



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 10:36 am BST

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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

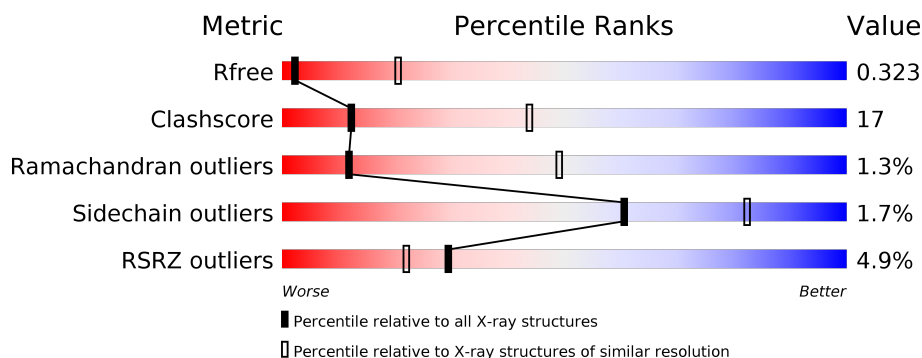
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 Å.

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











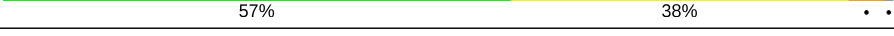


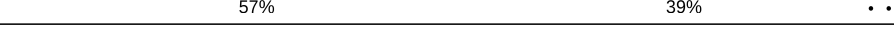

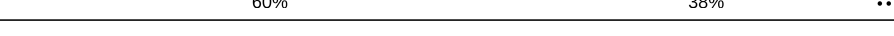


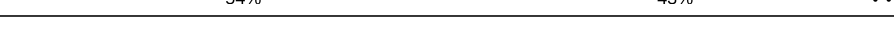

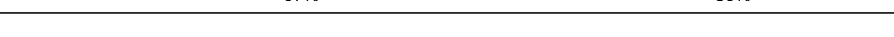
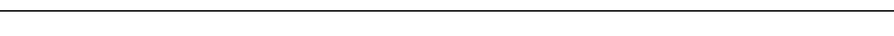

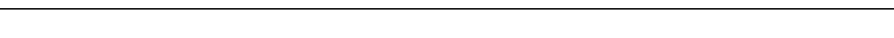



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	11	96	<div> <div>64%</div> <div>34%</div> <div>..</div> </div>
1	21	96	<div> <div>63%</div> <div>35%</div> <div>..</div> </div>
1	31	96	<div> <div>47%</div> <div>47%</div> <div>..</div> </div>
1	41	96	<div> <div>66%</div> <div>31%</div> <div>..</div> </div>
1	A1	96	<div> <div>53%</div> <div>43%</div> <div>..</div> </div>
1	B1	96	<div> <div>57%</div> <div>42%</div> <div>.</div> </div>

















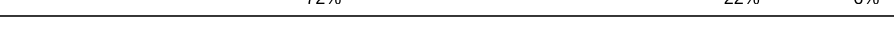

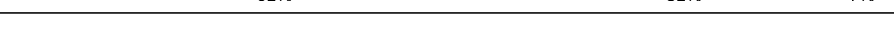
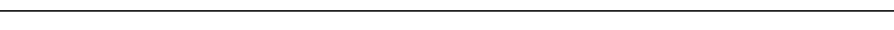
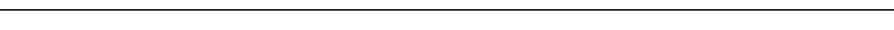
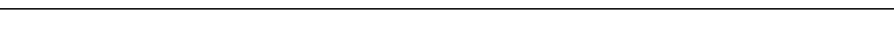
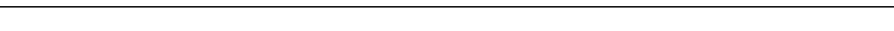
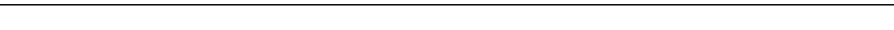

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Mol	Chain	Length	Quality of chain
1	C1	96	
1	D1	96	
1	E1	96	
1	F1	96	
1	G1	96	
1	H1	96	
1	I1	96	
1	J1	96	
1	K1	96	
1	L1	96	
1	M1	96	
1	N1	96	
1	O1	96	
1	P1	96	
1	Q1	96	
1	R1	96	
1	S1	96	
1	T1	96	
1	U1	96	
1	V1	96	
1	W1	96	
1	X1	96	
1	Y1	96	
1	Z1	96	
2	12	99	


























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Mol	Chain	Length	Quality of chain
2	13	99	
2	14	99	
2	15	99	
2	16	99	
2	17	99	
2	22	99	
2	23	99	
2	24	99	
2	25	99	
2	26	99	
2	27	99	
2	32	99	
2	33	99	
2	34	99	
2	35	99	
2	36	99	
2	37	99	
2	42	99	
2	43	99	
2	44	99	
2	45	99	
2	46	99	
2	47	99	
2	A2	99	
2	A3	99	


























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Mol	Chain	Length	Quality of chain
2	A4	99	
2	A5	99	
2	A6	99	
2	A7	99	
2	B2	99	
2	B3	99	
2	B4	99	
2	B5	99	
2	B6	99	
2	B7	99	
2	C2	99	
2	C3	99	
2	C4	99	
2	C5	99	
2	C6	99	
2	C7	99	
2	D2	99	
2	D3	99	
2	D4	99	
2	D5	99	
2	D6	99	
2	D7	99	
2	E2	99	
2	E3	99	
2	E4	99	

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Mol	Chain	Length	Quality of chain
2	E5	99	
2	E6	99	
2	E7	99	
2	F2	99	
2	F3	99	
2	F4	99	
2	F5	99	
2	F6	99	
2	F7	99	
2	G2	99	
2	G3	99	
2	G4	99	
2	G5	99	
2	G6	99	
2	G7	99	
2	H2	99	
2	H3	99	
2	H4	99	
2	H5	99	
2	H6	99	
2	H7	99	
2	I2	99	
2	I3	99	
2	I4	99	
2	I5	99	

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Mol	Chain	Length	Quality of chain
2	I6	99	
2	I7	99	
2	J2	99	
2	J3	99	
2	J4	99	
2	J5	99	
2	J6	99	
2	J7	99	
2	K2	99	
2	K3	99	
2	K4	99	
2	K5	99	
2	K6	99	
2	K7	99	
2	L2	99	
2	L3	99	
2	L4	99	
2	L5	99	
2	L6	99	
2	L7	99	
2	M2	99	
2	M3	99	
2	M4	99	
2	M5	99	
2	M6	99	









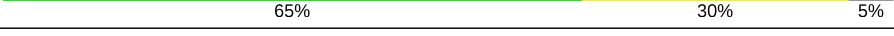


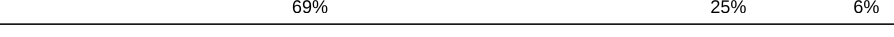

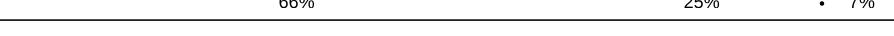


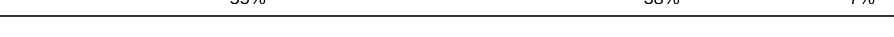

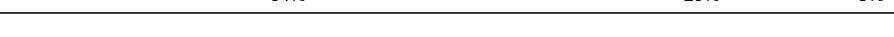
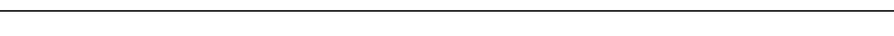

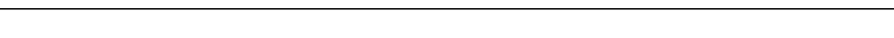
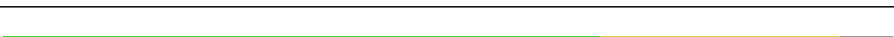


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Mol	Chain	Length	Quality of chain
2	M7	99	
2	N2	99	
2	N3	99	
2	N4	99	
2	N5	99	
2	N6	99	
2	N7	99	
2	O2	99	
2	O3	99	
2	O4	99	
2	O5	99	
2	O6	99	
2	O7	99	
2	P2	99	
2	P3	99	
2	P4	99	
2	P5	99	
2	P6	99	
2	P7	99	
2	Q2	99	
2	Q3	99	
2	Q4	99	
2	Q5	99	
2	Q6	99	
2	Q7	99	

















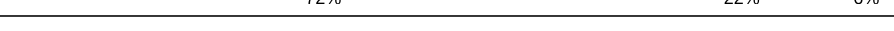

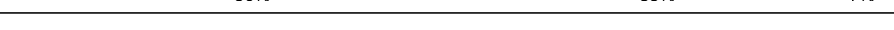
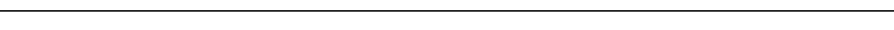
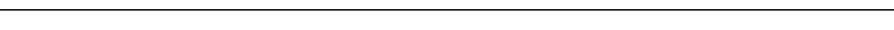
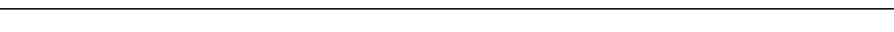
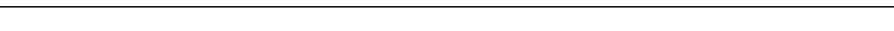
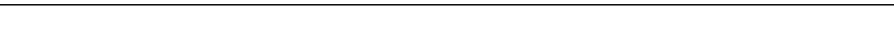

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Mol	Chain	Length	Quality of chain
2	R2	99	 70% 22% 5%
2	R3	99	 59% 32% 7%
2	R4	99	 73% 22% 5%
2	R5	99	 62% 30% 6%
2	R6	99	 65% 26% 7%
2	R7	99	 70% 24% 6%
2	S2	99	 68% 24% 5%
2	S3	99	 64% 27% 7%
2	S4	99	 65% 30% 5%
2	S5	99	 69% 24% 6%
2	S6	99	 66% 27% 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%
2	V2	99	 64% 29% 5%

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Mol	Chain	Length	Quality of chain
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%
2	Z3	99	 60% 32% • 7%

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Mol	Chain	Length	Quality of chain
2	Z4	99	
2	Z5	99	
2	Z6	99	
2	Z7	99	
3	18	212	
3	19	212	
3	28	212	
3	29	212	
3	38	212	
3	39	212	
3	48	212	
3	49	212	
3	A8	212	
3	A9	212	
3	B8	212	
3	B9	212	
3	C8	212	
3	C9	212	
3	D8	212	
3	D9	212	
3	E8	212	
3	E9	212	
3	F8	212	
3	F9	212	
3	G8	212	

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Mol	Chain	Length	Quality of chain
3	G9	212	
3	H8	212	
3	H9	212	
3	I8	212	
3	I9	212	
3	J8	212	
3	J9	212	
3	K8	212	
3	K9	212	
3	L8	212	
3	L9	212	
3	M8	212	
3	M9	212	
3	N8	212	
3	N9	212	
3	O8	212	
3	O9	212	
3	P8	212	
3	P9	212	
3	Q8	212	
3	Q9	212	
3	R8	212	
3	R9	212	
3	S8	212	
3	S9	212	

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

2 Entry composition

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

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

- Molecule 1 is a protein called Ethanolamine utilization protein EutN/carboxysome structural protein Ccml.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q1	95	Total	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 658	C 413	N 120	O 122	S 3	0	0	0
2	L5	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	L6	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	L7	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	M2	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	M3	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	M4	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	M5	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	M6	91	Total 653	C 410	N 119	O 121	S 3	0	0	0
2	M7	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	N2	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	N3	91	Total 653	C 410	N 119	O 121	S 3	0	0	0
2	N4	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	N5	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	N6	91	Total 653	C 410	N 119	O 121	S 3	0	0	0
2	N7	92	Total 657	C 412	N 120	O 122	S 3	0	0	0
2	O2	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	O3	92	Total 658	C 413	N 120	O 122	S 3	0	0	0
2	O4	94	Total 670	C 420	N 122	O 124	S 4	0	0	0
2	O5	93	Total 662	C 415	N 121	O 123	S 3	0	0	0
2	O6	92	Total 658	C 413	N 120	O 122	S 3	0	0	0

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

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

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

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

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

- Molecule 3 is a protein called Microcompartments protein.

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

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

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

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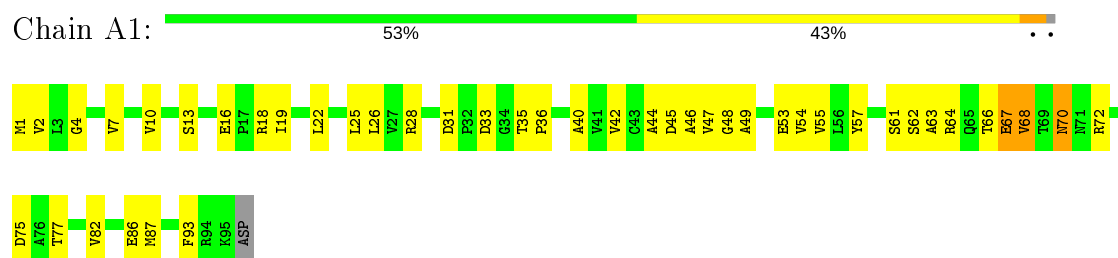
Continued from previous page...

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

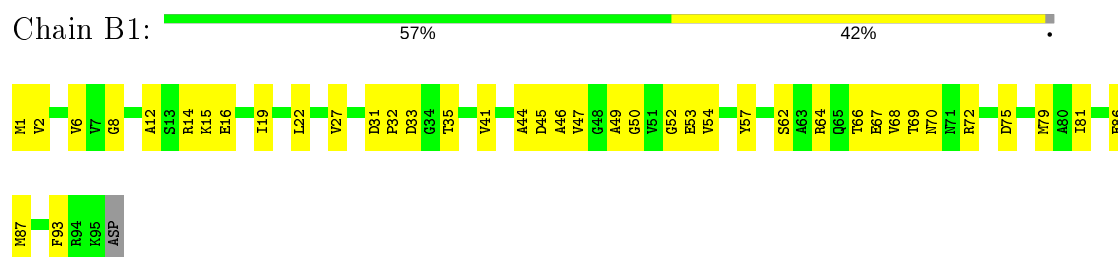
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

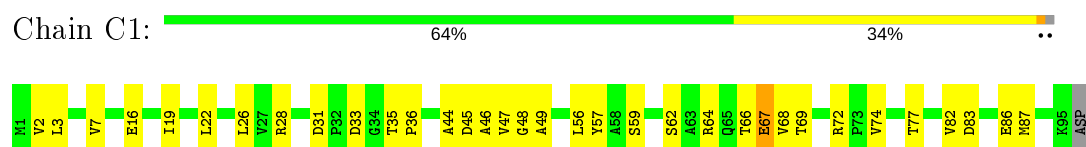
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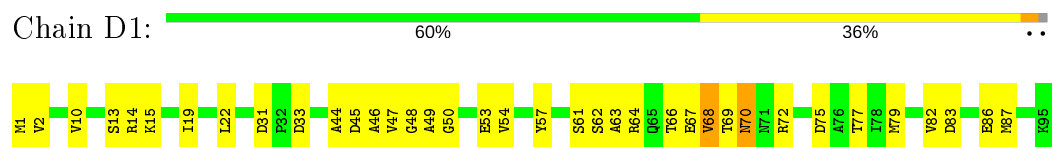
- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



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

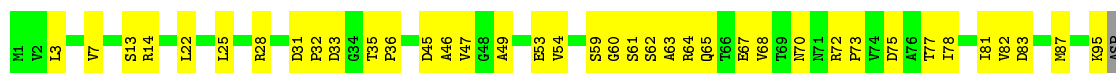


- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



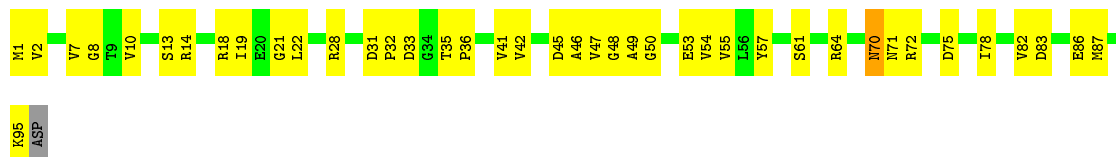
- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI





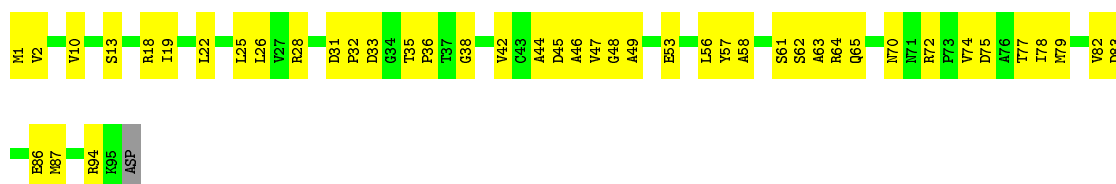
- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

Chain F1: 56% 42% ..



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

Chain G1: 53% 46% .



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

Chain H1: 59% 38% ..



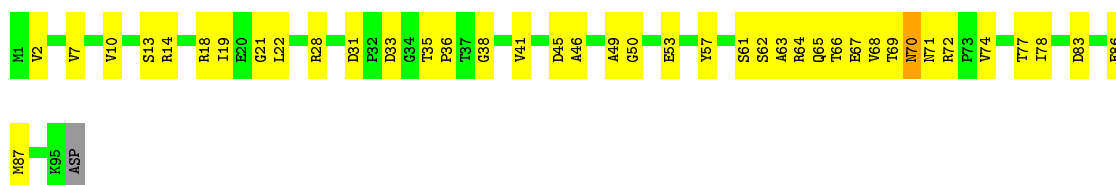
- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

Chain I1: 59% 36% ..

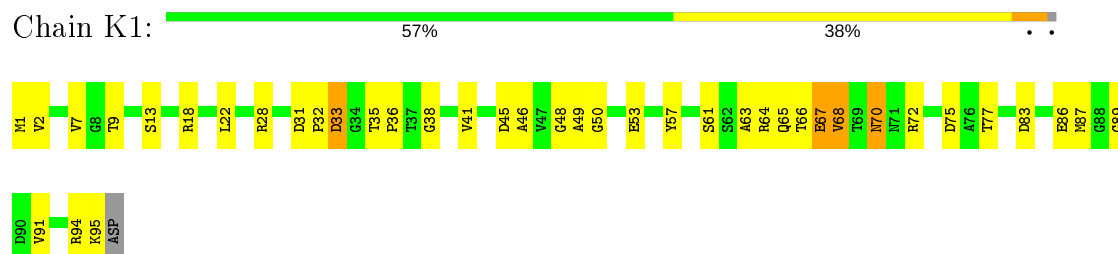


- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

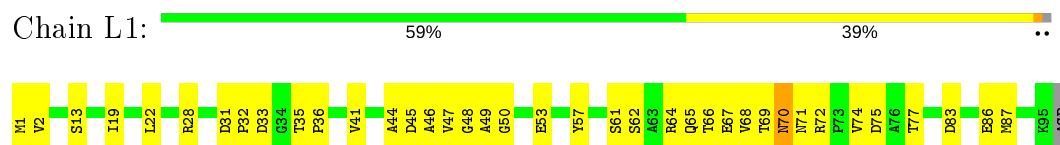
Chain J1: 57% 41% ..



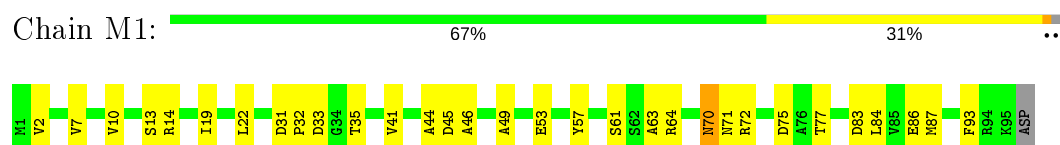
- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



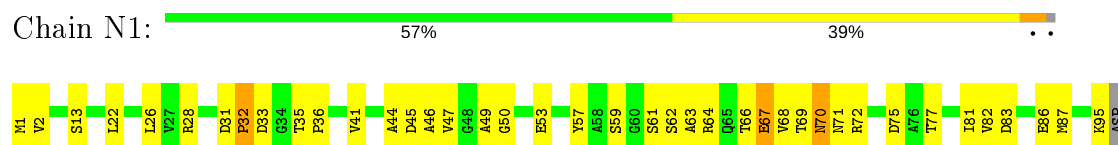
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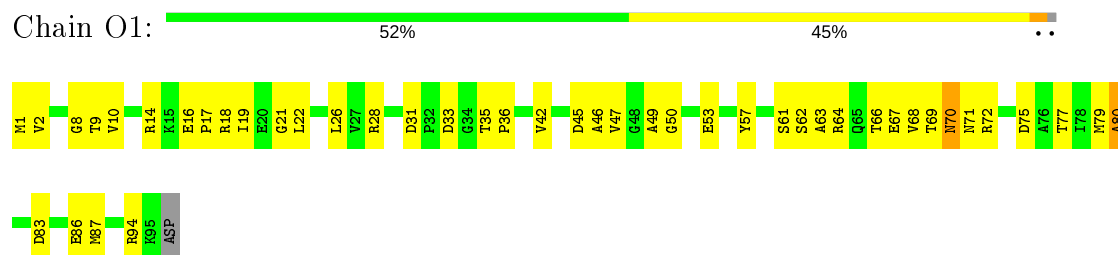
- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



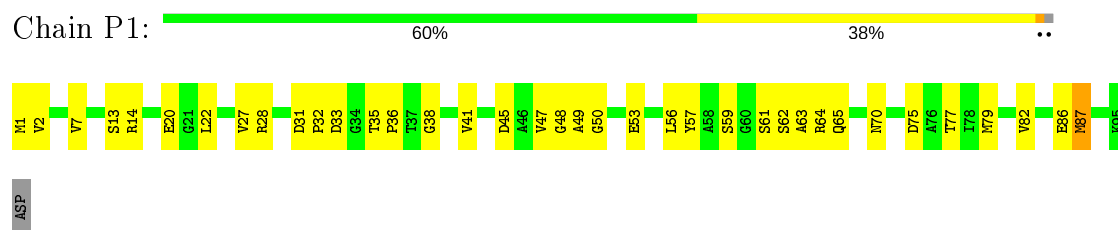
- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI



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



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



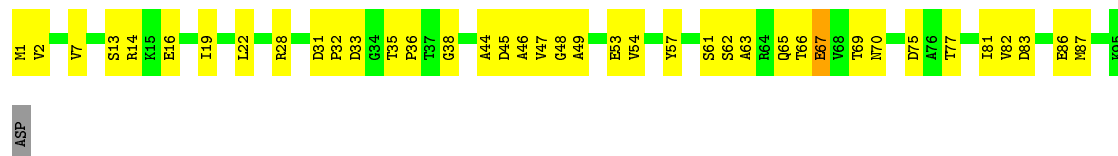
- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

Chain Q1:  61% 36% ..



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

Chain R1:  58% 40% ..



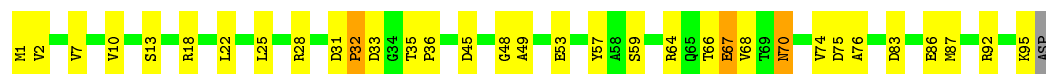
- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

Chain S1:  54% 43% ..



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

Chain T1:  65% 31% ..



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

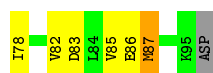
Chain U1:  67% 30% ..



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

Chain V1:  52% 45% ..





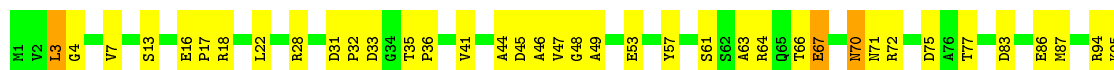
- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

Chain W1: 58% 39% ..



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

Chain X1: 59% 36% ..



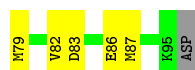
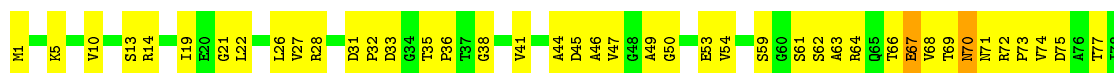
- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

Chain Y1: 63% 35% ..



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

Chain Z1: 50% 47% ..



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

Chain 11: 64% 34% ..



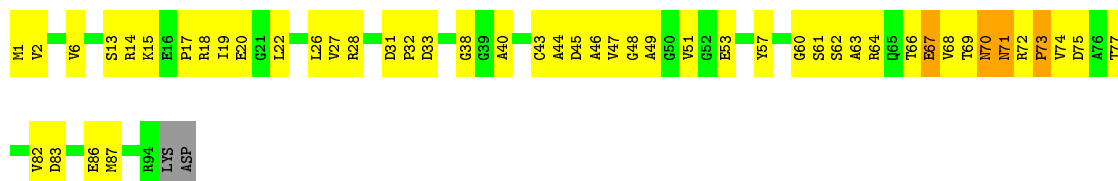
- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

Chain 21:  63% 35% ..



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

Chain 31:  47% 47% . .



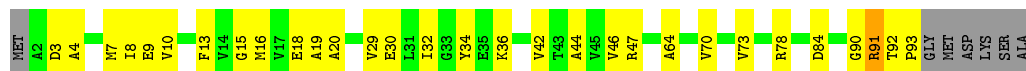
- Molecule 1: Ethanolamine utilization protein EutN/carboxysome structural protein CcmI

Chain 41:  66% 31% ..



- Molecule 2: Microcompartments protein

Chain A2:  63% 29% . 7%



- Molecule 2: Microcompartments protein

Chain A3:  64% 27% . 7%



- Molecule 2: Microcompartments protein

Chain A4:  68% 26% 6%



- Molecule 2: Microcompartments protein

Chain A5:  61% 31% . 7%



ASP
LYS
SER
ALA

• Molecule 2: Microcompartments protein

Chain A6: 71% 21% 7%

MET A2 E9 V10 F13 F14 G15 M16 V17 K25 E30 L31 L32 G33 Y34 E35 K36 T37 A44 V45 V46 R47 P79 D84 L89 G90 R91 T92 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain A7: 65% 27% 7%

MET A2 D3 A4 M7 I8 E9 V10 F13 F14 G15 M16 V17 E18 A19 A20 A21 D21 A22 K23 V24 K25 A26 A27 K28 V29 E30 L31 Y34 E35 K36 A44 R47 G48 D49 V50 A51 A52 A56 G60 A64 R78 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain B2: 61% 30% 8%

MET A2 D3 I8 E9 V10 R11 G12 F13 F14 G15 M16 V17 E18 A19 A20 E30 L31 I32 G33 Y34 E35 K36 G40 T43 A44 V45 V46 R47 A64 V70 V73 H74 R78 P79 D84 L89 G90 R91 T92 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain B3: 54% 38% 7%

MET A2 D3 L5 G6 M7 I8 V10 R11 G12 G15 M16 V17 E18 A19 A20 A21 V24 K25 G33 A36 A27 E30 L31 I32 G33 Y34 E35 K36 T43 R47 G48 A52 V53 A56 T57 A64 V73 H74 V75 R78 P79 D84 G90 R91 T92 P93 GLY

MET
ASP
LYS
SER
ALA

• Molecule 2: Microcompartments protein

Chain B4: 72% 21% 7%

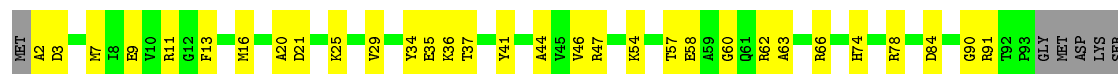
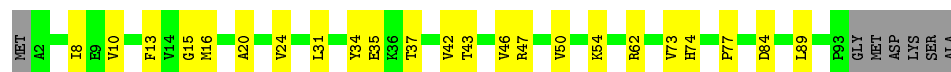
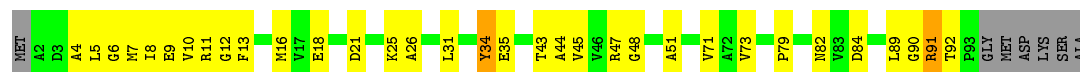
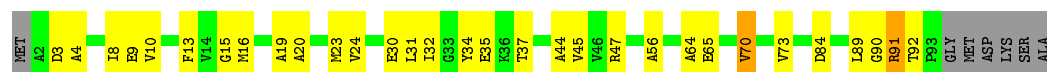
MET A2 V10 F13 F14 G15 M16 V17 E18 A19 A20 L31 Y34 E35 V42 T43 A44 R47 V50 T57 R62 H74 V75 I76 P77 R78 N82 L89 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain B5: 57% 35% 7%

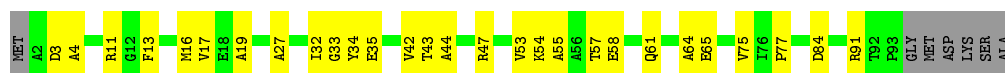
MET A2 D3 L5 I8 E9 V10 F13 F14 G15 M16 V17 E18 V29 E30 Y34 E35 K36 T37 A44 V45 V46 R47 V50 A51 A52 A56 T57 E58 A59 G60 Q61 R62 R66 V73 H74 P77 R78 D84 L89 G90 R91 T92 P93 GLY MET ASP

LYS
SER
ALA



ALA

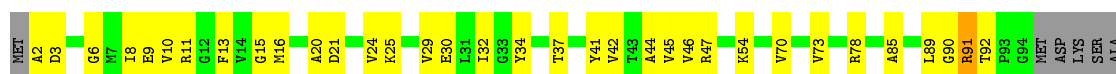




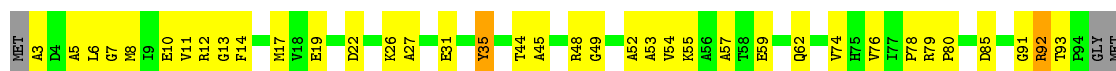
- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



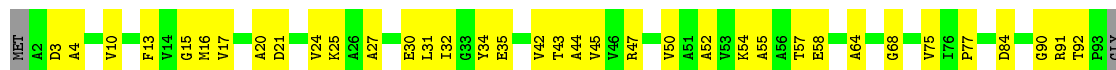
- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



MET
ASP
LYS
SER
ALA

- Molecule 2: Microcompartments protein

Chain D7:  71% 23% 6%

MET A2 M7 I8 E9 V10 G15 M16 V17 A20 P23 A27 E28 L31 Y34 E35 K36 T37 D49 V50 A51 A52 V53 A56 V73 P77 R78 T92 P93 G94 MET ASP LYS SER ALA

- Molecule 2: Microcompartments protein

Chain E2:  66% 27% 5%

MET A2 D3 A4 I8 E9 V10 F13 M16 G15 M16 A19 E30 L31 T32 G33 Y34 E35 K36 T37 Y41 V42 T43 A44 R47 A64 G68 E69 V70 V71 A72 V73 D84 G90 R91 T92 R95 GLY ASP LYS SER ALA

- Molecule 2: Microcompartments protein

Chain E3:  65% 27% 7%

MET A2 L5 M7 T8 E9 G12 E18 A19 A26 T32 G33 Y34 E35 T43 A44 V45 V46 R47 V53 A64 V71 A72 V73 R78 P79 R82 T83 D84 L89 G90 R91 T92 P93 GLY MET ASP LYS SER ALA

- Molecule 2: Microcompartments protein

Chain E4:  71% 24% 5%

MET A2 D3 E9 V10 F13 V14 G15 M16 E30 L31 Y34 V42 T43 A44 V45 V46 R47 V50 T57 R62 R66 V73 H74 P77 R78 L89 G90 R91 R95 ASP LYS SER ALA

- Molecule 2: Microcompartments protein

Chain E5:  64% 28% 7%

MET A2 M7 I8 E9 V10 G11 G12 F13 V14 G15 M16 V17 E18 E30 A19 A20 D21 V24 K25 I32 G33 Y34 E35 T37 T43 A44 R47 T57 G60 R66 V73 P77 R78 D84 G90 R91 T92 P93 GLY MET ASP LYS SER ALA

- Molecule 2: Microcompartments protein

Chain E6:  57% 36% 7%

MET A2 L5 G6 M7 I8 E9 V10 G15 M16 V17 E18 E30 L31 T32 G33 Y34 E35 K36 G40 Y41 V42 T43 A44 V45 V46 R47 A51 A52 V53 K54 A55 A56 T57 G60 Q61 A64 E65 V73 H74 V75 I76 P79 D84 G90 R91 T92 P93 GLY

MET
ASP
LYS
SER
ALA

- Molecule 2: Microcompartments protein

Chain E7:  64% 29% 7%



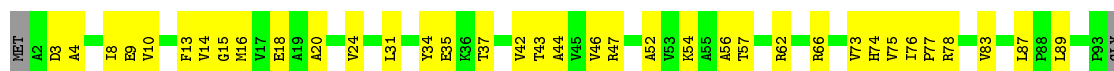
- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



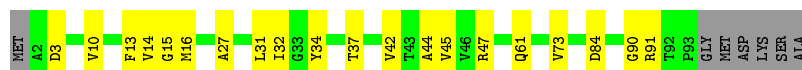
- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein




- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



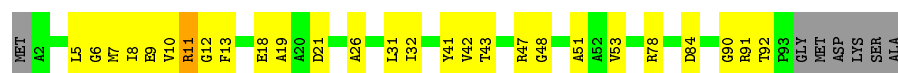
- Molecule 2: Microcompartments protein

Chain G2: 



- Molecule 2: Microcompartments protein

Chain G3: 



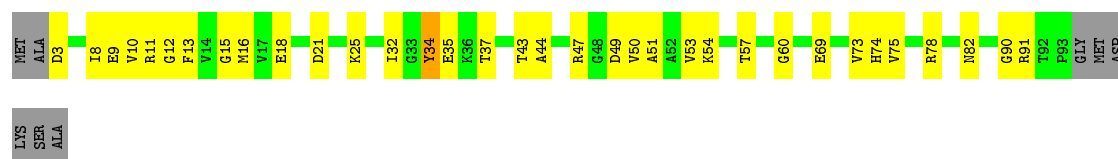
- Molecule 2: Microcompartments protein

Chain G4: 



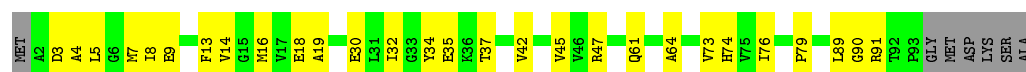
- Molecule 2: Microcompartments protein

Chain G5: 



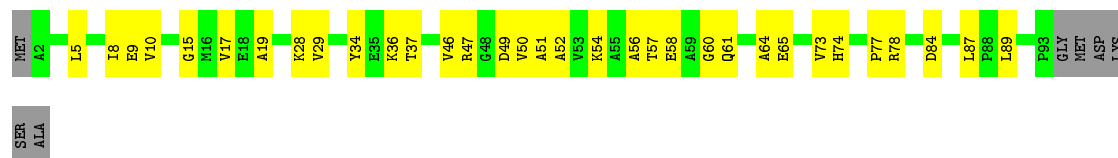
- Molecule 2: Microcompartments protein

Chain G6: 



- Molecule 2: Microcompartments protein

Chain G7: 



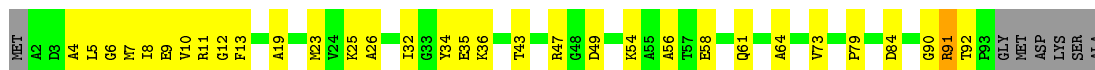
- Molecule 2: Microcompartments protein

Chain H2: 



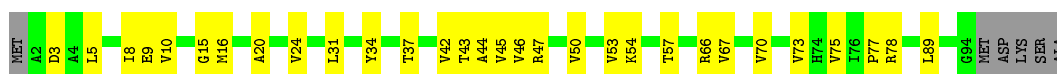
- Molecule 2: Microcompartments protein

Chain H3: 61% 31% 7%



- Molecule 2: Microcompartments protein

Chain H4: 64% 30% 6%



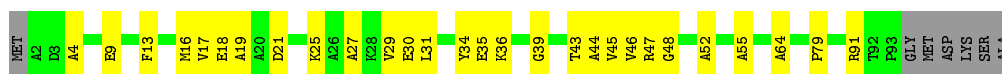
- Molecule 2: Microcompartments protein

Chain H5: 63% 28% 8%



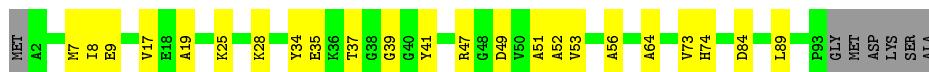
- Molecule 2: Microcompartments protein

Chain H6: 65% 28% 7%



- Molecule 2: Microcompartments protein

Chain H7: 70% 23% 7%



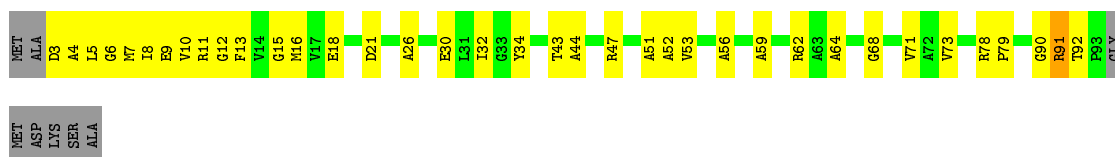
- Molecule 2: Microcompartments protein

Chain I2: 60% 31% 7%



- Molecule 2: Microcompartments protein

Chain I3: 55% 36% 8%



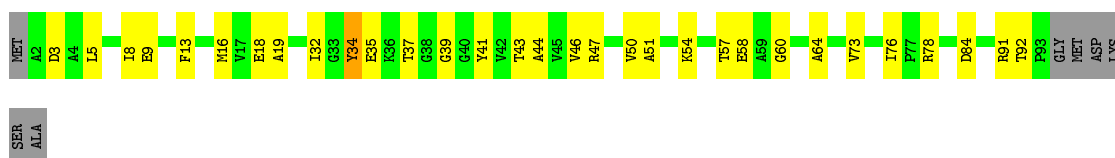
- Molecule 2: Microcompartments protein

Chain I4: 63% 30% 7%



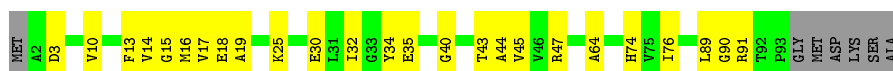
- Molecule 2: Microcompartments protein

Chain I5: 62% 30% 7%



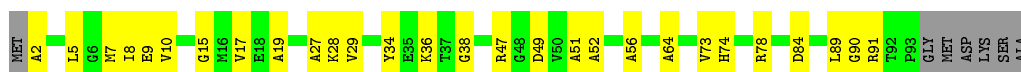
- Molecule 2: Microcompartments protein

Chain I6: 68% 25% 7%



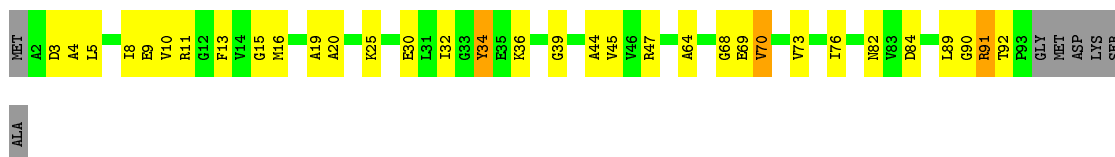
- Molecule 2: Microcompartments protein

Chain I7: 65% 28% 7%



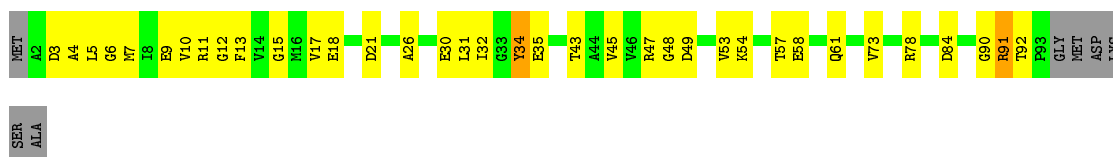
- Molecule 2: Microcompartments protein

Chain J2: 60% 30% 7%



- Molecule 2: Microcompartments protein

Chain J3: 57% 34% 7%



• Molecule 2: Microcompartments protein

Chain J4: 65% 28% 7%



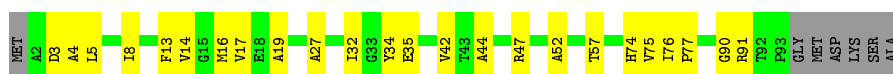
• Molecule 2: Microcompartments protein

Chain J5: 66% 25% 8%



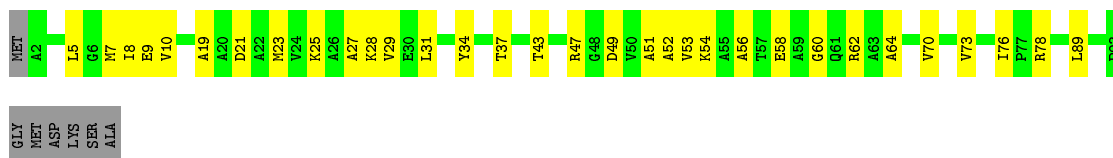
• Molecule 2: Microcompartments protein

Chain J6: 69% 24% 7%



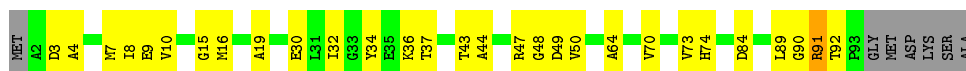
• Molecule 2: Microcompartments protein

Chain J7: 61% 32% 7%



• Molecule 2: Microcompartments protein

Chain K2: 64% 28% 7%



• Molecule 2: Microcompartments protein

Chain K3: 72% 20% 7%



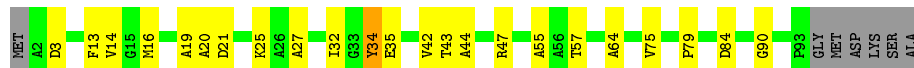
• Molecule 2: Microcompartments protein

Chain K4:  69% 23% 7%


• Molecule 2: Microcompartments protein

Chain K5:  73% 20% 6%

• Molecule 2: Microcompartments protein

Chain K6:  70% 22% 7%

• Molecule 2: Microcompartments protein

Chain K7:  73% 21% 6%

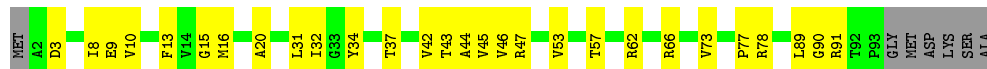
• Molecule 2: Microcompartments protein

Chain L2:  62% 31% 5%

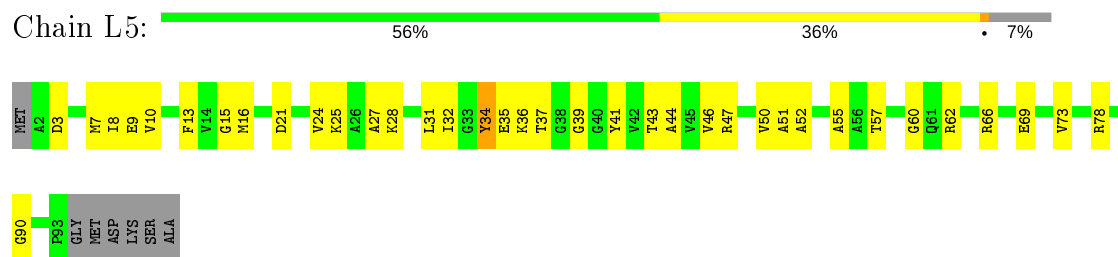
• Molecule 2: Microcompartments protein

Chain L3:  68% 24% 7%

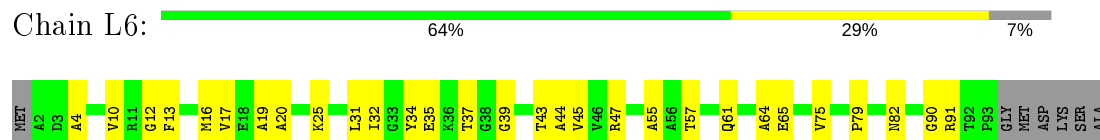
• Molecule 2: Microcompartments protein

Chain L4:  65% 28% 7%

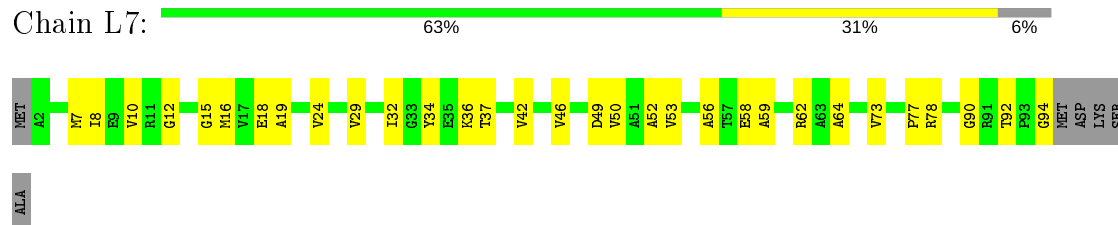
• Molecule 2: Microcompartments protein



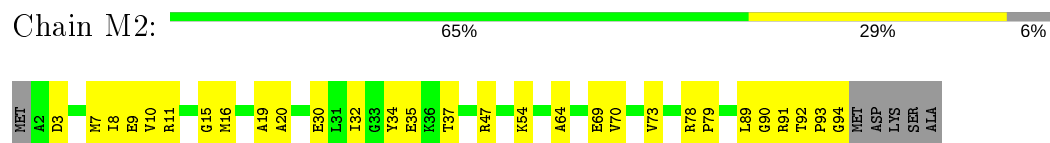
- Molecule 2: Microcompartments protein



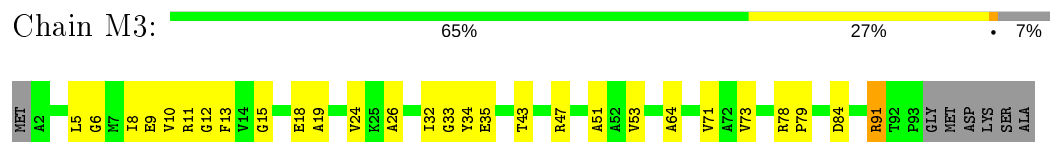
- Molecule 2: Microcompartments protein



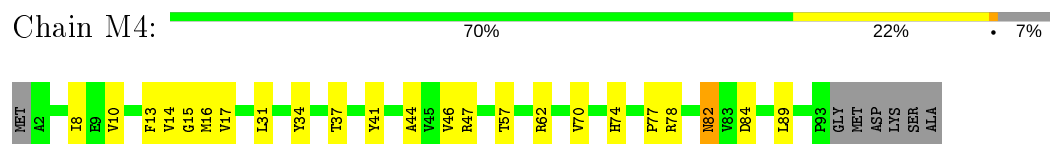
- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein

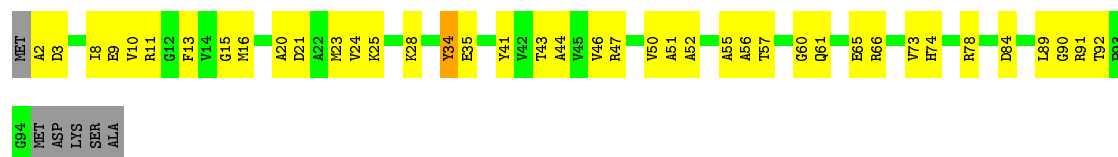


- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein





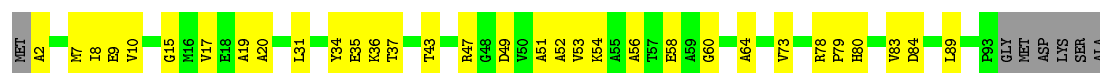
- Molecule 2: Microcompartments protein

Chain M6:



- Molecule 2: Microcompartments protein

Chain M7:



- Molecule 2: Microcompartments protein

Chain N2:



- Molecule 2: Microcompartments protein

Chain N3:



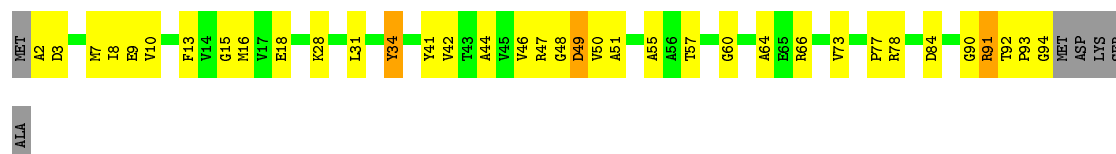
- Molecule 2: Microcompartments protein

Chain N4:



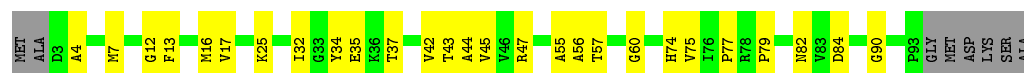
- Molecule 2: Microcompartments protein

Chain N5:



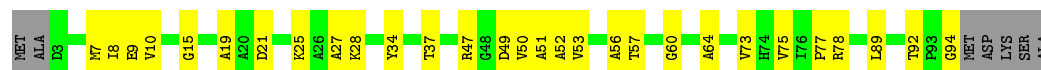
- Molecule 2: Microcompartments protein

Chain N6: 



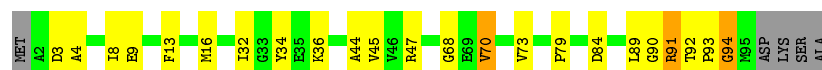
- Molecule 2: Microcompartments protein

Chain N7: 



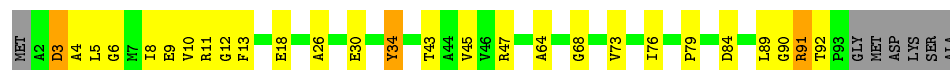
- Molecule 2: Microcompartments protein

Chain O2: 




- Molecule 2: Microcompartments protein

Chain O3: 



- Molecule 2: Microcompartments protein

Chain O4: 



- Molecule 2: Microcompartments protein

Chain O5: 



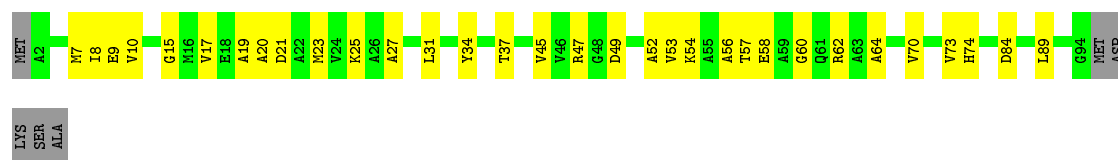
- Molecule 2: Microcompartments protein

Chain O6: 



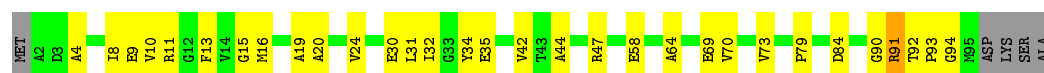
- Molecule 2: Microcompartments protein

Chain O7: 



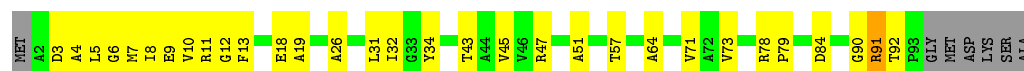
- Molecule 2: Microcompartments protein

Chain P2: 



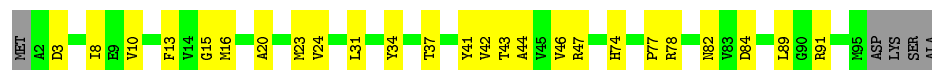
- Molecule 2: Microcompartments protein

Chain P3: 



- Molecule 2: Microcompartments protein

Chain P4: 



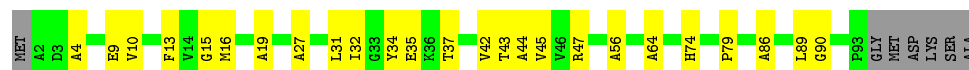
- Molecule 2: Microcompartments protein

Chain P5: 



- Molecule 2: Microcompartments protein

Chain P6: 

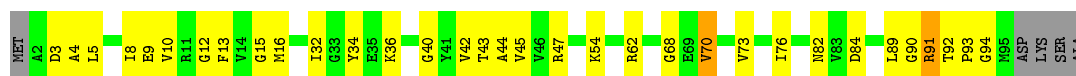


- Molecule 2: Microcompartments protein

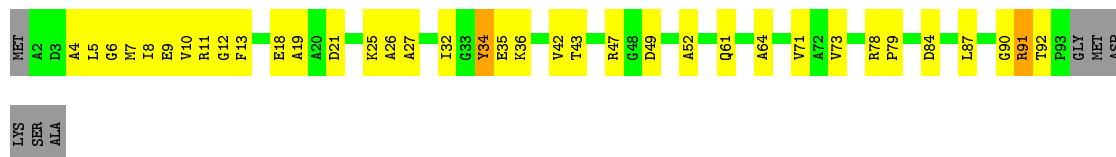
Chain P7: 




• Molecule 2: Microcompartments protein

Chain Q2:  62% 31% 5%

• Molecule 2: Microcompartments protein

Chain Q3:  57% 34% 7%


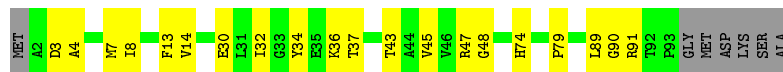
• Molecule 2: Microcompartments protein

Chain Q4:  % 70% 25% 5%

• Molecule 2: Microcompartments protein

Chain Q5:  62% 32% 6%

• Molecule 2: Microcompartments protein

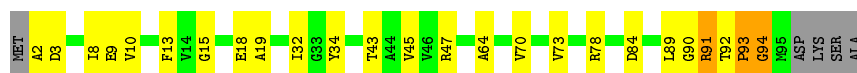
Chain Q6:  73% 20% 7%

• Molecule 2: Microcompartments protein

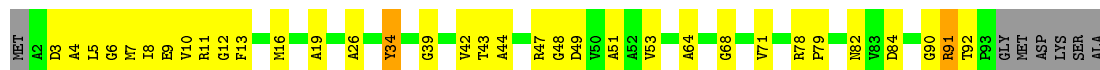
Chain Q7:  68% 26% 6%

• Molecule 2: Microcompartments protein

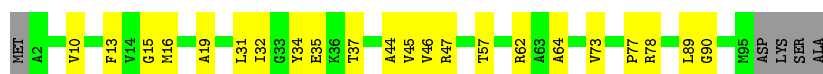
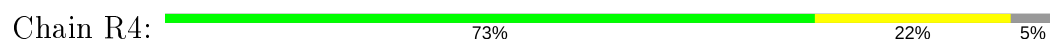
Chain R2:  70% 22% 5%



• Molecule 2: Microcompartments protein



• Molecule 2: Microcompartments protein



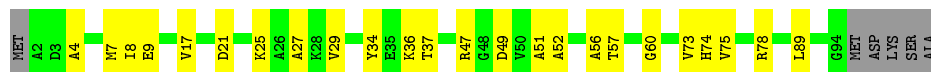
• Molecule 2: Microcompartments protein



• Molecule 2: Microcompartments protein



• Molecule 2: Microcompartments protein

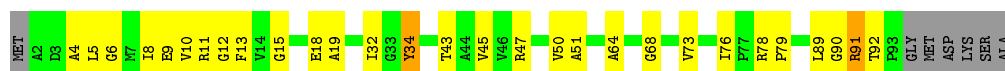


• Molecule 2: Microcompartments protein



• Molecule 2: Microcompartments protein





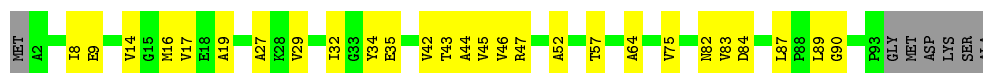
- Molecule 2: Microcompartments protein



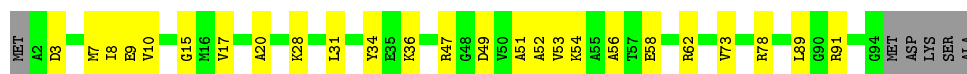
- Molecule 2: Microcompartments protein



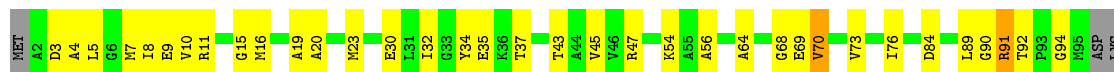
- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



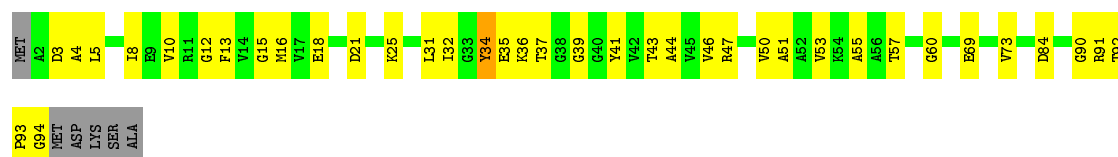
- Molecule 2: Microcompartments protein

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: 



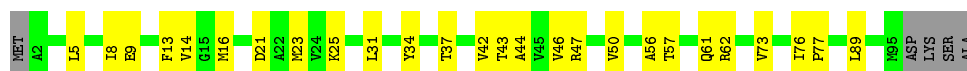
- Molecule 2: Microcompartments protein

Chain U3: 



- Molecule 2: Microcompartments protein

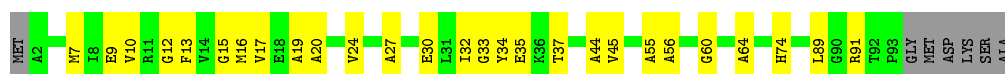
Chain U4: 



- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein

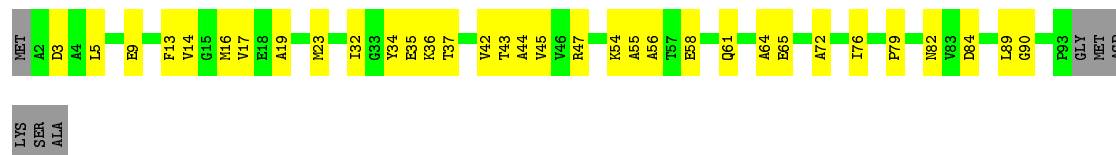


- Molecule 2: Microcompartments protein





- Molecule 2: Microcompartments protein



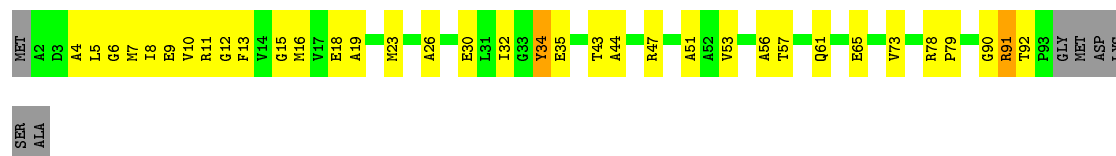
- Molecule 2: Microcompartments protein



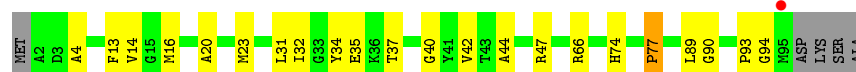
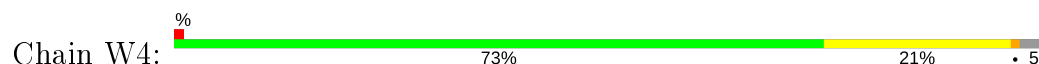
- Molecule 2: Microcompartments protein



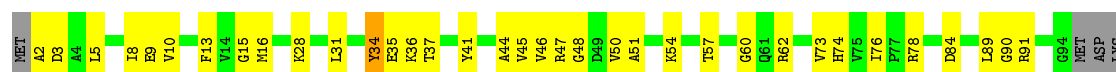
- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



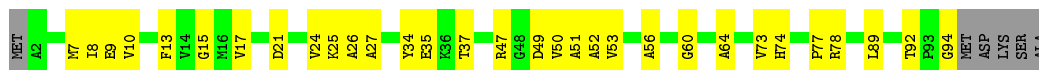
SER
ALA

- Molecule 2: Microcompartments protein

Chain W6:  66% 27% 7%

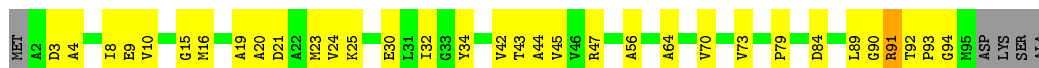

Residue map for Chain W6 showing quality scores for each residue. The map includes residues from MET to ALA, with colors indicating quality: green (good), yellow (moderate), and grey (poor).

- Molecule 2: Microcompartments protein

Chain W7:  63% 31% 6%


Residue map for Chain W7 showing quality scores for each residue. The map includes residues from MET to ALA, with colors indicating quality: green (good), yellow (moderate), and grey (poor).

- Molecule 2: Microcompartments protein

Chain X2:  62% 32% 5%


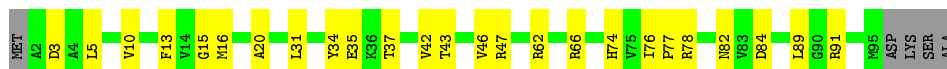
Residue map for Chain X2 showing quality scores for each residue. The map includes residues from MET to ALA, with colors indicating quality: green (good), yellow (moderate), and grey (poor).

- Molecule 2: Microcompartments protein

Chain X3:  61% 30% 7%

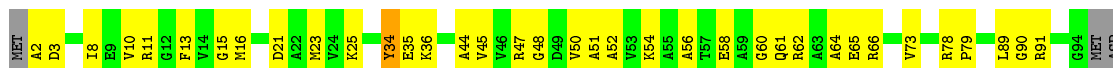

Residue map for Chain X3 showing quality scores for each residue. The map includes residues from MET to ALA, with colors indicating quality: green (good), yellow (moderate), and grey (poor).

- Molecule 2: Microcompartments protein

Chain X4:  70% 25% 5%


Residue map for Chain X4 showing quality scores for each residue. The map includes residues from MET to ALA, with colors indicating quality: green (good), yellow (moderate), and grey (poor).

- Molecule 2: Microcompartments protein

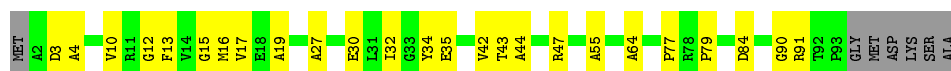
Chain X5:  58% 35% 6%


Residue map for Chain X5 showing quality scores for each residue. The map includes residues from MET to ASP, with colors indicating quality: green (good), yellow (moderate), and grey (poor).

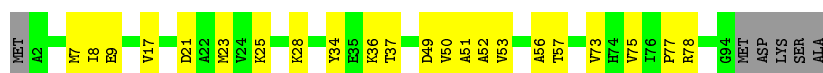
LYS
SER
ALA

- Molecule 2: Microcompartments protein

Chain X6:  68% 25% 7%



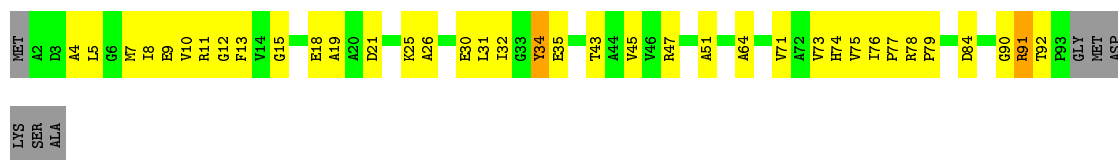
- Molecule 2: Microcompartments protein



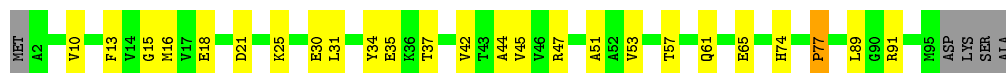
- Molecule 2: Microcompartments protein



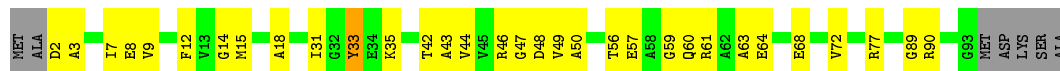
- Molecule 2: Microcompartments protein



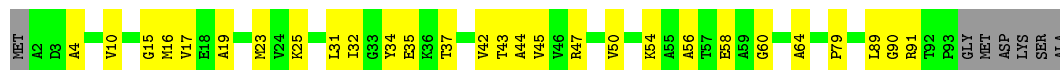
- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein

Chain Y7:  72% 22% 6%



- Molecule 2: Microcompartments protein

Chain Z2:  68% 25% 5%




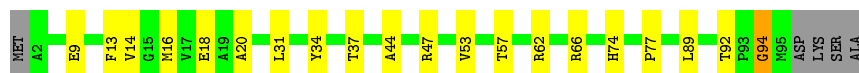
- Molecule 2: Microcompartments protein

Chain Z3:  60% 32% 7%



- Molecule 2: Microcompartments protein

Chain Z4:  75% 19% 5%



- Molecule 2: Microcompartments protein

Chain Z5:  69% 25% 6%



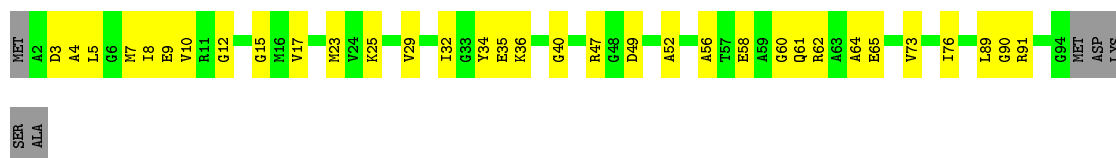
- Molecule 2: Microcompartments protein

Chain Z6:  70% 23% 7%



- Molecule 2: Microcompartments protein

Chain Z7:  61% 33% 6%



- Molecule 2: Microcompartments protein

Chain 12:  62% 30% 5%




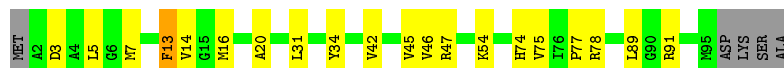
- Molecule 2: Microcompartments protein

Chain 13:  60% 32% 7%



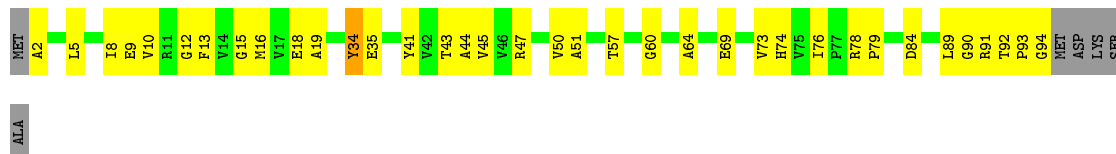
- Molecule 2: Microcompartments protein

Chain 14:  75% 19% 5%



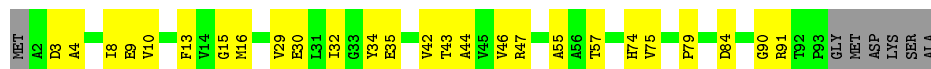
- Molecule 2: Microcompartments protein

Chain 15:  58% 35% 6%




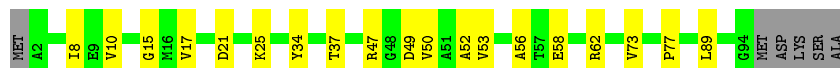
- Molecule 2: Microcompartments protein

Chain 16:  67% 26% 7%



- Molecule 2: Microcompartments protein

Chain 17:  75% 19% 6%

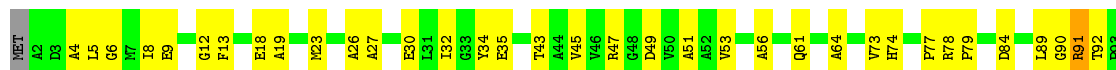


- Molecule 2: Microcompartments protein

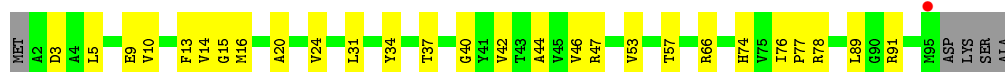
Chain 22:  68% 25% 5%



- Molecule 2: Microcompartments protein



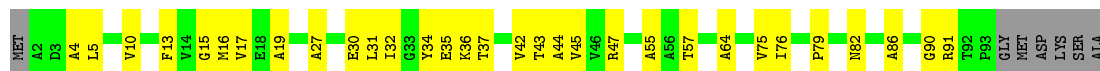
- Molecule 2: Microcompartments protein



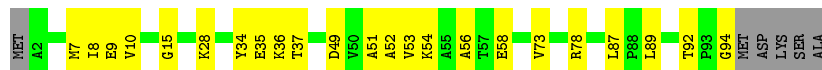
- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein



- Molecule 2: Microcompartments protein

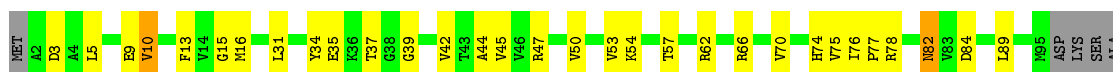


SER
ALA

• Molecule 2: Microcompartments protein

Chain 33:  63% 28% 7%

• Molecule 2: Microcompartments protein

Chain 34:  64% 29% 5%

• Molecule 2: Microcompartments protein

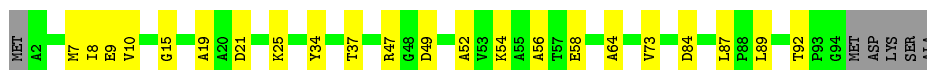
Chain 35:  61% 32% 6%

ALA

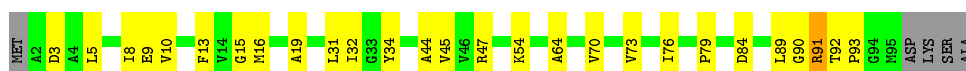
• Molecule 2: Microcompartments protein

Chain 36:  69% 24% 7%

• Molecule 2: Microcompartments protein

Chain 37:  72% 22% 6%

• Molecule 2: Microcompartments protein

Chain 42:  68% 26% 5%

• Molecule 2: Microcompartments protein

Chain 43:  61% 31% 7%



- Molecule 2: Microcompartments protein

Chain 44: 75% 20% 5%



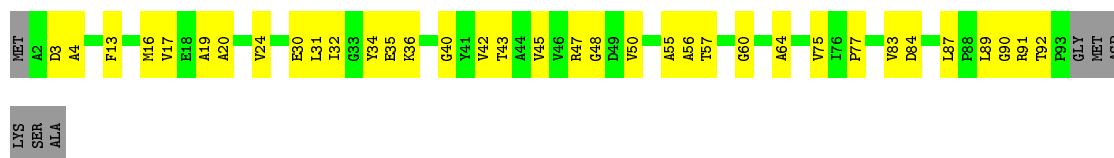
- Molecule 2: Microcompartments protein

Chain 45: 66% 25% 6%



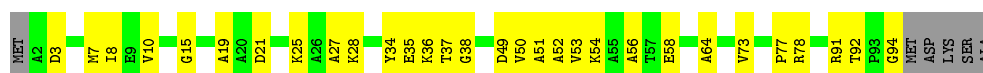
- Molecule 2: Microcompartments protein

Chain 46: 58% 35% 7%



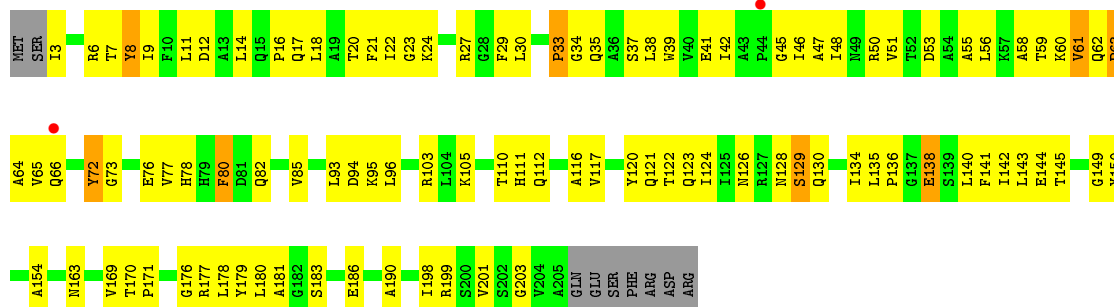
- Molecule 2: Microcompartments protein

Chain 47: 64% 30% 6%

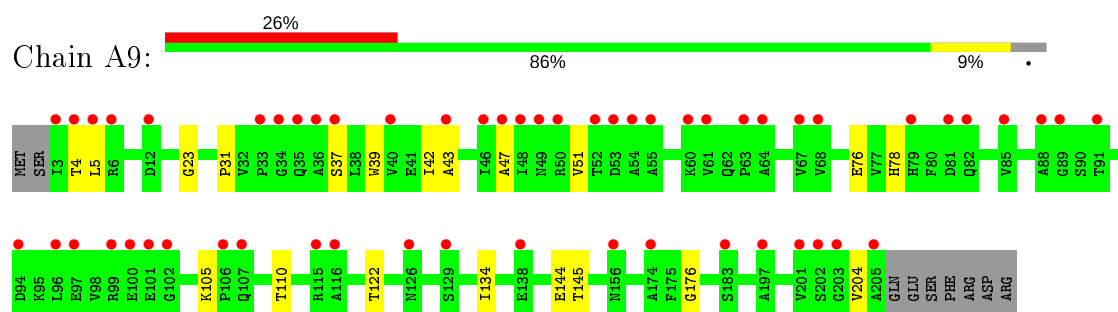


- Molecule 3: Microcompartments protein

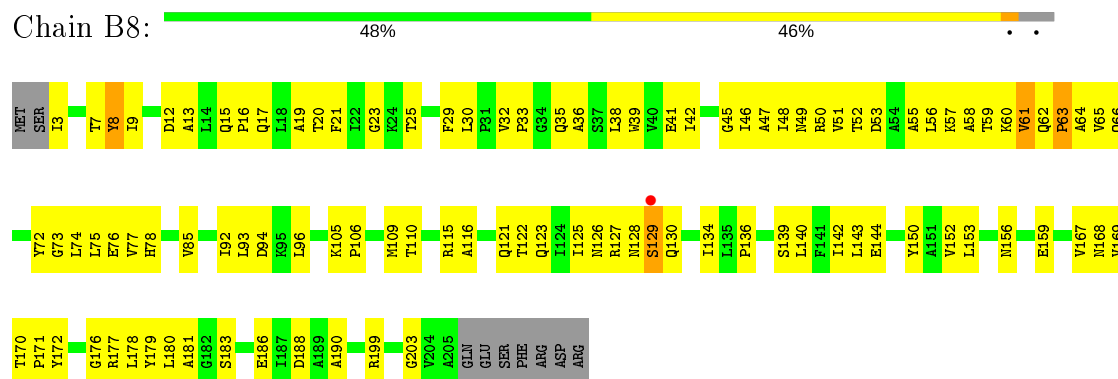
Chain A8: 47% 45% 6%



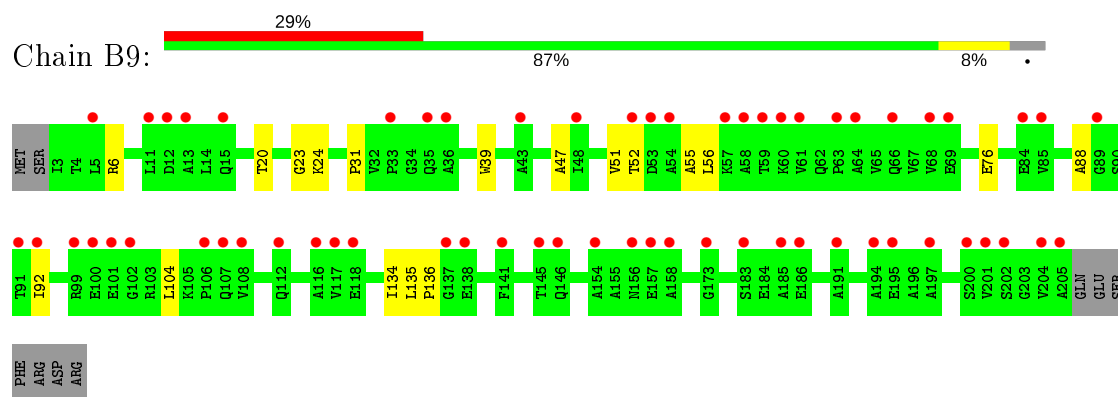
- Molecule 3: Microcompartments protein



• Molecule 3: Microcompartments protein



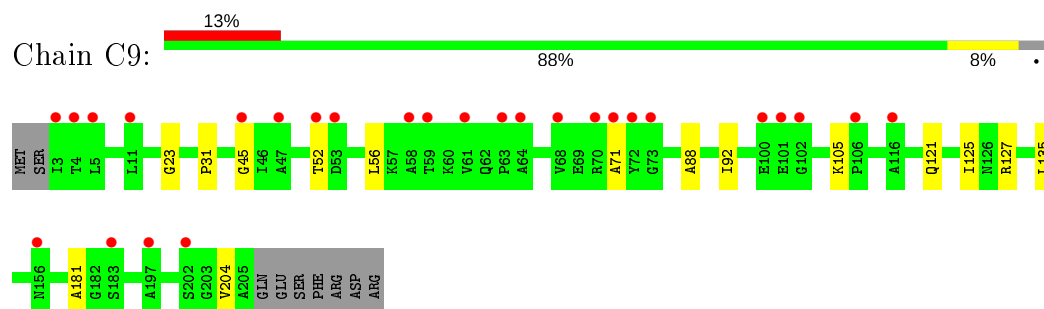
• Molecule 3: Microcompartments protein



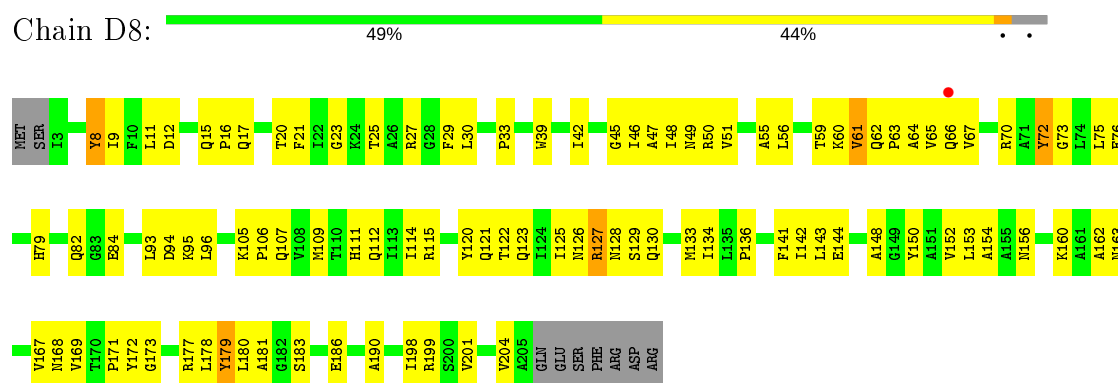
• Molecule 3: Microcompartments protein



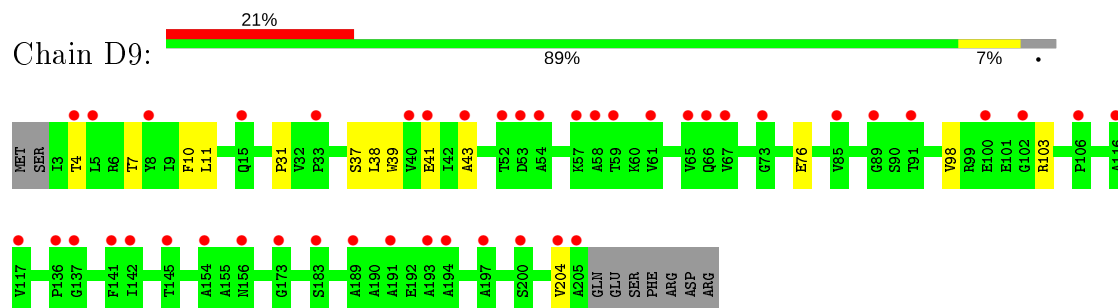
- Molecule 3: Microcompartments protein



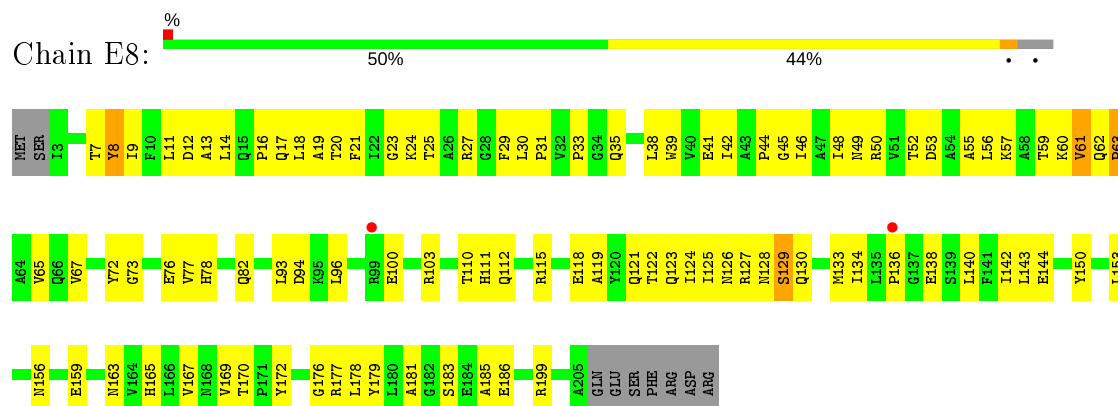
- Molecule 3: Microcompartments protein



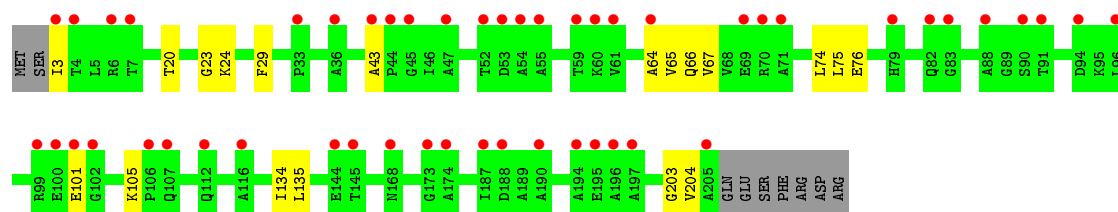
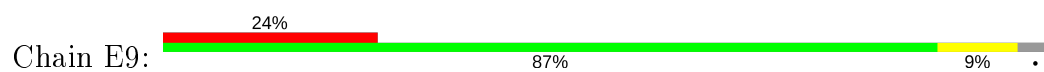
- Molecule 3: Microcompartments protein



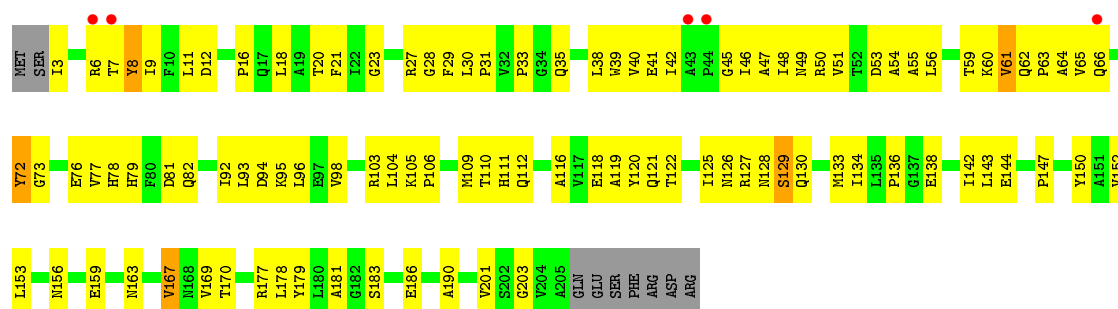
- Molecule 3: Microcompartments protein



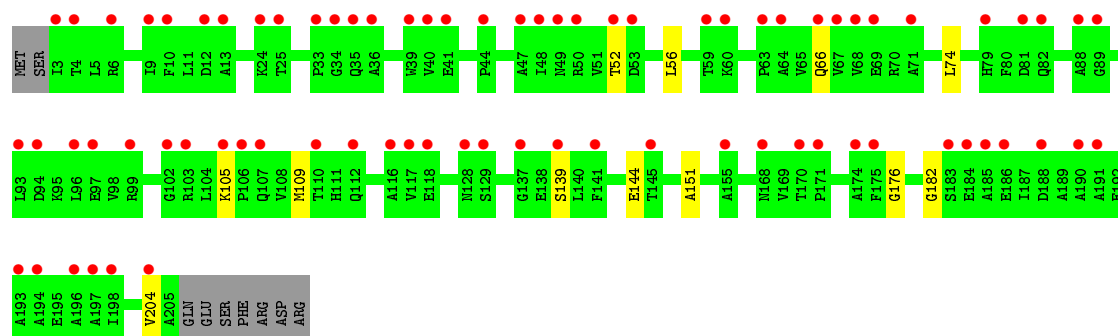
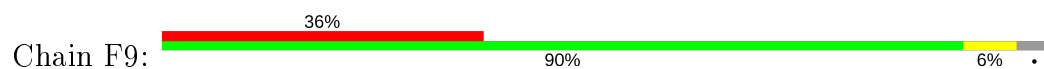
- Molecule 3: Microcompartments protein



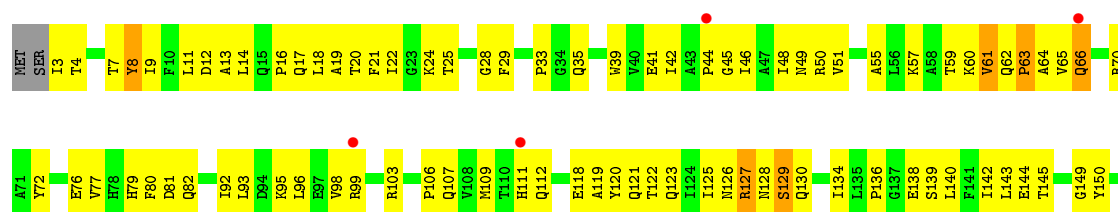
• Molecule 3: Microcompartments protein



• Molecule 3: Microcompartments protein

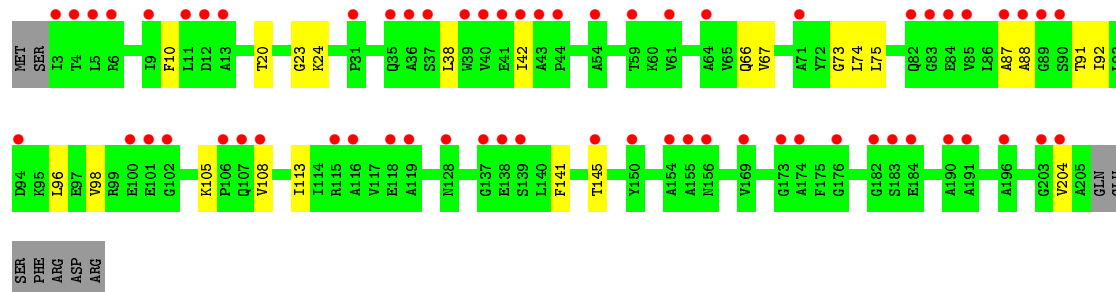
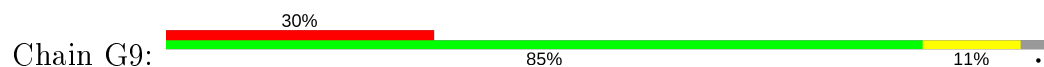


• Molecule 3: Microcompartments protein

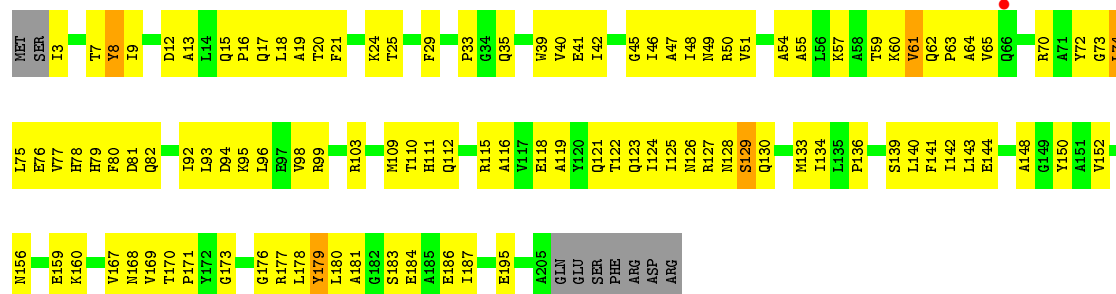




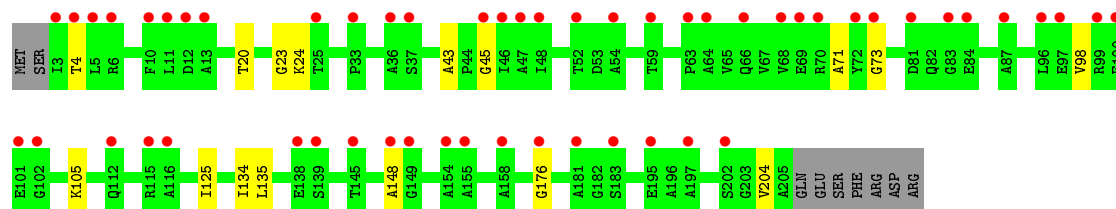
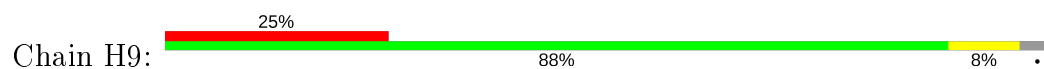
• Molecule 3: Microcompartments protein



• Molecule 3: Microcompartments protein

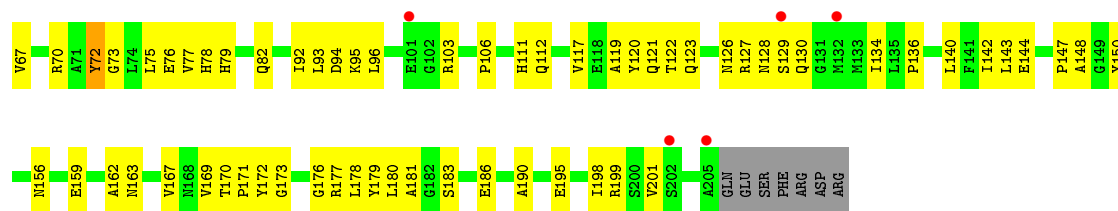


• Molecule 3: Microcompartments protein

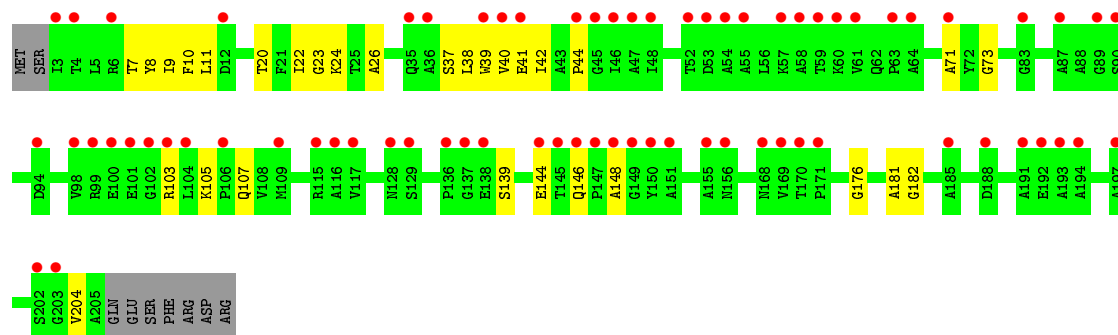
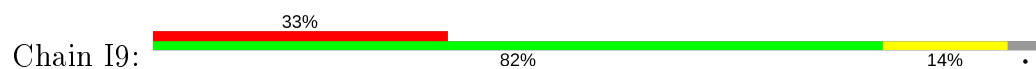


• Molecule 3: Microcompartments protein

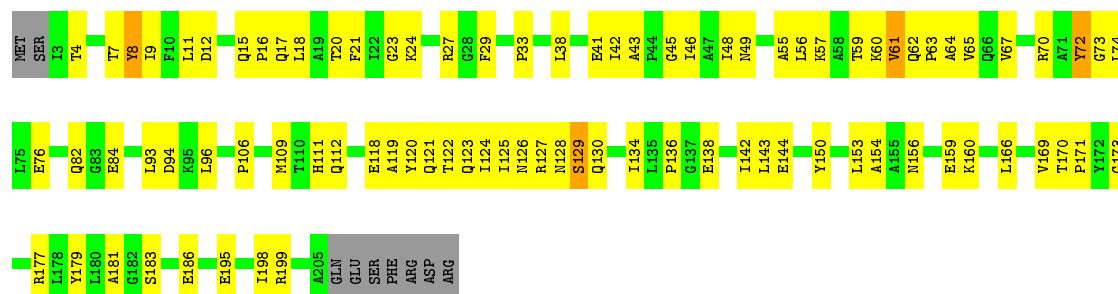




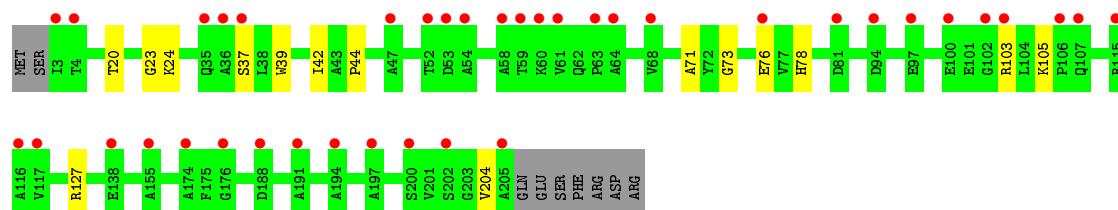
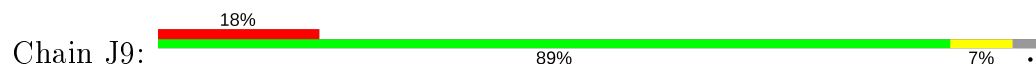
• Molecule 3: Microcompartment protein



• Molecule 3: Microcompartment protein

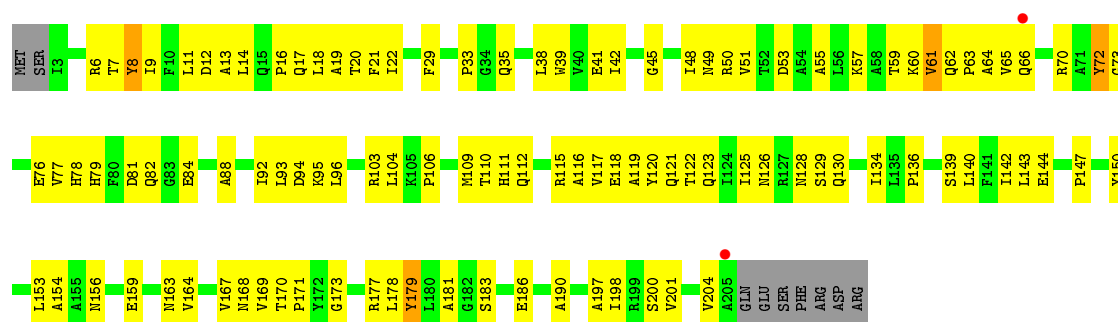


• Molecule 3: Microcompartment protein

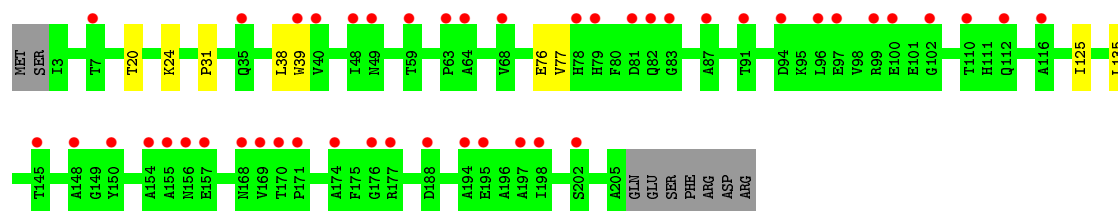


• Molecule 3: Microcompartment protein

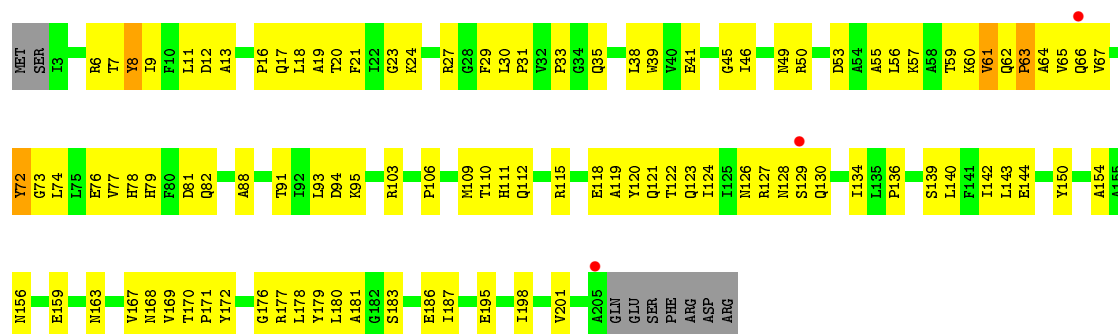




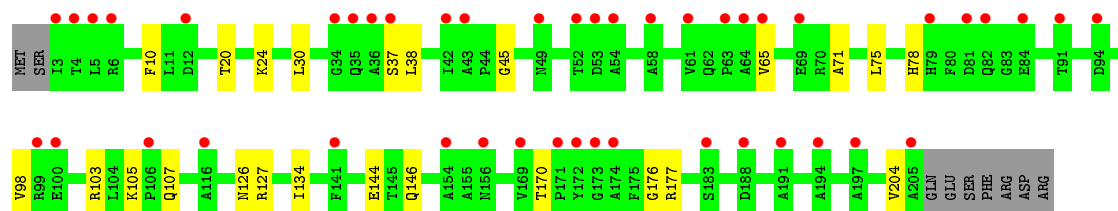
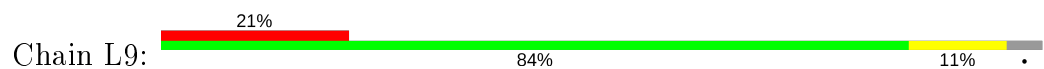
• Molecule 3: Microcompartments protein



• Molecule 3: Microcompartments protein

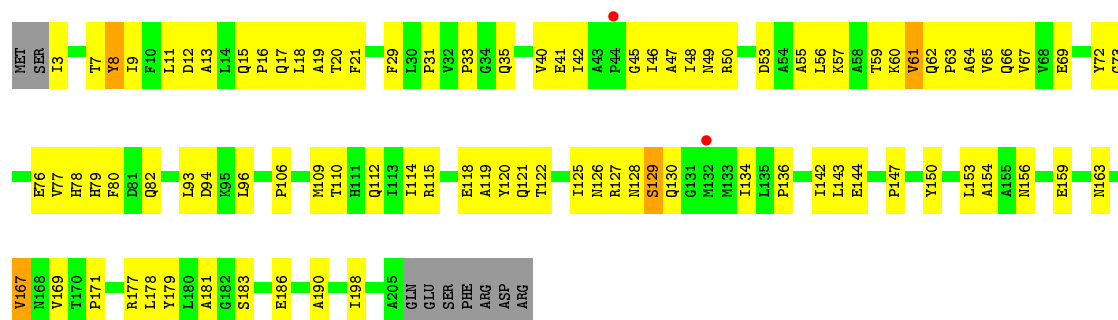


• Molecule 3: Microcompartments protein

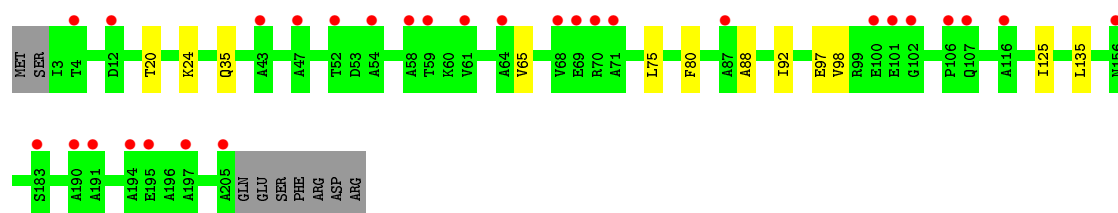
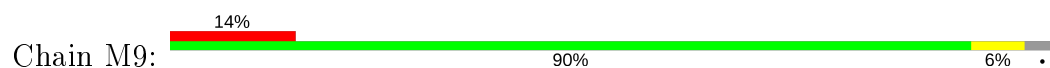


• Molecule 3: Microcompartments protein

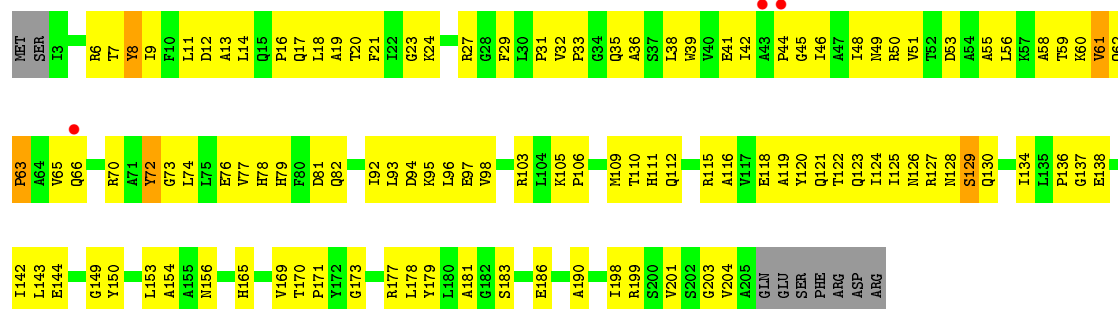




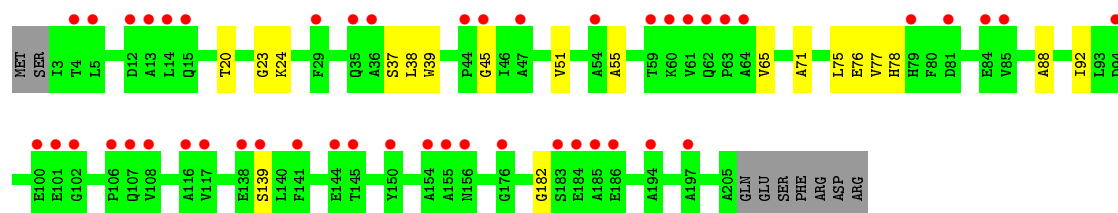
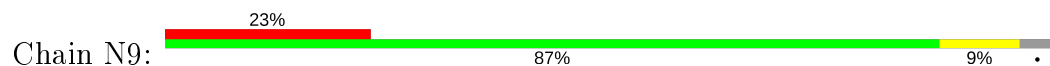
- Molecule 3: Microcompartments protein



- Molecule 3: Microcompartments protein

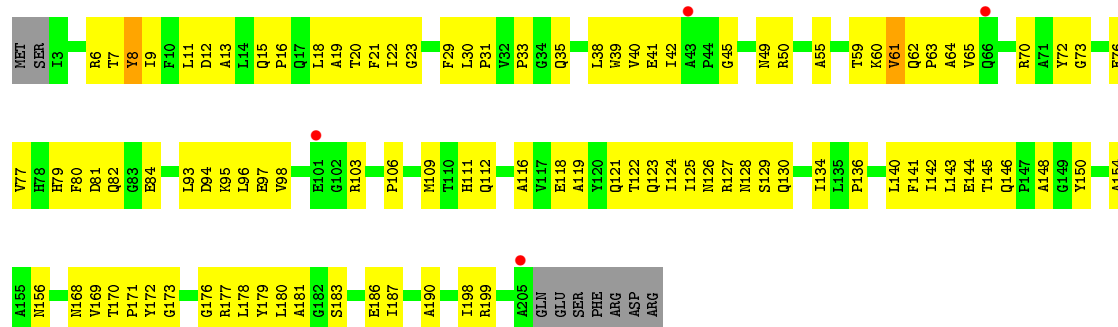


- Molecule 3: Microcompartments protein

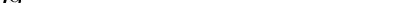


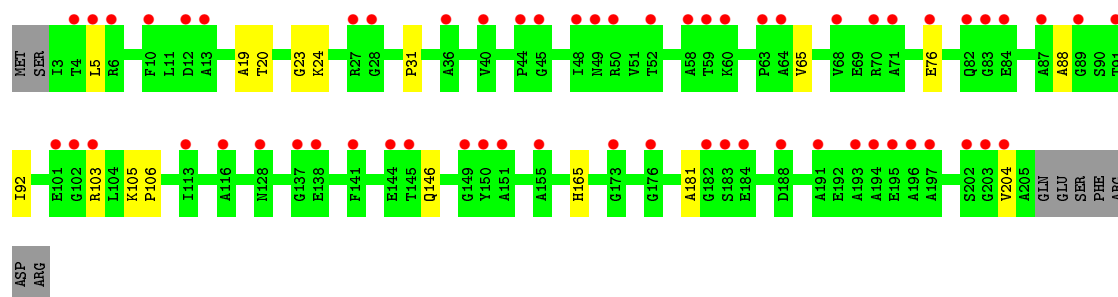
- Molecule 3: Microcompartments protein





- Molecule 3: Microcompartments protein

Chain Q9:  29% 88% 8%




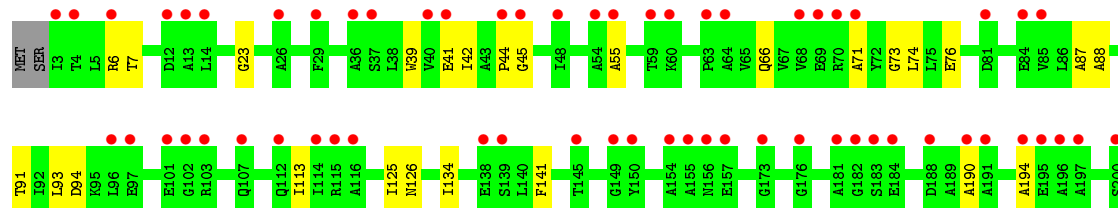
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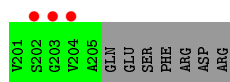
Chain R8:  2% 39% 54% . .



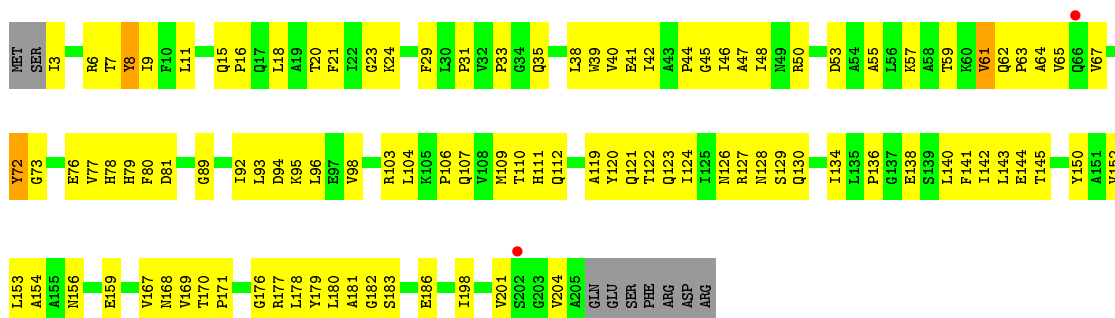
- Molecule 3: Microcompartments protein

Chain R9:  30% 83% 12%

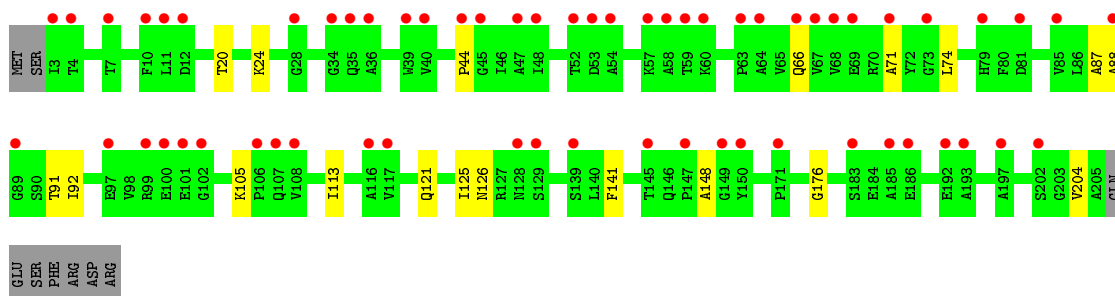
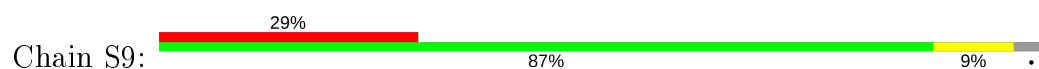




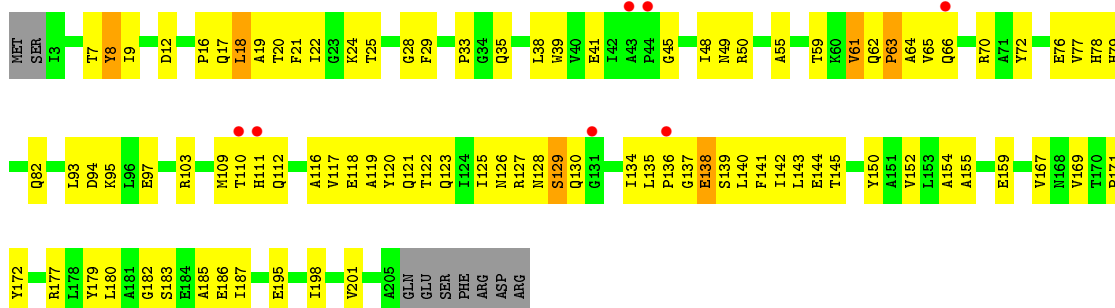
• Molecule 3: Microcompartments protein



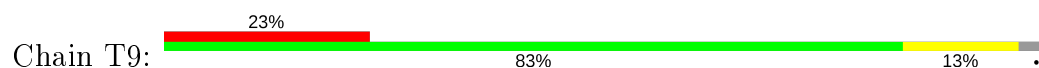
• Molecule 3: Microcompartments protein



• Molecule 3: Microcompartments protein



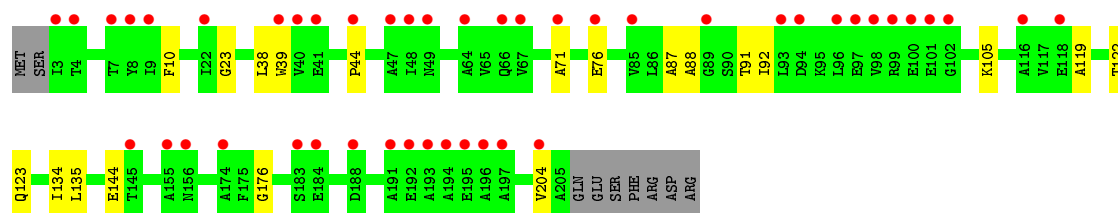
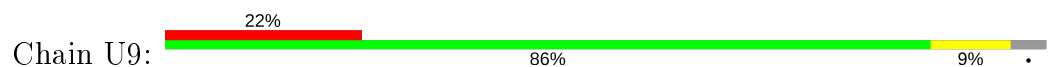
• Molecule 3: Microcompartments protein



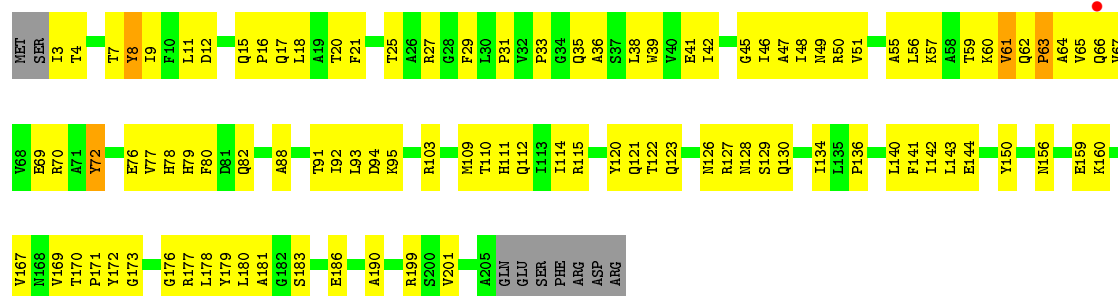
- Molecule 3: Microcompartments protein



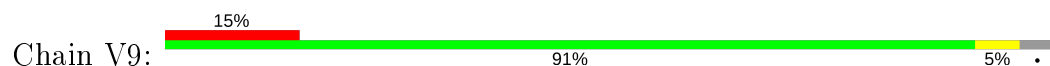
- Molecule 3: Microcompartments protein

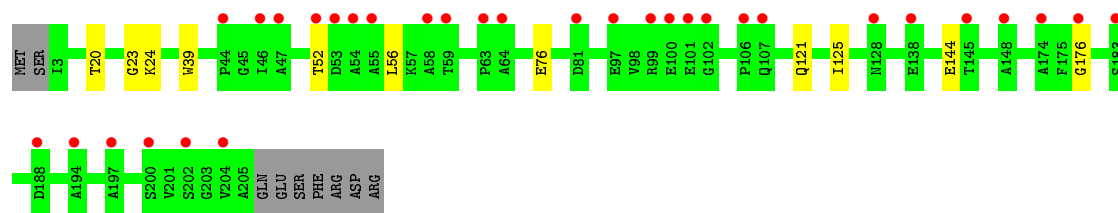


- Molecule 3: Microcompartments protein

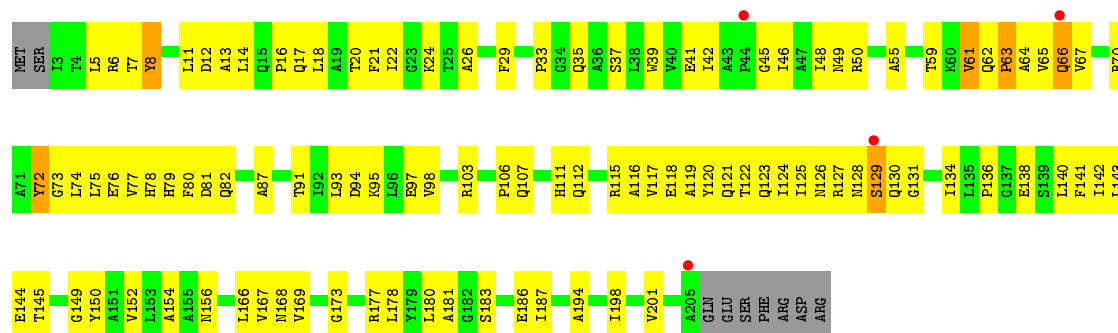


- Molecule 3: Microcompartments protein

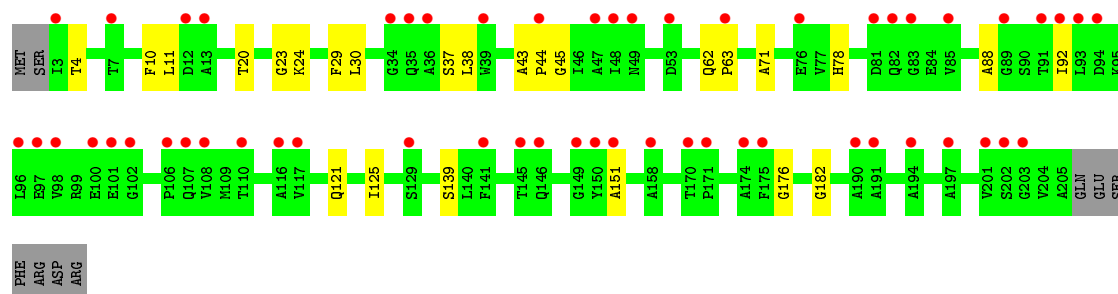
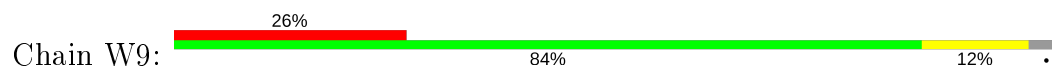




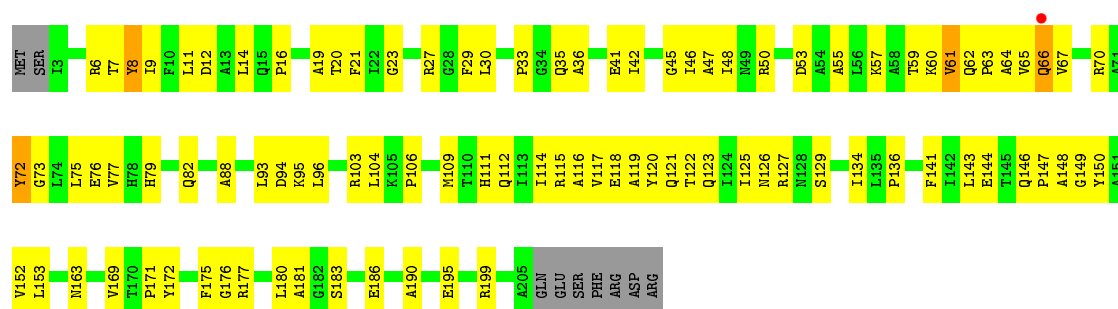
• Molecule 3: Microcompartments protein



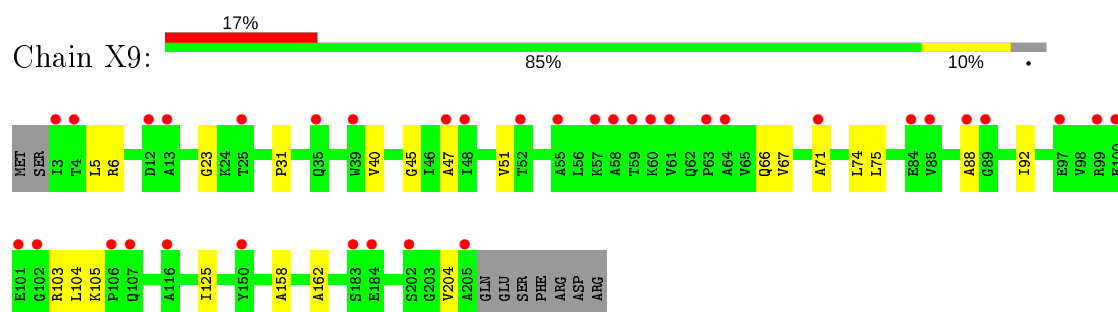
• Molecule 3: Microcompartments protein



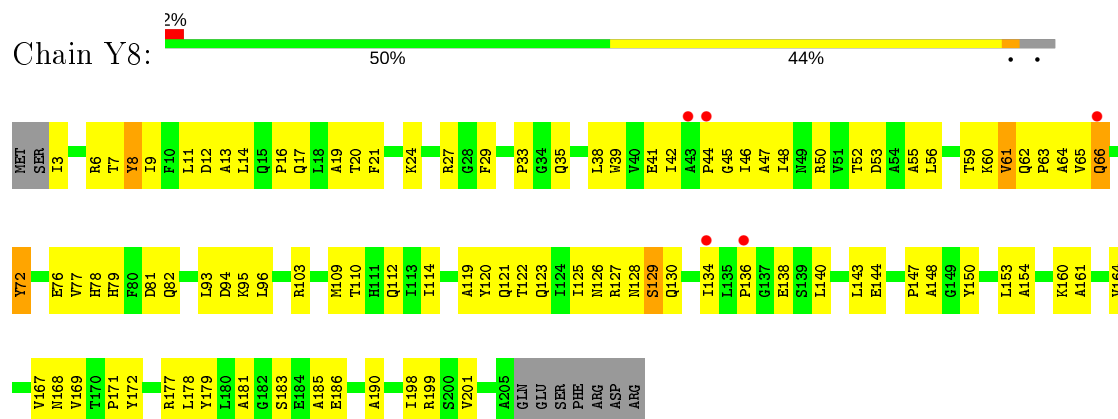
• Molecule 3: Microcompartments protein



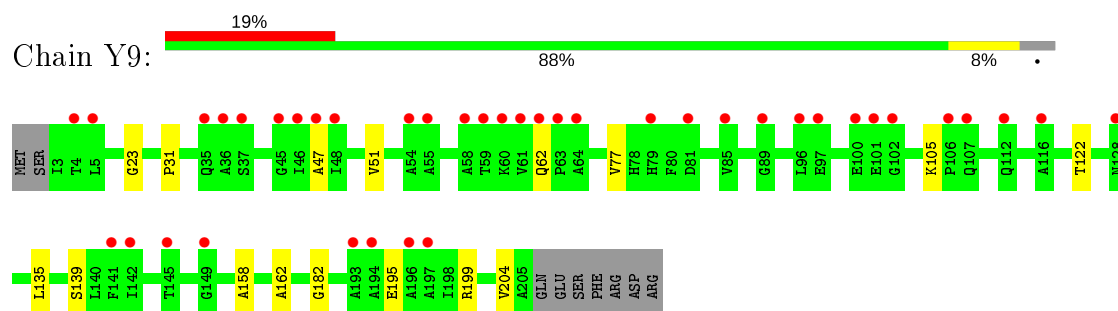
• Molecule 3: Microcompartments protein



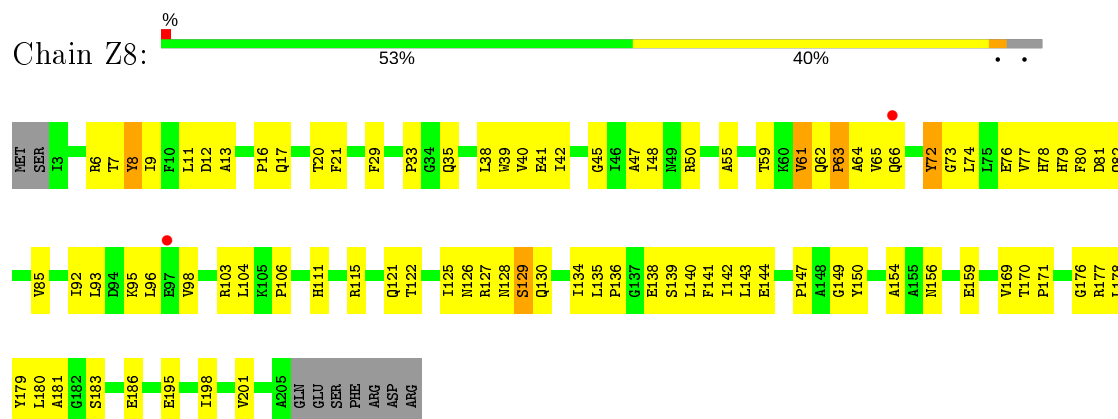
- Molecule 3: Microcompartments protein



- Molecule 3: Microcompartments protein

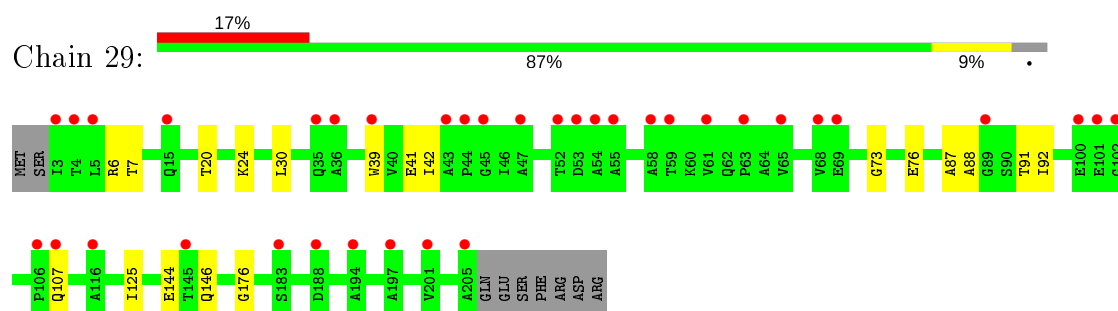


- Molecule 3: Microcompartments protein



- Molecule 3: Microcompartments protein

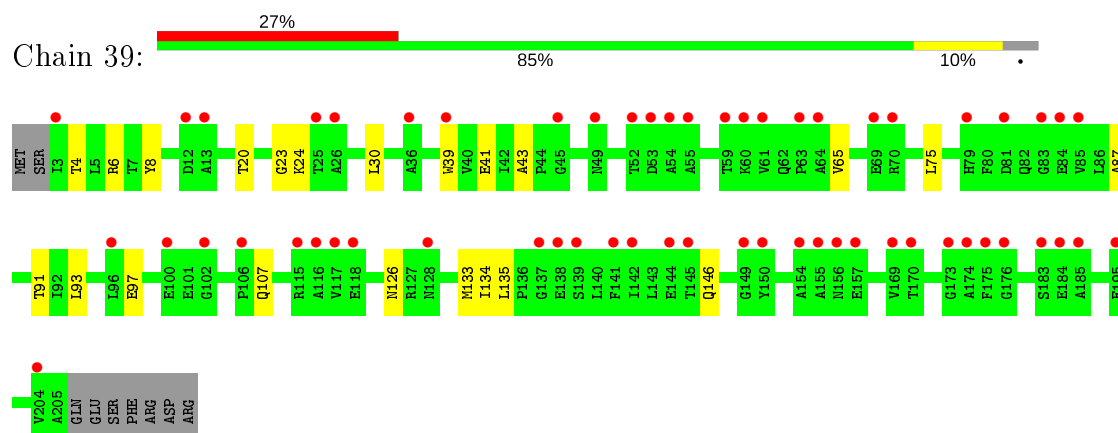
- Molecule 3: Microcompartments protein



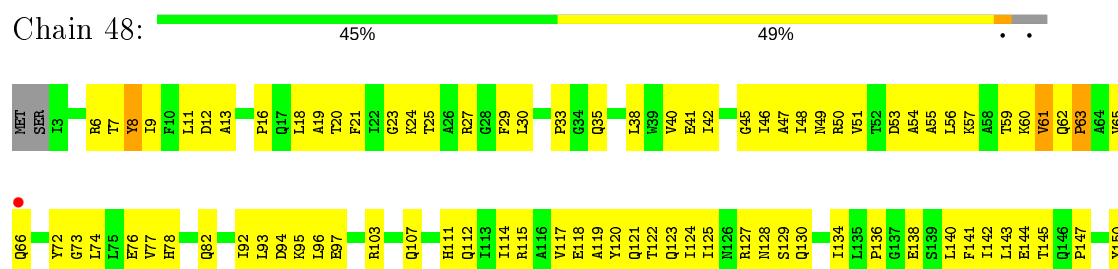
- Molecule 3: Microcompartments protein



- Molecule 3: Microcompartments protein

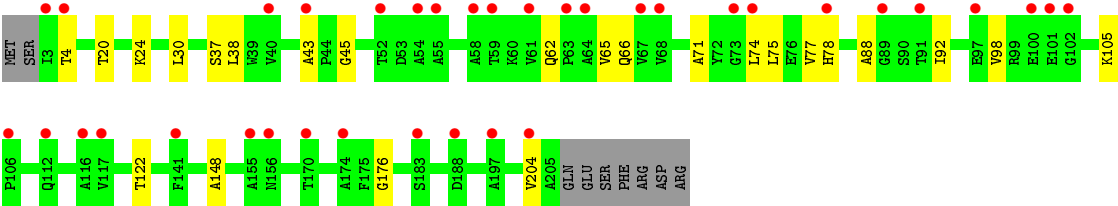
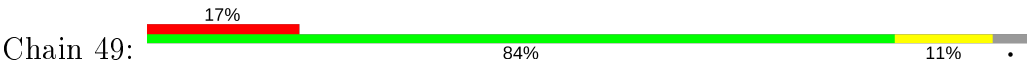


- Molecule 3: Microcompartments protein





● Molecule 3: Microcompartments protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	394.34Å 638.09Å 642.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.85 – 3.51 39.85 – 3.51	Depositor EDS
% Data completeness (in resolution range)	88.6 (39.85-3.51) 69.1 (39.85-3.51)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.48Å)	Xtriage
Refinement program	PHENIX dev_2650	Depositor
R, R_{free}	0.279 , 0.323 0.279 , 0.323	Depositor DCC
R_{free} test set	20031 reflections (2.28%)	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	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	11	0.34	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(°)	Ideal(°)
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 ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I1	678	0	705	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 ⓘ

5.3.1 Protein backbone ⓘ

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 ⓘ

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
2	N6	82	ASN
2	R2	34	TYR
3	28	127	ARG
3	N8	179	TYR
2	P3	34	TYR

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

Mol	Chain	Res	Type
3	L8	17	GLN
3	P8	78	HIS
3	18	78	HIS
3	M8	121	GLN
3	Q8	66	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	11	95/96 (98%)	-0.57	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	55, 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 3	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 carbohydrates 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.