wwPDB X-ray Structure Validation Summary Report (i)

Nov 4, 2023 – 09:53 PM EDT

PDB ID	:	5V74
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 (i) 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 (i)) were used in the production of this report:

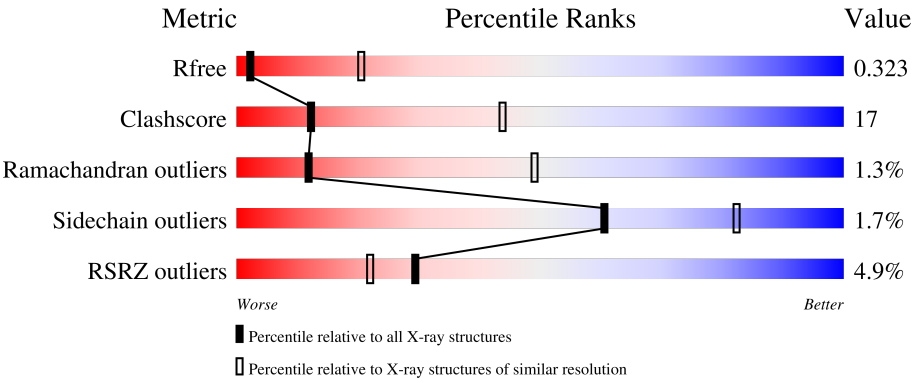
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
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}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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 <=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	64% 34%
1	21	96	63% 35%
1	31	96	47% 47%
1	41	96	66% 31%
1	A1	96	53% 43%

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Mol	Chain	Length	Quality of chain
1	B1	96	57% 42%
1	C1	96	64% 34%
1	D1	96	60% 36%
1	E1	96	59% 40%
1	F1	96	56% 42%
1	G1	96	53% 46%
1	H1	96	59% 38%
1	I1	96	59% 36%
1	J1	96	57% 41%
1	K1	96	57% 38%
1	L1	96	59% 39%
1	M1	96	67% 31%
1	N1	96	57% 39%
1	O1	96	52% 45%
1	P1	96	60% 38%
1	Q1	96	61% 36%
1	R1	96	58% 40%
1	S1	96	54% 43%
1	T1	96	65% 31%
1	U1	96	67% 30%
1	V1	96	52% 45%
1	W1	96	58% 39%
1	X1	96	59% 36%
1	Y1	96	63% 35%
1	Z1	96	50% 47%

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Mol	Chain	Length	Quality of chain
2	12	99	62% 30% • 5%
2	13	99	60% 32% • 7%
2	14	99	75% 19% • 5%
2	15	99	58% 35% • 6%
2	16	99	67% 26% 7%
2	17	99	75% 19% 6%
2	22	99	68% 25% • 5%
2	23	99	58% 34% • 7%
2	24	99	% 68% 27% 5%
2	25	99	59% 34% • 6%
2	26	99	62% 31% 7%
2	27	99	71% 23% 6%
2	32	99	60% 32% • 5%
2	33	99	63% 28% • 7%
2	34	99	64% 29% • 5%
2	35	99	61% 32% • 6%
2	36	99	69% 24% 7%
2	37	99	72% 22% 6%
2	42	99	68% 26% • 5%
2	43	99	61% 31% • 7%
2	44	99	75% 20% 5%
2	45	99	66% 25% • 6%
2	46	99	58% 35% 7%
2	47	99	64% 30% 6%
2	A2	99	63% 29% • 7%

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Mol	Chain	Length	Quality of chain
2	A3	99	64% 27% 7%
2	A4	99	68% 26% 6%
2	A5	99	61% 31% 7%
2	A6	99	71% 21% 7%
2	A7	99	65% 27% 7%
2	B2	99	61% 30% 8%
2	B3	99	54% 38% 7%
2	B4	99	72% 21% 7%
2	B5	99	57% 35% 7%
2	B6	99	69% 24% 7%
2	B7	99	66% 27% 7%
2	C2	99	62% 29% 7%
2	C3	99	60% 31% 7%
2	C4	99	70% 23% 7%
2	C5	99	62% 31% 7%
2	C6	99	65% 28% 7%
2	C7	99	65% 29% 6%
2	D2	99	60% 33% 6%
2	D3	99	56% 35% 7%
2	D4	99	59% 32% 7%
2	D5	99	61% 31% 7%
2	D6	99	57% 36% 7%
2	D7	99	71% 23% 6%
2	E2	99	66% 27% 5%
2	E3	99	65% 27% 7%

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Mol	Chain	Length	Quality of chain
2	E4	99	71% 24% 5%
2	E5	99	64% 28% 7%
2	E6	99	57% 36% 7%
2	E7	99	64% 29% 7%
2	F2	99	63% 30% 5%
2	F3	99	63% 28% 7%
2	F4	99	57% 36% 7%
2	F5	99	64% 29% 7%
2	F6	99	73% 20% 7%
2	F7	99	66% 28% 6%
2	G2	99	63% 30% 7%
2	G3	99	66% 26% 7%
2	G4	99	66% 26% 7%
2	G5	99	58% 33% 8%
2	G6	99	65% 28% 7%
2	G7	99	60% 33% 7%
2	H2	99	65% 28% 7%
2	H3	99	61% 31% 7%
2	H4	99	64% 30% 6%
2	H5	99	63% 28% 8%
2	H6	99	65% 28% 7%
2	H7	99	70% 23% 7%
2	I2	99	60% 31% 7%
2	I3	99	55% 36% 8%
2	I4	99	63% 30% 7%

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Mol	Chain	Length	Quality of chain
2	I5	99	62% 30% • 7%
2	I6	99	68% 25% 7%
2	I7	99	65% 28% 7%
2	J2	99	60% 30% • 7%
2	J3	99	57% 34% • 7%
2	J4	99	65% 28% 7%
2	J5	99	66% 25% • 8%
2	J6	99	69% 24% 7%
2	J7	99	61% 32% 7%
2	K2	99	64% 28% • 7%
2	K3	99	72% 20% • 7%
2	K4	99	69% 23% • 7%
2	K5	99	73% 20% • 6%
2	K6	99	70% 22% • 7%
2	K7	99	73% 21% 6%
2	L2	99	62% 31% • 5%
2	L3	99	68% 24% • 7%
2	L4	99	65% 28% 7%
2	L5	99	56% 36% • 7%
2	L6	99	64% 29% 7%
2	L7	99	63% 31% 6%
2	M2	99	65% 29% 6%
2	M3	99	65% 27% • 7%
2	M4	99	70% 22% • 7%
2	M5	99	54% 39% • 6%

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Mol	Chain	Length	Quality of chain
2	M6	99	69% 23% 8%
2	M7	99	61% 32% 7%
2	N2	99	63% 29% 7%
2	N3	99	60% 30% 8%
2	N4	99	67% 26% 7%
2	N5	99	58% 33% 6%
2	N6	99	65% 27% 8%
2	N7	99	64% 29% 7%
2	O2	99	72% 20% 5%
2	O3	99	66% 24% 7%
2	O4	99	76% 19% 5%
2	O5	99	66% 27% 6%
2	O6	99	65% 28% 7%
2	O7	99	62% 32% 6%
2	P2	99	64% 30% 5%
2	P3	99	62% 30% 7%
2	P4	99	70% 25% 5%
2	P5	99	64% 29% 6%
2	P6	99	68% 25% 7%
2	P7	99	63% 28% 8%
2	Q2	99	62% 31% 5%
2	Q3	99	57% 34% 7%
2	Q4	99	% 70% 25% 5%
2	Q5	99	62% 32% 6%
2	Q6	99	73% 20% 7%

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Mol	Chain	Length	Quality of chain
2	Q7	99	68% 26% 6%
2	R2	99	70% 22% 5%
2	R3	99	59% 32% 7%
2	R4	99	73% 22% 5%
2	R5	99	62% 30% 6%
2	R6	99	65% 26% 7%
2	R7	99	70% 24% 6%
2	S2	99	68% 24% 5%
2	S3	99	64% 27% 7%
2	S4	99	65% 30% 5%
2	S5	99	69% 24% 6%
2	S6	99	66% 27% 7%
2	S7	99	69% 25% 6%
2	T2	99	60% 33% 5%
2	T3	99	66% 25% 7%
2	T4	99	67% 28% 5%
2	T5	99	56% 37% 6%
2	T6	99	55% 38% 7%
2	T7	99	69% 25% 6%
2	U2	99	64% 29% 5%
2	U3	99	70% 22% 7%
2	U4	99	69% 26% 5%
2	U5	99	64% 29% 6%
2	U6	99	66% 27% 7%
2	U7	99	67% 27% 6%

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Mol	Chain	Length	Quality of chain
2	V2	99	64% 29% • 5%
2	V3	99	63% 29% • 7%
2	V4	99	66% 28% • 5%
2	V5	99	66% 27% • 6%
2	V6	99	60% 33% 7%
2	V7	99	61% 33% 6%
2	W2	99	62% 32% • 5%
2	W3	99	58% 33% • 7%
2	W4	99	% 73% 21% • 5%
2	W5	99	59% 34% • 6%
2	W6	99	66% 27% 7%
2	W7	99	63% 31% 6%
2	X2	99	62% 32% • 5%
2	X3	99	61% 30% • 7%
2	X4	99	70% 25% 5%
2	X5	99	58% 35% • 6%
2	X6	99	68% 25% 7%
2	X7	99	72% 22% 6%
2	Y2	99	63% 30% • 5%
2	Y3	99	56% 35% • 7%
2	Y4	99	70% 24% • 5%
2	Y5	99	61% 31% • 7%
2	Y6	99	65% 28% 7%
2	Y7	99	72% 22% 6%
2	Z2	99	68% 25% • 5%

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Mol	Chain	Length	Quality of chain
2	Z3	99	60% 32% 7%
2	Z4	99	75% 19% 5%
2	Z5	99	69% 25% 6%
2	Z6	99	70% 23% 7%
2	Z7	99	61% 33% 6%
3	18	212	50% 43%
3	19	212	27% 83% 9% 7%
3	28	212	49% 45%
3	29	212	17% 87% 9%
3	38	212	48% 45%
3	39	212	27% 85% 10%
3	48	212	45% 49%
3	49	212	17% 84% 11%
3	A8	212	% 47% 45%
3	A9	212	26% 86% 9%
3	B8	212	48% 46%
3	B9	212	29% 87% 8%
3	C8	212	43% 50%
3	C9	212	13% 88% 8%
3	D8	212	49% 44%
3	D9	212	21% 89% 7%
3	E8	212	% 50% 44%
3	E9	212	24% 87% 9%
3	F8	212	2% 47% 46%
3	F9	212	36% 90% 6%

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Mol	Chain	Length	Quality of chain
3	G8	212	2% 47% 46%
3	G9	212	30% 85% 11%
3	H8	212	44% 49%
3	H9	212	25% 88% 8%
3	I8	212	3% 46% 48%
3	I9	212	33% 82% 14%
3	J8	212	54% 40%
3	J9	212	18% 89% 7%
3	K8	212	% 45% 49%
3	K9	212	22% 92%
3	L8	212	% 47% 47%
3	L9	212	21% 84% 11%
3	M8	212	% 52% 42%
3	M9	212	14% 90% 6%
3	N8	212	% 42% 51%
3	N9	212	23% 87% 9%
3	O8	212	2% 48% 47%
3	O9	212	26% 88% 8%
3	P8	212	% 44% 50%
3	P9	212	19% 85% 11%
3	Q8	212	% 50% 44%
3	Q9	212	29% 88% 8%
3	R8	212	2% 39% 54%
3	R9	212	30% 83% 12%
3	S8	212	% 47% 48%

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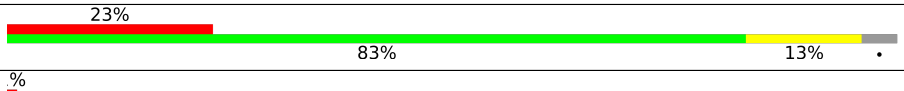
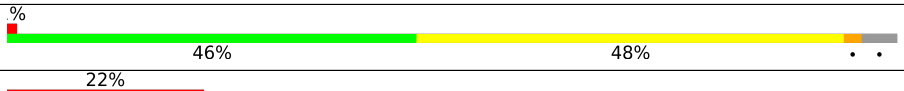
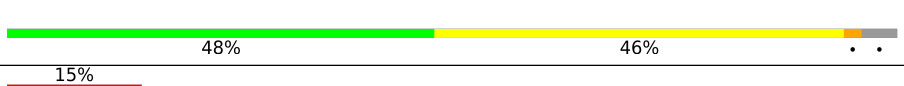
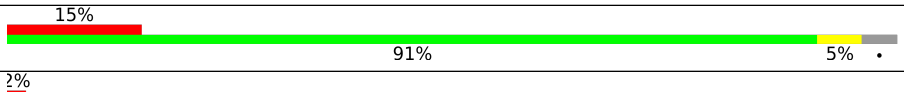
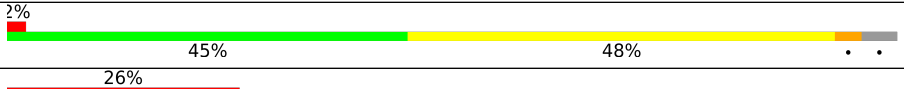
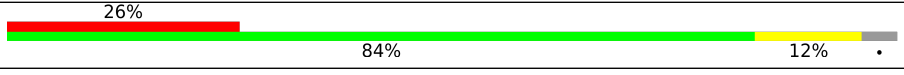
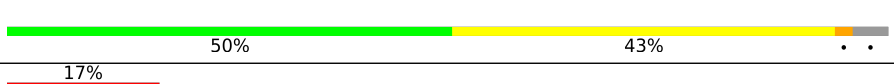
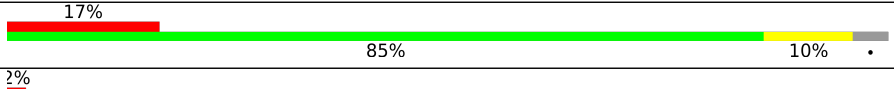
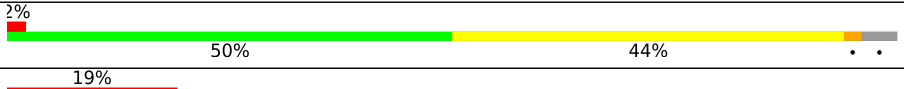
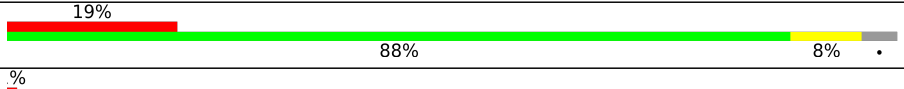
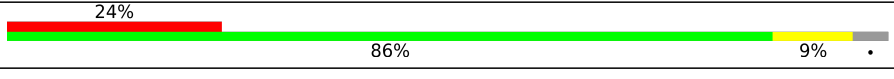
Mol	Chain	Length	Quality of chain
3	S9	212	
3	T8	212	
3	T9	212	
3	U8	212	
3	U9	212	
3	V8	212	
3	V9	212	
3	W8	212	
3	W9	212	
3	X8	212	
3	X9	212	
3	Y8	212	
3	Y9	212	
3	Z8	212	
3	Z9	212	

2 Entry composition (i)

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	C	N	O	S	0	0	0
			678	419	122	132	5			
1	R1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	S1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	T1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	U1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	V1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	W1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	X1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	Y1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	Z1	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	11	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	21	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			
1	31	94	Total	C	N	O	S	0	0	0
			669	413	120	131	5			
1	41	95	Total	C	N	O	S	0	0	0
			678	419	122	132	5			

- Molecule 2 is a protein called Microcompartments protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A2	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	A3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	A4	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	A5	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	A6	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	A7	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	B2	91	Total	C	N	O	S	0	0	0
			651	408	119	121	3			
2	B3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	B4	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	B5	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	B6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	B7	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	C2	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	C3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	C4	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	C5	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	C6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	C7	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	D2	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	D3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	D4	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	D5	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	D6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	D7	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	E2	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	E3	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	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	C	N	O	S	0	0	0
			658	413	120	122	3			
2	L5	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	L6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	L7	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	M2	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	M3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	M4	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	M5	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	M6	91	Total	C	N	O	S	0	0	0
			653	410	119	121	3			
2	M7	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	N2	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	N3	91	Total	C	N	O	S	0	0	0
			653	410	119	121	3			
2	N4	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	N5	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	N6	91	Total	C	N	O	S	0	0	0
			653	410	119	121	3			
2	N7	92	Total	C	N	O	S	0	0	0
			657	412	120	122	3			
2	O2	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	O3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	O4	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	O5	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	O6	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	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	C	N	O	S	0	0	0
			670	420	122	124	4			
2	S5	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	S6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	S7	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	T2	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	T3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	T4	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	T5	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	T6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	T7	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	U2	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	U3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	U4	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	U5	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	U6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	U7	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	V2	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	V3	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	V4	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	V5	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	V6	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	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	C	N	O	S	0	0	0
			670	420	122	124	4			
2	Z5	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	Z6	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	Z7	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	12	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	13	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	14	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	15	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	16	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	17	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	22	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	23	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	24	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	25	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	26	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	27	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	32	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	33	92	Total	C	N	O	S	0	0	0
			658	413	120	122	3			
2	34	94	Total	C	N	O	S	0	0	0
			670	420	122	124	4			
2	35	93	Total	C	N	O	S	0	0	0
			662	415	121	123	3			
2	36	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	37	93	Total C N O S 662 415 121 123 3	0	0	0
2	42	94	Total C N O S 670 420 122 124 4	0	0	0
2	43	92	Total C N O S 658 413 120 122 3	0	0	0
2	44	94	Total C N O S 670 420 122 124 4	0	0	0
2	45	93	Total C N O S 662 415 121 123 3	0	0	0
2	46	92	Total C N O S 658 413 120 122 3	0	0	0
2	47	93	Total C N O S 662 415 121 123 3	0	0	0

- Molecule 3 is a protein called Microcompartments protein.

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

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

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

Continued on next page...

Continued from previous page...

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

3 Residue-property plots (i)

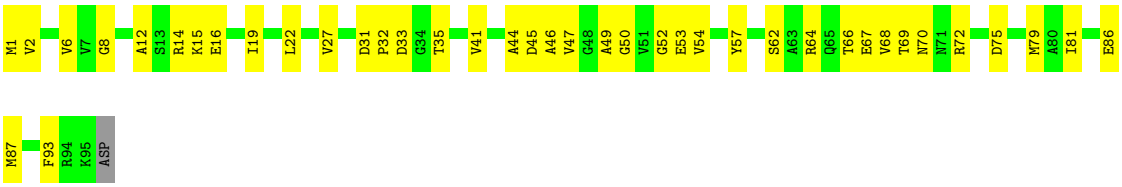
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 Ccml

Chain A1:

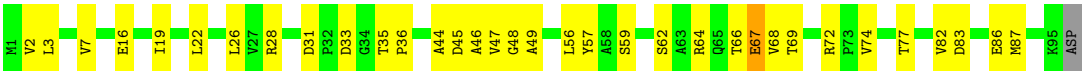
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain B1:



• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain C1:

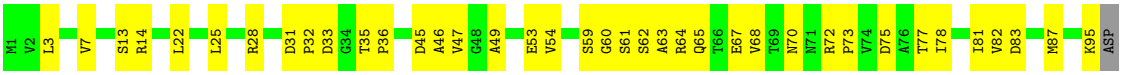


• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain D1:

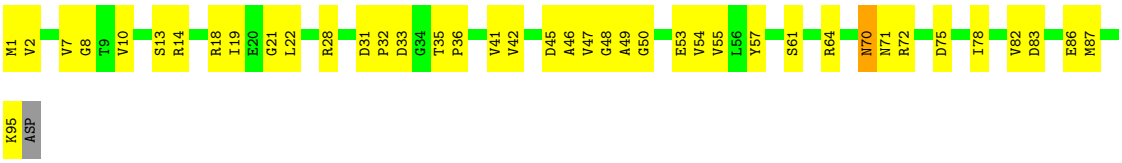
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain E1:



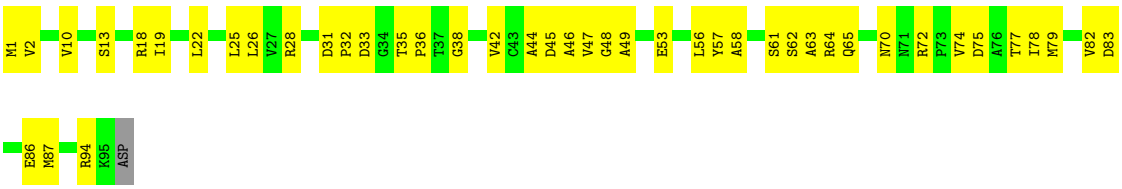
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain F1:



• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain G1:



• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

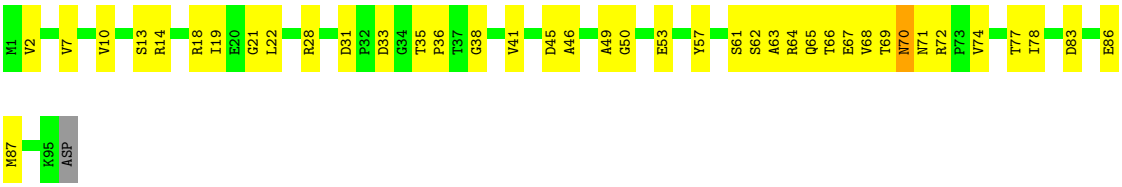
Chain H1:

• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain I1:

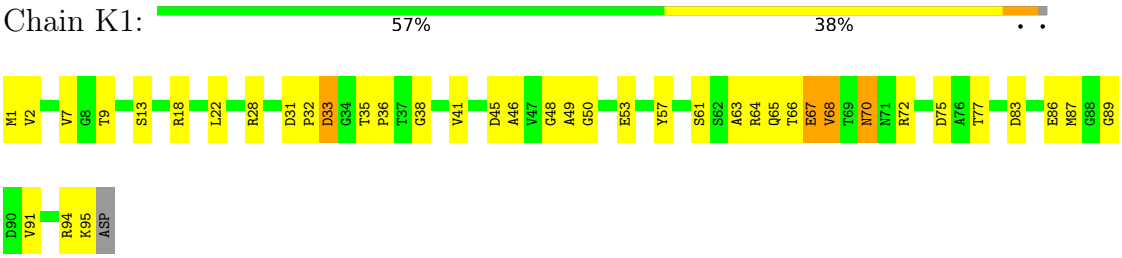
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain J1:



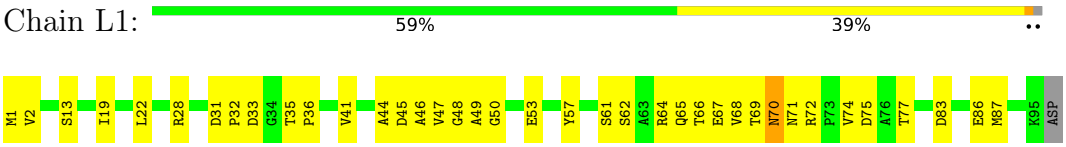
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain K1:



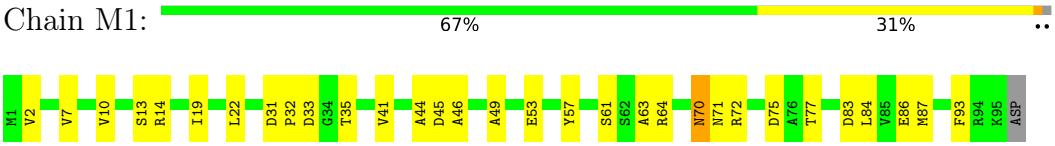
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain L1:



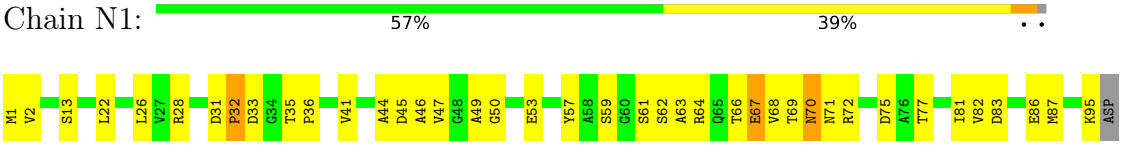
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain M1:



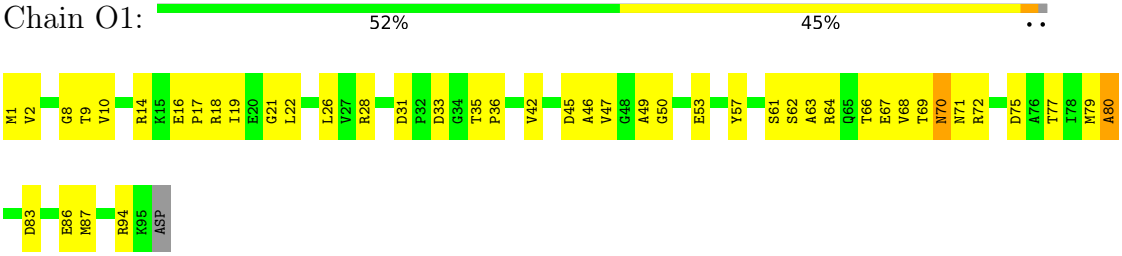
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain N1:



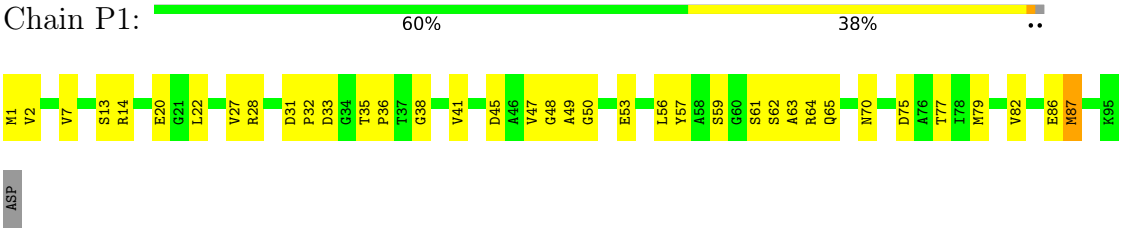
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain O1:



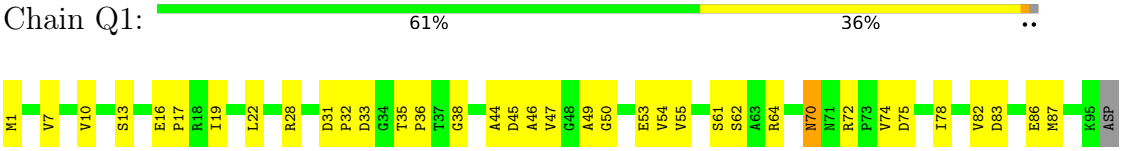
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain P1:



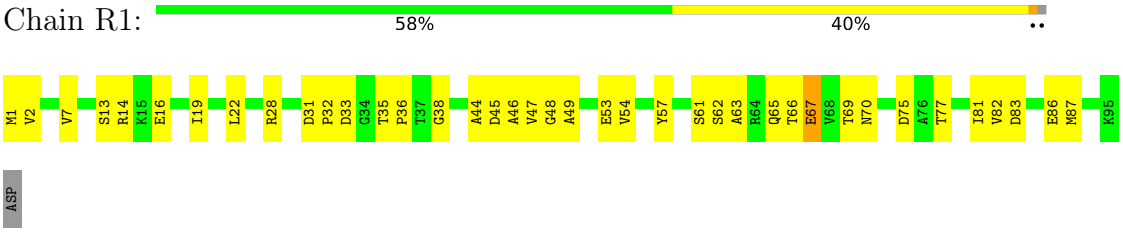
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain Q1:



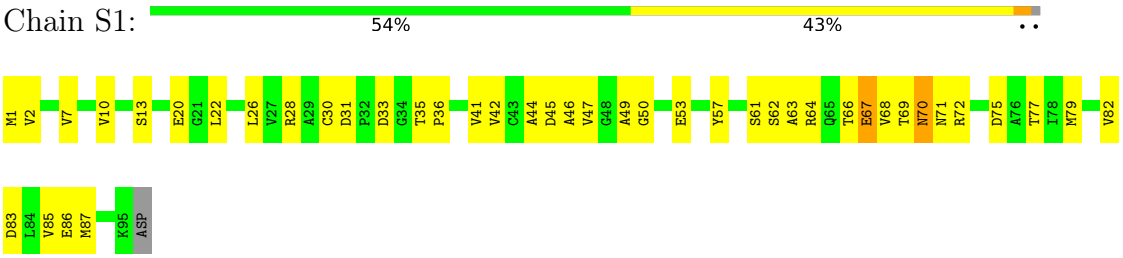
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain R1:



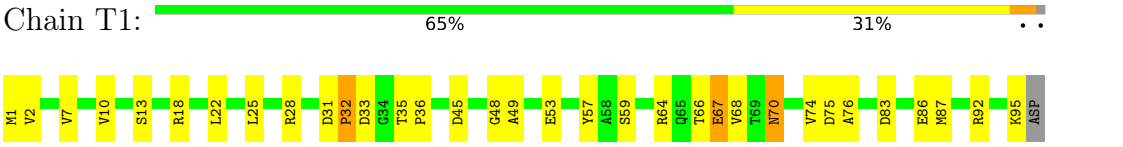
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain S1:



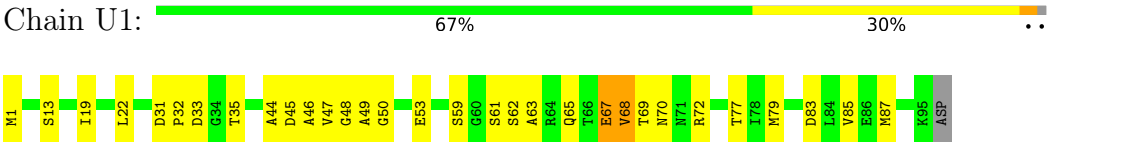
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain T1:



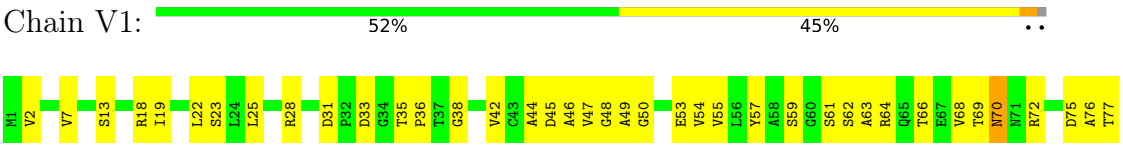
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

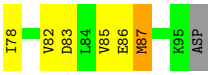
Chain U1:



• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

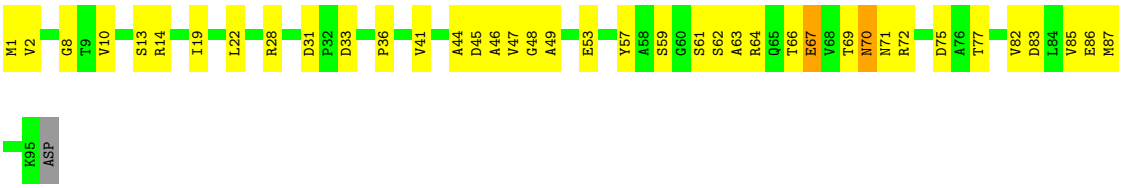
Chain V1:





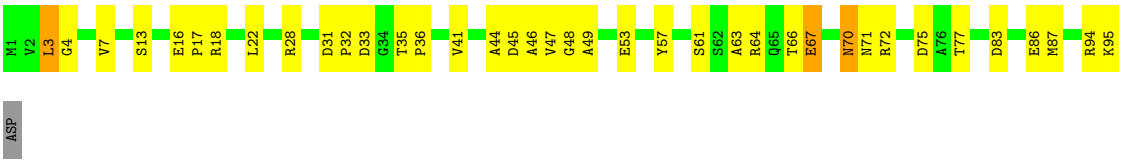
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain W1:



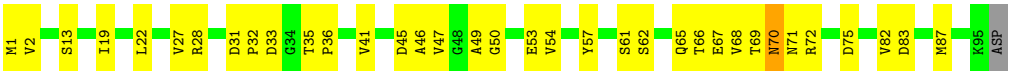
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain X1:



• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain Y1:

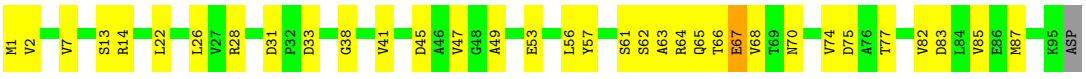


• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain Z1:

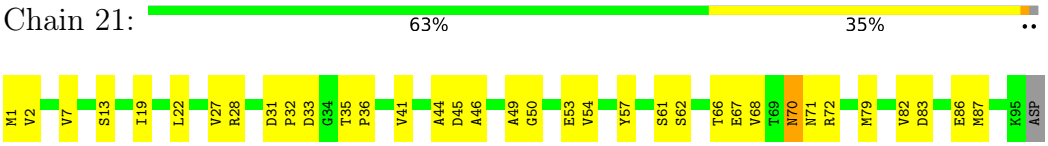
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain 11:



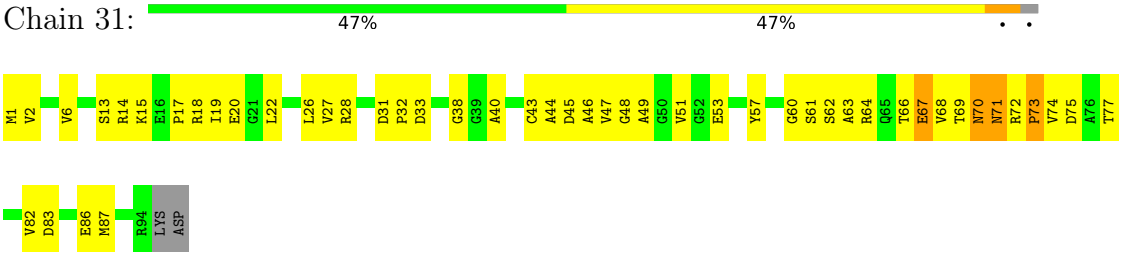
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain 21:



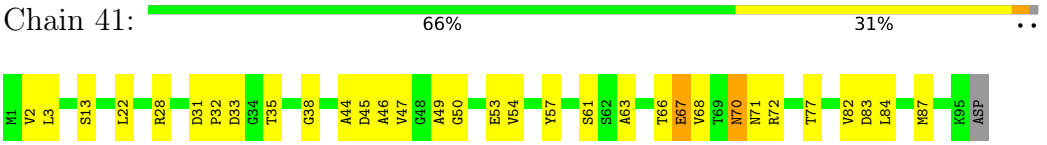
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain 31:



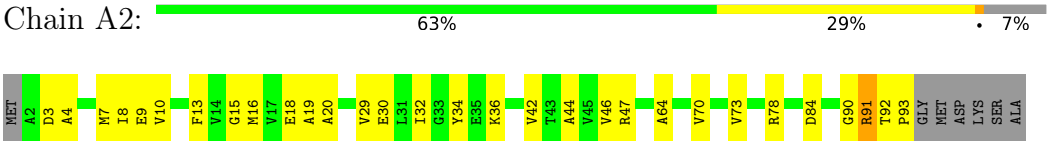
• Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein Ccml

Chain 41:



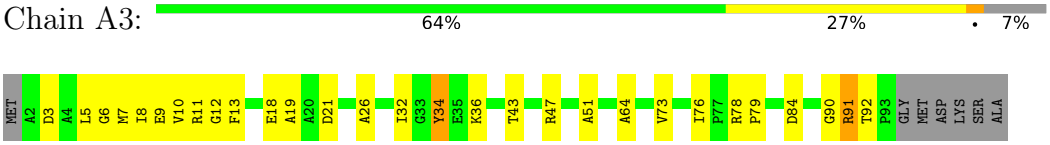
• Molecule 2: Microcompartments protein

Chain A2:



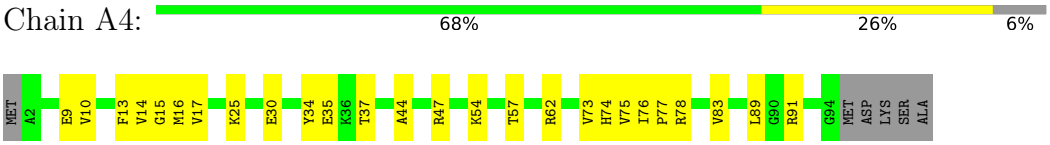
• Molecule 2: Microcompartments protein

Chain A3:



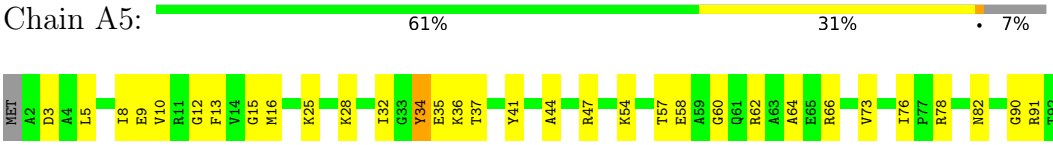
• Molecule 2: Microcompartments protein

Chain A4:



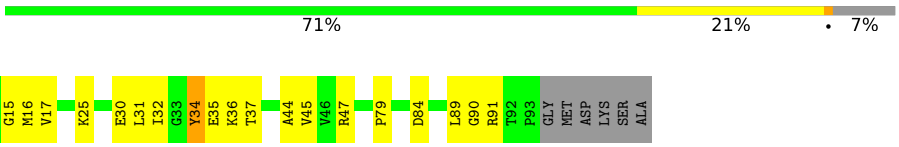
• Molecule 2: Microcompartments protein

Chain A5:



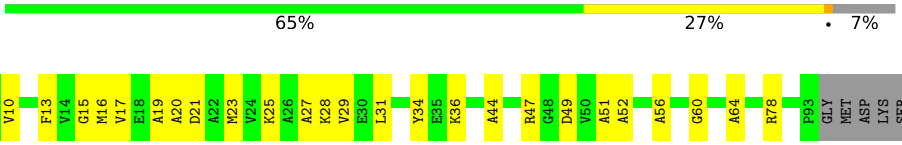
• Molecule 2: Microcompartments protein

Chain A6:



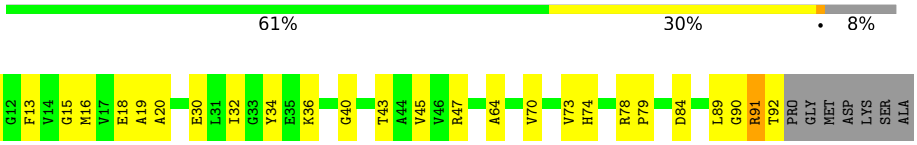
• Molecule 2: Microcompartments protein

Chain A7:



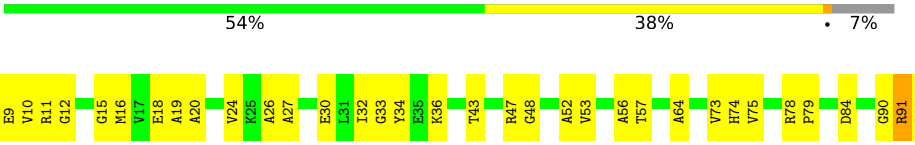
• Molecule 2: Microcompartments protein

Chain B2:



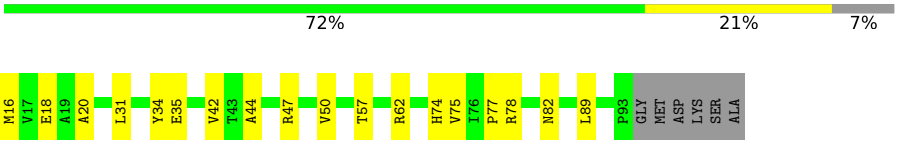
• Molecule 2: Microcompartments protein

Chain B3:



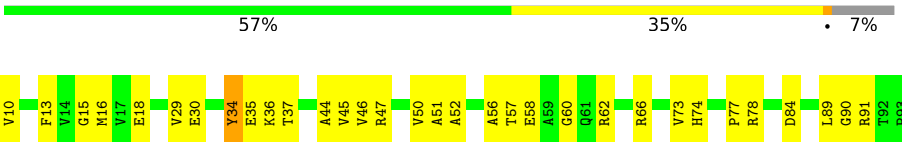
• Molecule 2: Microcompartments protein

Chain B4:



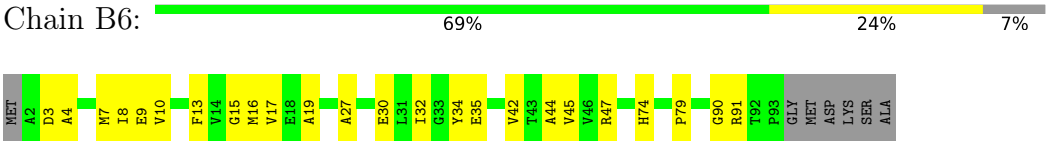
• Molecule 2: Microcompartments protein

Chain B5:



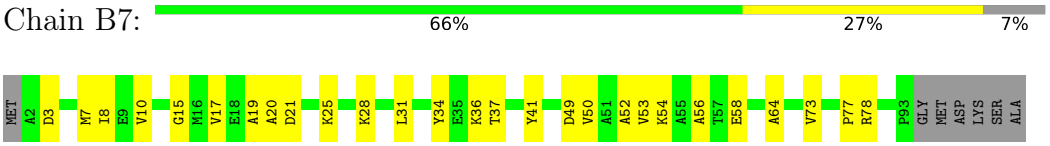
• Molecule 2: Microcompartments protein

Chain B6:



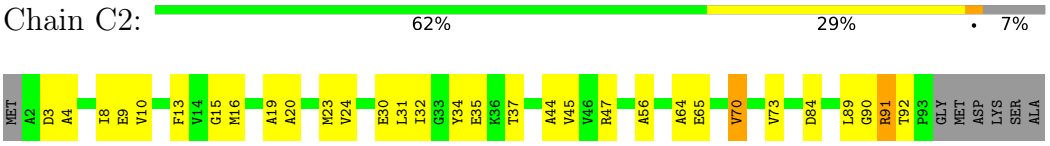
• Molecule 2: Microcompartments protein

Chain B7:



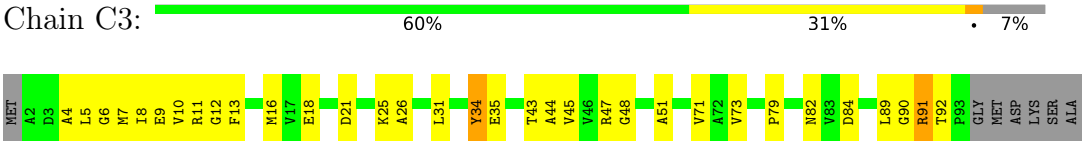
• Molecule 2: Microcompartments protein

Chain C2:



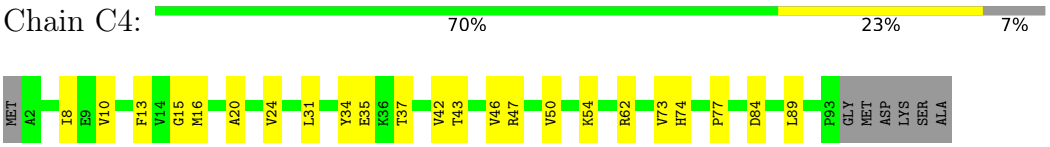
• Molecule 2: Microcompartments protein

Chain C3:



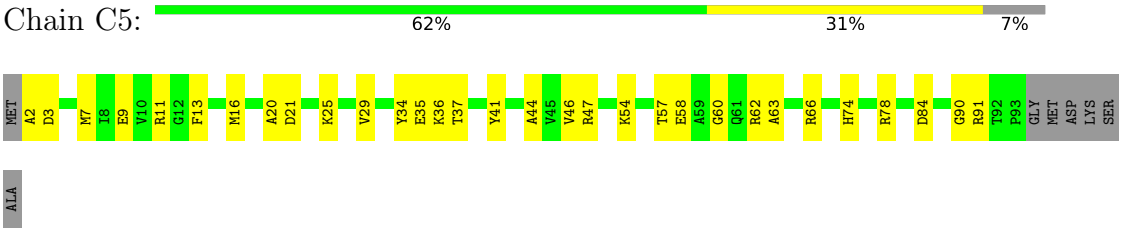
• Molecule 2: Microcompartments protein

Chain C4:



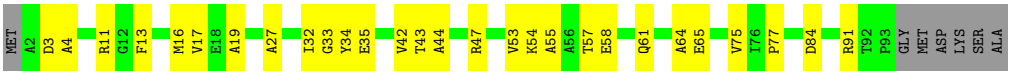
• Molecule 2: Microcompartments protein

Chain C5:



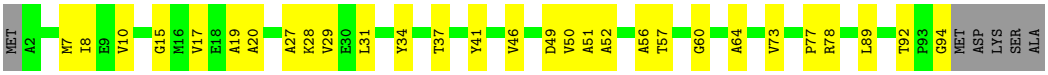
• Molecule 2: Microcompartments protein

Chain C6:



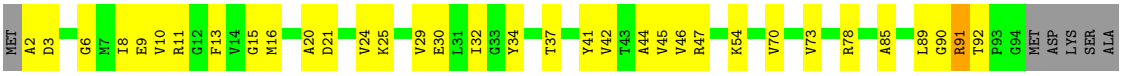
• Molecule 2: Microcompartments protein

Chain C7:



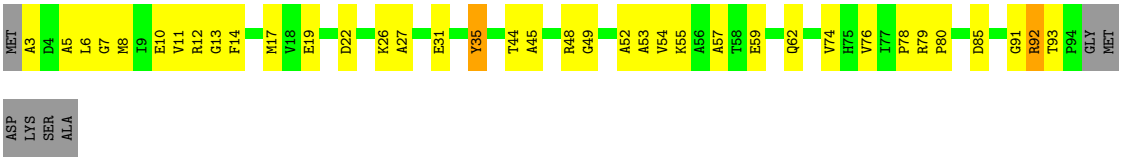
• Molecule 2: Microcompartments protein

Chain D2:



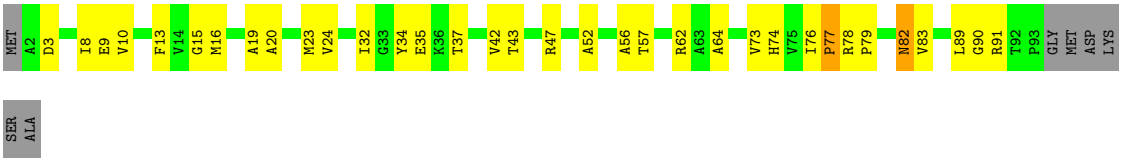
• Molecule 2: Microcompartments protein

Chain D3:



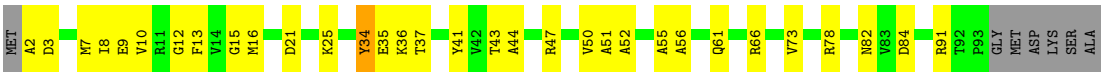
• Molecule 2: Microcompartments protein

Chain D4:



• Molecule 2: Microcompartments protein

Chain D5:

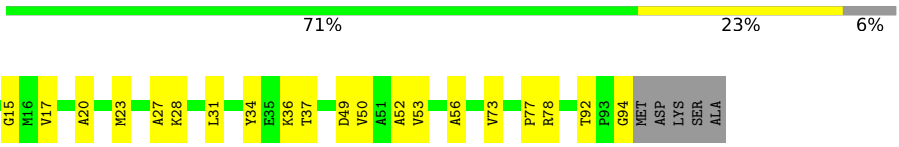


• Molecule 2: Microcompartments protein

Chain D6:

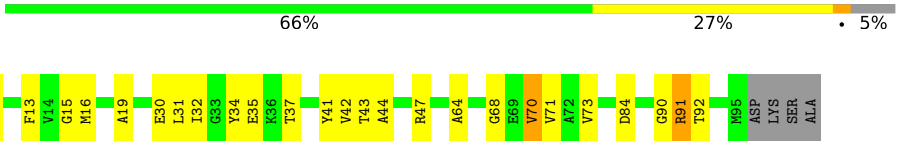
• Molecule 2: Microcompartments protein

Chain D7:



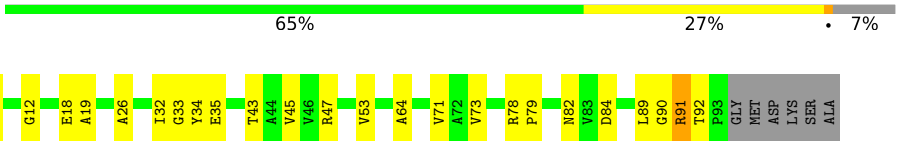
• Molecule 2: Microcompartments protein

Chain E2:



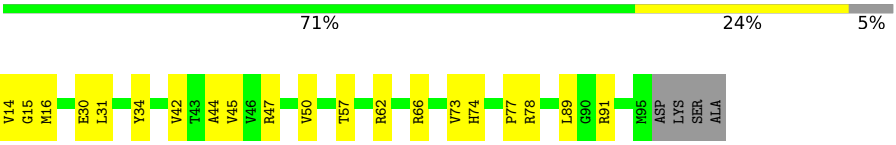
• Molecule 2: Microcompartments protein

Chain E3:



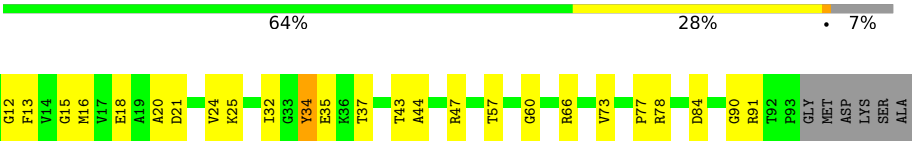
• Molecule 2: Microcompartments protein

Chain E4:



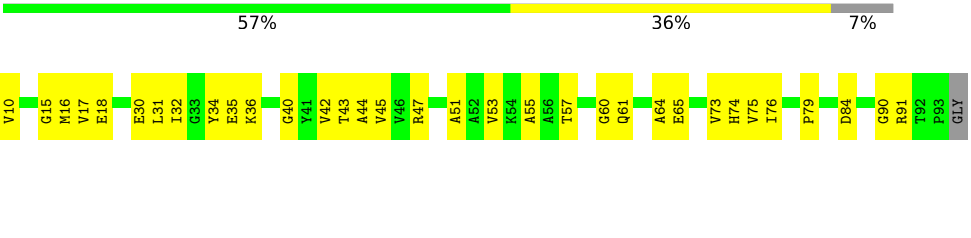
• Molecule 2: Microcompartments protein

Chain E5:



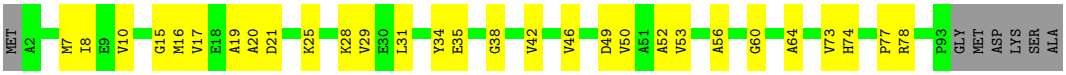
• Molecule 2: Microcompartments protein

Chain E6:



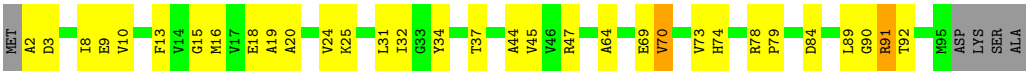
• Molecule 2: Microcompartments protein

Chain E7:



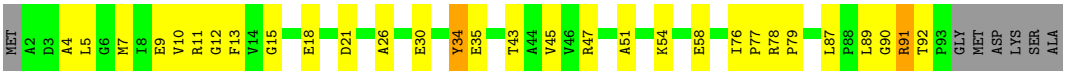
• Molecule 2: Microcompartments protein

Chain F2:



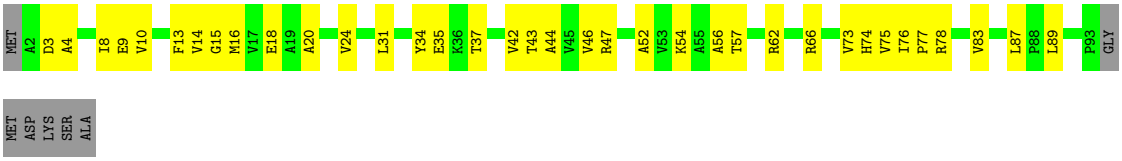
• Molecule 2: Microcompartments protein

Chain F3:



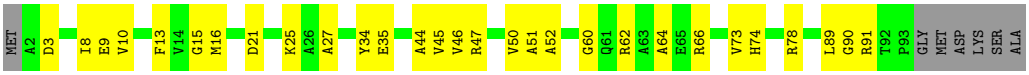
• Molecule 2: Microcompartments protein

Chain F4:



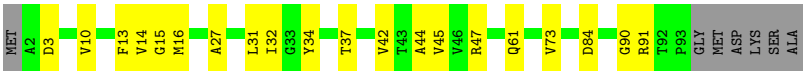
• Molecule 2: Microcompartments protein

Chain F5:



• Molecule 2: Microcompartments protein

Chain F6:

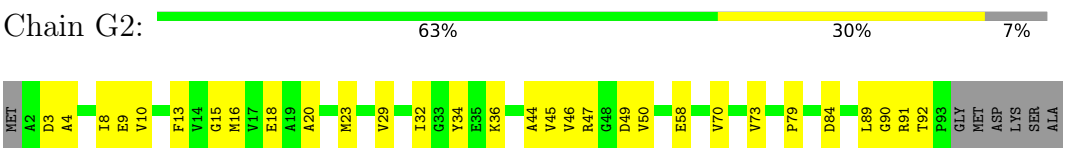


• Molecule 2: Microcompartments protein

Chain F7:

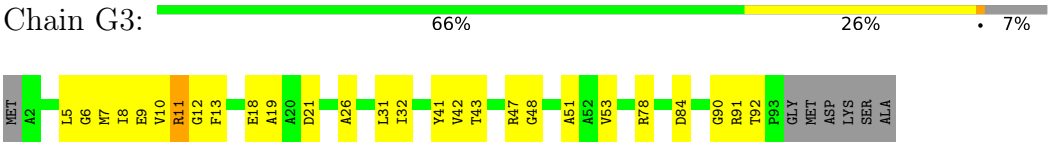
• Molecule 2: Microcompartments protein

Chain G2:



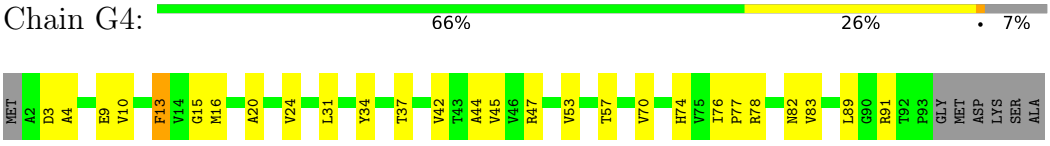
• Molecule 2: Microcompartments protein

Chain G3:



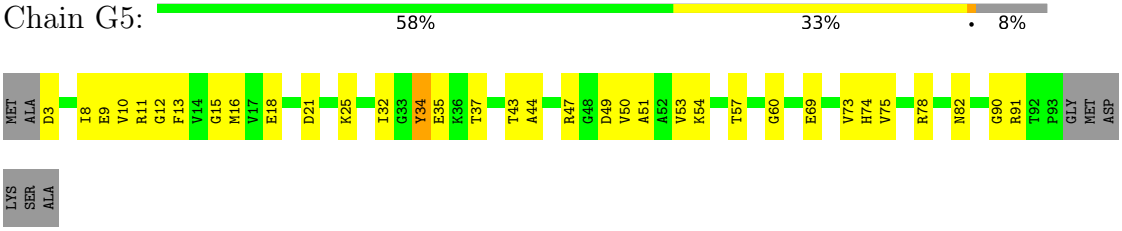
• Molecule 2: Microcompartments protein

Chain G4:



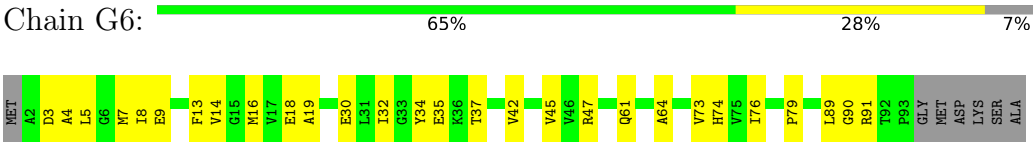
• Molecule 2: Microcompartments protein

Chain G5:



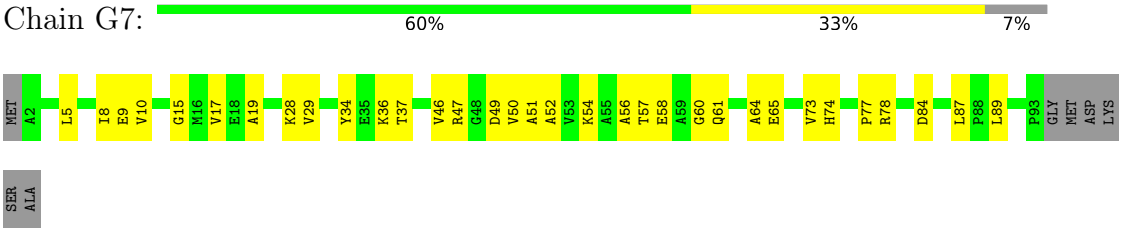
• Molecule 2: Microcompartments protein

Chain G6:



• Molecule 2: Microcompartments protein

Chain G7:

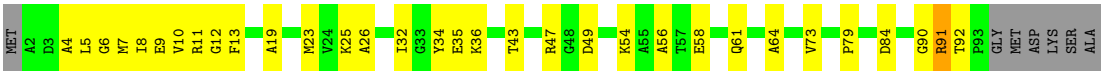


• Molecule 2: Microcompartments protein

Chain H2:

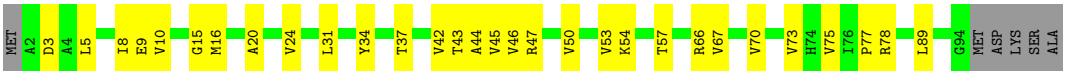
• Molecule 2: Microcompartments protein

Chain H3:



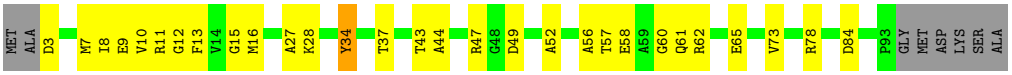
• Molecule 2: Microcompartments protein

Chain H4:



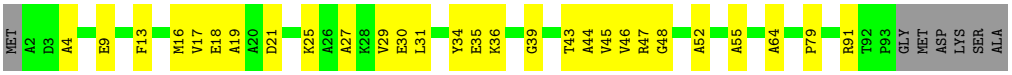
• Molecule 2: Microcompartments protein

Chain H5:



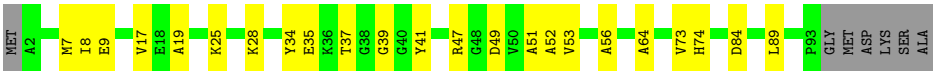
• Molecule 2: Microcompartments protein

Chain H6:



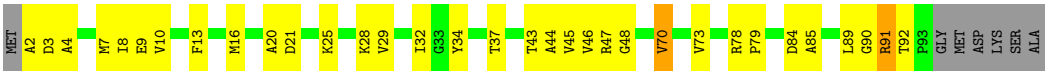
• Molecule 2: Microcompartments protein

Chain H7:



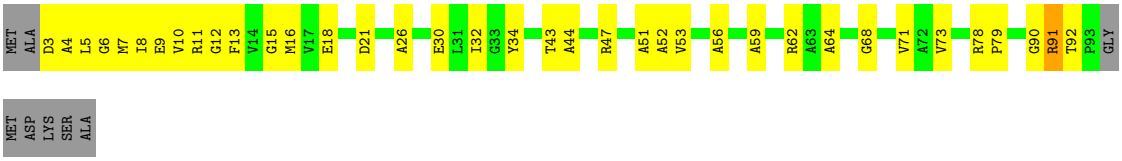
• Molecule 2: Microcompartments protein

Chain I2:



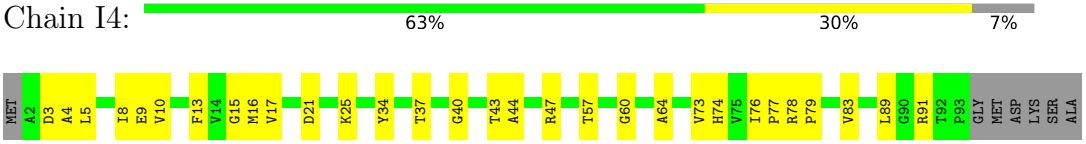
• Molecule 2: Microcompartments protein

Chain I3:



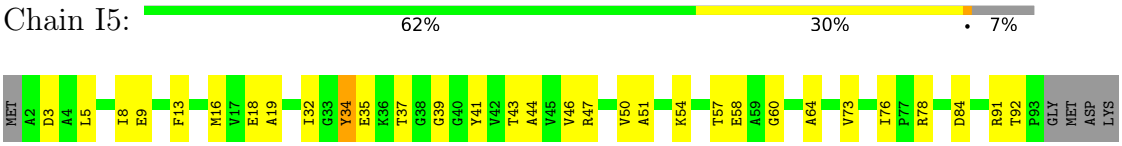
• Molecule 2: Microcompartments protein

Chain I4:



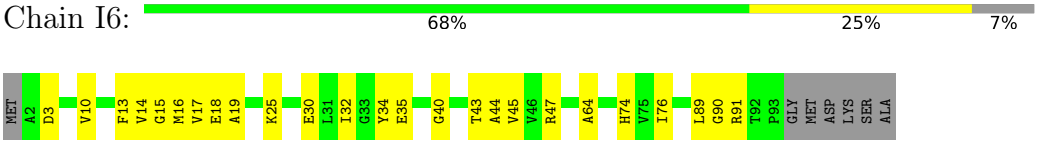
• Molecule 2: Microcompartments protein

Chain I5:



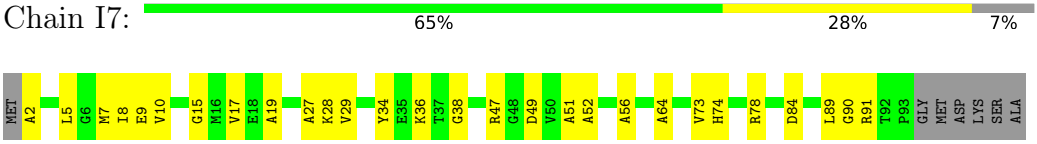
• Molecule 2: Microcompartments protein

Chain I6:



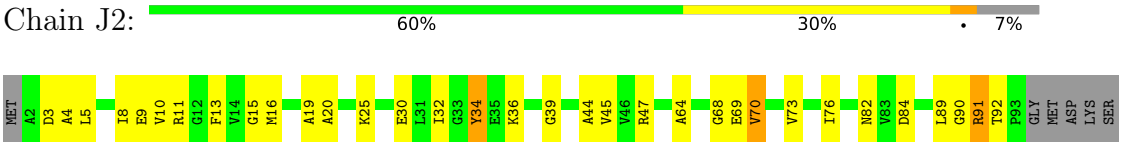
• Molecule 2: Microcompartments protein

Chain I7:



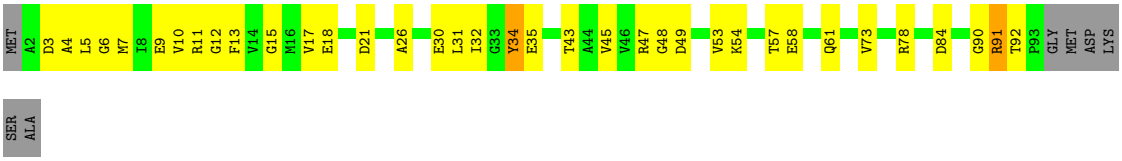
• Molecule 2: Microcompartments protein

Chain J2:



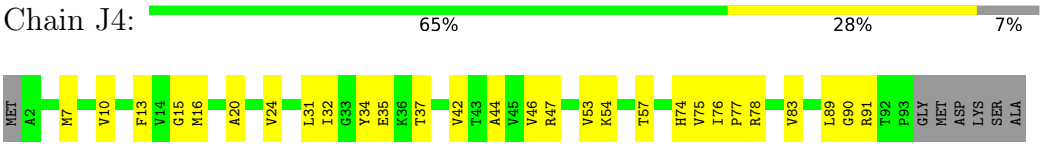
• Molecule 2: Microcompartments protein

Chain J3:



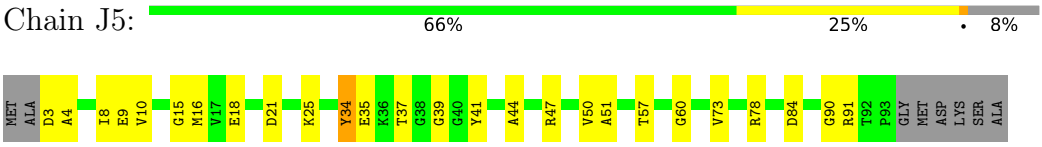
• Molecule 2: Microcompartments protein

Chain J4:



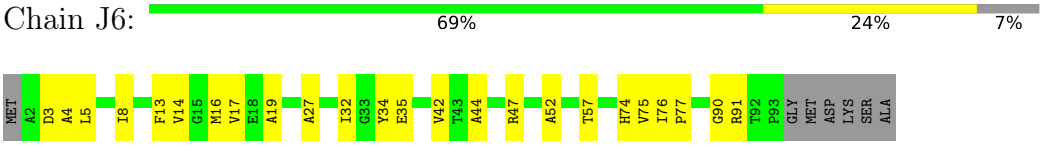
• Molecule 2: Microcompartments protein

Chain J5:



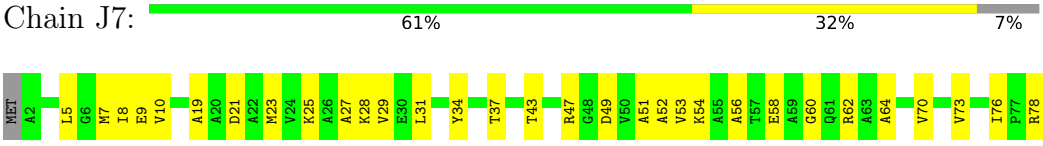
• Molecule 2: Microcompartments protein

Chain J6:



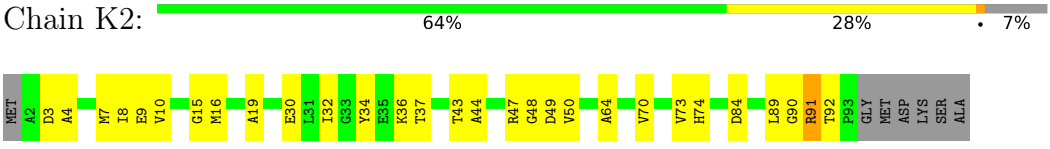
• Molecule 2: Microcompartments protein

Chain J7:



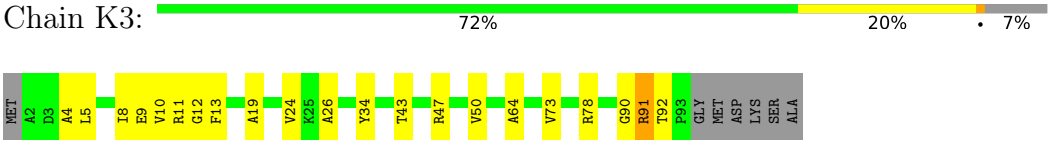
• Molecule 2: Microcompartments protein

Chain K2:



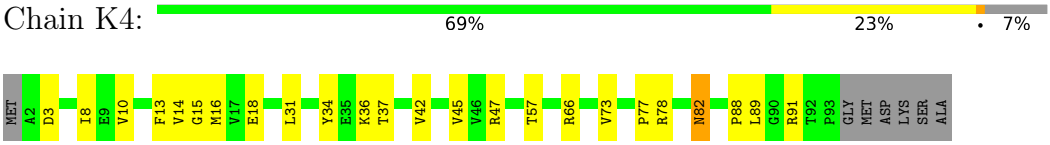
• Molecule 2: Microcompartments protein

Chain K3:



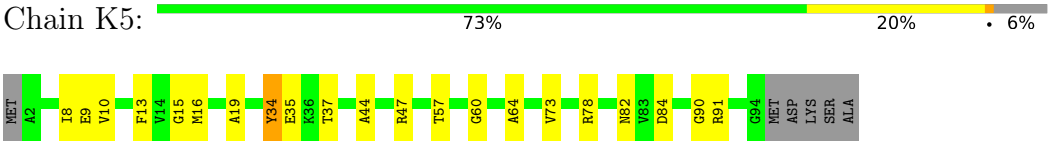
• Molecule 2: Microcompartments protein

Chain K4:



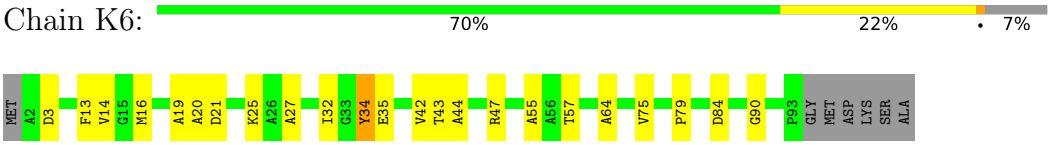
• Molecule 2: Microcompartments protein

Chain K5:



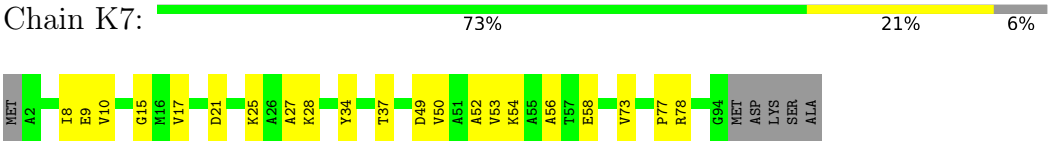
• Molecule 2: Microcompartments protein

Chain K6:



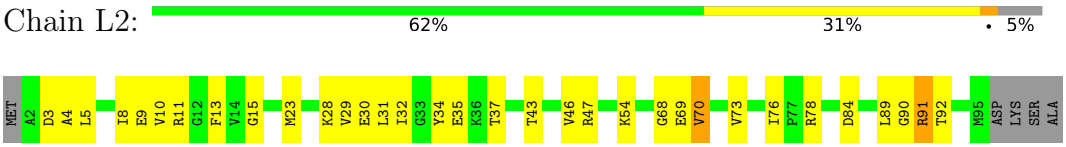
• Molecule 2: Microcompartments protein

Chain K7:



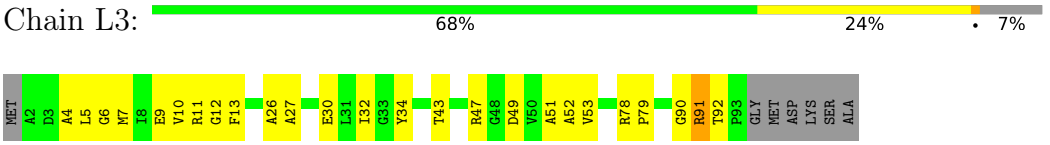
• Molecule 2: Microcompartments protein

Chain L2:



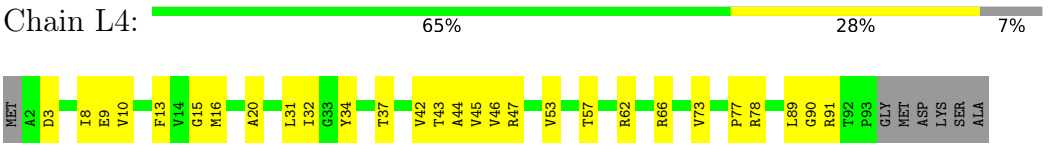
• Molecule 2: Microcompartments protein

Chain L3:



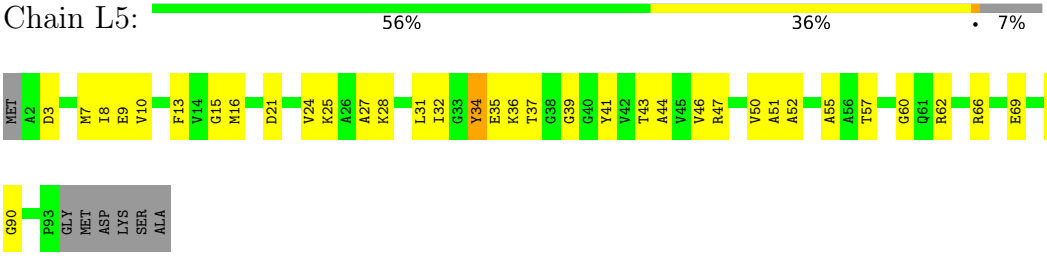
• Molecule 2: Microcompartments protein

Chain L4:



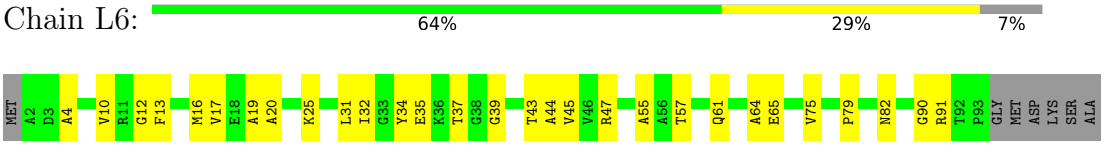
• Molecule 2: Microcompartments protein

Chain L5:



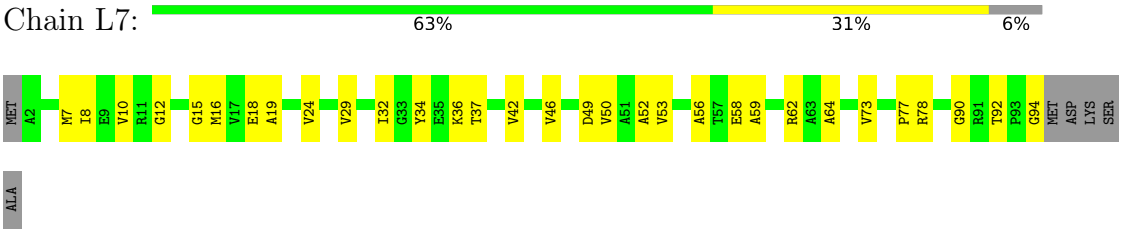
• Molecule 2: Microcompartments protein

Chain L6:



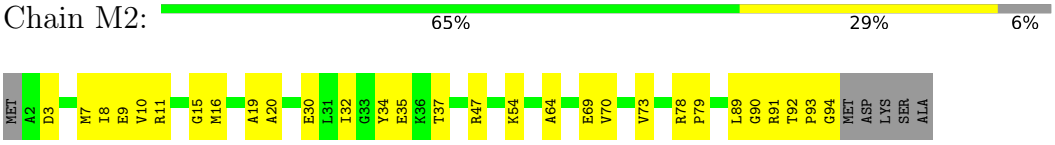
• Molecule 2: Microcompartments protein

Chain L7:



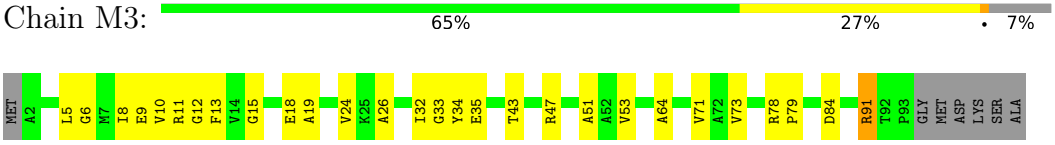
• Molecule 2: Microcompartments protein

Chain M2:



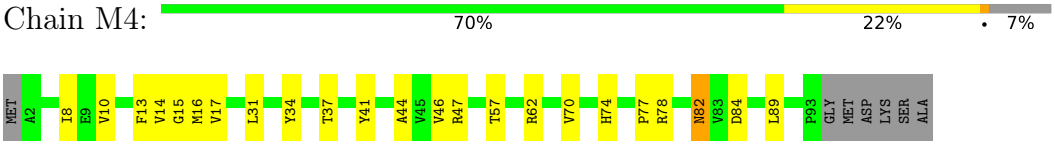
• Molecule 2: Microcompartments protein

Chain M3:



• Molecule 2: Microcompartments protein

Chain M4:

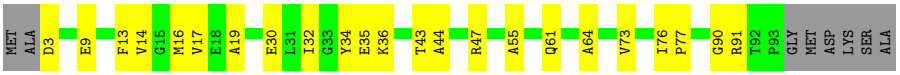


• Molecule 2: Microcompartments protein

Chain M5:

• Molecule 2: Microcompartments protein

Chain M6:



• Molecule 2: Microcompartments protein

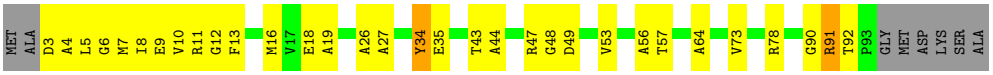
Chain M7:

• Molecule 2: Microcompartments protein

Chain N2:

• Molecule 2: Microcompartments protein

Chain N3:

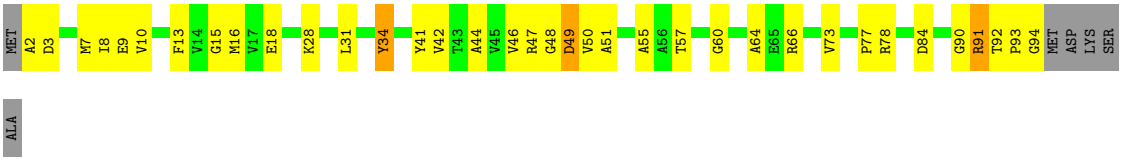


• Molecule 2: Microcompartments protein

Chain N4:

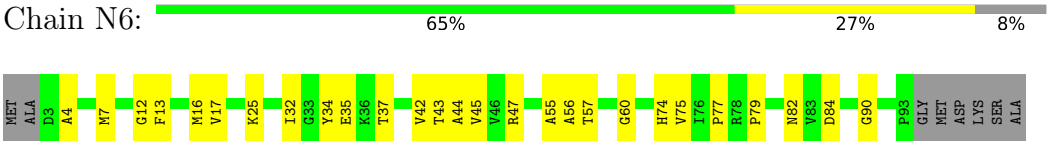
• Molecule 2: Microcompartments protein

Chain N5:



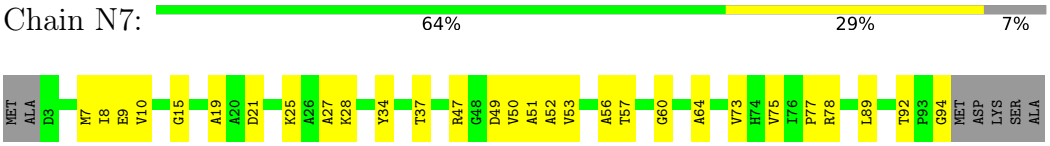
• Molecule 2: Microcompartments protein

Chain N6:



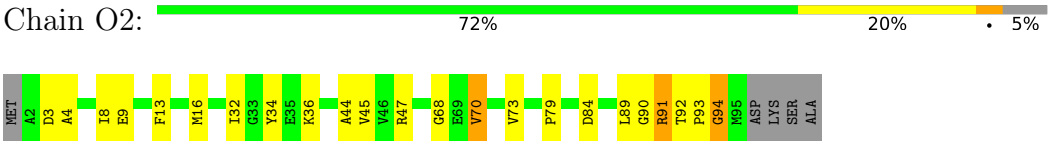
• Molecule 2: Microcompartments protein

Chain N7:



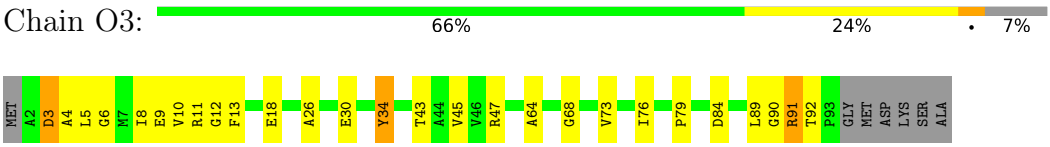
• Molecule 2: Microcompartments protein

Chain O2:



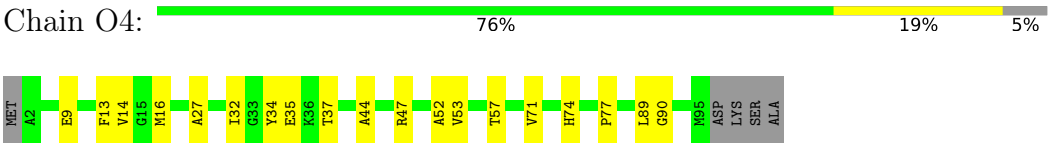
• Molecule 2: Microcompartments protein

Chain O3:



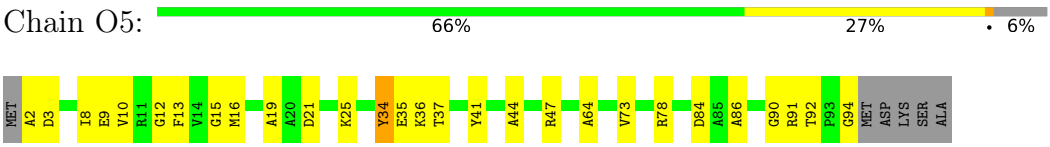
• Molecule 2: Microcompartments protein

Chain O4:



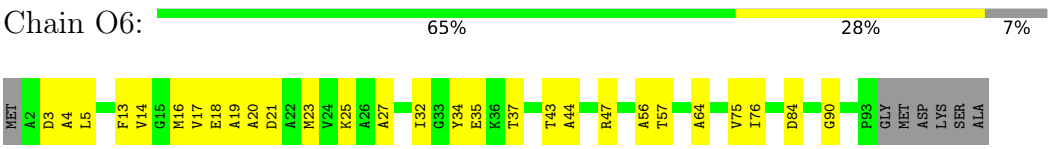
• Molecule 2: Microcompartments protein

Chain O5:



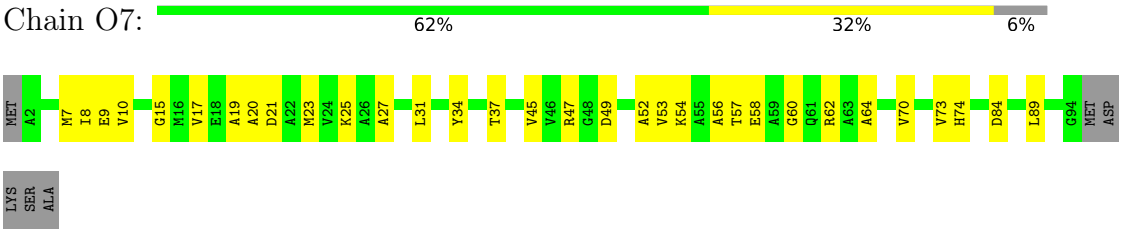
• Molecule 2: Microcompartments protein

Chain O6:



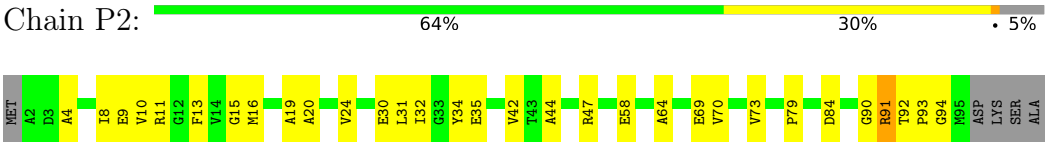
• Molecule 2: Microcompartments protein

Chain O7:



• Molecule 2: Microcompartments protein

Chain P2:



• Molecule 2: Microcompartments protein

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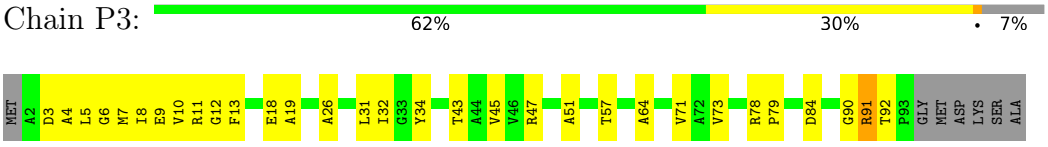
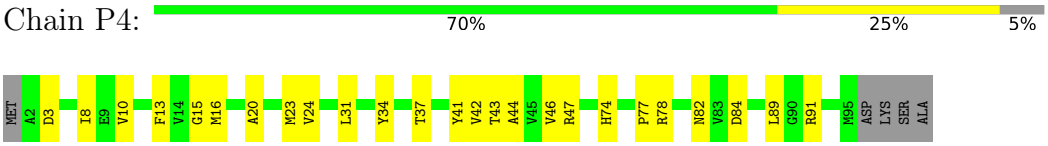


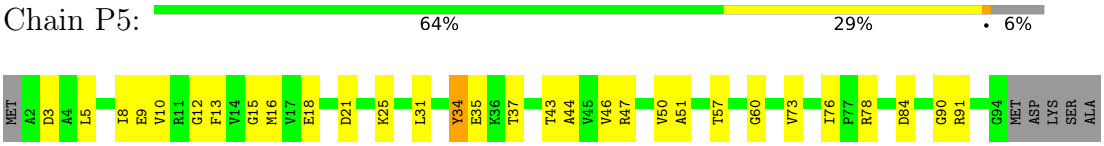
• Molecule 2: Microcompartments protein

Chain P4:



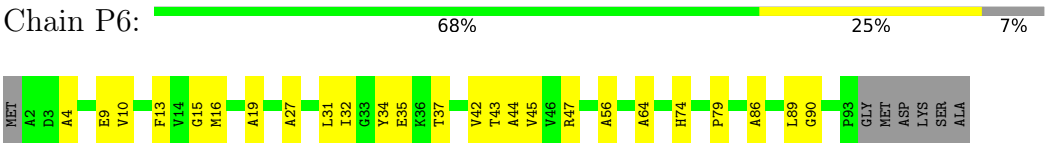
• Molecule 2: Microcompartments protein

Chain P5:



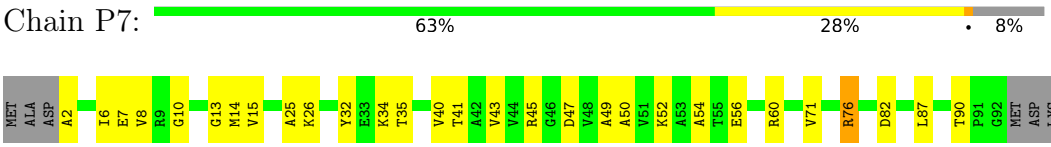
• Molecule 2: Microcompartments protein

Chain P6:



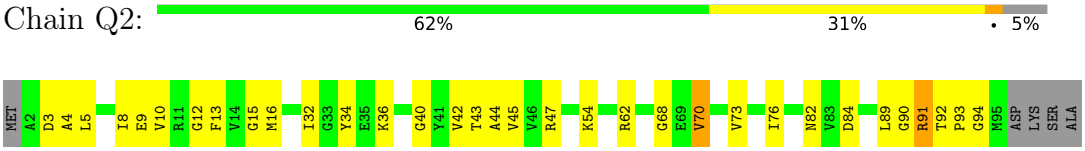
• Molecule 2: Microcompartments protein

Chain P7:



• Molecule 2: Microcompartments protein

Chain Q2:



• Molecule 2: Microcompartments protein

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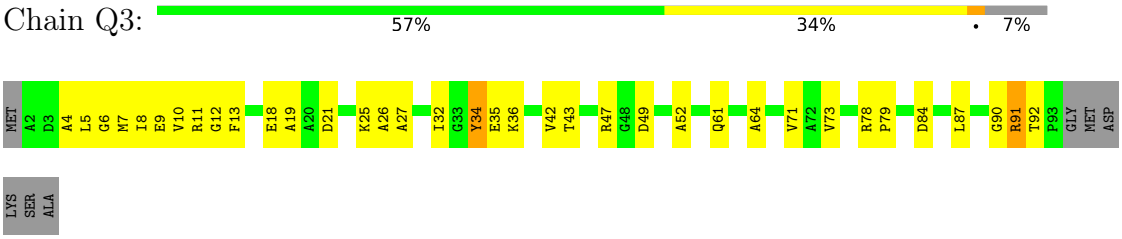
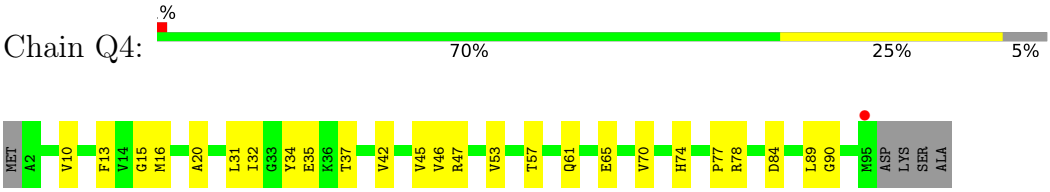


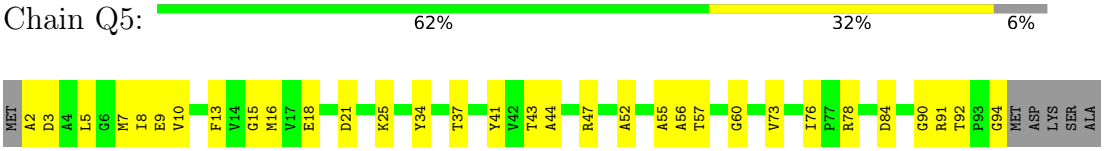
• Molecule 2: Microcompartments protein

Chain Q4:



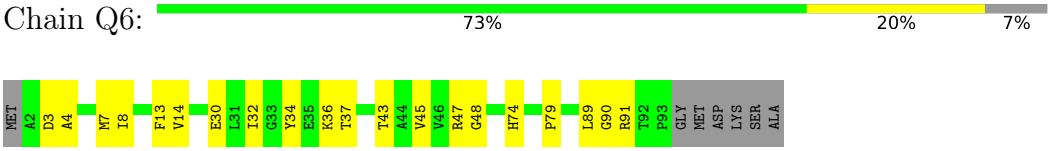
• Molecule 2: Microcompartments protein

Chain Q5:



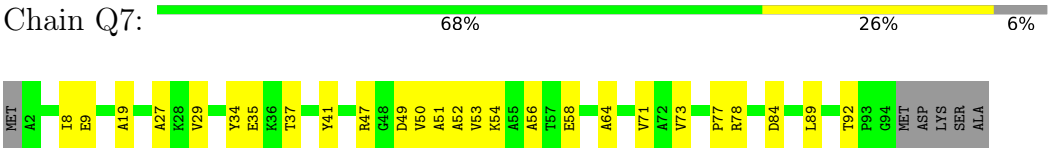
• Molecule 2: Microcompartments protein

Chain Q6:



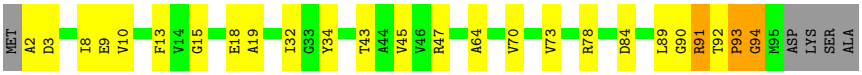
• Molecule 2: Microcompartments protein

Chain Q7:



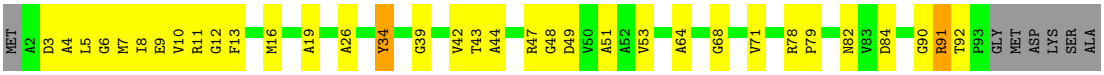
• Molecule 2: Microcompartments protein

Chain R2:



• Molecule 2: Microcompartments protein

Chain R3:



• Molecule 2: Microcompartments protein

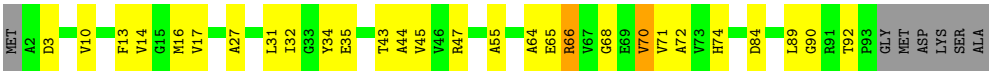
Chain R4:

• Molecule 2: Microcompartments protein

Chain R5:

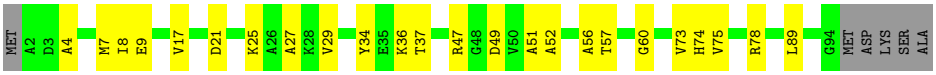
• Molecule 2: Microcompartments protein

Chain R6:



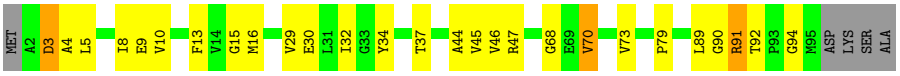
• Molecule 2: Microcompartments protein

Chain R7:



• Molecule 2: Microcompartments protein

Chain S2:



• Molecule 2: Microcompartments protein

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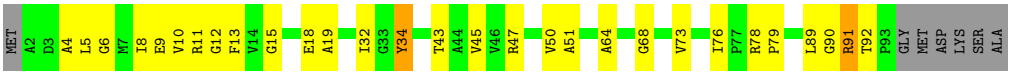
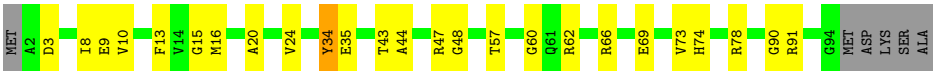


• Molecule 2: Microcompartments protein

Chain S4:

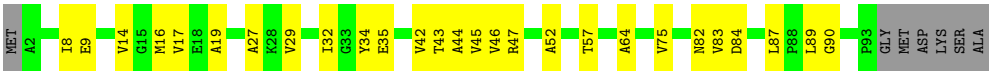
• Molecule 2: Microcompartments protein

Chain S5:



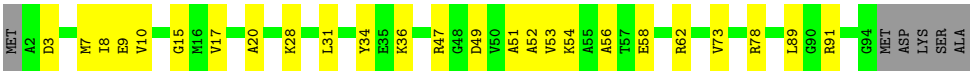
• Molecule 2: Microcompartments protein

Chain S6:



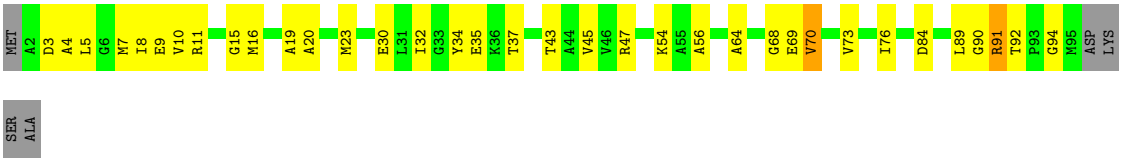
• Molecule 2: Microcompartments protein

Chain S7:



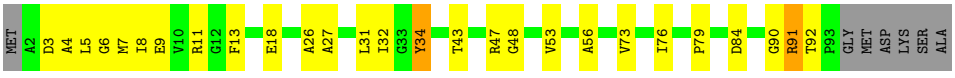
• Molecule 2: Microcompartments protein

Chain T2:



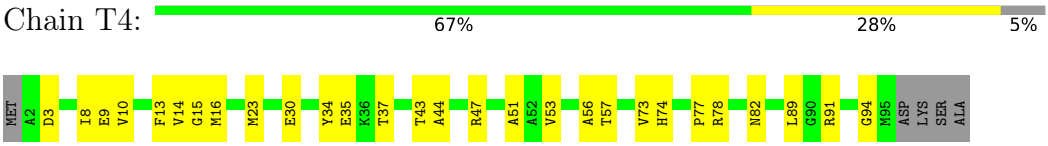
• Molecule 2: Microcompartments protein

Chain T3:



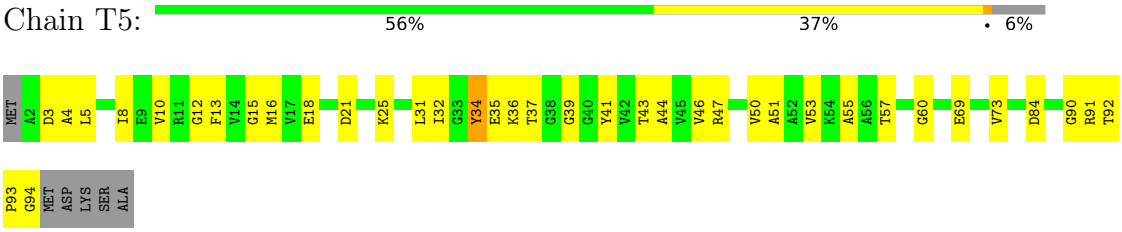
• Molecule 2: Microcompartments protein

Chain T4:



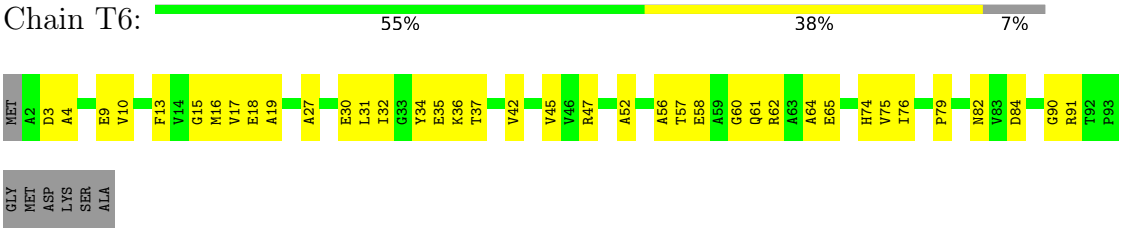
• Molecule 2: Microcompartments protein

Chain T5:



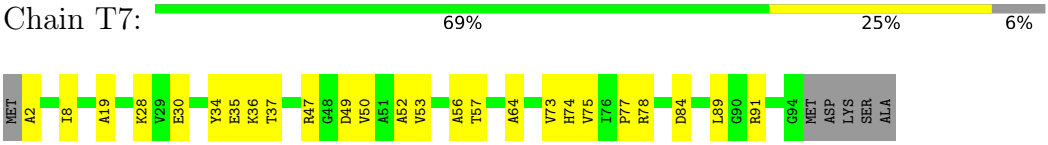
• Molecule 2: Microcompartments protein

Chain T6:



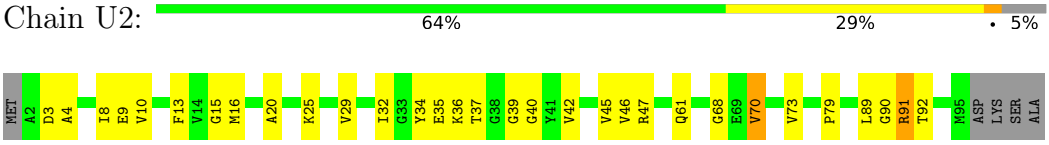
• Molecule 2: Microcompartments protein

Chain T7:



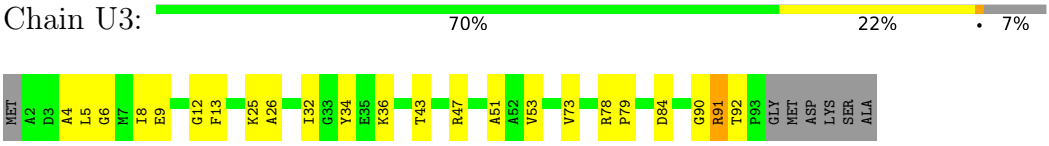
• Molecule 2: Microcompartments protein

Chain U2:



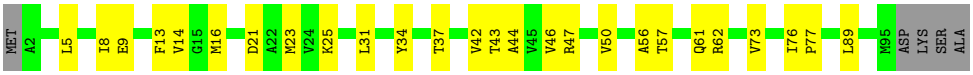
• Molecule 2: Microcompartments protein

Chain U3:



• Molecule 2: Microcompartments protein

Chain U4:



• Molecule 2: Microcompartments protein

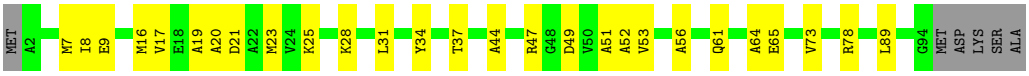
Chain U5:

• Molecule 2: Microcompartments protein

Chain U6:

• Molecule 2: Microcompartments protein

Chain U7:

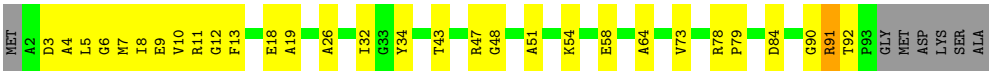


• Molecule 2: Microcompartments protein

Chain V2:

• Molecule 2: Microcompartments protein

Chain V3:



• Molecule 2: Microcompartments protein

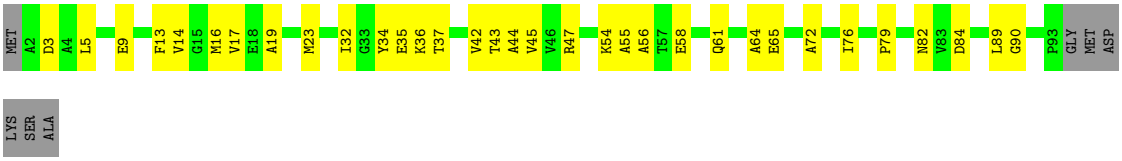
Chain V4:

• Molecule 2: Microcompartments protein

Chain V5:

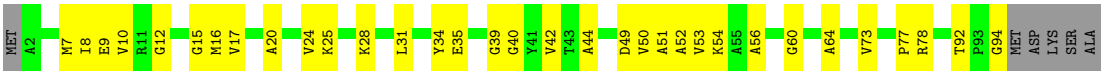
• Molecule 2: Microcompartments protein

Chain V6:



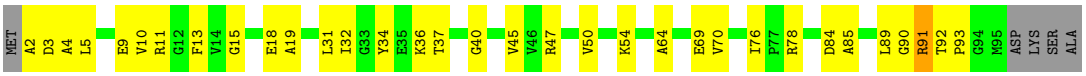
• Molecule 2: Microcompartments protein

Chain V7:



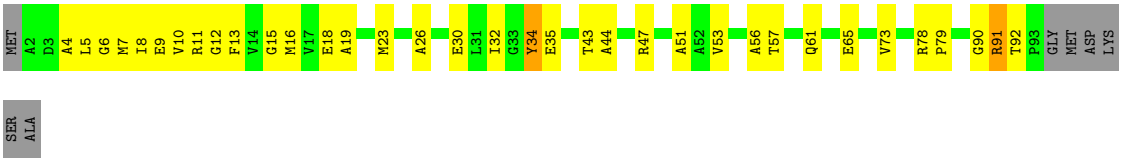
• Molecule 2: Microcompartments protein

Chain W2:



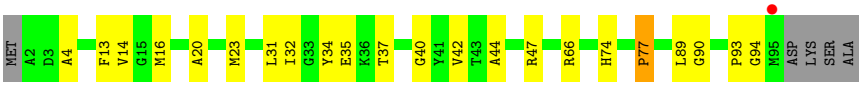
• Molecule 2: Microcompartments protein

Chain W3:



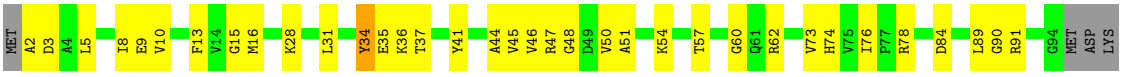
• Molecule 2: Microcompartments protein

Chain W4:



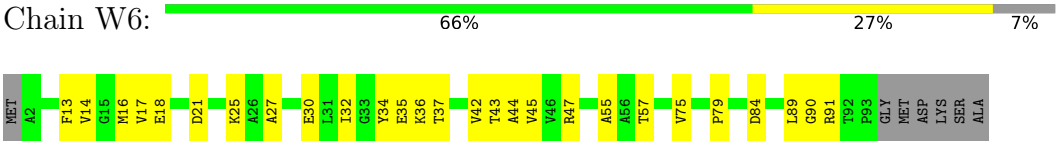
• Molecule 2: Microcompartments protein

Chain W5:



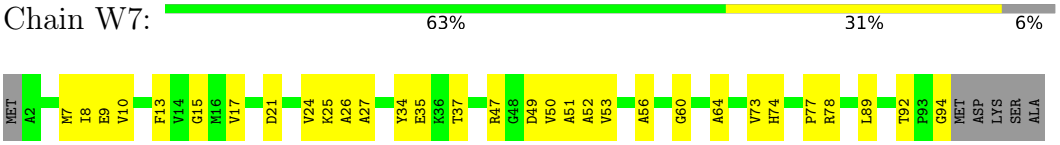
• Molecule 2: Microcompartments protein

Chain W6:



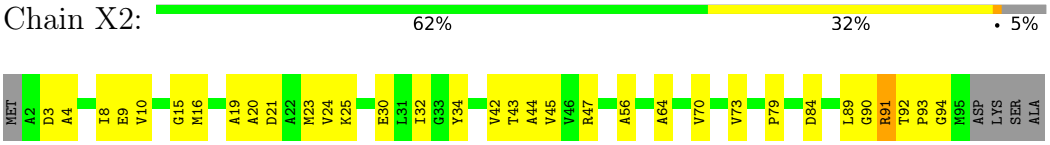
• Molecule 2: Microcompartments protein

Chain W7:



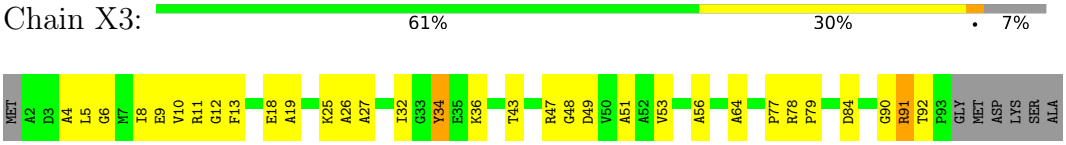
• Molecule 2: Microcompartments protein

Chain X2:



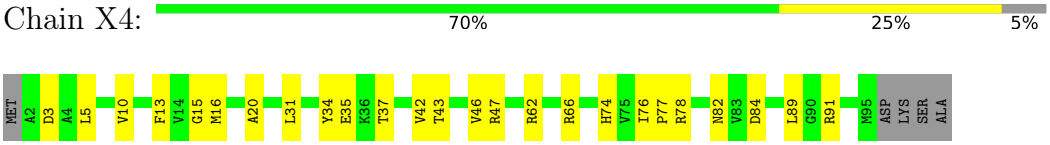
• Molecule 2: Microcompartments protein

Chain X3:



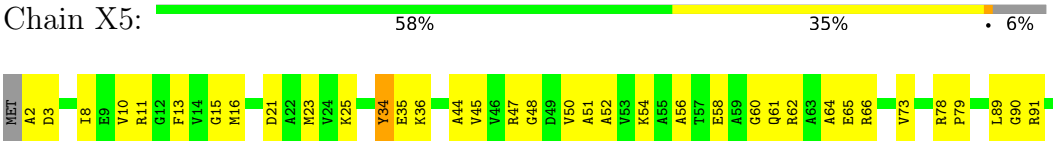
• Molecule 2: Microcompartments protein

Chain X4:



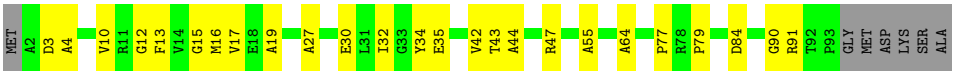
• Molecule 2: Microcompartments protein

Chain X5:



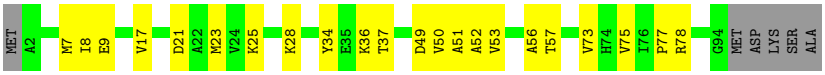
• Molecule 2: Microcompartments protein

Chain X6:



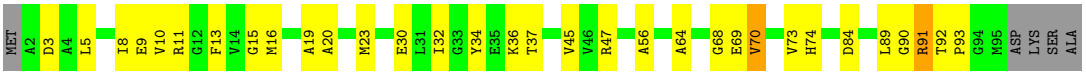
• Molecule 2: Microcompartments protein

Chain X7:



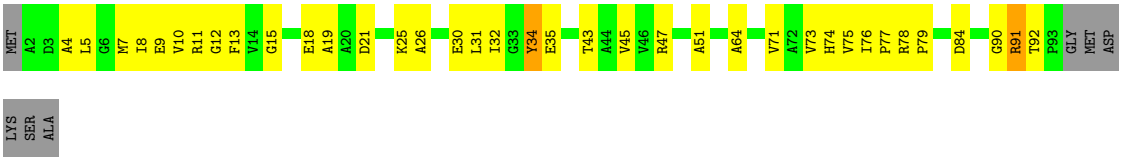
• Molecule 2: Microcompartments protein

Chain Y2:



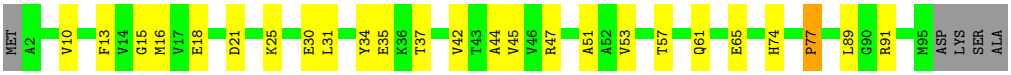
• Molecule 2: Microcompartments protein

Chain Y3:



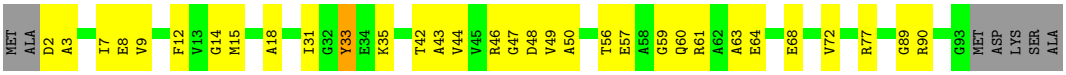
• Molecule 2: Microcompartments protein

Chain Y4:



• Molecule 2: Microcompartments protein

Chain Y5:

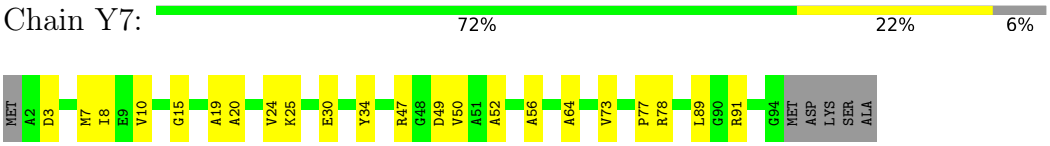


• Molecule 2: Microcompartments protein

Chain Y6:

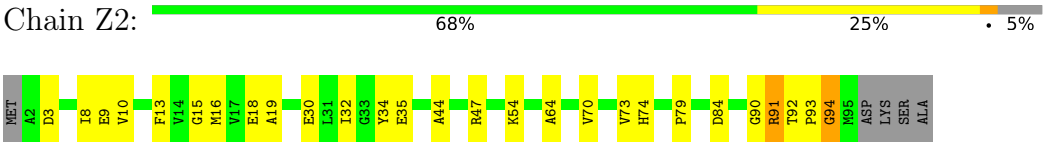
• Molecule 2: Microcompartments protein

Chain Y7:



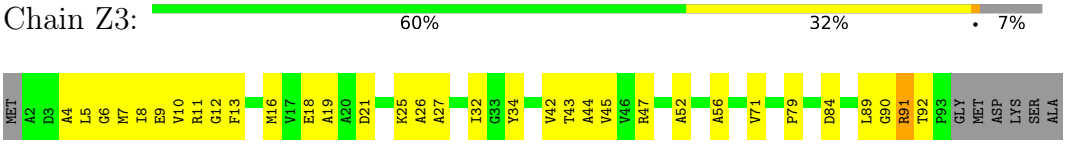
• Molecule 2: Microcompartments protein

Chain Z2:



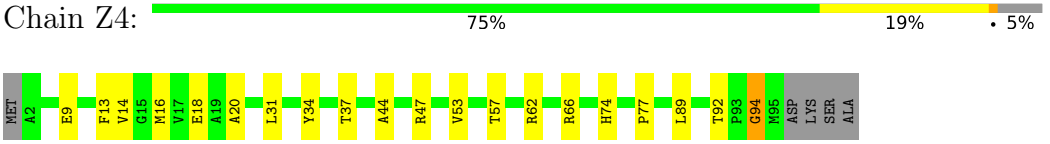
• Molecule 2: Microcompartments protein

Chain Z3:



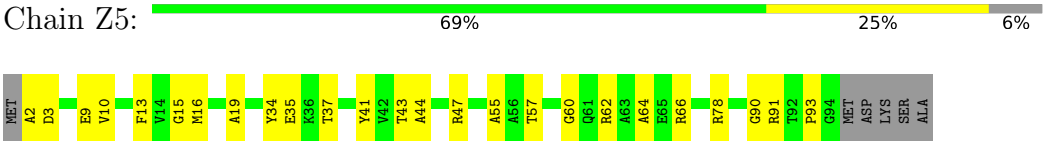
• Molecule 2: Microcompartments protein

Chain Z4:



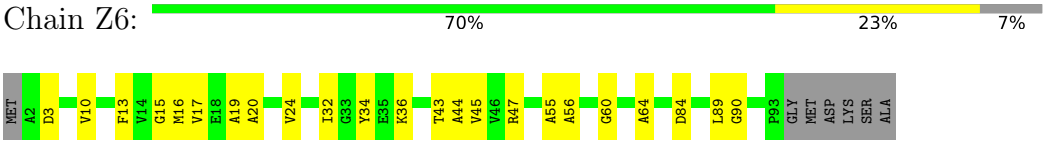
• Molecule 2: Microcompartments protein

Chain Z5:



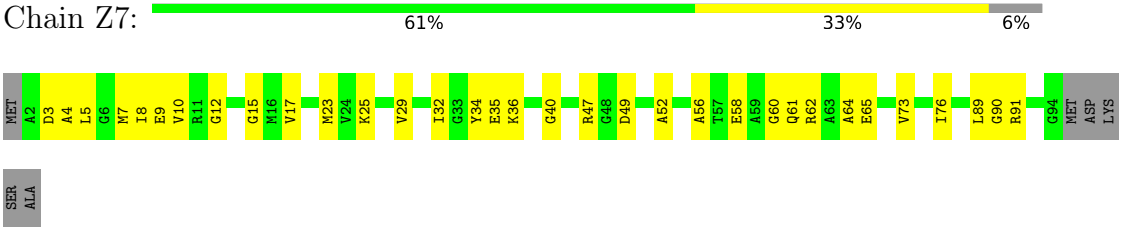
• Molecule 2: Microcompartments protein

Chain Z6:



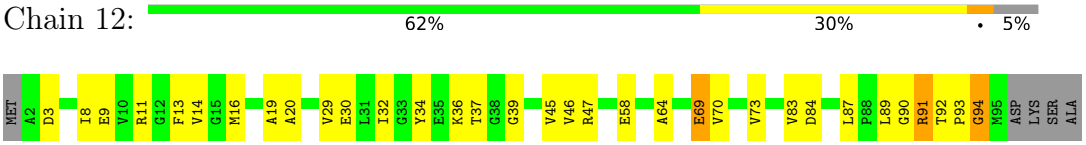
• Molecule 2: Microcompartments protein

Chain Z7:



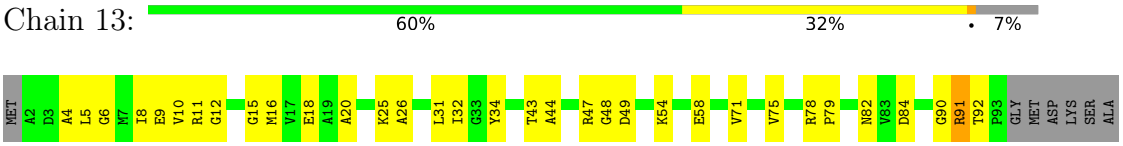
• Molecule 2: Microcompartments protein

Chain 12:



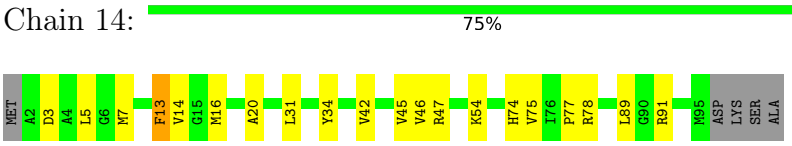
• Molecule 2: Microcompartments protein

Chain 13:



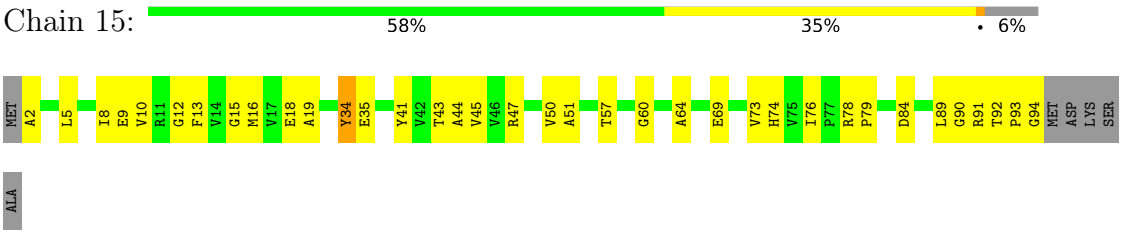
• Molecule 2: Microcompartments protein

Chain 14:



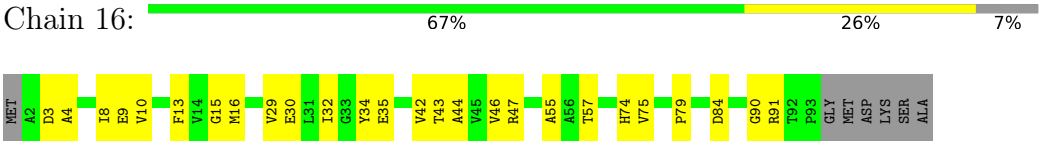
• Molecule 2: Microcompartments protein

Chain 15:



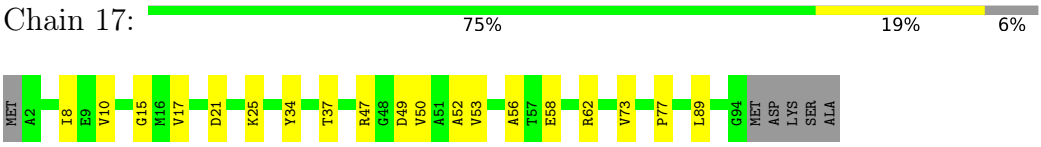
• Molecule 2: Microcompartments protein

Chain 16:



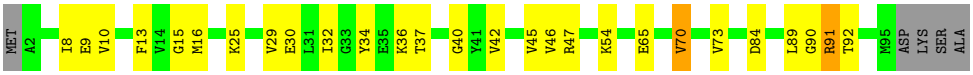
• Molecule 2: Microcompartments protein

Chain 17:



• Molecule 2: Microcompartments protein

Chain 22:



• Molecule 2: Microcompartments protein

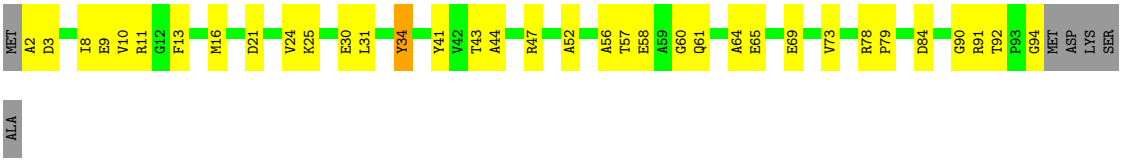
Chain 23:

• Molecule 2: Microcompartments protein

Chain 24:

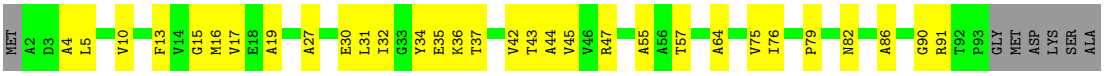
• Molecule 2: Microcompartments protein

Chain 25:



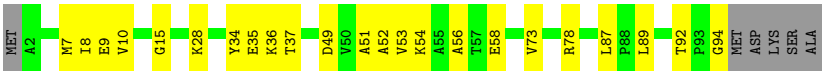
• Molecule 2: Microcompartments protein

Chain 26:



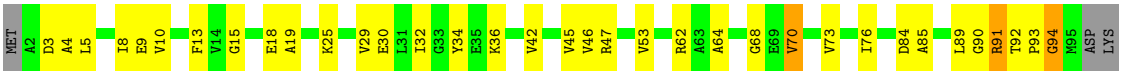
• Molecule 2: Microcompartments protein

Chain 27:



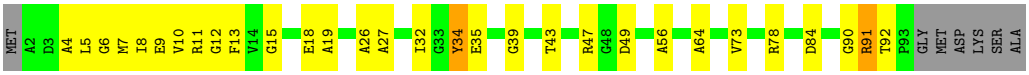
• Molecule 2: Microcompartments protein

Chain 32:



• Molecule 2: Microcompartments protein

Chain 33:



• Molecule 2: Microcompartments protein

Chain 34:

• Molecule 2: Microcompartments protein

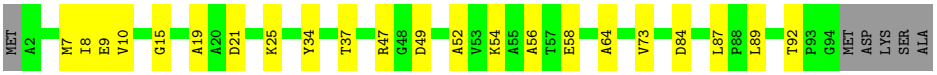
Chain 35:

• Molecule 2: Microcompartments protein

Chain 36:

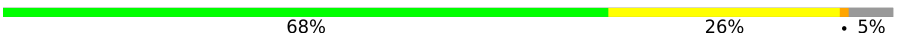
• Molecule 2: Microcompartments protein

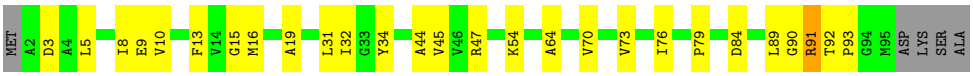
Chain 37:



• Molecule 2: Microcompartments protein

Chain 42:



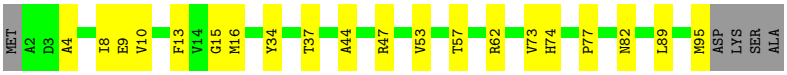


• Molecule 2: Microcompartments protein

Chain 43:

• Molecule 2: Microcompartments protein

Chain 44:

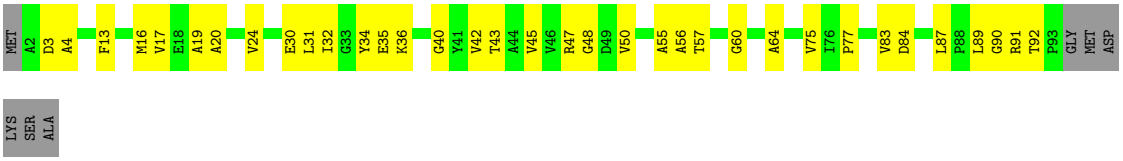


• Molecule 2: Microcompartments protein

Chain 45:

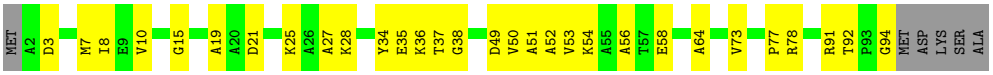
• Molecule 2: Microcompartments protein

Chain 46:



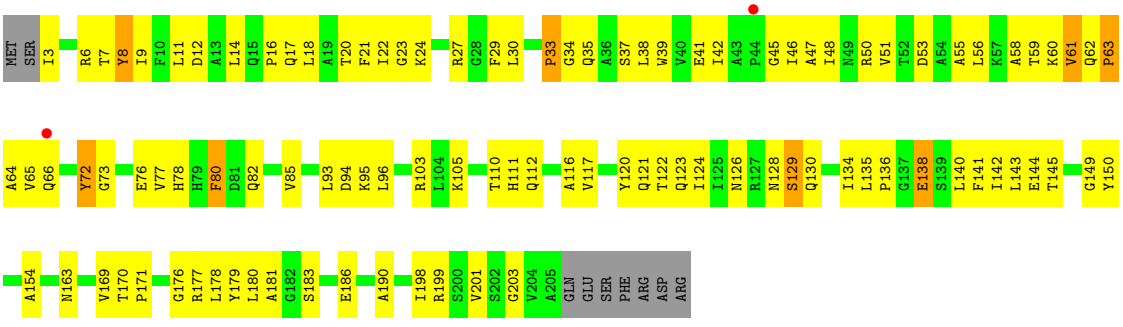
• Molecule 2: Microcompartments protein

Chain 47:



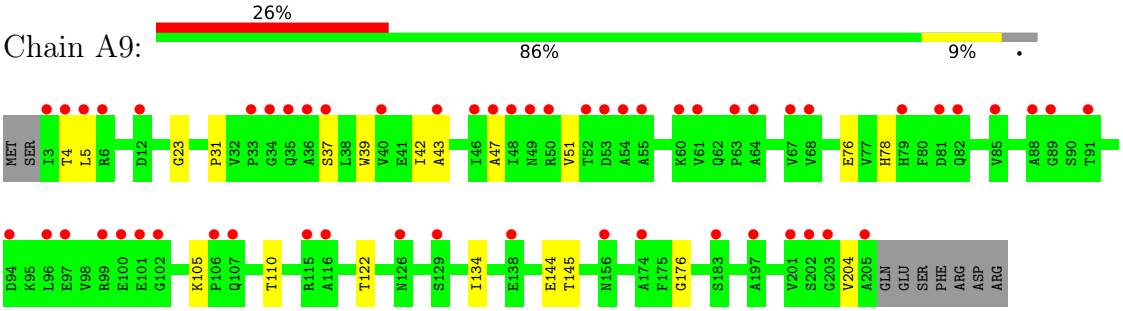
• Molecule 3: Microcompartments protein

Chain A8:



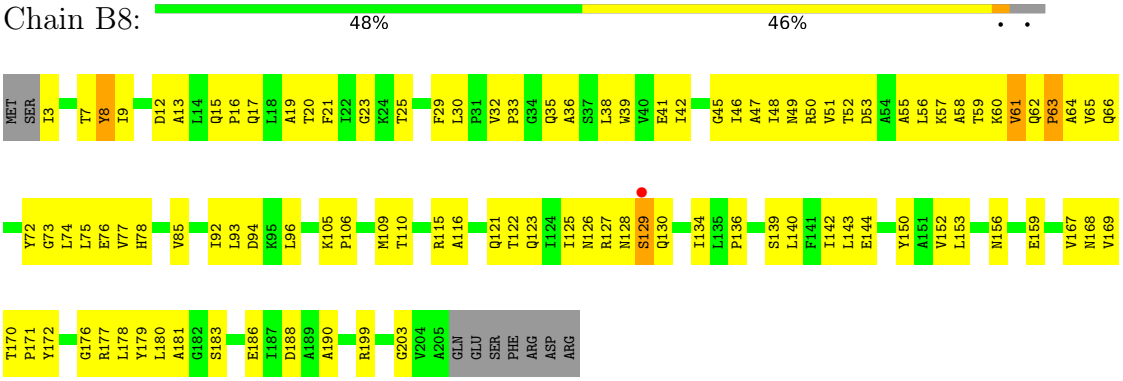
• Molecule 3: Microcompartments protein

Chain A9:



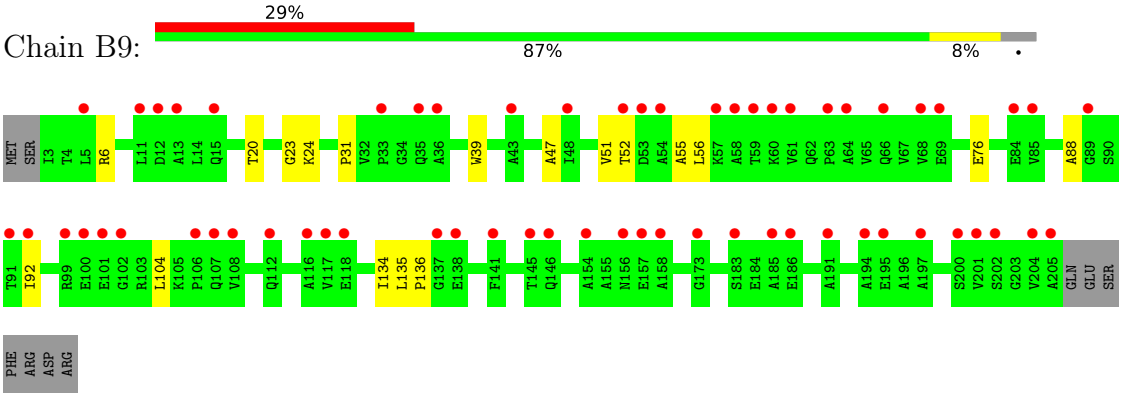
• Molecule 3: Microcompartments protein

Chain B8:



• Molecule 3: Microcompartments protein

Chain B9:

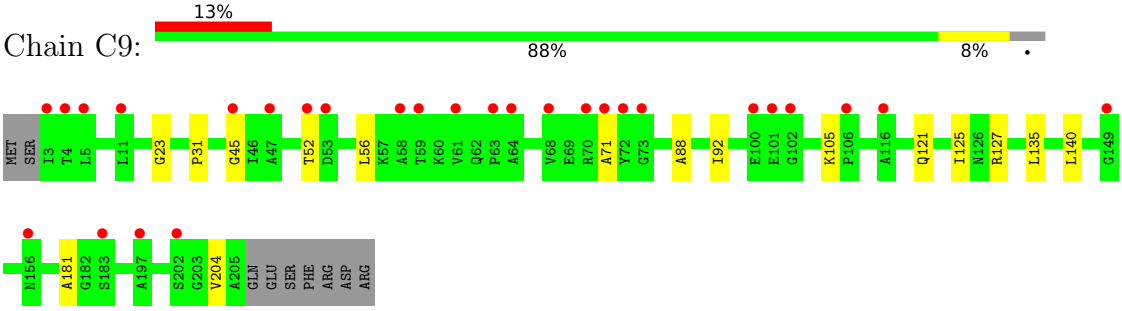


• Molecule 3: Microcompartments protein

Chain C8:

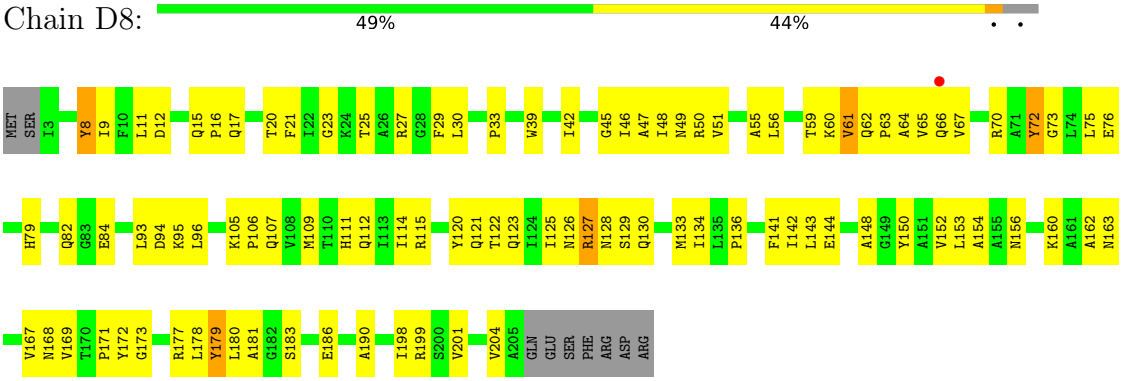
• Molecule 3: Microcompartments protein

Chain C9:



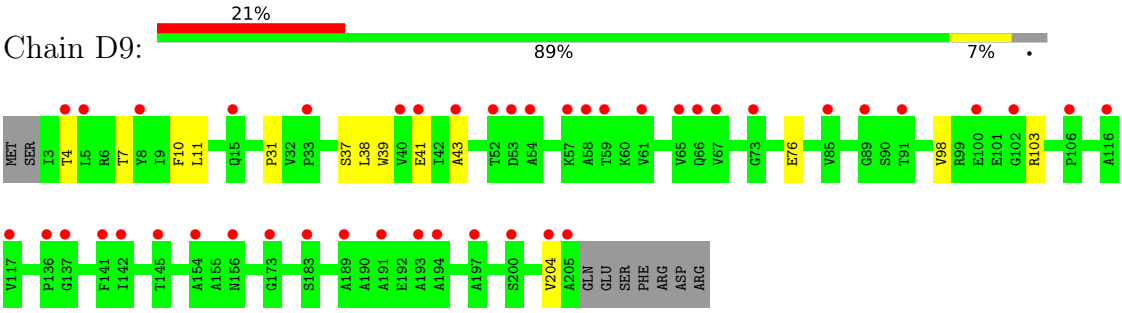
• Molecule 3: Microcompartments protein

Chain D8:



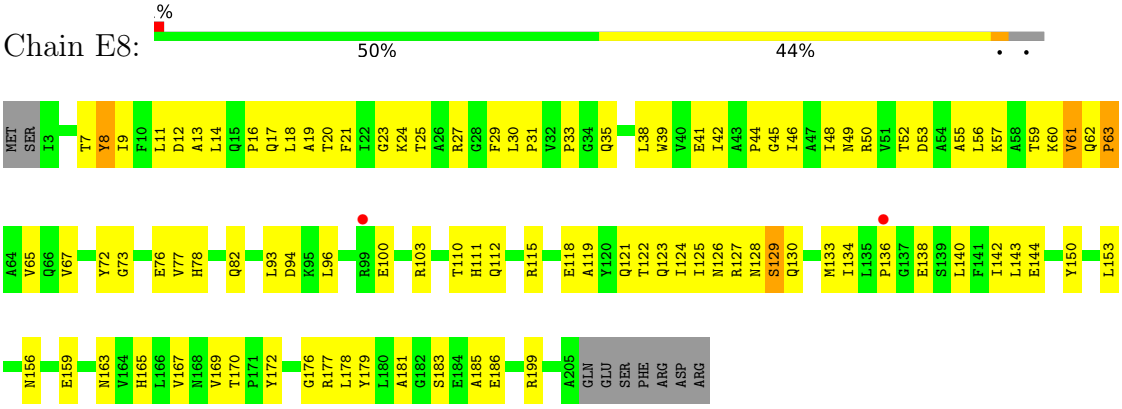
• Molecule 3: Microcompartments protein

Chain D9:



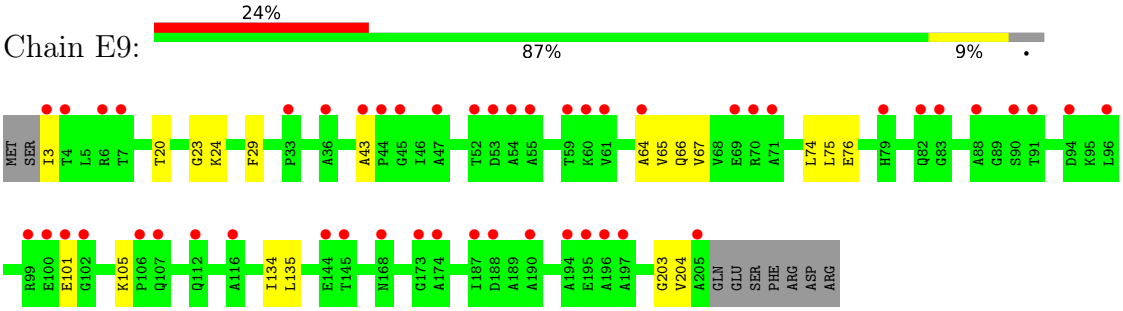
• Molecule 3: Microcompartments protein

Chain E8:



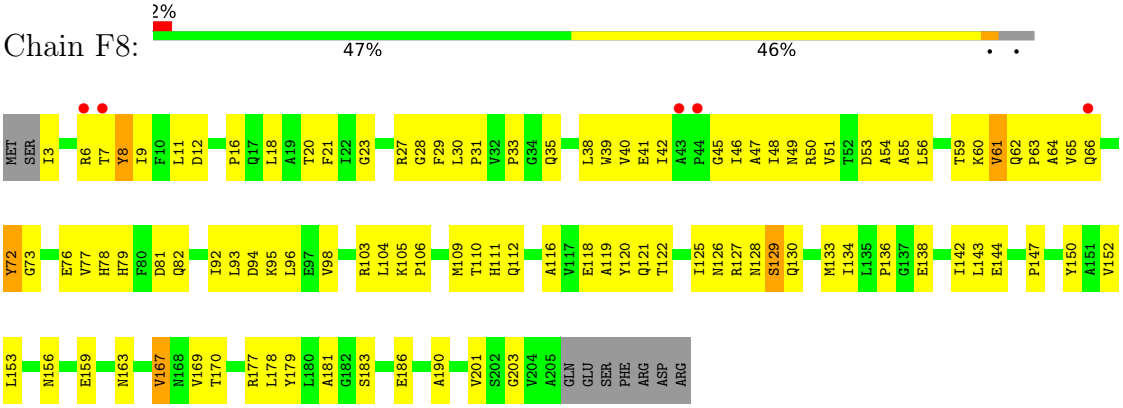
• Molecule 3: Microcompartments protein

Chain E9:



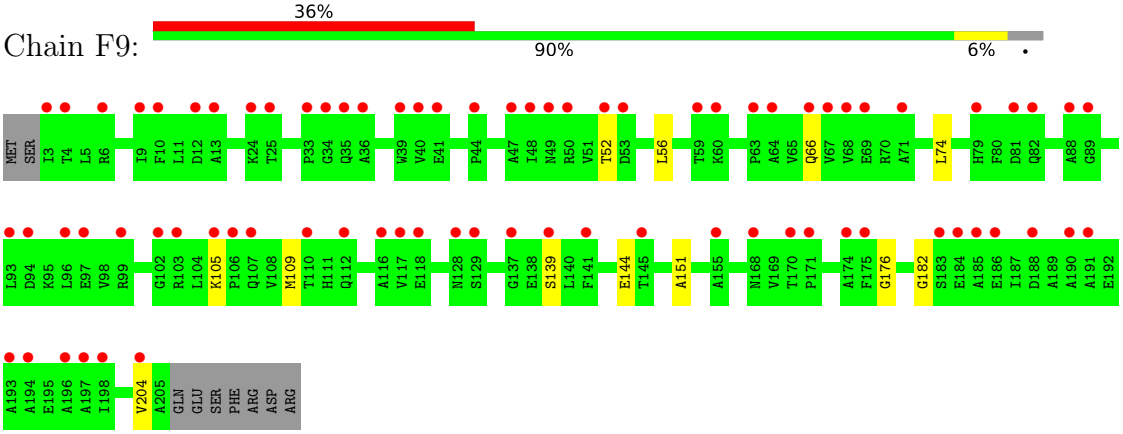
• Molecule 3: Microcompartments protein

Chain F8:



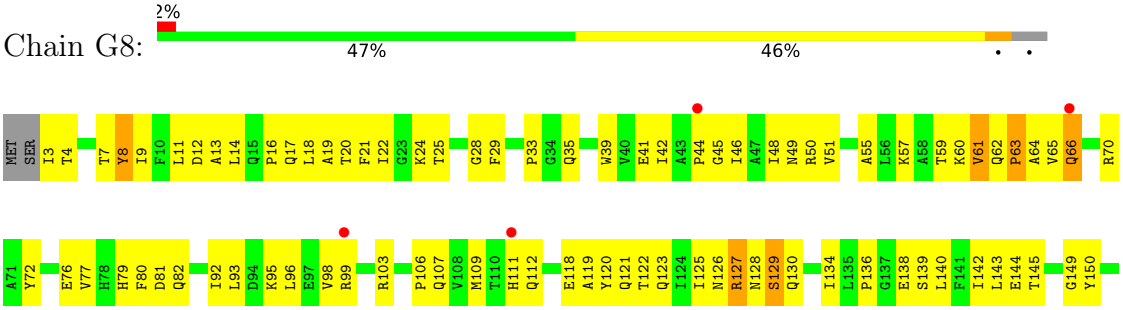
• Molecule 3: Microcompartments protein

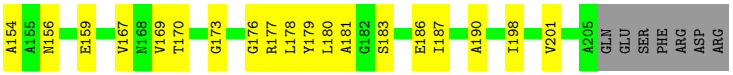
Chain F9:



• Molecule 3: Microcompartments protein

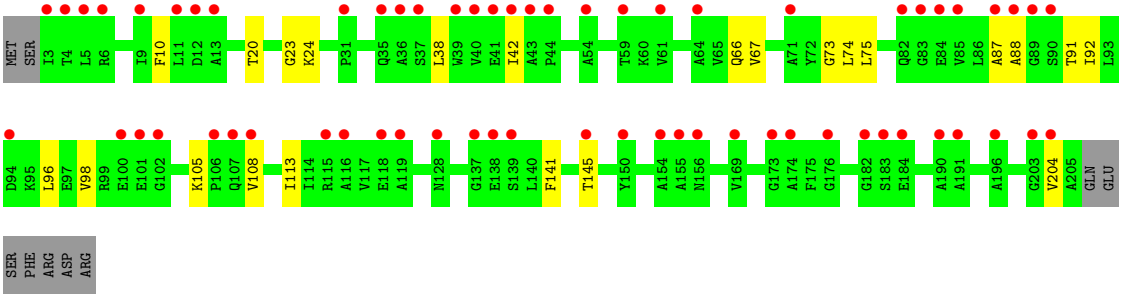
Chain G8:





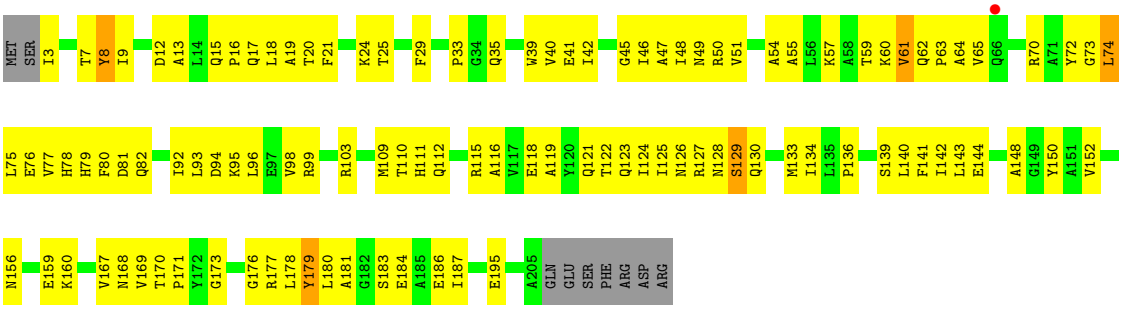
• Molecule 3: Microcompartments protein

Chain G9:



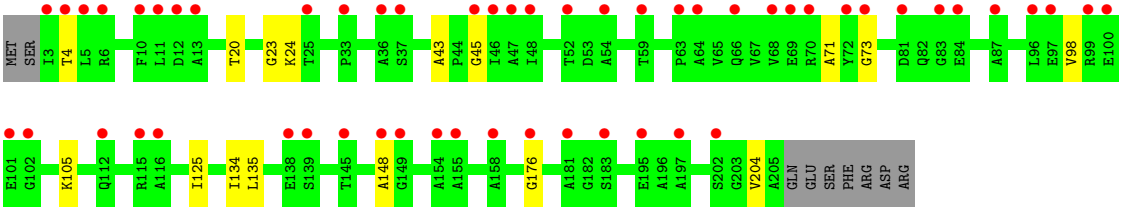
• Molecule 3: Microcompartments protein

Chain H8:



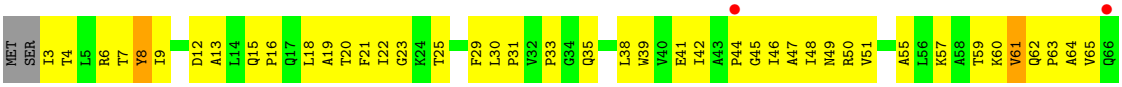
• Molecule 3: Microcompartments protein

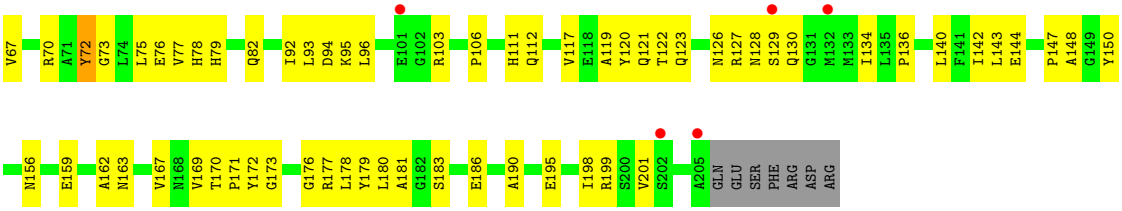
Chain H9:



• Molecule 3: Microcompartments protein

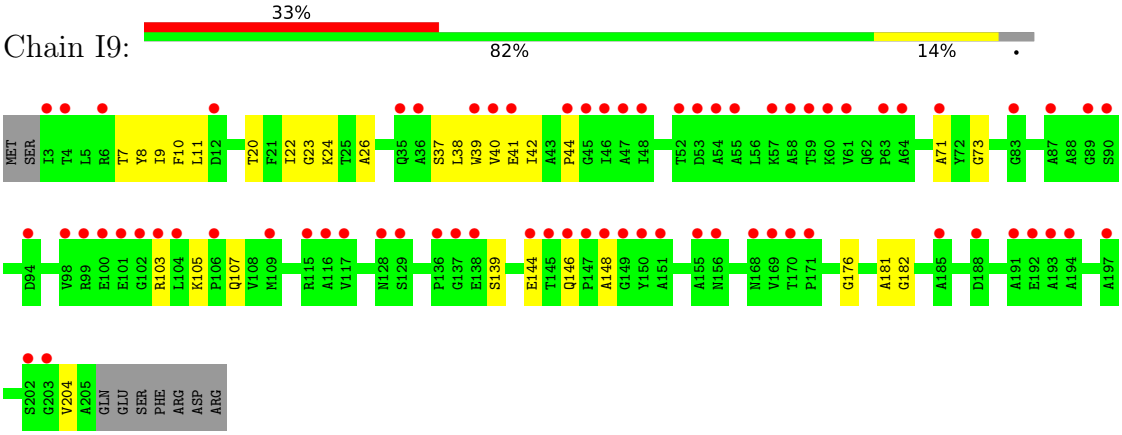
Chain I8:





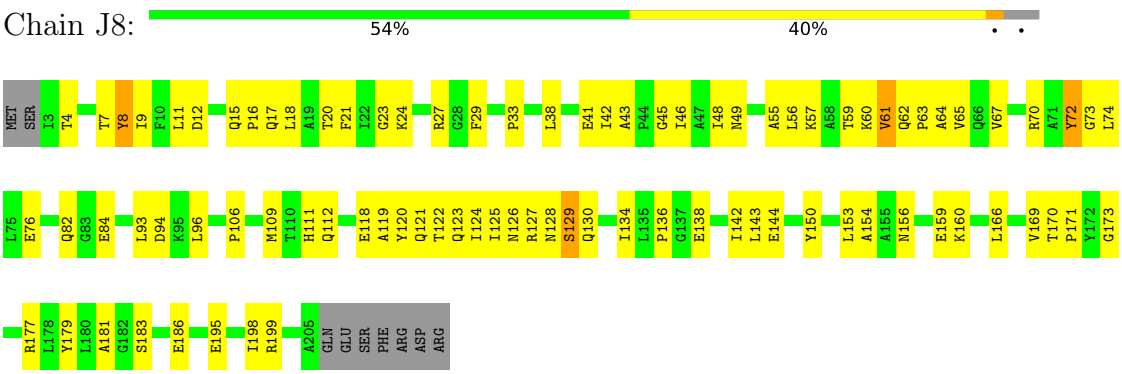
• Molecule 3: Microcompartments protein

Chain I9:



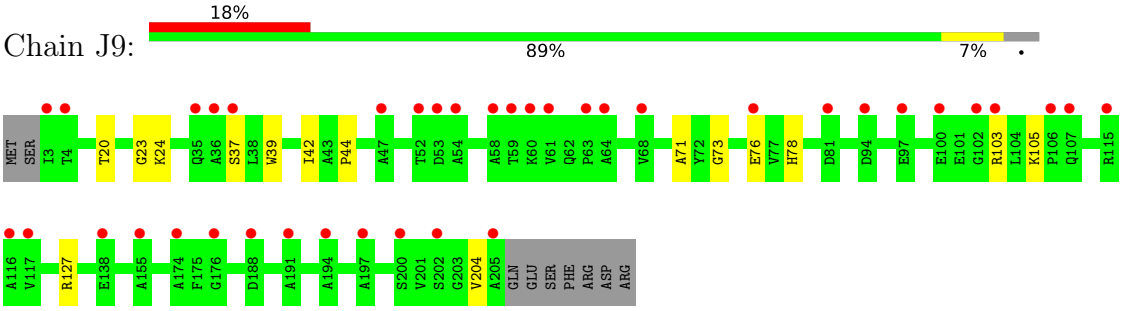
• Molecule 3: Microcompartments protein

Chain J8:



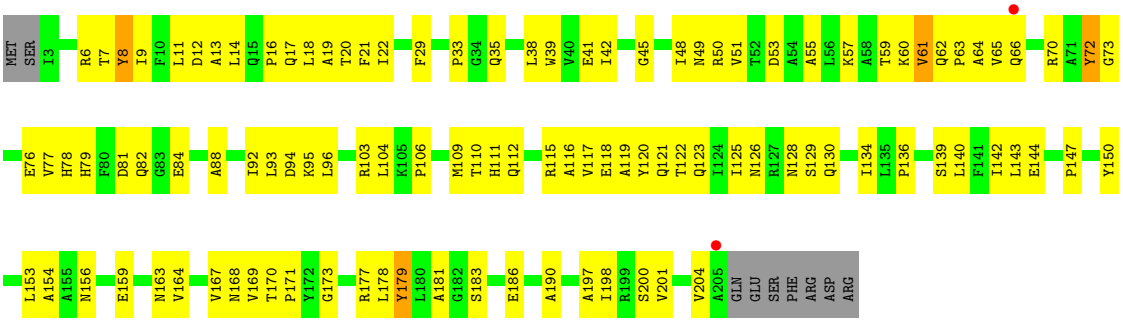
• Molecule 3: Microcompartments protein

Chain J9:



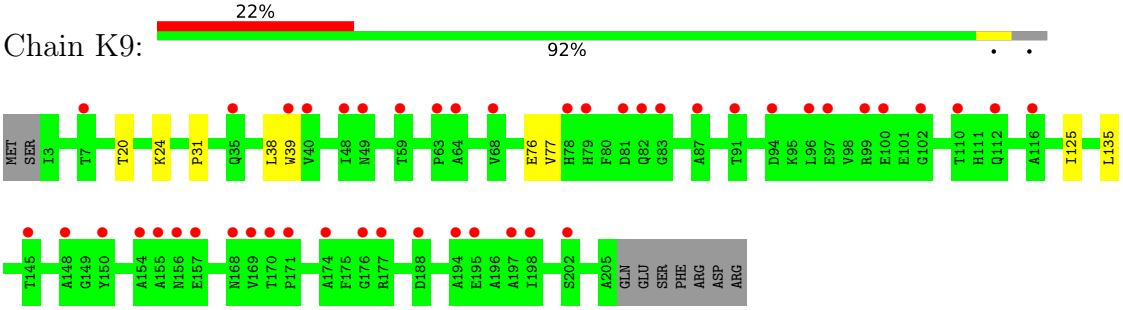
• Molecule 3: Microcompartments protein

Chain K8:



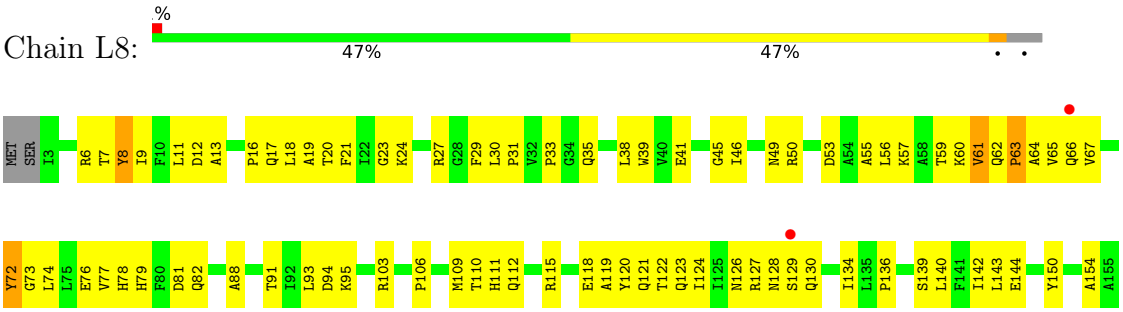
• Molecule 3: Microcompartments protein

Chain K9:



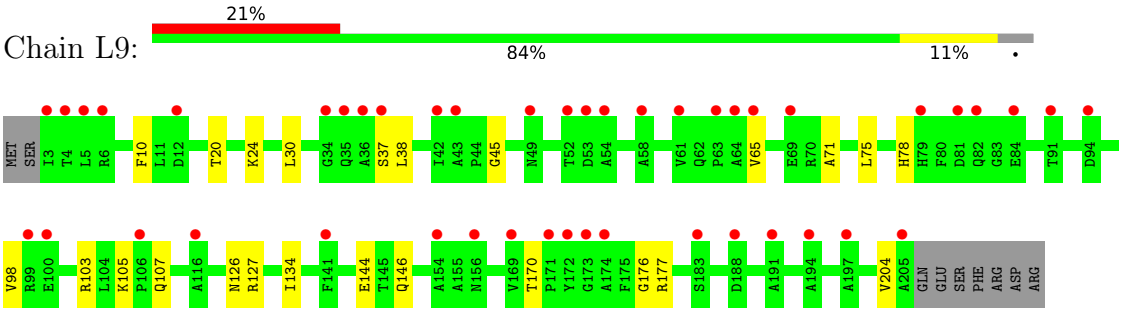
• Molecule 3: Microcompartments protein

Chain L8:



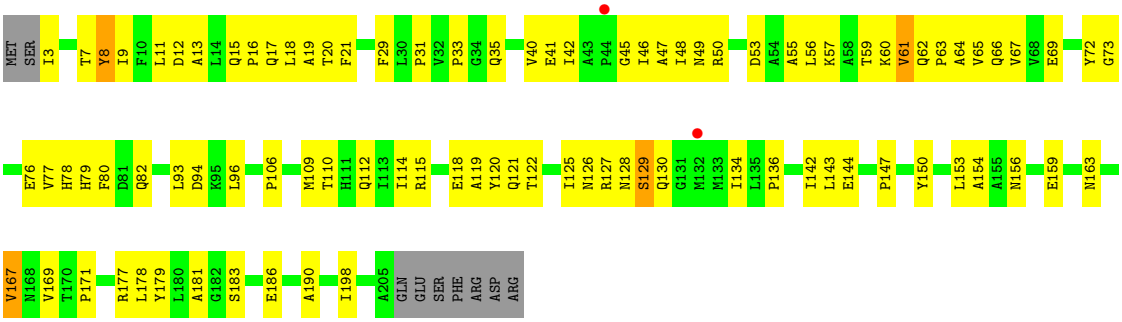
• Molecule 3: Microcompartments protein

Chain L9:



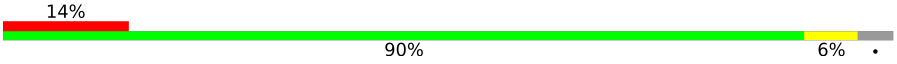
• Molecule 3: Microcompartments protein

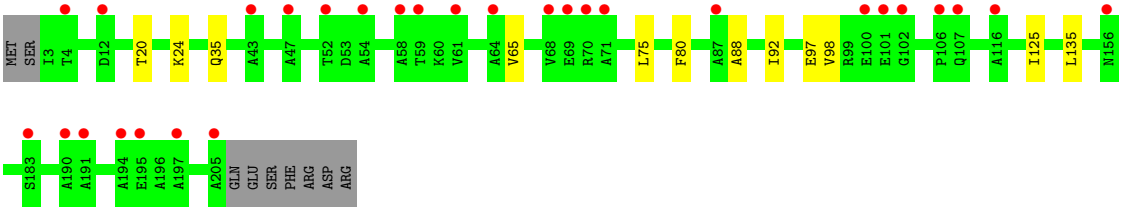
Chain M8:



• Molecule 3: Microcompartments protein

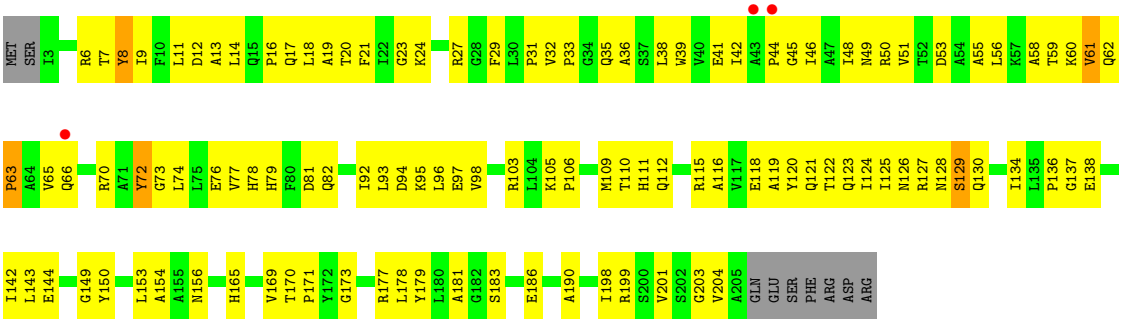
Chain M9:





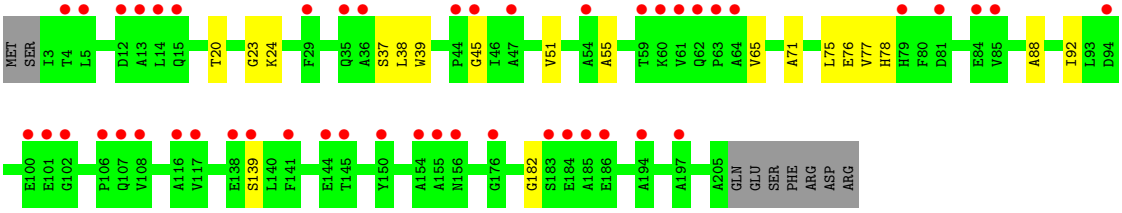
• Molecule 3: Microcompartments protein

Chain N8:



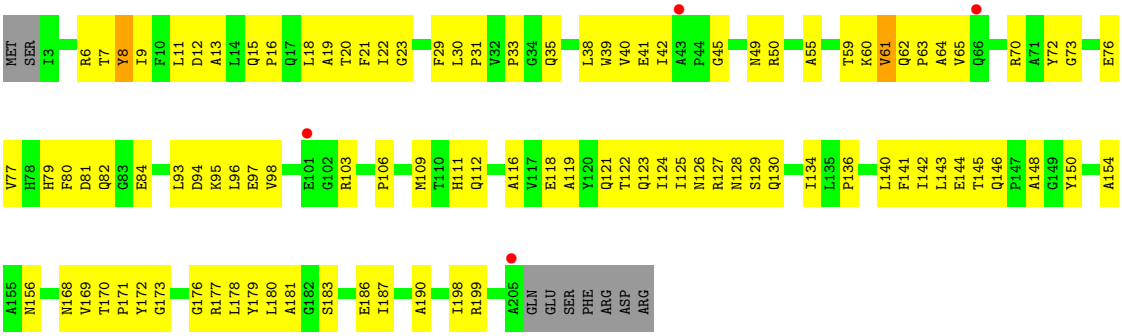
• Molecule 3: Microcompartments protein

Chain N9:



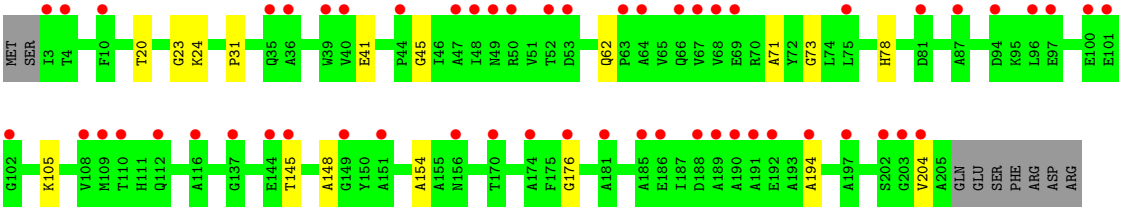
• Molecule 3: Microcompartments protein

Chain O8:



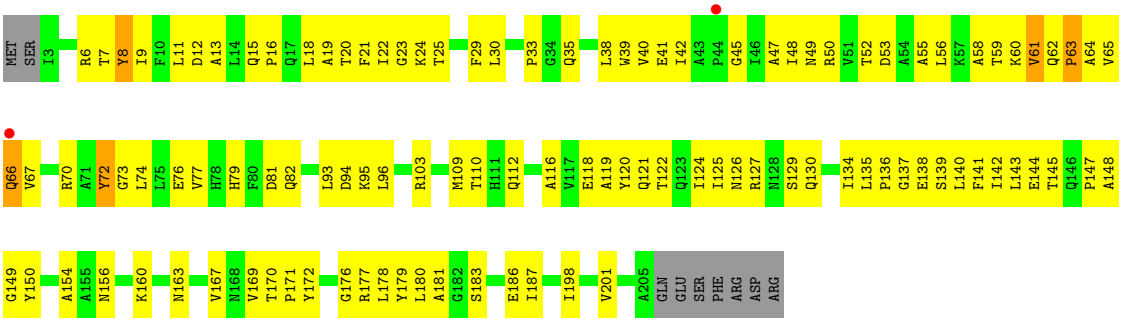
• Molecule 3: Microcompartments protein

Chain O9:



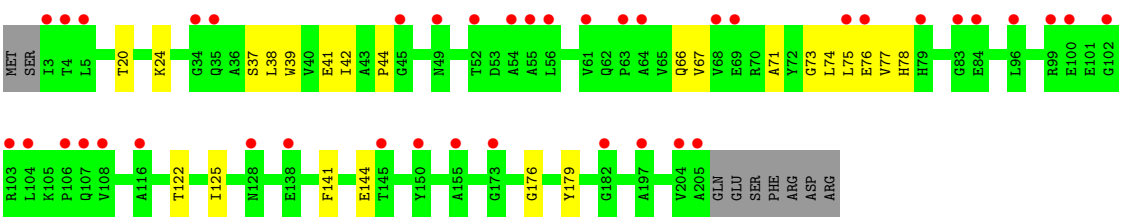
• Molecule 3: Microcompartments protein

Chain P8:



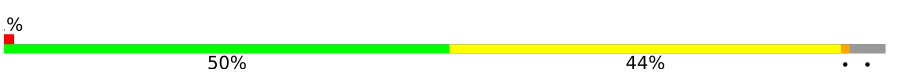
• Molecule 3: Microcompartments protein

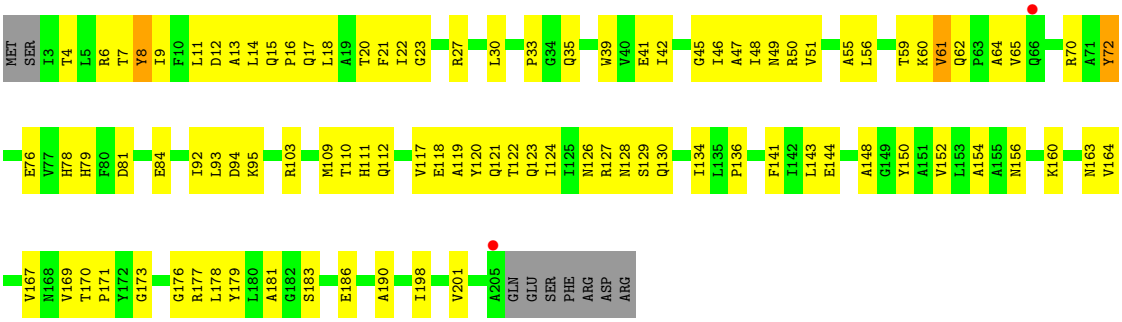
Chain P9:



• Molecule 3: Microcompartments protein

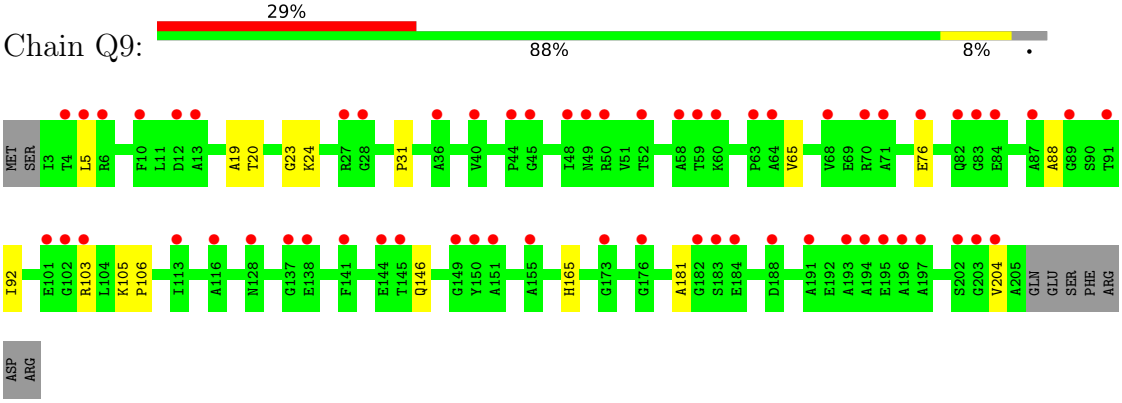
Chain Q8:





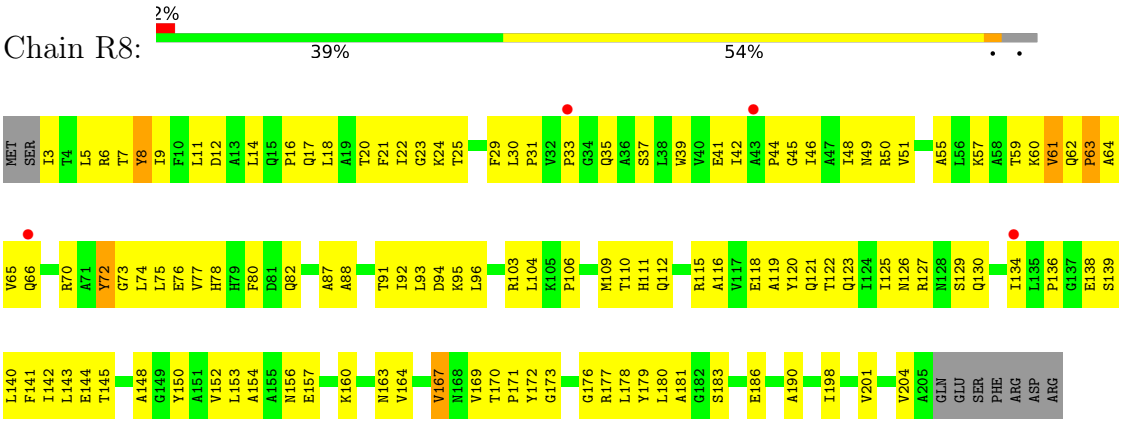
• Molecule 3: Microcompartments protein

Chain Q9:



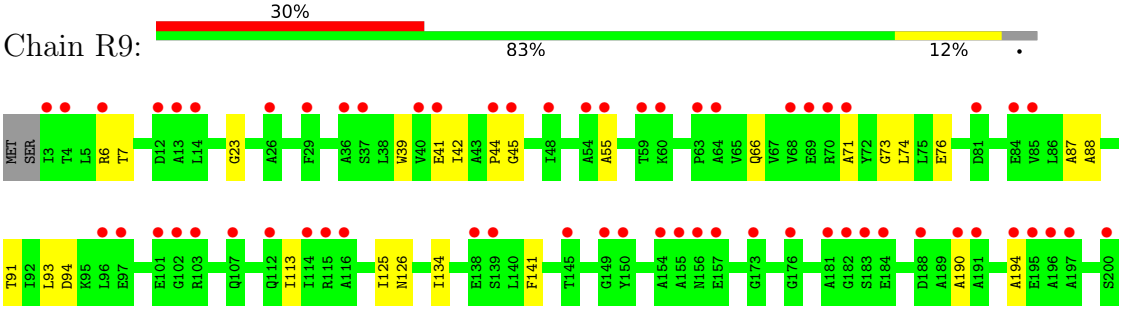
• Molecule 3: Microcompartments protein

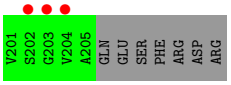
Chain R8:



• Molecule 3: Microcompartments protein

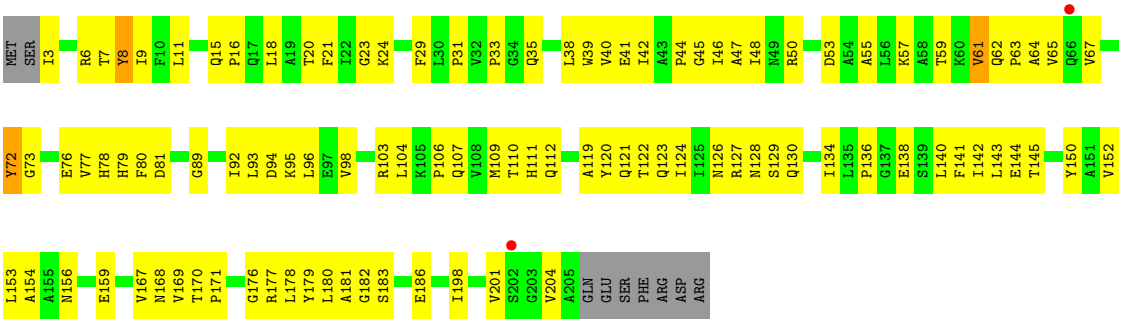
Chain R9:





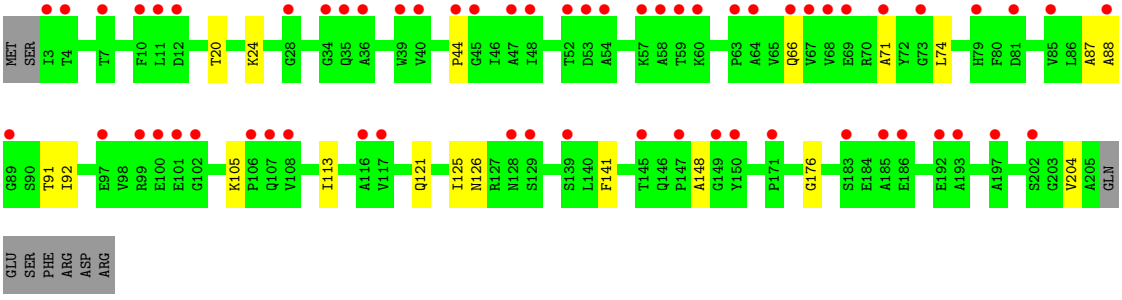
• Molecule 3: Microcompartments protein

Chain S8:



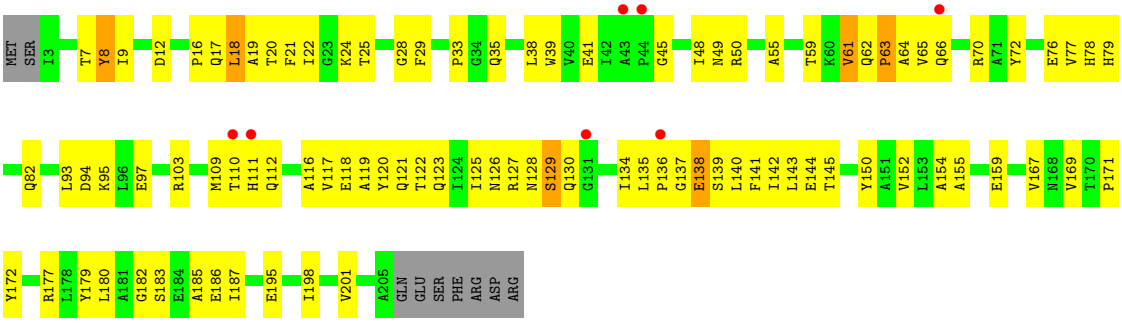
• Molecule 3: Microcompartments protein

Chain S9:



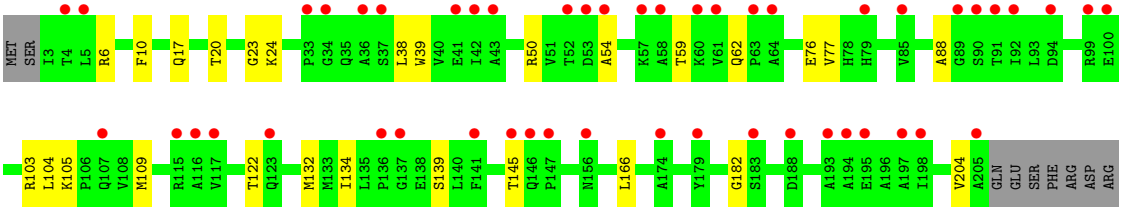
• Molecule 3: Microcompartments protein

Chain T8:



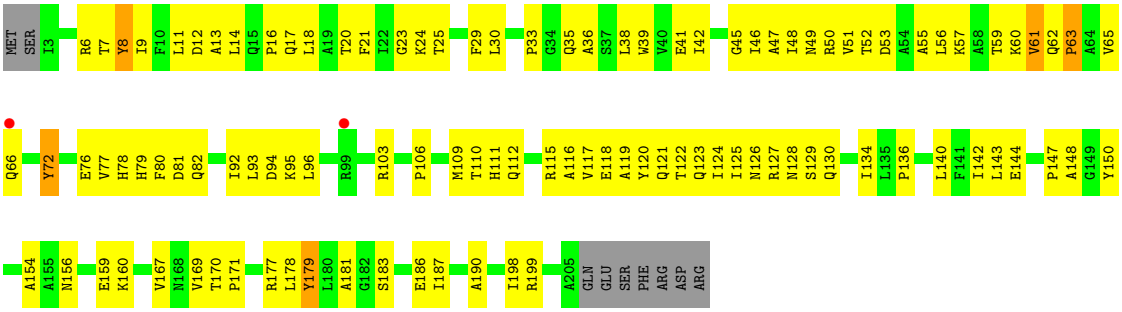
• Molecule 3: Microcompartments protein

Chain T9:



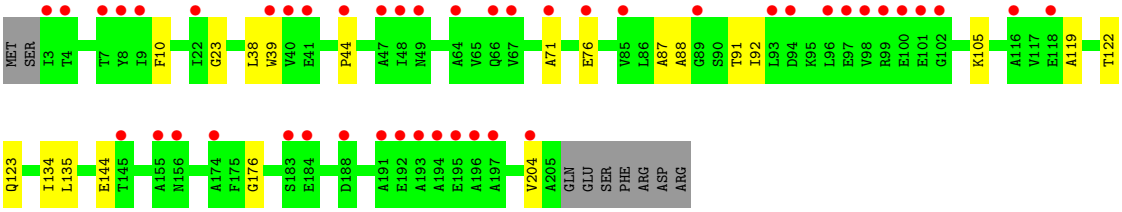
• Molecule 3: Microcompartments protein

Chain U8:



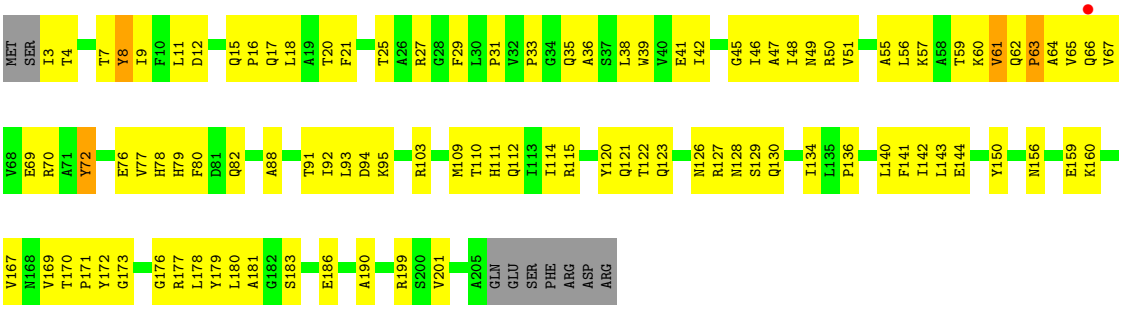
• Molecule 3: Microcompartments protein

Chain U9:



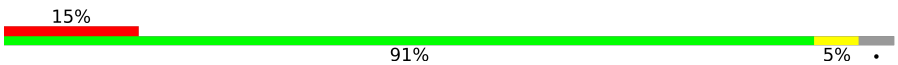
• Molecule 3: Microcompartments protein

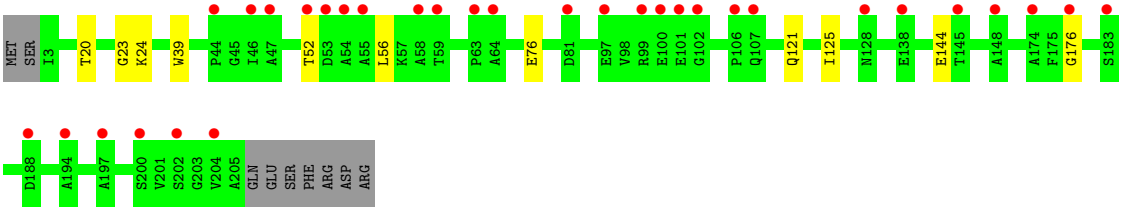
Chain V8:



• Molecule 3: Microcompartments protein

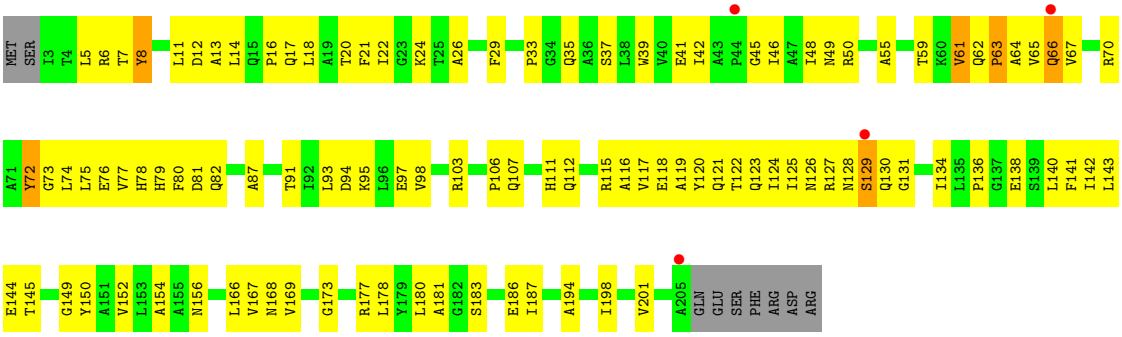
Chain V9:





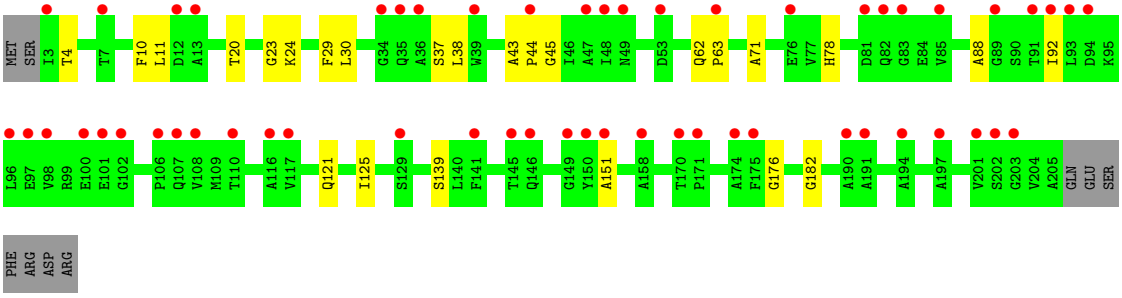
• Molecule 3: Microcompartments protein

Chain W8:



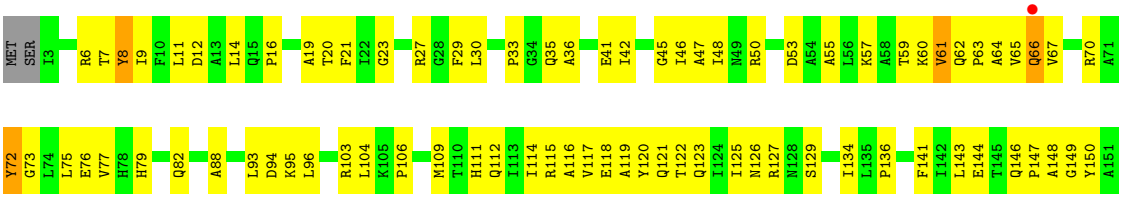
• Molecule 3: Microcompartments protein

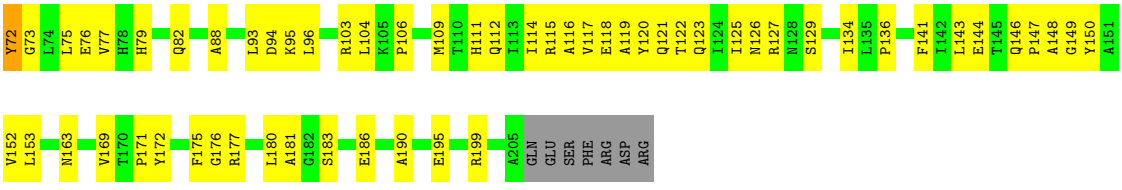
Chain W9:



• Molecule 3: Microcompartments protein

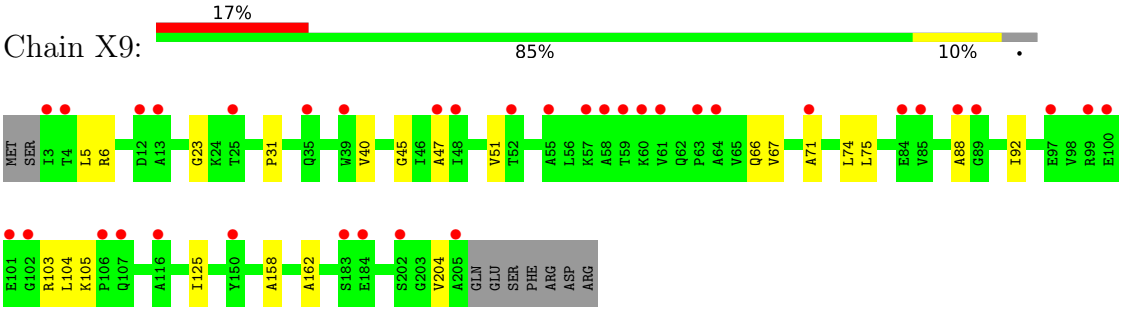
Chain X8:





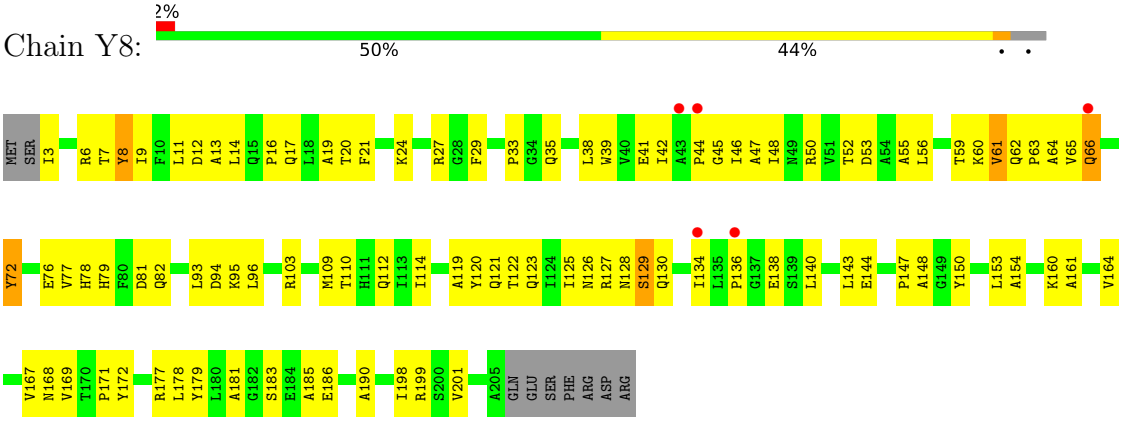
• Molecule 3: Microcompartments protein

Chain X9:



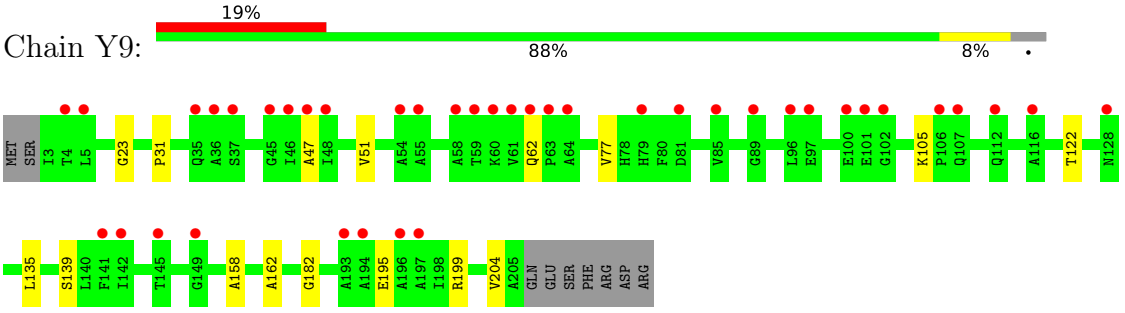
• Molecule 3: Microcompartments protein

Chain Y8:



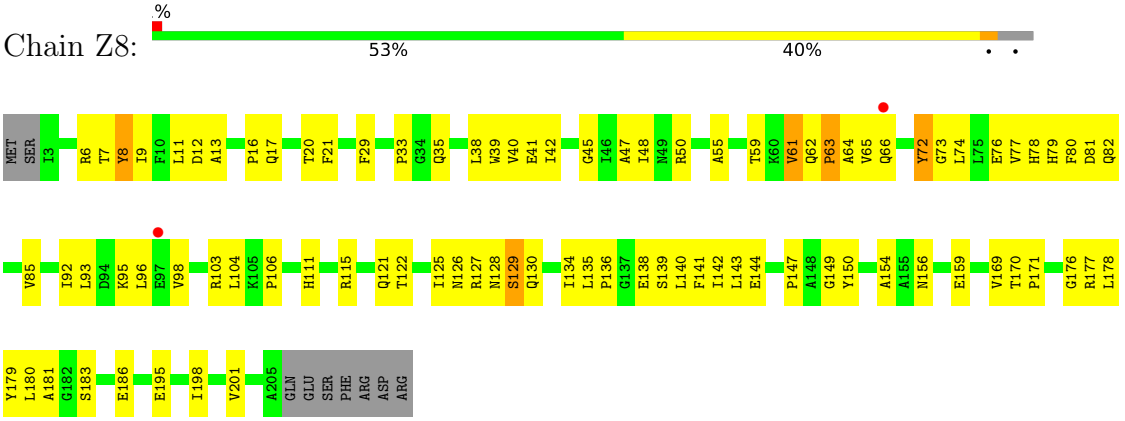
• Molecule 3: Microcompartments protein

Chain Y9:



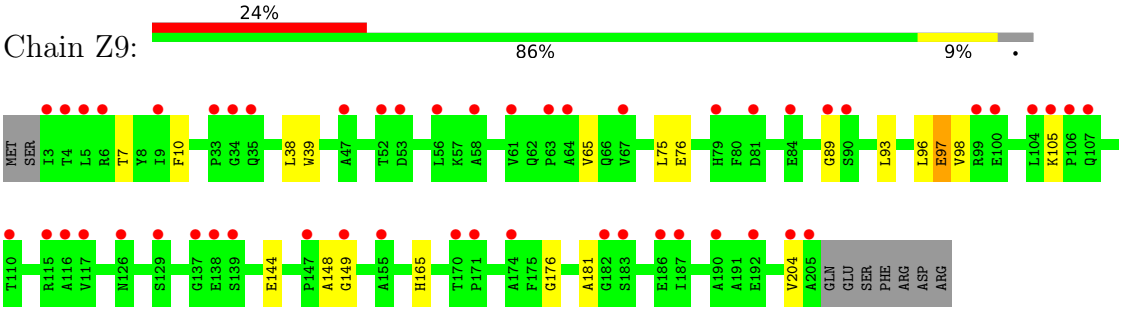
• Molecule 3: Microcompartments protein

Chain Z8:



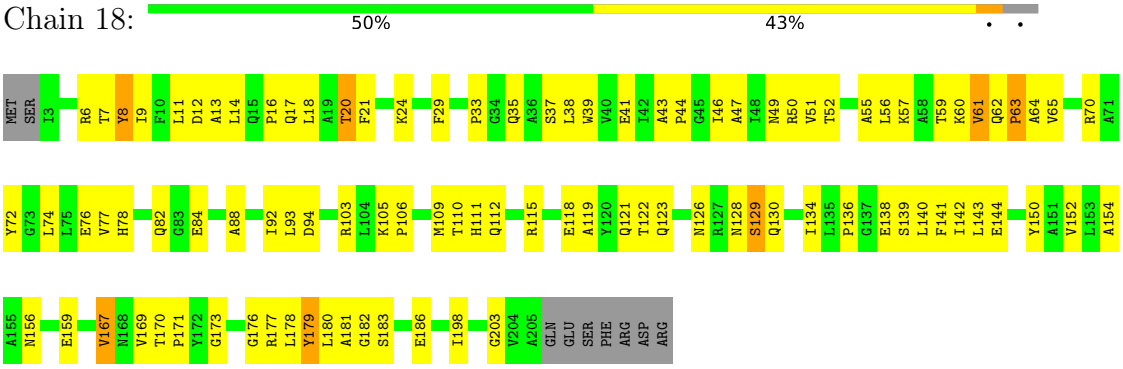
• Molecule 3: Microcompartments protein

Chain Z9:



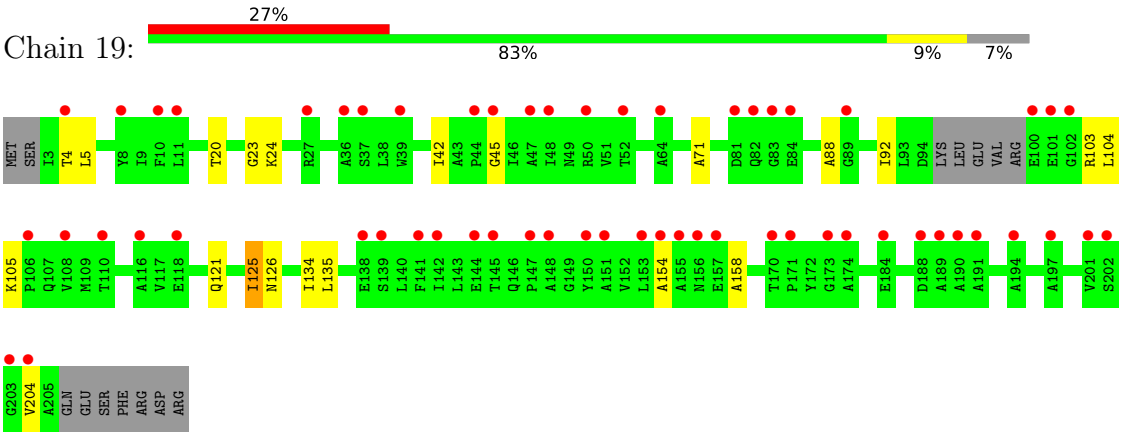
• Molecule 3: Microcompartments protein

Chain 18:



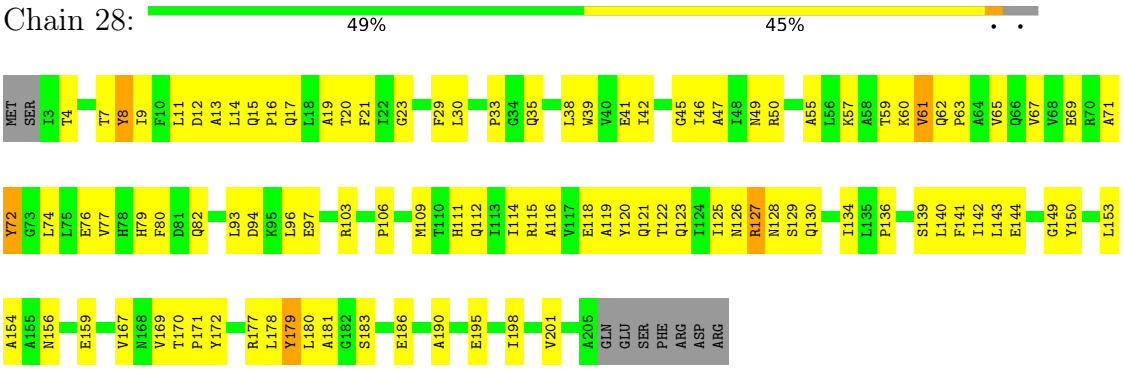
• Molecule 3: Microcompartments protein

Chain 19:



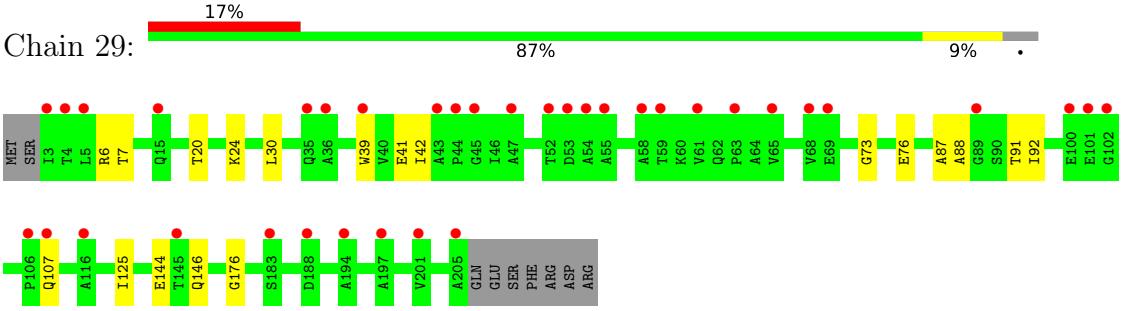
• Molecule 3: Microcompartments protein

Chain 28:



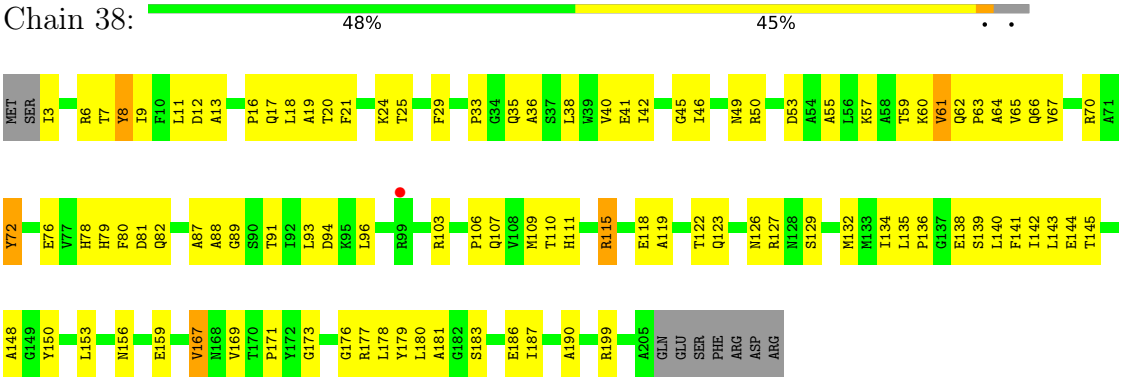
• Molecule 3: Microcompartments protein

Chain 29:



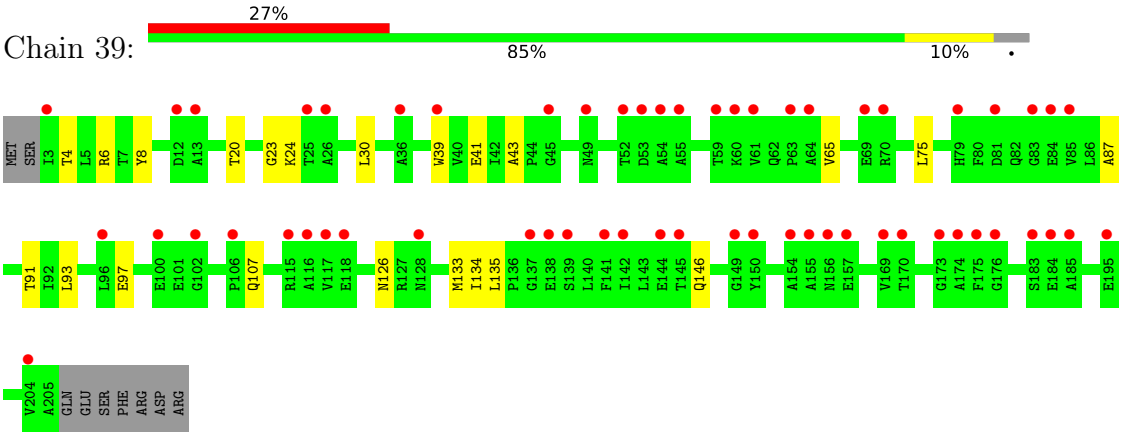
• Molecule 3: Microcompartments protein

Chain 38:



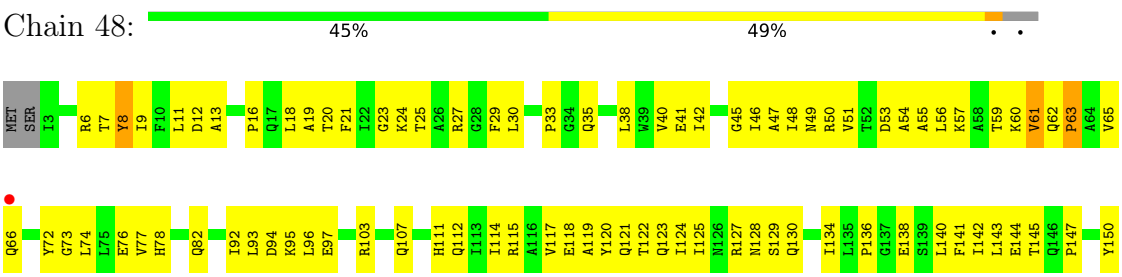
• Molecule 3: Microcompartments protein

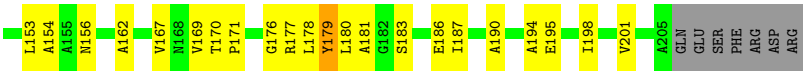
Chain 39:



• Molecule 3: Microcompartments protein

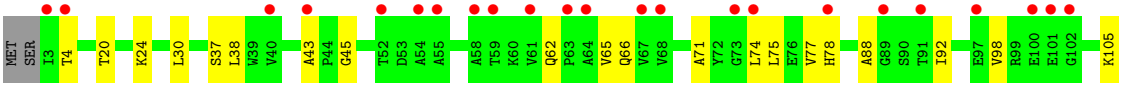
Chain 48:

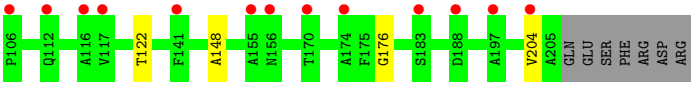




• Molecule 3: Microcompartments protein

Chain 49:





4 Data and refinement statistics (i)

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) 69.1 (39.85-3.51)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (2.28%)	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)	0.27 , 80.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.34	0/683	0.62	0/926
1	21	0.36	0/683	0.64	0/926
1	31	0.36	0/674	0.63	0/915
1	41	0.34	0/683	0.62	0/926
1	A1	0.31	0/683	0.60	0/926
1	B1	0.34	0/683	0.61	0/926
1	C1	0.31	0/683	0.59	0/926
1	D1	0.35	0/683	0.62	0/926
1	E1	0.32	0/683	0.60	0/926
1	F1	0.33	0/683	0.60	0/926
1	G1	0.33	0/683	0.60	0/926
1	H1	0.33	0/683	0.63	0/926
1	I1	0.35	0/683	0.61	0/926
1	J1	0.32	0/683	0.60	0/926
1	K1	0.34	0/683	0.61	0/926
1	L1	0.35	0/683	0.61	0/926
1	M1	0.35	0/683	0.64	0/926
1	N1	0.35	0/683	0.61	0/926
1	O1	0.32	0/683	0.63	0/926
1	P1	0.33	0/683	0.61	0/926
1	Q1	0.33	0/683	0.61	0/926
1	R1	0.32	0/683	0.63	0/926
1	S1	0.31	0/683	0.63	0/926
1	T1	0.34	0/683	0.64	0/926
1	U1	0.34	0/683	0.61	0/926
1	V1	0.31	0/683	0.61	0/926
1	W1	0.32	0/683	0.63	0/926
1	X1	0.33	0/683	0.63	0/926
1	Y1	0.34	0/683	0.60	0/926
1	Z1	0.34	0/683	0.61	0/926
2	12	0.31	0/678	0.51	0/919
2	13	0.29	0/666	0.55	0/904
2	14	0.29	0/678	0.55	0/919
2	15	0.30	0/670	0.53	0/909

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	16	0.29	0/666	0.54	0/904
2	17	0.29	0/670	0.54	0/909
2	22	0.30	0/678	0.55	0/919
2	23	0.31	0/666	0.57	0/904
2	24	0.29	0/678	0.54	0/919
2	25	0.32	0/670	0.59	0/909
2	26	0.29	0/666	0.53	0/904
2	27	0.29	0/670	0.53	0/909
2	32	0.29	0/678	0.53	0/919
2	33	0.29	0/666	0.56	0/904
2	34	0.29	0/678	0.56	0/919
2	35	0.30	0/670	0.55	0/909
2	36	0.29	0/666	0.55	0/904
2	37	0.29	0/670	0.50	0/909
2	42	0.29	0/678	0.53	0/919
2	43	0.29	0/666	0.55	0/904
2	44	0.29	0/678	0.52	0/919
2	45	0.29	0/670	0.55	0/909
2	46	0.30	0/666	0.56	0/904
2	47	0.29	0/670	0.49	0/909
2	A2	0.29	0/666	0.56	0/904
2	A3	0.29	0/666	0.59	0/904
2	A4	0.28	0/670	0.53	0/909
2	A5	0.31	0/666	0.57	0/904
2	A6	0.31	0/666	0.52	0/904
2	A7	0.28	0/666	0.52	0/904
2	B2	0.31	0/658	0.55	0/892
2	B3	0.29	0/666	0.55	0/904
2	B4	0.29	0/666	0.56	0/904
2	B5	0.30	0/666	0.58	0/904
2	B6	0.30	0/666	0.54	0/904
2	B7	0.29	0/666	0.53	0/904
2	C2	0.29	0/666	0.54	0/904
2	C3	0.28	0/666	0.54	0/904
2	C4	0.29	0/666	0.54	0/904
2	C5	0.31	0/666	0.55	0/904
2	C6	0.28	0/666	0.53	0/904
2	C7	0.30	0/670	0.53	0/909
2	D2	0.30	0/670	0.53	0/909
2	D3	0.28	0/666	0.55	0/904
2	D4	0.29	0/666	0.55	0/904
2	D5	0.30	0/666	0.53	0/904
2	D6	0.30	0/666	0.54	0/904

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
2	D7	0.29	0/670	0.53	0/909
2	E2	0.31	0/678	0.51	0/919
2	E3	0.28	0/666	0.51	0/904
2	E4	0.28	0/678	0.51	0/919
2	E5	0.29	0/666	0.50	0/904
2	E6	0.30	0/666	0.55	0/904
2	E7	0.28	0/666	0.52	0/904
2	F2	0.29	0/678	0.53	0/919
2	F3	0.28	0/666	0.53	0/904
2	F4	0.30	0/666	0.54	0/904
2	F5	0.28	0/666	0.54	0/904
2	F6	0.28	0/666	0.50	0/904
2	F7	0.30	0/670	0.51	0/909
2	G2	0.28	0/666	0.50	0/904
2	G3	0.29	0/666	0.55	0/904
2	G4	0.30	0/666	0.55	0/904
2	G5	0.28	0/661	0.52	0/897
2	G6	0.28	0/666	0.51	0/904
2	G7	0.29	0/666	0.54	0/904
2	H2	0.29	0/666	0.55	0/904
2	H3	0.30	0/666	0.56	0/904
2	H4	0.30	0/670	0.55	0/909
2	H5	0.30	0/661	0.53	0/897
2	H6	0.31	0/666	0.53	0/904
2	H7	0.29	0/666	0.52	0/904
2	I2	0.31	0/666	0.56	0/904
2	I3	0.27	0/661	0.53	0/897
2	I4	0.30	0/666	0.52	0/904
2	I5	0.30	0/666	0.54	0/904
2	I6	0.31	0/666	0.56	0/904
2	I7	0.28	0/666	0.53	0/904
2	J2	0.30	0/666	0.53	0/904
2	J3	0.29	0/666	0.58	0/904
2	J4	0.28	0/666	0.51	0/904
2	J5	0.32	0/661	0.57	0/897
2	J6	0.29	0/666	0.55	0/904
2	J7	0.28	0/666	0.52	0/904
2	K2	0.32	0/666	0.54	0/904
2	K3	0.28	0/666	0.53	0/904
2	K4	0.28	0/666	0.53	0/904
2	K5	0.30	0/670	0.54	0/909
2	K6	0.28	0/666	0.55	0/904
2	K7	0.29	0/670	0.52	0/909

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
2	L2	0.31	0/678	0.54	0/919
2	L3	0.33	0/666	0.56	0/904
2	L4	0.28	0/666	0.54	0/904
2	L5	0.30	0/666	0.53	0/904
2	L6	0.29	0/666	0.56	0/904
2	L7	0.31	0/670	0.55	0/909
2	M2	0.31	0/670	0.55	0/909
2	M3	0.29	0/666	0.56	0/904
2	M4	0.30	0/666	0.52	0/904
2	M5	0.30	0/670	0.52	0/909
2	M6	0.31	0/661	0.55	0/897
2	M7	0.30	0/666	0.54	0/904
2	N2	0.30	0/666	0.50	0/904
2	N3	0.29	0/661	0.54	0/897
2	N4	0.30	0/666	0.55	0/904
2	N5	0.32	0/670	0.54	0/909
2	N6	0.29	0/661	0.53	0/897
2	N7	0.29	0/665	0.52	0/902
2	O2	0.30	0/678	0.50	0/919
2	O3	0.28	0/666	0.55	0/904
2	O4	0.29	0/678	0.51	0/919
2	O5	0.30	0/670	0.54	0/909
2	O6	0.28	0/666	0.56	0/904
2	O7	0.28	0/670	0.51	0/909
2	P2	0.31	0/678	0.53	0/919
2	P3	0.28	0/666	0.53	0/904
2	P4	0.30	0/678	0.54	0/919
2	P5	0.30	0/670	0.57	0/909
2	P6	0.29	0/666	0.53	0/904
2	P7	0.30	0/657	0.54	0/891
2	Q2	0.29	0/678	0.50	0/919
2	Q3	0.30	0/666	0.56	0/904
2	Q4	0.28	0/678	0.53	0/919
2	Q5	0.30	0/670	0.54	0/909
2	Q6	0.29	0/666	0.56	0/904
2	Q7	0.28	0/670	0.52	0/909
2	R2	0.28	0/678	0.49	0/919
2	R3	0.31	0/666	0.58	0/904
2	R4	0.27	0/678	0.53	0/919
2	R5	0.29	0/670	0.55	0/909
2	R6	0.29	0/666	0.55	0/904
2	R7	0.29	0/670	0.51	0/909
2	S2	0.31	0/678	0.53	0/919

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
2	S3	0.29	0/666	0.52	0/904
2	S4	0.29	0/678	0.53	0/919
2	S5	0.30	0/670	0.56	0/909
2	S6	0.29	0/666	0.55	0/904
2	S7	0.29	0/670	0.52	0/909
2	T2	0.32	0/678	0.58	0/919
2	T3	0.29	0/666	0.57	0/904
2	T4	0.29	0/678	0.56	0/919
2	T5	0.34	0/670	0.61	0/909
2	T6	0.29	0/666	0.59	0/904
2	T7	0.29	0/670	0.55	0/909
2	U2	0.31	0/678	0.56	0/919
2	U3	0.30	0/666	0.55	0/904
2	U4	0.28	0/678	0.56	0/919
2	U5	0.30	0/670	0.52	0/909
2	U6	0.30	0/666	0.55	0/904
2	U7	0.30	0/670	0.51	0/909
2	V2	0.29	0/678	0.53	0/919
2	V3	0.31	0/666	0.56	0/904
2	V4	0.31	0/678	0.56	0/919
2	V5	0.31	0/670	0.56	0/909
2	V6	0.29	0/666	0.54	0/904
2	V7	0.28	0/670	0.51	0/909
2	W2	0.32	0/678	0.53	0/919
2	W3	0.28	0/666	0.56	0/904
2	W4	0.28	0/678	0.53	0/919
2	W5	0.29	0/670	0.54	0/909
2	W6	0.29	0/666	0.56	0/904
2	W7	0.29	0/670	0.53	0/909
2	X2	0.29	0/678	0.51	0/919
2	X3	0.28	0/666	0.55	0/904
2	X4	0.28	0/678	0.53	0/919
2	X5	0.31	0/670	0.53	0/909
2	X6	0.30	0/666	0.55	0/904
2	X7	0.30	0/670	0.50	0/909
2	Y2	0.30	0/678	0.51	0/919
2	Y3	0.29	0/666	0.58	0/904
2	Y4	0.29	0/678	0.52	0/919
2	Y5	0.32	0/665	0.62	0/902
2	Y6	0.29	0/666	0.53	0/904
2	Y7	0.29	0/670	0.50	0/909
2	Z2	0.29	0/678	0.51	0/919
2	Z3	0.29	0/666	0.54	0/904

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
2	Z4	0.28	0/678	0.52	0/919
2	Z5	0.28	0/670	0.53	0/909
2	Z6	0.29	0/666	0.55	0/904
2	Z7	0.29	0/670	0.53	0/909
3	18	0.31	0/1559	0.58	0/2122
3	19	0.24	0/973	0.46	0/1350
3	28	0.30	0/1559	0.58	0/2122
3	29	0.25	0/999	0.45	0/1388
3	38	0.30	0/1559	0.58	0/2122
3	39	0.25	0/999	0.48	0/1388
3	48	0.31	0/1559	0.55	0/2122
3	49	0.24	0/999	0.44	0/1388
3	A8	0.31	0/1559	0.58	0/2122
3	A9	0.25	0/999	0.45	1/1388 (0.1%)
3	B8	0.31	0/1559	0.57	0/2122
3	B9	0.24	0/999	0.48	1/1388 (0.1%)
3	C8	0.31	0/1559	0.57	0/2122
3	C9	0.25	0/999	0.46	0/1388
3	D8	0.32	0/1559	0.59	0/2122
3	D9	0.24	0/999	0.49	0/1388
3	E8	0.30	0/1559	0.57	0/2122
3	E9	0.24	0/999	0.48	0/1388
3	F8	0.31	0/1559	0.58	0/2122
3	F9	0.24	0/999	0.47	0/1388
3	G8	0.30	0/1559	0.58	0/2122
3	G9	0.25	0/999	0.47	0/1388
3	H8	0.30	0/1559	0.60	1/2122 (0.0%)
3	H9	0.24	0/999	0.47	0/1388
3	I8	0.32	0/1559	0.57	0/2122
3	I9	0.25	0/999	0.45	0/1388
3	J8	0.29	0/1559	0.58	0/2122
3	J9	0.25	0/999	0.44	0/1388
3	K8	0.31	0/1559	0.58	0/2122
3	K9	0.24	0/999	0.46	0/1388
3	L8	0.31	0/1559	0.56	0/2122
3	L9	0.24	0/999	0.46	1/1388 (0.1%)
3	M8	0.30	0/1559	0.57	0/2122
3	M9	0.24	0/999	0.44	0/1388
3	N8	0.31	0/1559	0.60	0/2122
3	N9	0.25	0/999	0.46	0/1388
3	O8	0.31	0/1559	0.58	0/2122
3	O9	0.25	0/999	0.44	0/1388
3	P8	0.31	0/1559	0.58	0/2122

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	P9	0.25	0/999	0.48	0/1388
3	Q8	0.31	0/1559	0.58	0/2122
3	Q9	0.25	0/999	0.46	0/1388
3	R8	0.32	0/1559	0.57	0/2122
3	R9	0.25	0/999	0.45	0/1388
3	S8	0.31	0/1559	0.58	0/2122
3	S9	0.24	0/999	0.45	0/1388
3	T8	0.30	0/1559	0.58	0/2122
3	T9	0.25	0/999	0.49	0/1388
3	U8	0.31	0/1559	0.56	0/2122
3	U9	0.25	0/999	0.44	0/1388
3	V8	0.30	0/1559	0.58	0/2122
3	V9	0.24	0/999	0.44	0/1388
3	W8	0.31	0/1559	0.58	0/2122
3	W9	0.25	0/999	0.46	0/1388
3	X8	0.31	0/1559	0.57	0/2122
3	X9	0.24	0/999	0.47	0/1388
3	Y8	0.30	0/1559	0.58	0/2122
3	Y9	0.25	0/999	0.44	0/1388
3	Z8	0.32	0/1559	0.58	0/2122
3	Z9	0.24	0/999	0.45	0/1388
All	All	0.30	0/217621	0.55	4/296423 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H8	74	LEU	CB-CG-CD1	-5.80	101.14	111.00
3	B9	134	ILE	C-N-CA	-5.49	107.98	121.70
3	L9	134	ILE	C-N-CA	-5.02	109.16	121.70
3	A9	134	ILE	C-N-CA	-5.01	109.18	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	11	678	0	705	34	0
1	21	678	0	705	29	1
1	31	669	0	692	44	0
1	41	678	0	705	19	1
1	A1	678	0	705	37	0
1	B1	678	0	705	37	0
1	C1	678	0	705	33	0
1	D1	678	0	705	36	0
1	E1	678	0	705	34	0
1	F1	678	0	705	41	0
1	G1	678	0	705	45	0
1	H1	678	0	705	39	0
1	I1	678	0	705	38	0
1	J1	678	0	705	43	0
1	K1	678	0	705	31	2
1	L1	678	0	705	42	0
1	M1	678	0	705	25	1
1	N1	678	0	705	34	2
1	O1	678	0	705	47	0
1	P1	678	0	705	44	0
1	Q1	678	0	705	38	0
1	R1	678	0	705	37	0
1	S1	678	0	705	44	0
1	T1	678	0	705	30	2
1	U1	678	0	705	29	0
1	V1	678	0	705	42	0
1	W1	678	0	705	37	0
1	X1	678	0	705	31	1
1	Y1	678	0	705	30	2
1	Z1	678	0	705	51	0
2	12	670	0	690	26	0
2	13	658	0	678	28	0
2	14	670	0	690	17	0
2	15	662	0	681	25	0
2	16	658	0	678	23	0
2	17	662	0	681	11	0
2	22	670	0	690	23	0
2	23	658	0	678	36	0
2	24	670	0	690	19	0
2	25	662	0	681	26	0
2	26	658	0	678	23	0
2	27	662	0	681	21	1
2	32	670	0	690	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	33	658	0	678	28	0
2	34	670	0	690	24	0
2	35	662	0	681	31	0
2	36	658	0	678	20	0
2	37	662	0	681	15	0
2	42	670	0	690	22	0
2	43	658	0	678	29	0
2	44	670	0	690	14	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	36	0
2	A3	658	0	678	35	0
2	A4	662	0	681	21	0
2	A5	658	0	678	28	0
2	A6	658	0	678	20	0
2	A7	658	0	678	24	0
2	B2	651	0	671	28	0
2	B3	658	0	678	32	0
2	B4	658	0	678	16	0
2	B5	658	0	678	32	0
2	B6	658	0	678	21	0
2	B7	658	0	678	24	0
2	C2	658	0	678	26	0
2	C3	658	0	678	27	0
2	C4	658	0	678	18	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	32	0
2	D3	658	0	678	38	0
2	D4	658	0	678	26	0
2	D5	658	0	678	27	0
2	D6	658	0	678	24	0
2	D7	662	0	681	18	0
2	E2	670	0	690	30	0
2	E3	658	0	678	22	0
2	E4	670	0	690	21	0
2	E5	658	0	678	24	0
2	E6	658	0	678	27	0
2	E7	658	0	678	25	0
2	F2	670	0	690	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F3	658	0	678	32	0
2	F4	658	0	678	34	0
2	F5	658	0	678	21	0
2	F6	658	0	678	17	0
2	F7	662	0	681	25	0
2	G2	658	0	678	24	0
2	G3	658	0	678	29	0
2	G4	658	0	678	22	0
2	G5	653	0	673	28	0
2	G6	658	0	678	26	0
2	G7	658	0	678	28	0
2	H2	658	0	678	22	0
2	H3	658	0	678	27	0
2	H4	662	0	681	22	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	31	0
2	I3	653	0	673	30	0
2	I4	658	0	678	25	0
2	I5	658	0	678	27	0
2	I6	658	0	678	24	0
2	I7	658	0	678	26	0
2	J2	658	0	678	32	0
2	J3	658	0	678	33	0
2	J4	658	0	678	21	0
2	J5	653	0	673	18	0
2	J6	658	0	678	19	0
2	J7	658	0	678	26	0
2	K2	658	0	678	23	0
2	K3	658	0	678	15	1
2	K4	658	0	678	19	0
2	K5	662	0	681	15	0
2	K6	658	0	678	18	0
2	K7	662	0	681	18	0
2	L2	670	0	690	35	0
2	L3	658	0	678	27	0
2	L4	658	0	678	26	0
2	L5	658	0	678	36	0
2	L6	658	0	678	27	0
2	L7	662	0	681	24	0
2	M2	662	0	681	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M3	658	0	678	21	1
2	M4	658	0	678	18	0
2	M5	662	0	681	32	0
2	M6	653	0	673	16	0
2	M7	658	0	678	26	0
2	N2	658	0	678	26	0
2	N3	653	0	673	22	0
2	N4	658	0	678	18	0
2	N5	662	0	681	28	0
2	N6	653	0	673	22	0
2	N7	657	0	676	21	0
2	O2	670	0	690	22	0
2	O3	658	0	678	23	0
2	O4	670	0	690	13	0
2	O5	662	0	681	23	0
2	O6	658	0	678	21	0
2	O7	662	0	681	24	1
2	P2	670	0	690	28	0
2	P3	658	0	678	28	0
2	P4	670	0	690	17	0
2	P5	662	0	681	23	0
2	P6	658	0	678	20	0
2	P7	649	0	672	28	0
2	Q2	670	0	690	27	0
2	Q3	658	0	678	32	0
2	Q4	670	0	690	18	0
2	Q5	662	0	681	24	0
2	Q6	658	0	678	17	0
2	Q7	662	0	681	20	0
2	R2	670	0	690	21	0
2	R3	658	0	678	28	0
2	R4	670	0	690	15	0
2	R5	662	0	681	21	0
2	R6	658	0	678	19	0
2	R7	662	0	681	20	0
2	S2	670	0	690	21	0
2	S3	658	0	678	24	0
2	S4	670	0	690	22	0
2	S5	662	0	681	24	0
2	S6	658	0	678	20	0
2	S7	662	0	681	19	0
2	T2	670	0	690	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T3	658	0	678	28	0
2	T4	670	0	690	21	0
2	T5	662	0	681	35	0
2	T6	658	0	678	28	0
2	T7	662	0	681	18	0
2	U2	670	0	690	29	0
2	U3	658	0	678	26	0
2	U4	670	0	690	21	0
2	U5	662	0	681	22	0
2	U6	658	0	678	21	0
2	U7	662	0	681	24	0
2	V2	670	0	690	27	0
2	V3	658	0	678	29	0
2	V4	670	0	690	24	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	30	0
2	W3	658	0	678	27	0
2	W4	670	0	690	14	0
2	W5	662	0	681	35	0
2	W6	658	0	678	26	0
2	W7	662	0	681	27	0
2	X2	670	0	690	25	0
2	X3	658	0	678	29	1
2	X4	670	0	690	19	0
2	X5	662	0	681	28	0
2	X6	658	0	678	21	0
2	X7	662	0	681	22	0
2	Y2	670	0	690	23	0
2	Y3	658	0	678	33	0
2	Y4	670	0	690	17	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	20	0
2	Z3	658	0	678	26	0
2	Z4	670	0	690	17	0
2	Z5	662	0	681	19	0
2	Z6	658	0	678	17	0
2	Z7	662	0	681	21	0
3	18	1533	0	1560	92	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	92	0
3	39	1000	0	510	14	0
3	48	1533	0	1560	95	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	113	0
3	B9	1000	0	510	12	0
3	C8	1533	0	1560	111	0
3	C9	1000	0	510	11	0
3	D8	1533	0	1560	95	0
3	D9	1000	0	510	7	0
3	E8	1533	0	1560	94	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	106	0
3	H9	1000	0	510	10	0
3	I8	1533	0	1560	101	0
3	I9	1000	0	510	18	0
3	J8	1533	0	1560	96	0
3	J9	1000	0	510	9	0
3	K8	1533	0	1560	101	2
3	K9	1000	0	510	5	0
3	L8	1533	0	1560	105	0
3	L9	1000	0	510	14	0
3	M8	1533	0	1560	85	0
3	M9	1000	0	510	5	0
3	N8	1533	0	1560	103	0
3	N9	1000	0	510	10	0
3	O8	1533	0	1560	82	4
3	O9	1000	0	510	10	0
3	P8	1533	0	1560	99	0
3	P9	1000	0	510	13	0
3	Q8	1533	0	1560	90	0
3	Q9	1000	0	510	11	0
3	R8	1533	0	1560	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R9	1000	0	510	17	0
3	S8	1533	0	1560	92	0
3	S9	1000	0	510	10	0
3	T8	1533	0	1560	76	1
3	T9	1000	0	510	17	0
3	U8	1533	0	1560	100	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	87	0
3	W9	1000	0	510	14	0
3	X8	1533	0	1560	87	0
3	X9	1000	0	510	12	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	11	0
All	All	215283	0	205772	7154	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 17.

The worst 5 of 7154 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%)	4 31
1	21	93/96 (97%)	79 (85%)	12 (13%)	2 (2%)	6 38
1	31	92/96 (96%)	77 (84%)	10 (11%)	5 (5%)	2 19
1	41	93/96 (97%)	77 (83%)	11 (12%)	5 (5%)	2 19
1	A1	93/96 (97%)	79 (85%)	11 (12%)	3 (3%)	4 31
1	B1	93/96 (97%)	78 (84%)	13 (14%)	2 (2%)	6 38
1	C1	93/96 (97%)	80 (86%)	12 (13%)	1 (1%)	14 53
1	D1	93/96 (97%)	79 (85%)	12 (13%)	2 (2%)	6 38
1	E1	93/96 (97%)	79 (85%)	10 (11%)	4 (4%)	2 23
1	F1	93/96 (97%)	80 (86%)	10 (11%)	3 (3%)	4 31
1	G1	93/96 (97%)	79 (85%)	13 (14%)	1 (1%)	14 53
1	H1	93/96 (97%)	80 (86%)	11 (12%)	2 (2%)	6 38
1	I1	93/96 (97%)	79 (85%)	11 (12%)	3 (3%)	4 31
1	J1	93/96 (97%)	79 (85%)	12 (13%)	2 (2%)	6 38
1	K1	93/96 (97%)	78 (84%)	10 (11%)	5 (5%)	2 19
1	L1	93/96 (97%)	79 (85%)	12 (13%)	2 (2%)	6 38
1	M1	93/96 (97%)	80 (86%)	11 (12%)	2 (2%)	6 38
1	N1	93/96 (97%)	79 (85%)	9 (10%)	5 (5%)	2 19
1	O1	93/96 (97%)	79 (85%)	11 (12%)	3 (3%)	4 31
1	P1	93/96 (97%)	80 (86%)	12 (13%)	1 (1%)	14 53
1	Q1	93/96 (97%)	79 (85%)	13 (14%)	1 (1%)	14 53
1	R1	93/96 (97%)	79 (85%)	12 (13%)	2 (2%)	6 38
1	S1	93/96 (97%)	80 (86%)	10 (11%)	3 (3%)	4 31
1	T1	93/96 (97%)	78 (84%)	11 (12%)	4 (4%)	2 23
1	U1	93/96 (97%)	78 (84%)	12 (13%)	3 (3%)	4 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	V1	93/96 (97%)	78 (84%)	14 (15%)	1 (1%)	14 53
1	W1	93/96 (97%)	79 (85%)	11 (12%)	3 (3%)	4 31
1	X1	93/96 (97%)	78 (84%)	11 (12%)	4 (4%)	2 23
1	Y1	93/96 (97%)	79 (85%)	11 (12%)	3 (3%)	4 31
1	Z1	93/96 (97%)	79 (85%)	10 (11%)	4 (4%)	2 23
2	12	92/99 (93%)	79 (86%)	8 (9%)	5 (5%)	2 19
2	13	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	6 38
2	14	92/99 (93%)	85 (92%)	6 (6%)	1 (1%)	14 53
2	15	91/99 (92%)	84 (92%)	5 (6%)	2 (2%)	6 38
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%)	6 38
2	23	90/99 (91%)	83 (92%)	6 (7%)	1 (1%)	14 53
2	24	92/99 (93%)	85 (92%)	6 (6%)	1 (1%)	14 53
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%)	2 19
2	33	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	6 38
2	34	92/99 (93%)	82 (89%)	7 (8%)	3 (3%)	4 30
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%)	4 30
2	43	90/99 (91%)	80 (89%)	8 (9%)	2 (2%)	6 38
2	44	92/99 (93%)	85 (92%)	6 (6%)	1 (1%)	14 53
2	45	91/99 (92%)	82 (90%)	7 (8%)	2 (2%)	6 38
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%)	6 38
2	A3	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	6 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A4	91/99 (92%)	84 (92%)	6 (7%)	1 (1%)	14 53
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%)	14 53
2	B2	89/99 (90%)	80 (90%)	7 (8%)	2 (2%)	6 38
2	B3	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	6 38
2	B4	90/99 (91%)	85 (94%)	4 (4%)	1 (1%)	14 53
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%)	6 38
2	C3	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	6 38
2	C4	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	14 53
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%)	6 38
2	D3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	6 38
2	D4	90/99 (91%)	83 (92%)	6 (7%)	1 (1%)	14 53
2	D5	90/99 (91%)	85 (94%)	5 (6%)	0	100 100
2	D6	90/99 (91%)	81 (90%)	8 (9%)	1 (1%)	14 53
2	D7	91/99 (92%)	85 (93%)	6 (7%)	0	100 100
2	E2	92/99 (93%)	82 (89%)	8 (9%)	2 (2%)	6 38
2	E3	90/99 (91%)	81 (90%)	8 (9%)	1 (1%)	14 53
2	E4	92/99 (93%)	83 (90%)	8 (9%)	1 (1%)	14 53
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%)	6 38
2	F3	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	6 38
2	F4	90/99 (91%)	84 (93%)	4 (4%)	2 (2%)	6 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	6 38
2	G3	90/99 (91%)	79 (88%)	8 (9%)	3 (3%)	4 30
2	G4	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	14 53
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%)	6 38
2	H3	90/99 (91%)	83 (92%)	5 (6%)	2 (2%)	6 38
2	H4	91/99 (92%)	82 (90%)	7 (8%)	2 (2%)	6 38
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%)	6 38
2	I3	89/99 (90%)	82 (92%)	5 (6%)	2 (2%)	6 38
2	I4	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	14 53
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%)	6 38
2	J3	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	6 38
2	J4	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	14 53
2	J5	89/99 (90%)	83 (93%)	5 (6%)	1 (1%)	14 53
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%)	6 38
2	K3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	6 38
2	K4	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	14 53
2	K5	91/99 (92%)	83 (91%)	8 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	6	38
2	L3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	6	38
2	L4	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	14	53
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%)	6	38
2	M3	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	6	38
2	M4	90/99 (91%)	83 (92%)	6 (7%)	1 (1%)	14	53
2	M5	91/99 (92%)	82 (90%)	8 (9%)	1 (1%)	14	53
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%)	14	53
2	N3	89/99 (90%)	81 (91%)	5 (6%)	3 (3%)	3	30
2	N4	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	14	53
2	N5	91/99 (92%)	82 (90%)	5 (6%)	4 (4%)	2	23
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	23
2	O3	90/99 (91%)	81 (90%)	6 (7%)	3 (3%)	4	30
2	O4	92/99 (93%)	86 (94%)	5 (5%)	1 (1%)	14	53
2	O5	91/99 (92%)	85 (93%)	6 (7%)	0	100	100
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%)	4	30
2	P3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	6	38
2	P4	92/99 (93%)	86 (94%)	5 (5%)	1 (1%)	14	53
2	P5	91/99 (92%)	84 (92%)	7 (8%)	0	100	100
2	P6	90/99 (91%)	82 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	P7	89/99 (90%)	84 (94%)	4 (4%)	1 (1%)	14 53
2	Q2	92/99 (93%)	80 (87%)	9 (10%)	3 (3%)	4 30
2	Q3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	6 38
2	Q4	92/99 (93%)	86 (94%)	5 (5%)	1 (1%)	14 53
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 23
2	R3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	6 38
2	R4	92/99 (93%)	85 (92%)	6 (6%)	1 (1%)	14 53
2	R5	91/99 (92%)	83 (91%)	7 (8%)	1 (1%)	14 53
2	R6	90/99 (91%)	78 (87%)	7 (8%)	5 (6%)	2 18
2	R7	91/99 (92%)	86 (94%)	4 (4%)	1 (1%)	14 53
2	S2	92/99 (93%)	81 (88%)	7 (8%)	4 (4%)	2 23
2	S3	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	6 38
2	S4	92/99 (93%)	85 (92%)	6 (6%)	1 (1%)	14 53
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%)	6 38
2	T3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	6 38
2	T4	92/99 (93%)	84 (91%)	5 (5%)	3 (3%)	4 30
2	T5	91/99 (92%)	86 (94%)	3 (3%)	2 (2%)	6 38
2	T6	90/99 (91%)	82 (91%)	8 (9%)	0	100 100
2	T7	91/99 (92%)	87 (96%)	4 (4%)	0	100 100
2	U2	92/99 (93%)	80 (87%)	10 (11%)	2 (2%)	6 38
2	U3	90/99 (91%)	83 (92%)	6 (7%)	1 (1%)	14 53
2	U4	92/99 (93%)	85 (92%)	6 (6%)	1 (1%)	14 53
2	U5	91/99 (92%)	85 (93%)	5 (6%)	1 (1%)	14 53
2	U6	90/99 (91%)	83 (92%)	7 (8%)	0	100 100
2	U7	91/99 (92%)	85 (93%)	6 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	V2	92/99 (93%)	81 (88%)	8 (9%)	3 (3%)	4 30
2	V3	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	6 38
2	V4	92/99 (93%)	84 (91%)	6 (6%)	2 (2%)	6 38
2	V5	91/99 (92%)	86 (94%)	5 (6%)	0	100 100
2	V6	90/99 (91%)	81 (90%)	8 (9%)	1 (1%)	14 53
2	V7	91/99 (92%)	85 (93%)	6 (7%)	0	100 100
2	W2	92/99 (93%)	81 (88%)	8 (9%)	3 (3%)	4 30
2	W3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	6 38
2	W4	92/99 (93%)	83 (90%)	6 (6%)	3 (3%)	4 30
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%)	6 38
2	X3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	6 38
2	X4	92/99 (93%)	86 (94%)	5 (5%)	1 (1%)	14 53
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%)	4 30
2	Y3	90/99 (91%)	83 (92%)	5 (6%)	2 (2%)	6 38
2	Y4	92/99 (93%)	83 (90%)	8 (9%)	1 (1%)	14 53
2	Y5	90/99 (91%)	82 (91%)	6 (7%)	2 (2%)	6 38
2	Y6	90/99 (91%)	83 (92%)	7 (8%)	0	100 100
2	Y7	91/99 (92%)	85 (93%)	6 (7%)	0	100 100
2	Z2	92/99 (93%)	80 (87%)	8 (9%)	4 (4%)	2 23
2	Z3	90/99 (91%)	81 (90%)	7 (8%)	2 (2%)	6 38
2	Z4	92/99 (93%)	83 (90%)	7 (8%)	2 (2%)	6 38
2	Z5	91/99 (92%)	84 (92%)	6 (7%)	1 (1%)	14 53
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%)	5 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	19	194/212 (92%)	183 (94%)	10 (5%)	1 (0%)	29 67
3	28	201/212 (95%)	174 (87%)	26 (13%)	1 (0%)	29 67
3	29	201/212 (95%)	187 (93%)	13 (6%)	1 (0%)	29 67
3	38	201/212 (95%)	174 (87%)	25 (12%)	2 (1%)	15 54
3	39	201/212 (95%)	187 (93%)	14 (7%)	0	100 100
3	48	201/212 (95%)	174 (87%)	23 (11%)	4 (2%)	7 41
3	49	201/212 (95%)	188 (94%)	12 (6%)	1 (0%)	29 67
3	A8	201/212 (95%)	168 (84%)	28 (14%)	5 (2%)	5 35
3	A9	201/212 (95%)	190 (94%)	11 (6%)	0	100 100
3	B8	201/212 (95%)	175 (87%)	23 (11%)	3 (2%)	10 46
3	B9	201/212 (95%)	185 (92%)	16 (8%)	0	100 100
3	C8	201/212 (95%)	172 (86%)	27 (13%)	2 (1%)	15 54
3	C9	201/212 (95%)	187 (93%)	14 (7%)	0	100 100
3	D8	201/212 (95%)	172 (86%)	28 (14%)	1 (0%)	29 67
3	D9	201/212 (95%)	185 (92%)	15 (8%)	1 (0%)	29 67
3	E8	201/212 (95%)	173 (86%)	24 (12%)	4 (2%)	7 41
3	E9	201/212 (95%)	190 (94%)	11 (6%)	0	100 100
3	F8	201/212 (95%)	173 (86%)	24 (12%)	4 (2%)	7 41
3	F9	201/212 (95%)	189 (94%)	12 (6%)	0	100 100
3	G8	201/212 (95%)	173 (86%)	24 (12%)	4 (2%)	7 41
3	G9	201/212 (95%)	185 (92%)	15 (8%)	1 (0%)	29 67
3	H8	201/212 (95%)	172 (86%)	27 (13%)	2 (1%)	15 54
3	H9	201/212 (95%)	188 (94%)	11 (6%)	2 (1%)	15 54
3	I8	201/212 (95%)	174 (87%)	26 (13%)	1 (0%)	29 67
3	I9	201/212 (95%)	187 (93%)	14 (7%)	0	100 100
3	J8	201/212 (95%)	168 (84%)	30 (15%)	3 (2%)	10 46
3	J9	201/212 (95%)	189 (94%)	12 (6%)	0	100 100
3	K8	201/212 (95%)	175 (87%)	25 (12%)	1 (0%)	29 67
3	K9	201/212 (95%)	188 (94%)	12 (6%)	1 (0%)	29 67
3	L8	201/212 (95%)	173 (86%)	26 (13%)	2 (1%)	15 54
3	L9	201/212 (95%)	187 (93%)	13 (6%)	1 (0%)	29 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	M8	201/212 (95%)	173 (86%)	25 (12%)	3 (2%)	10 46
3	M9	201/212 (95%)	186 (92%)	12 (6%)	3 (2%)	10 46
3	N8	201/212 (95%)	171 (85%)	26 (13%)	4 (2%)	7 41
3	N9	201/212 (95%)	185 (92%)	16 (8%)	0	100 100
3	O8	201/212 (95%)	173 (86%)	27 (13%)	1 (0%)	29 67
3	O9	201/212 (95%)	188 (94%)	13 (6%)	0	100 100
3	P8	201/212 (95%)	172 (86%)	27 (13%)	2 (1%)	15 54
3	P9	201/212 (95%)	186 (92%)	14 (7%)	1 (0%)	29 67
3	Q8	201/212 (95%)	173 (86%)	27 (13%)	1 (0%)	29 67
3	Q9	201/212 (95%)	188 (94%)	13 (6%)	0	100 100
3	R8	201/212 (95%)	171 (85%)	26 (13%)	4 (2%)	7 41
3	R9	201/212 (95%)	182 (90%)	16 (8%)	3 (2%)	10 46
3	S8	201/212 (95%)	173 (86%)	27 (13%)	1 (0%)	29 67
3	S9	201/212 (95%)	189 (94%)	12 (6%)	0	100 100
3	T8	201/212 (95%)	175 (87%)	21 (10%)	5 (2%)	5 35
3	T9	201/212 (95%)	191 (95%)	10 (5%)	0	100 100
3	U8	201/212 (95%)	173 (86%)	25 (12%)	3 (2%)	10 46
3	U9	201/212 (95%)	189 (94%)	12 (6%)	0	100 100
3	V8	201/212 (95%)	172 (86%)	27 (13%)	2 (1%)	15 54
3	V9	201/212 (95%)	187 (93%)	14 (7%)	0	100 100
3	W8	201/212 (95%)	173 (86%)	23 (11%)	5 (2%)	5 35
3	W9	201/212 (95%)	188 (94%)	13 (6%)	0	100 100
3	X8	201/212 (95%)	174 (87%)	26 (13%)	1 (0%)	29 67
3	X9	201/212 (95%)	186 (92%)	14 (7%)	1 (0%)	29 67
3	Y8	201/212 (95%)	171 (85%)	27 (13%)	3 (2%)	10 46
3	Y9	201/212 (95%)	186 (92%)	15 (8%)	0	100 100
3	Z8	201/212 (95%)	170 (85%)	28 (14%)	3 (2%)	10 46
3	Z9	201/212 (95%)	185 (92%)	15 (8%)	1 (0%)	29 67
All	All	31147/33420 (93%)	28065 (90%)	2692 (9%)	390 (1%)	12 49

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 (i)

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%)	72 (99%)	1 (1%)	67	85
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%)	72 (99%)	1 (1%)	67	85
1	P1	73/74 (99%)	72 (99%)	1 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	72 (99%)	1 (1%)	67	85
1	W1	73/74 (99%)	73 (100%)	0	100	100
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%)	63 (98%)	1 (2%)	62	83
2	13	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	14	64/68 (94%)	62 (97%)	2 (3%)	40	70
2	15	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	16	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	17	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	22	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	23	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	24	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	25	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	26	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	27	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	32	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	33	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	34	64/68 (94%)	62 (97%)	2 (3%)	40	70
2	35	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	36	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	37	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	42	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	43	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	44	64/68 (94%)	63 (98%)	1 (2%)	62	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	45	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	46	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	47	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	A2	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	A3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	A4	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	A5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	A6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	A7	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	B2	62/68 (91%)	61 (98%)	1 (2%)	62	83
2	B3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	B4	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	B5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	B6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	B7	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	C2	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	C3	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	C4	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	C5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	C6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	C7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	D2	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	D3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	D4	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	D5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	D6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	D7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	E2	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	E3	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	E4	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	E5	63/68 (93%)	62 (98%)	1 (2%)	62	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	E7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	F2	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	F3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	F4	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	F5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	F6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	F7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	G2	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	G3	63/68 (93%)	63 (100%)	0	100	100
2	G4	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	G5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	G6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	G7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	H2	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	H3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	H4	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	H5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	H6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	H7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	I2	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	I3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	I4	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	I5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	I6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	I7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	J2	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	J3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	J4	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	J5	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	J6	63/68 (93%)	62 (98%)	1 (2%)	62	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	K2	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	K3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	K4	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	K5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	K6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	K7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	L2	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	L3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	L4	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	L5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	L6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	L7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	M2	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	M3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	M4	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	M5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	M6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	M7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	N2	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	N3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	N4	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	N5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	N6	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	N7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	O2	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	O3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	O4	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	O5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	O6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	O7	63/68 (93%)	62 (98%)	1 (2%)	62	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P2	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	P3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	P4	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	P5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	P6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	P7	62/68 (91%)	61 (98%)	1 (2%)	62	83
2	Q2	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	Q3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	Q4	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	Q5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	Q6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	Q7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	R2	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	R3	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	R4	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	R5	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	R6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	R7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	S2	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	S3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	S4	64/68 (94%)	62 (97%)	2 (3%)	40	70
2	S5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	S6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	S7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	T2	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	T3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	T4	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	T5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	T6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	T7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	U2	64/68 (94%)	63 (98%)	1 (2%)	62	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	U3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	U4	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	U5	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	U6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	U7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	V2	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	V3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	V4	64/68 (94%)	62 (97%)	2 (3%)	40	70
2	V5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	V6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	V7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	W2	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	W3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	W4	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	W5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	W6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	W7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	X2	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	X3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	X4	64/68 (94%)	62 (97%)	2 (3%)	40	70
2	X5	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	X6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	X7	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	Y2	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	Y3	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	Y4	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	Y5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	Y6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	Y7	63/68 (93%)	61 (97%)	2 (3%)	39	69
2	Z2	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	Z3	63/68 (93%)	62 (98%)	1 (2%)	62	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z4	64/68 (94%)	63 (98%)	1 (2%)	62	83
2	Z5	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	Z6	63/68 (93%)	62 (98%)	1 (2%)	62	83
2	Z7	63/68 (93%)	62 (98%)	1 (2%)	62	83
3	18	155/164 (94%)	153 (99%)	2 (1%)	69	86
3	28	155/164 (94%)	151 (97%)	4 (3%)	46	74
3	38	155/164 (94%)	150 (97%)	5 (3%)	39	69
3	48	155/164 (94%)	152 (98%)	3 (2%)	57	80
3	A8	155/164 (94%)	150 (97%)	5 (3%)	39	69
3	B8	155/164 (94%)	152 (98%)	3 (2%)	57	80
3	C8	155/164 (94%)	150 (97%)	5 (3%)	39	69
3	D8	155/164 (94%)	149 (96%)	6 (4%)	32	65
3	E8	155/164 (94%)	152 (98%)	3 (2%)	57	80
3	F8	155/164 (94%)	153 (99%)	2 (1%)	69	86
3	G8	155/164 (94%)	151 (97%)	4 (3%)	46	74
3	H8	155/164 (94%)	152 (98%)	3 (2%)	57	80
3	I8	155/164 (94%)	152 (98%)	3 (2%)	57	80
3	J8	155/164 (94%)	151 (97%)	4 (3%)	46	74
3	K8	155/164 (94%)	151 (97%)	4 (3%)	46	74
3	L8	155/164 (94%)	153 (99%)	2 (1%)	69	86
3	M8	155/164 (94%)	152 (98%)	3 (2%)	57	80
3	N8	155/164 (94%)	151 (97%)	4 (3%)	46	74
3	O8	155/164 (94%)	153 (99%)	2 (1%)	69	86
3	P8	155/164 (94%)	152 (98%)	3 (2%)	57	80
3	Q8	155/164 (94%)	153 (99%)	2 (1%)	69	86
3	R8	155/164 (94%)	153 (99%)	2 (1%)	69	86
3	S8	155/164 (94%)	153 (99%)	2 (1%)	69	86
3	T8	155/164 (94%)	151 (97%)	4 (3%)	46	74
3	U8	155/164 (94%)	151 (97%)	4 (3%)	46	74
3	V8	155/164 (94%)	151 (97%)	4 (3%)	46	74
3	W8	155/164 (94%)	152 (98%)	3 (2%)	57	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	X8	155/164 (94%)	151 (97%)	4 (3%)	46 74
3	Y8	155/164 (94%)	151 (97%)	4 (3%)	46 74
3	Z8	155/164 (94%)	151 (97%)	4 (3%)	46 74
All	All	18213/19380 (94%)	17905 (98%)	308 (2%)	60 82

5 of 308 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	W8	66	GLN
2	32	34	TYR
2	X5	79	PRO
2	Z6	34	TYR
2	43	82	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
3	T8	121	GLN
3	Z8	156	ASN
2	V6	82	ASN
3	W8	123	GLN
3	28	123	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 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, 95^{th} 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%)	-0.57	0	100	100	65, 89, 126, 149	0
1	21	95/96 (98%)	-0.68	0	100	100	49, 75, 109, 126	0
1	31	94/96 (97%)	-0.57	0	100	100	64, 91, 139, 160	0
1	41	95/96 (98%)	-0.63	0	100	100	57, 84, 118, 140	0
1	A1	95/96 (98%)	-0.57	0	100	100	61, 83, 112, 131	0
1	B1	95/96 (98%)	-0.62	0	100	100	63, 87, 122, 134	0
1	C1	95/96 (98%)	-0.62	0	100	100	63, 89, 115, 132	0
1	D1	95/96 (98%)	-0.65	0	100	100	60, 86, 114, 130	0
1	E1	95/96 (98%)	-0.64	0	100	100	53, 87, 115, 136	0
1	F1	95/96 (98%)	-0.58	0	100	100	71, 94, 123, 140	0
1	G1	95/96 (98%)	-0.55	0	100	100	76, 94, 126, 159	0
1	H1	95/96 (98%)	-0.62	0	100	100	63, 91, 130, 148	0
1	I1	95/96 (98%)	-0.54	0	100	100	67, 89, 125, 137	0
1	J1	95/96 (98%)	-0.66	0	100	100	63, 88, 123, 151	0
1	K1	95/96 (98%)	-0.65	0	100	100	55, 80, 112, 131	0
1	L1	95/96 (98%)	-0.64	0	100	100	52, 79, 109, 120	0
1	M1	95/96 (98%)	-0.67	0	100	100	55, 79, 111, 122	0
1	N1	95/96 (98%)	-0.67	0	100	100	54, 80, 110, 118	0
1	O1	95/96 (98%)	-0.51	0	100	100	66, 91, 126, 147	0
1	P1	95/96 (98%)	-0.60	0	100	100	65, 91, 116, 137	0
1	Q1	95/96 (98%)	-0.55	0	100	100	62, 89, 125, 150	0
1	R1	95/96 (98%)	-0.55	0	100	100	70, 95, 124, 145	0
1	S1	95/96 (98%)	-0.57	0	100	100	57, 94, 118, 139	0
1	T1	95/96 (98%)	-0.60	0	100	100	55, 82, 110, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	U1	95/96 (98%)	-0.62	0	100	100	54, 82, 111, 126	0
1	V1	95/96 (98%)	-0.58	0	100	100	72, 94, 124, 138	0
1	W1	95/96 (98%)	-0.55	0	100	100	73, 94, 126, 135	0
1	X1	95/96 (98%)	-0.68	0	100	100	54, 80, 110, 120	0
1	Y1	95/96 (98%)	-0.62	0	100	100	50, 82, 112, 134	0
1	Z1	95/96 (98%)	-0.59	0	100	100	66, 92, 123, 141	0
2	12	94/99 (94%)	-0.68	0	100	100	58, 82, 113, 128	0
2	13	92/99 (92%)	-0.67	0	100	100	58, 82, 110, 131	0
2	14	94/99 (94%)	-0.60	0	100	100	54, 80, 113, 150	0
2	15	93/99 (93%)	-0.65	0	100	100	54, 81, 112, 140	0
2	16	92/99 (92%)	-0.66	0	100	100	58, 79, 111, 132	0
2	17	93/99 (93%)	-0.64	0	100	100	57, 81, 114, 128	0
2	22	94/99 (94%)	-0.67	0	100	100	47, 71, 103, 133	0
2	23	92/99 (92%)	-0.65	0	100	100	45, 76, 104, 115	0
2	24	94/99 (94%)	-0.62	1 (1%)	80	69	39, 70, 102, 124	0
2	25	93/99 (93%)	-0.67	0	100	100	44, 70, 99, 131	0
2	26	92/99 (92%)	-0.65	0	100	100	43, 73, 99, 119	0
2	27	93/99 (93%)	-0.66	0	100	100	54, 74, 107, 123	0
2	32	94/99 (94%)	-0.64	0	100	100	61, 81, 111, 135	0
2	33	92/99 (92%)	-0.63	0	100	100	48, 84, 113, 129	0
2	34	94/99 (94%)	-0.63	0	100	100	57, 81, 113, 137	0
2	35	93/99 (93%)	-0.60	0	100	100	65, 83, 113, 121	0
2	36	92/99 (92%)	-0.64	0	100	100	63, 85, 110, 122	0
2	37	93/99 (93%)	-0.66	0	100	100	58, 79, 113, 124	0
2	42	94/99 (94%)	-0.67	0	100	100	49, 76, 105, 134	0
2	43	92/99 (92%)	-0.60	0	100	100	54, 80, 113, 131	0
2	44	94/99 (94%)	-0.56	0	100	100	58, 81, 111, 147	0
2	45	93/99 (93%)	-0.64	0	100	100	59, 82, 111, 140	0
2	46	92/99 (92%)	-0.62	0	100	100	54, 77, 101, 115	0
2	47	93/99 (93%)	-0.64	0	100	100	53, 76, 108, 123	0
2	A2	92/99 (92%)	-0.60	0	100	100	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%)	-0.60	0	100	100	56, 84, 110, 128	0
2	A4	93/99 (93%)	-0.61	0	100	100	55, 85, 112, 142	0
2	A5	92/99 (92%)	-0.63	0	100	100	54, 85, 111, 126	0
2	A6	92/99 (92%)	-0.62	0	100	100	60, 86, 112, 122	0
2	A7	92/99 (92%)	-0.61	0	100	100	54, 84, 112, 128	0
2	B2	91/99 (91%)	-0.67	0	100	100	54, 73, 105, 125	0
2	B3	92/99 (92%)	-0.68	0	100	100	51, 81, 103, 123	0
2	B4	92/99 (92%)	-0.62	0	100	100	57, 77, 107, 116	0
2	B5	92/99 (92%)	-0.67	0	100	100	58, 82, 109, 123	0
2	B6	92/99 (92%)	-0.66	0	100	100	58, 77, 105, 116	0
2	B7	92/99 (92%)	-0.64	0	100	100	57, 80, 104, 114	0
2	C2	92/99 (92%)	-0.66	0	100	100	53, 77, 104, 114	0
2	C3	92/99 (92%)	-0.66	0	100	100	63, 81, 113, 122	0
2	C4	92/99 (92%)	-0.68	0	100	100	54, 75, 100, 122	0
2	C5	92/99 (92%)	-0.67	0	100	100	55, 79, 105, 121	0
2	C6	92/99 (92%)	-0.67	0	100	100	50, 76, 106, 120	0
2	C7	93/99 (93%)	-0.68	0	100	100	54, 75, 102, 131	0
2	D2	93/99 (93%)	-0.65	0	100	100	50, 78, 111, 118	0
2	D3	92/99 (92%)	-0.60	0	100	100	60, 84, 112, 123	0
2	D4	92/99 (92%)	-0.59	0	100	100	54, 80, 108, 121	0
2	D5	92/99 (92%)	-0.62	0	100	100	60, 83, 109, 133	0
2	D6	92/99 (92%)	-0.66	0	100	100	45, 76, 104, 122	0
2	D7	93/99 (93%)	-0.59	0	100	100	48, 77, 108, 119	0
2	E2	94/99 (94%)	-0.62	0	100	100	58, 80, 112, 128	0
2	E3	92/99 (92%)	-0.60	0	100	100	68, 87, 112, 124	0
2	E4	94/99 (94%)	-0.59	0	100	100	61, 82, 114, 128	0
2	E5	92/99 (92%)	-0.61	0	100	100	59, 83, 108, 131	0
2	E6	92/99 (92%)	-0.65	0	100	100	63, 81, 105, 122	0
2	E7	92/99 (92%)	-0.62	0	100	100	53, 81, 109, 125	0
2	F2	94/99 (94%)	-0.59	0	100	100	66, 87, 116, 135	0
2	F3	92/99 (92%)	-0.58	0	100	100	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%)	-0.67	0	100	100	64, 83, 111, 130	0
2	F5	92/99 (92%)	-0.64	0	100	100	67, 86, 109, 129	0
2	F6	92/99 (92%)	-0.64	0	100	100	62, 83, 108, 118	0
2	F7	93/99 (93%)	-0.67	0	100	100	62, 84, 111, 131	0
2	G2	92/99 (92%)	-0.58	0	100	100	65, 90, 113, 121	0
2	G3	92/99 (92%)	-0.56	0	100	100	63, 88, 119, 129	0
2	G4	92/99 (92%)	-0.58	0	100	100	60, 86, 113, 127	0
2	G5	91/99 (91%)	-0.58	0	100	100	65, 84, 111, 127	0
2	G6	92/99 (92%)	-0.61	0	100	100	66, 87, 110, 126	0
2	G7	92/99 (92%)	-0.62	0	100	100	55, 83, 122, 137	0
2	H2	92/99 (92%)	-0.63	0	100	100	58, 79, 104, 111	0
2	H3	92/99 (92%)	-0.62	0	100	100	58, 84, 117, 126	0
2	H4	93/99 (93%)	-0.56	0	100	100	57, 83, 112, 135	0
2	H5	91/99 (91%)	-0.60	0	100	100	59, 84, 112, 121	0
2	H6	92/99 (92%)	-0.58	0	100	100	58, 82, 105, 121	0
2	H7	92/99 (92%)	-0.60	0	100	100	61, 83, 108, 127	0
2	I2	92/99 (92%)	-0.66	0	100	100	54, 81, 107, 123	0
2	I3	91/99 (91%)	-0.69	0	100	100	64, 85, 109, 130	0
2	I4	92/99 (92%)	-0.63	0	100	100	58, 83, 106, 117	0
2	I5	92/99 (92%)	-0.57	0	100	100	59, 87, 115, 125	0
2	I6	92/99 (92%)	-0.57	0	100	100	60, 87, 111, 121	0
2	I7	92/99 (92%)	-0.61	0	100	100	62, 83, 107, 131	0
2	J2	92/99 (92%)	-0.57	0	100	100	65, 84, 110, 125	0
2	J3	92/99 (92%)	-0.63	0	100	100	59, 81, 112, 123	0
2	J4	92/99 (92%)	-0.64	0	100	100	59, 79, 109, 119	0
2	J5	91/99 (91%)	-0.66	0	100	100	51, 78, 107, 121	0
2	J6	92/99 (92%)	-0.62	0	100	100	51, 81, 105, 123	0
2	J7	92/99 (92%)	-0.70	0	100	100	56, 80, 103, 121	0
2	K2	92/99 (92%)	-0.65	0	100	100	43, 79, 106, 119	0
2	K3	92/99 (92%)	-0.66	0	100	100	60, 83, 115, 134	0
2	K4	92/99 (92%)	-0.69	0	100	100	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%)	-0.63	0	100	100	42, 80, 102, 136	0
2	K6	92/99 (92%)	-0.69	0	100	100	53, 78, 104, 119	0
2	K7	93/99 (93%)	-0.67	0	100	100	50, 78, 112, 121	0
2	L2	94/99 (94%)	-0.63	0	100	100	46, 78, 105, 126	0
2	L3	92/99 (92%)	-0.65	0	100	100	52, 80, 112, 126	0
2	L4	92/99 (92%)	-0.62	0	100	100	53, 79, 101, 116	0
2	L5	92/99 (92%)	-0.68	0	100	100	54, 76, 107, 128	0
2	L6	92/99 (92%)	-0.64	0	100	100	53, 79, 105, 135	0
2	L7	93/99 (93%)	-0.62	0	100	100	47, 71, 93, 116	0
2	M2	93/99 (93%)	-0.71	0	100	100	47, 69, 94, 107	0
2	M3	92/99 (92%)	-0.69	0	100	100	54, 76, 108, 121	0
2	M4	92/99 (92%)	-0.68	0	100	100	44, 75, 94, 122	0
2	M5	93/99 (93%)	-0.70	0	100	100	48, 71, 99, 122	0
2	M6	91/99 (91%)	-0.65	0	100	100	50, 71, 99, 114	0
2	M7	92/99 (92%)	-0.64	0	100	100	49, 75, 105, 123	0
2	N2	92/99 (92%)	-0.70	0	100	100	50, 71, 100, 114	0
2	N3	91/99 (91%)	-0.63	0	100	100	42, 76, 101, 133	0
2	N4	92/99 (92%)	-0.62	0	100	100	50, 73, 100, 121	0
2	N5	93/99 (93%)	-0.60	0	100	100	57, 75, 105, 115	0
2	N6	91/99 (91%)	-0.66	0	100	100	55, 76, 98, 106	0
2	N7	92/99 (92%)	-0.68	0	100	100	50, 75, 106, 118	0
2	O2	94/99 (94%)	-0.62	0	100	100	62, 84, 117, 131	0
2	O3	92/99 (92%)	-0.63	0	100	100	56, 81, 114, 124	0
2	O4	94/99 (94%)	-0.64	0	100	100	56, 83, 114, 130	0
2	O5	93/99 (93%)	-0.66	0	100	100	59, 85, 113, 130	0
2	O6	92/99 (92%)	-0.62	0	100	100	57, 78, 103, 122	0
2	O7	93/99 (93%)	-0.62	0	100	100	63, 81, 106, 121	0
2	P2	94/99 (94%)	-0.62	0	100	100	59, 84, 115, 130	0
2	P3	92/99 (92%)	-0.65	0	100	100	56, 82, 112, 122	0
2	P4	94/99 (94%)	-0.62	0	100	100	53, 82, 112, 128	0
2	P5	93/99 (93%)	-0.59	0	100	100	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%)	-0.52	0	100	100	59, 82, 108, 117	0
2	P7	91/99 (91%)	-0.63	0	100	100	49, 79, 110, 114	0
2	Q2	94/99 (94%)	-0.58	0	100	100	51, 83, 118, 129	0
2	Q3	92/99 (92%)	-0.59	0	100	100	62, 83, 107, 129	0
2	Q4	94/99 (94%)	-0.52	1 (1%)	80	69	56, 84, 109, 133	0
2	Q5	93/99 (93%)	-0.63	0	100	100	61, 82, 113, 119	0
2	Q6	92/99 (92%)	-0.62	0	100	100	56, 82, 112, 123	0
2	Q7	93/99 (93%)	-0.57	0	100	100	63, 85, 115, 130	0
2	R2	94/99 (94%)	-0.64	0	100	100	61, 83, 110, 144	0
2	R3	92/99 (92%)	-0.59	0	100	100	51, 82, 113, 126	0
2	R4	94/99 (94%)	-0.58	0	100	100	56, 82, 116, 143	0
2	R5	93/99 (93%)	-0.68	0	100	100	62, 86, 115, 143	0
2	R6	92/99 (92%)	-0.58	0	100	100	62, 87, 115, 132	0
2	R7	93/99 (93%)	-0.59	0	100	100	62, 82, 114, 127	0
2	S2	94/99 (94%)	-0.55	0	100	100	53, 84, 112, 139	0
2	S3	92/99 (92%)	-0.63	0	100	100	65, 83, 116, 123	0
2	S4	94/99 (94%)	-0.61	0	100	100	65, 83, 105, 152	0
2	S5	93/99 (93%)	-0.61	0	100	100	34, 83, 108, 117	0
2	S6	92/99 (92%)	-0.58	0	100	100	46, 81, 107, 119	0
2	S7	93/99 (93%)	-0.62	0	100	100	51, 79, 108, 123	0
2	T2	94/99 (94%)	-0.58	0	100	100	45, 72, 105, 155	0
2	T3	92/99 (92%)	-0.64	0	100	100	46, 78, 108, 137	0
2	T4	94/99 (94%)	-0.61	0	100	100	53, 78, 113, 141	0
2	T5	93/99 (93%)	-0.65	0	100	100	40, 75, 103, 125	0
2	T6	92/99 (92%)	-0.64	0	100	100	53, 80, 108, 124	0
2	T7	93/99 (93%)	-0.61	0	100	100	54, 79, 109, 125	0
2	U2	94/99 (94%)	-0.63	0	100	100	42, 71, 101, 121	0
2	U3	92/99 (92%)	-0.64	0	100	100	57, 86, 117, 129	0
2	U4	94/99 (94%)	-0.57	0	100	100	46, 76, 112, 127	0
2	U5	93/99 (93%)	-0.61	0	100	100	60, 77, 110, 131	0
2	U6	92/99 (92%)	-0.62	0	100	100	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%)	-0.57	0	100	100	44, 79, 110, 136	0
2	V2	94/99 (94%)	-0.58	0	100	100	59, 85, 112, 136	0
2	V3	92/99 (92%)	-0.63	0	100	100	56, 80, 109, 126	0
2	V4	94/99 (94%)	-0.53	0	100	100	60, 82, 106, 125	0
2	V5	93/99 (93%)	-0.60	0	100	100	55, 85, 112, 124	0
2	V6	92/99 (92%)	-0.57	0	100	100	57, 79, 107, 117	0
2	V7	93/99 (93%)	-0.63	0	100	100	60, 79, 102, 116	0
2	W2	94/99 (94%)	-0.60	0	100	100	61, 87, 116, 125	0
2	W3	92/99 (92%)	-0.57	0	100	100	63, 87, 117, 134	0
2	W4	94/99 (94%)	-0.55	1 (1%)	80	69	62, 84, 110, 157	0
2	W5	93/99 (93%)	-0.59	0	100	100	60, 84, 114, 142	0
2	W6	92/99 (92%)	-0.57	0	100	100	64, 83, 107, 131	0
2	W7	93/99 (93%)	-0.60	0	100	100	47, 79, 108, 134	0
2	X2	94/99 (94%)	-0.61	0	100	100	51, 76, 107, 137	0
2	X3	92/99 (92%)	-0.64	0	100	100	52, 80, 112, 128	0
2	X4	94/99 (94%)	-0.63	0	100	100	46, 76, 109, 129	0
2	X5	93/99 (93%)	-0.62	0	100	100	51, 80, 107, 137	0
2	X6	92/99 (92%)	-0.65	0	100	100	57, 80, 101, 132	0
2	X7	93/99 (93%)	-0.65	0	100	100	57, 79, 108, 121	0
2	Y2	94/99 (94%)	-0.64	0	100	100	58, 78, 109, 122	0
2	Y3	92/99 (92%)	-0.59	0	100	100	52, 82, 105, 125	0
2	Y4	94/99 (94%)	-0.54	0	100	100	44, 83, 113, 133	0
2	Y5	92/99 (92%)	-0.61	0	100	100	50, 75, 104, 130	0
2	Y6	92/99 (92%)	-0.60	0	100	100	49, 80, 103, 119	0
2	Y7	93/99 (93%)	-0.62	0	100	100	55, 81, 105, 128	0
2	Z2	94/99 (94%)	-0.64	0	100	100	58, 82, 113, 130	0
2	Z3	92/99 (92%)	-0.62	0	100	100	62, 85, 111, 126	0
2	Z4	94/99 (94%)	-0.64	0	100	100	60, 80, 110, 141	0
2	Z5	93/99 (93%)	-0.69	0	100	100	59, 82, 114, 122	0
2	Z6	92/99 (92%)	-0.61	0	100	100	57, 81, 112, 129	0
2	Z7	93/99 (93%)	-0.63	0	100	100	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%)	-0.15	0 100 100	71, 120, 149, 157	0
3	19	198/212 (93%)	1.51	58 (29%) 0 0	121, 155, 174, 192	0
3	28	203/212 (95%)	-0.20	0 100 100	68, 116, 146, 163	0
3	29	203/212 (95%)	1.10	36 (17%) 1 1	106, 145, 172, 190	0
3	38	203/212 (95%)	-0.07	1 (0%) 91 84	72, 120, 152, 175	0
3	39	203/212 (95%)	1.58	58 (28%) 0 0	124, 156, 176, 190	0
3	48	203/212 (95%)	-0.18	1 (0%) 91 84	73, 117, 147, 161	0
3	49	203/212 (95%)	1.20	36 (17%) 1 1	110, 149, 171, 189	0
3	A8	203/212 (95%)	-0.10	2 (0%) 82 71	76, 121, 149, 163	0
3	A9	203/212 (95%)	1.44	56 (27%) 0 0	118, 156, 177, 196	0
3	B8	203/212 (95%)	-0.09	1 (0%) 91 84	73, 116, 145, 172	0
3	B9	203/212 (95%)	1.32	61 (30%) 0 0	103, 148, 172, 194	0
3	C8	203/212 (95%)	-0.17	1 (0%) 91 84	74, 115, 147, 170	0
3	C9	203/212 (95%)	1.03	28 (13%) 2 3	100, 147, 171, 203	0
3	D8	203/212 (95%)	-0.11	1 (0%) 91 84	79, 115, 144, 172	0
3	D9	203/212 (95%)	1.23	44 (21%) 0 0	111, 145, 170, 181	0
3	E8	203/212 (95%)	-0.07	2 (0%) 82 71	85, 124, 152, 168	0
3	E9	203/212 (95%)	1.36	50 (24%) 0 0	115, 156, 177, 184	0
3	F8	203/212 (95%)	-0.06	5 (2%) 57 43	71, 125, 155, 178	0
3	F9	203/212 (95%)	1.70	77 (37%) 0 0	116, 157, 181, 202	0
3	G8	203/212 (95%)	-0.09	4 (1%) 65 52	74, 122, 150, 184	0
3	G9	203/212 (95%)	1.53	63 (31%) 0 0	124, 159, 180, 197	0
3	H8	203/212 (95%)	-0.13	1 (0%) 91 84	68, 121, 150, 161	0
3	H9	203/212 (95%)	1.44	54 (26%) 0 0	111, 156, 178, 194	0
3	I8	203/212 (95%)	-0.01	7 (3%) 45 34	84, 121, 150, 171	0
3	I9	203/212 (95%)	1.58	71 (34%) 0 0	112, 156, 177, 195	0
3	J8	203/212 (95%)	-0.14	0 100 100	72, 118, 145, 168	0
3	J9	203/212 (95%)	1.16	39 (19%) 1 1	105, 149, 173, 188	0
3	K8	203/212 (95%)	-0.11	2 (0%) 82 71	72, 119, 148, 167	0
3	K9	203/212 (95%)	1.28	46 (22%) 0 0	113, 152, 172, 197	0
3	L8	203/212 (95%)	-0.16	3 (1%) 73 61	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%)	1.24	45 (22%) 0 0	109, 150, 173, 191	0
3	M8	203/212 (95%)	-0.16	2 (0%) 82 71	68, 114, 148, 168	0
3	M9	203/212 (95%)	1.09	29 (14%) 2 2	105, 145, 174, 181	0
3	N8	203/212 (95%)	-0.12	3 (1%) 73 61	62, 117, 152, 164	0
3	N9	203/212 (95%)	1.26	48 (23%) 0 0	103, 150, 175, 189	0
3	O8	203/212 (95%)	-0.06	4 (1%) 65 52	80, 118, 150, 183	0
3	O9	203/212 (95%)	1.51	56 (27%) 0 0	111, 154, 178, 188	0
3	P8	203/212 (95%)	-0.16	2 (0%) 82 71	76, 117, 141, 155	0
3	P9	203/212 (95%)	1.25	41 (20%) 1 1	119, 149, 173, 195	0
3	Q8	203/212 (95%)	-0.06	2 (0%) 82 71	71, 121, 152, 172	0
3	Q9	203/212 (95%)	1.48	61 (30%) 0 0	113, 157, 183, 201	0
3	R8	203/212 (95%)	-0.07	4 (1%) 65 52	70, 122, 152, 174	0
3	R9	203/212 (95%)	1.52	64 (31%) 0 0	116, 157, 177, 185	0
3	S8	203/212 (95%)	-0.10	2 (0%) 82 71	78, 121, 149, 172	0
3	S9	203/212 (95%)	1.49	61 (30%) 0 0	122, 156, 176, 186	0
3	T8	203/212 (95%)	-0.05	7 (3%) 45 34	68, 114, 149, 169	0
3	T9	203/212 (95%)	1.41	49 (24%) 0 0	109, 153, 179, 195	0
3	U8	203/212 (95%)	-0.16	2 (0%) 82 71	73, 118, 150, 162	0
3	U9	203/212 (95%)	1.28	46 (22%) 0 0	100, 153, 175, 188	0
3	V8	203/212 (95%)	-0.13	1 (0%) 91 84	75, 118, 149, 166	0
3	V9	203/212 (95%)	1.12	32 (15%) 2 2	108, 148, 170, 179	0
3	W8	203/212 (95%)	-0.13	4 (1%) 65 52	80, 121, 148, 167	0
3	W9	203/212 (95%)	1.41	55 (27%) 0 0	112, 155, 178, 190	0
3	X8	203/212 (95%)	-0.15	1 (0%) 91 84	77, 116, 149, 165	0
3	X9	203/212 (95%)	1.14	36 (17%) 1 1	107, 150, 175, 195	0
3	Y8	203/212 (95%)	-0.06	5 (2%) 57 43	66, 118, 153, 163	0
3	Y9	203/212 (95%)	1.20	40 (19%) 1 1	114, 151, 175, 184	0
3	Z8	203/212 (95%)	-0.09	2 (0%) 82 71	74, 121, 151, 167	0
3	Z9	203/212 (95%)	1.32	51 (25%) 0 0	115, 155, 175, 184	0
All	All	31689/33420 (94%)	-0.15	1566 (4%) 29 22	34, 95, 163, 203	0

The worst 5 of 1566 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	39	116	ALA	7.0
3	Z9	116	ALA	6.8
3	O9	67	VAL	6.3
3	O9	116	ALA	5.8
3	C9	3	ILE	5.8

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 monosaccharides 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.