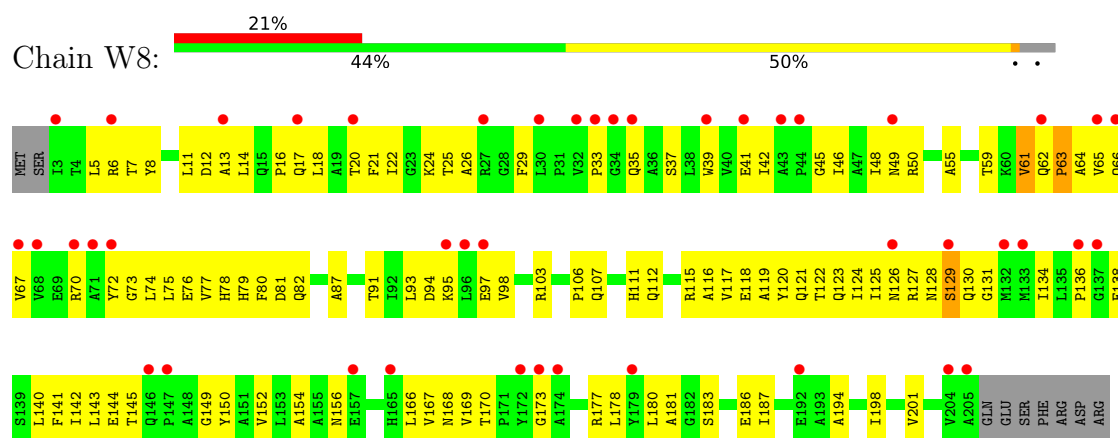




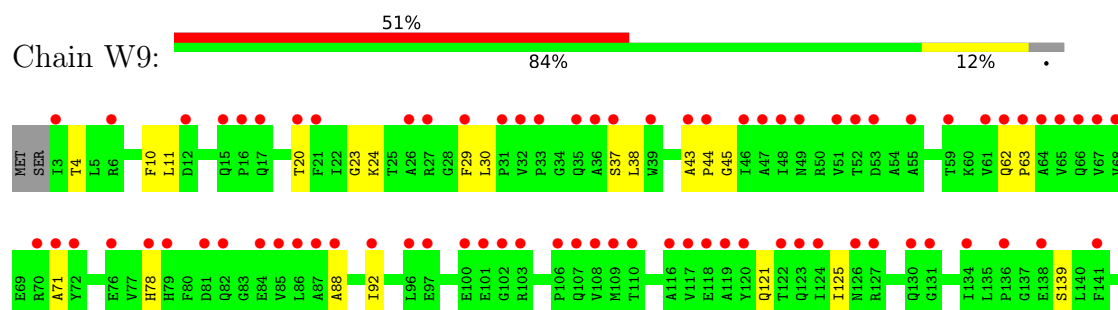
• Molecule 3: Microcompartments protein



• Molecule 3: Microcompartments protein

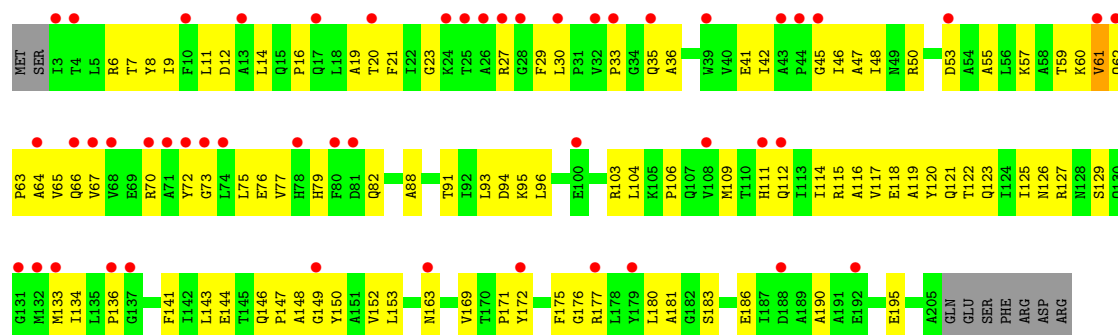


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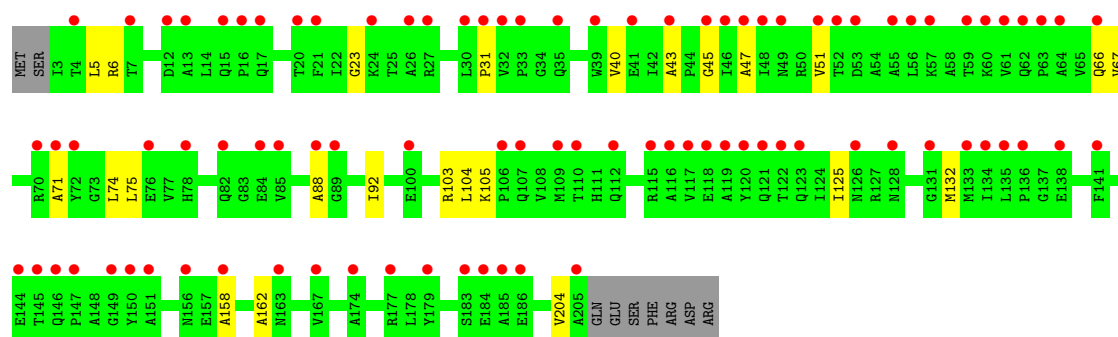
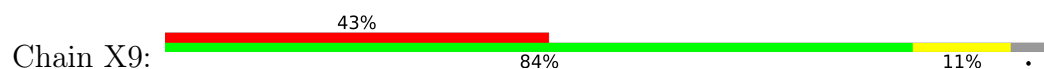




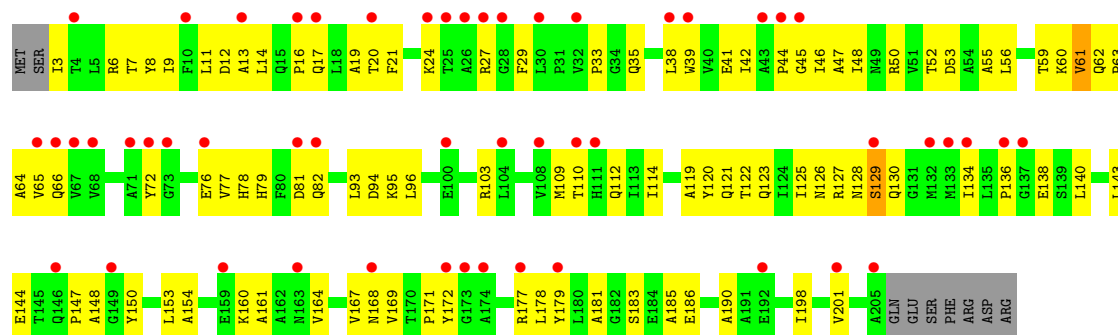
• Molecule 3: Microcompartments protein



• Molecule 3: Microcompartments protein

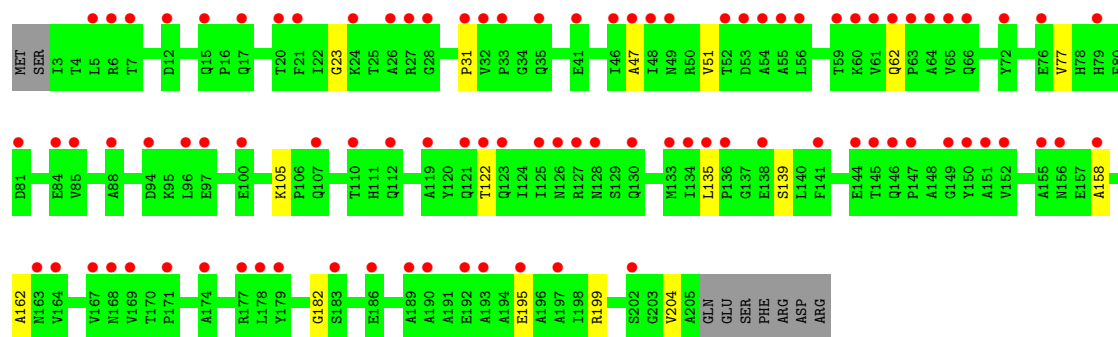


• Molecule 3: Microcompartments protein

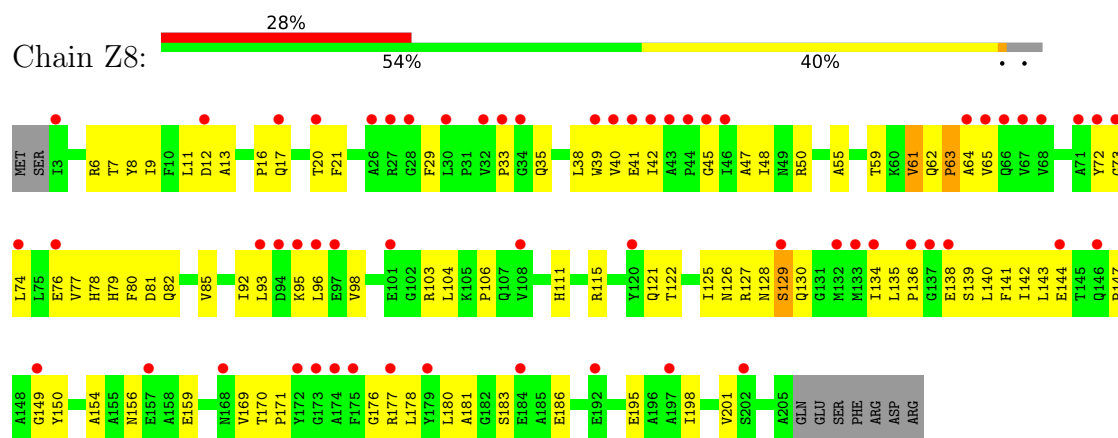


• Molecule 3: Microcompartments protein

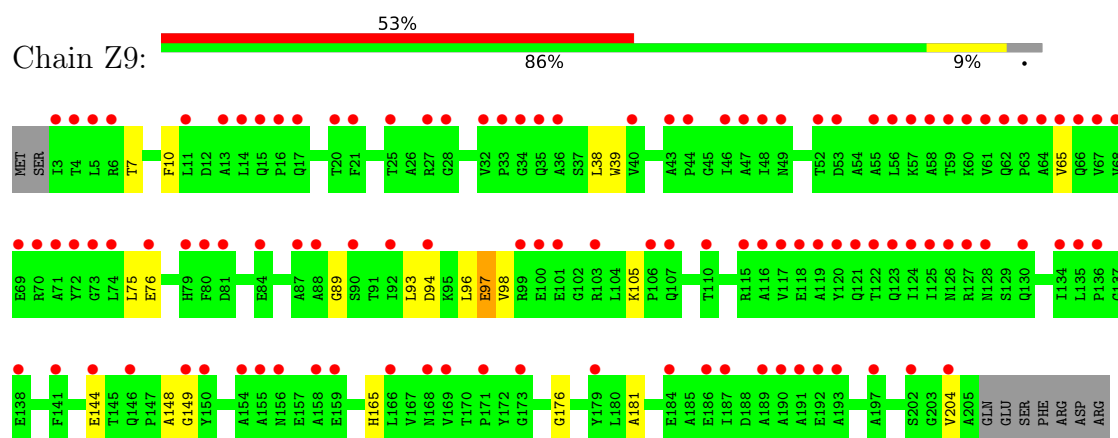




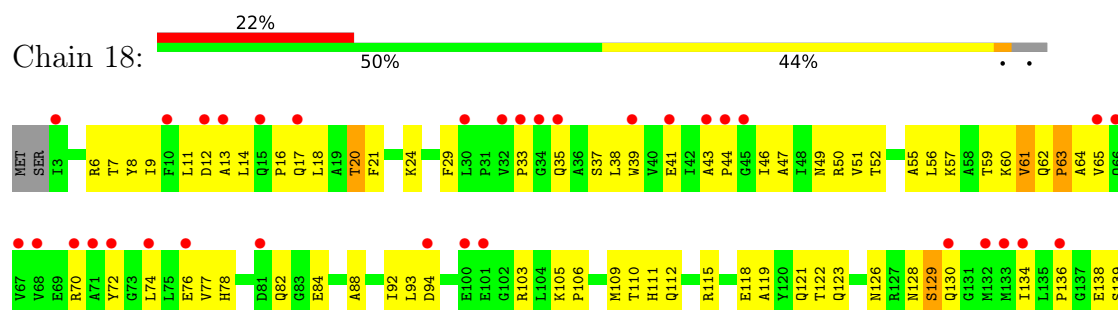
- Molecule 3: Microcompartments protein



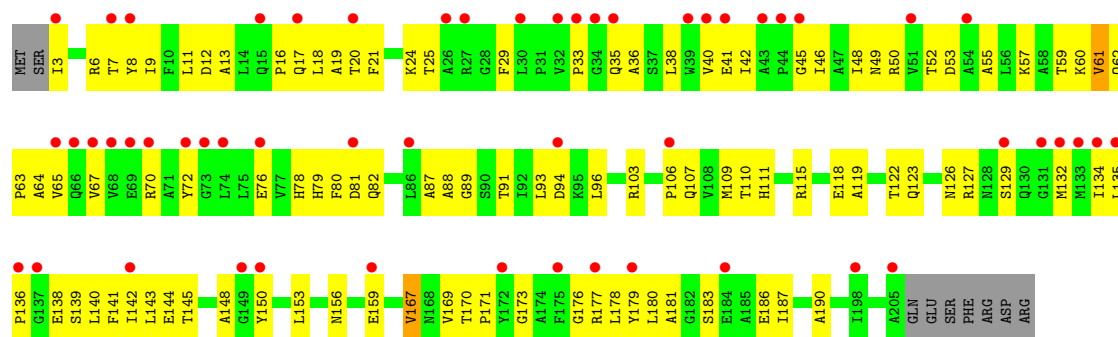
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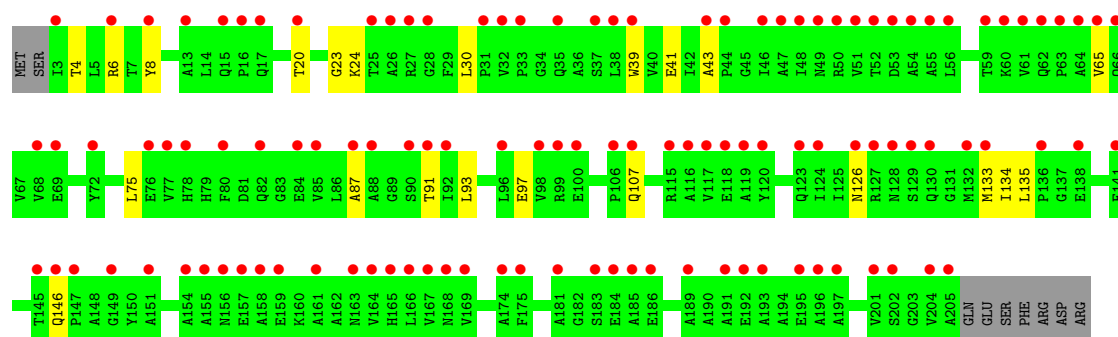
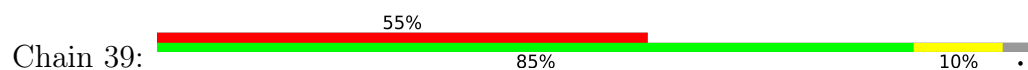
- Molecule 3: Microcompartments protein



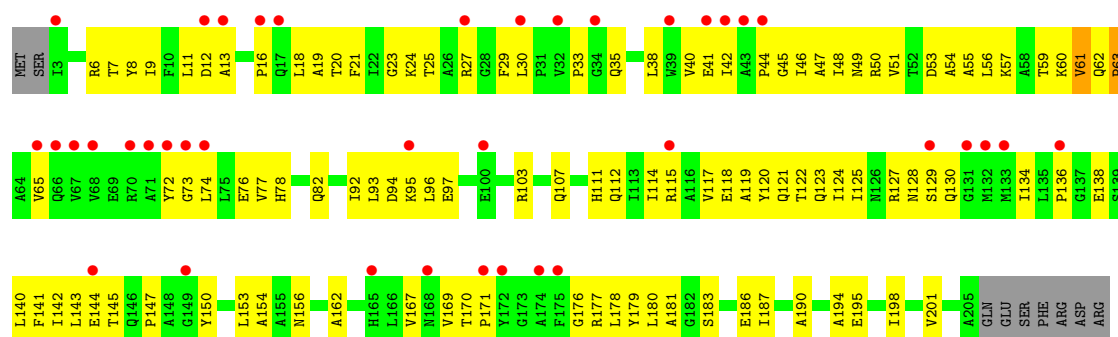




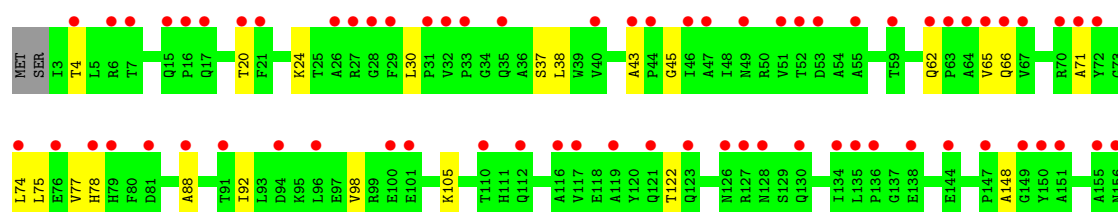
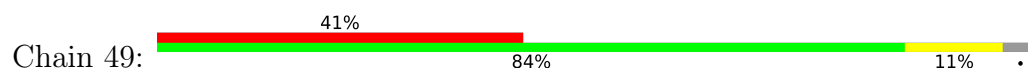
• Molecule 3: Microcompartments protein

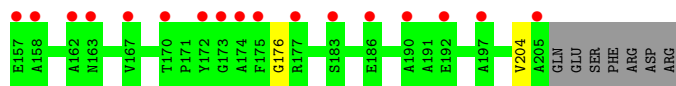


• Molecule 3: Microcompartments protein



• Molecule 3: Microcompartments protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	394.34Å 638.09Å 642.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.85 – 3.51 39.85 – 3.51	Depositor EDS
% Data completeness (in resolution range)	88.6 (39.85-3.51) 69.0 (39.85-3.51)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.48Å)	Xtriage
Refinement program	PHENIX dev_2650	Depositor
R, R_{free}	0.279 , 0.323 0.279 , 0.323	Depositor DCC
R_{free} test set	20031 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 80.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	215283	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3423e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	11	0.26	0/683	0.58	0/926
1	21	0.28	0/683	0.59	0/926
1	31	0.28	0/674	0.59	0/915
1	41	0.27	0/683	0.56	0/926
1	A1	0.24	0/683	0.55	0/926
1	B1	0.25	0/683	0.59	0/926
1	C1	0.24	0/683	0.55	0/926
1	D1	0.27	0/683	0.58	0/926
1	E1	0.24	0/683	0.56	0/926
1	F1	0.25	0/683	0.57	0/926
1	G1	0.25	0/683	0.55	0/926
1	H1	0.25	0/683	0.58	0/926
1	I1	0.27	0/683	0.57	0/926
1	J1	0.23	0/683	0.56	0/926
1	K1	0.27	0/683	0.57	0/926
1	L1	0.26	0/683	0.57	0/926
1	M1	0.28	0/683	0.60	0/926
1	N1	0.26	0/683	0.57	0/926
1	O1	0.23	0/683	0.59	0/926
1	P1	0.25	0/683	0.57	0/926
1	Q1	0.25	0/683	0.57	0/926
1	R1	0.24	0/683	0.59	0/926
1	S1	0.23	0/683	0.59	0/926
1	T1	0.27	0/683	0.61	0/926
1	U1	0.26	0/683	0.57	1/926 (0.1%)
1	V1	0.23	0/683	0.55	0/926
1	W1	0.26	0/683	0.61	0/926
1	X1	0.24	0/683	0.58	0/926
1	Y1	0.27	0/683	0.55	0/926
1	Z1	0.27	0/683	0.58	0/926
2	12	0.23	0/678	0.52	0/919
2	13	0.21	0/666	0.48	0/904
2	14	0.20	0/678	0.47	0/919
2	15	0.22	0/670	0.52	0/909

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	16	0.22	0/666	0.49	0/904
2	17	0.20	0/670	0.47	0/909
2	22	0.25	0/678	0.54	0/919
2	23	0.25	0/666	0.49	0/904
2	24	0.20	0/678	0.48	0/919
2	25	0.24	0/670	0.54	0/909
2	26	0.22	0/666	0.47	0/904
2	27	0.21	0/670	0.47	0/909
2	32	0.21	0/678	0.54	1/919 (0.1%)
2	33	0.21	0/666	0.50	0/904
2	34	0.23	0/678	0.54	0/919
2	35	0.22	0/670	0.55	0/909
2	36	0.22	0/666	0.47	0/904
2	37	0.21	0/670	0.42	0/909
2	42	0.22	0/678	0.52	0/919
2	43	0.21	0/666	0.52	0/904
2	44	0.21	0/678	0.48	0/919
2	45	0.22	0/670	0.54	0/909
2	46	0.23	0/666	0.52	0/904
2	47	0.21	0/670	0.42	0/909
2	A2	0.22	0/666	0.52	0/904
2	A3	0.22	0/666	0.52	0/904
2	A4	0.20	0/670	0.45	0/909
2	A5	0.22	0/666	0.56	0/904
2	A6	0.24	0/666	0.48	0/904
2	A7	0.21	0/666	0.47	0/904
2	B2	0.24	0/658	0.54	0/892
2	B3	0.21	0/666	0.48	0/904
2	B4	0.21	0/666	0.49	0/904
2	B5	0.22	0/666	0.54	0/904
2	B6	0.23	0/666	0.50	0/904
2	B7	0.22	0/666	0.48	0/904
2	C2	0.21	0/666	0.51	0/904
2	C3	0.21	0/666	0.48	0/904
2	C4	0.21	0/666	0.49	0/904
2	C5	0.22	0/666	0.54	0/904
2	C6	0.20	0/666	0.47	0/904
2	C7	0.21	0/670	0.46	0/909
2	D2	0.23	0/670	0.52	0/909
2	D3	0.22	0/666	0.50	0/904
2	D4	0.21	0/666	0.51	0/904
2	D5	0.21	0/666	0.50	0/904
2	D6	0.22	0/666	0.50	0/904

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	D7	0.22	0/670	0.49	0/909
2	E2	0.22	0/678	0.48	0/919
2	E3	0.21	0/666	0.46	0/904
2	E4	0.20	0/678	0.46	0/919
2	E5	0.20	0/666	0.45	0/904
2	E6	0.22	0/666	0.51	0/904
2	E7	0.21	0/666	0.44	0/904
2	F2	0.21	0/678	0.51	0/919
2	F3	0.20	0/666	0.47	0/904
2	F4	0.21	0/666	0.52	0/904
2	F5	0.20	0/666	0.48	0/904
2	F6	0.20	0/666	0.44	0/904
2	F7	0.21	0/670	0.43	0/909
2	G2	0.19	0/666	0.51	0/904
2	G3	0.21	0/666	0.50	0/904
2	G4	0.21	0/666	0.47	0/904
2	G5	0.22	0/661	0.51	0/897
2	G6	0.19	0/666	0.44	0/904
2	G7	0.21	0/666	0.43	0/904
2	H2	0.22	0/666	0.53	0/904
2	H3	0.23	0/666	0.51	0/904
2	H4	0.21	0/670	0.47	0/909
2	H5	0.22	0/661	0.52	0/897
2	H6	0.22	0/666	0.48	0/904
2	H7	0.20	0/666	0.46	0/904
2	I2	0.23	0/666	0.50	0/904
2	I3	0.21	0/661	0.46	0/897
2	I4	0.21	0/666	0.47	0/904
2	I5	0.23	0/666	0.51	0/904
2	I6	0.23	0/666	0.51	0/904
2	I7	0.20	0/666	0.46	0/904
2	J2	0.22	0/666	0.53	0/904
2	J3	0.22	0/666	0.54	0/904
2	J4	0.20	0/666	0.45	0/904
2	J5	0.25	0/661	0.55	0/897
2	J6	0.24	0/666	0.51	0/904
2	J7	0.21	0/666	0.47	0/904
2	K2	0.23	0/666	0.52	0/904
2	K3	0.21	0/666	0.48	0/904
2	K4	0.20	0/666	0.48	0/904
2	K5	0.22	0/670	0.54	0/909
2	K6	0.20	0/666	0.51	0/904
2	K7	0.20	0/670	0.45	0/909

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	L2	0.23	0/678	0.53	0/919
2	L3	0.25	0/666	0.49	0/904
2	L4	0.19	0/666	0.48	0/904
2	L5	0.22	0/666	0.50	0/904
2	L6	0.21	0/666	0.51	0/904
2	L7	0.23	0/670	0.47	0/909
2	M2	0.24	0/670	0.52	0/909
2	M3	0.22	0/666	0.49	0/904
2	M4	0.22	0/666	0.46	0/904
2	M5	0.22	0/670	0.50	0/909
2	M6	0.24	0/661	0.51	0/897
2	M7	0.23	0/666	0.50	0/904
2	N2	0.22	0/666	0.47	0/904
2	N3	0.21	0/661	0.51	0/897
2	N4	0.22	0/666	0.51	0/904
2	N5	0.24	0/670	0.55	0/909
2	N6	0.22	0/661	0.46	0/897
2	N7	0.21	0/665	0.45	0/902
2	O2	0.22	0/678	0.50	1/919 (0.1%)
2	O3	0.20	0/666	0.50	0/904
2	O4	0.21	0/678	0.47	0/919
2	O5	0.21	0/670	0.49	0/909
2	O6	0.20	0/666	0.47	0/904
2	O7	0.21	0/670	0.46	0/909
2	P2	0.23	0/678	0.49	0/919
2	P3	0.21	0/666	0.48	0/904
2	P4	0.22	0/678	0.46	0/919
2	P5	0.23	0/670	0.53	0/909
2	P6	0.21	0/666	0.48	0/904
2	P7	0.23	0/657	0.49	0/891
2	Q2	0.21	0/678	0.51	0/919
2	Q3	0.23	0/666	0.51	0/904
2	Q4	0.20	0/678	0.46	0/919
2	Q5	0.22	0/670	0.53	0/909
2	Q6	0.22	0/666	0.49	0/904
2	Q7	0.20	0/670	0.45	0/909
2	R2	0.21	0/678	0.47	0/919
2	R3	0.24	0/666	0.53	0/904
2	R4	0.20	0/678	0.48	0/919
2	R5	0.21	0/670	0.52	0/909
2	R6	0.23	0/666	0.56	0/904
2	R7	0.20	0/670	0.43	0/909
2	S2	0.25	0/678	0.52	0/919

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	S3	0.22	0/666	0.48	0/904
2	S4	0.22	0/678	0.50	0/919
2	S5	0.22	0/670	0.53	0/909
2	S6	0.21	0/666	0.49	0/904
2	S7	0.23	0/670	0.46	0/909
2	T2	0.25	0/678	0.59	0/919
2	T3	0.22	0/666	0.54	0/904
2	T4	0.22	0/678	0.53	0/919
2	T5	0.26	0/670	0.60	0/909
2	T6	0.22	0/666	0.53	0/904
2	T7	0.22	0/670	0.49	0/909
2	U2	0.24	0/678	0.55	0/919
2	U3	0.22	0/666	0.48	0/904
2	U4	0.21	0/678	0.48	0/919
2	U5	0.22	0/670	0.49	0/909
2	U6	0.22	0/666	0.49	0/904
2	U7	0.22	0/670	0.46	0/909
2	V2	0.22	0/678	0.49	0/919
2	V3	0.24	0/666	0.52	0/904
2	V4	0.24	0/678	0.52	0/919
2	V5	0.22	0/670	0.51	0/909
2	V6	0.22	0/666	0.47	0/904
2	V7	0.21	0/670	0.47	0/909
2	W2	0.23	0/678	0.52	0/919
2	W3	0.21	0/666	0.50	0/904
2	W4	0.20	0/678	0.51	0/919
2	W5	0.21	0/670	0.52	0/909
2	W6	0.21	0/666	0.49	0/904
2	W7	0.21	0/670	0.50	0/909
2	X2	0.22	0/678	0.49	0/919
2	X3	0.21	0/666	0.50	0/904
2	X4	0.20	0/678	0.46	0/919
2	X5	0.24	0/670	0.51	0/909
2	X6	0.21	0/666	0.50	0/904
2	X7	0.21	0/670	0.43	0/909
2	Y2	0.24	0/678	0.51	0/919
2	Y3	0.22	0/666	0.53	0/904
2	Y4	0.22	0/678	0.46	0/919
2	Y5	0.24	0/665	0.64	0/902
2	Y6	0.22	0/666	0.45	0/904
2	Y7	0.20	0/670	0.44	0/909
2	Z2	0.22	0/678	0.48	0/919
2	Z3	0.21	0/666	0.49	0/904

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Z4	0.21	0/678	0.47	0/919
2	Z5	0.21	0/670	0.49	0/909
2	Z6	0.21	0/666	0.49	0/904
2	Z7	0.22	0/670	0.48	0/909
3	18	0.23	0/1559	0.57	0/2122
3	19	0.13	0/973	0.41	0/1350
3	28	0.22	0/1559	0.58	0/2122
3	29	0.13	0/999	0.38	0/1388
3	38	0.24	0/1559	0.56	0/2122
3	39	0.15	0/999	0.46	0/1388
3	48	0.23	0/1559	0.55	0/2122
3	49	0.13	0/999	0.37	0/1388
3	A8	0.25	0/1559	0.56	0/2122
3	A9	0.13	0/999	0.35	0/1388
3	B8	0.22	0/1559	0.57	0/2122
3	B9	0.13	0/999	0.42	0/1388
3	C8	0.23	0/1559	0.57	0/2122
3	C9	0.14	0/999	0.37	0/1388
3	D8	0.28	1/1559 (0.1%)	0.59	0/2122
3	D9	0.14	0/999	0.50	2/1388 (0.1%)
3	E8	0.22	0/1559	0.55	0/2122
3	E9	0.13	0/999	0.45	2/1388 (0.1%)
3	F8	0.23	0/1559	0.57	0/2122
3	F9	0.13	0/999	0.43	0/1388
3	G8	0.22	0/1559	0.55	0/2122
3	G9	0.14	0/999	0.41	0/1388
3	H8	0.23	0/1559	0.61	0/2122
3	H9	0.13	0/999	0.44	2/1388 (0.1%)
3	I8	0.23	0/1559	0.56	0/2122
3	I9	0.15	0/999	0.40	0/1388
3	J8	0.21	0/1559	0.58	0/2122
3	J9	0.13	0/999	0.36	0/1388
3	K8	0.23	0/1559	0.58	0/2122
3	K9	0.13	0/999	0.39	0/1388
3	L8	0.22	0/1559	0.55	0/2122
3	L9	0.14	0/999	0.40	0/1388
3	M8	0.22	0/1559	0.58	0/2122
3	M9	0.13	0/999	0.36	0/1388
3	N8	0.23	0/1559	0.59	0/2122
3	N9	0.13	0/999	0.39	0/1388
3	O8	0.23	0/1559	0.58	0/2122
3	O9	0.14	0/999	0.37	0/1388
3	P8	0.27	1/1559 (0.1%)	0.57	0/2122

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	P9	0.14	0/999	0.41	0/1388
3	Q8	0.28	1/1559 (0.1%)	0.57	0/2122
3	Q9	0.13	0/999	0.44	2/1388 (0.1%)
3	R8	0.24	0/1559	0.57	0/2122
3	R9	0.13	0/999	0.40	0/1388
3	S8	0.23	0/1559	0.58	0/2122
3	S9	0.12	0/999	0.40	0/1388
3	T8	0.22	0/1559	0.57	0/2122
3	T9	0.15	0/999	0.49	0/1388
3	U8	0.22	0/1559	0.54	0/2122
3	U9	0.13	0/999	0.38	0/1388
3	V8	0.22	0/1559	0.57	0/2122
3	V9	0.13	0/999	0.37	0/1388
3	W8	0.23	0/1559	0.58	0/2122
3	W9	0.14	0/999	0.40	0/1388
3	X8	0.22	0/1559	0.55	0/2122
3	X9	0.13	0/999	0.44	2/1388 (0.1%)
3	Y8	0.22	0/1559	0.56	0/2122
3	Y9	0.15	0/999	0.39	0/1388
3	Z8	0.24	0/1559	0.56	0/2122
3	Z9	0.13	0/999	0.40	0/1388
All	All	0.22	3/217621 (0.0%)	0.51	13/296423 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P8	175	PHE	C-N	6.21	1.36	1.33
3	Q8	175	PHE	C-N	5.98	1.36	1.33
3	D8	175	PHE	C-N	5.94	1.36	1.33

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	32	67	VAL	N-CA-C	-6.81	105.95	111.81
1	U1	69	THR	CA-C-O	-6.28	111.52	120.51
3	D9	43	ALA	CA-C-N	6.27	142.06	127.00
3	D9	43	ALA	C-N-CA	6.27	142.06	127.00
3	E9	146	GLN	CA-C-N	6.09	141.62	127.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I1	678	0	705	40	0
1	21	678	0	705	30	1
1	31	669	0	692	43	0
1	41	678	0	705	21	1
1	A1	678	0	705	40	0
1	B1	678	0	705	39	0
1	C1	678	0	705	38	0
1	D1	678	0	705	38	0
1	E1	678	0	705	38	0
1	F1	678	0	705	46	0
1	G1	678	0	705	48	0
1	H1	678	0	705	40	0
1	I1	678	0	705	39	0
1	J1	678	0	705	49	0
1	K1	678	0	705	33	2
1	L1	678	0	705	46	0
1	M1	678	0	705	25	1
1	N1	678	0	705	37	2
1	O1	678	0	705	52	0
1	P1	678	0	705	45	0
1	Q1	678	0	705	36	0
1	R1	678	0	705	39	0
1	S1	678	0	705	43	0
1	T1	678	0	705	34	2
1	U1	678	0	705	30	0
1	V1	678	0	705	46	0
1	W1	678	0	705	40	0
1	X1	678	0	705	34	1
1	Y1	678	0	705	31	2
1	Z1	678	0	705	54	0
2	12	670	0	690	29	0
2	13	658	0	678	32	0
2	14	670	0	690	19	0
2	15	662	0	681	28	0
2	16	658	0	678	25	0
2	17	662	0	681	13	0
2	22	670	0	690	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	23	658	0	678	41	0
2	24	670	0	690	21	0
2	25	662	0	681	27	0
2	26	658	0	678	22	0
2	27	662	0	681	20	1
2	32	670	0	690	28	0
2	33	658	0	678	29	0
2	34	670	0	690	26	0
2	35	662	0	681	32	0
2	36	658	0	678	22	0
2	37	662	0	681	16	0
2	42	670	0	690	23	0
2	43	658	0	678	33	0
2	44	670	0	690	16	0
2	45	662	0	681	22	0
2	46	658	0	678	24	0
2	47	662	0	681	23	1
2	A2	658	0	678	35	0
2	A3	658	0	678	37	0
2	A4	662	0	681	23	0
2	A5	658	0	678	29	0
2	A6	658	0	678	19	0
2	A7	658	0	678	24	0
2	B2	651	0	671	30	0
2	B3	658	0	678	33	0
2	B4	658	0	678	17	0
2	B5	658	0	678	34	0
2	B6	658	0	678	23	0
2	B7	658	0	678	25	0
2	C2	658	0	678	26	0
2	C3	658	0	678	32	0
2	C4	658	0	678	19	0
2	C5	658	0	678	27	0
2	C6	658	0	678	20	0
2	C7	662	0	681	26	0
2	D2	662	0	681	34	0
2	D3	658	0	678	41	0
2	D4	658	0	678	28	0
2	D5	658	0	678	27	0
2	D6	658	0	678	23	0
2	D7	662	0	681	20	0
2	E2	670	0	690	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E3	658	0	678	24	0
2	E4	670	0	690	23	0
2	E5	658	0	678	24	0
2	E6	658	0	678	26	0
2	E7	658	0	678	26	0
2	F2	670	0	690	29	0
2	F3	658	0	678	34	0
2	F4	658	0	678	35	0
2	F5	658	0	678	23	0
2	F6	658	0	678	19	0
2	F7	662	0	681	28	0
2	G2	658	0	678	27	0
2	G3	658	0	678	32	0
2	G4	658	0	678	24	0
2	G5	653	0	673	29	0
2	G6	658	0	678	28	0
2	G7	658	0	678	32	0
2	H2	658	0	678	26	0
2	H3	658	0	678	29	0
2	H4	662	0	681	23	0
2	H5	653	0	673	28	0
2	H6	658	0	678	23	0
2	H7	658	0	678	21	0
2	I2	658	0	678	32	0
2	I3	653	0	673	31	0
2	I4	658	0	678	28	0
2	I5	658	0	678	30	0
2	I6	658	0	678	22	0
2	I7	658	0	678	22	0
2	J2	658	0	678	34	0
2	J3	658	0	678	35	0
2	J4	658	0	678	22	0
2	J5	653	0	673	21	0
2	J6	658	0	678	21	0
2	J7	658	0	678	28	0
2	K2	658	0	678	26	0
2	K3	658	0	678	16	1
2	K4	658	0	678	22	0
2	K5	662	0	681	18	0
2	K6	658	0	678	19	0
2	K7	662	0	681	19	0
2	L2	670	0	690	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L3	658	0	678	28	0
2	L4	658	0	678	28	0
2	L5	658	0	678	36	0
2	L6	658	0	678	27	0
2	L7	662	0	681	26	0
2	M2	662	0	681	24	0
2	M3	658	0	678	23	1
2	M4	658	0	678	20	0
2	M5	662	0	681	34	0
2	M6	653	0	673	16	0
2	M7	658	0	678	28	0
2	N2	658	0	678	28	0
2	N3	653	0	673	24	0
2	N4	658	0	678	20	0
2	N5	662	0	681	31	0
2	N6	653	0	673	24	0
2	N7	657	0	676	21	0
2	O2	670	0	690	27	0
2	O3	658	0	678	26	0
2	O4	670	0	690	15	0
2	O5	662	0	681	26	0
2	O6	658	0	678	22	0
2	O7	662	0	681	25	1
2	P2	670	0	690	30	0
2	P3	658	0	678	32	0
2	P4	670	0	690	22	0
2	P5	662	0	681	24	0
2	P6	658	0	678	22	0
2	P7	649	0	672	30	0
2	Q2	670	0	690	30	0
2	Q3	658	0	678	36	0
2	Q4	670	0	690	19	0
2	Q5	662	0	681	25	0
2	Q6	658	0	678	17	0
2	Q7	662	0	681	23	0
2	R2	670	0	690	22	0
2	R3	658	0	678	31	0
2	R4	670	0	690	16	0
2	R5	662	0	681	21	0
2	R6	658	0	678	18	0
2	R7	662	0	681	21	0
2	S2	670	0	690	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S3	658	0	678	27	0
2	S4	670	0	690	24	0
2	S5	662	0	681	26	0
2	S6	658	0	678	21	0
2	S7	662	0	681	20	0
2	T2	670	0	690	32	0
2	T3	658	0	678	28	0
2	T4	670	0	690	23	0
2	T5	662	0	681	37	0
2	T6	658	0	678	30	0
2	T7	662	0	681	20	0
2	U2	670	0	690	30	0
2	U3	658	0	678	28	0
2	U4	670	0	690	22	0
2	U5	662	0	681	23	0
2	U6	658	0	678	20	0
2	U7	662	0	681	26	0
2	V2	670	0	690	29	0
2	V3	658	0	678	32	0
2	V4	670	0	690	26	0
2	V5	662	0	681	24	0
2	V6	658	0	678	29	0
2	V7	662	0	681	29	0
2	W2	670	0	690	33	0
2	W3	658	0	678	31	0
2	W4	670	0	690	15	0
2	W5	662	0	681	37	0
2	W6	658	0	678	27	0
2	W7	662	0	681	28	0
2	X2	670	0	690	26	0
2	X3	658	0	678	33	1
2	X4	670	0	690	21	0
2	X5	662	0	681	30	0
2	X6	658	0	678	20	0
2	X7	662	0	681	21	0
2	Y2	670	0	690	25	0
2	Y3	658	0	678	34	0
2	Y4	670	0	690	19	0
2	Y5	657	0	676	20	0
2	Y6	658	0	678	23	0
2	Y7	662	0	681	16	0
2	Z2	670	0	690	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z3	658	0	678	27	0
2	Z4	670	0	690	19	0
2	Z5	662	0	681	21	0
2	Z6	658	0	678	17	0
2	Z7	662	0	681	22	0
3	18	1533	0	1560	94	2
3	19	975	0	499	13	0
3	28	1533	0	1560	101	0
3	29	1000	0	510	10	0
3	38	1533	0	1560	95	0
3	39	1000	0	510	14	0
3	48	1533	0	1560	97	0
3	49	1000	0	510	13	0
3	A8	1533	0	1560	95	0
3	A9	1000	0	510	13	0
3	B8	1533	0	1560	117	0
3	B9	1000	0	510	13	0
3	C8	1533	0	1560	112	0
3	C9	1000	0	510	11	0
3	D8	1533	0	1560	96	0
3	D9	1000	0	510	7	0
3	E8	1533	0	1560	95	0
3	E9	1000	0	510	11	0
3	F8	1533	0	1560	97	0
3	F9	1000	0	510	7	0
3	G8	1533	0	1560	96	0
3	G9	1000	0	510	12	0
3	H8	1533	0	1560	107	0
3	H9	1000	0	510	11	0
3	I8	1533	0	1560	104	0
3	I9	1000	0	510	18	0
3	J8	1533	0	1560	98	0
3	J9	1000	0	510	9	0
3	K8	1533	0	1560	102	2
3	K9	1000	0	510	5	0
3	L8	1533	0	1560	108	0
3	L9	1000	0	510	15	0
3	M8	1533	0	1560	86	0
3	M9	1000	0	510	5	0
3	N8	1533	0	1560	103	0
3	N9	1000	0	510	11	0
3	O8	1533	0	1560	84	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O9	1000	0	510	10	0
3	P8	1533	0	1560	101	0
3	P9	1000	0	510	13	0
3	Q8	1533	0	1560	90	0
3	Q9	1000	0	510	13	0
3	R8	1533	0	1560	110	0
3	R9	1000	0	510	17	0
3	S8	1533	0	1560	93	0
3	S9	1000	0	510	10	0
3	T8	1533	0	1560	77	1
3	T9	1000	0	510	18	0
3	U8	1533	0	1560	102	0
3	U9	1000	0	510	12	0
3	V8	1533	0	1560	89	0
3	V9	1000	0	510	6	0
3	W8	1533	0	1560	89	0
3	W9	1000	0	510	14	0
3	X8	1533	0	1560	89	0
3	X9	1000	0	510	13	0
3	Y8	1533	0	1560	94	0
3	Y9	1000	0	510	11	0
3	Z8	1533	0	1560	77	1
3	Z9	1000	0	510	12	0
All	All	215283	0	205772	7422	14

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 7422 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C3:35:GLU:OE2	2:D7:36:LYS:NZ	1.66	1.28
2:A7:36:LYS:NZ	2:E3:35:GLU:OE2	1.73	1.20
2:G7:36:LYS:NZ	2:W3:35:GLU:OE2	1.79	1.14
2:P5:3:ASP:OD2	2:P5:91:ARG:NH1	1.82	1.12
2:K7:54:LYS:NZ	2:K7:58:GLU:OE2	1.84	1.09

The worst 5 of 14 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X1:83:ASP:OD2	1:41:13:SER:OG[3_455]	1.82	0.38
2:M3:35:GLU:OE2	2:27:36:LYS:NZ[3_455]	1.86	0.34
1:M1:83:ASP:OD2	1:21:13:SER:OG[3_455]	1.93	0.27
1:T1:83:ASP:OD2	1:Y1:13:SER:OG[3_455]	1.93	0.27
2:X3:36:LYS:O	2:47:36:LYS:NZ[3_455]	1.96	0.24

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 X-ray entries followed by that with respect to entries of similar resolution.

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	11	93/96 (97%)	80 (86%)	10 (11%)	3 (3%)	3	24
1	21	93/96 (97%)	79 (85%)	12 (13%)	2 (2%)	5	30
1	31	92/96 (96%)	77 (84%)	10 (11%)	5 (5%)	1	13
1	41	93/96 (97%)	77 (83%)	11 (12%)	5 (5%)	1	13
1	A1	93/96 (97%)	79 (85%)	11 (12%)	3 (3%)	3	24
1	B1	93/96 (97%)	78 (84%)	13 (14%)	2 (2%)	5	30
1	C1	93/96 (97%)	80 (86%)	12 (13%)	1 (1%)	11	44
1	D1	93/96 (97%)	79 (85%)	12 (13%)	2 (2%)	5	30
1	E1	93/96 (97%)	79 (85%)	10 (11%)	4 (4%)	2	18
1	F1	93/96 (97%)	80 (86%)	10 (11%)	3 (3%)	3	24
1	G1	93/96 (97%)	79 (85%)	13 (14%)	1 (1%)	11	44
1	H1	93/96 (97%)	80 (86%)	11 (12%)	2 (2%)	5	30
1	I1	93/96 (97%)	79 (85%)	11 (12%)	3 (3%)	3	24
1	J1	93/96 (97%)	79 (85%)	12 (13%)	2 (2%)	5	30
1	K1	93/96 (97%)	78 (84%)	10 (11%)	5 (5%)	1	13
1	L1	93/96 (97%)	79 (85%)	12 (13%)	2 (2%)	5	30
1	M1	93/96 (97%)	80 (86%)	11 (12%)	2 (2%)	5	30
1	N1	93/96 (97%)	79 (85%)	9 (10%)	5 (5%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O1	93/96 (97%)	79 (85%)	11 (12%)	3 (3%)	3	24
1	P1	93/96 (97%)	80 (86%)	12 (13%)	1 (1%)	11	44
1	Q1	93/96 (97%)	79 (85%)	13 (14%)	1 (1%)	11	44
1	R1	93/96 (97%)	79 (85%)	12 (13%)	2 (2%)	5	30
1	S1	93/96 (97%)	80 (86%)	10 (11%)	3 (3%)	3	24
1	T1	93/96 (97%)	78 (84%)	11 (12%)	4 (4%)	2	18
1	U1	93/96 (97%)	78 (84%)	12 (13%)	3 (3%)	3	24
1	V1	93/96 (97%)	78 (84%)	14 (15%)	1 (1%)	11	44
1	W1	93/96 (97%)	79 (85%)	11 (12%)	3 (3%)	3	24
1	X1	93/96 (97%)	78 (84%)	11 (12%)	4 (4%)	2	18
1	Y1	93/96 (97%)	79 (85%)	11 (12%)	3 (3%)	3	24
1	Z1	93/96 (97%)	79 (85%)	10 (11%)	4 (4%)	2	18
2	12	92/99 (93%)	79 (86%)	8 (9%)	5 (5%)	1	13
2	13	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	5	30
2	14	92/99 (93%)	85 (92%)	6 (6%)	1 (1%)	11	44
2	15	91/99 (92%)	84 (92%)	5 (6%)	2 (2%)	5	30
2	16	90/99 (91%)	83 (92%)	7 (8%)	0	100	100
2	17	91/99 (92%)	86 (94%)	5 (6%)	0	100	100
2	22	92/99 (93%)	84 (91%)	6 (6%)	2 (2%)	5	30
2	23	90/99 (91%)	83 (92%)	6 (7%)	1 (1%)	11	44
2	24	92/99 (93%)	85 (92%)	6 (6%)	1 (1%)	11	44
2	25	91/99 (92%)	85 (93%)	6 (7%)	0	100	100
2	26	90/99 (91%)	82 (91%)	8 (9%)	0	100	100
2	27	91/99 (92%)	84 (92%)	7 (8%)	0	100	100
2	32	92/99 (93%)	80 (87%)	7 (8%)	5 (5%)	1	13
2	33	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	5	30
2	34	92/99 (93%)	82 (89%)	7 (8%)	3 (3%)	3	23
2	35	91/99 (92%)	83 (91%)	8 (9%)	0	100	100
2	36	90/99 (91%)	82 (91%)	8 (9%)	0	100	100
2	37	91/99 (92%)	84 (92%)	7 (8%)	0	100	100
2	42	92/99 (93%)	80 (87%)	9 (10%)	3 (3%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	43	90/99 (91%)	80 (89%)	8 (9%)	2 (2%)	5	30
2	44	92/99 (93%)	85 (92%)	6 (6%)	1 (1%)	11	44
2	45	91/99 (92%)	82 (90%)	7 (8%)	2 (2%)	5	30
2	46	90/99 (91%)	82 (91%)	8 (9%)	0	100	100
2	47	91/99 (92%)	85 (93%)	6 (7%)	0	100	100
2	A2	90/99 (91%)	80 (89%)	8 (9%)	2 (2%)	5	30
2	A3	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	5	30
2	A4	91/99 (92%)	84 (92%)	6 (7%)	1 (1%)	11	44
2	A5	90/99 (91%)	83 (92%)	7 (8%)	0	100	100
2	A6	90/99 (91%)	82 (91%)	8 (9%)	0	100	100
2	A7	90/99 (91%)	85 (94%)	4 (4%)	1 (1%)	11	44
2	B2	89/99 (90%)	80 (90%)	7 (8%)	2 (2%)	5	30
2	B3	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	5	30
2	B4	90/99 (91%)	85 (94%)	4 (4%)	1 (1%)	11	44
2	B5	90/99 (91%)	84 (93%)	6 (7%)	0	100	100
2	B6	90/99 (91%)	82 (91%)	8 (9%)	0	100	100
2	B7	90/99 (91%)	85 (94%)	5 (6%)	0	100	100
2	C2	90/99 (91%)	79 (88%)	9 (10%)	2 (2%)	5	30
2	C3	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	5	30
2	C4	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	11	44
2	C5	90/99 (91%)	84 (93%)	6 (7%)	0	100	100
2	C6	90/99 (91%)	82 (91%)	8 (9%)	0	100	100
2	C7	91/99 (92%)	86 (94%)	5 (6%)	0	100	100
2	D2	91/99 (92%)	80 (88%)	9 (10%)	2 (2%)	5	30
2	D3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	5	30
2	D4	90/99 (91%)	83 (92%)	6 (7%)	1 (1%)	11	44
2	D5	90/99 (91%)	85 (94%)	5 (6%)	0	100	100
2	D6	90/99 (91%)	81 (90%)	8 (9%)	1 (1%)	11	44
2	D7	91/99 (92%)	85 (93%)	6 (7%)	0	100	100
2	E2	92/99 (93%)	82 (89%)	8 (9%)	2 (2%)	5	30
2	E3	90/99 (91%)	81 (90%)	8 (9%)	1 (1%)	11	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E4	92/99 (93%)	83 (90%)	8 (9%)	1 (1%)	11	44
2	E5	90/99 (91%)	86 (96%)	4 (4%)	0	100	100
2	E6	90/99 (91%)	82 (91%)	8 (9%)	0	100	100
2	E7	90/99 (91%)	86 (96%)	4 (4%)	0	100	100
2	F2	92/99 (93%)	82 (89%)	8 (9%)	2 (2%)	5	30
2	F3	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	5	30
2	F4	90/99 (91%)	84 (93%)	4 (4%)	2 (2%)	5	30
2	F5	90/99 (91%)	85 (94%)	5 (6%)	0	100	100
2	F6	90/99 (91%)	82 (91%)	8 (9%)	0	100	100
2	F7	91/99 (92%)	85 (93%)	6 (7%)	0	100	100
2	G2	90/99 (91%)	80 (89%)	8 (9%)	2 (2%)	5	30
2	G3	90/99 (91%)	79 (88%)	8 (9%)	3 (3%)	3	23
2	G4	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	11	44
2	G5	89/99 (90%)	83 (93%)	6 (7%)	0	100	100
2	G6	90/99 (91%)	83 (92%)	7 (8%)	0	100	100
2	G7	90/99 (91%)	85 (94%)	5 (6%)	0	100	100
2	H2	90/99 (91%)	78 (87%)	10 (11%)	2 (2%)	5	30
2	H3	90/99 (91%)	83 (92%)	5 (6%)	2 (2%)	5	30
2	H4	91/99 (92%)	82 (90%)	7 (8%)	2 (2%)	5	30
2	H5	89/99 (90%)	84 (94%)	5 (6%)	0	100	100
2	H6	90/99 (91%)	82 (91%)	8 (9%)	0	100	100
2	H7	90/99 (91%)	86 (96%)	4 (4%)	0	100	100
2	I2	90/99 (91%)	79 (88%)	9 (10%)	2 (2%)	5	30
2	I3	89/99 (90%)	82 (92%)	5 (6%)	2 (2%)	5	30
2	I4	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	11	44
2	I5	90/99 (91%)	85 (94%)	5 (6%)	0	100	100
2	I6	90/99 (91%)	82 (91%)	8 (9%)	0	100	100
2	I7	90/99 (91%)	86 (96%)	4 (4%)	0	100	100
2	J2	90/99 (91%)	80 (89%)	8 (9%)	2 (2%)	5	30
2	J3	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	5	30
2	J4	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	11	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J5	89/99 (90%)	83 (93%)	5 (6%)	1 (1%)	11	44
2	J6	90/99 (91%)	82 (91%)	8 (9%)	0	100	100
2	J7	90/99 (91%)	85 (94%)	5 (6%)	0	100	100
2	K2	90/99 (91%)	80 (89%)	8 (9%)	2 (2%)	5	30
2	K3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	5	30
2	K4	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	11	44
2	K5	91/99 (92%)	83 (91%)	8 (9%)	0	100	100
2	K6	90/99 (91%)	82 (91%)	8 (9%)	0	100	100
2	K7	91/99 (92%)	86 (94%)	5 (6%)	0	100	100
2	L2	92/99 (93%)	83 (90%)	7 (8%)	2 (2%)	5	30
2	L3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	5	30
2	L4	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	11	44
2	L5	90/99 (91%)	84 (93%)	6 (7%)	0	100	100
2	L6	90/99 (91%)	81 (90%)	9 (10%)	0	100	100
2	L7	91/99 (92%)	86 (94%)	5 (6%)	0	100	100
2	M2	91/99 (92%)	80 (88%)	9 (10%)	2 (2%)	5	30
2	M3	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	5	30
2	M4	90/99 (91%)	83 (92%)	6 (7%)	1 (1%)	11	44
2	M5	91/99 (92%)	82 (90%)	8 (9%)	1 (1%)	11	44
2	M6	89/99 (90%)	81 (91%)	8 (9%)	0	100	100
2	M7	90/99 (91%)	85 (94%)	5 (6%)	0	100	100
2	N2	90/99 (91%)	82 (91%)	7 (8%)	1 (1%)	11	44
2	N3	89/99 (90%)	81 (91%)	5 (6%)	3 (3%)	3	23
2	N4	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	11	44
2	N5	91/99 (92%)	82 (90%)	5 (6%)	4 (4%)	2	17
2	N6	89/99 (90%)	81 (91%)	8 (9%)	0	100	100
2	N7	90/99 (91%)	85 (94%)	5 (6%)	0	100	100
2	O2	92/99 (93%)	81 (88%)	7 (8%)	4 (4%)	2	18
2	O3	90/99 (91%)	81 (90%)	6 (7%)	3 (3%)	3	23
2	O4	92/99 (93%)	86 (94%)	5 (5%)	1 (1%)	11	44
2	O5	91/99 (92%)	85 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O6	90/99 (91%)	81 (90%)	9 (10%)	0	100	100
2	O7	91/99 (92%)	85 (93%)	6 (7%)	0	100	100
2	P2	92/99 (93%)	80 (87%)	9 (10%)	3 (3%)	3	23
2	P3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	5	30
2	P4	92/99 (93%)	86 (94%)	5 (5%)	1 (1%)	11	44
2	P5	91/99 (92%)	84 (92%)	7 (8%)	0	100	100
2	P6	90/99 (91%)	82 (91%)	8 (9%)	0	100	100
2	P7	89/99 (90%)	84 (94%)	4 (4%)	1 (1%)	11	44
2	Q2	92/99 (93%)	80 (87%)	9 (10%)	3 (3%)	3	23
2	Q3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	5	30
2	Q4	92/99 (93%)	86 (94%)	5 (5%)	1 (1%)	11	44
2	Q5	91/99 (92%)	83 (91%)	8 (9%)	0	100	100
2	Q6	90/99 (91%)	81 (90%)	9 (10%)	0	100	100
2	Q7	91/99 (92%)	85 (93%)	6 (7%)	0	100	100
2	R2	92/99 (93%)	80 (87%)	8 (9%)	4 (4%)	2	18
2	R3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	5	30
2	R4	92/99 (93%)	85 (92%)	6 (6%)	1 (1%)	11	44
2	R5	91/99 (92%)	83 (91%)	7 (8%)	1 (1%)	11	44
2	R6	90/99 (91%)	78 (87%)	7 (8%)	5 (6%)	1	13
2	R7	91/99 (92%)	86 (94%)	4 (4%)	1 (1%)	11	44
2	S2	92/99 (93%)	81 (88%)	7 (8%)	4 (4%)	2	18
2	S3	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	5	30
2	S4	92/99 (93%)	85 (92%)	6 (6%)	1 (1%)	11	44
2	S5	91/99 (92%)	84 (92%)	7 (8%)	0	100	100
2	S6	90/99 (91%)	82 (91%)	8 (9%)	0	100	100
2	S7	91/99 (92%)	86 (94%)	5 (6%)	0	100	100
2	T2	92/99 (93%)	81 (88%)	9 (10%)	2 (2%)	5	30
2	T3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	5	30
2	T4	92/99 (93%)	84 (91%)	5 (5%)	3 (3%)	3	23
2	T5	91/99 (92%)	86 (94%)	3 (3%)	2 (2%)	5	30
2	T6	90/99 (91%)	82 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T7	91/99 (92%)	87 (96%)	4 (4%)	0	100	100
2	U2	92/99 (93%)	80 (87%)	10 (11%)	2 (2%)	5	30
2	U3	90/99 (91%)	83 (92%)	6 (7%)	1 (1%)	11	44
2	U4	92/99 (93%)	85 (92%)	6 (6%)	1 (1%)	11	44
2	U5	91/99 (92%)	85 (93%)	5 (6%)	1 (1%)	11	44
2	U6	90/99 (91%)	83 (92%)	7 (8%)	0	100	100
2	U7	91/99 (92%)	85 (93%)	6 (7%)	0	100	100
2	V2	92/99 (93%)	81 (88%)	8 (9%)	3 (3%)	3	23
2	V3	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	5	30
2	V4	92/99 (93%)	84 (91%)	6 (6%)	2 (2%)	5	30
2	V5	91/99 (92%)	86 (94%)	5 (6%)	0	100	100
2	V6	90/99 (91%)	81 (90%)	8 (9%)	1 (1%)	11	44
2	V7	91/99 (92%)	85 (93%)	6 (7%)	0	100	100
2	W2	92/99 (93%)	81 (88%)	8 (9%)	3 (3%)	3	23
2	W3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	5	30
2	W4	92/99 (93%)	83 (90%)	6 (6%)	3 (3%)	3	23
2	W5	91/99 (92%)	83 (91%)	8 (9%)	0	100	100
2	W6	90/99 (91%)	81 (90%)	9 (10%)	0	100	100
2	W7	91/99 (92%)	85 (93%)	6 (7%)	0	100	100
2	X2	92/99 (93%)	80 (87%)	10 (11%)	2 (2%)	5	30
2	X3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	5	30
2	X4	92/99 (93%)	86 (94%)	5 (5%)	1 (1%)	11	44
2	X5	91/99 (92%)	84 (92%)	7 (8%)	0	100	100
2	X6	90/99 (91%)	82 (91%)	8 (9%)	0	100	100
2	X7	91/99 (92%)	86 (94%)	5 (6%)	0	100	100
2	Y2	92/99 (93%)	81 (88%)	8 (9%)	3 (3%)	3	23
2	Y3	90/99 (91%)	83 (92%)	5 (6%)	2 (2%)	5	30
2	Y4	92/99 (93%)	83 (90%)	8 (9%)	1 (1%)	11	44
2	Y5	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	5	30
2	Y6	90/99 (91%)	83 (92%)	7 (8%)	0	100	100
2	Y7	91/99 (92%)	85 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Z2	92/99 (93%)	80 (87%)	8 (9%)	4 (4%)	2	18
2	Z3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	5	30
2	Z4	92/99 (93%)	83 (90%)	7 (8%)	2 (2%)	5	30
2	Z5	91/99 (92%)	84 (92%)	6 (7%)	1 (1%)	11	44
2	Z6	90/99 (91%)	82 (91%)	8 (9%)	0	100	100
2	Z7	91/99 (92%)	84 (92%)	7 (8%)	0	100	100
3	18	201/212 (95%)	174 (87%)	22 (11%)	5 (2%)	4	28
3	19	194/212 (92%)	183 (94%)	10 (5%)	1 (0%)	24	58
3	28	201/212 (95%)	174 (87%)	26 (13%)	1 (0%)	24	58
3	29	201/212 (95%)	187 (93%)	13 (6%)	1 (0%)	24	58
3	38	201/212 (95%)	174 (87%)	25 (12%)	2 (1%)	12	45
3	39	201/212 (95%)	187 (93%)	14 (7%)	0	100	100
3	48	201/212 (95%)	174 (87%)	23 (11%)	4 (2%)	6	32
3	49	201/212 (95%)	188 (94%)	12 (6%)	1 (0%)	24	58
3	A8	201/212 (95%)	168 (84%)	28 (14%)	5 (2%)	4	28
3	A9	201/212 (95%)	190 (94%)	11 (6%)	0	100	100
3	B8	201/212 (95%)	175 (87%)	23 (11%)	3 (2%)	8	37
3	B9	201/212 (95%)	185 (92%)	16 (8%)	0	100	100
3	C8	201/212 (95%)	172 (86%)	27 (13%)	2 (1%)	12	45
3	C9	201/212 (95%)	187 (93%)	14 (7%)	0	100	100
3	D8	201/212 (95%)	172 (86%)	28 (14%)	1 (0%)	24	58
3	D9	201/212 (95%)	185 (92%)	15 (8%)	1 (0%)	24	58
3	E8	201/212 (95%)	173 (86%)	24 (12%)	4 (2%)	6	32
3	E9	201/212 (95%)	190 (94%)	11 (6%)	0	100	100
3	F8	201/212 (95%)	173 (86%)	24 (12%)	4 (2%)	6	32
3	F9	201/212 (95%)	189 (94%)	12 (6%)	0	100	100
3	G8	201/212 (95%)	173 (86%)	24 (12%)	4 (2%)	6	32
3	G9	201/212 (95%)	185 (92%)	15 (8%)	1 (0%)	24	58
3	H8	201/212 (95%)	172 (86%)	27 (13%)	2 (1%)	12	45
3	H9	201/212 (95%)	188 (94%)	11 (6%)	2 (1%)	12	45
3	I8	201/212 (95%)	174 (87%)	26 (13%)	1 (0%)	24	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I9	201/212 (95%)	187 (93%)	14 (7%)	0	100	100
3	J8	201/212 (95%)	168 (84%)	30 (15%)	3 (2%)	8	37
3	J9	201/212 (95%)	189 (94%)	12 (6%)	0	100	100
3	K8	201/212 (95%)	175 (87%)	25 (12%)	1 (0%)	24	58
3	K9	201/212 (95%)	188 (94%)	12 (6%)	1 (0%)	24	58
3	L8	201/212 (95%)	173 (86%)	26 (13%)	2 (1%)	12	45
3	L9	201/212 (95%)	187 (93%)	13 (6%)	1 (0%)	24	58
3	M8	201/212 (95%)	173 (86%)	25 (12%)	3 (2%)	8	37
3	M9	201/212 (95%)	186 (92%)	12 (6%)	3 (2%)	8	37
3	N8	201/212 (95%)	171 (85%)	26 (13%)	4 (2%)	6	32
3	N9	201/212 (95%)	185 (92%)	16 (8%)	0	100	100
3	O8	201/212 (95%)	173 (86%)	27 (13%)	1 (0%)	24	58
3	O9	201/212 (95%)	188 (94%)	13 (6%)	0	100	100
3	P8	201/212 (95%)	172 (86%)	27 (13%)	2 (1%)	12	45
3	P9	201/212 (95%)	186 (92%)	14 (7%)	1 (0%)	24	58
3	Q8	201/212 (95%)	173 (86%)	27 (13%)	1 (0%)	24	58
3	Q9	201/212 (95%)	188 (94%)	13 (6%)	0	100	100
3	R8	201/212 (95%)	171 (85%)	26 (13%)	4 (2%)	6	32
3	R9	201/212 (95%)	182 (90%)	16 (8%)	3 (2%)	8	37
3	S8	201/212 (95%)	173 (86%)	27 (13%)	1 (0%)	24	58
3	S9	201/212 (95%)	189 (94%)	12 (6%)	0	100	100
3	T8	201/212 (95%)	175 (87%)	21 (10%)	5 (2%)	4	28
3	T9	201/212 (95%)	191 (95%)	10 (5%)	0	100	100
3	U8	201/212 (95%)	173 (86%)	25 (12%)	3 (2%)	8	37
3	U9	201/212 (95%)	189 (94%)	12 (6%)	0	100	100
3	V8	201/212 (95%)	172 (86%)	27 (13%)	2 (1%)	12	45
3	V9	201/212 (95%)	187 (93%)	14 (7%)	0	100	100
3	W8	201/212 (95%)	173 (86%)	23 (11%)	5 (2%)	4	28
3	W9	201/212 (95%)	188 (94%)	13 (6%)	0	100	100
3	X8	201/212 (95%)	174 (87%)	26 (13%)	1 (0%)	24	58
3	X9	201/212 (95%)	186 (92%)	14 (7%)	1 (0%)	24	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Y8	201/212 (95%)	171 (85%)	27 (13%)	3 (2%)	8	37
3	Y9	201/212 (95%)	186 (92%)	15 (8%)	0	100	100
3	Z8	201/212 (95%)	170 (85%)	28 (14%)	3 (2%)	8	37
3	Z9	201/212 (95%)	185 (92%)	15 (8%)	1 (0%)	24	58
All	All	31147/33420 (93%)	28065 (90%)	2692 (9%)	390 (1%)	9	40

5 of 390 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A1	70	ASN
2	A2	91	ARG
2	A3	11	ARG
1	B1	70	ASN
2	B2	91	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	11	73/74 (99%)	73 (100%)	0	100	100
1	21	73/74 (99%)	73 (100%)	0	100	100
1	31	72/74 (97%)	72 (100%)	0	100	100
1	41	73/74 (99%)	73 (100%)	0	100	100
1	A1	73/74 (99%)	73 (100%)	0	100	100
1	B1	73/74 (99%)	73 (100%)	0	100	100
1	C1	73/74 (99%)	73 (100%)	0	100	100
1	D1	73/74 (99%)	73 (100%)	0	100	100
1	E1	73/74 (99%)	73 (100%)	0	100	100
1	F1	73/74 (99%)	73 (100%)	0	100	100
1	G1	73/74 (99%)	73 (100%)	0	100	100
1	H1	73/74 (99%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I1	73/74 (99%)	73 (100%)	0	100	100
1	J1	73/74 (99%)	73 (100%)	0	100	100
1	K1	73/74 (99%)	73 (100%)	0	100	100
1	L1	73/74 (99%)	73 (100%)	0	100	100
1	M1	73/74 (99%)	73 (100%)	0	100	100
1	N1	73/74 (99%)	73 (100%)	0	100	100
1	O1	73/74 (99%)	73 (100%)	0	100	100
1	P1	73/74 (99%)	73 (100%)	0	100	100
1	Q1	73/74 (99%)	73 (100%)	0	100	100
1	R1	73/74 (99%)	73 (100%)	0	100	100
1	S1	73/74 (99%)	73 (100%)	0	100	100
1	T1	73/74 (99%)	73 (100%)	0	100	100
1	U1	73/74 (99%)	73 (100%)	0	100	100
1	V1	73/74 (99%)	73 (100%)	0	100	100
1	W1	73/74 (99%)	72 (99%)	1 (1%)	59	72
1	X1	73/74 (99%)	73 (100%)	0	100	100
1	Y1	73/74 (99%)	73 (100%)	0	100	100
1	Z1	73/74 (99%)	73 (100%)	0	100	100
2	12	64/68 (94%)	64 (100%)	0	100	100
2	13	63/68 (93%)	63 (100%)	0	100	100
2	14	64/68 (94%)	64 (100%)	0	100	100
2	15	63/68 (93%)	63 (100%)	0	100	100
2	16	63/68 (93%)	63 (100%)	0	100	100
2	17	63/68 (93%)	63 (100%)	0	100	100
2	22	64/68 (94%)	64 (100%)	0	100	100
2	23	63/68 (93%)	63 (100%)	0	100	100
2	24	64/68 (94%)	64 (100%)	0	100	100
2	25	63/68 (93%)	63 (100%)	0	100	100
2	26	63/68 (93%)	63 (100%)	0	100	100
2	27	63/68 (93%)	63 (100%)	0	100	100
2	32	64/68 (94%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	33	63/68 (93%)	63 (100%)	0	100	100
2	34	64/68 (94%)	64 (100%)	0	100	100
2	35	63/68 (93%)	63 (100%)	0	100	100
2	36	63/68 (93%)	62 (98%)	1 (2%)	55	70
2	37	63/68 (93%)	62 (98%)	1 (2%)	55	70
2	42	64/68 (94%)	64 (100%)	0	100	100
2	43	63/68 (93%)	63 (100%)	0	100	100
2	44	64/68 (94%)	63 (98%)	1 (2%)	55	70
2	45	63/68 (93%)	63 (100%)	0	100	100
2	46	63/68 (93%)	63 (100%)	0	100	100
2	47	63/68 (93%)	63 (100%)	0	100	100
2	A2	63/68 (93%)	63 (100%)	0	100	100
2	A3	63/68 (93%)	63 (100%)	0	100	100
2	A4	63/68 (93%)	63 (100%)	0	100	100
2	A5	63/68 (93%)	63 (100%)	0	100	100
2	A6	63/68 (93%)	63 (100%)	0	100	100
2	A7	63/68 (93%)	63 (100%)	0	100	100
2	B2	62/68 (91%)	62 (100%)	0	100	100
2	B3	63/68 (93%)	63 (100%)	0	100	100
2	B4	63/68 (93%)	63 (100%)	0	100	100
2	B5	63/68 (93%)	63 (100%)	0	100	100
2	B6	63/68 (93%)	63 (100%)	0	100	100
2	B7	63/68 (93%)	63 (100%)	0	100	100
2	C2	63/68 (93%)	63 (100%)	0	100	100
2	C3	63/68 (93%)	63 (100%)	0	100	100
2	C4	63/68 (93%)	63 (100%)	0	100	100
2	C5	63/68 (93%)	63 (100%)	0	100	100
2	C6	63/68 (93%)	63 (100%)	0	100	100
2	C7	63/68 (93%)	63 (100%)	0	100	100
2	D2	63/68 (93%)	63 (100%)	0	100	100
2	D3	63/68 (93%)	63 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D4	63/68 (93%)	63 (100%)	0	100	100
2	D5	63/68 (93%)	63 (100%)	0	100	100
2	D6	63/68 (93%)	63 (100%)	0	100	100
2	D7	63/68 (93%)	63 (100%)	0	100	100
2	E2	64/68 (94%)	64 (100%)	0	100	100
2	E3	63/68 (93%)	62 (98%)	1 (2%)	55	70
2	E4	64/68 (94%)	64 (100%)	0	100	100
2	E5	63/68 (93%)	63 (100%)	0	100	100
2	E6	63/68 (93%)	63 (100%)	0	100	100
2	E7	63/68 (93%)	62 (98%)	1 (2%)	55	70
2	F2	64/68 (94%)	63 (98%)	1 (2%)	55	70
2	F3	63/68 (93%)	63 (100%)	0	100	100
2	F4	63/68 (93%)	63 (100%)	0	100	100
2	F5	63/68 (93%)	63 (100%)	0	100	100
2	F6	63/68 (93%)	63 (100%)	0	100	100
2	F7	63/68 (93%)	63 (100%)	0	100	100
2	G2	63/68 (93%)	63 (100%)	0	100	100
2	G3	63/68 (93%)	63 (100%)	0	100	100
2	G4	63/68 (93%)	63 (100%)	0	100	100
2	G5	63/68 (93%)	63 (100%)	0	100	100
2	G6	63/68 (93%)	63 (100%)	0	100	100
2	G7	63/68 (93%)	63 (100%)	0	100	100
2	H2	63/68 (93%)	63 (100%)	0	100	100
2	H3	63/68 (93%)	63 (100%)	0	100	100
2	H4	63/68 (93%)	63 (100%)	0	100	100
2	H5	63/68 (93%)	63 (100%)	0	100	100
2	H6	63/68 (93%)	63 (100%)	0	100	100
2	H7	63/68 (93%)	63 (100%)	0	100	100
2	I2	63/68 (93%)	63 (100%)	0	100	100
2	I3	63/68 (93%)	63 (100%)	0	100	100
2	I4	63/68 (93%)	62 (98%)	1 (2%)	55	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I5	63/68 (93%)	63 (100%)	0	100	100
2	I6	63/68 (93%)	63 (100%)	0	100	100
2	I7	63/68 (93%)	63 (100%)	0	100	100
2	J2	63/68 (93%)	63 (100%)	0	100	100
2	J3	63/68 (93%)	63 (100%)	0	100	100
2	J4	63/68 (93%)	63 (100%)	0	100	100
2	J5	63/68 (93%)	63 (100%)	0	100	100
2	J6	63/68 (93%)	63 (100%)	0	100	100
2	J7	63/68 (93%)	63 (100%)	0	100	100
2	K2	63/68 (93%)	63 (100%)	0	100	100
2	K3	63/68 (93%)	63 (100%)	0	100	100
2	K4	63/68 (93%)	63 (100%)	0	100	100
2	K5	63/68 (93%)	63 (100%)	0	100	100
2	K6	63/68 (93%)	63 (100%)	0	100	100
2	K7	63/68 (93%)	63 (100%)	0	100	100
2	L2	64/68 (94%)	64 (100%)	0	100	100
2	L3	63/68 (93%)	63 (100%)	0	100	100
2	L4	63/68 (93%)	63 (100%)	0	100	100
2	L5	63/68 (93%)	63 (100%)	0	100	100
2	L6	63/68 (93%)	63 (100%)	0	100	100
2	L7	63/68 (93%)	63 (100%)	0	100	100
2	M2	63/68 (93%)	63 (100%)	0	100	100
2	M3	63/68 (93%)	63 (100%)	0	100	100
2	M4	63/68 (93%)	63 (100%)	0	100	100
2	M5	63/68 (93%)	63 (100%)	0	100	100
2	M6	63/68 (93%)	63 (100%)	0	100	100
2	M7	63/68 (93%)	63 (100%)	0	100	100
2	N2	63/68 (93%)	63 (100%)	0	100	100
2	N3	63/68 (93%)	63 (100%)	0	100	100
2	N4	63/68 (93%)	63 (100%)	0	100	100
2	N5	63/68 (93%)	63 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N6	63/68 (93%)	63 (100%)	0	100	100
2	N7	63/68 (93%)	63 (100%)	0	100	100
2	O2	64/68 (94%)	64 (100%)	0	100	100
2	O3	63/68 (93%)	63 (100%)	0	100	100
2	O4	64/68 (94%)	64 (100%)	0	100	100
2	O5	63/68 (93%)	63 (100%)	0	100	100
2	O6	63/68 (93%)	63 (100%)	0	100	100
2	O7	63/68 (93%)	63 (100%)	0	100	100
2	P2	64/68 (94%)	64 (100%)	0	100	100
2	P3	63/68 (93%)	63 (100%)	0	100	100
2	P4	64/68 (94%)	64 (100%)	0	100	100
2	P5	63/68 (93%)	63 (100%)	0	100	100
2	P6	63/68 (93%)	63 (100%)	0	100	100
2	P7	62/68 (91%)	62 (100%)	0	100	100
2	Q2	64/68 (94%)	64 (100%)	0	100	100
2	Q3	63/68 (93%)	63 (100%)	0	100	100
2	Q4	64/68 (94%)	64 (100%)	0	100	100
2	Q5	63/68 (93%)	63 (100%)	0	100	100
2	Q6	63/68 (93%)	63 (100%)	0	100	100
2	Q7	63/68 (93%)	63 (100%)	0	100	100
2	R2	64/68 (94%)	64 (100%)	0	100	100
2	R3	63/68 (93%)	63 (100%)	0	100	100
2	R4	64/68 (94%)	64 (100%)	0	100	100
2	R5	63/68 (93%)	63 (100%)	0	100	100
2	R6	63/68 (93%)	63 (100%)	0	100	100
2	R7	63/68 (93%)	62 (98%)	1 (2%)	55	70
2	S2	64/68 (94%)	64 (100%)	0	100	100
2	S3	63/68 (93%)	63 (100%)	0	100	100
2	S4	64/68 (94%)	63 (98%)	1 (2%)	55	70
2	S5	63/68 (93%)	63 (100%)	0	100	100
2	S6	63/68 (93%)	63 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S7	63/68 (93%)	63 (100%)	0	100	100
2	T2	64/68 (94%)	64 (100%)	0	100	100
2	T3	63/68 (93%)	63 (100%)	0	100	100
2	T4	64/68 (94%)	64 (100%)	0	100	100
2	T5	63/68 (93%)	63 (100%)	0	100	100
2	T6	63/68 (93%)	63 (100%)	0	100	100
2	T7	63/68 (93%)	62 (98%)	1 (2%)	55	70
2	U2	64/68 (94%)	64 (100%)	0	100	100
2	U3	63/68 (93%)	63 (100%)	0	100	100
2	U4	64/68 (94%)	64 (100%)	0	100	100
2	U5	63/68 (93%)	63 (100%)	0	100	100
2	U6	63/68 (93%)	63 (100%)	0	100	100
2	U7	63/68 (93%)	63 (100%)	0	100	100
2	V2	64/68 (94%)	64 (100%)	0	100	100
2	V3	63/68 (93%)	63 (100%)	0	100	100
2	V4	64/68 (94%)	64 (100%)	0	100	100
2	V5	63/68 (93%)	63 (100%)	0	100	100
2	V6	63/68 (93%)	63 (100%)	0	100	100
2	V7	63/68 (93%)	63 (100%)	0	100	100
2	W2	64/68 (94%)	64 (100%)	0	100	100
2	W3	63/68 (93%)	63 (100%)	0	100	100
2	W4	64/68 (94%)	64 (100%)	0	100	100
2	W5	63/68 (93%)	63 (100%)	0	100	100
2	W6	63/68 (93%)	63 (100%)	0	100	100
2	W7	63/68 (93%)	63 (100%)	0	100	100
2	X2	64/68 (94%)	64 (100%)	0	100	100
2	X3	63/68 (93%)	63 (100%)	0	100	100
2	X4	64/68 (94%)	64 (100%)	0	100	100
2	X5	63/68 (93%)	62 (98%)	1 (2%)	55	70
2	X6	63/68 (93%)	63 (100%)	0	100	100
2	X7	63/68 (93%)	63 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Y2	64/68 (94%)	64 (100%)	0	100	100
2	Y3	63/68 (93%)	63 (100%)	0	100	100
2	Y4	64/68 (94%)	64 (100%)	0	100	100
2	Y5	63/68 (93%)	63 (100%)	0	100	100
2	Y6	63/68 (93%)	63 (100%)	0	100	100
2	Y7	63/68 (93%)	62 (98%)	1 (2%)	55	70
2	Z2	64/68 (94%)	64 (100%)	0	100	100
2	Z3	63/68 (93%)	63 (100%)	0	100	100
2	Z4	64/68 (94%)	64 (100%)	0	100	100
2	Z5	63/68 (93%)	63 (100%)	0	100	100
2	Z6	63/68 (93%)	63 (100%)	0	100	100
2	Z7	63/68 (93%)	63 (100%)	0	100	100
3	18	155/164 (94%)	155 (100%)	0	100	100
3	28	155/164 (94%)	155 (100%)	0	100	100
3	38	155/164 (94%)	155 (100%)	0	100	100
3	48	155/164 (94%)	155 (100%)	0	100	100
3	A8	155/164 (94%)	155 (100%)	0	100	100
3	B8	155/164 (94%)	155 (100%)	0	100	100
3	C8	155/164 (94%)	155 (100%)	0	100	100
3	D8	155/164 (94%)	155 (100%)	0	100	100
3	E8	155/164 (94%)	155 (100%)	0	100	100
3	F8	155/164 (94%)	155 (100%)	0	100	100
3	G8	155/164 (94%)	155 (100%)	0	100	100
3	H8	155/164 (94%)	155 (100%)	0	100	100
3	I8	155/164 (94%)	155 (100%)	0	100	100
3	J8	155/164 (94%)	155 (100%)	0	100	100
3	K8	155/164 (94%)	155 (100%)	0	100	100
3	L8	155/164 (94%)	155 (100%)	0	100	100
3	M8	155/164 (94%)	155 (100%)	0	100	100
3	N8	155/164 (94%)	155 (100%)	0	100	100
3	O8	155/164 (94%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P8	155/164 (94%)	155 (100%)	0	100	100
3	Q8	155/164 (94%)	155 (100%)	0	100	100
3	R8	155/164 (94%)	155 (100%)	0	100	100
3	S8	155/164 (94%)	155 (100%)	0	100	100
3	T8	155/164 (94%)	155 (100%)	0	100	100
3	U8	155/164 (94%)	155 (100%)	0	100	100
3	V8	155/164 (94%)	155 (100%)	0	100	100
3	W8	155/164 (94%)	155 (100%)	0	100	100
3	X8	155/164 (94%)	155 (100%)	0	100	100
3	Y8	155/164 (94%)	155 (100%)	0	100	100
3	Z8	155/164 (94%)	155 (100%)	0	100	100
All	All	18213/19380 (94%)	18200 (100%)	13 (0%)	88	87

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W1	19	ILE
2	X5	42	VAL
2	44	57	THR
2	36	57	THR
2	37	43	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
3	V8	17	GLN
2	14	82	ASN
1	W1	65	GLN
3	Z8	17	GLN
3	28	62	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	11	95/96 (98%)	0.61	3 (3%)	50	28	65, 89, 126, 149	0
1	21	95/96 (98%)	0.51	5 (5%)	32	18	49, 75, 109, 126	0
1	31	94/96 (97%)	0.67	4 (4%)	40	21	64, 91, 139, 160	0
1	41	95/96 (98%)	0.58	3 (3%)	50	28	57, 84, 118, 140	0
1	A1	95/96 (98%)	0.72	5 (5%)	32	18	61, 83, 112, 131	0
1	B1	95/96 (98%)	0.63	5 (5%)	32	18	63, 87, 122, 134	0
1	C1	95/96 (98%)	0.41	3 (3%)	50	28	63, 89, 115, 132	0
1	D1	95/96 (98%)	0.58	5 (5%)	32	18	60, 86, 114, 130	0
1	E1	95/96 (98%)	0.51	4 (4%)	40	21	53, 87, 115, 136	0
1	F1	95/96 (98%)	0.78	3 (3%)	50	28	71, 94, 123, 140	0
1	G1	95/96 (98%)	0.63	5 (5%)	32	18	76, 94, 126, 159	0
1	H1	95/96 (98%)	0.64	7 (7%)	20	13	63, 91, 130, 148	0
1	I1	95/96 (98%)	0.64	6 (6%)	26	16	67, 89, 125, 137	0
1	J1	95/96 (98%)	0.66	4 (4%)	40	21	63, 88, 123, 151	0
1	K1	95/96 (98%)	0.53	3 (3%)	50	28	55, 80, 112, 131	0
1	L1	95/96 (98%)	0.52	3 (3%)	50	28	52, 79, 109, 120	0
1	M1	95/96 (98%)	0.53	3 (3%)	50	28	55, 79, 111, 122	0
1	N1	95/96 (98%)	0.45	4 (4%)	40	21	54, 80, 110, 118	0
1	O1	95/96 (98%)	0.62	4 (4%)	40	21	66, 91, 126, 147	0
1	P1	95/96 (98%)	0.64	5 (5%)	32	18	65, 91, 116, 137	0
1	Q1	95/96 (98%)	0.64	5 (5%)	32	18	62, 89, 125, 150	0
1	R1	95/96 (98%)	0.63	3 (3%)	50	28	70, 95, 124, 145	0
1	S1	95/96 (98%)	0.66	6 (6%)	26	16	57, 94, 118, 139	0
1	T1	95/96 (98%)	0.58	7 (7%)	20	13	55, 82, 110, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	U1	95/96 (98%)	0.45	4 (4%)	40	21	54, 82, 111, 126	0
1	V1	95/96 (98%)	0.65	5 (5%)	32	18	72, 94, 124, 138	0
1	W1	95/96 (98%)	0.64	7 (7%)	20	13	73, 94, 126, 135	0
1	X1	95/96 (98%)	0.46	3 (3%)	50	28	54, 80, 110, 120	0
1	Y1	95/96 (98%)	0.51	4 (4%)	40	21	50, 82, 112, 134	0
1	Z1	95/96 (98%)	0.65	4 (4%)	40	21	66, 92, 123, 141	0
2	12	94/99 (94%)	0.30	1 (1%)	78	52	58, 82, 113, 128	0
2	13	92/99 (92%)	0.41	3 (3%)	49	27	58, 82, 110, 131	0
2	14	94/99 (94%)	0.33	4 (4%)	40	21	54, 80, 113, 150	0
2	15	93/99 (93%)	0.33	1 (1%)	78	52	54, 81, 112, 140	0
2	16	92/99 (92%)	0.31	1 (1%)	78	52	58, 79, 111, 132	0
2	17	93/99 (93%)	0.39	3 (3%)	50	28	57, 81, 114, 128	0
2	22	94/99 (94%)	0.31	2 (2%)	63	36	47, 71, 103, 133	0
2	23	92/99 (92%)	0.36	3 (3%)	49	27	45, 76, 104, 115	0
2	24	94/99 (94%)	0.21	0	100	100	39, 70, 102, 124	0
2	25	93/99 (93%)	0.22	1 (1%)	78	52	44, 70, 99, 131	0
2	26	92/99 (92%)	0.28	1 (1%)	78	52	43, 73, 99, 119	0
2	27	93/99 (93%)	0.32	3 (3%)	50	28	54, 74, 107, 123	0
2	32	94/99 (94%)	0.31	2 (2%)	63	36	61, 81, 111, 135	0
2	33	92/99 (92%)	0.39	3 (3%)	49	27	48, 84, 113, 129	0
2	34	94/99 (94%)	0.30	1 (1%)	78	52	57, 81, 113, 137	0
2	35	93/99 (93%)	0.28	1 (1%)	78	52	65, 83, 113, 121	0
2	36	92/99 (92%)	0.31	3 (3%)	49	27	63, 85, 110, 122	0
2	37	93/99 (93%)	0.39	5 (5%)	31	18	58, 79, 113, 124	0
2	42	94/99 (94%)	0.29	0	100	100	49, 76, 105, 134	0
2	43	92/99 (92%)	0.41	3 (3%)	49	27	54, 80, 113, 131	0
2	44	94/99 (94%)	0.29	3 (3%)	50	28	58, 81, 111, 147	0
2	45	93/99 (93%)	0.29	2 (2%)	62	35	59, 82, 111, 140	0
2	46	92/99 (92%)	0.31	3 (3%)	49	27	54, 77, 101, 115	0
2	47	93/99 (93%)	0.24	2 (2%)	62	35	53, 76, 108, 123	0
2	A2	92/99 (92%)	0.45	3 (3%)	49	27	59, 82, 109, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
2	A3	92/99 (92%)	0.37	0	100 100	56, 84, 110, 128	0
2	A4	93/99 (93%)	0.45	3 (3%)	50 28	55, 85, 112, 142	0
2	A5	92/99 (92%)	0.36	6 (6%)	25 15	54, 85, 111, 126	0
2	A6	92/99 (92%)	0.44	2 (2%)	62 35	60, 86, 112, 122	0
2	A7	92/99 (92%)	0.46	3 (3%)	49 27	54, 84, 112, 128	0
2	B2	91/99 (91%)	0.27	2 (2%)	62 35	54, 73, 105, 125	0
2	B3	92/99 (92%)	0.38	2 (2%)	62 35	51, 81, 103, 123	0
2	B4	92/99 (92%)	0.30	1 (1%)	78 52	57, 77, 107, 116	0
2	B5	92/99 (92%)	0.39	1 (1%)	78 52	58, 82, 109, 123	0
2	B6	92/99 (92%)	0.37	3 (3%)	49 27	58, 77, 105, 116	0
2	B7	92/99 (92%)	0.42	3 (3%)	49 27	57, 80, 104, 114	0
2	C2	92/99 (92%)	0.28	0	100 100	53, 77, 104, 114	0
2	C3	92/99 (92%)	0.32	2 (2%)	62 35	63, 81, 113, 122	0
2	C4	92/99 (92%)	0.18	1 (1%)	78 52	54, 75, 100, 122	0
2	C5	92/99 (92%)	0.29	1 (1%)	78 52	55, 79, 105, 121	0
2	C6	92/99 (92%)	0.28	1 (1%)	78 52	50, 76, 106, 120	0
2	C7	93/99 (93%)	0.30	1 (1%)	78 52	54, 75, 102, 131	0
2	D2	93/99 (93%)	0.28	0	100 100	50, 78, 111, 118	0
2	D3	92/99 (92%)	0.49	1 (1%)	78 52	60, 84, 112, 123	0
2	D4	92/99 (92%)	0.35	0	100 100	54, 80, 108, 121	0
2	D5	92/99 (92%)	0.26	1 (1%)	78 52	60, 83, 109, 133	0
2	D6	92/99 (92%)	0.38	3 (3%)	49 27	45, 76, 104, 122	0
2	D7	93/99 (93%)	0.39	2 (2%)	62 35	48, 77, 108, 119	0
2	E2	94/99 (94%)	0.35	4 (4%)	40 21	58, 80, 112, 128	0
2	E3	92/99 (92%)	0.49	3 (3%)	49 27	68, 87, 112, 124	0
2	E4	94/99 (94%)	0.27	1 (1%)	78 52	61, 82, 114, 128	0
2	E5	92/99 (92%)	0.37	3 (3%)	49 27	59, 83, 108, 131	0
2	E6	92/99 (92%)	0.38	4 (4%)	40 21	63, 81, 105, 122	0
2	E7	92/99 (92%)	0.28	1 (1%)	78 52	53, 81, 109, 125	0
2	F2	94/99 (94%)	0.38	1 (1%)	78 52	66, 87, 116, 135	0
2	F3	92/99 (92%)	0.43	5 (5%)	31 18	66, 87, 116, 127	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	F4	92/99 (92%)	0.27	2 (2%) 62 35	64, 83, 111, 130	0
2	F5	92/99 (92%)	0.38	1 (1%) 78 52	67, 86, 109, 129	0
2	F6	92/99 (92%)	0.31	1 (1%) 78 52	62, 83, 108, 118	0
2	F7	93/99 (93%)	0.31	2 (2%) 62 35	62, 84, 111, 131	0
2	G2	92/99 (92%)	0.50	4 (4%) 40 21	65, 90, 113, 121	0
2	G3	92/99 (92%)	0.47	3 (3%) 49 27	63, 88, 119, 129	0
2	G4	92/99 (92%)	0.44	4 (4%) 40 21	60, 86, 113, 127	0
2	G5	91/99 (91%)	0.36	1 (1%) 78 52	65, 84, 111, 127	0
2	G6	92/99 (92%)	0.43	2 (2%) 62 35	66, 87, 110, 126	0
2	G7	92/99 (92%)	0.39	3 (3%) 49 27	55, 83, 122, 137	0
2	H2	92/99 (92%)	0.39	1 (1%) 78 52	58, 79, 104, 111	0
2	H3	92/99 (92%)	0.39	2 (2%) 62 35	58, 84, 117, 126	0
2	H4	93/99 (93%)	0.34	1 (1%) 78 52	57, 83, 112, 135	0
2	H5	91/99 (91%)	0.43	4 (4%) 39 21	59, 84, 112, 121	0
2	H6	92/99 (92%)	0.42	1 (1%) 78 52	58, 82, 105, 121	0
2	H7	92/99 (92%)	0.39	4 (4%) 40 21	61, 83, 108, 127	0
2	I2	92/99 (92%)	0.38	1 (1%) 78 52	54, 81, 107, 123	0
2	I3	91/99 (91%)	0.35	4 (4%) 39 21	64, 85, 109, 130	0
2	I4	92/99 (92%)	0.34	2 (2%) 62 35	58, 83, 106, 117	0
2	I5	92/99 (92%)	0.54	4 (4%) 40 21	59, 87, 115, 125	0
2	I6	92/99 (92%)	0.39	3 (3%) 49 27	60, 87, 111, 121	0
2	I7	92/99 (92%)	0.46	3 (3%) 49 27	62, 83, 107, 131	0
2	J2	92/99 (92%)	0.38	1 (1%) 78 52	65, 84, 110, 125	0
2	J3	92/99 (92%)	0.42	3 (3%) 49 27	59, 81, 112, 123	0
2	J4	92/99 (92%)	0.27	1 (1%) 78 52	59, 79, 109, 119	0
2	J5	91/99 (91%)	0.33	2 (2%) 62 35	51, 78, 107, 121	0
2	J6	92/99 (92%)	0.37	1 (1%) 78 52	51, 81, 105, 123	0
2	J7	92/99 (92%)	0.22	1 (1%) 78 52	56, 80, 103, 121	0
2	K2	92/99 (92%)	0.37	2 (2%) 62 35	43, 79, 106, 119	0
2	K3	92/99 (92%)	0.32	3 (3%) 49 27	60, 83, 115, 134	0
2	K4	92/99 (92%)	0.17	3 (3%) 49 27	50, 77, 108, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	K5	93/99 (93%)	0.33	2 (2%) 62 35	42, 80, 102, 136	0
2	K6	92/99 (92%)	0.34	4 (4%) 40 21	53, 78, 104, 119	0
2	K7	93/99 (93%)	0.29	1 (1%) 78 52	50, 78, 112, 121	0
2	L2	94/99 (94%)	0.37	0 100 100	46, 78, 105, 126	0
2	L3	92/99 (92%)	0.37	2 (2%) 62 35	52, 80, 112, 126	0
2	L4	92/99 (92%)	0.25	2 (2%) 62 35	53, 79, 101, 116	0
2	L5	92/99 (92%)	0.22	2 (2%) 62 35	54, 76, 107, 128	0
2	L6	92/99 (92%)	0.33	3 (3%) 49 27	53, 79, 105, 135	0
2	L7	93/99 (93%)	0.38	2 (2%) 62 35	47, 71, 93, 116	0
2	M2	93/99 (93%)	0.30	1 (1%) 78 52	47, 69, 94, 107	0
2	M3	92/99 (92%)	0.28	2 (2%) 62 35	54, 76, 108, 121	0
2	M4	92/99 (92%)	0.20	0 100 100	44, 75, 94, 122	0
2	M5	93/99 (93%)	0.33	2 (2%) 62 35	48, 71, 99, 122	0
2	M6	91/99 (91%)	0.27	2 (2%) 62 35	50, 71, 99, 114	0
2	M7	92/99 (92%)	0.39	2 (2%) 62 35	49, 75, 105, 123	0
2	N2	92/99 (92%)	0.17	2 (2%) 62 35	50, 71, 100, 114	0
2	N3	91/99 (91%)	0.42	4 (4%) 39 21	42, 76, 101, 133	0
2	N4	92/99 (92%)	0.24	2 (2%) 62 35	50, 73, 100, 121	0
2	N5	93/99 (93%)	0.35	4 (4%) 40 21	57, 75, 105, 115	0
2	N6	91/99 (91%)	0.29	1 (1%) 78 52	55, 76, 98, 106	0
2	N7	92/99 (92%)	0.24	1 (1%) 78 52	50, 75, 106, 118	0
2	O2	94/99 (94%)	0.33	2 (2%) 63 36	62, 84, 117, 131	0
2	O3	92/99 (92%)	0.37	1 (1%) 78 52	56, 81, 114, 124	0
2	O4	94/99 (94%)	0.22	3 (3%) 50 28	56, 83, 114, 130	0
2	O5	93/99 (93%)	0.29	2 (2%) 62 35	59, 85, 113, 130	0
2	O6	92/99 (92%)	0.24	2 (2%) 62 35	57, 78, 103, 122	0
2	O7	93/99 (93%)	0.43	3 (3%) 50 28	63, 81, 106, 121	0
2	P2	94/99 (94%)	0.35	1 (1%) 78 52	59, 84, 115, 130	0
2	P3	92/99 (92%)	0.37	4 (4%) 40 21	56, 82, 112, 122	0
2	P4	94/99 (94%)	0.20	0 100 100	53, 82, 112, 128	0
2	P5	93/99 (93%)	0.51	2 (2%) 62 35	55, 82, 113, 123	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	P6	92/99 (92%)	0.36	2 (2%) 62 35	59, 82, 108, 117	0
2	P7	91/99 (91%)	0.46	2 (2%) 62 35	49, 79, 110, 114	0
2	Q2	94/99 (94%)	0.51	5 (5%) 32 18	51, 83, 118, 129	0
2	Q3	92/99 (92%)	0.50	5 (5%) 31 18	62, 83, 107, 129	0
2	Q4	94/99 (94%)	0.36	3 (3%) 50 28	56, 84, 109, 133	0
2	Q5	93/99 (93%)	0.41	0 100 100	61, 82, 113, 119	0
2	Q6	92/99 (92%)	0.27	4 (4%) 40 21	56, 82, 112, 123	0
2	Q7	93/99 (93%)	0.47	4 (4%) 40 21	63, 85, 115, 130	0
2	R2	94/99 (94%)	0.28	3 (3%) 50 28	61, 83, 110, 144	0
2	R3	92/99 (92%)	0.47	3 (3%) 49 27	51, 82, 113, 126	0
2	R4	94/99 (94%)	0.33	2 (2%) 63 36	56, 82, 116, 143	0
2	R5	93/99 (93%)	0.30	3 (3%) 50 28	62, 86, 115, 143	0
2	R6	92/99 (92%)	0.44	3 (3%) 49 27	62, 87, 115, 132	0
2	R7	93/99 (93%)	0.42	2 (2%) 62 35	62, 82, 114, 127	0
2	S2	94/99 (94%)	0.46	2 (2%) 63 36	53, 84, 112, 139	0
2	S3	92/99 (92%)	0.46	2 (2%) 62 35	65, 83, 116, 123	0
2	S4	94/99 (94%)	0.30	1 (1%) 78 52	65, 83, 105, 152	0
2	S5	93/99 (93%)	0.51	4 (4%) 40 21	34, 83, 108, 117	0
2	S6	92/99 (92%)	0.38	1 (1%) 78 52	46, 81, 107, 119	0
2	S7	93/99 (93%)	0.38	1 (1%) 78 52	51, 79, 108, 123	0
2	T2	94/99 (94%)	0.50	2 (2%) 63 36	45, 72, 105, 155	0
2	T3	92/99 (92%)	0.46	2 (2%) 62 35	46, 78, 108, 137	0
2	T4	94/99 (94%)	0.18	2 (2%) 63 36	53, 78, 113, 141	0
2	T5	93/99 (93%)	0.39	2 (2%) 62 35	40, 75, 103, 125	0
2	T6	92/99 (92%)	0.39	5 (5%) 31 18	53, 80, 108, 124	0
2	T7	93/99 (93%)	0.38	3 (3%) 50 28	54, 79, 109, 125	0
2	U2	94/99 (94%)	0.30	1 (1%) 78 52	42, 71, 101, 121	0
2	U3	92/99 (92%)	0.45	3 (3%) 49 27	57, 86, 117, 129	0
2	U4	94/99 (94%)	0.44	5 (5%) 32 18	46, 76, 112, 127	0
2	U5	93/99 (93%)	0.25	1 (1%) 78 52	60, 77, 110, 131	0
2	U6	92/99 (92%)	0.33	2 (2%) 62 35	55, 76, 98, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
2	U7	93/99 (93%)	0.54	8 (8%)	16 11	44, 79, 110, 136	0
2	V2	94/99 (94%)	0.44	2 (2%)	63 36	59, 85, 112, 136	0
2	V3	92/99 (92%)	0.40	3 (3%)	49 27	56, 80, 109, 126	0
2	V4	94/99 (94%)	0.44	1 (1%)	78 52	60, 82, 106, 125	0
2	V5	93/99 (93%)	0.55	1 (1%)	78 52	55, 85, 112, 124	0
2	V6	92/99 (92%)	0.39	2 (2%)	62 35	57, 79, 107, 117	0
2	V7	93/99 (93%)	0.33	0 100 100		60, 79, 102, 116	0
2	W2	94/99 (94%)	0.36	1 (1%)	78 52	61, 87, 116, 125	0
2	W3	92/99 (92%)	0.55	3 (3%)	49 27	63, 87, 117, 134	0
2	W4	94/99 (94%)	0.30	4 (4%)	40 21	62, 84, 110, 157	0
2	W5	93/99 (93%)	0.37	5 (5%)	31 18	60, 84, 114, 142	0
2	W6	92/99 (92%)	0.32	4 (4%)	40 21	64, 83, 107, 131	0
2	W7	93/99 (93%)	0.39	2 (2%)	62 35	47, 79, 108, 134	0
2	X2	94/99 (94%)	0.39	3 (3%)	50 28	51, 76, 107, 137	0
2	X3	92/99 (92%)	0.38	2 (2%)	62 35	52, 80, 112, 128	0
2	X4	94/99 (94%)	0.22	3 (3%)	50 28	46, 76, 109, 129	0
2	X5	93/99 (93%)	0.41	5 (5%)	31 18	51, 80, 107, 137	0
2	X6	92/99 (92%)	0.28	3 (3%)	49 27	57, 80, 101, 132	0
2	X7	93/99 (93%)	0.35	3 (3%)	50 28	57, 79, 108, 121	0
2	Y2	94/99 (94%)	0.32	3 (3%)	50 28	58, 78, 109, 122	0
2	Y3	92/99 (92%)	0.54	3 (3%)	49 27	52, 82, 105, 125	0
2	Y4	94/99 (94%)	0.42	6 (6%)	25 15	44, 83, 113, 133	0
2	Y5	92/99 (92%)	0.44	2 (2%)	62 35	50, 75, 104, 130	0
2	Y6	92/99 (92%)	0.40	2 (2%)	62 35	49, 80, 103, 119	0
2	Y7	93/99 (93%)	0.36	3 (3%)	50 28	55, 81, 105, 128	0
2	Z2	94/99 (94%)	0.29	1 (1%)	78 52	58, 82, 113, 130	0
2	Z3	92/99 (92%)	0.42	4 (4%)	40 21	62, 85, 111, 126	0
2	Z4	94/99 (94%)	0.20	2 (2%)	63 36	60, 80, 110, 141	0
2	Z5	93/99 (93%)	0.25	1 (1%)	78 52	59, 82, 114, 122	0
2	Z6	92/99 (92%)	0.30	1 (1%)	78 52	57, 81, 112, 129	0
2	Z7	93/99 (93%)	0.48	4 (4%)	40 21	55, 74, 106, 123	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
3	18	203/212 (95%)	1.43	46 (22%)	2	2	71, 120, 149, 157	0
3	19	198/212 (93%)	2.31	103 (52%)	0	0	121, 155, 174, 192	0
3	28	203/212 (95%)	1.37	44 (21%)	2	2	68, 116, 146, 163	0
3	29	203/212 (95%)	1.70	68 (33%)	1	1	106, 145, 172, 190	0
3	38	203/212 (95%)	1.50	54 (26%)	1	2	72, 120, 152, 175	0
3	39	203/212 (95%)	2.31	116 (57%)	0	0	124, 156, 176, 190	0
3	48	203/212 (95%)	1.33	39 (19%)	3	3	73, 117, 147, 161	0
3	49	203/212 (95%)	1.96	86 (42%)	0	1	110, 149, 171, 189	0
3	A8	203/212 (95%)	1.34	42 (20%)	2	3	76, 121, 149, 163	0
3	A9	203/212 (95%)	2.21	105 (51%)	0	1	118, 156, 177, 196	0
3	B8	203/212 (95%)	1.50	57 (28%)	1	2	73, 116, 145, 172	0
3	B9	203/212 (95%)	2.20	110 (54%)	0	0	103, 148, 172, 194	0
3	C8	203/212 (95%)	1.36	44 (21%)	2	2	74, 115, 147, 170	0
3	C9	203/212 (95%)	1.91	82 (40%)	0	1	100, 147, 171, 203	0
3	D8	203/212 (95%)	1.52	53 (26%)	1	2	79, 115, 144, 172	0
3	D9	203/212 (95%)	2.14	104 (51%)	0	1	111, 145, 170, 181	0
3	E8	203/212 (95%)	1.51	54 (26%)	1	2	85, 124, 152, 168	0
3	E9	203/212 (95%)	2.05	94 (46%)	0	1	115, 156, 177, 184	0
3	F8	203/212 (95%)	1.48	56 (27%)	1	2	71, 125, 155, 178	0
3	F9	203/212 (95%)	2.36	123 (60%)	0	0	116, 157, 181, 202	0
3	G8	203/212 (95%)	1.43	51 (25%)	1	2	74, 122, 150, 184	0
3	G9	203/212 (95%)	2.33	123 (60%)	0	0	124, 159, 180, 197	0
3	H8	203/212 (95%)	1.54	57 (28%)	1	2	68, 121, 150, 161	0
3	H9	203/212 (95%)	2.19	101 (49%)	0	1	111, 156, 178, 194	0
3	I8	203/212 (95%)	1.48	55 (27%)	1	2	84, 121, 150, 171	0
3	I9	203/212 (95%)	2.25	115 (56%)	0	0	112, 156, 177, 195	0
3	J8	203/212 (95%)	1.40	53 (26%)	1	2	72, 118, 145, 168	0
3	J9	203/212 (95%)	2.09	105 (51%)	0	1	105, 149, 173, 188	0
3	K8	203/212 (95%)	1.43	48 (23%)	2	2	72, 119, 148, 167	0
3	K9	203/212 (95%)	2.05	101 (49%)	0	1	113, 152, 172, 197	0
3	L8	203/212 (95%)	1.28	41 (20%)	3	3	73, 116, 146, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)		Q<0.9
3	L9	203/212 (95%)	2.04	90 (44%)	0	1	109, 150, 173, 191
3	M8	203/212 (95%)	1.37	40 (19%)	3	3	68, 114, 148, 168
3	M9	203/212 (95%)	1.78	69 (33%)	1	1	105, 145, 174, 181
3	N8	203/212 (95%)	1.50	48 (23%)	2	2	62, 117, 152, 164
3	N9	203/212 (95%)	2.01	98 (48%)	0	1	103, 150, 175, 189
3	O8	203/212 (95%)	1.39	47 (23%)	2	2	80, 118, 150, 183
3	O9	203/212 (95%)	2.18	106 (52%)	0	0	111, 154, 178, 188
3	P8	203/212 (95%)	1.39	45 (22%)	2	2	76, 117, 141, 155
3	P9	203/212 (95%)	2.06	100 (49%)	0	1	119, 149, 173, 195
3	Q8	203/212 (95%)	1.42	51 (25%)	1	2	71, 121, 152, 172
3	Q9	203/212 (95%)	2.19	108 (53%)	0	0	113, 157, 183, 201
3	R8	203/212 (95%)	1.46	45 (22%)	2	2	70, 122, 152, 174
3	R9	203/212 (95%)	2.23	114 (56%)	0	0	116, 157, 177, 185
3	S8	203/212 (95%)	1.48	57 (28%)	1	2	78, 121, 149, 172
3	S9	203/212 (95%)	2.17	101 (49%)	0	1	122, 156, 176, 186
3	T8	203/212 (95%)	1.58	61 (30%)	1	2	68, 114, 149, 169
3	T9	203/212 (95%)	2.46	119 (58%)	0	0	109, 153, 179, 195
3	U8	203/212 (95%)	1.48	56 (27%)	1	2	73, 118, 150, 162
3	U9	203/212 (95%)	2.21	105 (51%)	0	1	100, 153, 175, 188
3	V8	203/212 (95%)	1.42	49 (24%)	2	2	75, 118, 149, 166
3	V9	203/212 (95%)	2.04	98 (48%)	0	1	108, 148, 170, 179
3	W8	203/212 (95%)	1.40	44 (21%)	2	2	80, 121, 148, 167
3	W9	203/212 (95%)	2.15	109 (53%)	0	0	112, 155, 178, 190
3	X8	203/212 (95%)	1.40	50 (24%)	2	2	77, 116, 149, 165
3	X9	203/212 (95%)	1.97	91 (44%)	0	1	107, 150, 175, 195
3	Y8	203/212 (95%)	1.43	52 (25%)	1	2	66, 118, 153, 163
3	Y9	203/212 (95%)	2.05	93 (45%)	0	1	114, 151, 175, 184
3	Z8	203/212 (95%)	1.52	59 (29%)	1	2	74, 121, 151, 167
3	Z9	203/212 (95%)	2.22	112 (55%)	0	0	115, 155, 175, 184
All	All	31689/33420 (94%)	0.93	5092 (16%)	4	4	34, 95, 163, 203

The worst 5 of 5092 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	19	84	GLU	8.1
3	Z9	84	GLU	7.4
3	T9	61	VAL	7.3
3	G9	123	GLN	6.7
3	J9	17	GLN	6.6

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.