



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 03:45 AM UTC

PDB ID : 9LY9 / pdb_00009ly9
EMDB ID : EMD-62529
Title : Cryo-EM structure of carboxysomal mid-shell: T = 16 shell under C1 symmetry.
Authors : Li, J.X.; Li, T.P.; Wang, S.M.; Zhang, Y.Z.; Liu, L.N.; Wang, P.
Deposited on : 2025-02-19
Resolution : 3.71 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

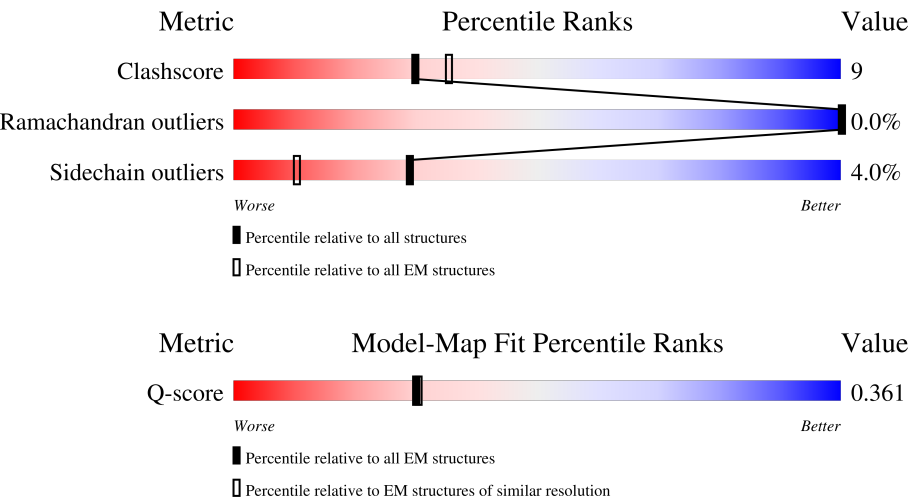
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.71 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10534 (3.21 - 4.21)

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

Mol	Chain	Length	Quality of chain
1	A0	98	56%33%5%6%
1	A1	98	58%31%5%6%
1	A2	98	56%33%5%6%
1	A3	98	56%32%6%6%

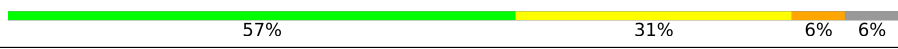
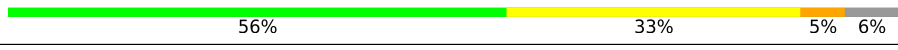
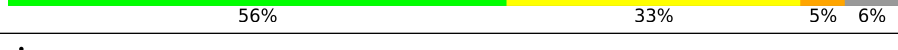
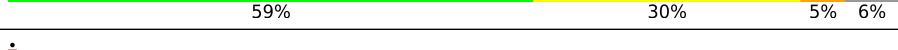
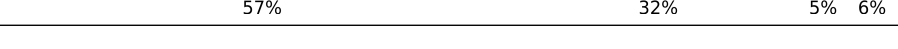
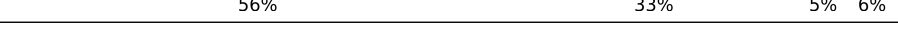
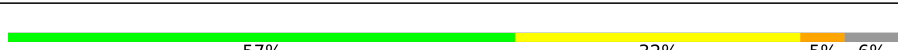
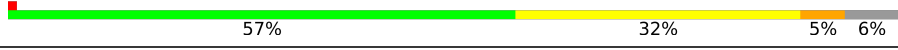
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	A4	98	
1	A5	98	
1	A6	98	
1	A7	98	
1	A8	98	
1	A9	98	
1	AA	98	
1	AB	98	
1	AC	98	
1	AD	98	
1	AE	98	
1	AF	98	
1	AG	98	
1	AH	98	
1	AI	98	
1	AJ	98	
1	AK	98	
1	AL	98	
1	AM	98	
1	AN	98	
1	AO	98	
1	AP	98	
1	AQ	98	
1	AR	98	
1	AS	98	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AT	98	
1	AU	98	
1	AV	98	
1	AW	98	
1	AX	98	
1	AY	98	
1	AZ	98	
1	Aa	98	
1	Ab	98	
1	Ac	98	
1	Ad	98	
1	Ae	98	
1	Af	98	
1	Ag	98	
1	Ah	98	
1	Ai	98	
1	Aj	98	
1	Ak	98	
1	Al	98	
1	Am	98	
1	An	98	
1	Ao	98	
1	Ap	98	
1	Aq	98	
1	Ar	98	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	As	98	
1	At	98	
1	Au	98	
1	Av	98	
1	Aw	98	
1	Ax	98	
1	B0	98	
1	B1	98	
1	B2	98	
1	B3	98	
1	B4	98	
1	B5	98	
1	B6	98	
1	B7	98	
1	B8	98	
1	B9	98	
1	BA	98	
1	BB	98	
1	BC	98	
1	BD	98	
1	BE	98	
1	BF	98	
1	BG	98	
1	BH	98	
1	BI	98	

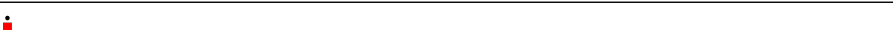
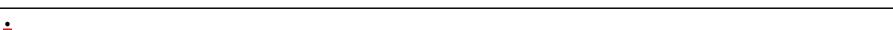
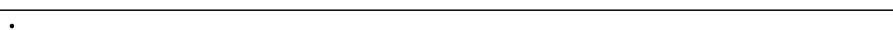
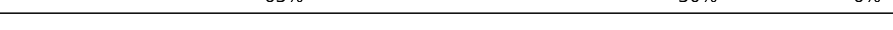
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	BJ	98	
1	BK	98	
1	BL	98	
1	BM	98	
1	BN	98	
1	BO	98	
1	BP	98	
1	BQ	98	
1	BR	98	
1	BS	98	
1	BT	98	
1	BU	98	
1	BV	98	
1	BW	98	
1	BX	98	
1	BY	98	
1	BZ	98	
1	Ba	98	
1	Bb	98	
1	Bc	98	
1	Bd	98	
1	Be	98	
1	Bf	98	
1	Bg	98	
1	Bh	98	

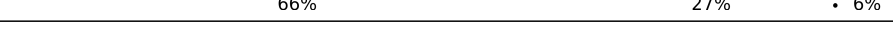
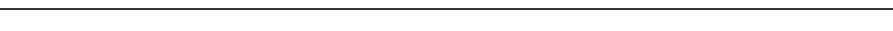
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Bi	98	 63% 30% • 6%
1	Bj	98	 64% 29% • 6%
1	Bk	98	 62% 31% • 6%
1	Bl	98	 63% 30% • 6%
1	Bm	98	 58% 35% • 6%
1	Bn	98	 62% 31% • 6%
1	Bo	98	 63% 30% • 6%
1	Bp	98	 61% 32% • 6%
1	Bq	98	 65% 28% • 6%
1	Br	98	 63% 30% • 6%
1	Bs	98	 62% 31% • 6%
1	Bt	98	 63% 30% • 6%
1	Bu	98	 63% 30% • 6%
1	Bv	98	 63% 30% • 6%
1	Bw	98	 62% 31% • 6%
1	Bx	98	 64% 29% • 6%
1	C0	98	 65% 28% • 6%
1	C1	98	 65% 28% • 6%
1	C2	98	 65% 28% • 6%
1	C3	98	 65% 28% • 6%
1	C4	98	 63% 30% • 6%
1	C5	98	 67% 26% • 6%
1	C6	98	 66% 27% • 6%
1	C7	98	 65% 28% • 6%
1	C8	98	 67% 26% • 6%

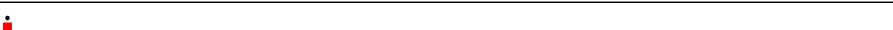
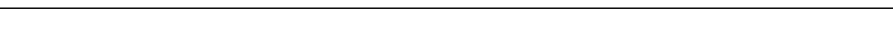
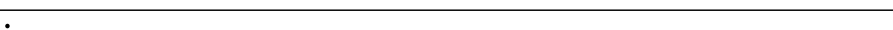
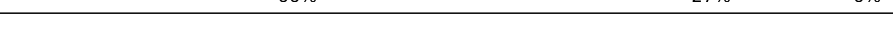
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	C9	98	 63% 30% • 6%
1	CA	98	 66% 27% • 6%
1	CB	98	 67% 26% • 6%
1	CC	98	 67% 26% • 6%
1	CD	98	 65% 28% • 6%
1	CE	98	 67% 26% • 6%
1	CF	98	 65% 28% • 6%
1	CG	98	 66% 27% • 6%
1	CH	98	 65% 28% • 6%
1	CI	98	 67% 24% • 6%
1	CJ	98	 64% 29% • 6%
1	CK	98	 67% 26% • 6%
1	CL	98	 66% 27% • 6%
1	CM	98	 66% 27% • 6%
1	CN	98	 66% 27% • 6%
1	CO	98	 63% 30% • 6%
1	CP	98	 66% 27% • 6%
1	CQ	98	 67% 26% • 6%
1	CR	98	 66% 27% • 6%
1	CS	98	 65% 28% • 6%
1	CT	98	 66% 27% • 6%
1	CU	98	 64% 29% • 6%
1	CV	98	 65% 28% • 6%
1	CW	98	 64% 29% • 6%
1	CX	98	 66% 27% • 6%

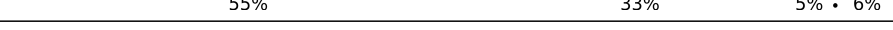
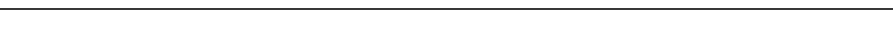
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	CY	98	 65% 28% • 6%
1	CZ	98	 68% 24% • 6%
1	Ca	98	 65% 28% • 6%
1	Cb	98	 66% 27% • 6%
1	Cc	98	 66% 26% • 6%
1	Cd	98	 65% 28% • 6%
1	Ce	98	 65% 28% • 6%
1	Cf	98	 66% 27% • 6%
1	Cg	98	 66% 26% • 6%
1	Ch	98	 64% 29% • 6%
1	Ci	98	 67% 26% • 6%
1	Cj	98	 66% 27% • 6%
1	Ck	98	 66% 27% • 6%
1	Cl	98	 66% 27% • 6%
1	Cm	98	 66% 26% • 6%
1	Cn	98	 65% 28% • 6%
1	Co	98	 68% 24% • 6%
1	Cp	98	 65% 28% • 6%
1	Cq	98	 65% 28% • 6%
1	Cr	98	 67% 24% • 6%
1	Cs	98	 65% 28% • 6%
1	Ct	98	 64% 29% • 6%
1	Cu	98	 66% 27% • 6%
1	Cv	98	 66% 26% • 6%
1	Cw	98	 64% 29% • 6%

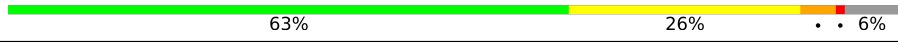
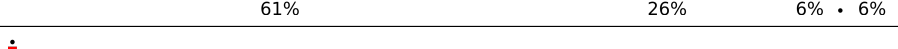
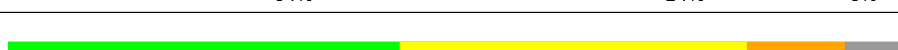
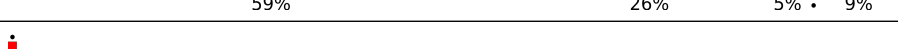
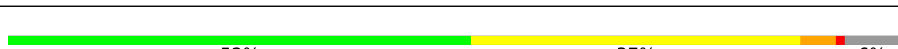
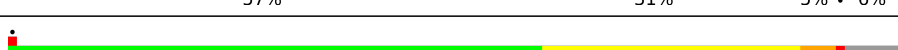
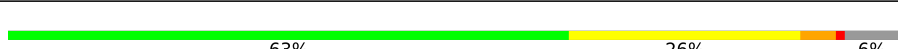
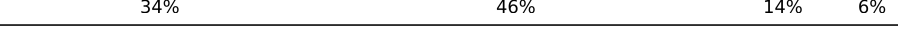
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Cx	98	
1	D0	98	
1	D1	98	
1	D2	98	
1	D3	98	
1	D4	98	
1	D5	98	
1	D6	98	
1	D7	98	
1	D8	98	
1	D9	98	
1	DA	98	
1	DB	98	
1	DC	98	
1	DD	98	
1	DE	98	
1	DF	98	
1	DG	98	
1	DH	98	
1	DI	98	
1	DJ	98	
1	DK	98	
1	DL	98	
1	DM	98	
1	DN	98	

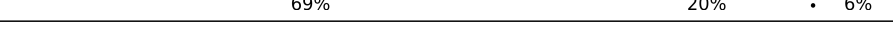
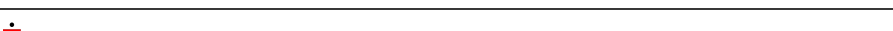
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	DO	98	
1	DP	98	
1	DQ	98	
1	DR	98	
1	DS	98	
1	DT	98	
1	DU	98	
1	DV	98	
1	DW	98	
1	DX	98	
1	DY	98	
1	DZ	98	
1	Da	98	
1	Db	98	
1	Dc	98	
1	Dd	98	
1	De	98	
1	Df	98	
1	Dg	98	
1	Dh	98	
1	Di	98	
1	Dj	98	
1	Dk	98	
1	Dl	98	
1	Dm	98	

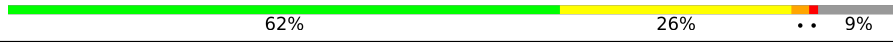
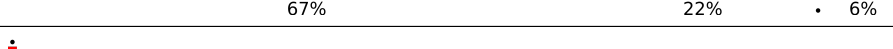
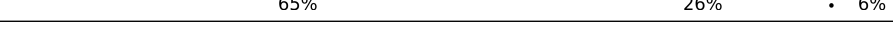
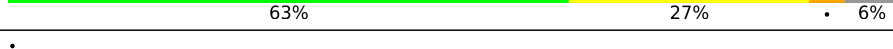
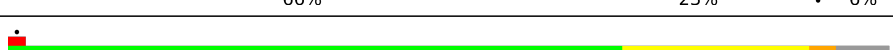
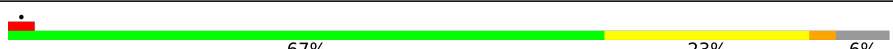
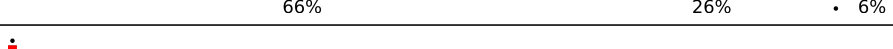
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Dn	98	
1	Do	98	
1	Dp	98	
1	Dq	98	
1	Dr	98	
1	Ds	98	
1	Dt	98	
1	Du	98	
1	Dv	98	
1	Dw	98	
1	Dx	98	
1	E0	98	
1	E1	98	
1	E2	98	
1	E3	98	
1	E4	98	
1	E5	98	
1	E6	98	
1	E7	98	
1	E8	98	
1	E9	98	
1	EA	98	
1	EB	98	
1	EC	98	
1	ED	98	

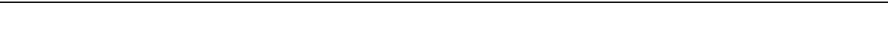
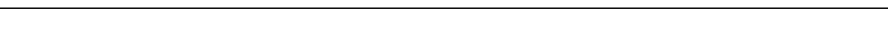
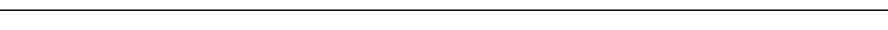
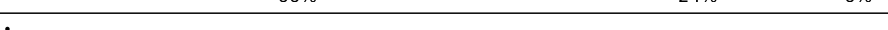
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	EE	98	
1	EF	98	
1	EG	98	
1	EH	98	
1	EI	98	
1	EJ	98	
1	EK	98	
1	EL	98	
1	EM	98	
1	EN	98	
1	EO	98	
1	EP	98	
1	EQ	98	
1	ER	98	
1	ES	98	
1	ET	98	
1	EU	98	
1	EV	98	
1	EW	98	
1	EX	98	
1	EY	98	
1	EZ	98	
1	Ea	98	
1	Eb	98	
1	Ec	98	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Ed	98	 67% 22% • 6%
1	Ee	98	 65% 26% • 6%
1	Ef	98	 65% 24% • 6%
1	Eg	98	 65% 27% • 6%
1	Eh	98	 67% 23% • 6%
1	Ei	98	 69% 21% • 6%
1	Ej	98	 67% 23% • 6%
1	Ek	98	 66% 24% • 6%
1	El	98	 69% 18% • 9%
1	Em	98	 64% 24% 5% 6%
1	En	98	 66% 23% • 6%
1	Eo	98	 65% 26% • 6%
1	Ep	98	 63% 27% • 6%
1	Eq	98	 66% 24% • 6%
1	Er	98	 69% 21% • 6%
1	Es	98	 66% 23% • 6%
1	Et	98	 65% 26% • 6%
1	Eu	98	 67% 21% 5% 6%
1	Ev	98	 63% 28% • 6%
1	Ew	98	 65% 26% • 6%
1	Ex	98	 69% 21% • 6%
1	F0	98	 60% 30% • 6%
1	F1	98	 63% 27% • 6%
1	F2	98	 60% 30% • 6%
1	F3	98	 63% 26% 5% 6%

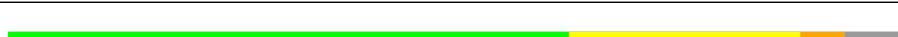
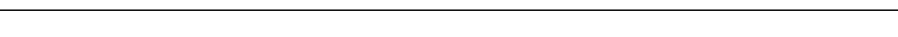
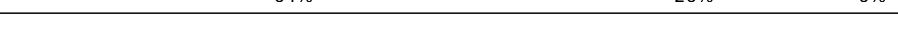
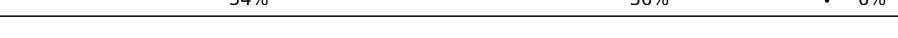
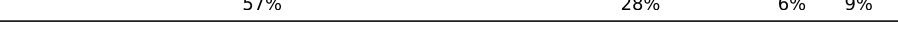
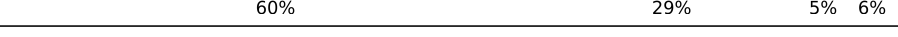
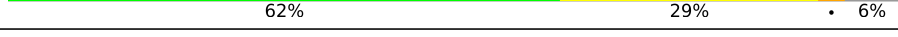
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F4	98	
1	F5	98	
1	F6	98	
1	F7	98	
1	F8	98	
1	F9	98	
1	FA	98	
1	FB	98	
1	FC	98	
1	FD	98	
1	FE	98	
1	FF	98	
1	FG	98	
1	FH	98	
1	FI	98	
1	FJ	98	
1	FK	98	
1	FL	98	
1	FM	98	
1	FN	98	
1	FO	98	
1	FP	98	
1	FQ	98	
1	FR	98	
1	FS	98	

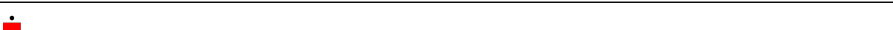
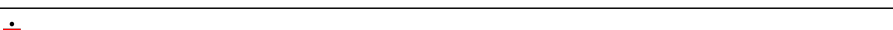
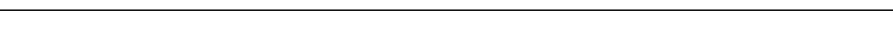
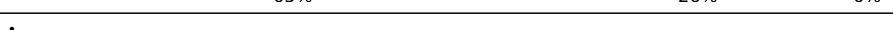
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FT	98	
1	FU	98	
1	FV	98	
1	FW	98	
1	FX	98	
1	FY	98	
1	FZ	98	
1	Fa	98	
1	Fb	98	
1	Fc	98	
1	Fd	98	
1	Fe	98	
1	Ff	98	
1	Fg	98	
1	Fh	98	
1	Fi	98	
1	Fj	98	
1	Fk	98	
1	Fl	98	
1	Fm	98	
1	Fn	98	
1	Fo	98	
1	Fp	98	
1	Fq	98	
1	Fr	98	

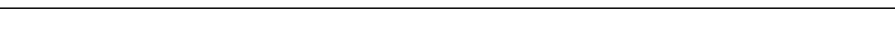
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Fs	98	 63% 27% • 6%
1	Ft	98	 62% 28% • 6%
1	Fu	98	 63% 27% • 6%
1	Fv	98	 63% 27% • 6%
1	Fw	98	 63% 26% 5% 6%
1	Fx	98	 64% 26% • 6%
1	G0	98	 58% 34% • 6%
1	G1	98	 65% 26% •• 6%
1	G2	98	 64% 28% • 6%
1	G3	98	 66% 23% •• 6%
1	G4	98	 65% 26% •• 6%
1	G5	98	 65% 26% •• 6%
1	G6	98	 65% 24% •• 6%
1	G7	98	 65% 26% •• 6%
1	G8	98	 66% 23% •• 6%
1	G9	98	 65% 26% •• 6%
1	GA	98	 65% 24% •• 6%
1	GB	98	 64% 28% • 6%
1	GC	98	 66% 23% •• 6%
1	GD	98	 65% 26% •• 6%
1	GE	98	 65% 26% •• 6%
1	GF	98	 58% 33% • 6%
1	GG	98	 65% 24% •• 6%
1	GH	98	 64% 28% • 6%
1	GI	98	 60% 30% •• 6%

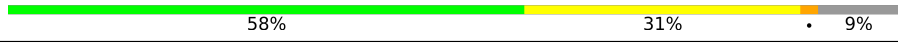
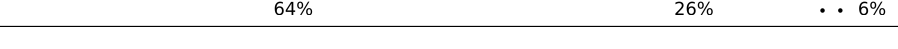
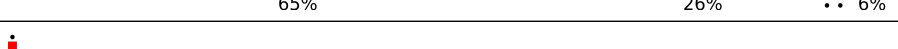
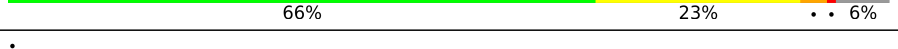
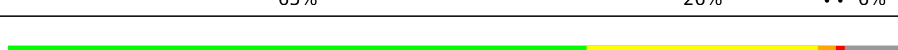
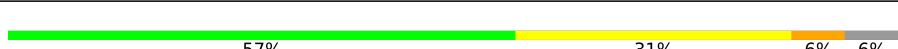
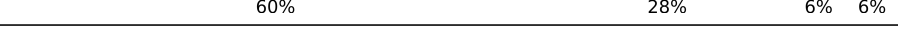
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	GJ	98	
1	GK	98	
1	GL	98	
1	GM	98	
1	GN	98	
1	GO	98	
1	GP	98	
1	GQ	98	
1	GR	98	
1	GS	98	
1	GT	98	
1	GU	98	
1	GV	98	
1	GW	98	
1	GX	98	
1	GY	98	
1	GZ	98	
1	Ga	98	
1	Gb	98	
1	Gc	98	
1	Gd	98	
1	Ge	98	
1	Gf	98	
1	Gg	98	
1	Gh	98	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Gi	98	
1	Gj	98	
1	Gk	98	
1	Gl	98	
1	Gm	98	
1	Gn	98	
1	Go	98	
1	Gp	98	
1	Gq	98	
1	Gr	98	
1	Gs	98	
1	Gt	98	
1	Gu	98	
1	Gv	98	
1	Gw	98	
1	Gx	98	
1	H0	98	
1	H1	98	
1	H2	98	
1	H3	98	
1	H4	98	
1	H5	98	
1	H6	98	
1	H7	98	
1	H8	98	

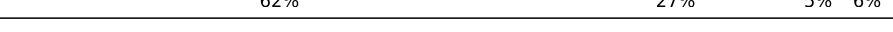
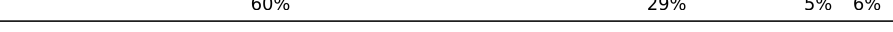
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H9	98	
1	HA	98	
1	HB	98	
1	HC	98	
1	HD	98	
1	HE	98	
1	HF	98	
1	HG	98	
1	HH	98	
1	HI	98	
1	HJ	98	
1	HK	98	
1	HL	98	
1	HM	98	
1	HN	98	
1	HO	98	
1	HP	98	
1	HQ	98	
1	HR	98	
1	HS	98	
1	HT	98	
1	HU	98	
1	HV	98	
1	HW	98	
1	HX	98	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	HY	98	
1	HZ	98	
1	Ha	98	
1	Hb	98	
1	Hc	98	
1	Hd	98	
1	He	98	
1	Hf	98	
1	Hg	98	
1	Hh	98	
1	Hi	98	
1	Hj	98	
1	Hk	98	
1	Hl	98	
1	Hm	98	
1	Hn	98	
1	Ho	98	
1	Hp	98	
1	Hq	98	
1	Hr	98	
1	Hs	98	
1	Ht	98	
1	Hu	98	
1	Hv	98	
1	Hw	98	

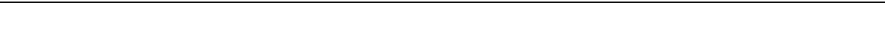
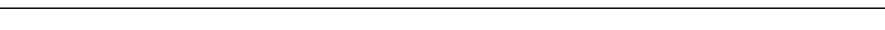
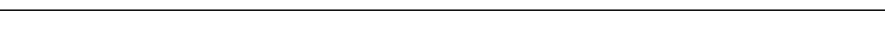
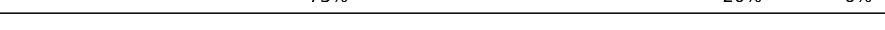
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Hx	98	
1	I0	98	
1	I1	98	
1	I2	98	
1	I3	98	
1	I4	98	
1	I5	98	
1	I6	98	
1	I7	98	
1	I8	98	
1	I9	98	
1	IA	98	
1	IB	98	
1	IC	98	
1	ID	98	
1	IE	98	
1	IF	98	
1	IG	98	
1	IH	98	
1	II	98	
1	IJ	98	
1	IK	98	
1	IL	98	
1	IM	98	
1	IN	98	

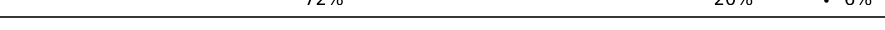
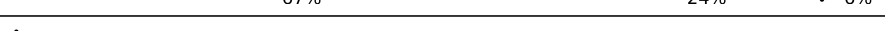
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	IO	98	
1	IP	98	
1	IQ	98	
1	IR	98	
1	IS	98	
1	IT	98	
1	IU	98	
1	IV	98	
1	IW	98	
1	IX	98	
1	IY	98	
1	IZ	98	
1	Ia	98	
1	Ib	98	
1	Ic	98	
1	Id	98	
1	Ie	98	
1	If	98	
1	Ig	98	
1	Ih	98	
1	Ii	98	
1	Ij	98	
1	Ik	98	
1	Il	98	
1	Im	98	

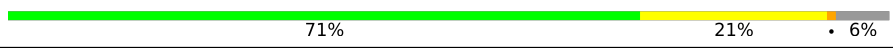
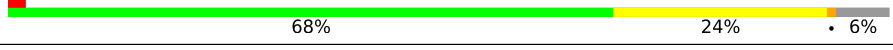
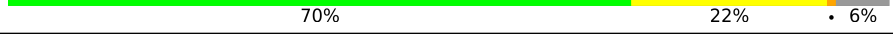
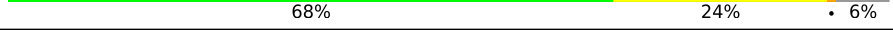
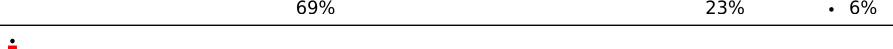
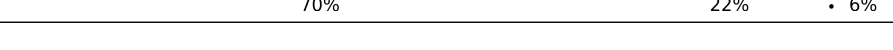
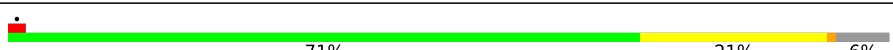
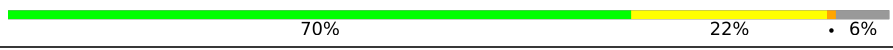
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	In	98	
1	Io	98	
1	Ip	98	
1	Iq	98	
1	Ir	98	
1	Is	98	
1	It	98	
1	Iu	98	
1	Iv	98	
1	Iw	98	
1	Ix	98	
1	J0	98	
1	J1	98	
1	J2	98	
1	J3	98	
1	J4	98	
1	J5	98	
1	J6	98	
1	J7	98	
1	J8	98	
1	J9	98	
1	JA	98	
1	JB	98	
1	JC	98	
1	JD	98	

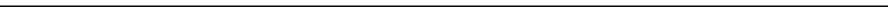
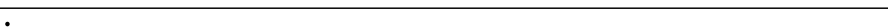
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	JE	98	
1	JF	98	
1	JG	98	
1	JH	98	
1	JI	98	
1	JJ	98	
1	JK	98	
1	JL	98	
1	JM	98	
1	JN	98	
1	JO	98	
1	JP	98	
1	JQ	98	
1	JR	98	
1	JS	98	
1	JT	98	
1	JU	98	
1	JV	98	
1	JW	98	
1	JX	98	
1	JY	98	
1	JZ	98	
1	Ja	98	
1	Jb	98	
1	Jc	98	

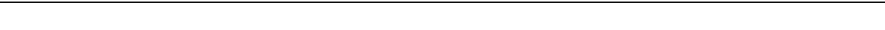
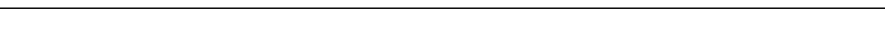
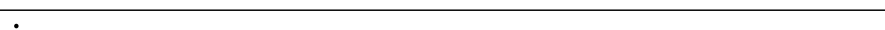
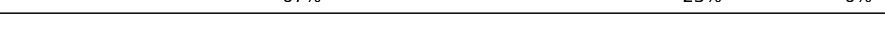
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Jd	98	
1	Je	98	
1	Jf	98	
1	Jg	98	
1	Jh	98	
1	Ji	98	
1	Jj	98	
1	Jk	98	
1	Jl	98	
1	Jm	98	
1	Jn	98	
1	Jo	98	
1	Jp	98	
1	Jq	98	
1	Jr	98	
1	Js	98	
1	Jt	98	
1	Ju	98	
1	Jv	98	
1	Jw	98	
1	Jx	98	
1	K0	98	
1	K1	98	
1	K2	98	
1	K3	98	

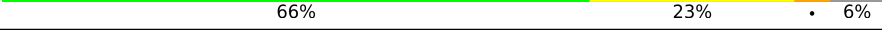
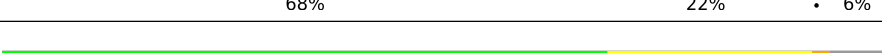
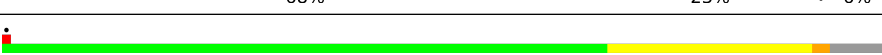
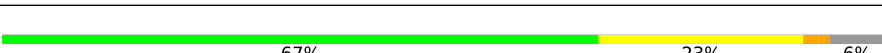
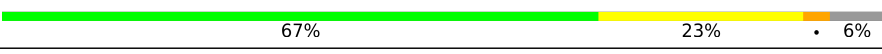
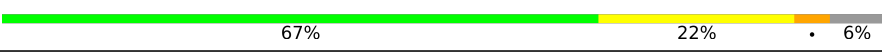
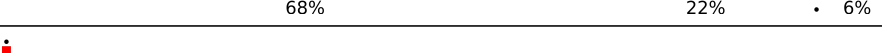
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K4	98	 67% 23% 6%
1	K5	98	 67% 23% 6%
1	K6	98	 66% 24% 6%
1	K7	98	 68% 22% 6%
1	K8	98	 66% 23% 6%
1	K9	98	 67% 23% 6%
1	KA	98	 66% 24% 6%
1	KB	98	 67% 23% 6%
1	KC	98	 68% 22% 6%
1	KD	98	 68% 22% 6%
1	KE	98	 67% 23% 6%
1	KF	98	 65% 26% 6%
1	KG	98	 66% 24% 6%
1	KH	98	 67% 23% 6%
1	KI	98	 68% 22% 6%
1	KJ	98	 68% 22% 6%
1	KK	98	 68% 22% 6%
1	KL	98	 68% 22% 6%
1	KM	98	 67% 23% 6%
1	KN	98	 69% 21% 6%
1	KO	98	 68% 22% 6%
1	KP	98	 66% 24% 6%
1	KQ	98	 67% 23% 6%
1	KR	98	 67% 23% 6%
1	KS	98	 68% 22% 6%

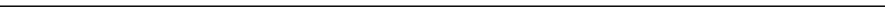
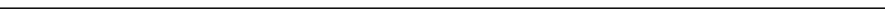
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	KT	98	
1	KU	98	
1	KV	98	
1	KW	98	
1	KX	98	
1	KY	98	
1	KZ	98	
1	Ka	98	
1	Kb	98	
1	Kc	98	
1	Kd	98	
1	Ke	98	
1	Kf	98	
1	Kg	98	
1	Kh	98	
1	Ki	98	
1	Kj	98	
1	Kk	98	
1	Kl	98	
1	Km	98	
1	Kn	98	
1	Ko	98	
1	Kp	98	
1	Kq	98	
1	Kr	98	

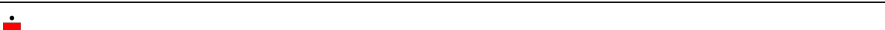
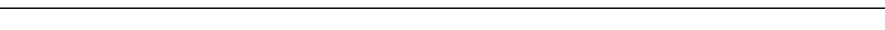
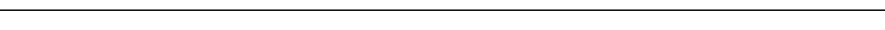
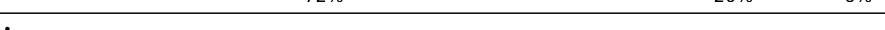
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Ks	98	 67% 22% 6%
1	Kt	98	 67% 23% 6%
1	Ku	98	 66% 23% 6%
1	Kv	98	 68% 22% 6%
1	Kw	98	 68% 22% 6%
1	Kx	98	 67% 23% 6%
1	L0	98	 72% 20% 6%
1	L1	98	 74% 18% 6%
1	L2	98	 72% 20% 6%
1	L3	98	 70% 23% 6%
1	L4	98	 74% 18% 6%
1	L5	98	 66% 27% 6%
1	L6	98	 72% 21% 6%
1	L7	98	 71% 20% 6%
1	L8	98	 68% 24% 6%
1	L9	98	 74% 19% 6%
1	LA	98	 72% 21% 6%
1	LB	98	 67% 26% 6%
1	LC	98	 71% 22% 6%
1	LD	98	 72% 20% 6%
1	LE	98	 72% 20% 6%
1	LF	98	 72% 20% 6%
1	LG	98	 76% 17% 6%
1	LH	98	 72% 20% 6%
1	LI	98	 68% 23% 6%

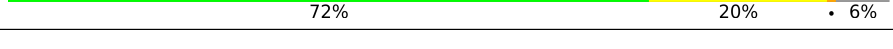
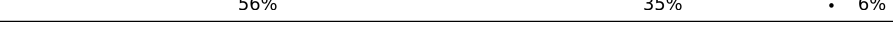
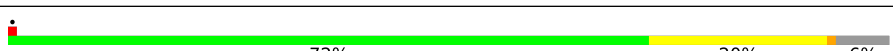
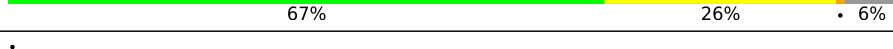
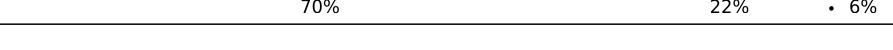
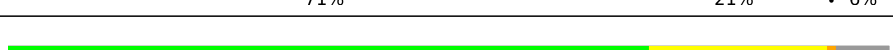
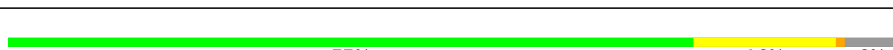
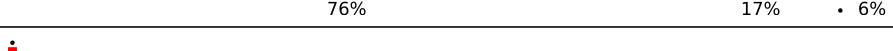
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	LJ	98	 74% 19% 6%
1	LK	98	 73% 19% 6%
1	LL	98	 71% 22% 6%
1	LM	98	 71% 20% 6%
1	LN	98	 69% 23% 6%
1	LO	98	 74% 18% 6%
1	LP	98	 72% 21% 6%
1	LQ	98	 67% 26% 6%
1	LR	98	 73% 19% 6%
1	LS	98	 70% 22% 6%
1	LT	98	 72% 20% 6%
1	LU	98	 72% 20% 6%
1	LV	98	 76% 18% 6%
1	LW	98	 72% 20% 6%
1	LX	98	 72% 21% 6%
1	LY	98	 73% 19% 6%
1	LZ	98	 73% 19% 6%
1	La	98	 70% 22% 6%
1	Lb	98	 73% 20% 6%
1	Lc	98	 70% 22% 6%
1	Ld	98	 74% 18% 6%
1	Le	98	 72% 21% 6%
1	Lf	98	 67% 26% 6%
1	Lg	98	 71% 21% 6%
1	Lh	98	 72% 20% 6%

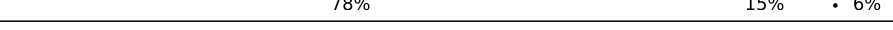
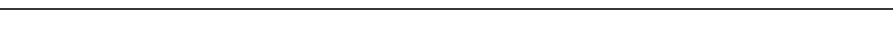
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Li	98	
1	Lj	98	
1	Lk	98	
1	Ll	98	
1	Lm	98	
1	Ln	98	
1	Lo	98	
1	Lp	98	
1	Lq	98	
1	Lr	98	
1	Ls	98	
1	Lt	98	
1	Lu	98	
1	Lv	98	
1	Lw	98	
1	Lx	98	
1	M0	98	
1	M1	98	
1	M2	98	
1	M3	98	
1	M4	98	
1	M5	98	
1	M6	98	
1	M7	98	
1	M8	98	

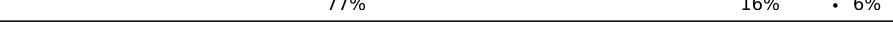
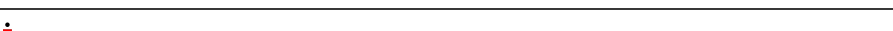
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M9	98	 76% 17% • 6%
1	MA	98	 77% 16% • 6%
1	MB	98	 74% 18% • 6%
1	MC	98	 76% 17% • 6%
1	MD	98	 80% 13% • 6%
1	ME	98	 78% 15% • 6%
1	MF	98	 72% 20% • 6%
1	MG	98	 78% 15% • 6%
1	MH	98	 77% 16% • 6%
1	MI	98	 78% 15% • 6%
1	MJ	98	 77% 16% • 6%
1	MK	98	 77% 16% • 6%
1	ML	98	 76% 17% • 6%
1	MM	98	 78% 15% • 6%
1	MN	98	 78% 15% • 6%
1	MO	98	 77% 16% • 6%
1	MP	98	 78% 15% • 6%
1	MQ	98	 77% 16% • 6%
1	MR	98	 76% 17% • 6%
1	MS	98	 79% 14% • 6%
1	MT	98	 78% 15% • 6%
1	MU	98	 78% 15% • 6%
1	MV	98	 76% 17% • 6%
1	MW	98	 78% 15% • 6%
1	MX	98	 77% 16% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	MY	98	 79% 14% • 6%
1	MZ	98	 77% 16% • 6%
1	Ma	98	 78% 15% • 6%
1	Mb	98	 79% 14% • 6%
1	Mc	98	 77% 16% • 6%
1	Md	98	 78% 15% • 6%
1	Me	98	 78% 15% • 6%
1	Mf	98	 79% 14% • 6%
1	Mg	98	 78% 15% • 6%
1	Mh	98	 77% 16% • 6%
1	Mi	98	 76% 17% • 6%
1	Mj	98	 78% 15% • 6%
1	Mk	98	 77% 16% • 6%
1	ML	98	 77% 16% • 6%
1	Mm	98	 71% 18% • 6%
1	Mn	98	 79% 14% • 6%
1	Mo	98	 78% 15% • 6%
1	Mp	98	 77% 16% • 6%
1	Mq	98	 78% 15% • 6%
1	Mr	98	 78% 15% • 6%
1	Ms	98	 77% 16% • 6%
1	Mt	98	 78% 15% • 6%
1	Mu	98	 78% 15% • 6%
1	Mv	98	 72% 20% • 6%
1	Mw	98	 77% 16% • 6%

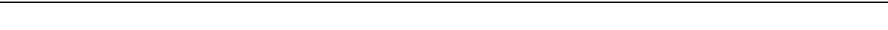
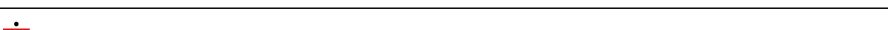
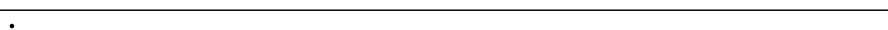
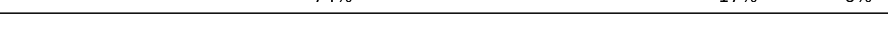
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Mx	98	
1	N0	98	
1	N1	98	
1	N2	98	
1	N3	98	
1	N4	98	
1	N5	98	
1	N6	98	
1	N7	98	
1	N8	98	
1	N9	98	
1	NA	98	
1	NB	98	
1	NC	98	
1	ND	98	
1	NE	98	
1	NF	98	
1	NG	98	
1	NH	98	
1	NI	98	
1	NJ	98	
1	NK	98	
1	NL	98	
1	NM	98	
1	NN	98	

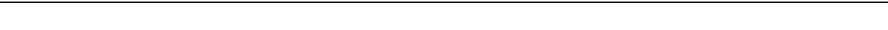
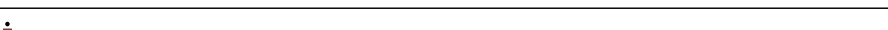
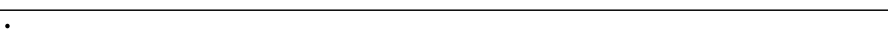
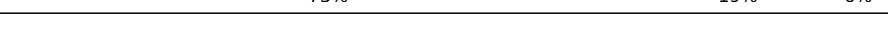
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	NO	98	 74%17%6%
1	NP	98	 74%17%6%
1	NQ	98	 73%18%6%
1	NR	98	 76%16%6%
1	NS	98	 76%16%6%
1	NT	98	 74%17%6%
1	NU	98	 76%16%6%
1	NV	98	 76%16%6%
1	NW	98	 77%15%6%
1	NX	98	 73%18%6%
1	NY	98	 73%17%6%
1	NZ	98	 78%14%6%
1	Na	98	 77%15%6%
1	Nb	98	 74%17%6%
1	Nc	98	 76%16%6%
1	Nd	98	 74%17%6%
1	Ne	98	 76%16%6%
1	Nf	98	 74%17%6%
1	Ng	98	 76%16%6%
1	Nh	98	 74%17%6%
1	Ni	98	 76%16%6%
1	Nj	98	 76%16%6%
1	Nk	98	 74%17%6%
1	Nl	98	 76%16%6%
1	Nm	98	 69%22%6%

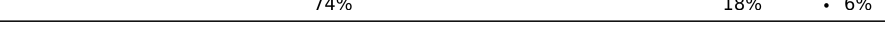
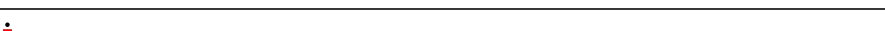
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Nn	98	 70% 20% 6%
1	No	98	 76% 16% 6%
1	Np	98	 76% 16% 6%
1	Nq	98	 73% 18% 6%
1	Nr	98	 78% 14% 6%
1	Ns	98	 74% 17% 6%
1	Nt	98	 74% 17% 6%
1	Nu	98	 74% 17% 6%
1	Nv	98	 73% 18% 6%
1	Nw	98	 76% 16% 6%
1	Nx	98	 76% 16% 6%
1	O0	98	 72% 20% 6%
1	O1	98	 73% 19% 6%
1	O2	98	 73% 19% 6%
1	O3	98	 72% 19% 6%
1	O4	98	 72% 20% 6%
1	O5	98	 74% 18% 6%
1	O6	98	 73% 19% 6%
1	O7	98	 73% 18% 6%
1	O8	98	 71% 21% 6%
1	O9	98	 72% 20% 6%
1	OA	98	 73% 19% 6%
1	OB	98	 74% 18% 6%
1	OC	98	 73% 18% 6%
1	OD	98	 73% 19% 6%

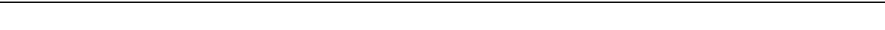
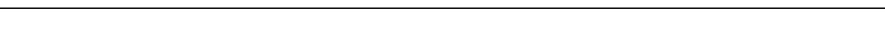
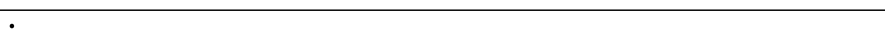
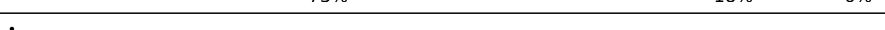
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	OE	98	 73% 19% • 6%
1	OF	98	 71% 21% • 6%
1	OG	98	 73% 19% • 6%
1	OH	98	 73% 19% • 6%
1	OI	98	 71% 21% • 6%
1	OJ	98	 72% 20% • 6%
1	OK	98	 73% 19% • 6%
1	OL	98	 72% 20% • 6%
1	OM	98	 73% 18% • 6%
1	ON	98	 71% 21% • 6%
1	OO	98	 72% 20% • 6%
1	OP	98	 73% 19% • 6%
1	OQ	98	 74% 18% • 6%
1	OR	98	 74% 18% • 6%
1	OS	98	 73% 19% • 6%
1	OT	98	 73% 19% • 6%
1	OU	98	 71% 21% • 6%
1	OV	98	 73% 19% • 6%
1	OW	98	 72% 20% • 6%
1	OX	98	 72% 20% • 6%
1	OY	98	 73% 19% • 6%
1	OZ	98	 74% 18% • 6%
1	Oa	98	 72% 20% • 6%
1	Ob	98	 73% 18% • 6%
1	Oc	98	 71% 21% • 6%

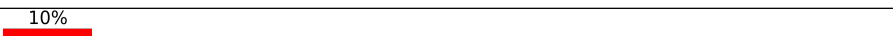
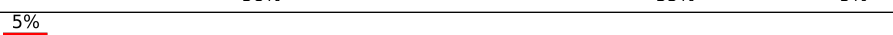
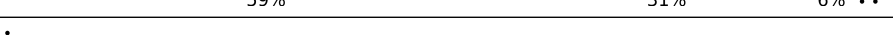
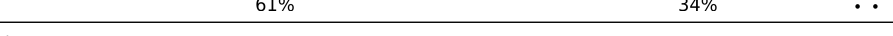
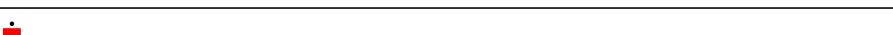
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Od	98	 73% 19% • 6%
1	Oe	98	 73% 19% • 6%
1	Of	98	 74% 18% • 6%
1	Og	98	 73% 19% • 6%
1	Oh	98	 73% 19% • 6%
1	Oi	98	 74% 18% • 6%
1	Oj	98	 71% 21% • 6%
1	Ok	98	 73% 19% • 6%
1	Ol	98	 73% 19% • 6%
1	Om	98	 72% 20% • 6%
1	On	98	 73% 19% • 6%
1	Oo	98	 74% 18% • 6%
1	Op	98	 71% 21% • 6%
1	Oq	98	 73% 18% • 6%
1	Or	98	 71% 21% • 6%
1	Os	98	 72% 20% • 6%
1	Ot	98	 73% 19% • 6%
1	Ou	98	 74% 18% • 6%
1	Ov	98	 68% 23% • 6%
1	Ow	98	 73% 19% • 6%
1	Ox	98	 74% 18% • 6%
2	P0	83	 60% 31% 5% ••
2	P1	83	 57% 36% 5% •
2	P2	83	 66% 27% 5% •
2	P3	83	 64% 29% 5% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	P4	83	
2	P5	83	
2	P6	83	
2	P7	83	
2	P8	83	
2	P9	83	
2	PA	83	
2	PB	83	
2	PC	83	
2	PD	83	
2	PE	83	
2	PF	83	
2	PG	83	
2	PH	83	
2	PI	83	
2	PJ	83	
2	PK	83	
2	PL	83	
2	PM	83	
2	PN	83	
2	PO	83	
2	PP	83	
2	PQ	83	
2	PR	83	
2	PS	83	

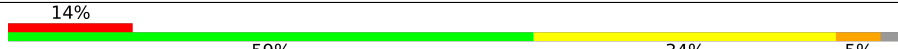
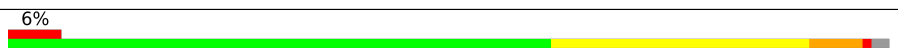
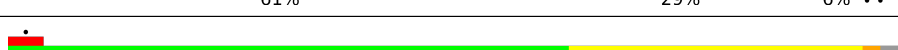
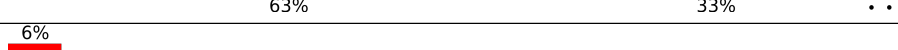
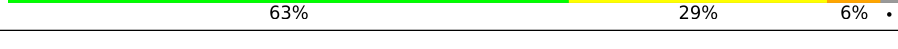
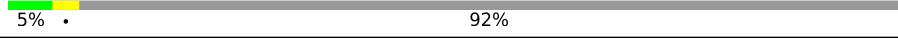
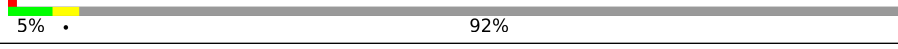
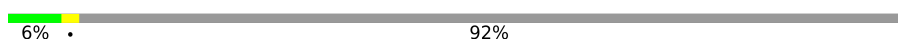
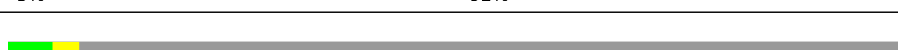
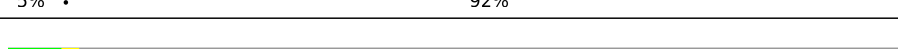
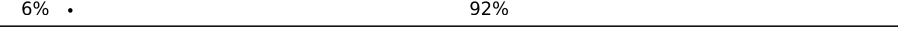
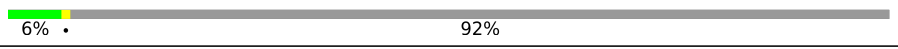
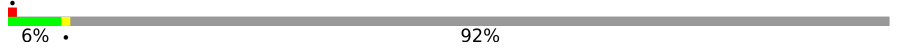
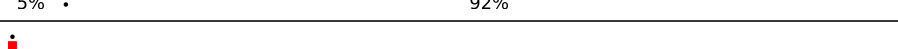
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	PT	83	
2	PU	83	
2	PV	83	
2	PW	83	
2	PX	83	
2	PY	83	
2	PZ	83	
2	Pa	83	
2	Pb	83	
2	Pc	83	
2	Pd	83	
2	Pe	83	
2	Pf	83	
2	Pg	83	
2	Ph	83	
2	Pi	83	
2	Pj	83	
2	Pk	83	
2	Pl	83	
2	Pm	83	
2	Pn	83	
2	Po	83	
2	Pp	83	
2	Pq	83	
2	Pr	83	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	Ps	83	
2	Pt	83	
2	Pu	83	
2	Pv	83	
2	Pw	83	
2	Px	83	
3	X0	869	
3	X1	869	
3	X2	869	
3	X3	869	
3	X4	869	
3	X5	869	
3	X6	869	
3	X7	869	
3	X8	869	
3	X9	869	
3	XA	869	
3	XB	869	
3	XC	869	
3	XD	869	
3	XE	869	
3	XF	869	
3	XG	869	
3	XH	869	
3	XI	869	

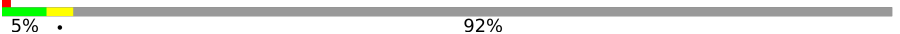
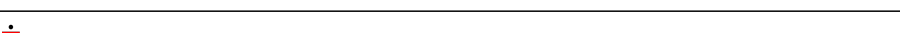
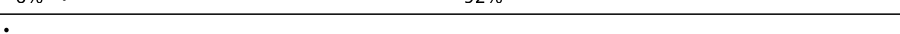
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
3	XJ	869		92%
3	XK	869		92%
3	XL	869		92%
3	XM	869		92%
3	XN	869		92%
3	XO	869		92%
3	XP	869		92%
3	XQ	869		92%
3	XR	869		92%
3	XS	869		92%
3	XT	869		92%
3	XU	869		92%
3	XV	869		92%
3	XW	869		92%
3	XX	869		92%
3	XY	869		92%
3	XZ	869		92%
3	Xa	869		92%
3	Xb	869		92%
3	Xc	869		92%
3	Xd	869		92%
3	Xe	869		92%
3	Xf	869		92%
3	Xg	869		92%
3	Xh	869		92%

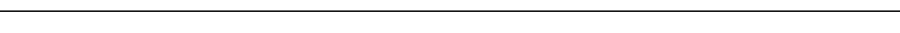
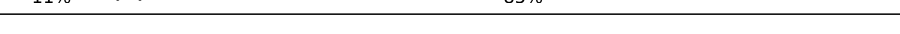
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Xi	869	 92%
3	Xj	869	 92%
3	Xk	869	 92%
3	Xl	869	 92%
3	Xm	869	 92%
3	Xn	869	 92%
3	Xo	869	 92%
3	Xp	869	 92%
3	Xq	869	 92%
3	Xr	869	 92%
3	Xs	869	 92%
3	Xt	869	 92%
3	Xu	869	 92%
3	Xv	869	 92%
3	Xw	869	 92%
3	Xx	869	 92%
3	Y0	869	 85%
3	Y1	869	 85%
3	Y2	869	 85%
3	Y3	869	 85%
3	Y4	869	 85%
3	Y5	869	 85%
3	Y6	869	 85%
3	Y7	869	 85%
3	Y8	869	 85%

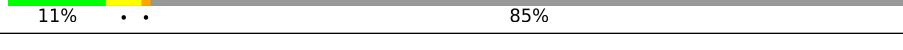
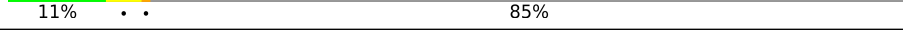
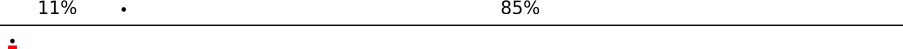
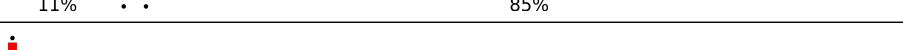
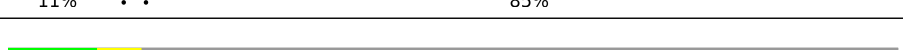
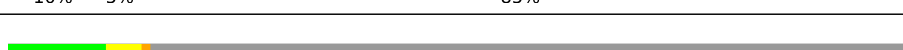
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Y9	869	 11% . . 85%
3	YA	869	 11% . . 85%
3	YB	869	 11% . . 85%
3	YC	869	 11% . 85%
3	YD	869	 11% . . 85%
3	YE	869	 10% . . 85%
3	YF	869	 10% 5% 85%
3	YG	869	 11% . . 85%
3	YH	869	 11% . 85%
3	YI	869	 10% . . 85%
3	YJ	869	 11% . . 85%
3	YK	869	 11% . . 85%
3	YL	869	 10% . 85%
3	YM	869	 10% . . 85%
3	YN	869	 11% . . 85%
3	YO	869	 11% . . 85%
3	YP	869	 11% . . 85%
3	YQ	869	 10% . . 85%
3	YR	869	 11% . 85%
3	YS	869	 11% . . 85%
3	YT	869	 10% . . 85%
3	YU	869	 10% 5% . 85%
3	YV	869	 11% . . 85%
3	YW	869	 10% . 85%
3	YX	869	 11% . . 85%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	YY	869	 11% 85%
3	YZ	869	 11% 85%
3	Ya	869	 11% 85%
3	Yb	869	 10% 5% 85%
3	Yc	869	 11% 85%
3	Yd	869	 11% 85%
3	Ye	869	 11% 85%
3	Yf	869	 11% 85%
3	Yg	869	 11% 85%
3	Yh	869	 11% 85%
3	Yi	869	 11% 85%
3	Yj	869	 10% 5% 85%
3	Yk	869	 11% 85%
3	Yl	869	 11% 85%
3	Ym	869	 10% 5% 85%
3	Yn	869	 11% 85%
3	Yo	869	 11% 85%
3	Yp	869	 11% 85%
3	Yq	869	 10% 85%
3	Yr	869	 11% 85%
3	Ys	869	 11% 85%
3	Yt	869	 11% 85%
3	Yu	869	 10% 85%
3	Yv	869	 11% 85%
3	Yw	869	 11% 85%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Yx	869	11% . 85%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 716166 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Major carboxysome shell protein CsoS1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AB	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AC	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AD	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AE	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BA	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BB	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BC	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BD	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BE	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CA	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CB	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CC	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CD	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CE	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DA	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DB	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	DC	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DE	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EA	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EB	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EC	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	ED	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EE	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FA	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FB	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FC	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FD	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FE	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GA	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GB	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GC	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GD	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GE	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HA	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HB	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HC	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HD	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	HE	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IA	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IB	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IC	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	ID	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IE	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JA	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JB	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JD	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JE	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KA	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KB	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KC	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KD	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KE	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LA	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LB	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LC	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LD	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LE	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MA	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	MB	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MC	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MD	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	ME	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NA	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NB	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NC	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	ND	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NE	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OA	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OB	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OC	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OD	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OE	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	A1	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	A2	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	A3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	A4	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	A5	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	B1	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	B2	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	B4	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	B5	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	C1	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	C2	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	C3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	C4	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	C5	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	D1	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	D2	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	D3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	D5	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	E1	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	E2	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	E4	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	E5	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	F1	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	F2	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	F3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	F4	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	F5	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G1	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	G2	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	G3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	G4	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	G5	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	H1	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	H2	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	H3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	H4	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	H5	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	I1	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	I2	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	I3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	I4	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	I5	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	J1	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	J2	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	J4	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	J5	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	K1	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	K2	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	K4	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	K5	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	L1	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	L2	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	L4	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	L5	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	M1	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	M2	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	M3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	M4	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	M5	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	N1	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	N2	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	N3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	N4	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	N5	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	O1	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	O2	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	O3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	O4	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O5	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	A0	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	A6	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	A7	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	A8	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	A9	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	B0	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	B6	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	B7	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	B8	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	B9	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	C0	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	C6	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	C7	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	C8	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	C9	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	D0	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	D8	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	D9	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	E0	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	E6	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E7	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	E8	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	E9	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	F0	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	F6	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	F7	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	F8	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	F9	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	G0	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	G6	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	G7	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	G8	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	G9	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	H0	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	H6	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	H7	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	H8	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	H9	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	I0	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	I6	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	I7	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I8	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	I9	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	J0	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	J7	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	J8	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	J9	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	K0	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	K6	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	K7	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	K8	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	K9	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	L0	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	L6	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	L7	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	L8	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	L9	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	M0	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	M6	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	M7	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	M8	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	M9	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N0	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	N6	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	N7	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	N8	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	N9	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	O0	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	O6	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	O7	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	O8	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	O9	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AP	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AQ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AR	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AS	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AT	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BP	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BQ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BR	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BS	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BT	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CP	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CQ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CR	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CS	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CT	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DP	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DQ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DT	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EP	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EQ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	ER	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	ES	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	ET	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FP	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FQ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FR	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FS	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FT	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GP	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GQ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GR	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GS	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	GT	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HP	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HQ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HR	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HS	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HT	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IP	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IQ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IR	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IS	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IT	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JP	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JQ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JR	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JS	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JT	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KP	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KQ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KR	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KS	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KT	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	LP	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LQ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LR	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LS	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LT	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MP	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MQ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MR	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MS	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MT	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NP	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NQ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NR	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NS	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NT	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OP	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OQ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OR	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OS	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OT	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AG	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AH	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AI	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AJ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AK	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BG	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BH	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BI	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BJ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BK	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CG	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CH	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CI	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CJ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CK	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DG	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DK	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EG	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EH	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EJ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EK	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FG	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	FH	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FI	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FJ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FK	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GG	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GH	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GI	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GJ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GK	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HG	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HH	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HI	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HJ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HK	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IG	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IH	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	II	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IJ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IK	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JG	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JH	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	JJ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JK	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KG	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KH	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KJ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KK	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LG	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LH	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LJ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LK	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MG	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MH	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MJ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NG	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NH	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NJ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NK	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OG	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OH	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OJ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OK	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AF	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AL	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AM	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AN	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AO	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BF	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BL	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BM	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BN	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BO	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CF	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CL	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CM	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CN	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CO	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DL	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DN	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DO	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EM	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EN	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EO	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	FM	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FN	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FO	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GF	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GL	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GM	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GN	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GO	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HF	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HL	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HM	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HN	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HO	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IF	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IL	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IM	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IN	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IO	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JL	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JM	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JN	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	JO	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KF	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KL	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KM	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KN	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KO	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LF	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LL	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LO	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	ML	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MM	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MN	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MO	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NF	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NM	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NN	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NO	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OF	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OL	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OM	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	ON	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	OO	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ae	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Af	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ag	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ah	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ai	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Be	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bf	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bg	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bh	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bi	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ce	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Cf	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Cg	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ch	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ci	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	De	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Dg	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Di	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ee	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ef	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Eg	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Eh	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ei	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fe	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ff	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fg	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fi	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ge	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gf	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gg	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gh	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gi	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	He	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hf	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hg	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hh	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hi	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ie	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	If	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ig	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ih	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ii	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Je	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jf	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jg	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jh	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ji	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ke	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Kf	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Kg	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Kh	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ki	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Le	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Lf	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Lg	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Lh	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Li	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Me	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mf	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mg	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mh	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mi	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ne	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Nf	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ng	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Nh	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ni	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Oe	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Of	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Og	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Oh	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Oi	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AV	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AW	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AX	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AY	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AZ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BV	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BW	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BX	89	Total 635	C 395	N 119	O 118	S 3	0	0
1	BY	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BZ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CV	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CW	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CX	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CY	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CZ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DV	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DW	89	Total 635	C 395	N 119	O 118	S 3	0	0
1	DX	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DZ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EV	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EW	89	Total 635	C 395	N 119	O 118	S 3	0	0
1	EX	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EY	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EZ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FV	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FW	89	Total 635	C 395	N 119	O 118	S 3	0	0
1	FX	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FZ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GV	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GW	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GX	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GY	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	GZ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HV	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HW	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HX	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HY	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HZ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IV	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IW	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IX	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IY	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IZ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JV	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JW	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JX	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JZ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KV	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KW	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KX	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KY	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KZ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LV	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	LW	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LX	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LY	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LZ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MV	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MW	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MX	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MY	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MZ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NV	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NW	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NX	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NY	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NZ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OV	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OW	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OX	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OY	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OZ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	AU	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Aa	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ab	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ac	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ad	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	BU	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ba	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bb	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bc	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bd	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	CU	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ca	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Cb	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Cc	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Cd	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Da	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Dc	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Dd	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EU	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ea	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Eb	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ec	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ed	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	FU	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fa	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fb	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fc	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fd	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	GU	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ga	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gb	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gc	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gd	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	HU	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ha	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hb	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hc	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hd	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	IU	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ia	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ib	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ic	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Id	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ja	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Jb	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jc	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jd	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	KU	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ka	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Kb	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Kc	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Kd	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LU	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	La	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Lb	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Lc	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ld	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MU	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ma	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mb	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mc	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Md	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NU	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Na	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Nb	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Nc	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Nd	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OU	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Oa	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ob	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Oc	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Od	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	At	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Au	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Av	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Aw	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ax	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bt	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bu	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bv	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bw	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bx	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ct	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Cu	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Cv	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Cw	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Cx	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Dt	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Du	89	Total 635	C 395	N 119	O 118	S 3	0	0
1	Dv	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Dx	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Et	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Eu	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ev	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ew	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ex	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ft	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fu	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fv	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fw	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fx	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gt	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gu	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gv	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gw	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gx	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ht	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Hu	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hv	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hw	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hx	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	It	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Iu	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Iv	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Iw	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ix	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jt	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ju	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jw	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jx	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Kt	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ku	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Kv	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Kw	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Kx	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Lt	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Lu	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Lv	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Lw	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Lx	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mt	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mu	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mv	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mw	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mx	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Nt	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Nu	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Nv	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Nw	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Nx	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ot	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ou	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ov	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ow	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ox	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ak	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Al	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Am	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	An	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ao	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bk	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bl	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bm	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bn	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bo	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ck	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Cl	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Cm	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Cn	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Co	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Dk	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Dm	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Do	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ek	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	En	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Eo	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fk	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fm	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fn	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fo	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Gk	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gl	89	Total 635	C 395	N 119	O 118	S 3	0	0
1	Gm	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gn	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Go	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hk	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hl	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hm	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hn	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ho	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ik	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Il	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Im	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	In	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Io	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jk	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jl	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jn	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jo	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Kk	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Kl	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Kn	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ko	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Lk	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ll	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ln	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Lo	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mk	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ml	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mn	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mo	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Nk	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Nl	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Nn	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	No	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ok	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ol	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	On	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Oo	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Aj	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ap	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Aq	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ar	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	As	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bj	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bp	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bq	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Br	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Bs	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Cj	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Cp	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Cq	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Cr	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Cs	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Dp	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Dr	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ds	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ej	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ep	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Eq	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Er	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Es	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fj	89	Total 635	C 395	N 119	O 118	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Fp	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fr	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fs	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gj	89	Total 635	C 395	N 119	O 118	S 3	0	0
1	Gp	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gq	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gr	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Gs	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hj	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hp	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hq	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hr	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Hs	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ij	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ip	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Iq	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ir	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Is	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jj	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jp	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jq	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Jr	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Js	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Kj	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Kp	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Kq	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Kr	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ks	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Lj	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Lp	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Lq	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Lr	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ls	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mj	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mp	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mq	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Mr	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Ms	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Nj	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Np	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Nq	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Nr	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ns	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Oj	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Op	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Oq	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Or	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Os	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DD	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JC	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	D4	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	J3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	D7	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	J6	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DS	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EI	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DM	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Dw	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jv	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Dn	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DR	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FL	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LM	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	LN	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NL	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Fh	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FY	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JY	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Dj	89	Total 635	C 395	N 119	O 118	S 3	0	0
1	Fq	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	EL	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Dh	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DY	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Db	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Dq	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	L3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Em	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DJ	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	E3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DH	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DI	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	D6	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Df	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JI	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	KI	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	LI	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MI	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	NI	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	OI	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	FF	89	Total 635	C 395	N 119	O 118	S 3	0	0
1	JU	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	El	89	Total 635	C 395	N 119	O 118	S 3	0	0
1	Fl	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Km	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Nm	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Om	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	DU	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Dl	89	Total 635	C 395	N 119	O 118	S 3	0	0
1	EF	89	Total 635	C 395	N 119	O 118	S 3	0	0
1	DF	89	Total 635	C 395	N 119	O 118	S 3	0	0
1	MK	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	JF	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Jm	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Lm	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	MF	92	Total 656	C 408	N 123	O 122	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Mm	92	Total	C	N	O	S	0	0
			656	408	123	122	3		

- Molecule 2 is a protein called Carboxysome shell vertex protein CsoS4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	PA	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	PB	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	PC	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	PD	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	PE	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	P1	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	P2	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	P3	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	P4	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	P5	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	P6	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	P7	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	P8	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	P9	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	P0	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	PP	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	PQ	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	PR	81	Total	C	N	O	S	0	0
			608	386	105	112	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	PS	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	PT	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	PG	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	PH	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	PI	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	PJ	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	PK	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	PL	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	PM	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	PN	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	PO	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	PF	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pe	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pf	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pg	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Ph	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pi	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	PV	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	PW	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	PX	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	PY	81	Total 608	C 386	N 105	O 112	S 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	PZ	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pa	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pb	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pc	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pd	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	PU	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pt	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pu	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pv	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pw	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Px	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pk	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pl	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pm	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pn	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Po	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pp	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pq	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pr	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Ps	81	Total 608	C 386	N 105	O 112	S 5	0	0
2	Pj	81	Total 608	C 386	N 105	O 112	S 5	0	0

- Molecule 3 is a protein called Carboxysome assembly protein CsoS2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	XA	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	XB	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	XC	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	XE	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	YA	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	YB	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	YC	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	YD	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	YE	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	X1	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	X2	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	Y1	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	Y2	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	Y4	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	Y5	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	X6	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	X9	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	X0	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	Y6	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	Y7	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	Y8	134	Total 980	C 591	N 191	O 193	S 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Y9	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	Y0	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	XP	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	XQ	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	XR	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	XT	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	YP	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	YQ	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	YR	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	YS	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	YT	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	XG	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	XH	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	XK	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	YG	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	YH	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	YI	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	YJ	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	YK	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	XL	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	XO	72	Total 513	C 314	N 86	O 110	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	XF	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	YL	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	YM	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	YN	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	YO	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	YF	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	Xe	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Xf	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Xg	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Xi	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Ye	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	Yf	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	Yg	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	Yh	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	Yi	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	XV	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	XW	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	XZ	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	YV	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	YW	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	YX	134	Total	C	N	O	S	0	0
			980	591	191	193	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	YY	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	YZ	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	Xd	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	XU	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Ya	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	Yb	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	Yc	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	Yd	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	YU	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	Xt	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Xu	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Xv	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Xx	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Yt	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	Yu	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	Yv	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	Yw	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	Yx	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	Xk	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Xl	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Xo	72	Total	C	N	O	S	0	0
			513	314	86	110	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Yk	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	Yl	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	Ym	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	Yn	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	Yo	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	Xp	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	Xs	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	Xj	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	Yp	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	Yq	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	Yr	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	Ys	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	Yj	134	Total 980	C 591	N 191	O 193	S 5	0	0
3	XD	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	X4	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	X7	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	X8	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	XS	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	Xh	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	XY	72	Total 513	C 314	N 86	O 110	S 3	0	0
3	Xb	72	Total 513	C 314	N 86	O 110	S 3	0	0

Continued on next page...

Continued from previous page...

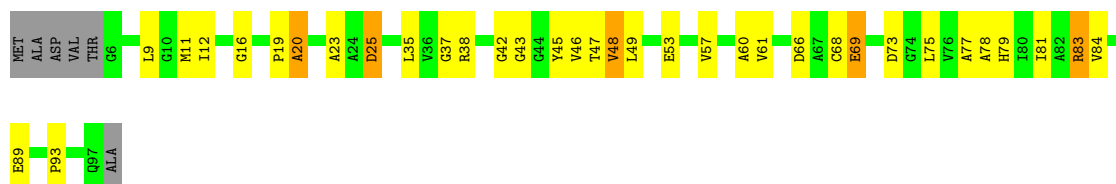
Mol	Chain	Residues	Atoms					AltConf	Trace
3	Xc	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Xw	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Xn	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Xq	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Xr	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	X5	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	XX	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	XJ	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	XM	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Y3	134	Total	C	N	O	S	0	0
			980	591	191	193	5		
3	Xa	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	XN	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	X3	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	XI	72	Total	C	N	O	S	0	0
			513	314	86	110	3		
3	Xm	72	Total	C	N	O	S	0	0
			513	314	86	110	3		

3 Residue-property plots [i](#)

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

- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AA: 



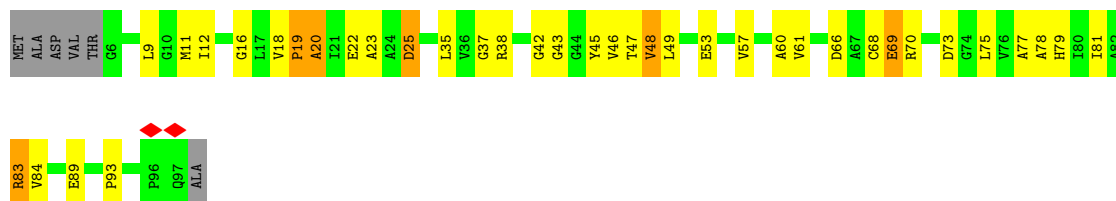
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AB: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AC: 



- Molecule 1: Major carboxysome shell protein CsoS1A

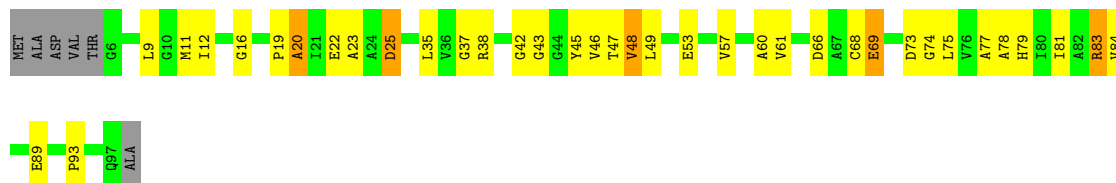
Chain AD: 





- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AE: 56% 33% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BA: 62% 31% 6% 6%



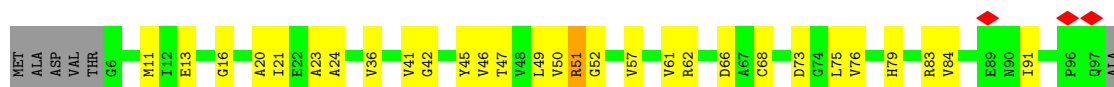
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BB: 63% 30% 6% 6%



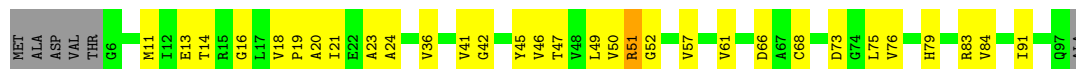
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BC: 64% 29% 6% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BD: 62% 31% 6% 6%



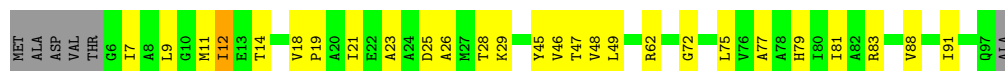
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BE: 64% 29% 6% 6%



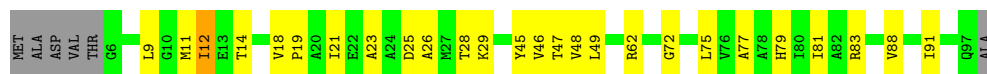
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CA:  66% 27% • 6%



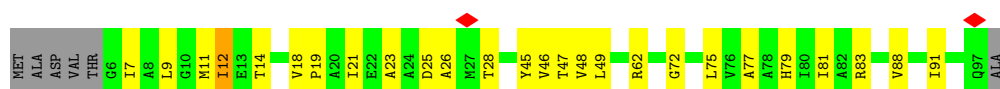
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CB:  67% 26% • 6%



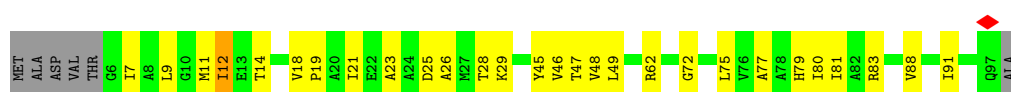
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CC:  67% 26% • 6%



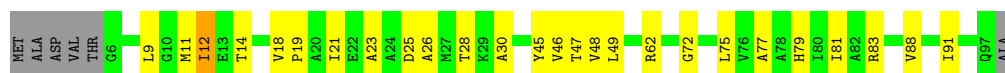
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CD:  65% 28% • 6%



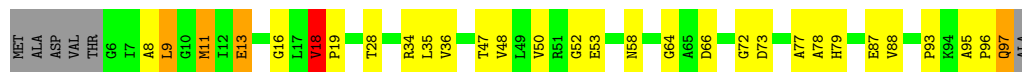
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CE:  67% 26% • 6%



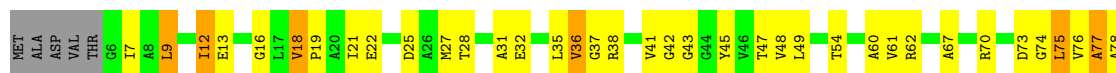
- Molecule 1: Major carboxysome shell protein CsoS1A

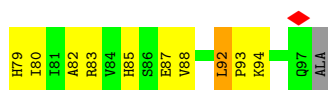
Chain DA:  63% 26% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DB:  46% 41% 7% 6%





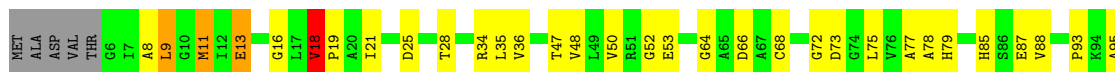
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DC: 55% 33% 5% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DE: 59% 30% • • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EA: 65% 24% • 6%



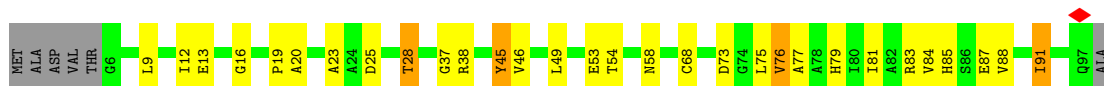
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EB: 70% 19% • 6%



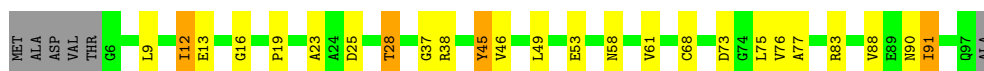
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EC: 63% 27% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain ED: 68% 21% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



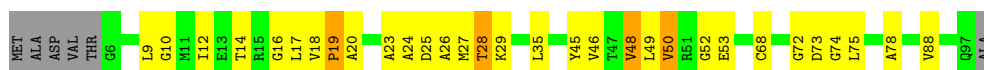
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A





- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



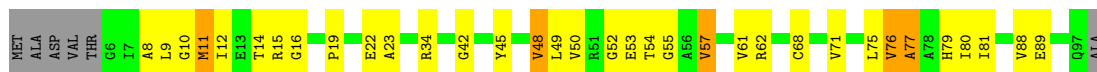
- Molecule 1: Major carboxysome shell protein CsoS1A



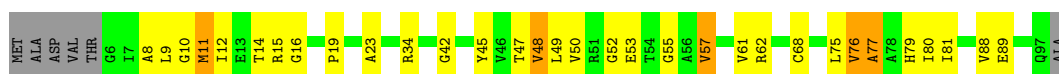
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

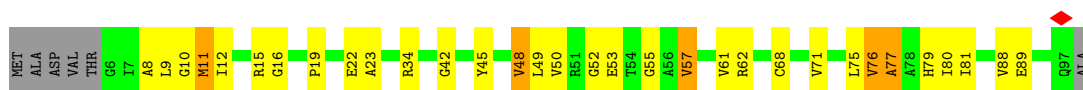


- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A





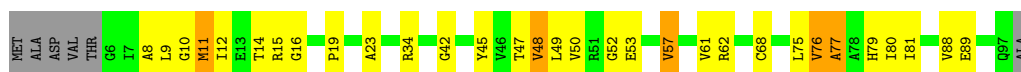
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HD: 63% 26% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HE: 62% 27% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IA: 73% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IB: 70% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IC: 72% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain ID: 74% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IE: 73% 20% 6%



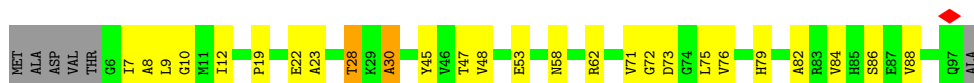
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JA: 72% 20% 6%



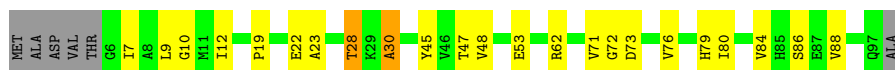
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JB: 67% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JD: 70% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JE: 71% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KA: 66% 24% 6%



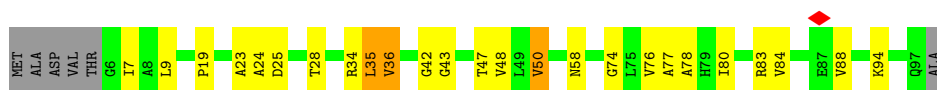
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KB: 67% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

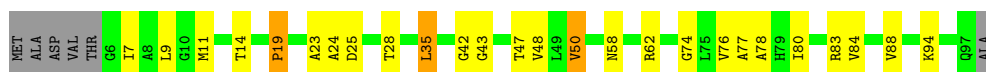
Chain KC: 68% 22% 6%



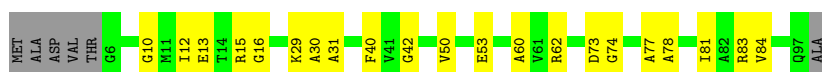
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



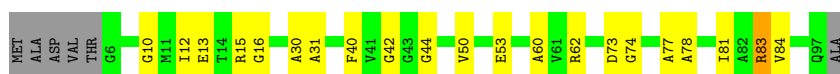
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

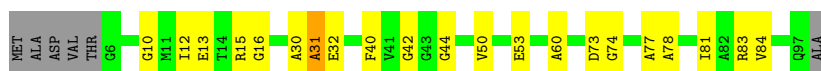


- Molecule 1: Major carboxysome shell protein CsoS1A

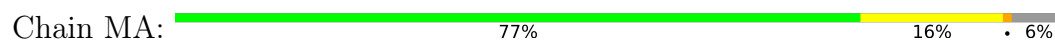


- Molecule 1: Major carboxysome shell protein CsoS1A

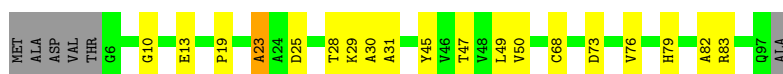
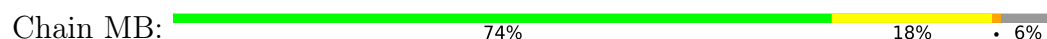




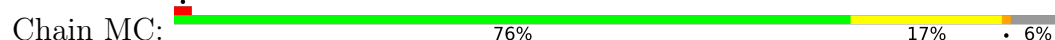
- Molecule 1: Major carboxysome shell protein CsoS1A



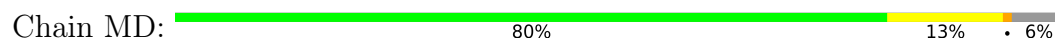
- Molecule 1: Major carboxysome shell protein CsoS1A



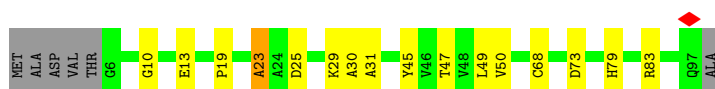
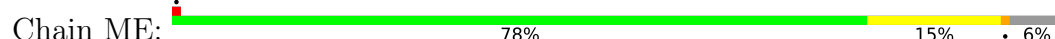
- Molecule 1: Major carboxysome shell protein CsoS1A



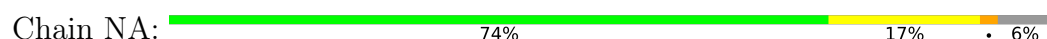
- Molecule 1: Major carboxysome shell protein CsoS1A



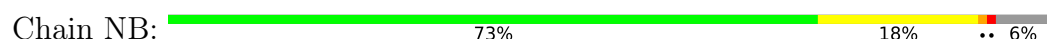
- Molecule 1: Major carboxysome shell protein CsoS1A

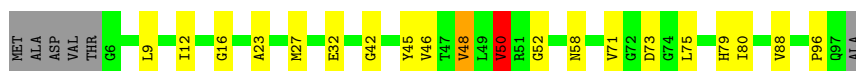


- Molecule 1: Major carboxysome shell protein CsoS1A

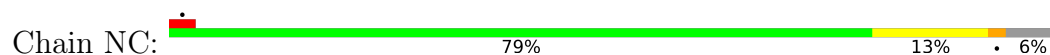


- Molecule 1: Major carboxysome shell protein CsoS1A

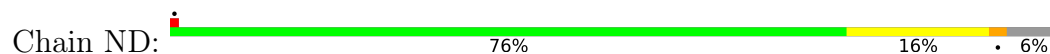




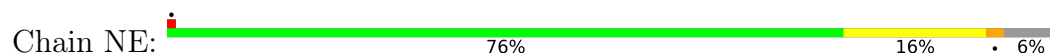
- Molecule 1: Major carboxysome shell protein CsoS1A



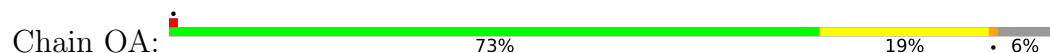
- Molecule 1: Major carboxysome shell protein CsoS1A



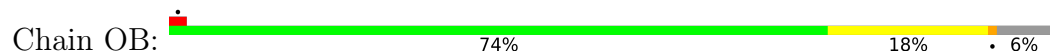
- Molecule 1: Major carboxysome shell protein CsoS1A



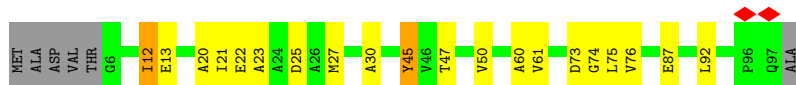
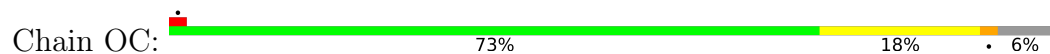
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OD:  73% 19% 6%



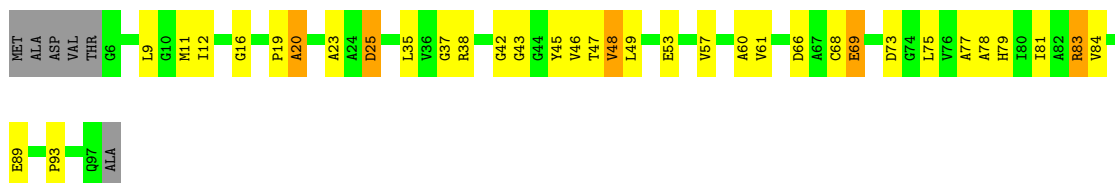
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OE:  73% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain A1:  58% 31% 5% 6%



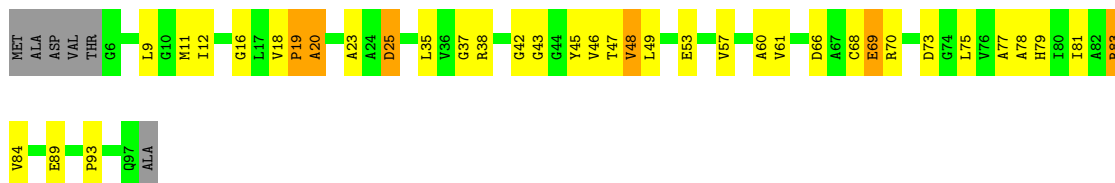
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain A2:  56% 33% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain A3:  56% 32% 6% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain A4:  57% 32% 5% 6%





- Molecule 1: Major carboxysome shell protein CsoS1A

Chain A5: 56% 33% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain B1: 62% 31% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain B2: 62% 31% • 6%



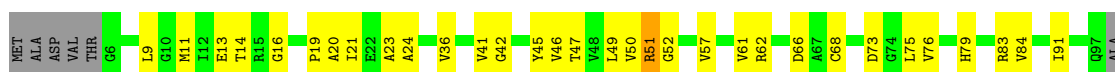
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain B3: 61% 32% • 6%



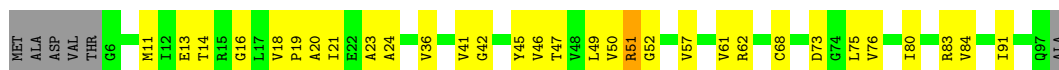
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain B4: 61% 32% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain B5: 62% 31% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain C1:  65% 28% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain C2:  65% 28% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain C3:  65% 28% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain C4:  63% 30% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain C5:  67% 26% • 6%



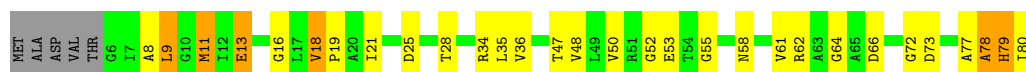
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain D1:  62% 27% • 6%



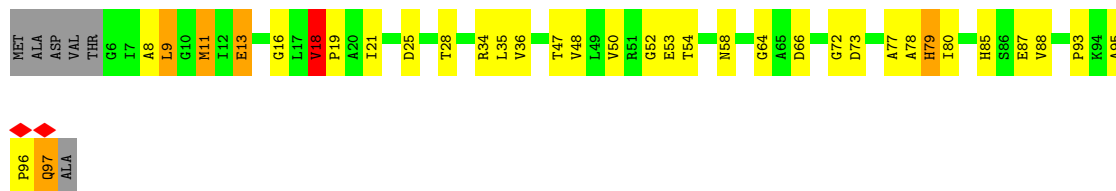
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain D2:  56% 31% 7% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain D3:  58% 30% 5% • 6%



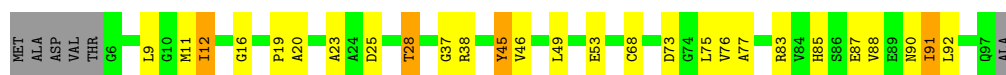
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain D5:  60% 29% • • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain E1:  66% 23% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain E2:  69% 20% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain E4:  69% 20% • 6%



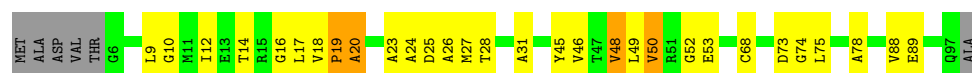
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain E5:  65% 26% • 6%



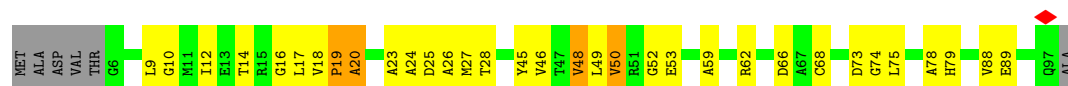
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain F1: 



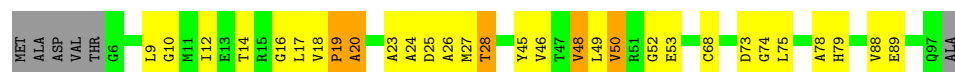
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain F2: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain F3: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain F4: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain F5: 



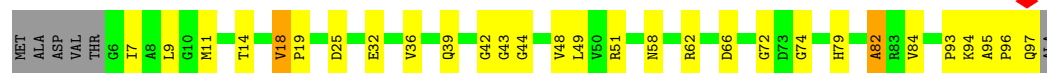
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain G1: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain G2: 



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



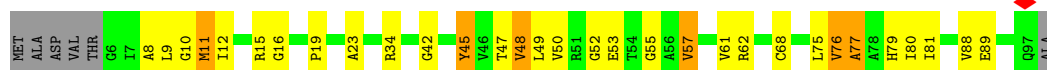
- Molecule 1: Major carboxysome shell protein CsoS1A



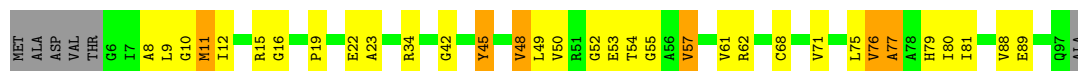
- Molecule 1: Major carboxysome shell protein CsoS1A



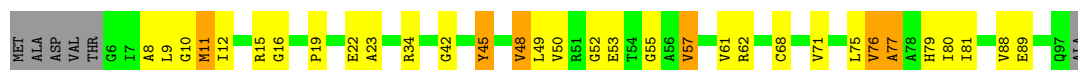
- Molecule 1: Major carboxysome shell protein CsoS1A



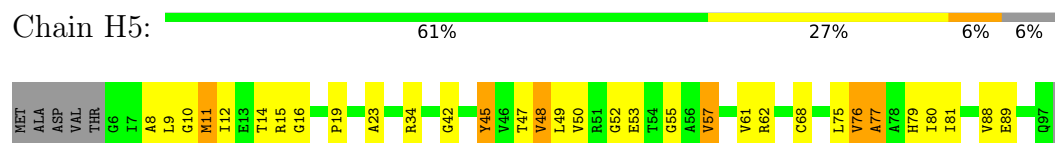
- Molecule 1: Major carboxysome shell protein CsoS1A



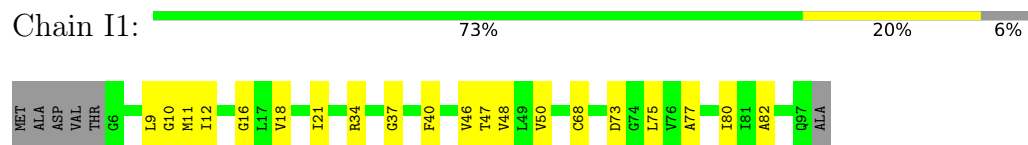
- Molecule 1: Major carboxysome shell protein CsoS1A



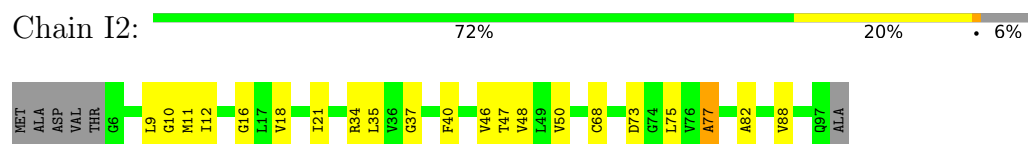
- Molecule 1: Major carboxysome shell protein CsoS1A



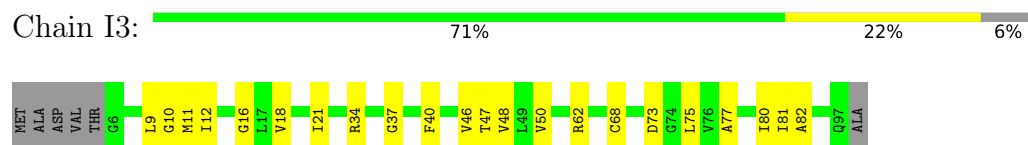
- Molecule 1: Major carboxysome shell protein CsoS1A



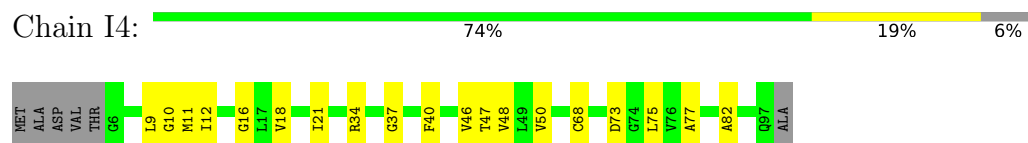
- Molecule 1: Major carboxysome shell protein CsoS1A



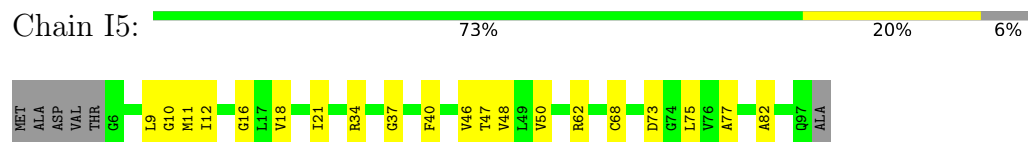
- Molecule 1: Major carboxysome shell protein CsoS1A



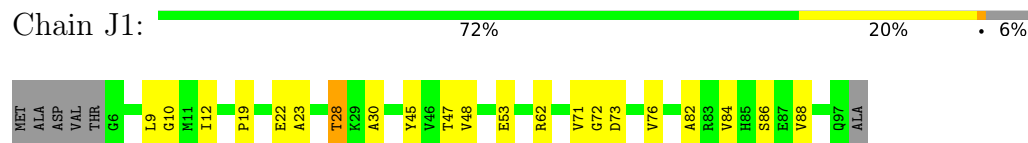
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



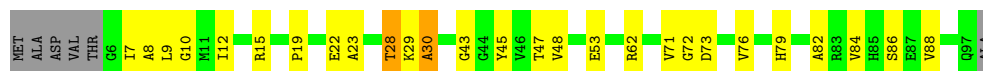
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain J2:  67% 26% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain J4:  66% 26% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain J5:  71% 21% • 6%



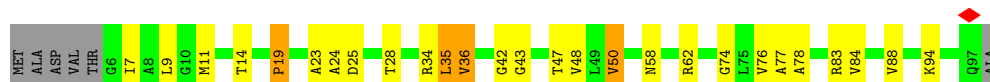
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain K1:  67% 23% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain K2:  66% 23% • 6%



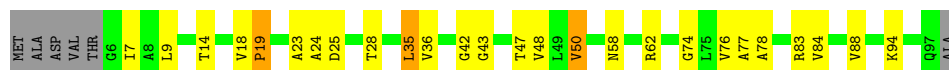
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain K3:  68% 22% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain K4:  67% 23% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain K5:  67% 23% 6%



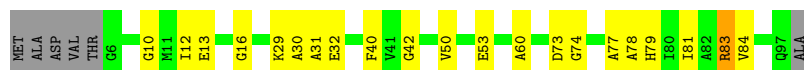
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain L1:  74% 18% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain L2:  72% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain L4:  74% 18% 6%



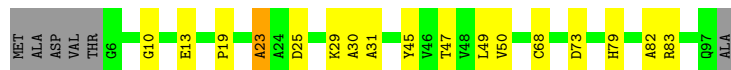
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain L5:  66% 27% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain M1:  77% 16% 6%

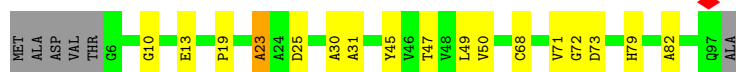
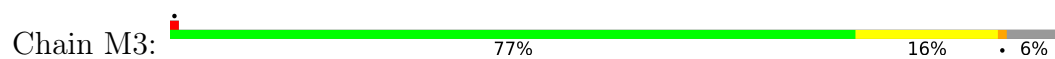


- Molecule 1: Major carboxysome shell protein CsoS1A

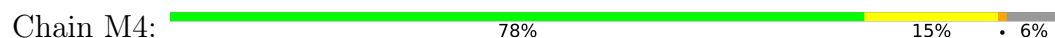
Chain M2:  77% 16% 6%



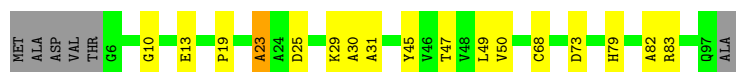
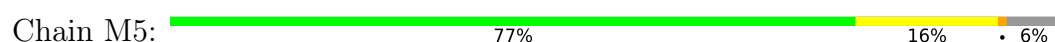
- Molecule 1: Major carboxysome shell protein CsoS1A



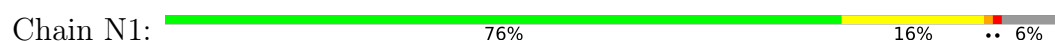
- Molecule 1: Major carboxysome shell protein CsoS1A



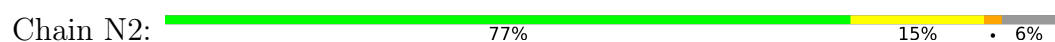
- Molecule 1: Major carboxysome shell protein CsoS1A



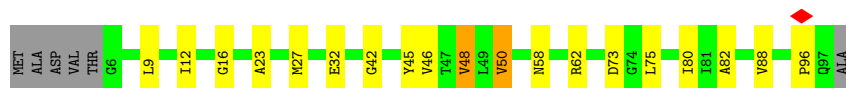
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



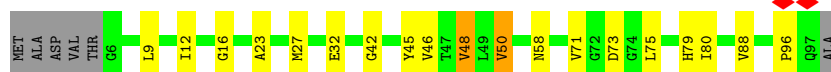
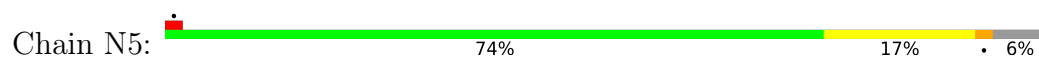
- Molecule 1: Major carboxysome shell protein CsoS1A



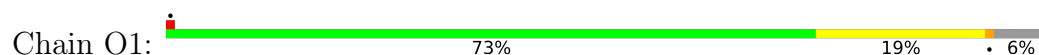
- Molecule 1: Major carboxysome shell protein CsoS1A



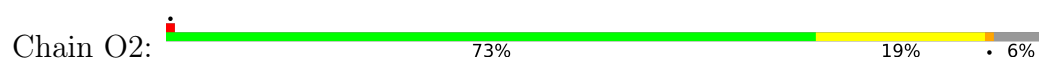
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



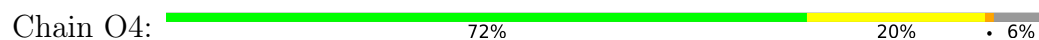
- Molecule 1: Major carboxysome shell protein CsoS1A



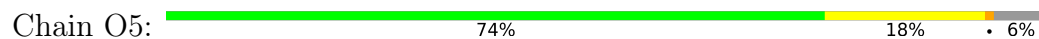
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



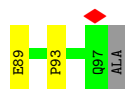
- Molecule 1: Major carboxysome shell protein CsoS1A





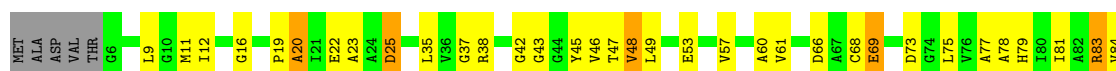
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain A6: 58% 31% 5% 6%



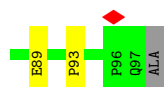
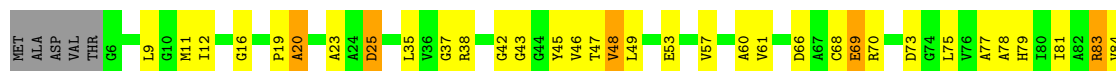
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain A7: 57% 32% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain A8: 57% 32% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain A9: 57% 32% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain B0: 62% 31% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain B6: 61% 32% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain B7: 65% 28% 6%



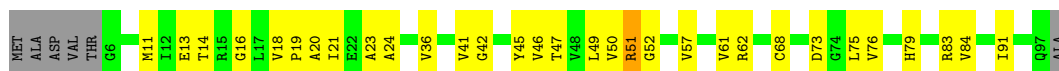
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain B8: 60% 33% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain B9: 62% 31% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain C0: 65% 28% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain C6: 66% 27% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain C7:  65% 28% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain C8:  67% 26% • 6%



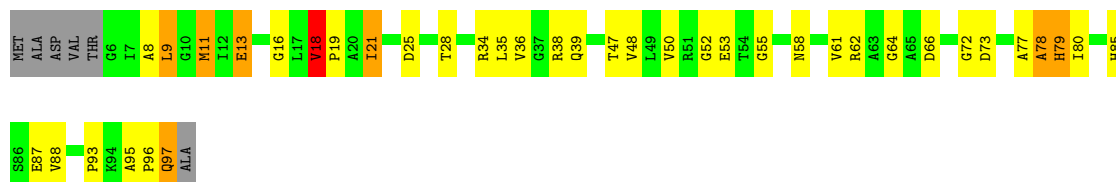
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain C9:  63% 30% • 6%



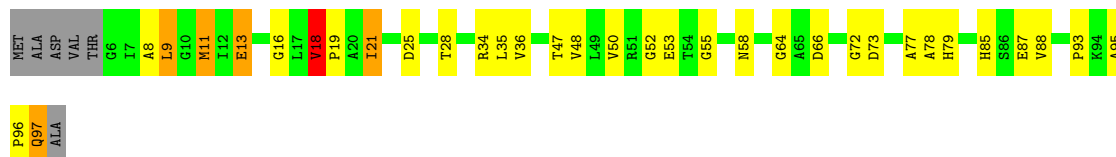
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain D0:  54% 32% 7% • 6%



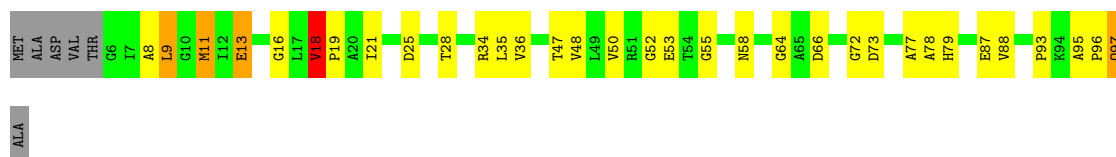
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain D8:  59% 29% 5% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain D9:  60% 29% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain E0:  70% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain E6:  69% 20% 6%



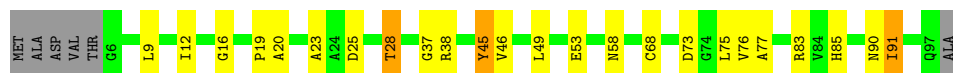
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain E7:  65% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain E8:  69% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain E9:  66% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain F0:  60% 30% 6%



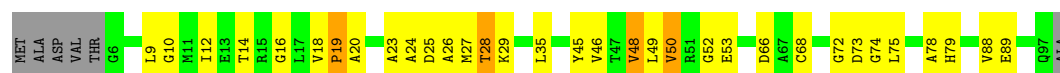
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain F6:  61% 29% 6%



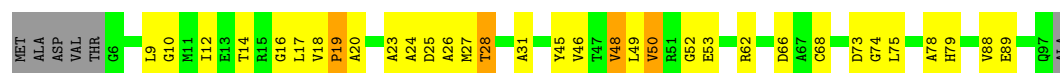
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain F7: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain F8: 



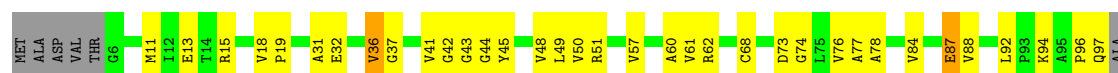
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain F9: 



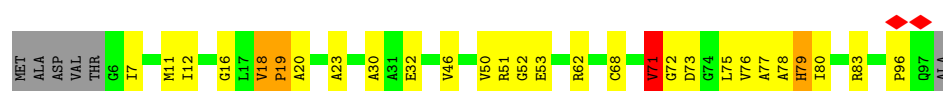
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain G0: 



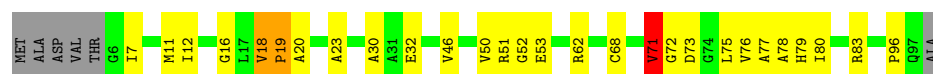
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain G6: 



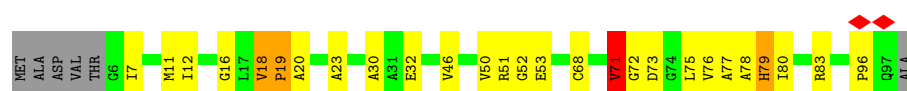
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain G7: 

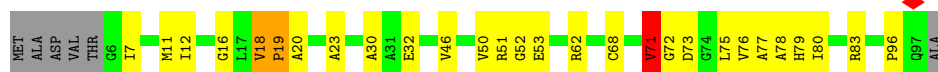


- Molecule 1: Major carboxysome shell protein CsoS1A

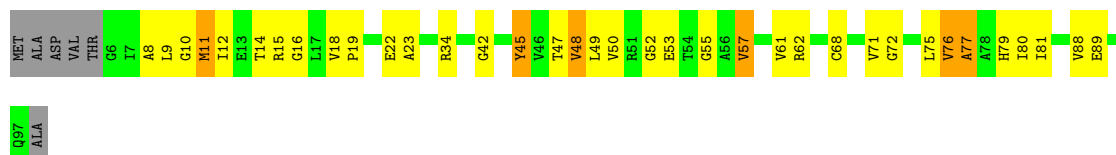
Chain G8: 



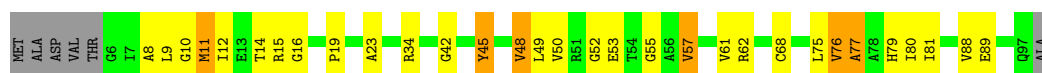
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



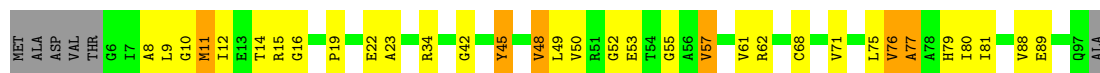
- Molecule 1: Major carboxysome shell protein CsoS1A



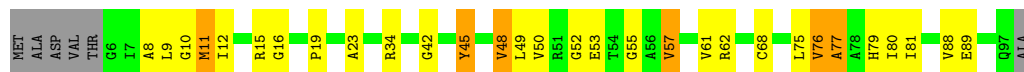
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain I6: 71% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain I7: 73% 20% 6%



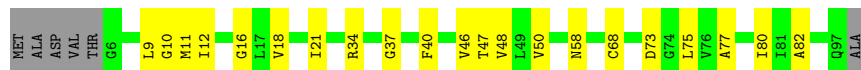
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain I8: 71% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain I9: 72% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain J0: 69% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain J7: 66% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain J8: 69% 23% 6%



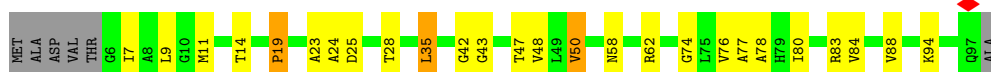
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain J9:  70% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain K0:  67% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain K6:  66% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain K7:  68% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain K8:  66% 23% 6%



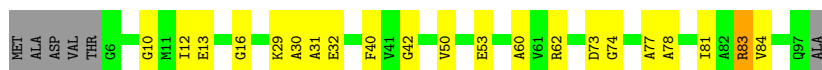
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain K9:  67% 23% 6%



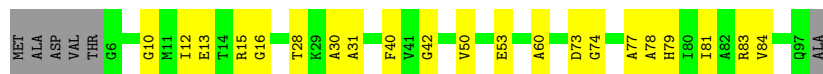
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain L0:  72% 20% 6%



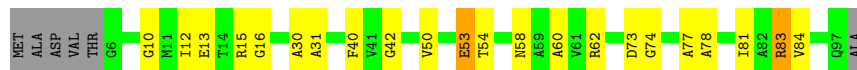
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain L6:  72% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain L7:  71% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain L8:  68% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain L9:  74% 19% 6%



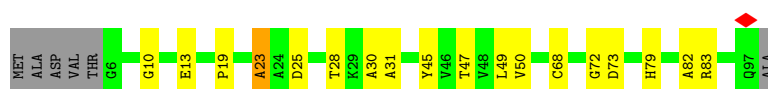
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain M0:  77% 16% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain M6:  76% 17% 6%



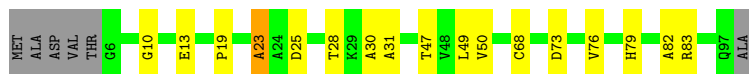
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain M7:  78% 15% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain M8:  77% 16% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain M9:  76% 17% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain N0:  76% 16% •• 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain N6:  76% 16% •• 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain N7:  74% 17% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain N8:  74% 17% •• 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain N9:  73% 18% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain O0:  72% 20% • 6%



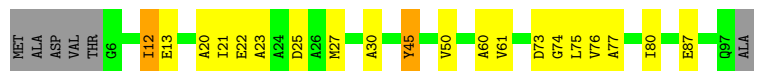
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain O6:  73% 19% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain O7:  73% 18% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain O8:  71% 21% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain O9:  72% 20% • 6%



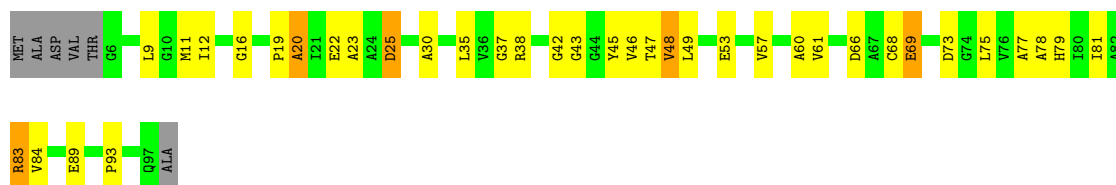
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AP:  57% 31% 6% 6%



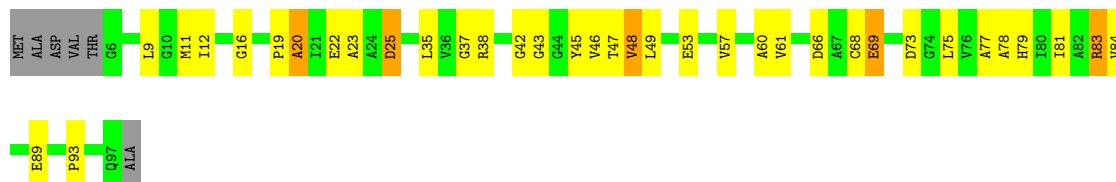
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AQ:  56% 33% 5% 6%



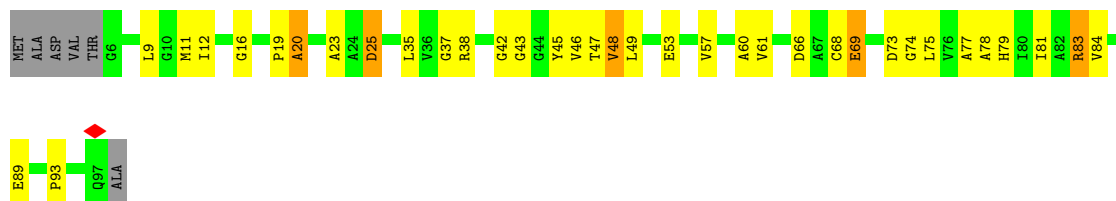
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AR: 57% 32% 5% 6%



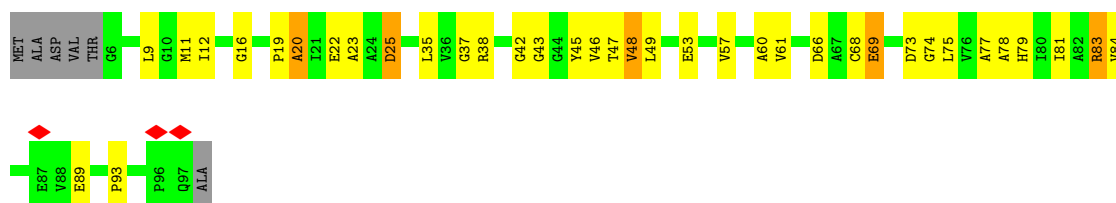
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AS: 57% 32% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AT: 56% 33% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BP: 61% 32% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BQ: 63% 30% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A



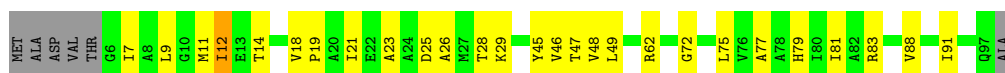
- Molecule 1: Major carboxysome shell protein CsoS1A



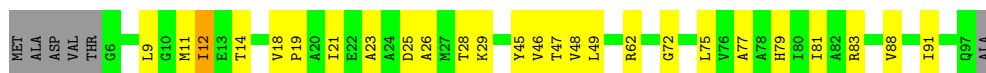
- Molecule 1: Major carboxysome shell protein CsoS1A



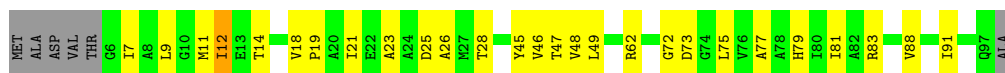
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

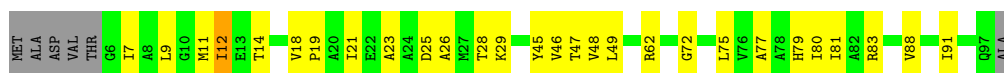


- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A





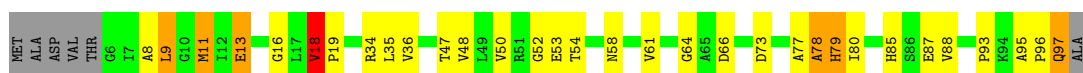
- Molecule 1: Major carboxysome shell protein CsoS1A



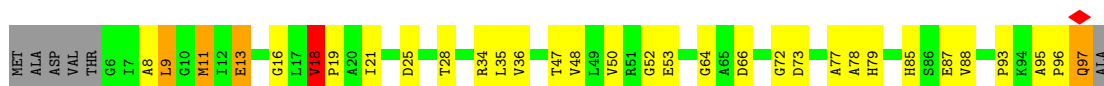
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



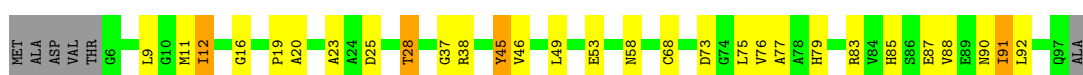
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A





- Molecule 1: Major carboxysome shell protein CsoS1A



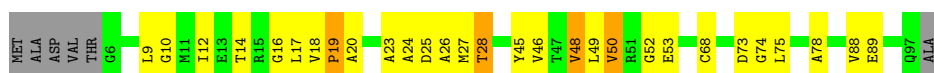
- Molecule 1: Major carboxysome shell protein CsoS1A



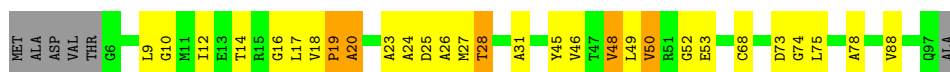
- Molecule 1: Major carboxysome shell protein CsoS1A



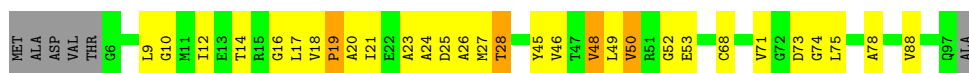
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

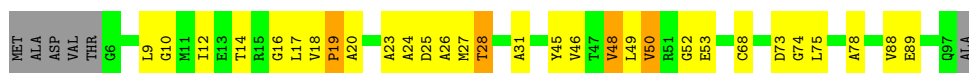


- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

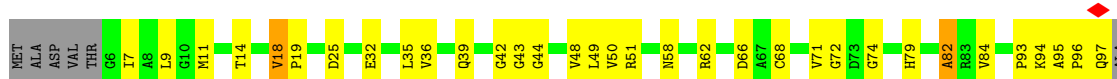




- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



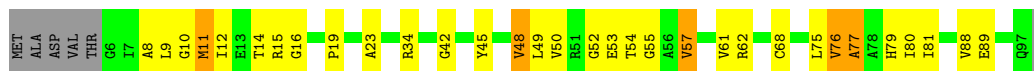
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



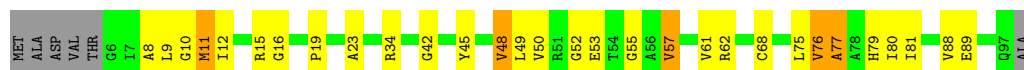
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HQ: 



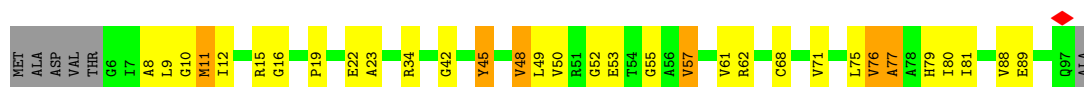
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HR: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HS: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HT: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IP: 



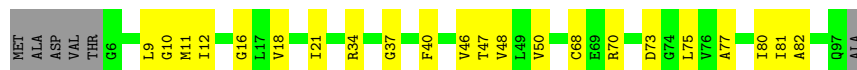
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IQ: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IR: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IS:  70% 23% 6%



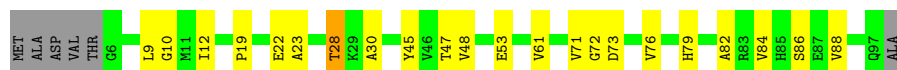
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IT:  73% 20% 6%



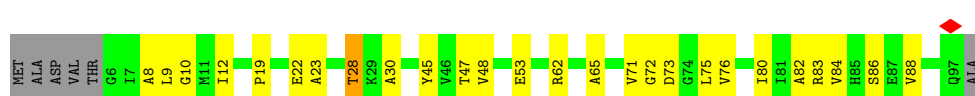
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JP:  71% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JQ:  67% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JR:  68% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JS:  68% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JT:  71% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KP:  66% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KQ:  67% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KR:  67% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KS:  68% 22% 6%



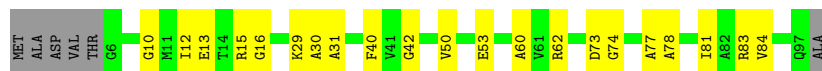
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KT:  64% 27% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain LP:  72% 21% 6%



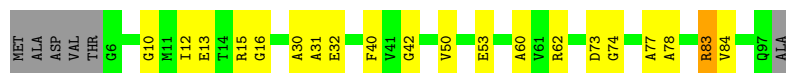
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain LQ:  67% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain LR:  73% 19% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain LS:  70% 22% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain LT:  72% 20% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain MP:  78% 15% • 6%



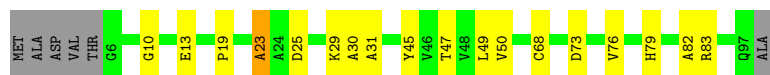
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain MQ:  77% 16% • 6%



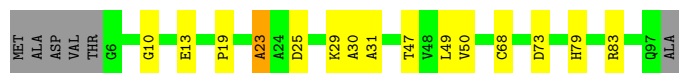
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain MR:  76% 17% • 6%



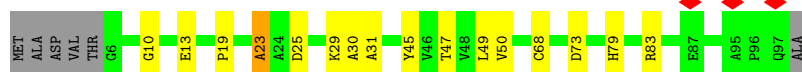
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain MS:  79% 14% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain MT:  78% 15% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NP:  74% 17% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NQ:  73% 18% •• 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NR:  76% 16% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NS:  76% 16% • 6%



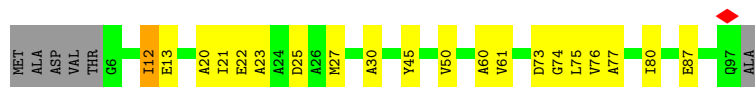
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NT:  74% 17% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OP:  73% 19% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OQ:  74% 18% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OR:  74% 18% • 6%



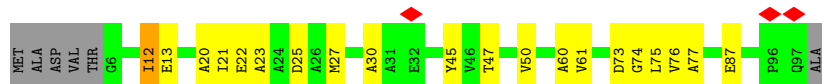
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OS:  73% 19% • 6%



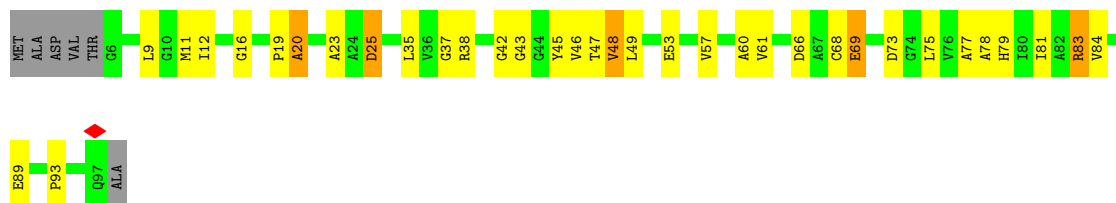
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OT:  73% 19% • 6%



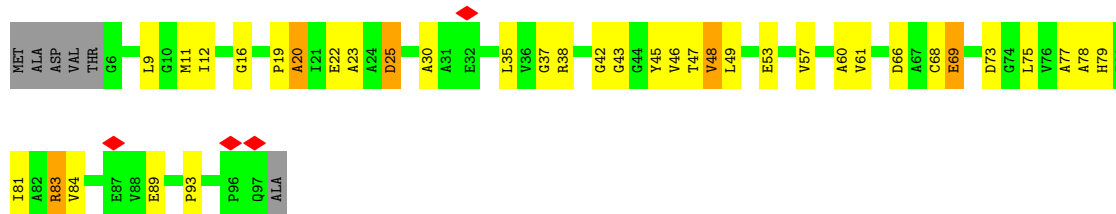
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AG:  58% 31% 5% 6%

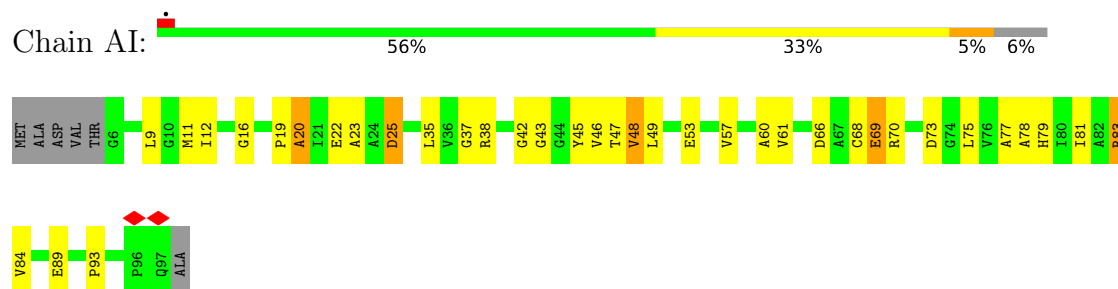


- Molecule 1: Major carboxysome shell protein CsoS1A

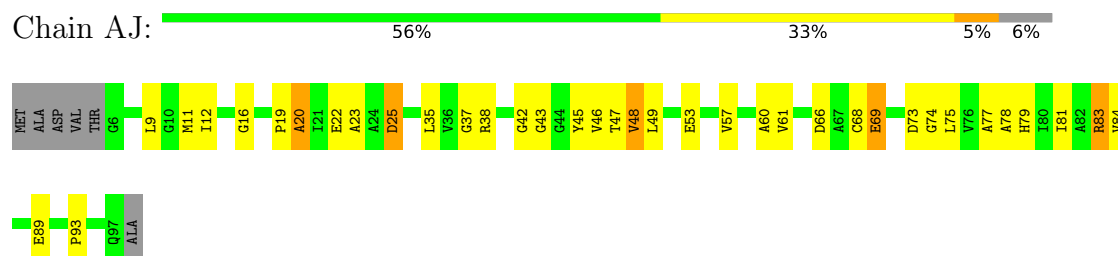
Chain AH:  56% 33% 5% 6%



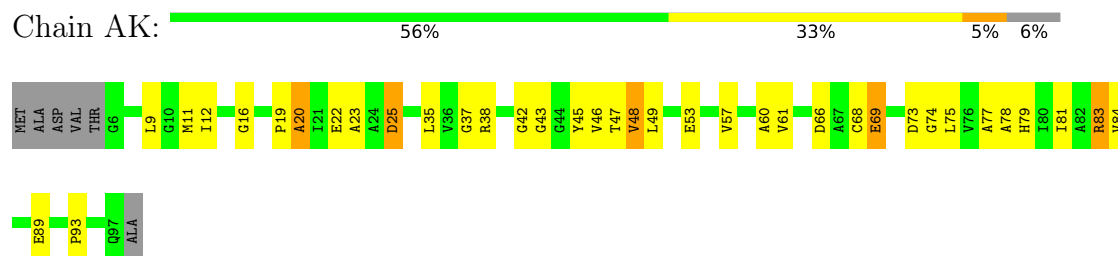
- Molecule 1: Major carboxysome shell protein CsoS1A



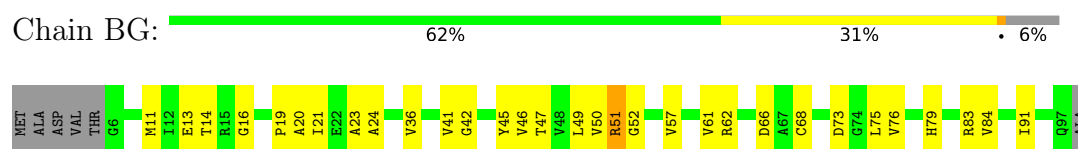
- Molecule 1: Major carboxysome shell protein CsoS1A



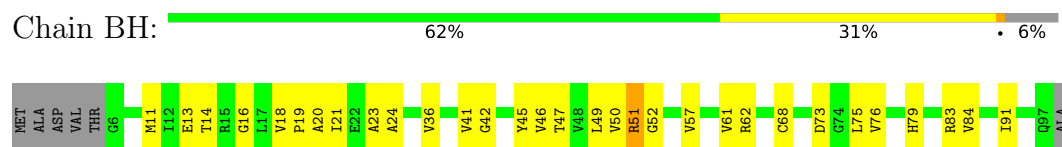
- Molecule 1: Major carboxysome shell protein CsoS1A



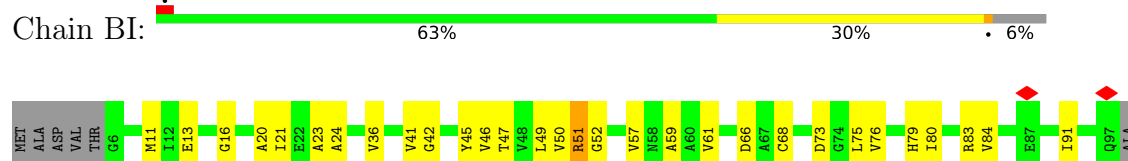
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BJ:  61% 32% • 6%



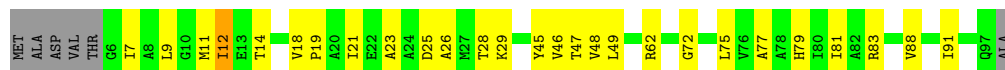
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BK:  64% 29% • 6%



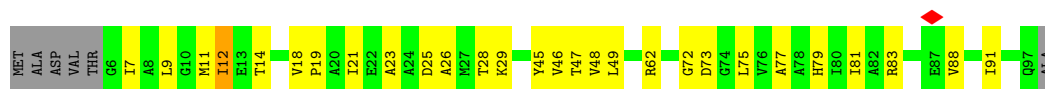
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CG:  66% 27% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CH:  65% 28% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CI:  67% 24% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CJ:  64% 29% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CK:  67% 26% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DG:  63% 26% 6%



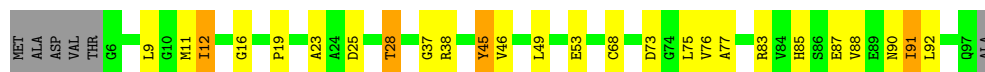
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DK:  60% 29% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EG:  67% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EH:  68% 21% 6%



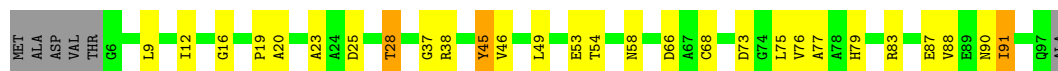
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EJ:  65% 24% 6%



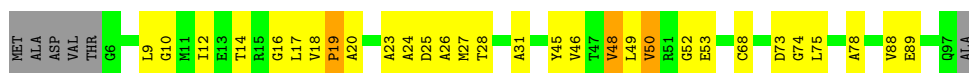
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EK:  65% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

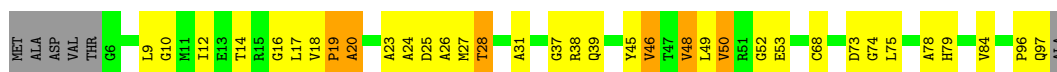
Chain FG:  63% 28% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



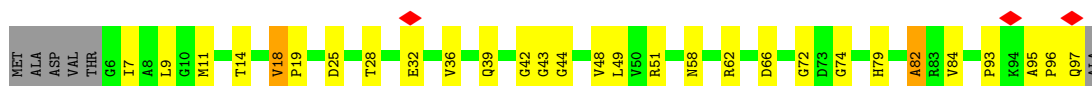
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

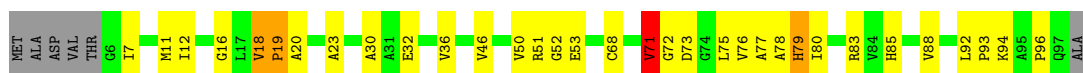


- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

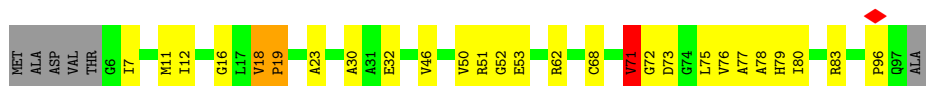




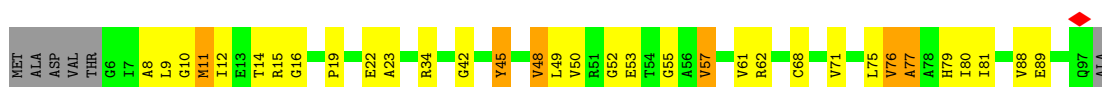
- Molecule 1: Major carboxysome shell protein CsoS1A



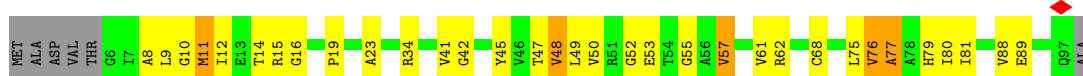
- Molecule 1: Major carboxysome shell protein CsoS1A



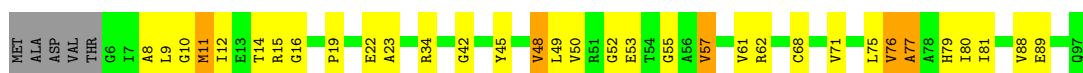
- Molecule 1: Major carboxysome shell protein CsoS1A



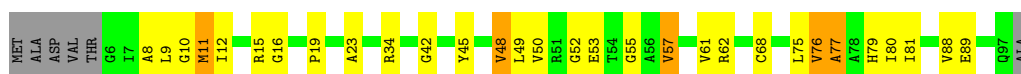
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

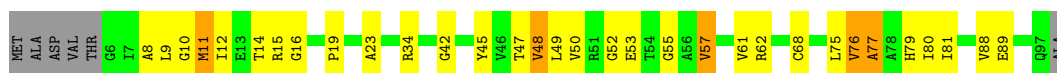


- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A





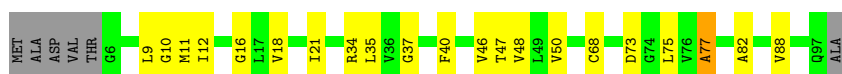
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IG: 73% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IH: 72% 20% 6%



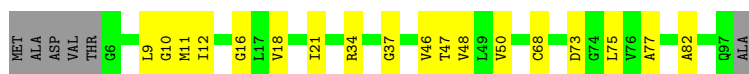
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain II: 71% 22% 6%



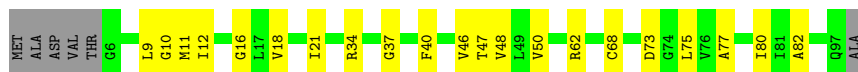
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IJ: 76% 18% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IK: 72% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JG: 71% 21% 6%



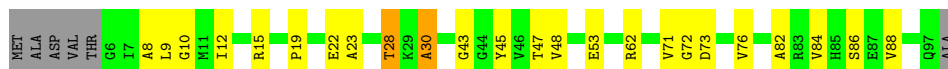
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JH: 68% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JJ: 69% 22% 6%



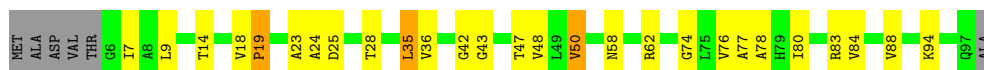
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JK: 70% 22% 6%



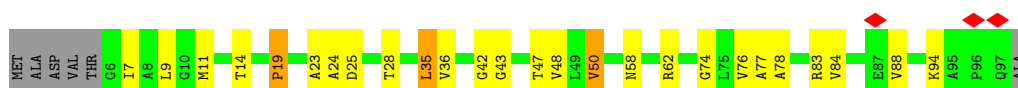
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KG: 66% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KH: 67% 23% 6%



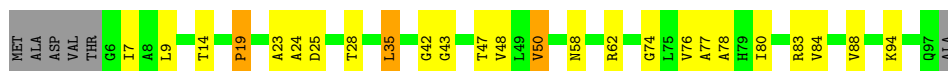
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KJ: 68% 22% 6%



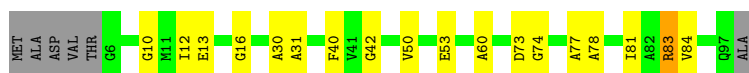
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KK: 68% 22% 6%

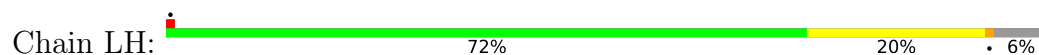


- Molecule 1: Major carboxysome shell protein CsoS1A

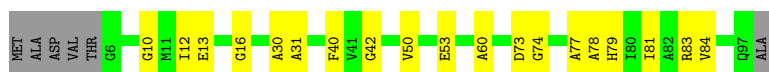
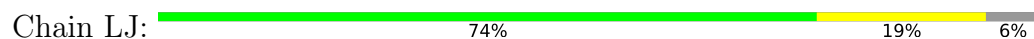
Chain LG: 76% 17% 6%



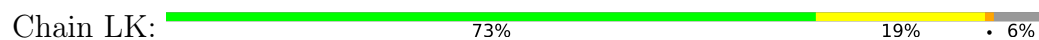
- Molecule 1: Major carboxysome shell protein CsoS1A



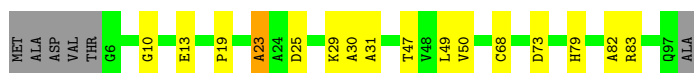
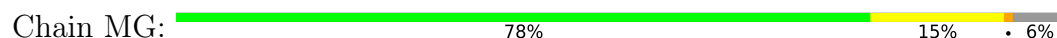
- Molecule 1: Major carboxysome shell protein CsoS1A



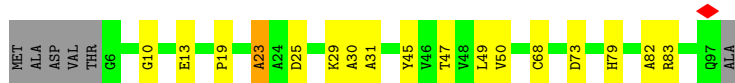
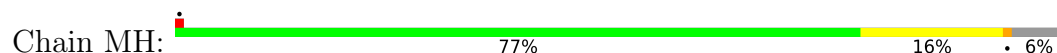
- Molecule 1: Major carboxysome shell protein CsoS1A



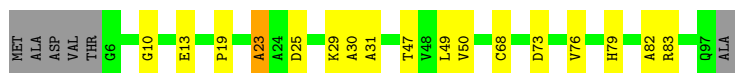
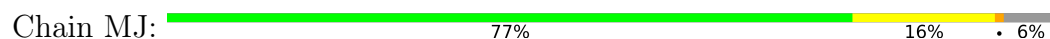
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

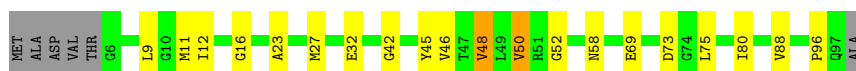


- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A





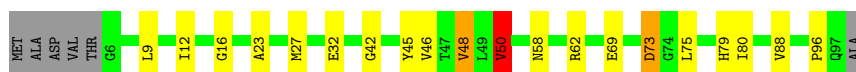
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NH: 77% 15% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NJ: 73% 17% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NK: 76% 16% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OG: 73% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OH: 73% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OJ: 72% 20% 6%



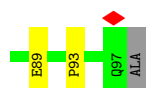
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OK:  73% 19% 6%



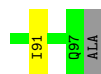
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AF:  56% 33% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AL:  59% 30% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AM:  56% 33% 5% 6%



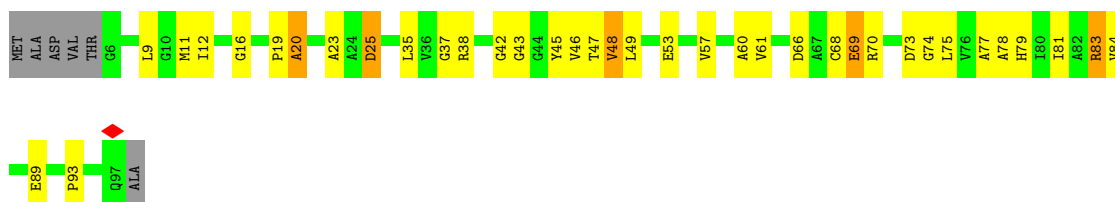
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AN:  57% 32% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

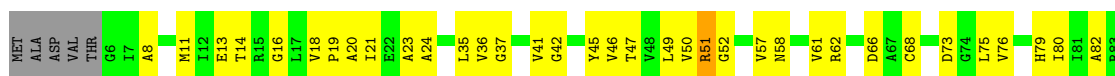
Chain AO:  56% 33% 5% 6%



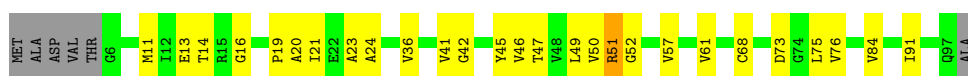
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



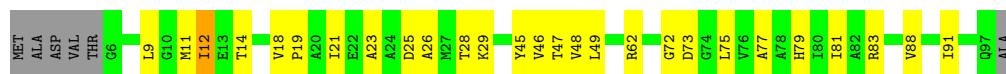
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CF:  65% 28% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CL:  66% 27% • 6%



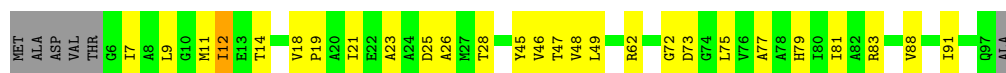
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CM:  66% 27% • 6%



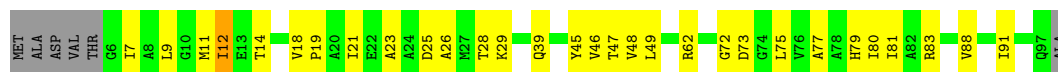
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CN:  66% 27% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CO:  63% 30% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

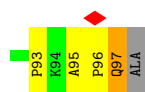
Chain DL:  59% 30% • • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DN:  57% 31% 5% • 6%

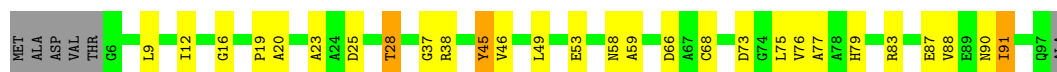




- Molecule 1: Major carboxysome shell protein CsoS1A



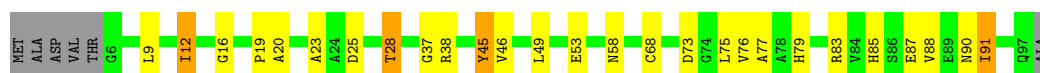
- Molecule 1: Major carboxysome shell protein CsoS1A



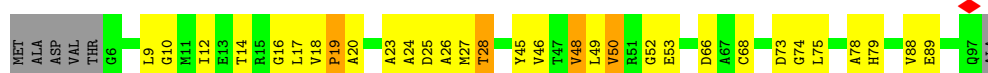
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A





- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GF: 58% 33% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GL: 65% 24% 6%



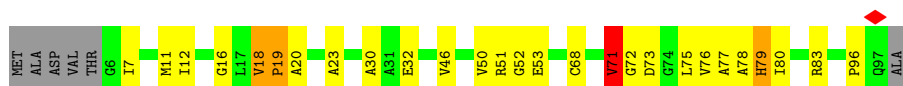
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GM: 65% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GN: 66% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GO: 65% 26% 6%



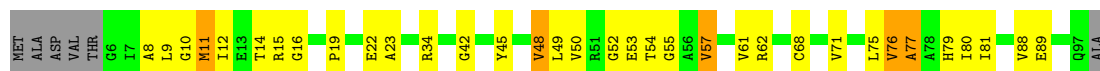
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HF: 60% 28% 6% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HL:  59% 30% 5% 6%



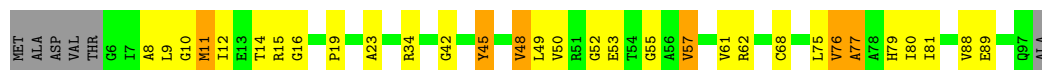
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HM:  59% 29% 6% 6%



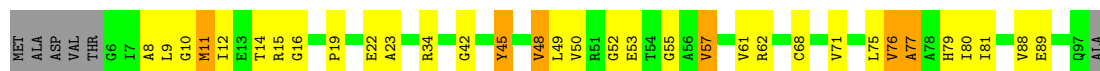
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HN:  62% 26% 6% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HO:  60% 28% 6% 6%



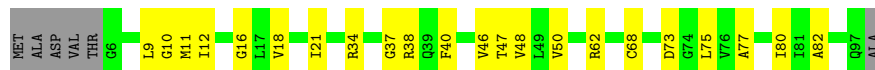
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IF:  70% 23% 6%



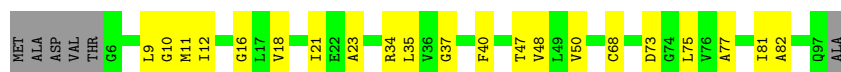
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IL:  71% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IM:  72% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IN: 



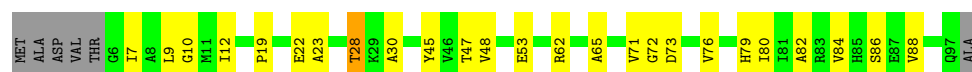
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IO: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JL: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JM: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JN: 



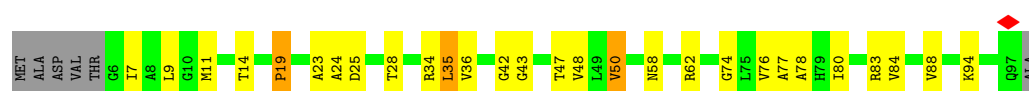
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JO: 



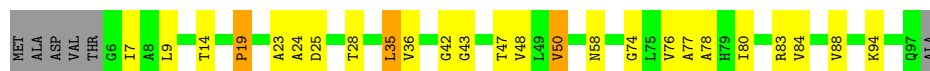
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KF: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KL:  68% 22% 6%



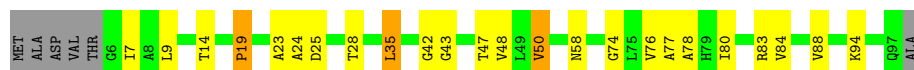
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KM:  67% 23% 6%



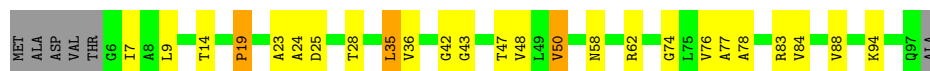
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KN:  69% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KO:  68% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain LF:  72% 20% 6%



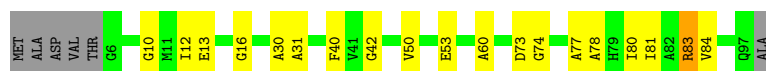
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain LL:  71% 22% 6%



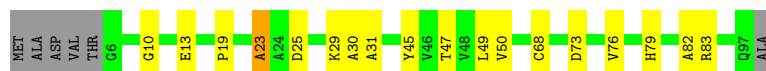
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain LO:  74% 18% 6%



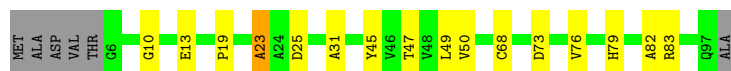
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain ML:  76% 17% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain MM:  78% 15% • 6%



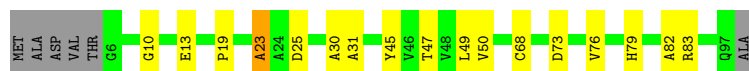
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain MN:  78% 15% • 6%



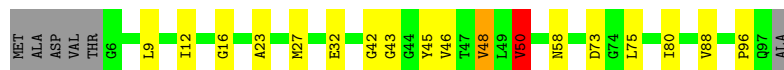
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain MO:  77% 16% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NF:  76% 16% •• 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NM:  72% 19% • 6%



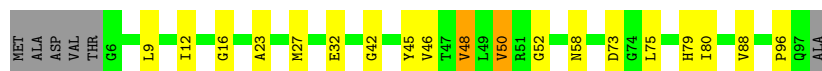
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NN:  76% 16% •• 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NO:  74% 17% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OF:  71% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OL:  72% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OM:  73% 18% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain ON:  71% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OO:  72% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

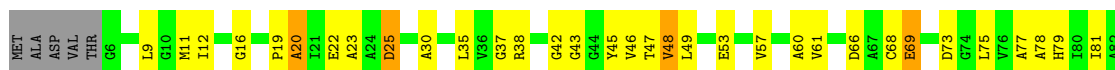
Chain Ae:  58% 31% 5% 6%





- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Af: 56% 33% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ag: 56% 33% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ah: 56% 33% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ai: 57% 32% 5% 6%

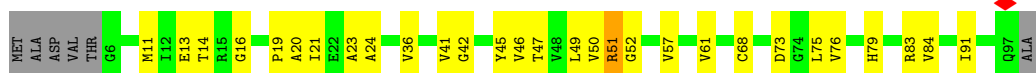


- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Be: 62% 31% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



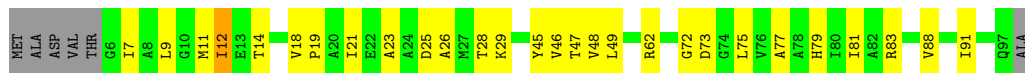
- Molecule 1: Major carboxysome shell protein CsoS1A



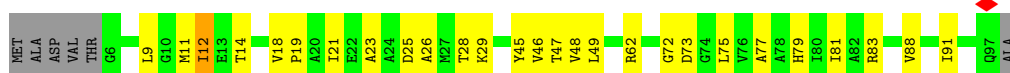
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A





- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ch: 64% 29% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ci: 67% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain De: 63% 26% 6%



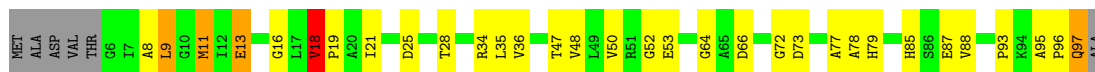
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dg: 57% 32% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Di: 61% 28% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ee: 65% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ef:  65% 24% 6%



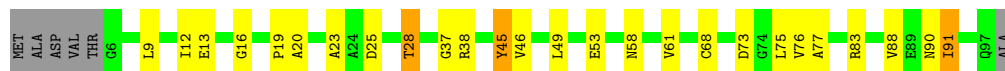
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Eg:  65% 27% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Eh:  67% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ei:  69% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fe:  62% 29% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ff:  63% 26% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fg:  64% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fi: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ge: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Gf: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Gg: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Gh: 



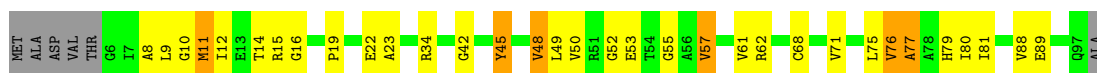
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Gi: 

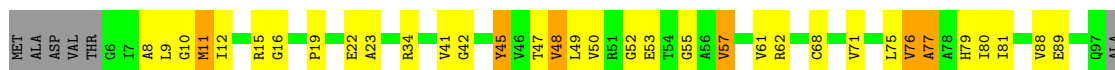


- Molecule 1: Major carboxysome shell protein CsoS1A

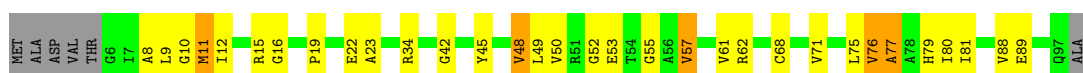
Chain He: 



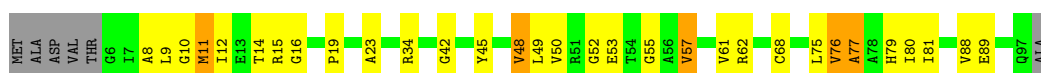
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



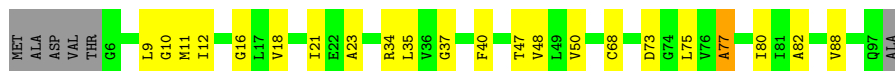
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

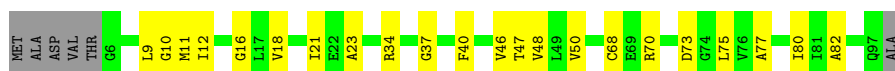


- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A





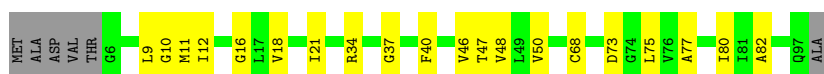
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ih:



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ii:



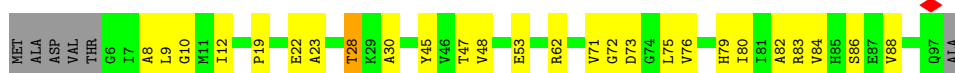
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Je:



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Jf:



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Jg:



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Jh:



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ji:



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ke: 67% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kf: 67% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kg: 67% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kh: 67% 22% 6%



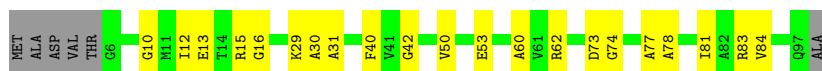
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ki: 66% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Le: 72% 21% 6%

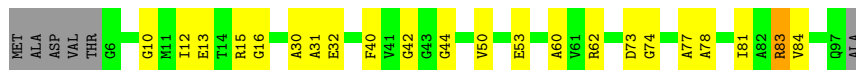


- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Lf: 67% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A



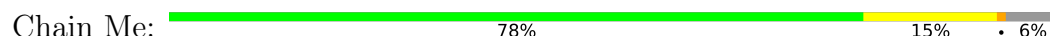
- Molecule 1: Major carboxysome shell protein CsoS1A



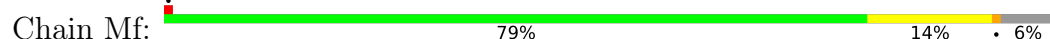
- Molecule 1: Major carboxysome shell protein CsoS1A



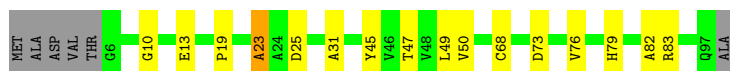
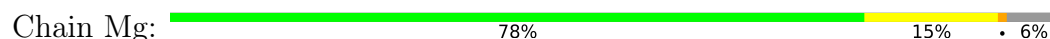
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

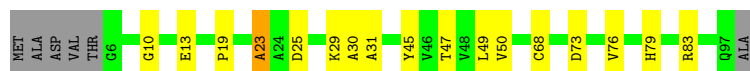


- Molecule 1: Major carboxysome shell protein CsoS1A



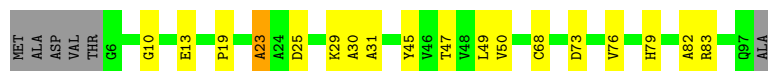
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Mh:  77% 16% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Mi:  76% 17% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ne:  76% 16% •• 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Nf:  74% 17% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ng:  76% 16% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Nh:  74% 17% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ni:  76% 16% •• 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Oe:  73% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Of:  74% 18% 6%



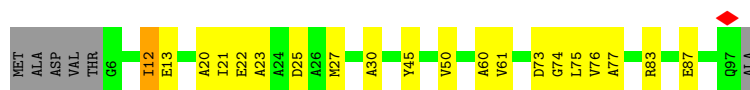
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Og:  73% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Oh:  73% 19% 6%



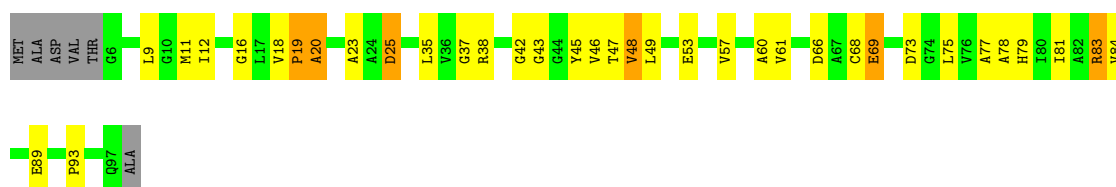
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Oi:  74% 18% 6%



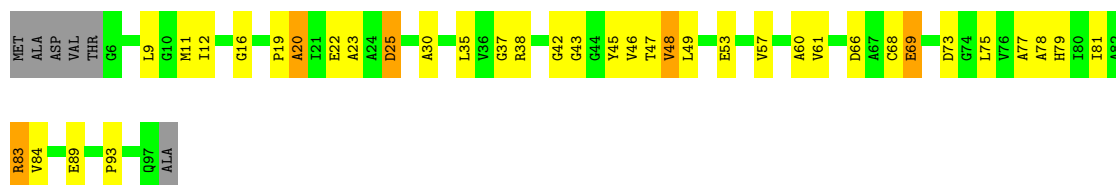
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AV:  57% 31% 6% 6%



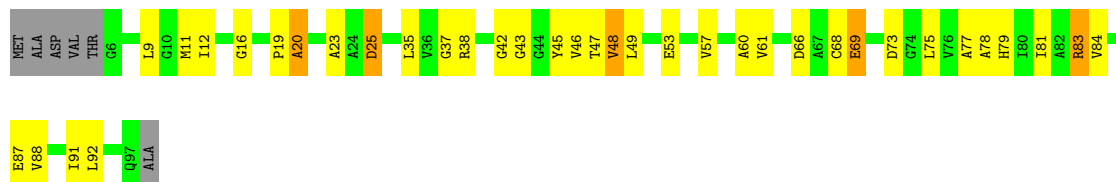
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AW:  56% 33% 5% 6%



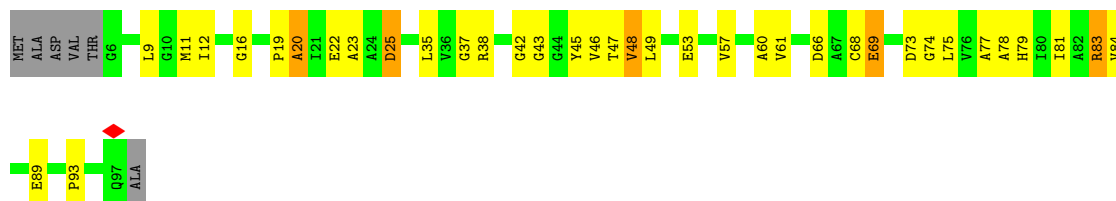
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AX: 56% 33% 5% 6%



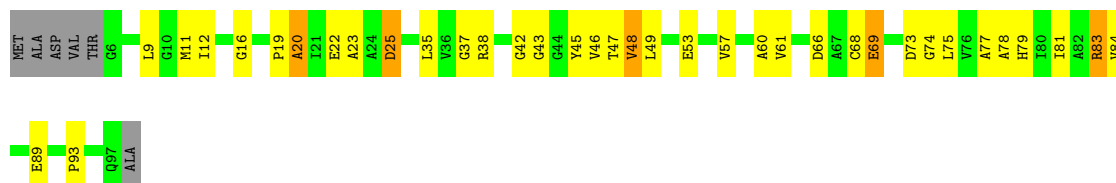
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AY: 56% 33% 5% 6%



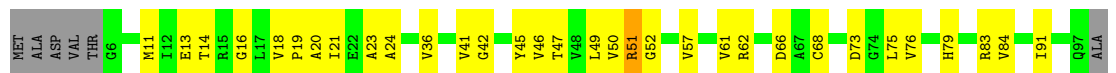
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AZ: 56% 33% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BV: 61% 32% 6%

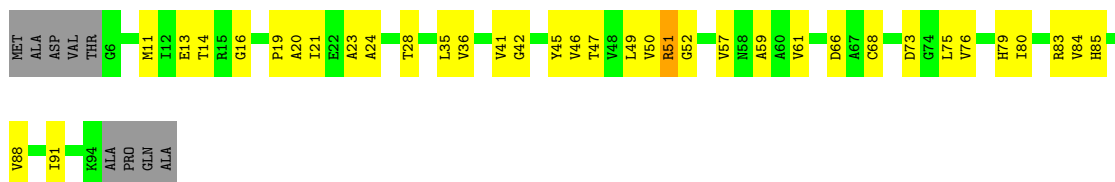


- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BW: 63% 30% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A



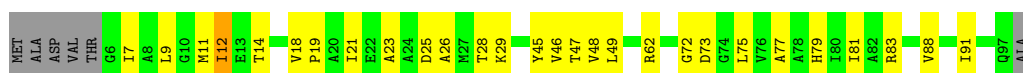
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

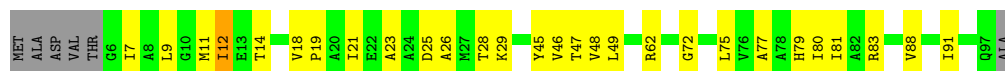


- Molecule 1: Major carboxysome shell protein CsoS1A



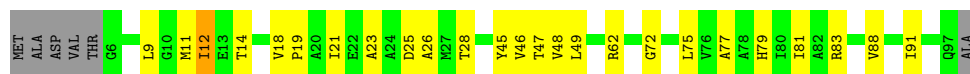
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CY:  65% 28% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CZ:  68% 24% • 6%



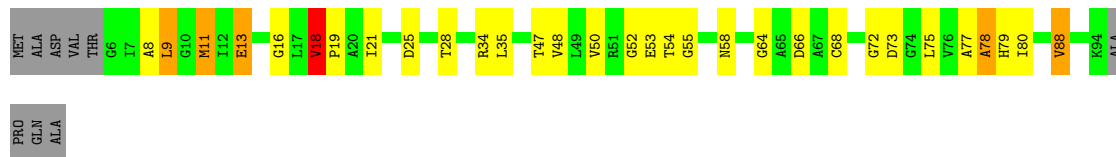
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DV:  60% 29% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DW:  59% 26% 5% • 9%



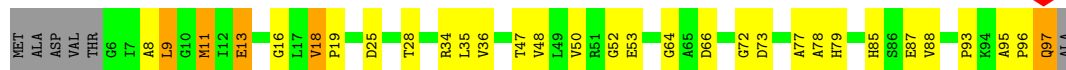
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DX:  54% 34% 6% • 6%



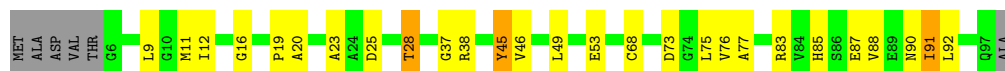
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DZ:  62% 27% 5% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EV:  66% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EW:  64% 22% 9%



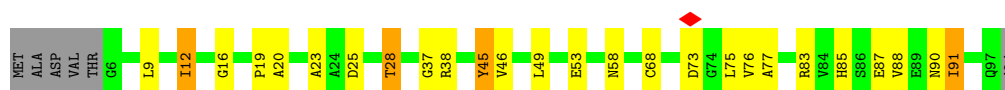
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EX:  66% 26% 6%



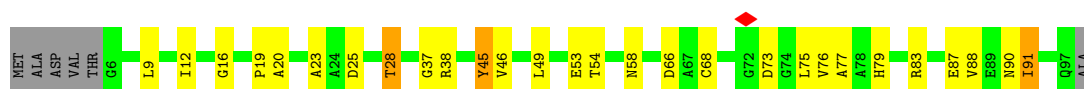
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EY:  67% 22% 6%



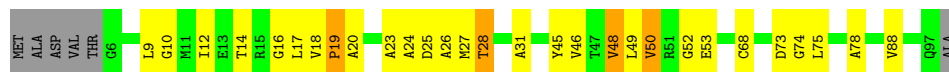
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EZ:  65% 26% 6%



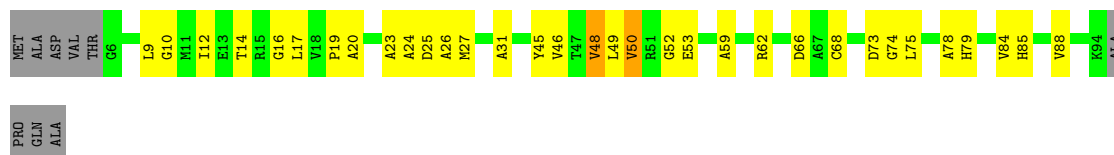
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FV:  64% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FW:  57% 32% 9%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FX:  62% 29% 6%



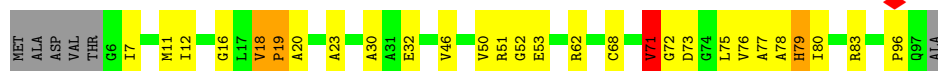
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FZ:  61% 29% 6%



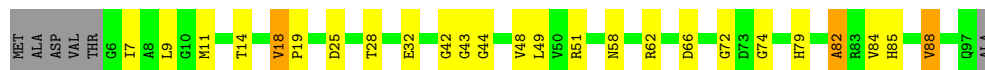
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GV:  65% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GW:  68% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GX:  66% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GY:  65% 26% 6%



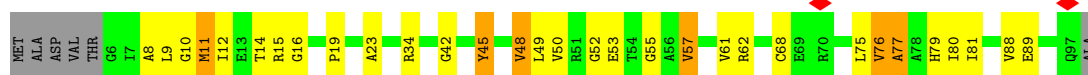
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GZ:  65% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HV: 



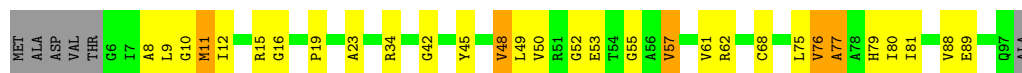
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HW: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HX: 



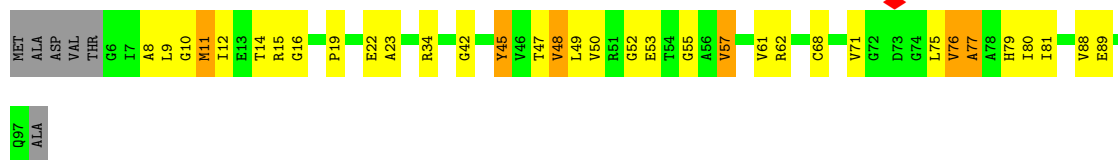
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HY: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HZ: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IV: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IW: 



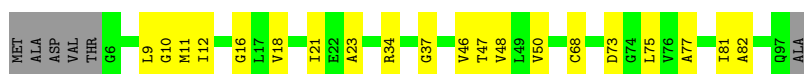
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IX: 71% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IY: 73% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain IZ: 71% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JV: 71% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JW: 68% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JX: 68% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JZ: 70% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KV: 67% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KW: 68% 23% 6%



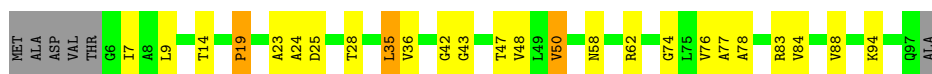
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KX: 66% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KY: 68% 22% 6%



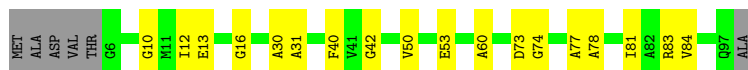
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KZ: 68% 23% 6%



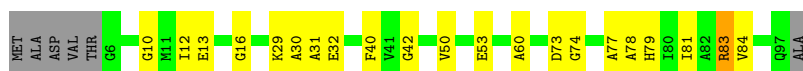
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain LV: 76% 18% 6%

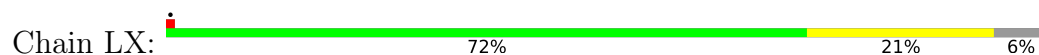


- Molecule 1: Major carboxysome shell protein CsoS1A

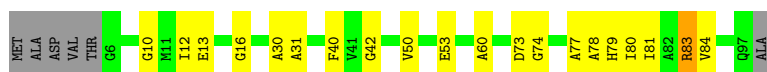
Chain LW: 72% 20% 6%



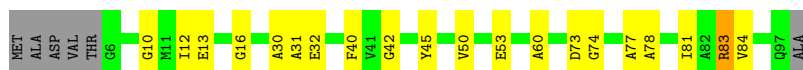
- Molecule 1: Major carboxysome shell protein CsoS1A



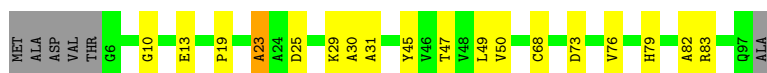
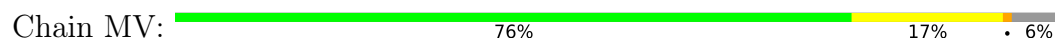
- Molecule 1: Major carboxysome shell protein CsoS1A



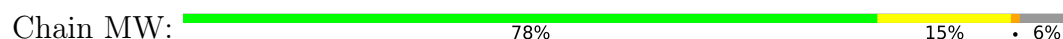
- Molecule 1: Major carboxysome shell protein CsoS1A



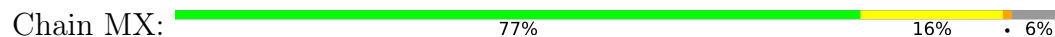
- Molecule 1: Major carboxysome shell protein CsoS1A



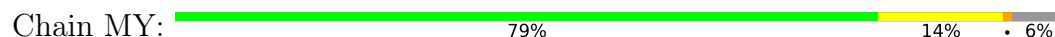
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



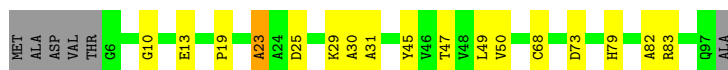
- Molecule 1: Major carboxysome shell protein CsoS1A





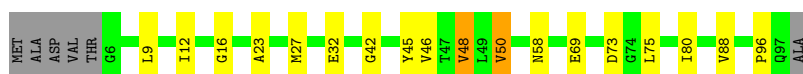
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain MZ: 77% 16% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NV: 76% 16% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NW: 77% 15% • 6%



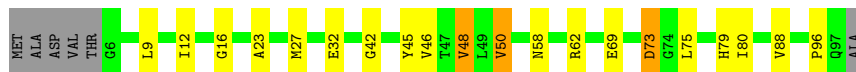
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NX: 73% 18% •• 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NY: 73% 17% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NZ: 78% 14% •• 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OV: 73% 19% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OW: 72% 20% 6%



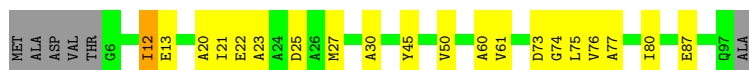
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OX: 72% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OY: 73% 19% 6%



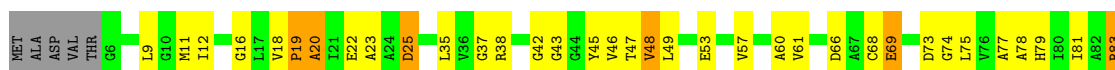
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OZ: 74% 18% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AU: 55% 33% 6% 6%



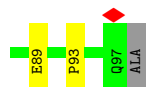
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Aa: 59% 30% 5% 6%





- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



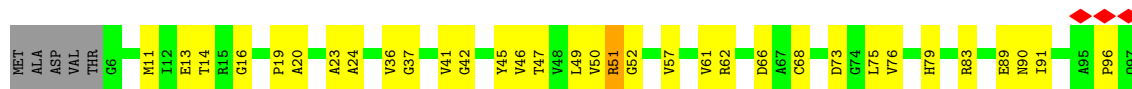
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



ALA

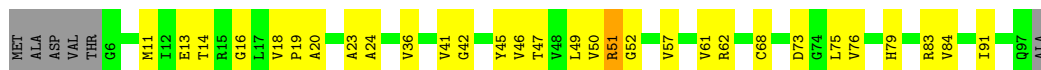
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bb:  64% 29% • 6%

- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bc:  62% 31% • 6%

- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bd:  63% 30% • 6%

- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CU:  64% 29% • 6%

- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ca:  65% 28% • 6%

- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cb:  66% 27% • 6%

- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cc:  66% 26% • 6%



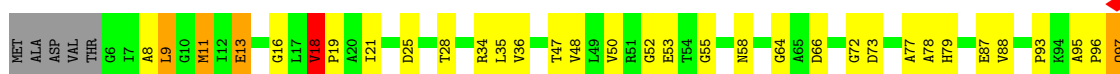
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cd: 65% 28% 6%



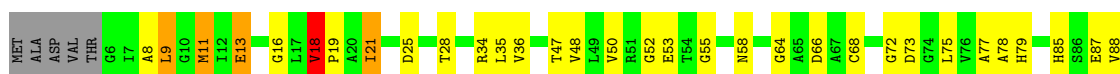
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Da: 60% 29% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dc: 57% 31% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dd: 60% 29% 6%



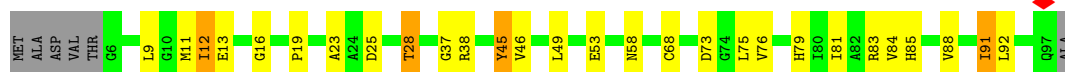
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EU: 67% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ea: 



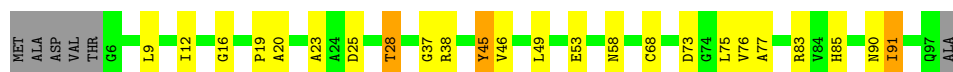
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Eb: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ec: 



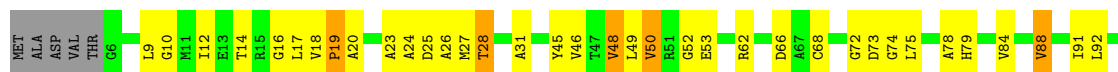
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ed: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FU: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fa: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fb: 



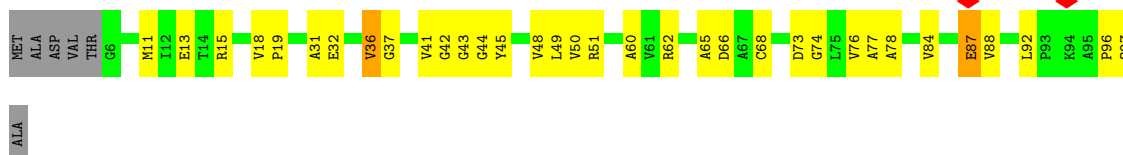
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



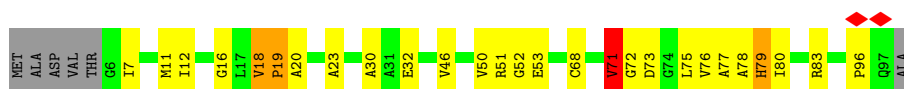
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



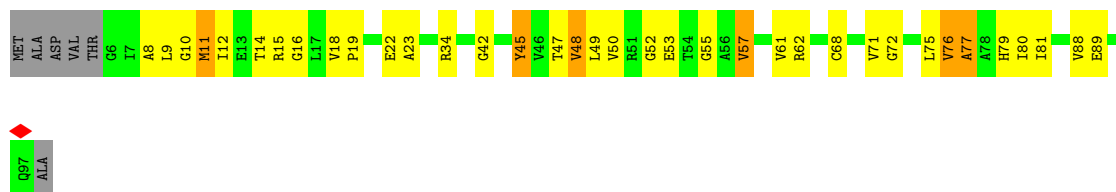
- Molecule 1: Major carboxysome shell protein CsoS1A



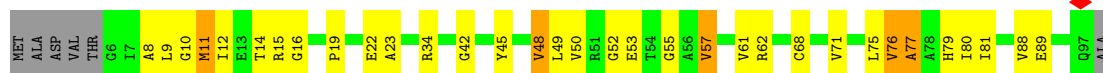
- Molecule 1: Major carboxysome shell protein CsoS1A



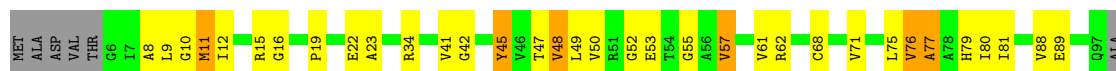
- Molecule 1: Major carboxysome shell protein CsoS1A



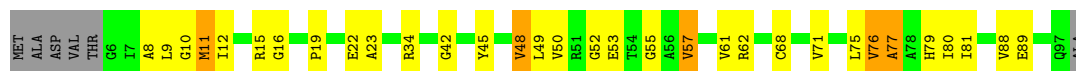
- Molecule 1: Major carboxysome shell protein CsoS1A



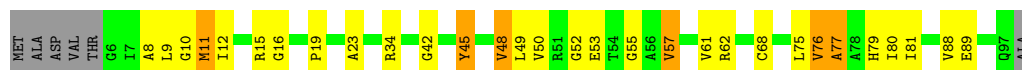
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



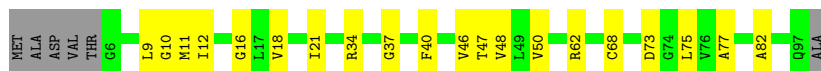
- Molecule 1: Major carboxysome shell protein CsoS1A





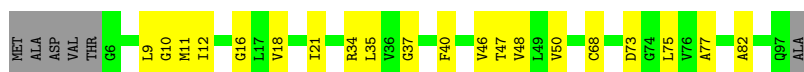
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ia: 73% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ib: 73% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ic: 71% 22% 6%



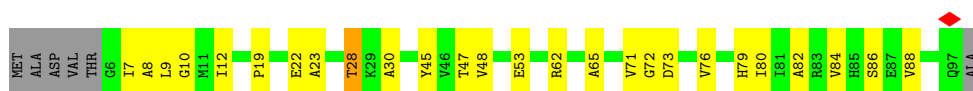
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Id: 73% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ja: 67% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Jb: 70% 21% 6%



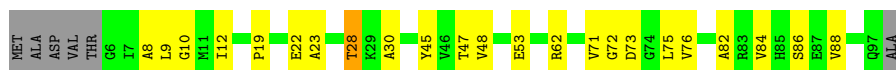
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Jc: 70% 22% 6%



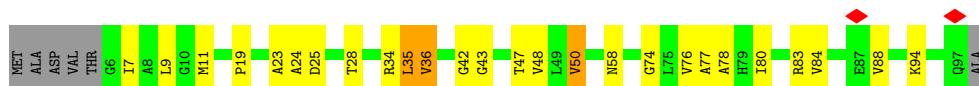
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Jd: 70% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain KU: 67% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ka: 68% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kb: 67% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kc: 68% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kd: 67% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

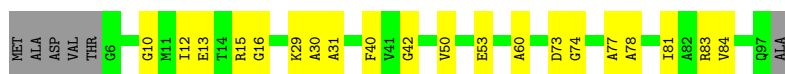
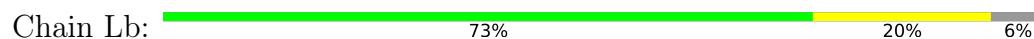
Chain LU: 72% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A



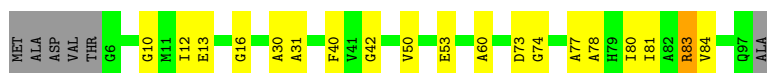
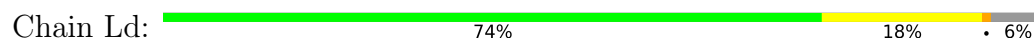
- Molecule 1: Major carboxysome shell protein CsoS1A



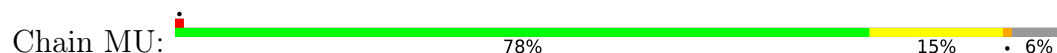
- Molecule 1: Major carboxysome shell protein CsoS1A



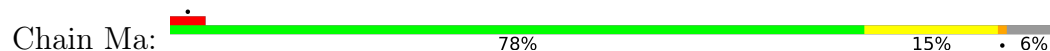
- Molecule 1: Major carboxysome shell protein CsoS1A



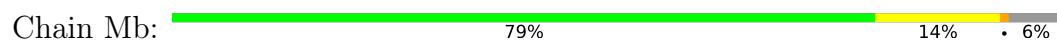
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A





- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Mc: 77% 16% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Md: 78% 15% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NU: 76% 16% • 6%



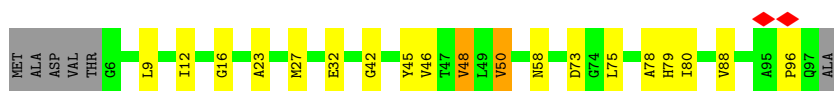
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Na: 77% 15% •• 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Nb: 74% 17% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Nc: 76% 16% •• 6%

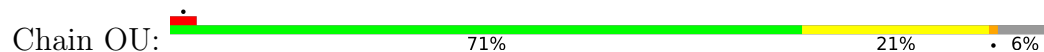


- Molecule 1: Major carboxysome shell protein CsoS1A

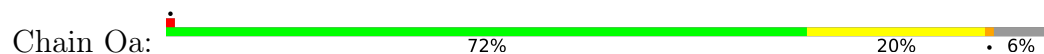
Chain Nd: 74% 17% • 6%



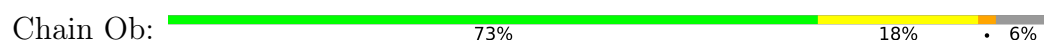
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



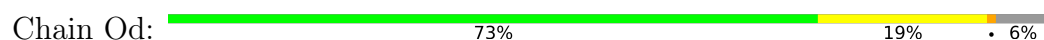
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

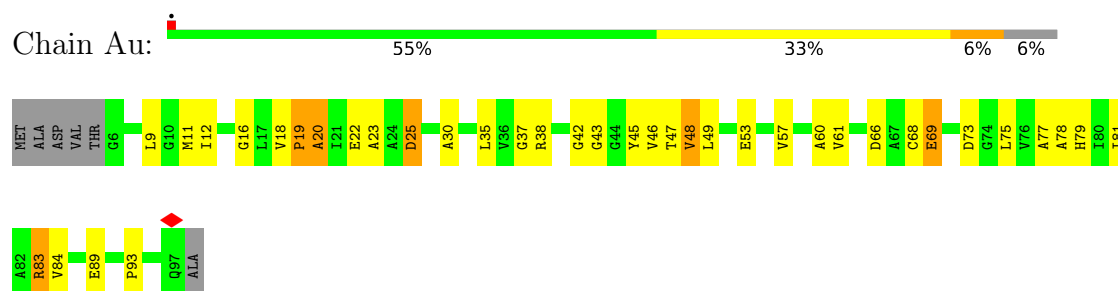


- Molecule 1: Major carboxysome shell protein CsoS1A

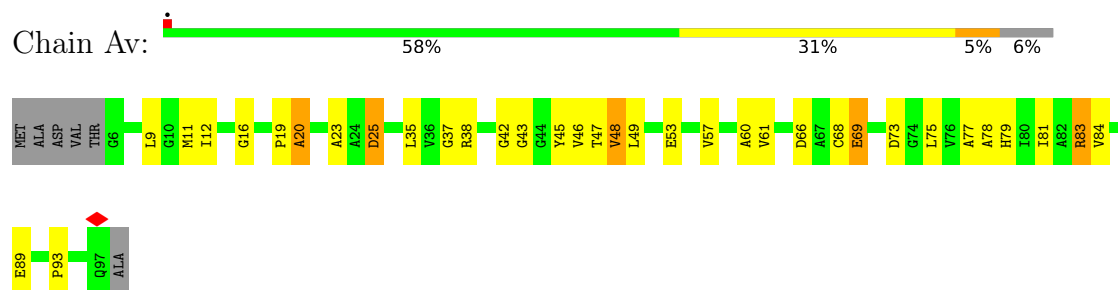


- Molecule 1: Major carboxysome shell protein CsoS1A

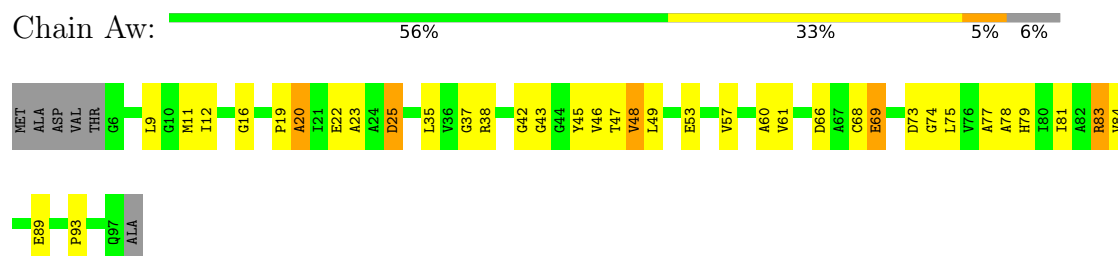




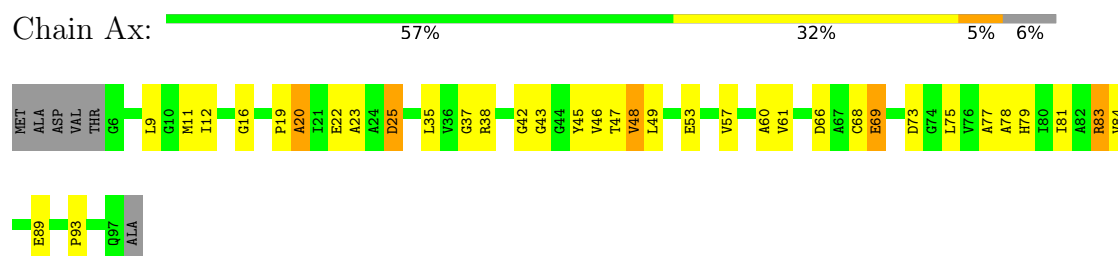
- Molecule 1: Major carboxysome shell protein CsoS1A



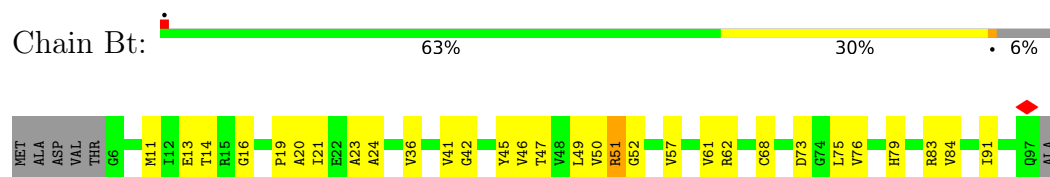
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bu:  63% 30% 6%



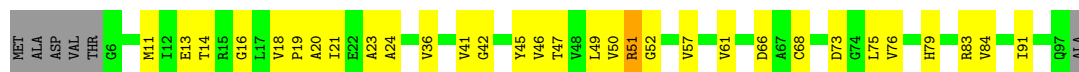
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bv:  63% 30% 6%



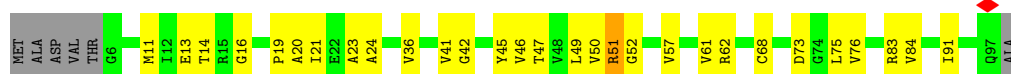
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bw:  62% 31% 6%



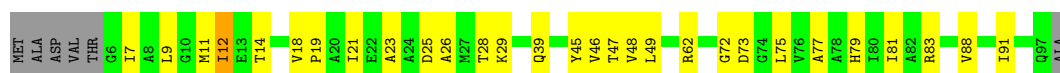
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bx:  64% 29% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ct:  64% 29% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cu:  66% 27% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cv:  66% 26% 6%



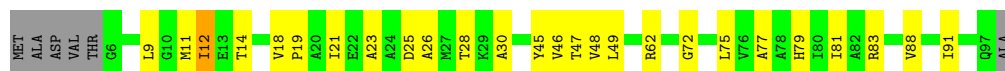
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cw:  64% 29% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cx:  67% 26% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dt:  62% 27% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Du:  61% 23% 5% • 9%



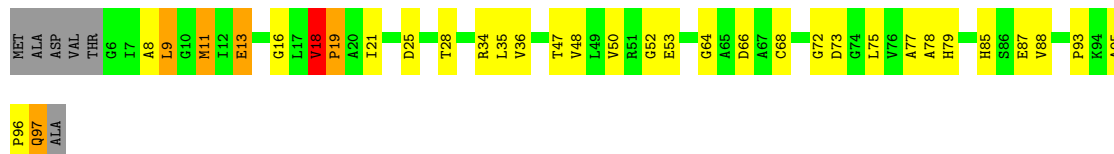
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dv:  57% 31% 5% • 6%



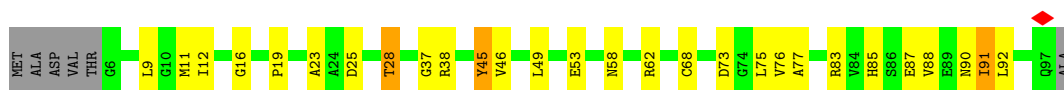
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dx:  59% 29% 5% • 6%



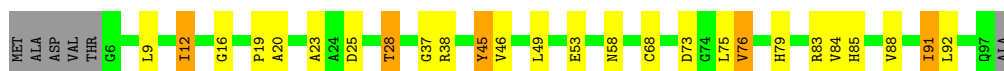
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Et:  65% 26% • 6%



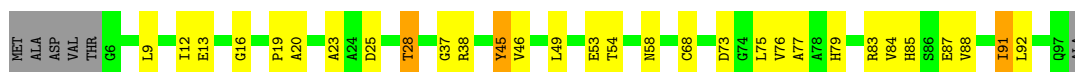
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Eu: 67% 21% 5% 6%



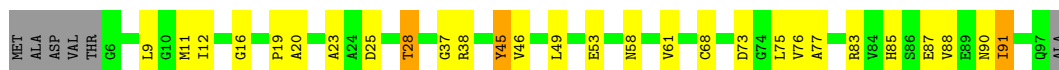
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ev: 63% 28% 6%



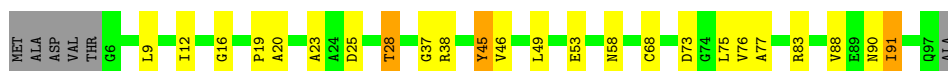
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ew: 65% 26% 6%



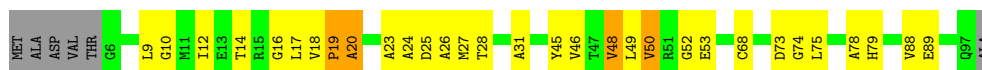
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ex: 69% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ft: 62% 28% 6%



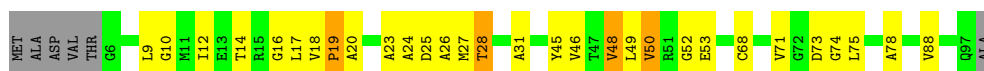
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fu: 63% 27% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

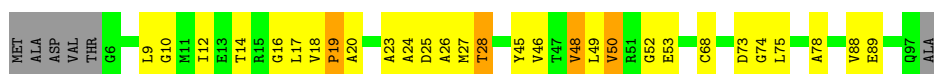
Chain Fv: 63% 27% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A



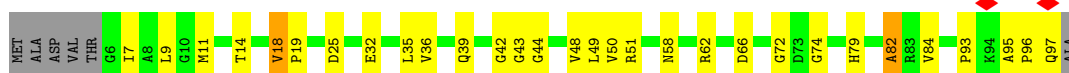
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



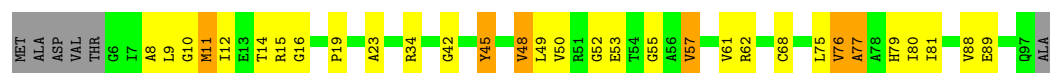
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Gx: 



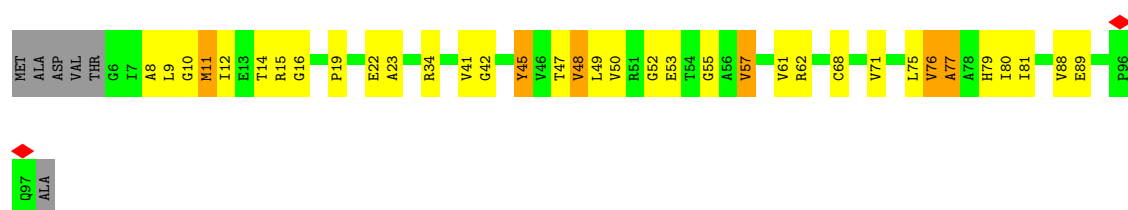
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ht: 



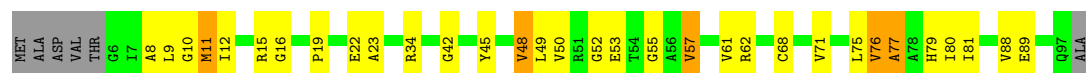
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Hu: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Hv: 



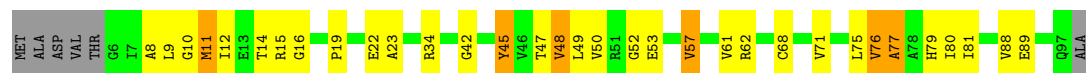
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Hw: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Hx: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain It: 



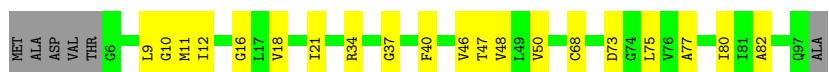
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Iu: 72% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Iv: 73% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Iw: 73% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ix: 73% 20% 6%



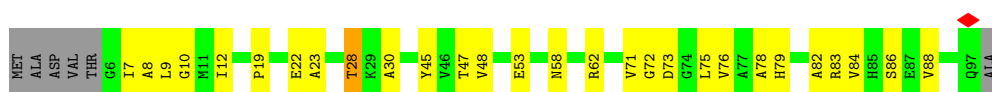
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Jt: 73% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ju: 65% 28% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Jw: 65% 26% 6%



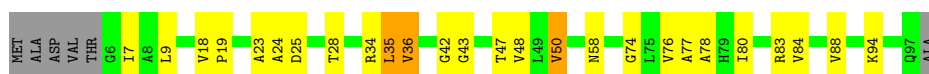
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Jx: 70% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kt: 67% 23% 6%



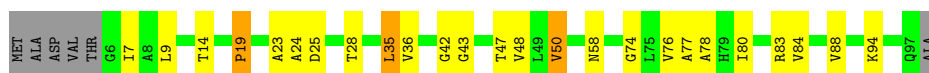
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ku: 66% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kv: 68% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kw: 68% 22% 6%



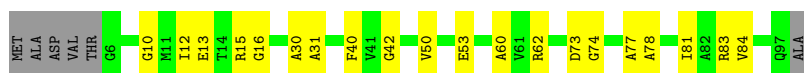
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kx: 67% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

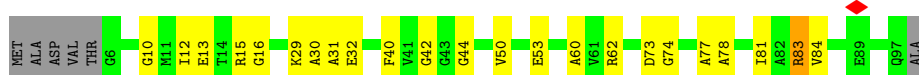
Chain Lt: 73% 20% 6%



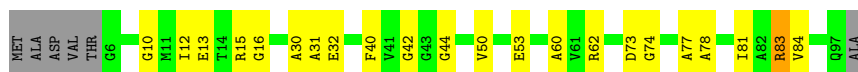
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



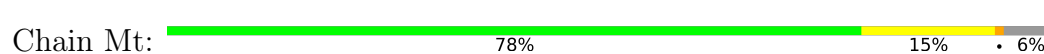
- Molecule 1: Major carboxysome shell protein CsoS1A



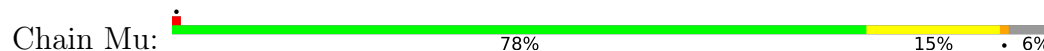
- Molecule 1: Major carboxysome shell protein CsoS1A



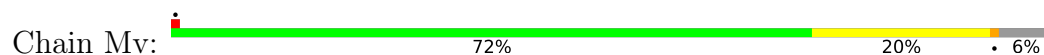
- Molecule 1: Major carboxysome shell protein CsoS1A

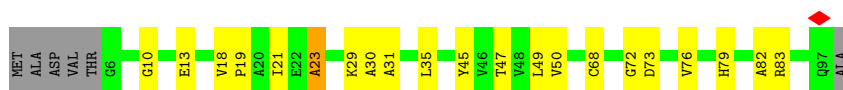


- Molecule 1: Major carboxysome shell protein CsoS1A

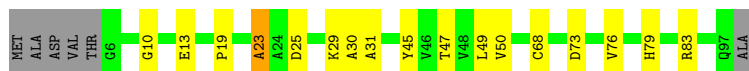
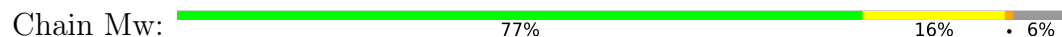


- Molecule 1: Major carboxysome shell protein CsoS1A

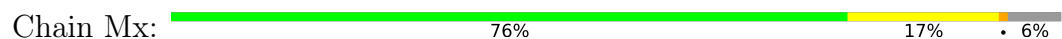




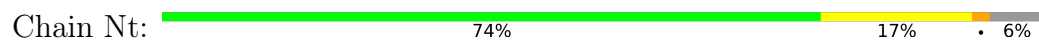
- Molecule 1: Major carboxysome shell protein CsoS1A



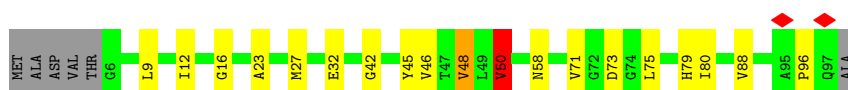
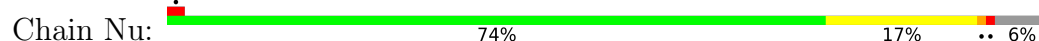
- Molecule 1: Major carboxysome shell protein CsoS1A



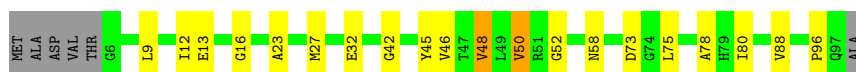
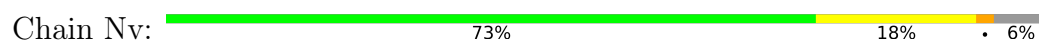
- Molecule 1: Major carboxysome shell protein CsoS1A



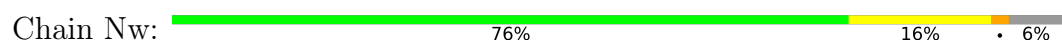
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

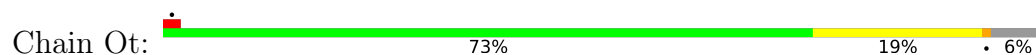


- Molecule 1: Major carboxysome shell protein CsoS1A

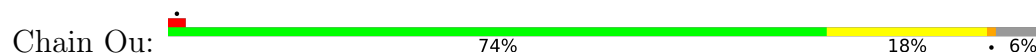




- Molecule 1: Major carboxysome shell protein CsoS1A



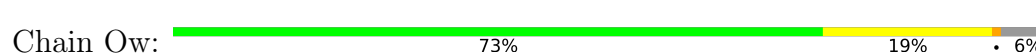
- Molecule 1: Major carboxysome shell protein CsoS1A



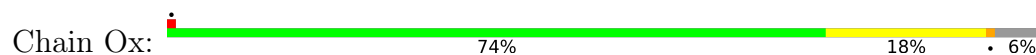
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



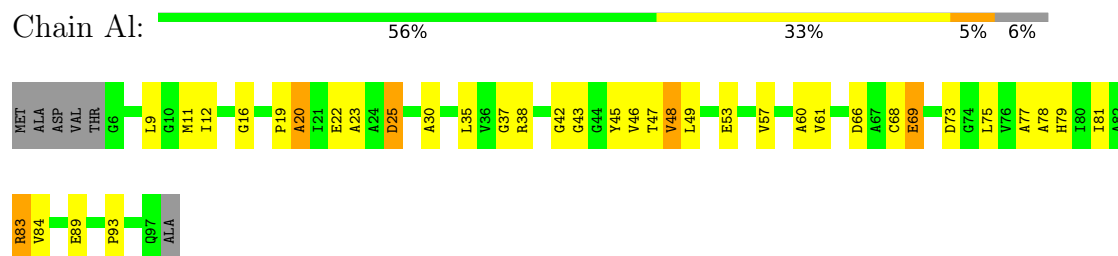
- Molecule 1: Major carboxysome shell protein CsoS1A



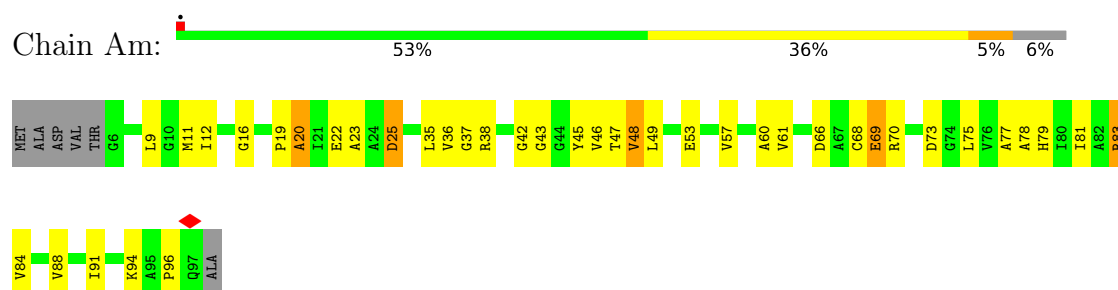
- Molecule 1: Major carboxysome shell protein CsoS1A



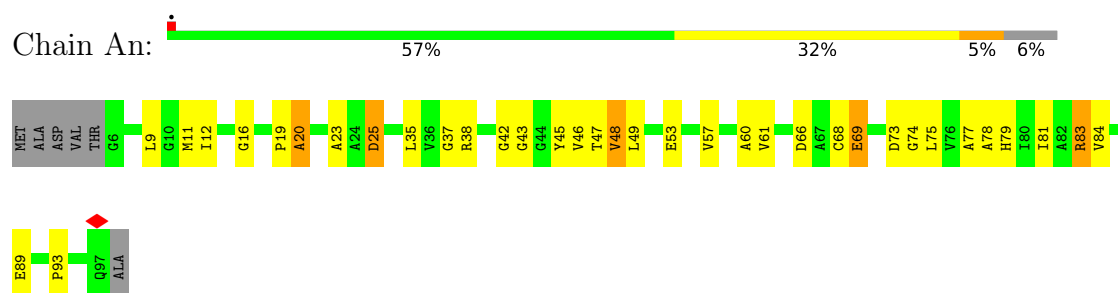
- Molecule 1: Major carboxysome shell protein CsoS1A



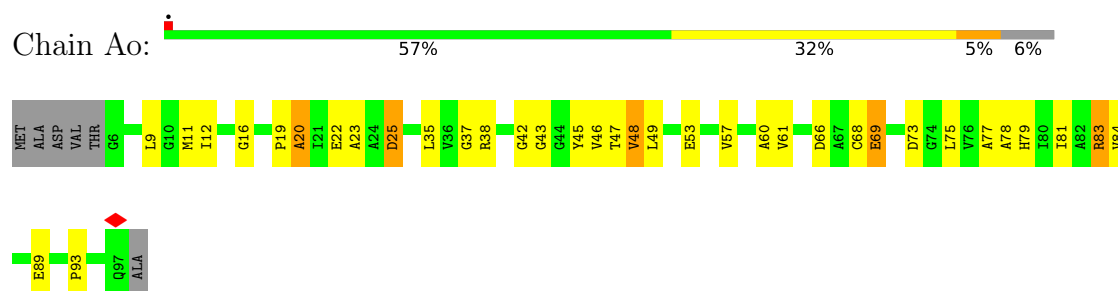
- Molecule 1: Major carboxysome shell protein CsoS1A



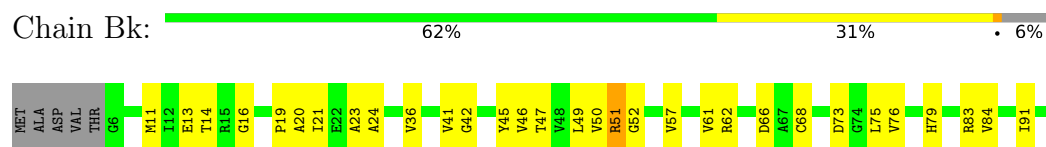
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bl: 



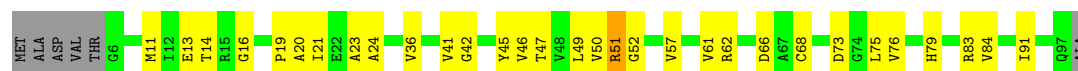
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bm: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bn: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bo: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ck: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cl: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cm: 



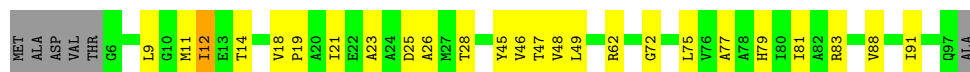
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cn:  65% 28% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Co:  68% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dk:  62% 27% 6%



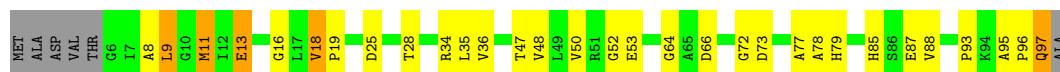
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dm:  53% 36% 6%



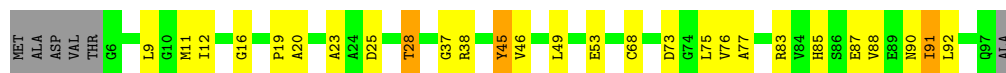
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Do:  62% 27% 5% 6%



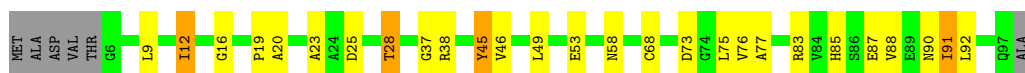
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ek:  66% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain En:  66% 23% 6%



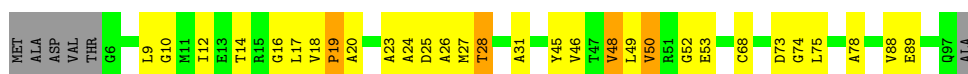
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Eo: 65% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fk: 63% 27% 6%



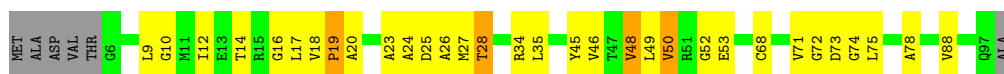
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fm: 62% 29% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fn: 61% 29% 6%



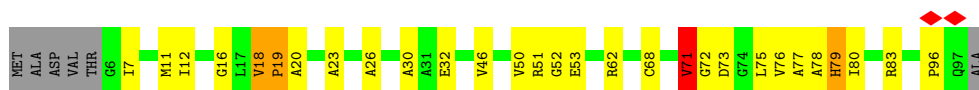
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fo: 61% 30% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Gk: 64% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Gl: 62% 27% 9%



- Molecule 1: Major carboxysome shell protein CsoS1A



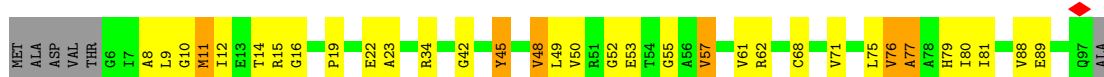
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

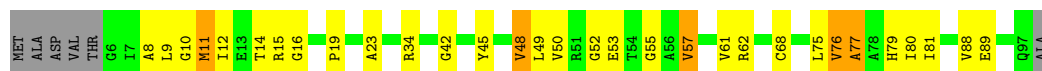


- Molecule 1: Major carboxysome shell protein CsoS1A



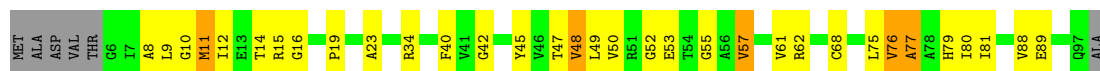
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Hn:  62% 27% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ho:  60% 29% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ik:  73% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Il:  74% 18% 6%



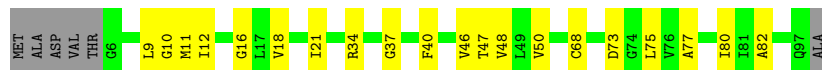
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Im:  72% 21% 6%



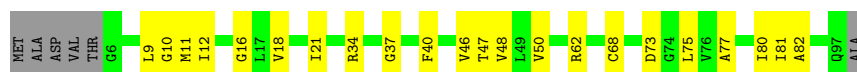
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain In:  73% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Io:  71% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Jk:  71% 21% 6%



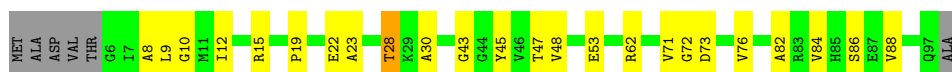
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Jl:  67% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Jn:  69% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Jo:  70% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kk:  67% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kl:  67% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kn:  67% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ko:  66% 24% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Lk:  76% 17% • 6%



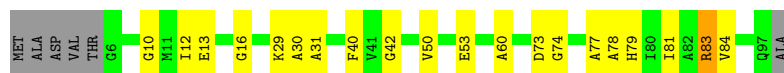
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ll:  72% 20% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ln:  73% 19% • 6%



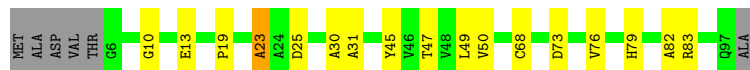
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Lo:  73% 19% • 6%



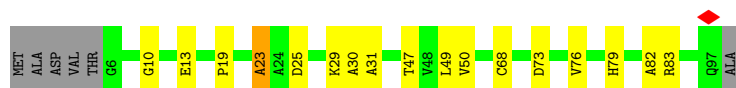
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Mk:  77% 16% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ml:  77% 16% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Mn:  79% 14% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Mo:  78% 15% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Nk:  74% 17% •• 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Nl:  76% 16% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Nn:  70% 20% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain No:  76% 16% •• 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ok:  73% 19% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ol:  73% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain On:  73% 19% 6%



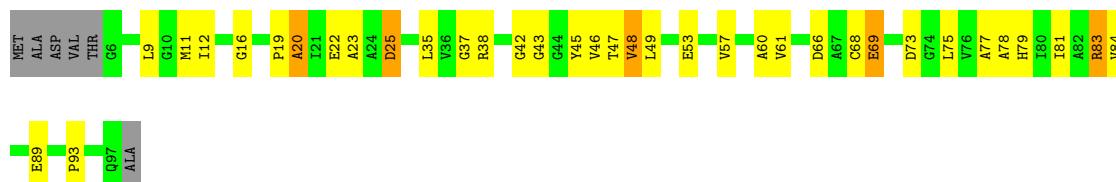
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Oo:  74% 18% 6%



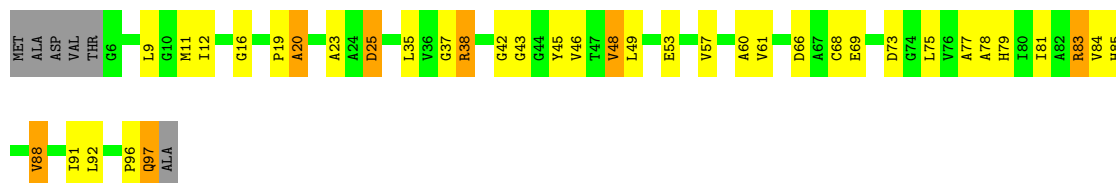
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Aj:  57% 32% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

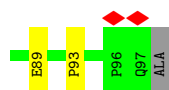
Chain Ap:  55% 32% 7% 6%



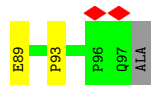
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Aq:  57% 32% 5% 6%

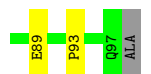




- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



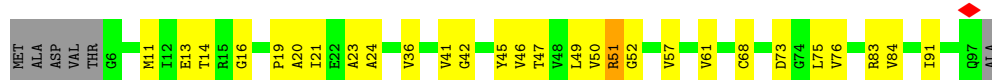
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

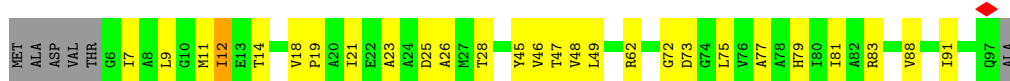




- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dp:  58% 31% • • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dr:  57% 31% 5% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ds:  58% 31% • • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ej:  67% 23% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ep:  63% 27% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Eq:  66% 24% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Er:  69% 21% 6%



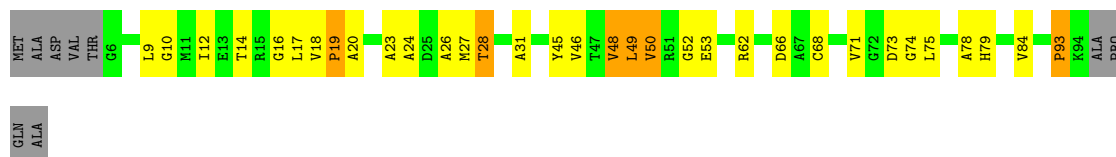
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Es:  66% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fj:  57% 28% 6% 9%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fp:  62% 29% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fr:  62% 28% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fs:  63% 27% 6%

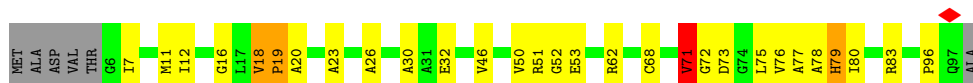


- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Gj:  58% 31% 9%



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



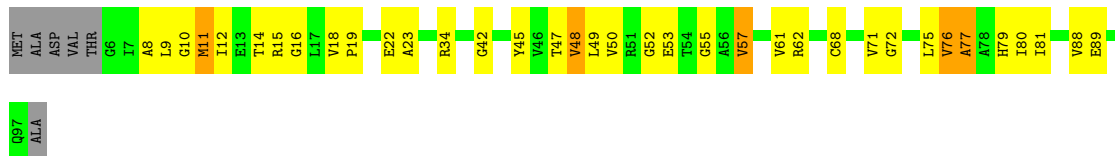
- Molecule 1: Major carboxysome shell protein CsoS1A



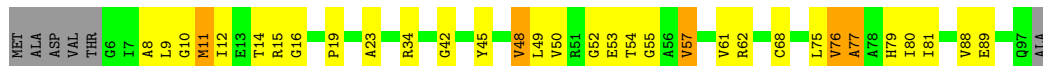
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

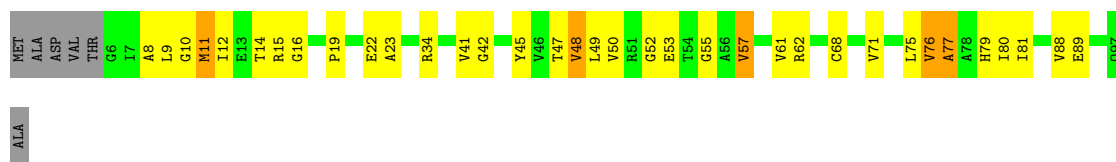


- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Hq:  58% 31% 5% 6%



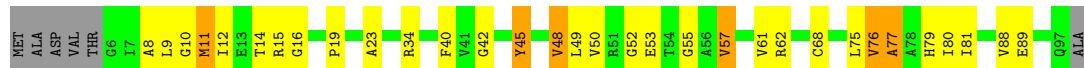
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Hr:  61% 28% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Hs:  61% 27% 6% 6%



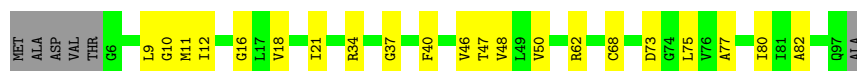
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ij:  70% 23% 6%



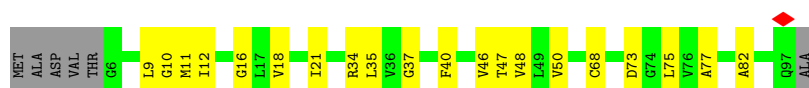
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ip:  72% 21% 6%



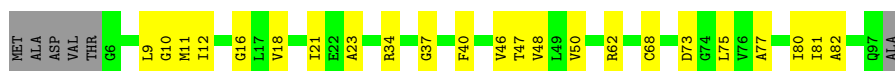
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Iq:  73% 20% 6%



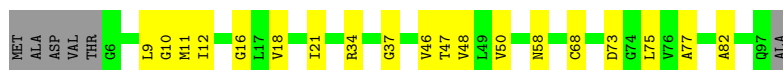
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ir:  70% 23% 6%



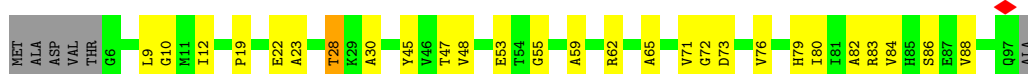
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ii: 74% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ij: 66% 27% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ip: 65% 28% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Iq: 66% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Jr: 70% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Js: 71% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kj:  68% 23% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kp:  65% 24% • 6%



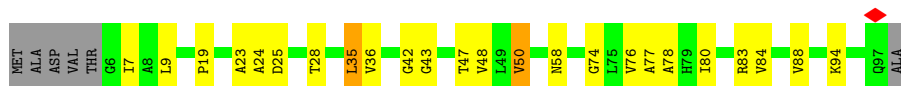
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kq:  68% 22% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Kr:  69% 22% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ks:  67% 22% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Lj:  73% 19% • 6%



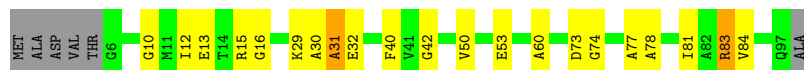
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Lp:  72% 20% • 6%



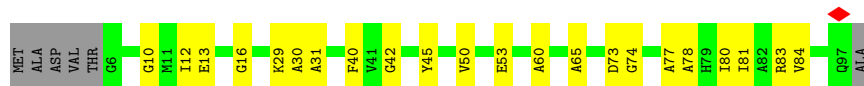
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Lq:  72% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Lr:  71% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ls:  74% 18% 6%



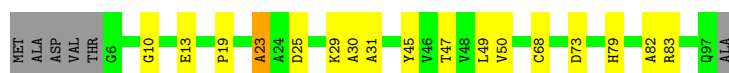
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Mj:  78% 15% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Mp:  77% 16% 6%



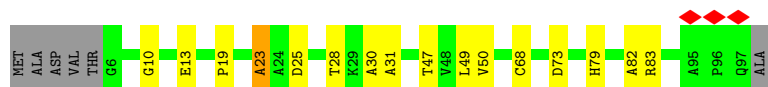
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Mq:  78% 15% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Mr:  78% 15% 6%



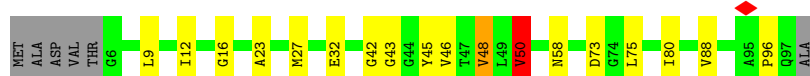
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ms:  77% 16% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Nj:  76% 16% •• 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Np:  76% 16% •• 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Nq:  73% 18% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Nr:  78% 14% •• 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ns:  74% 17% • 6%



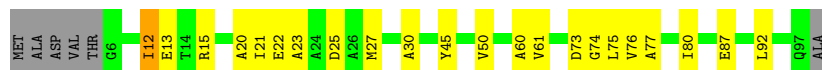
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Oj:  71% 21% • 6%



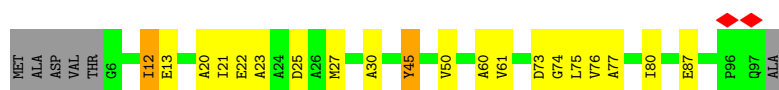
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Op:  71% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Oq:  73% 18% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Or:  71% 21% 6%



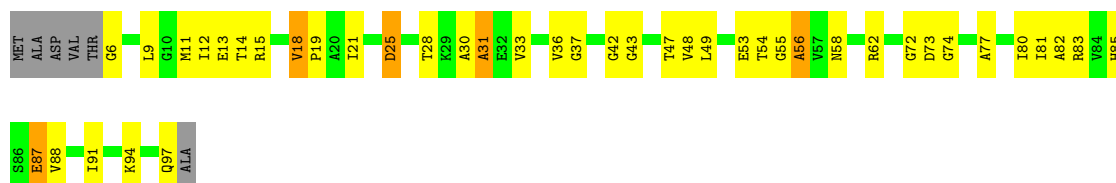
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Os:  72% 20% 6%



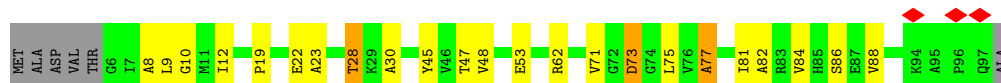
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DD:  51% 38% 5% 6%

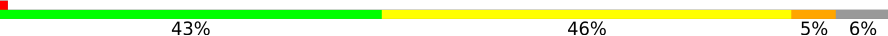


- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JC:  70% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain D4:  43% 46% 5% 6%



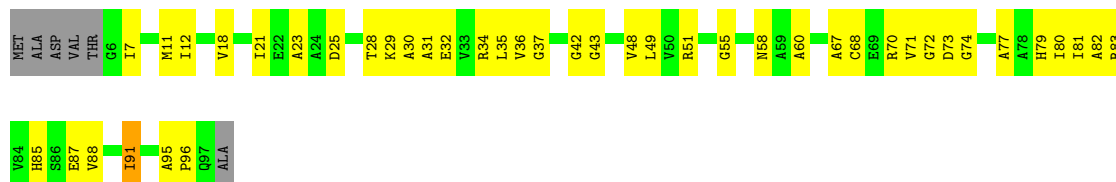
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain J3: 64% 24% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain D7: 50% 43% 6%



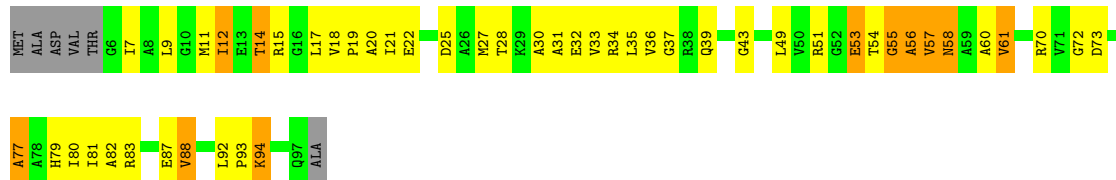
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain J6: 66% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DS: 44% 39% 11% 6%



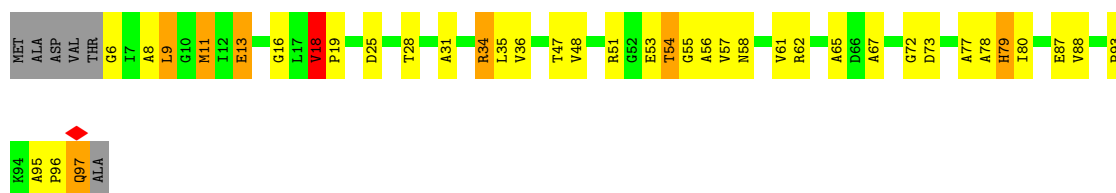
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EI: 66% 26% 6%

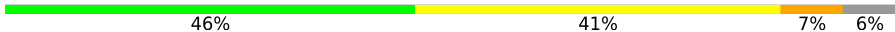


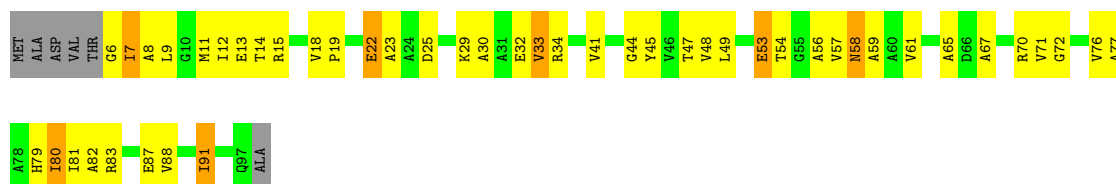
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DM: 



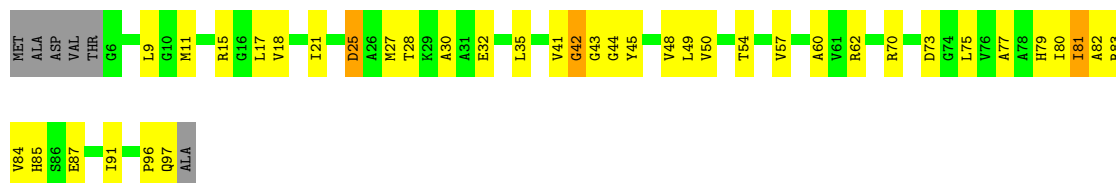
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dw: 



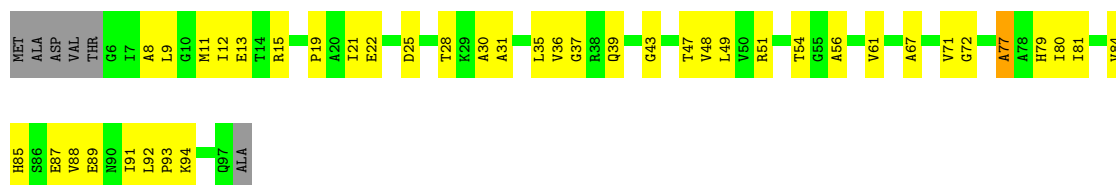
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Jv: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dn: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DR: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FL: 



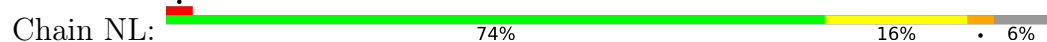
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

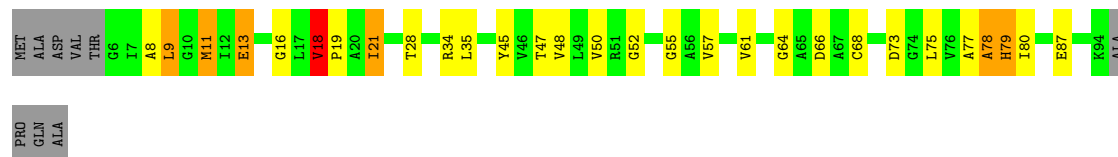


- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dj: 



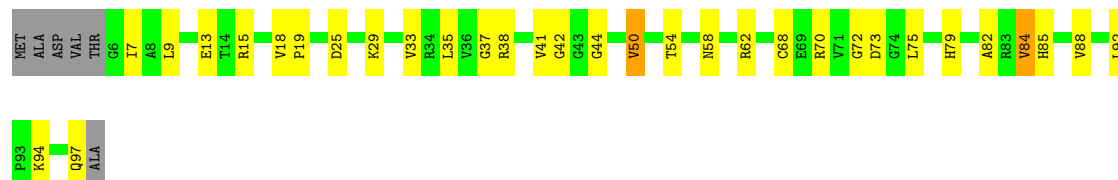
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fq: 

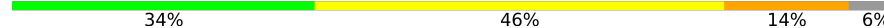


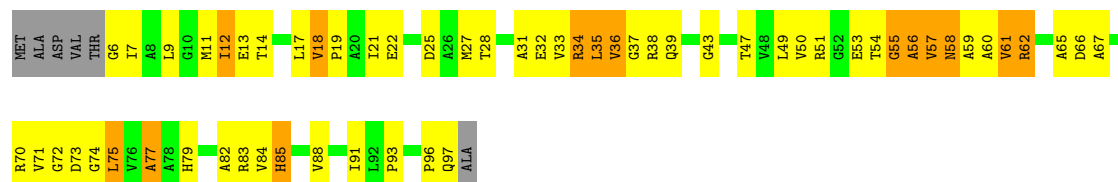
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EL: 



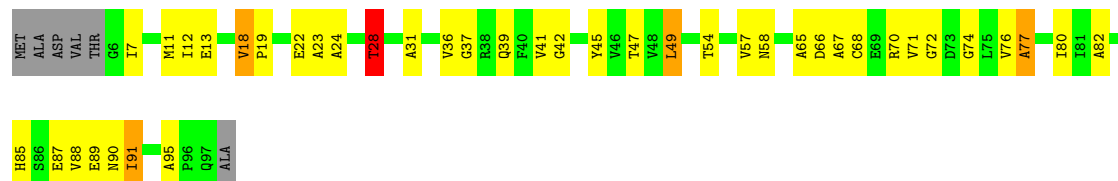
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dh: 



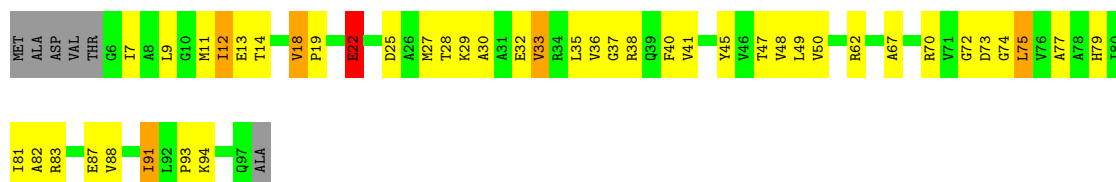
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DY: 

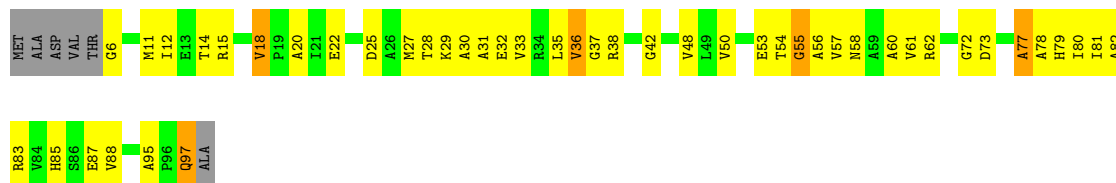


- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Db: 



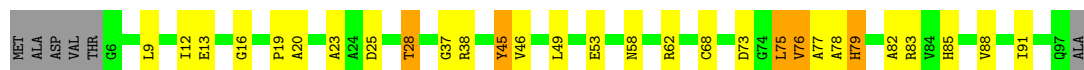
- Molecule 1: Major carboxysome shell protein CsoS1A



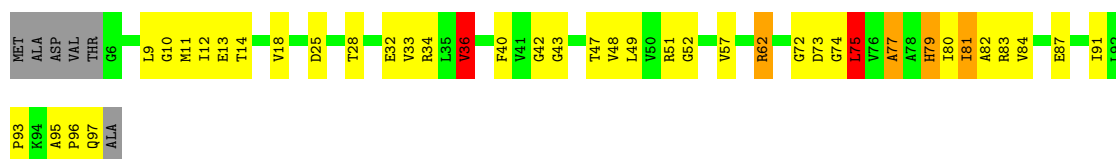
- Molecule 1: Major carboxysome shell protein CsoS1A



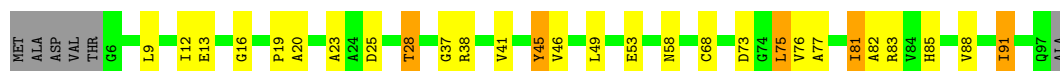
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

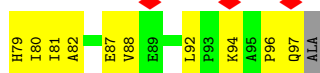
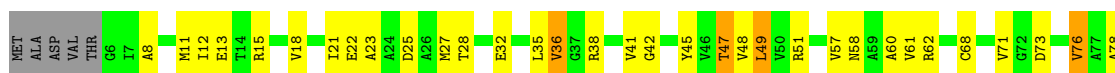


- Molecule 1: Major carboxysome shell protein CsoS1A

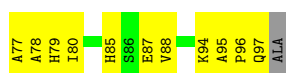


- Molecule 1: Major carboxysome shell protein CsoS1A

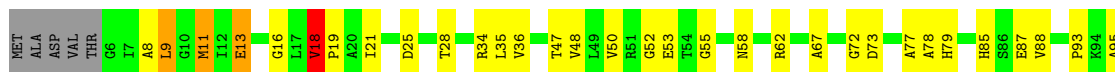




- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

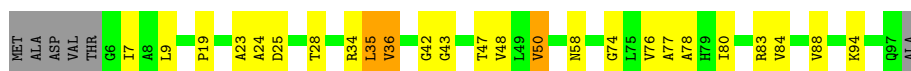


- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A





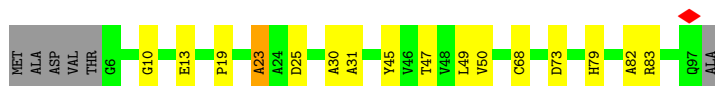
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain LI: 68% 23% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain MI: 78% 15% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain NI: 77% 15% • 6%



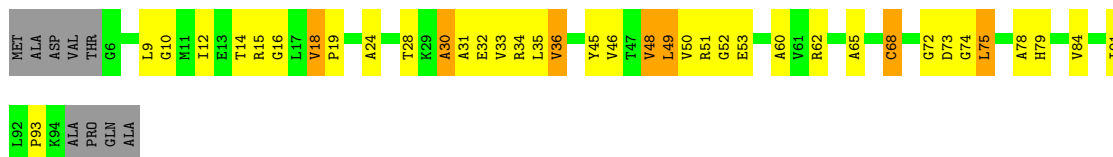
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain OI: 71% 21% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FF: 52% 32% 7% 9%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JU: 70% 21% • 6%



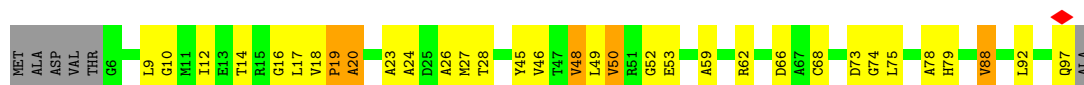
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain El: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fl: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Km: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Nm: 



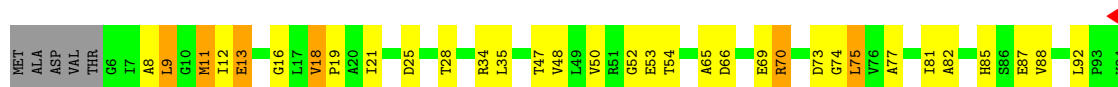
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Om: 



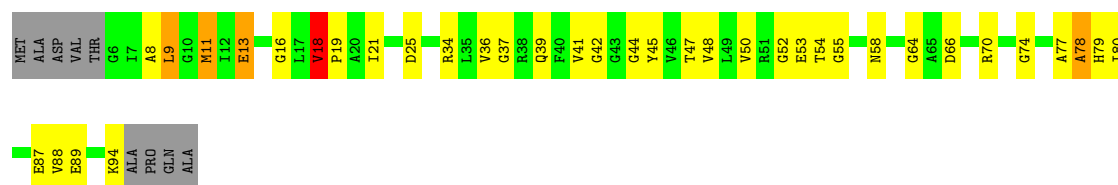
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DU: 



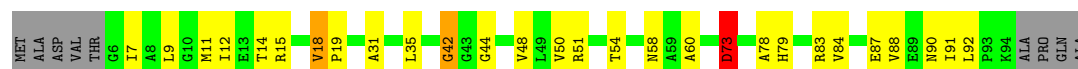
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DI:  53% 33% 9%



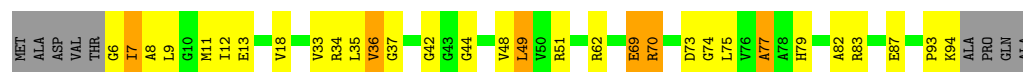
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EF:  62% 26% 9%



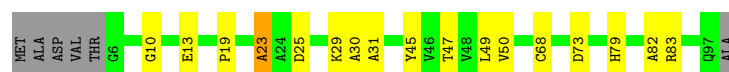
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DF:  59% 26% 6% 9%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain MK:  77% 16% 6%



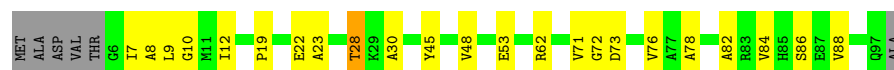
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain JF:  65% 27% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Jm:  70% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

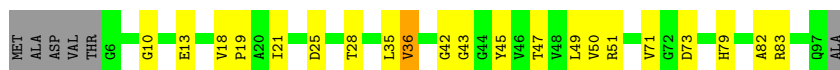
Chain Lm:  56% 35% 6%





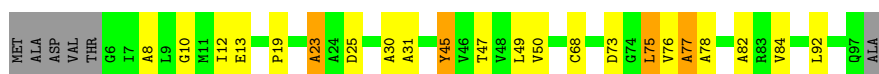
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain MF: 72% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Mm: 71% 18% 6%



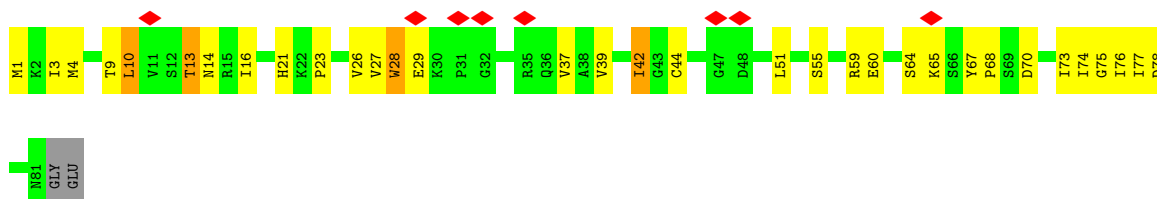
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain PA: 63% 30% 5%



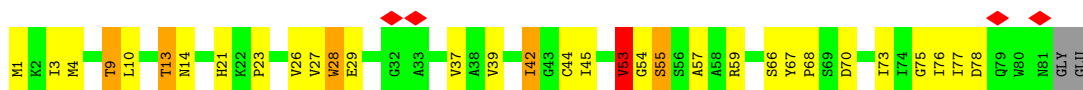
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain PB: 10% 58% 35% 5%



- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain PC: 5% 59% 31% 6%



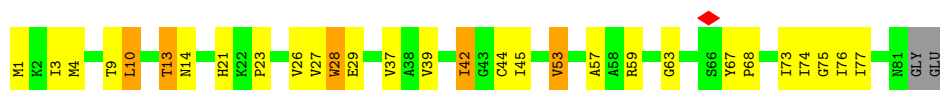
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain PD: 61% 34% 2%



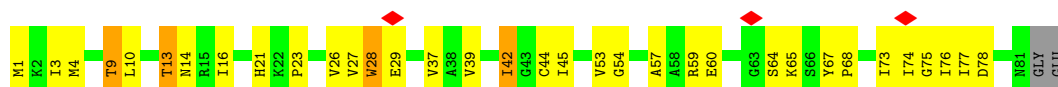
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain PE:  63% 29% 6% .



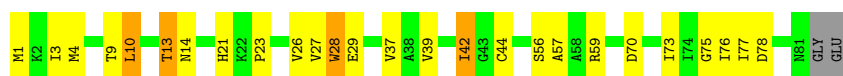
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain P1:  57% 36% 5% .



- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain P2:  66% 27% 5% .



- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain P3:  64% 29% 5% .



- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain P4:  67% 25% 5% .



- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain P5:  65% 29% . .



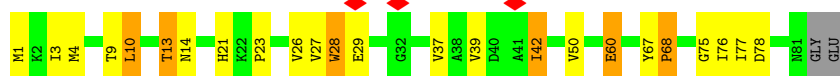
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain P6:  60% 31% 6% .



- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain P7: 69% 22% 7% .



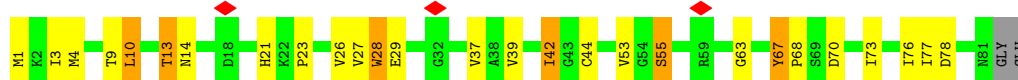
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain P8: 63% 28% 6% ..



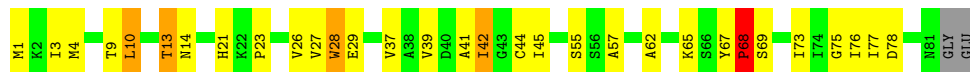
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain P9: 65% 25% 7% .



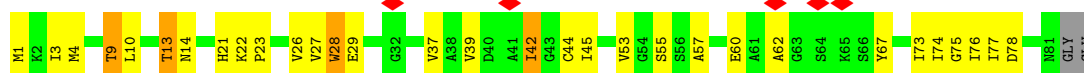
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain P0: 60% 31% 5% ..



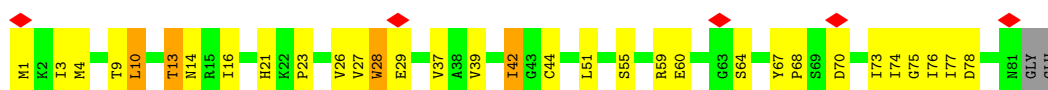
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain PP: 60% 33% 5% .



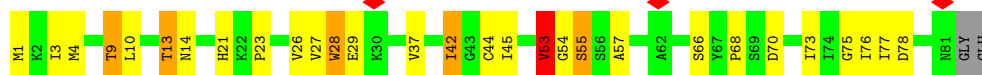
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain PQ: 59% 34% 5% .



- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain PR:  63% 28% 6% ..



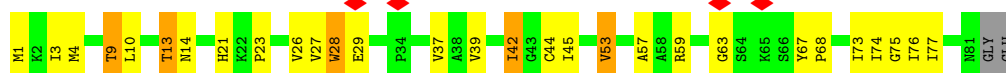
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain PS:  61% 34% 7% ..



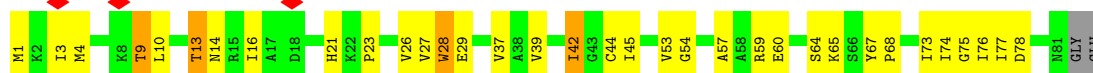
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain PT:  63% 29% 5% ..



- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain PG:  57% 36% 5% ..



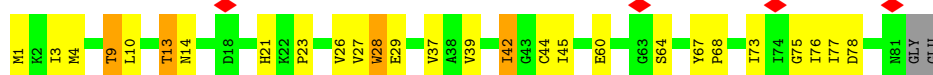
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain PH:  65% 28% 18% 5% ..



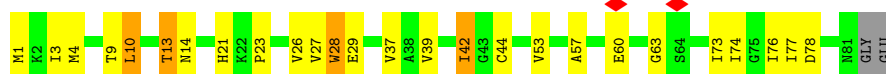
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain PI:  65% 28% 5% ..

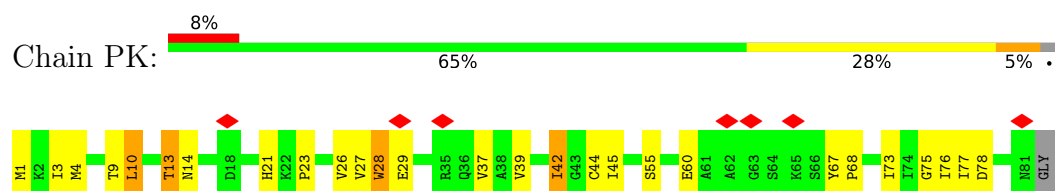


- Molecule 2: Carboxysome shell vertex protein CsoS4A

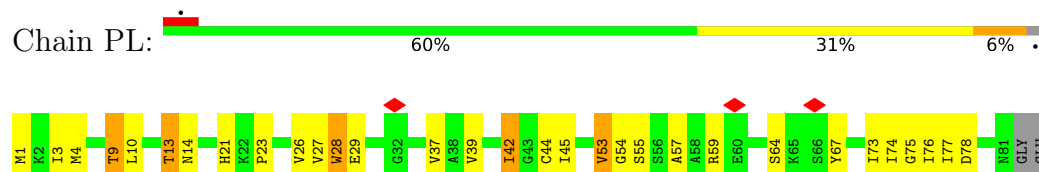
Chain PJ:  66% 27% 5% ..



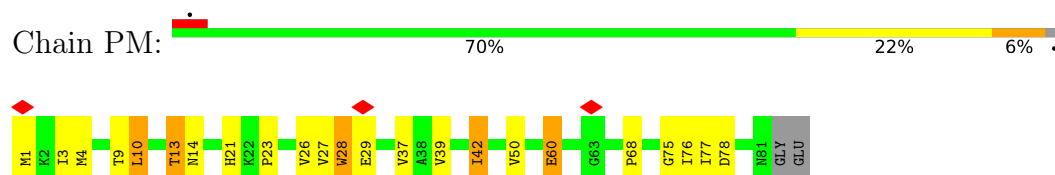
- Molecule 2: Carboxysome shell vertex protein CsoS4A



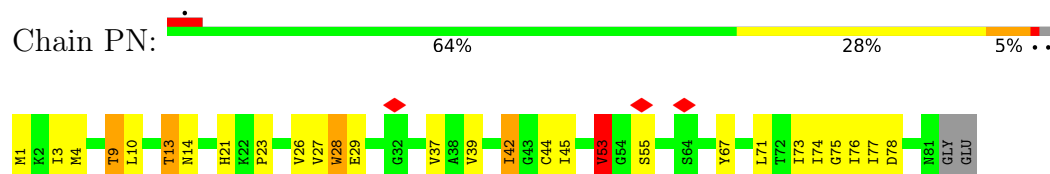
- Molecule 2: Carboxysome shell vertex protein CsoS4A



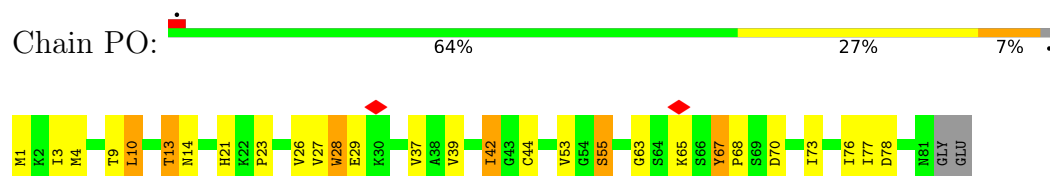
- Molecule 2: Carboxysome shell vertex protein CsoS4A



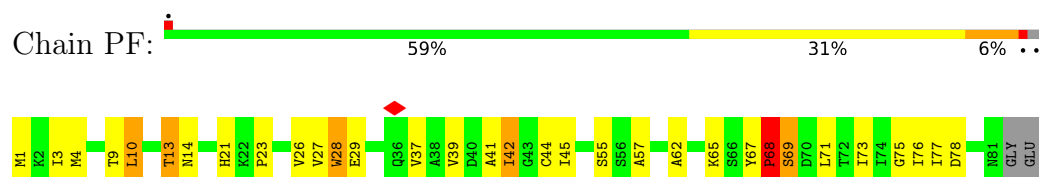
- Molecule 2: Carboxysome shell vertex protein CsoS4A



- Molecule 2: Carboxysome shell vertex protein CsoS4A

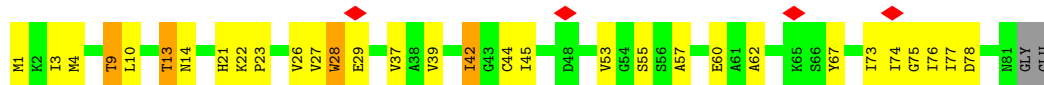


- Molecule 2: Carboxysome shell vertex protein CsoS4A



- Molecule 2: Carboxysome shell vertex protein CsoS4A

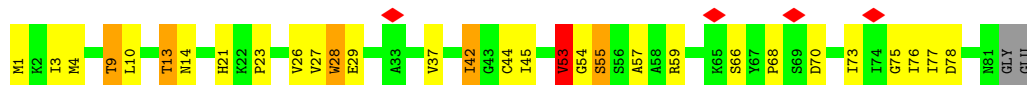




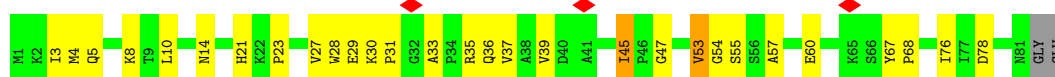
- Molecule 2: Carboxysome shell vertex protein CsoS4A



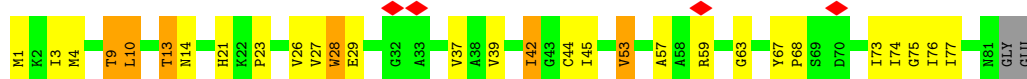
- Molecule 2: Carboxysome shell vertex protein CsoS4A



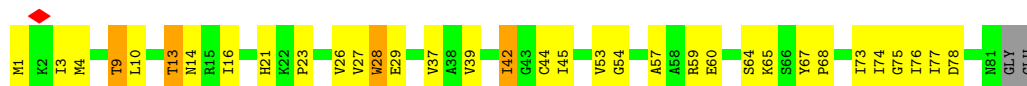
- Molecule 2: Carboxysome shell vertex protein CsoS4A



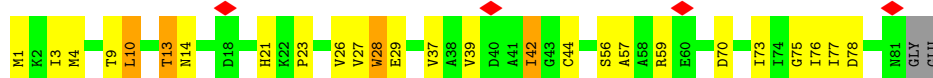
- Molecule 2: Carboxysome shell vertex protein CsoS4A



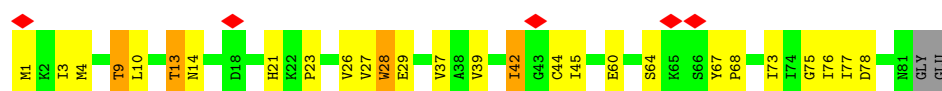
- Molecule 2: Carboxysome shell vertex protein CsoS4A



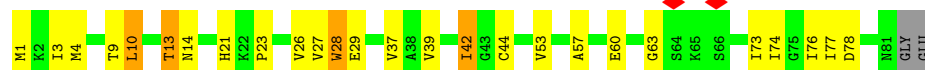
- Molecule 2: Carboxysome shell vertex protein CsoS4A



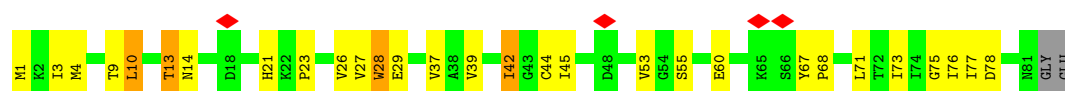
- Molecule 2: Carboxysome shell vertex protein CsoS4A



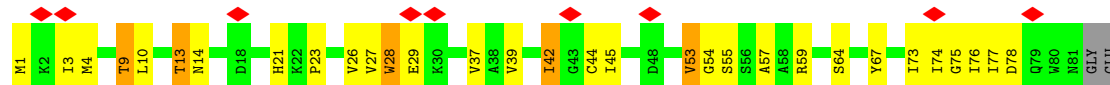
- Molecule 2: Carboxysome shell vertex protein CsoS4A



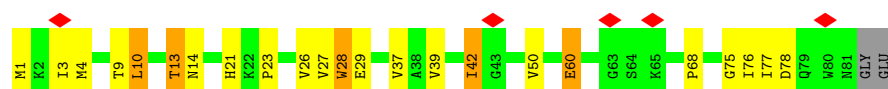
- Molecule 2: Carboxysome shell vertex protein CsoS4A



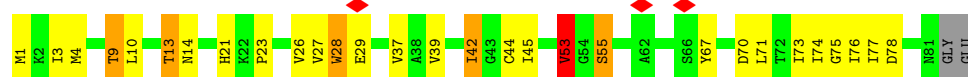
- Molecule 2: Carboxysome shell vertex protein CsoS4A



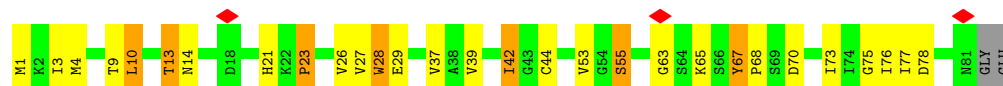
- Molecule 2: Carboxysome shell vertex protein CsoS4A



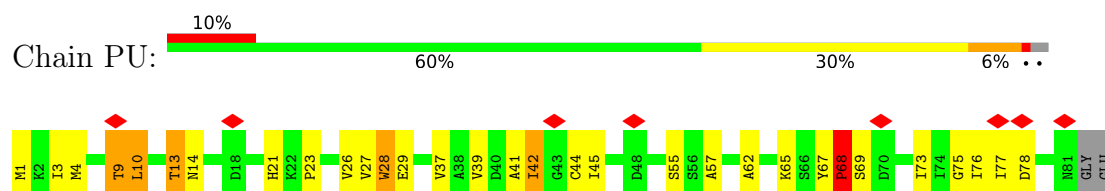
- Molecule 2: Carboxysome shell vertex protein CsoS4A



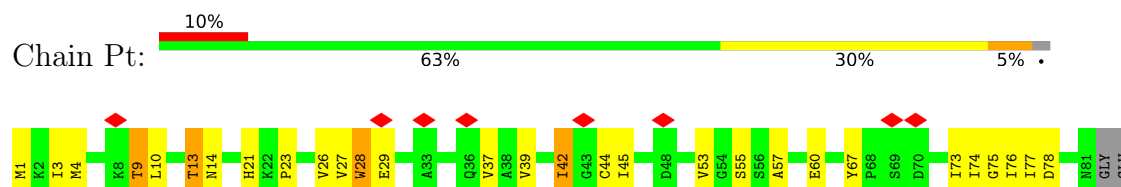
- Molecule 2: Carboxysome shell vertex protein CsoS4A



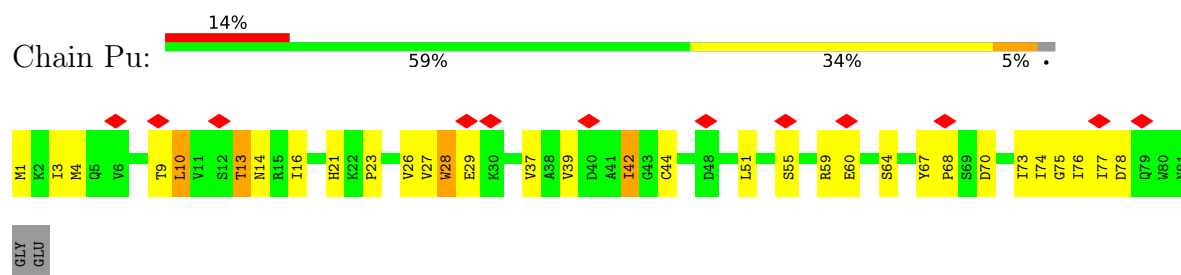
- Molecule 2: Carboxysome shell vertex protein CsoS4A



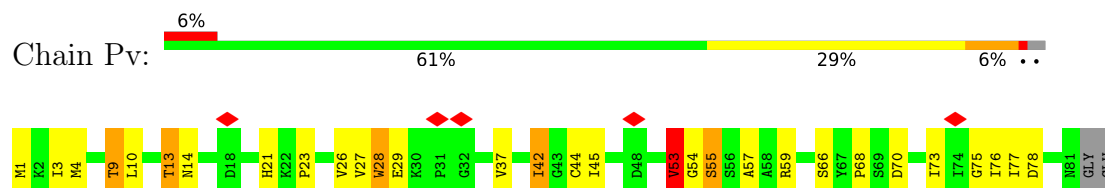
- Molecule 2: Carboxysome shell vertex protein CsoS4A



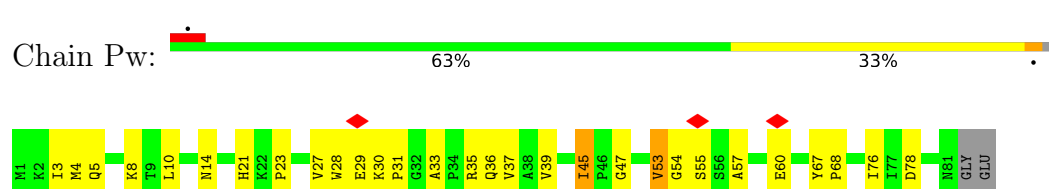
- Molecule 2: Carboxysome shell vertex protein CsoS4A



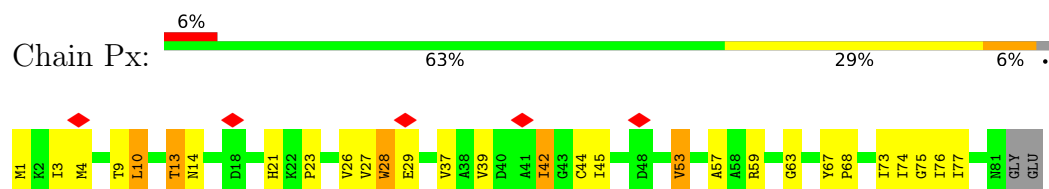
- Molecule 2: Carboxysome shell vertex protein CsoS4A



- Molecule 2: Carboxysome shell vertex protein CsoS4A

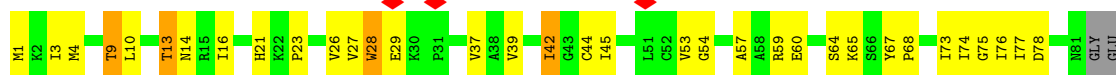


- Molecule 2: Carboxysome shell vertex protein CsoS4A



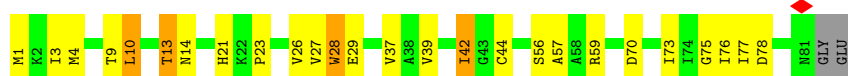
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain Pk:  57% 36% 5% .



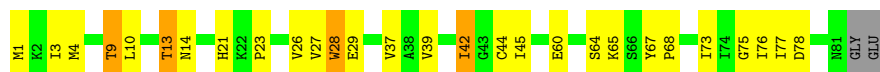
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain Pl:  66% 27% 5% .



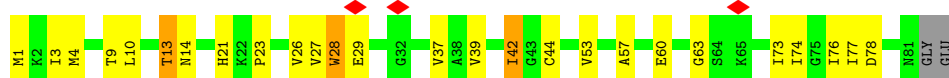
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain Pm:  64% 29% 5% .



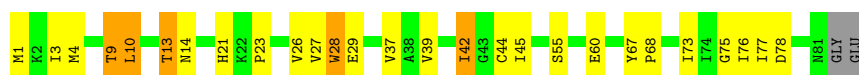
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain Pn:  66% 28% . .



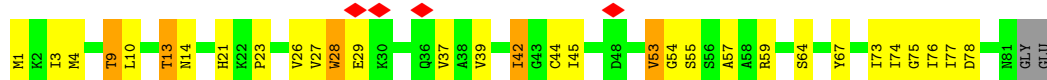
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain Po:  65% 27% 6% .



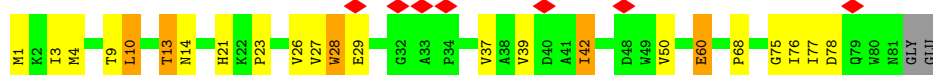
- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain Pp:  5% 60% 31% 6% .

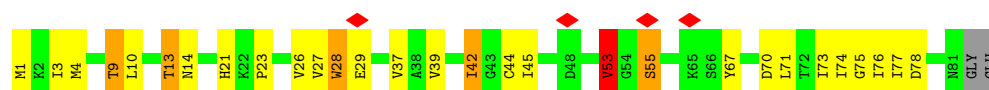


- Molecule 2: Carboxysome shell vertex protein CsoS4A

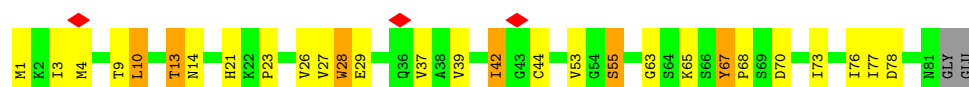
Chain Pq:  8% 70% 22% 6% .



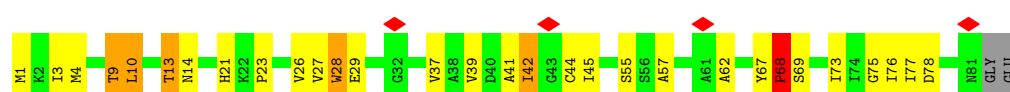
- Molecule 2: Carboxysome shell vertex protein CsoS4A



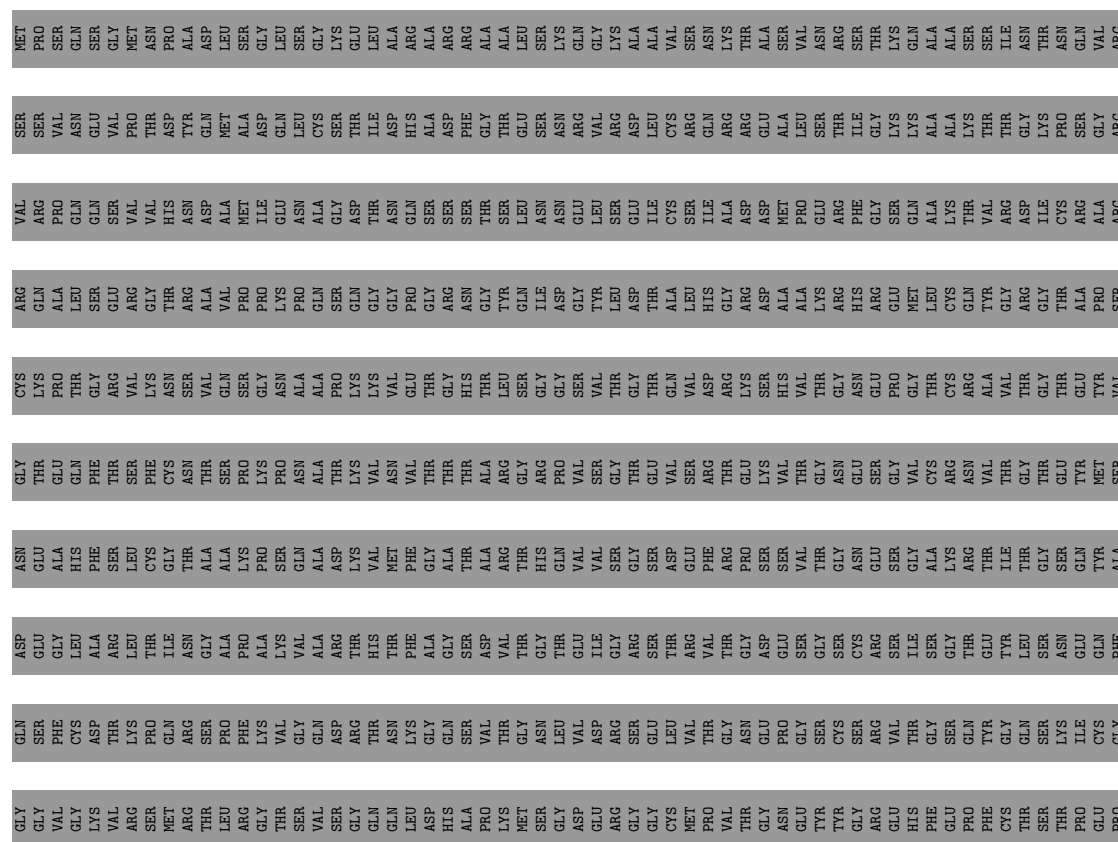
- Molecule 2: Carboxysome shell vertex protein CsoS4A

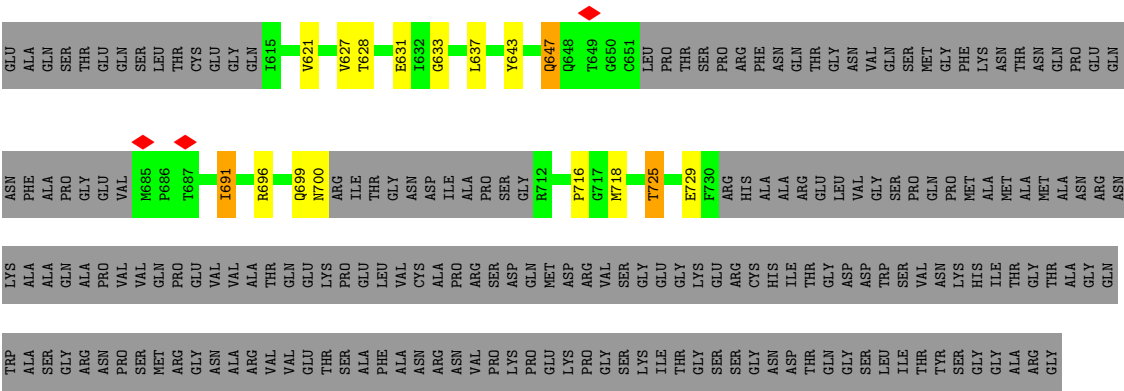


- Molecule 2: Carboxysome shell vertex protein CsoS4A



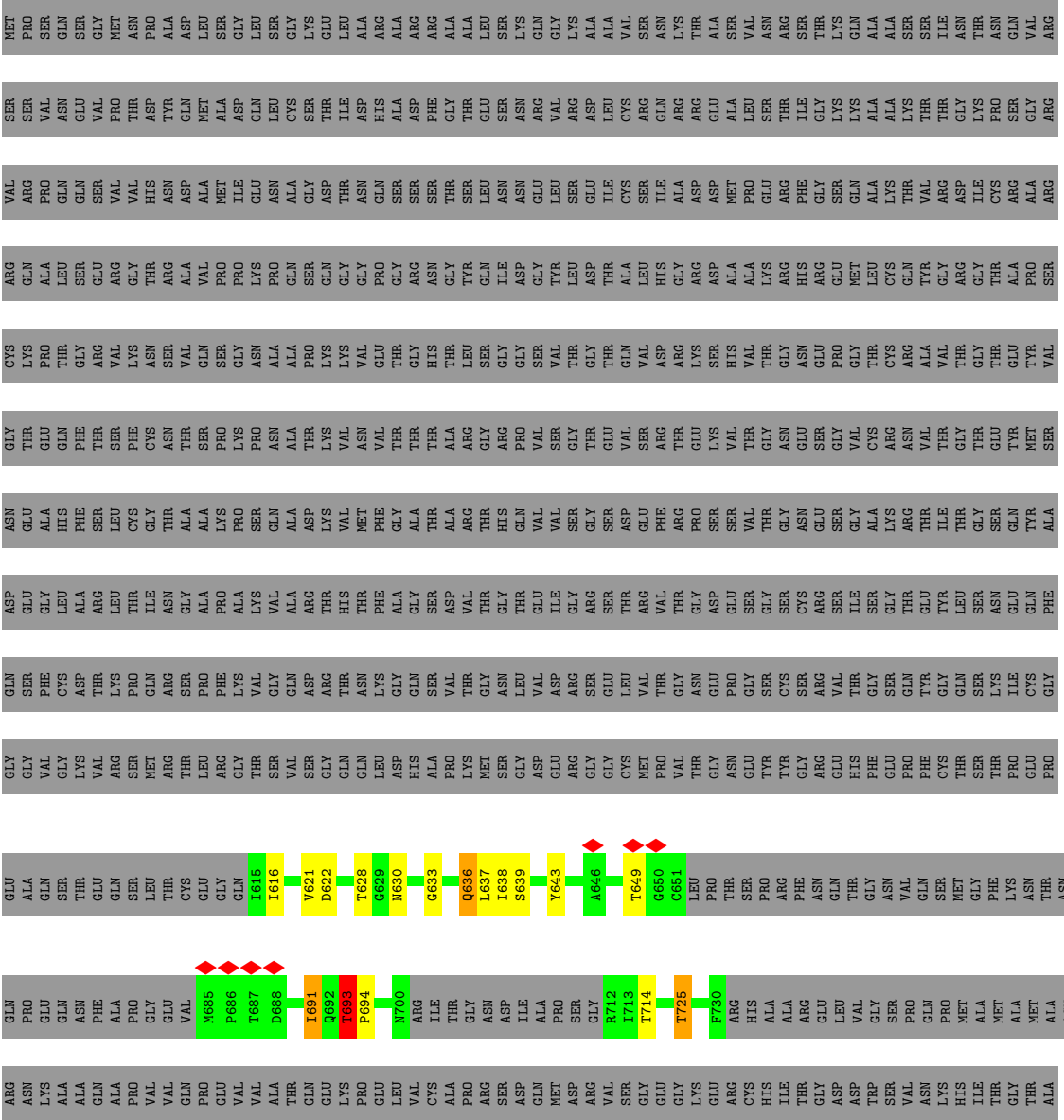
- Molecule 3: Carboxysome assembly protein CsoS2B



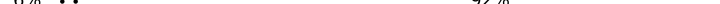


● Molecule 3: Carboxysome assembly protein CsoS2B

Chain XB: 6% 92%



- Molecule 3: Carboxysome assembly protein CsoS2B

Chain XC:  6% .. 92%

MET	PRO	SER	SER	GLN	SER	GLY	MET	ASN	ALA	PRO	ASP	LEU	SER	GLY	LEU	LYS	GLY	GLN	LEU	ALA	ALA	ARG	ARG	ARG	ALA	ALA	ALA	LEU	SER	LYS	GLN	GLY	LYS	ALA	ALA	VAL	VAL	SER	ASN	ASN	ARG	SER	SER	THR	THR	LYS	GLN	ALA	ALA	ALA	SER	SER	ILE	ASN	THR	ASN	GLN	VAL	PIC
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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

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

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

CYS	LYS	PRO	THR	GLY	ARG	VAL	LYS	ASN	SER	GLN	SER	GLY	ASN	ALA	ALA	PRO	LYS	LYS	VAL	GLU	THR	GLY	HIS	THR	LEU	SER	SER	GLY	GLY	SER	VAL	THR	THR	GLN	VAL	ASP	ARG	ASP	LYS	SER	SER	HIS	VAL	THR	GLY	ASN	GLU	PRO	GLY	THR	CYS	ARG	ALA	ALA	VAL	THR	GLY	THR	GLU	GLU	TYR	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLY	THR	GLU	GLU	GLN	PHE	THR	THR	SER	SER	PHE	CYS	ASN	THR	THR	PRO	PRO	PRO	ASN	ALA	THR	THR	LYS	VAL	ASN	VAL	THR	THR	THR	ALA	ARG	ARG	ARG	PRO	VAL	SER	SER	GLY	THR	THR	GLU	VAL	SER	THR	ARG	THR	GLY	LYS	GLU	VAL	THR	THR	GLY	ASN	GLU	GLY	SER	SER	VAL	CYS	ARG	ASN	VAL	THR	THR	GLY	THR	GLU	TYR	THR	MET	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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

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

GLN	SER	PHE	CYS	ASP	THR	LYS	PRO	GLN	ARG	SER	PRO	PHE	LYS	VAL	GLY	GLN	ASP	ARG	THR	ASN	LYS	GLY	GLN	SER	VAL	THR	GLY	ASN	LEU	VAL	ASP	ARG	SER	SER	GLU	LEU	VAL	THR	GLY	ASN	GLY	GLU	PRO	GLY	SER	CYS	SER	SER	ARG	VAL	THR	THR	SER	LYS	ILE	CYS	TYR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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

GLU	ALA	GLN	SER	THR	GLU	GLN	SER	LEU	THR	CYS	GLU	GLY	GLN	1615	1616	1617	1618	1619	1620	1621	1622	1623	1624	1627	1628	1629	1630	1634	1643	1644	1645	1646	1647	1648	1649	1650	1651	LEU	PRO	THR	SER	PRO	ARG	PHE	ASN	GLN	THR	GLY	ASN	VAL	GLN	SER	MET	GLY	PHE	YS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----

ASN	THR	ASN	GLN	PRO	GLU	GLN	ASN	PHE	ALA	PRO	GLY	GLU	VAL	M685	P696	T691	T693	P694	N700	ARG	ILE	THR	GLY	ASN	ASP	ILE	ALA	ALA	PRO	SER	GLY	R712	I713	T714	L719	T725	E729	F730	ARG	HIS	ALA	ALA	ARG	GLU	LEU	VAL	GLY	SER	PRO	GLN	PRO	MET	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ALA	MET	ALA	ALA	ASN	ARG	ASN	LYS	ALA	ALA	GLN	ALA	PRO	VAL	VAL	GLN	GLN	PRO	GLY	VAL	VAL	ALA	ALA	THR	GLN	GLN	GLU	LYS	CYS	VAL	ALA	PRO	ARG	SER	SER	ASP	GLN	MET	ASP	GLY	GLY	GLU	LYS	GLU	GLU	ARG	VAL	VAL	SER	SER	ASP	HIS	ILE	THR	GLY	GLY	ASP	ASN	LYS	ALA	HIS	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible]

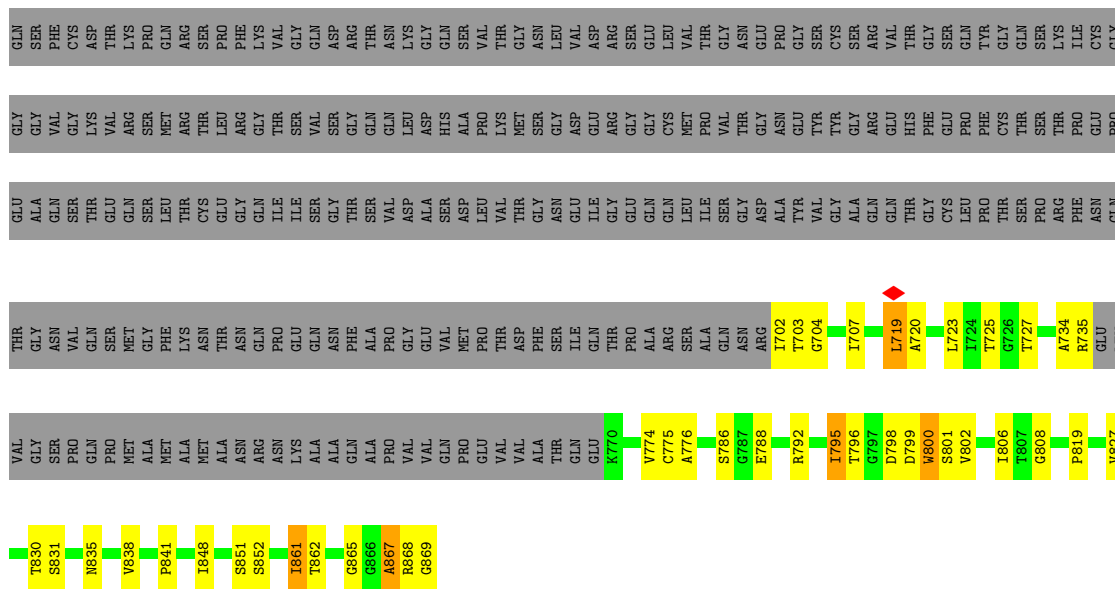
ALA
ARG
GLY

- Molecule 3: Carboxysome assembly protein CsoS2B

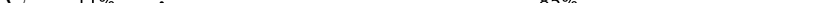
Chain XE: 6% .. 92%

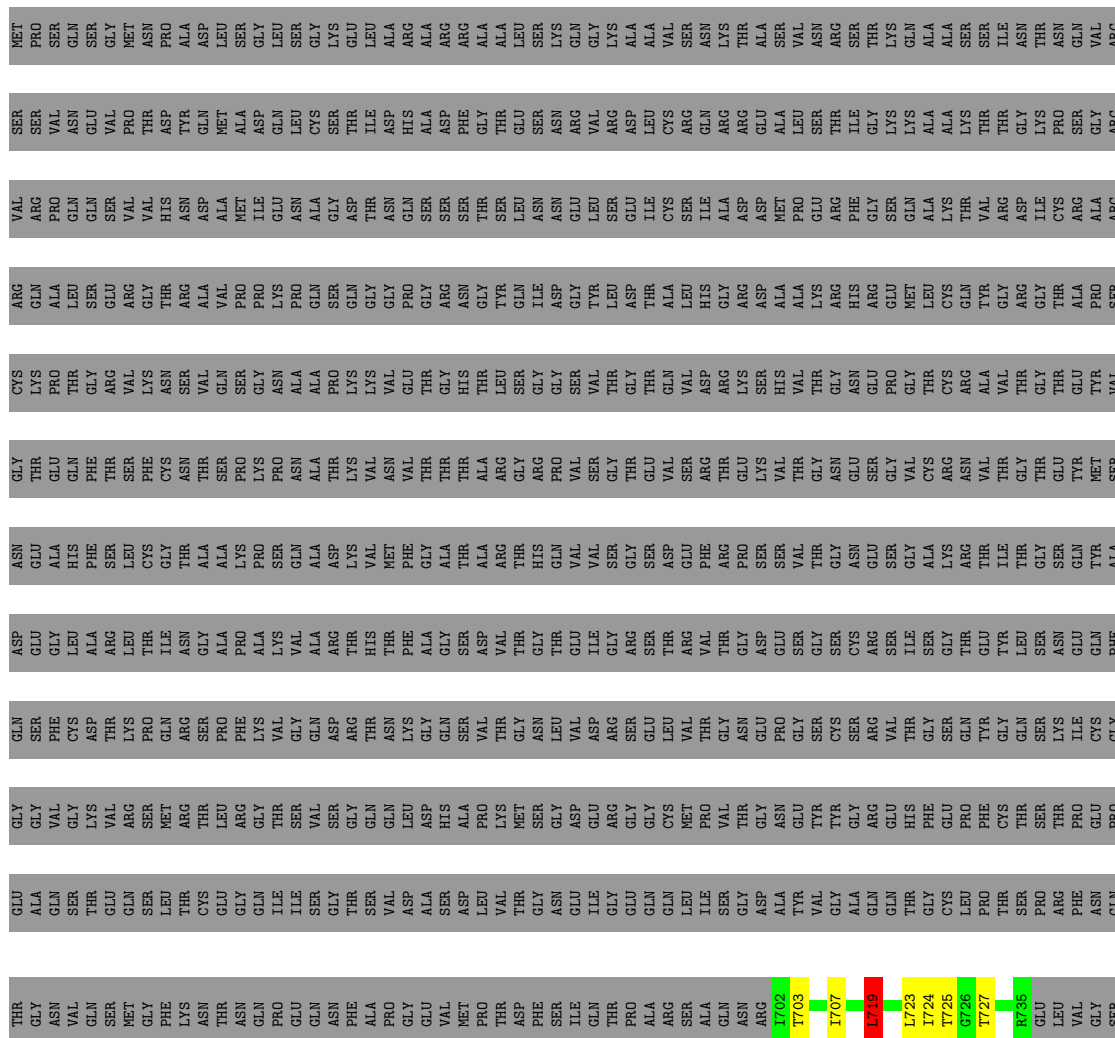
MET	PRO	SER	SER	GLN	SER	GLY	MET	ASN	ALA	PRO	ALA	ASP	LEU	SER	GLY	LEU	SER	GLY	LYS	GLU	LEU	ALA	ALA	ARG	ARG	ALA	ALA	LEU	SER	LYS	GLN	GLY	LYS	ALA	ALA	ALA	VAL	SER	ASN	ASN	ARG	SER	THR	THR	LYS	GLN	ALA	ALA	ALA	SER	SER	ILE	ASN	THR	ASN	GLN	VAL	ARG
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

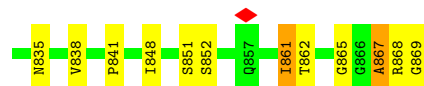




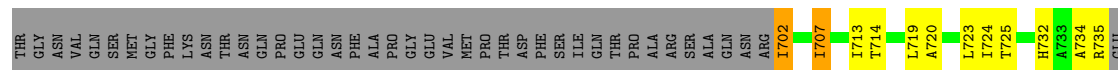
- Molecule 3: Carboxysome assembly protein CsoS2B

Chain YC:  11% 1% 85%





- Molecule 3: Carboxysome assembly protein CsoS2B



- Molecule 3: Carboxysome assembly protein CsoS2B

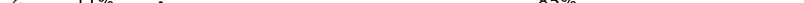
H732	THR	GLU	GLY	GLN	GLY	GLN	ASP	ASN	GLY	CYS	ARG	VAL	SER	MET	GLN	CYS	ARG	VAL	SER	MET
R735	ASN	ALA	GLY	GLN	VAL	PHE	GLY	GLY	GLU	SER	ARG	PRO	SER	GLY	GLN	GLY	PRO	ARG	SER	GLY
GLU	GLN	SER	GLY	GLN	GLY	CYS	ASP	HIS	PHE	GLY	GLN	THR	GLN	GLY	GLN	GLY	GLN	GLN	GLN	GLN
LEU	GLN	THR	GLY	THR	ASP	THR	ALA	SER	THR	ARG	VAL	ARG	GLY	THR	SER	GLY	SER	VAL	GLY	GLY
VAL	SER	GLU	VAL	GLN	ARG	LYS	THR	LEU	SER	THR	VAL	THR	THR	SER	GLY	VAL	VAL	SER	VAL	GLY
GLY	MET	GLN	ARG	GLY	THR	GLY	LEU	GLY	THR	GLY	GLY	GLY	THR	GLY	THR	GLY	GLY	GLY	GLY	GLY
SER	GLY	SER	SER	GLY	SER	PRO	THR	CYS	THR	PRO	GLY	VAL	GLY	PHE	GLY	VAL	GLY	VAL	THR	GLY
PRO	PHE	LEU	MET	GLY	GLY	GLN	ILE	GLY	GLY	ILE	GLY	THR	CYS	CYS	ASN	THR	THR	THR	THR	THR
GLN	LYS	THR	ARG	GLY	ARG	GLY	ASP	THR	GLY	ASN	ALA	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
PRO	ASN	CYS	THR	GLY	PRO	PRO	ALA	ALA	ALA	VAL	VAL	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
MET	ASN	GLY	LEU	GLY	ARG	PHE	GLY	GLY	GLY	GLY	GLY	GLY	SER	SER	PRO	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	ARG	GLY	GLY	THR	THR	GLY	THR	ARG	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
MET	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	GLY	GLY	GLN	GLY	GLY	THR	GLY	GL											

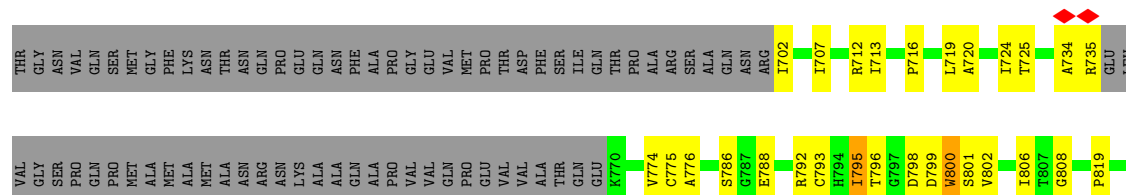
Chain X1: 5% 92%

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



- Molecule 3: Carboxysome assembly protein CsoS2B

Chain Y2:  11% 85%



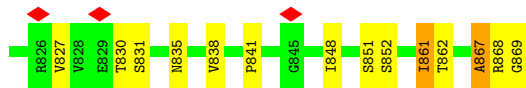


- Molecule 3: Carboxysome assembly protein CsoS2B

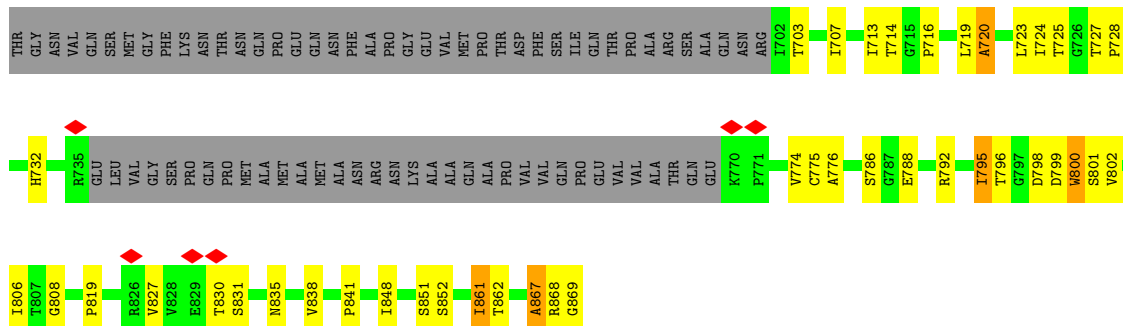








Chain Y7: 10% 85%



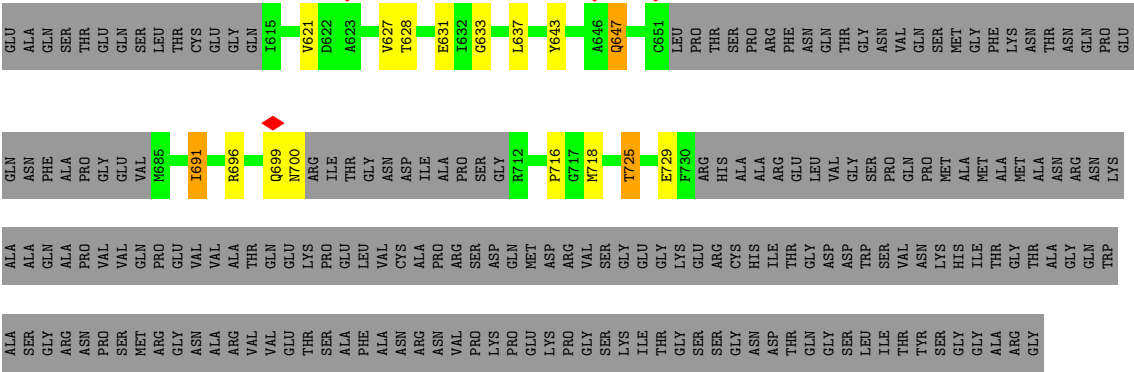
- Molecule 3: Carboxysome assembly protein CsoS2B

11% . .

- Molecule 3: Carboxysome assembly protein CsoS2B

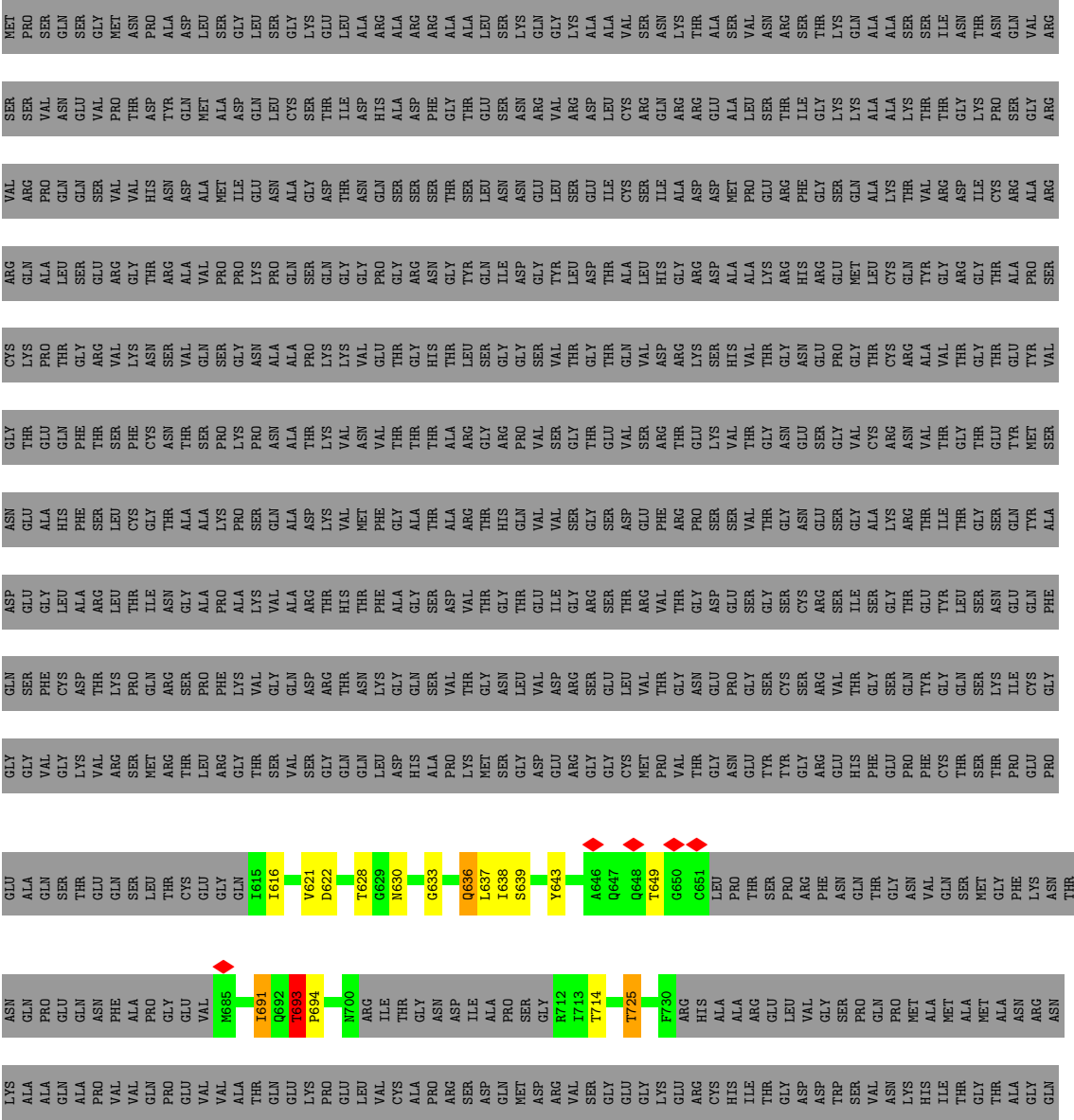
11% . .

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



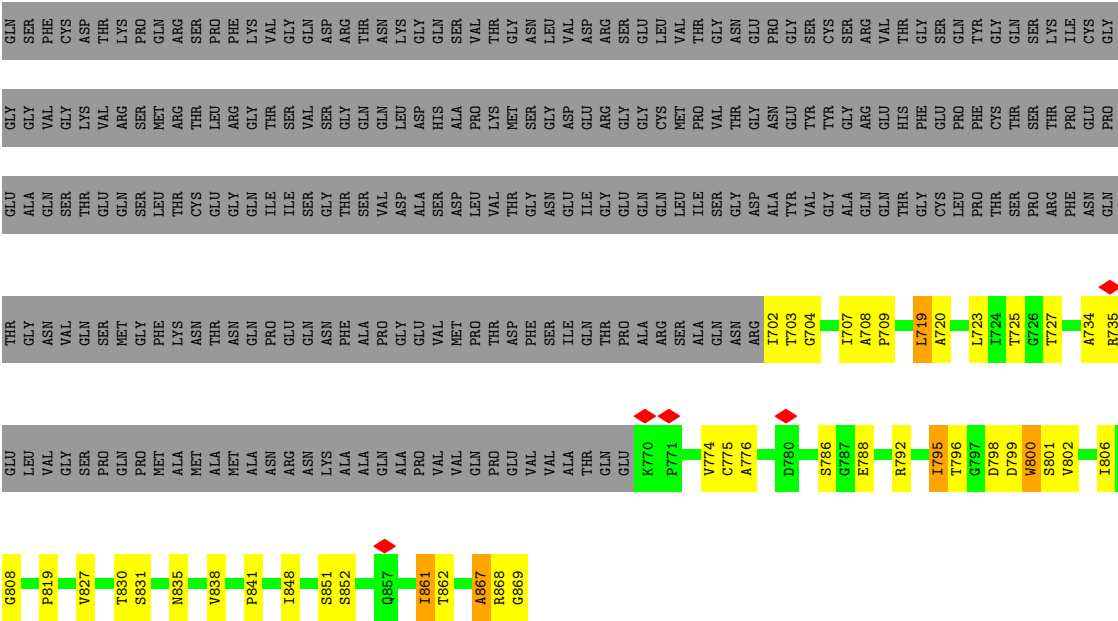
● Molecule 3: Carboxysome assembly protein CsoS2B

Chain XQ: 6% . 92%



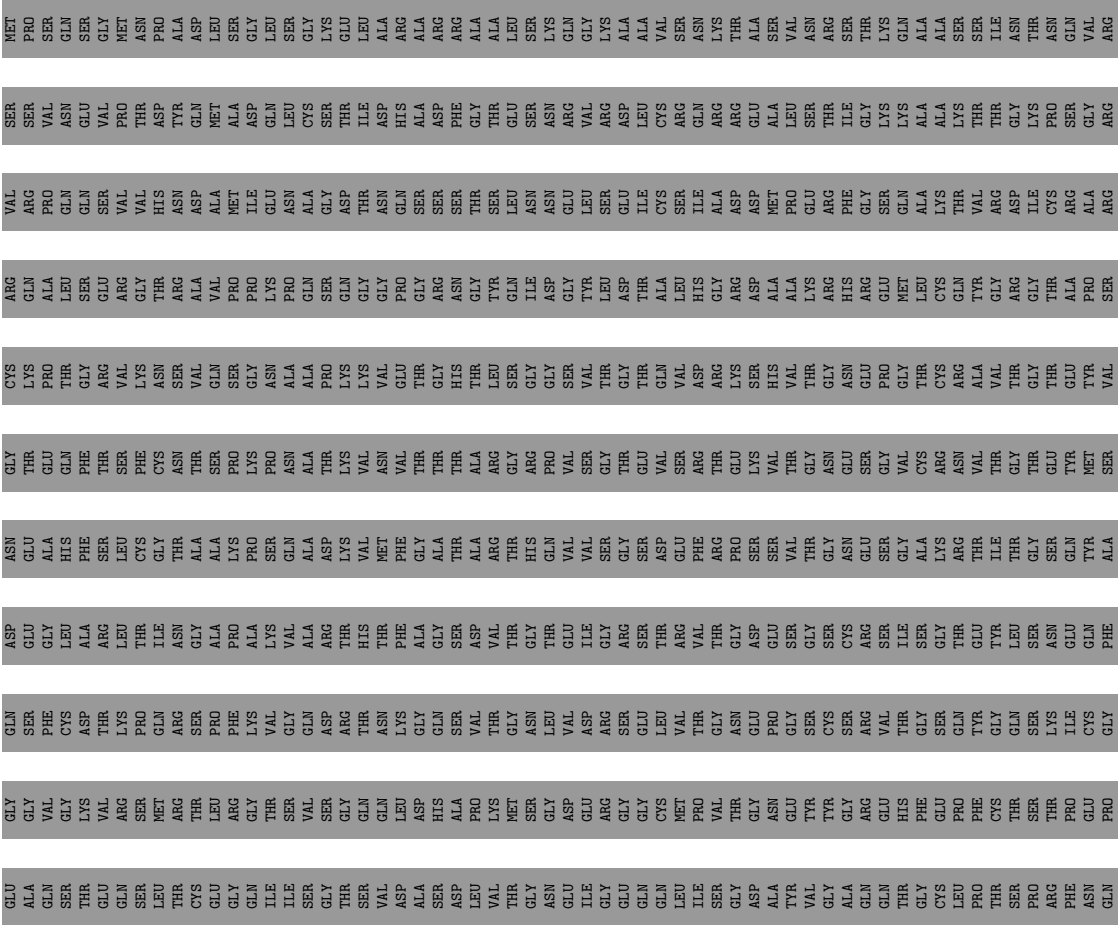
- Molecule 3: Carboxysome assembly protein CsoS2B

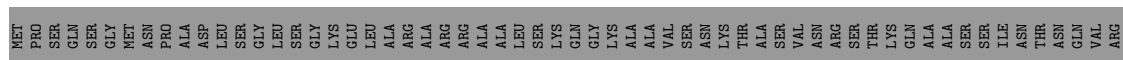


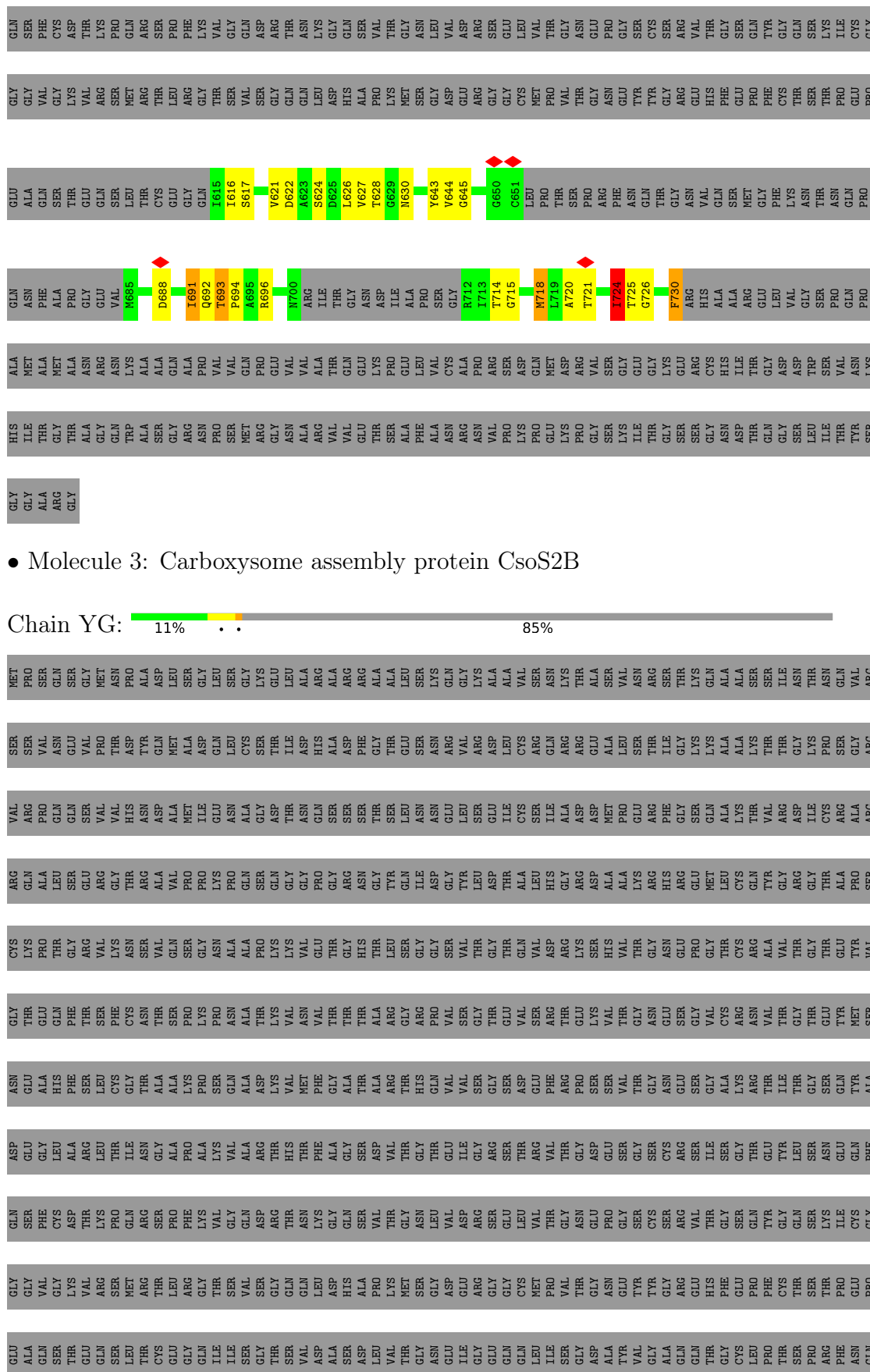


● Molecule 3: Carboxysome assembly protein CsoS2B

Chain YR: 11% . 85%

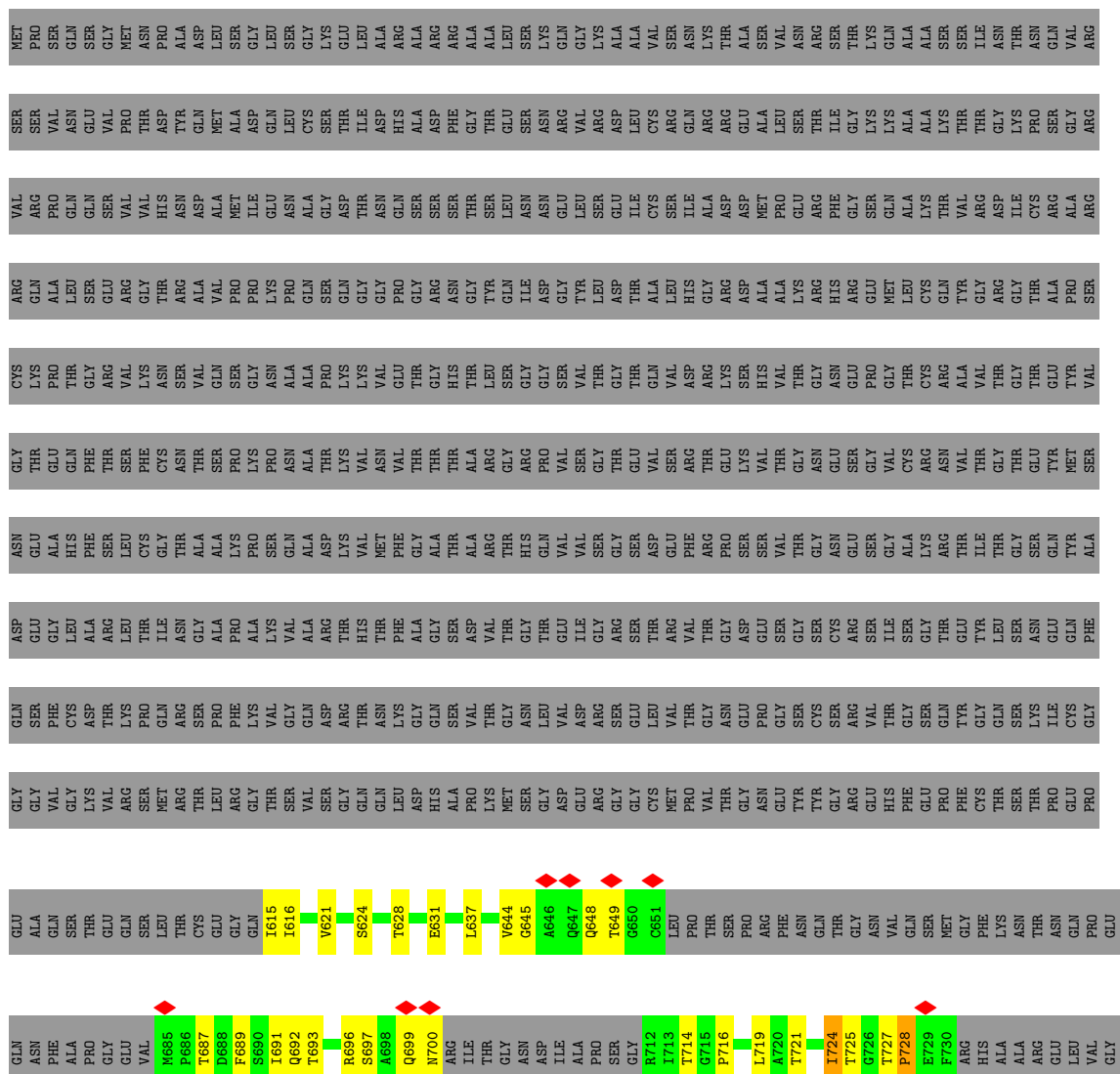




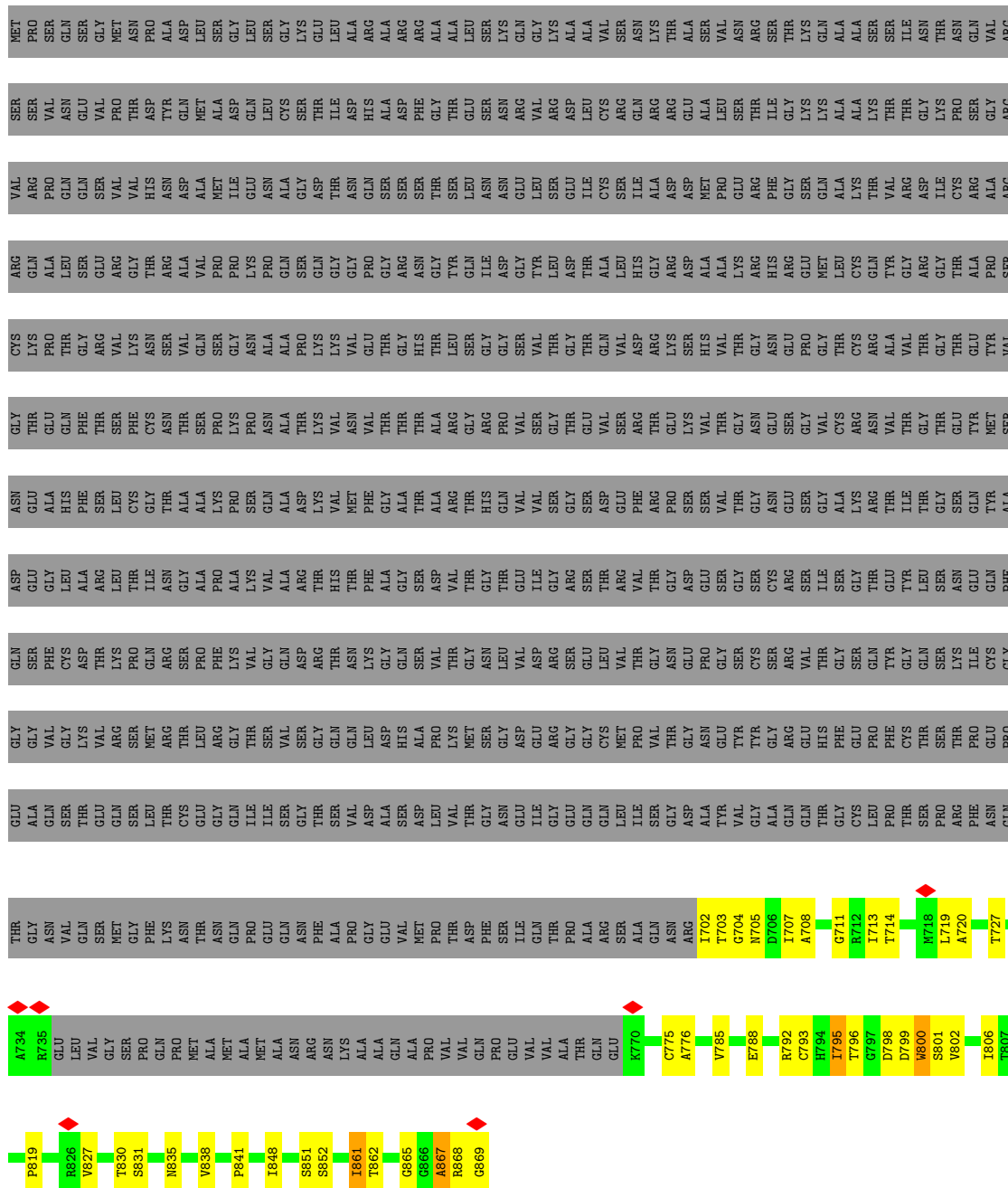




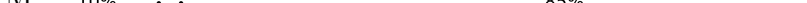
- Molecule 3: Carboxysome assembly protein CsoS2B



- Molecule 3: Carboxysome assembly protein CsoS2B

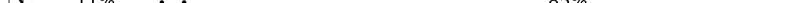


- Molecule 3: Carboxysome assembly protein CsoS2B

Chain YM: 

[illegible]

- Molecule 3: Carboxysome assembly protein CsoS2B

Chain YN: 

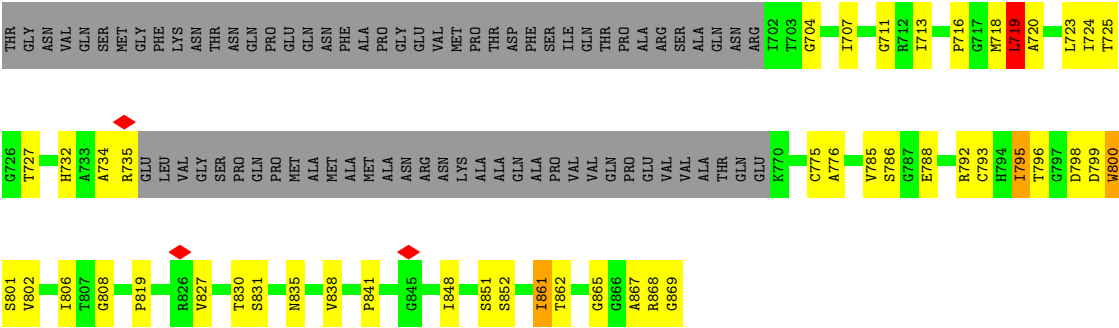
VAL	SER	MET
ARG	SER	PRO
PRO	VAL	SER
GLN	ASN	GLN
GLY	VAL	GLY
VAL	THR	MET
VAL	PRO	ASN
HIS	ASP	PRO
ASN	TYR	ALA
ASP	GLN	ASP
ALA	MET	LEU
MET	ALA	SER
ILE	ASP	GLY
GLU	GLN	LEU
ASN	LEU	SER
ALA	CYS	GLY
GLY	SER	LYS
ASP	THR	GLU
THR	ILE	LEU
ASN	ASP	ALA
GLN	HIS	ARG
GLM	ALA	ALA
SER	ASP	ARG
SER	PHE	ARG
THR	GLY	ALA
SER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

V827	T830	S831	N835	V838	P841	I848	S851	S852	I861	T862	G865	G866	A867	R868	G869
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

Chain YO: 11% 11% 11% 85%

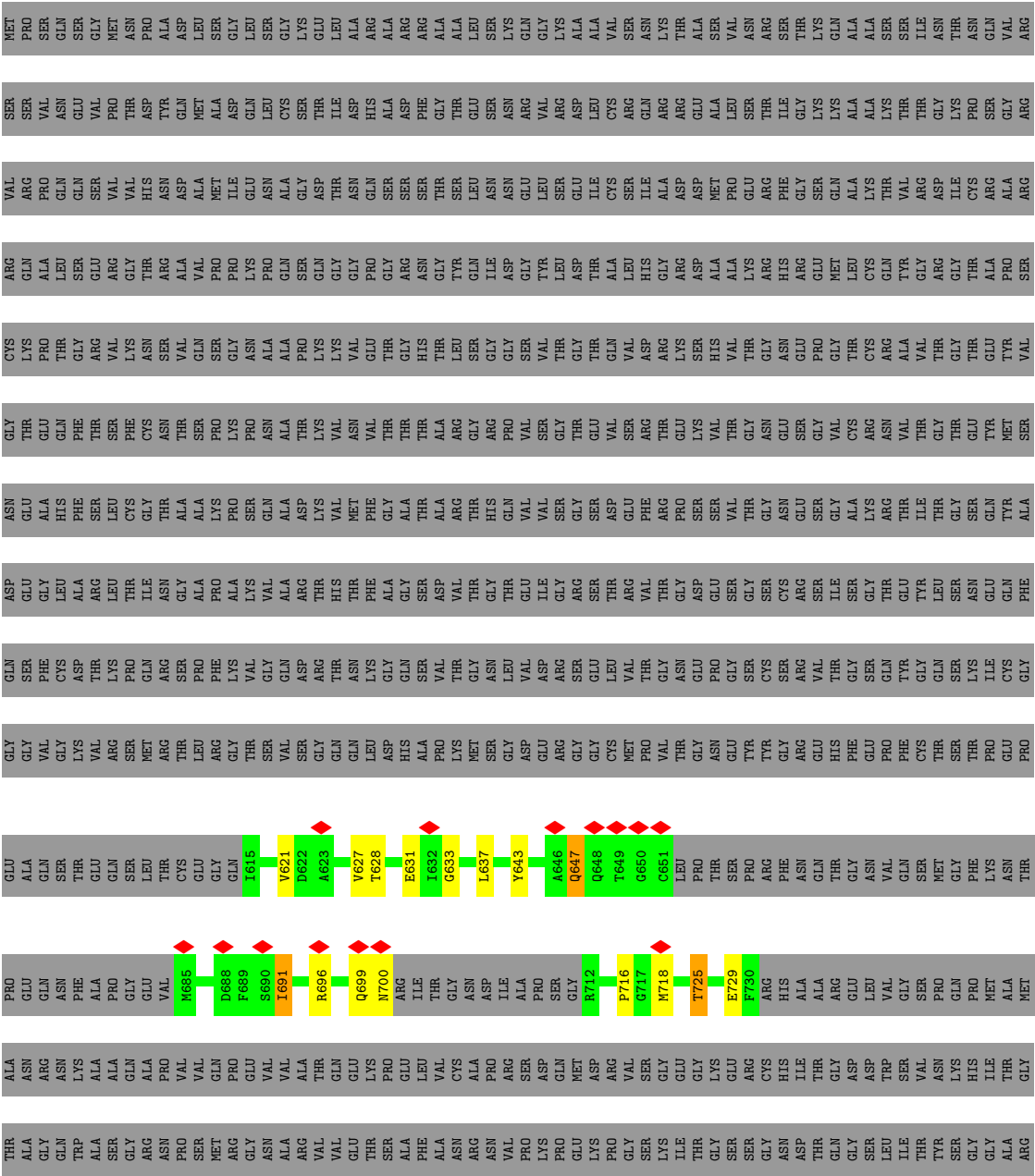






● Molecule 3: Carboxysome assembly protein CsoS2B

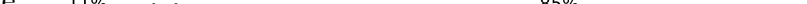
Chain Xc: 6% 92%



- Molecule 3: Carboxysome assembly protein CsoS2B

[illegible]

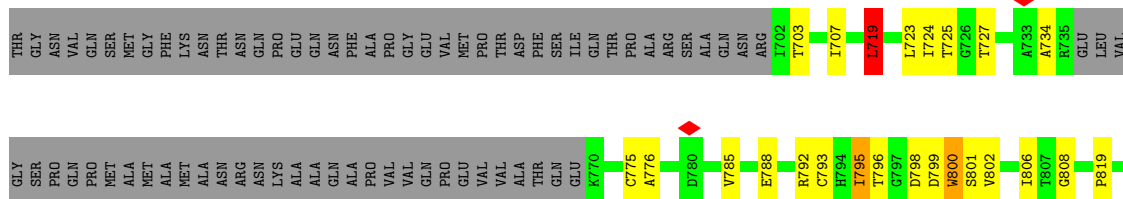
- Molecule 3: Carboxysome assembly protein CsoS2B

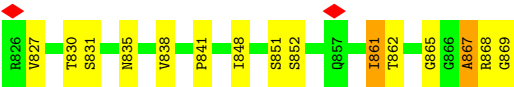
Chain Ye: 

[illegible]

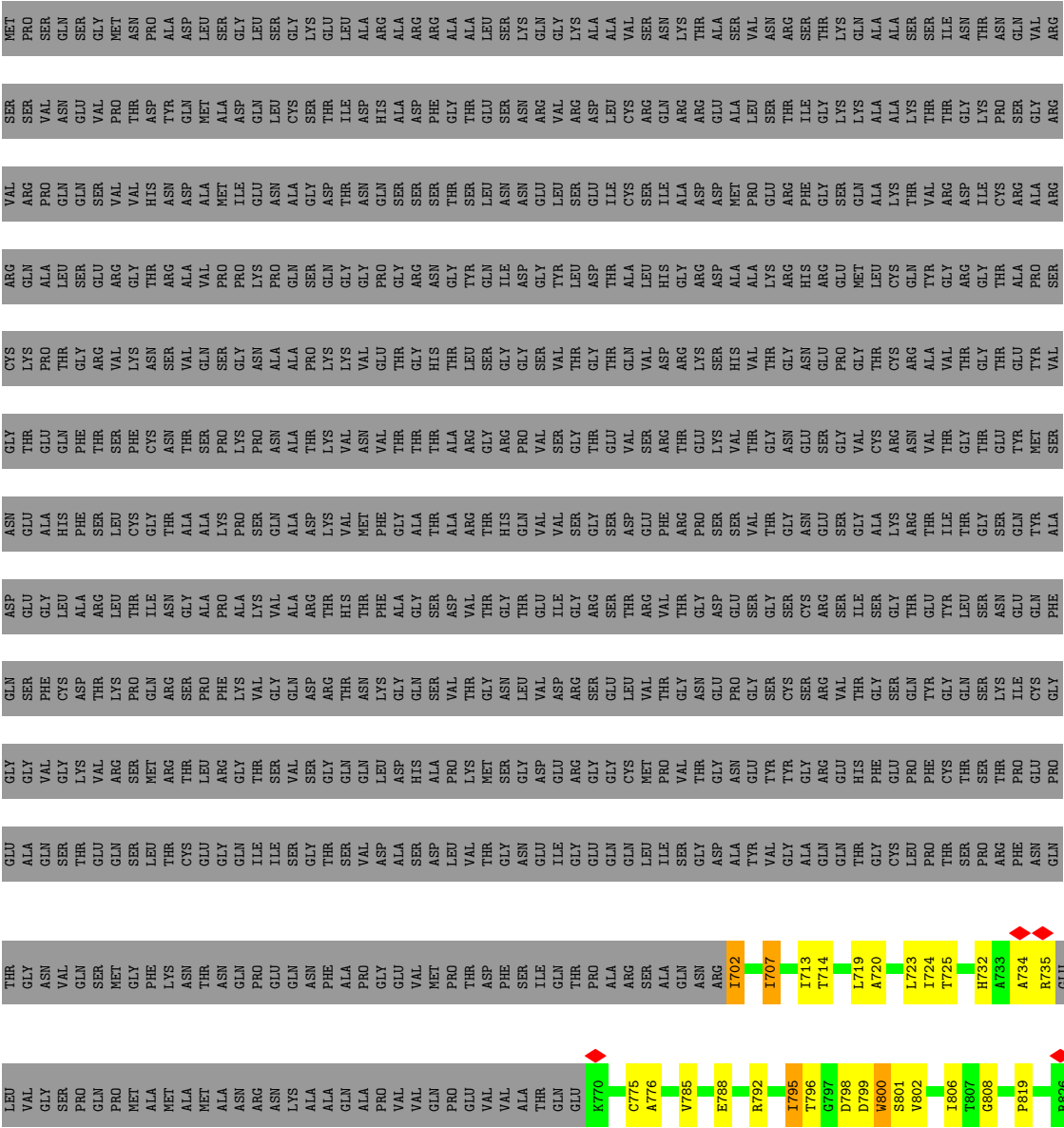


- Molecule 3: Carboxysome assembly protein CsoS2B





• Molecule 3: Carboxysome assembly protein CsoS2B

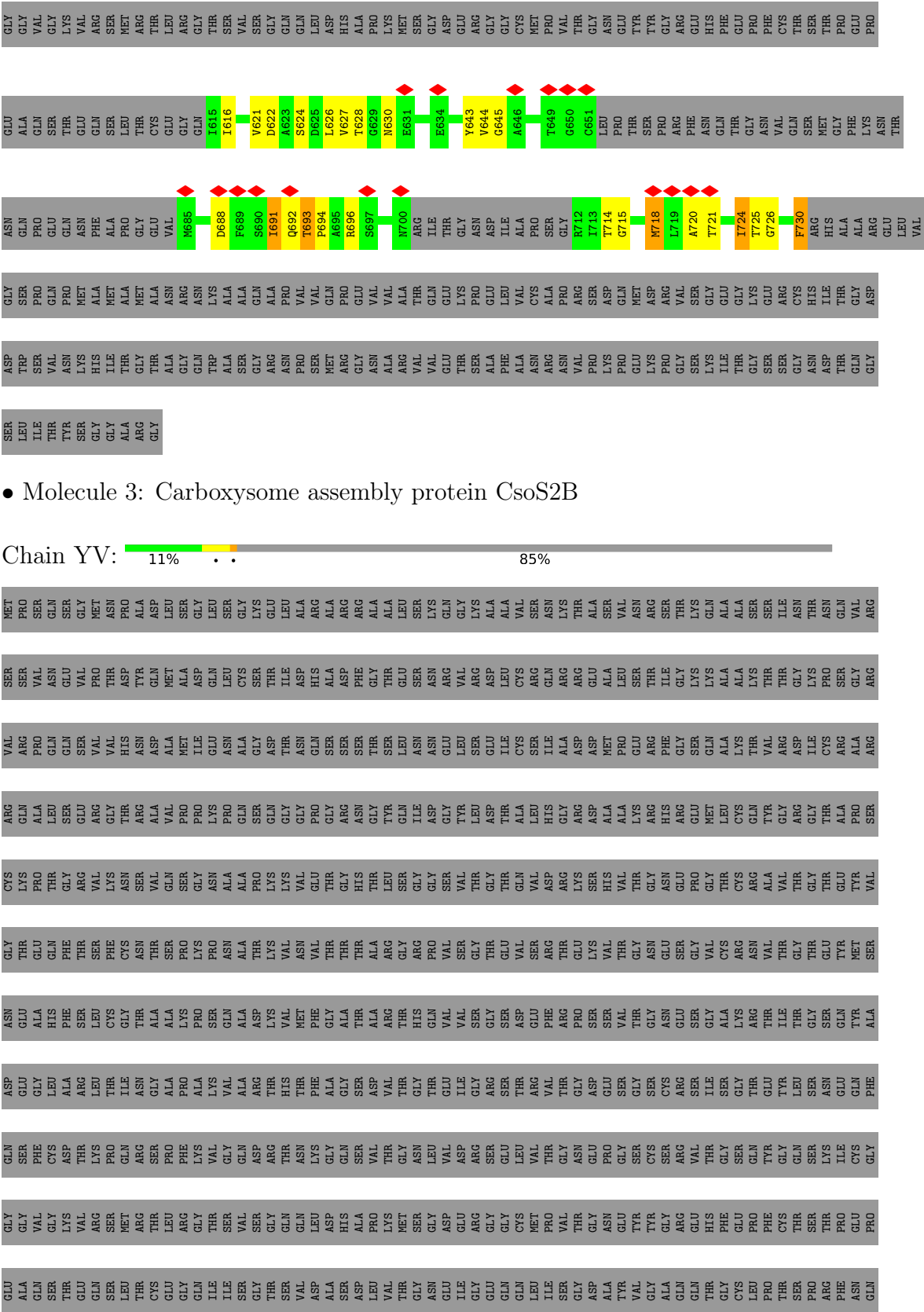


• Molecule 3: Carboxysome assembly protein CsoS2B

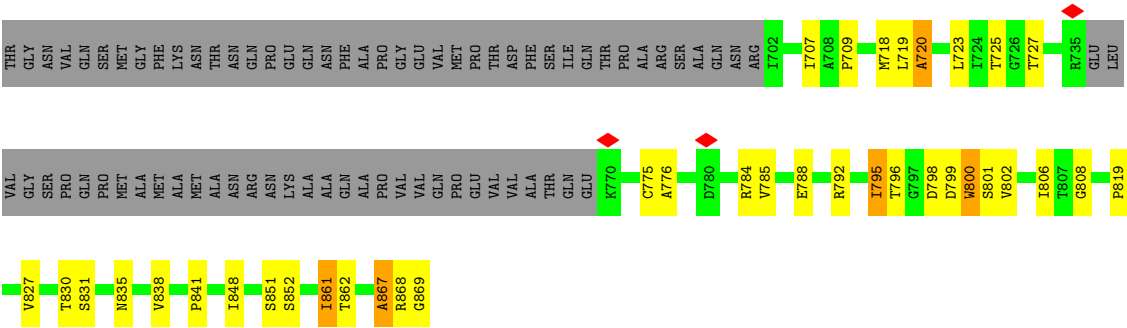


- Molecule 3: Carboxysome assembly protein CsoS2B



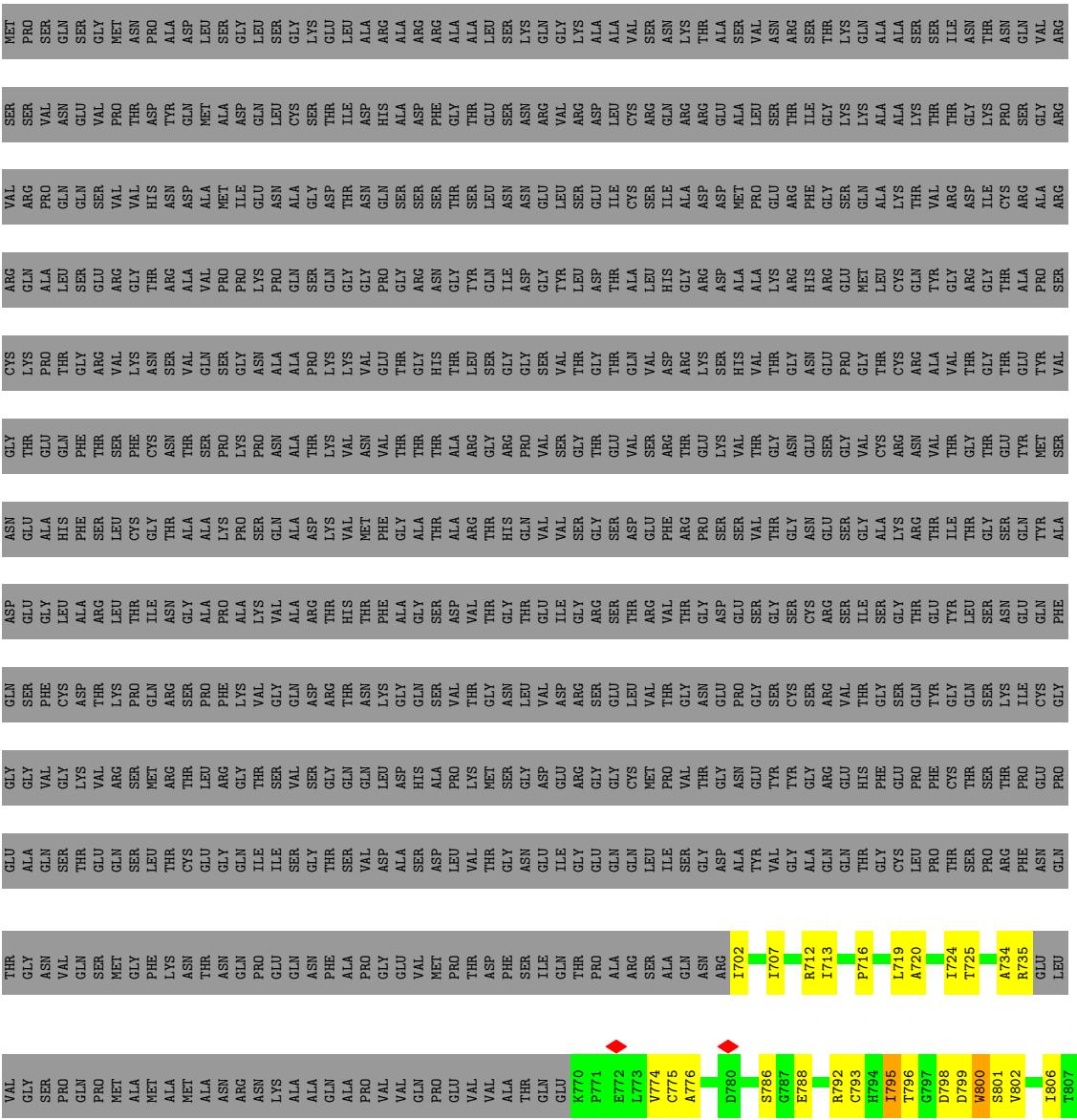


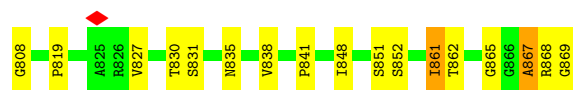
● Molecule 3: Carboxysome assembly protein CsoS2B



● Molecule 3: Carboxysome assembly protein CsoS2B

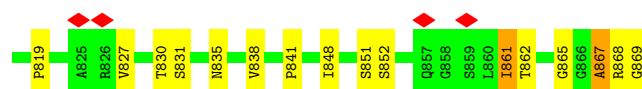
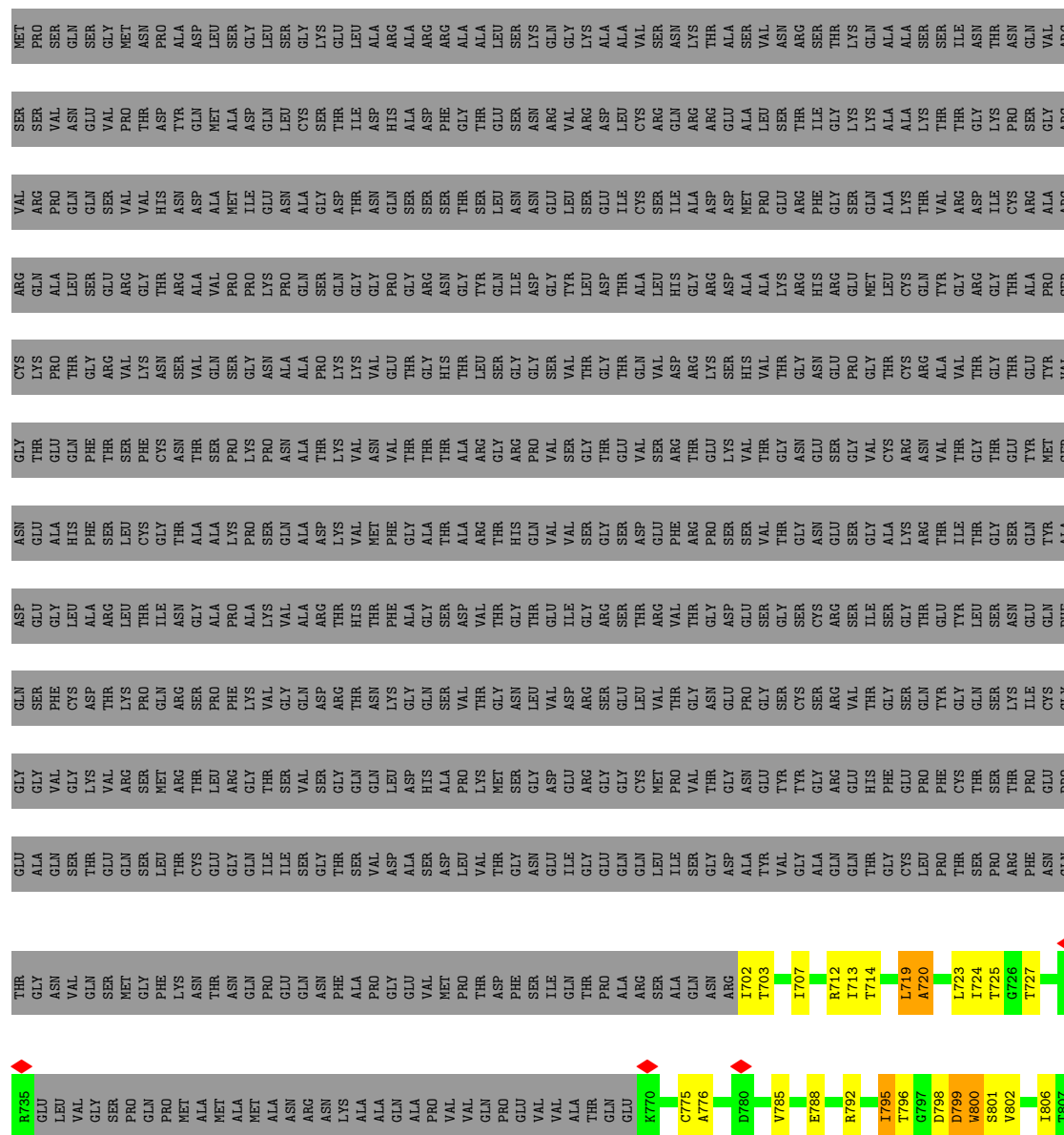
Chain YW: 10% 85%





• Molecule 3: Carboxysome assembly protein CsoS2B

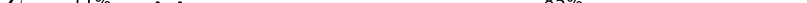
Chain YX: 11% . . 85%



• Molecule 3: Carboxysome assembly protein CsoS2B

Chain YY: 11% . 85%

- Molecule 3: Carboxysome assembly protein CsoS2B

Chain YZ:  11% 85%

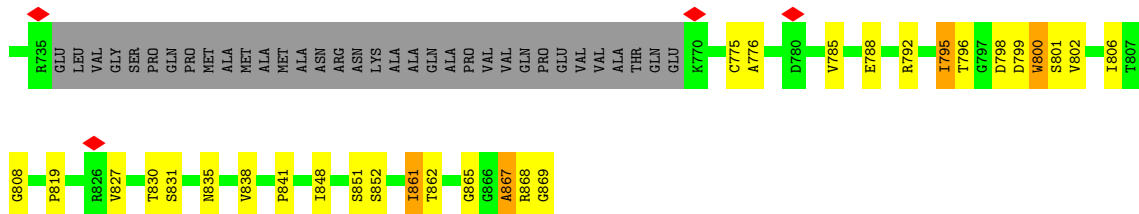
[illegible]

- Molecule 3: Carboxysome assembly protein CsoS2B

[illegible]



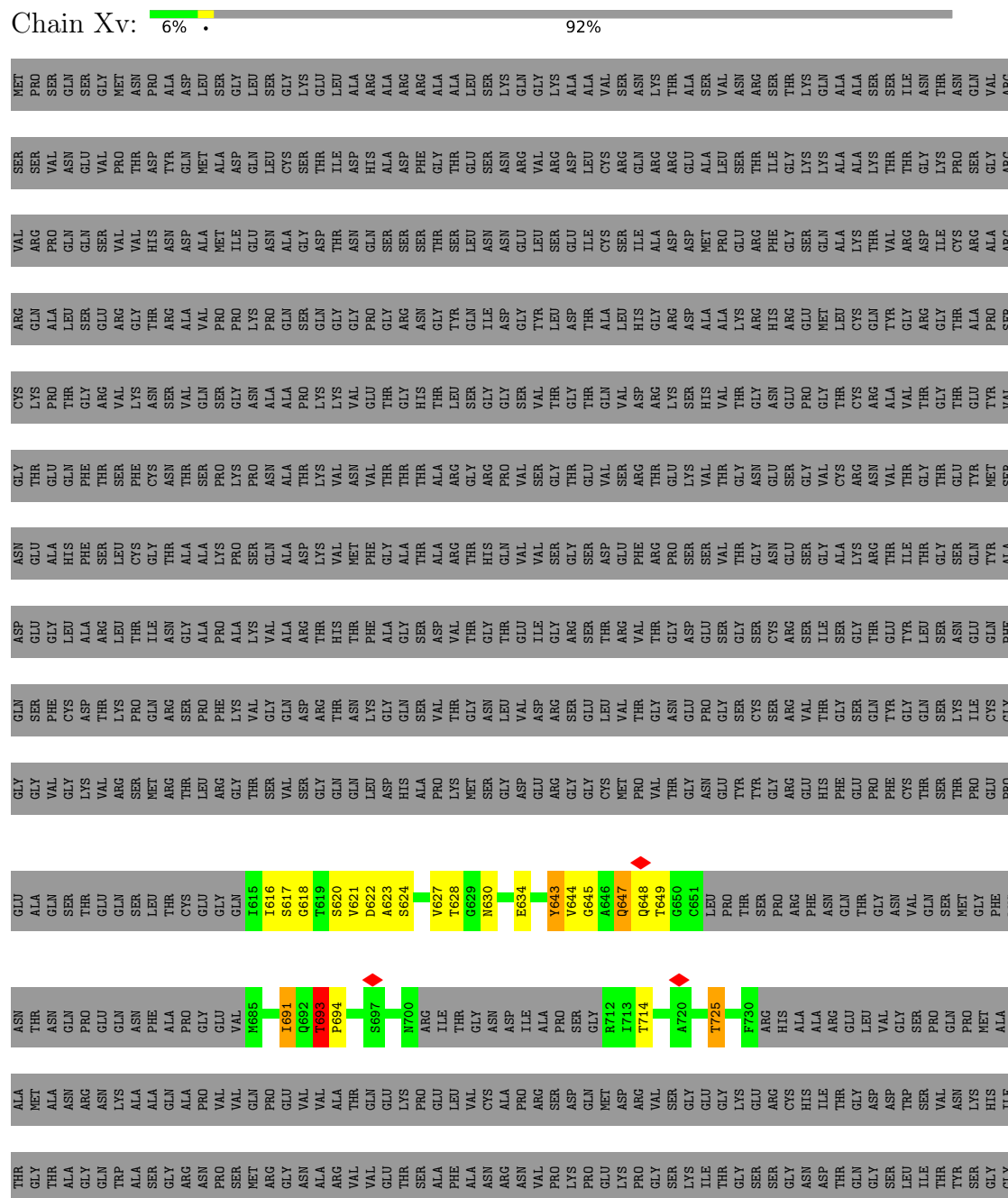








- Molecule 3: Carboxysome assembly protein CsoS2B



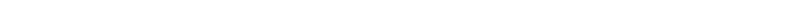


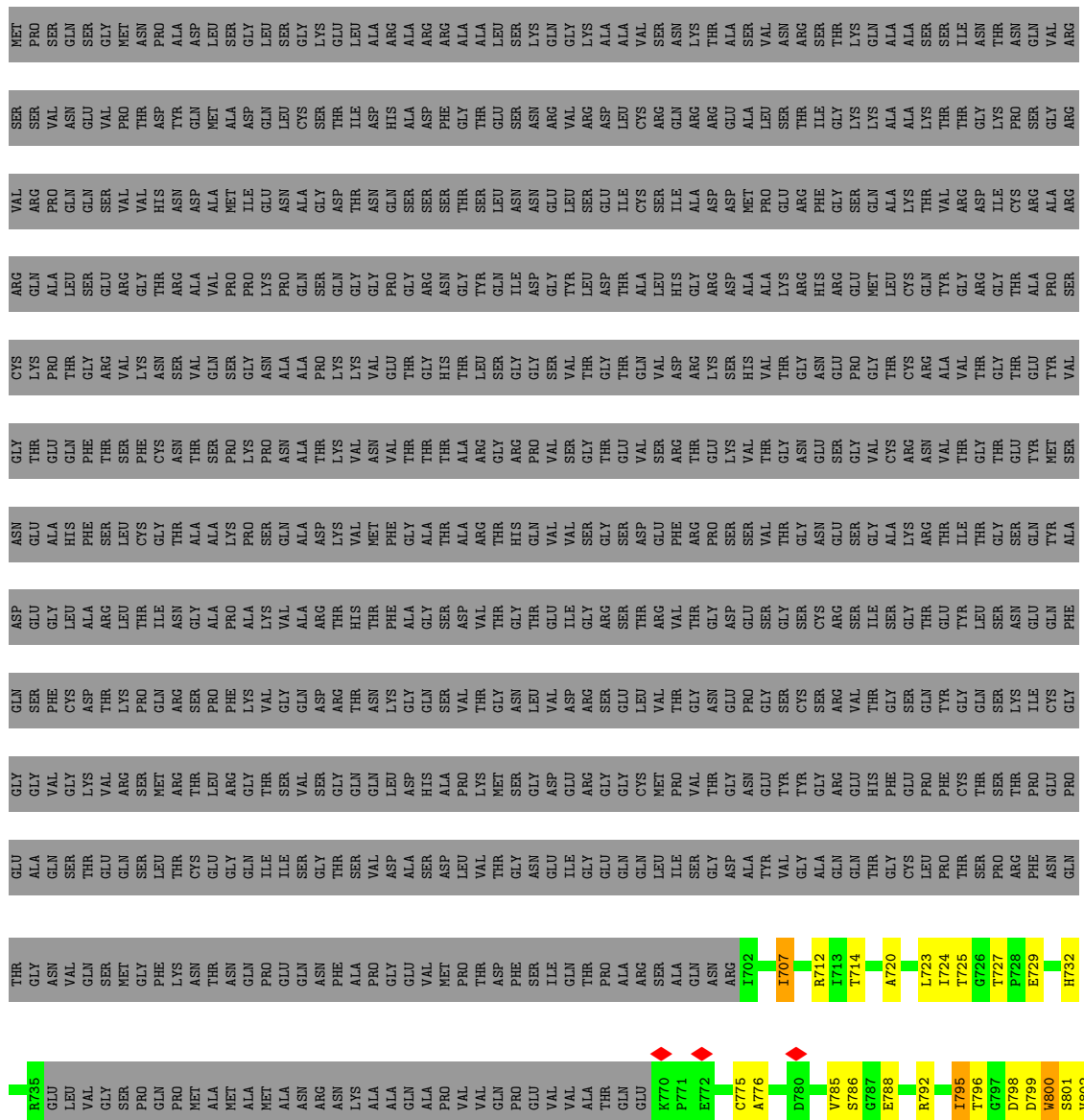
- Molecule 3: Carboxysome assembly protein CsoS2B

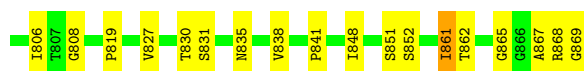
ARG	GLN	ARG	VAL	SER	MET
GLN	ALA	PRO	ARG	SER	PRO
ALA	LEU	PRO	GLN	VAL	ASN
LEU	SER	GLN	GLN	ASN	GLN
GLI	SER	GLN	SER	VAL	GLY
ARG	GLY	VAL	VAL	PRO	MET
GLY	THR	VAL	VAL	THR	ASN
THR	HIS	HIS	ASP	TYR	PRO
ARG	ARG	ASN	ASP	TYR	ALA
ALA	ALA	ASP	GLN	GLN	ASP
VAL	VAL	ALA	ALA	MET	LEU
VAL	PRO	MET	MET	ALA	SER
PRO	PRO	ILE	ILE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



- Molecule 3: Carboxysome assembly protein CsoS2B

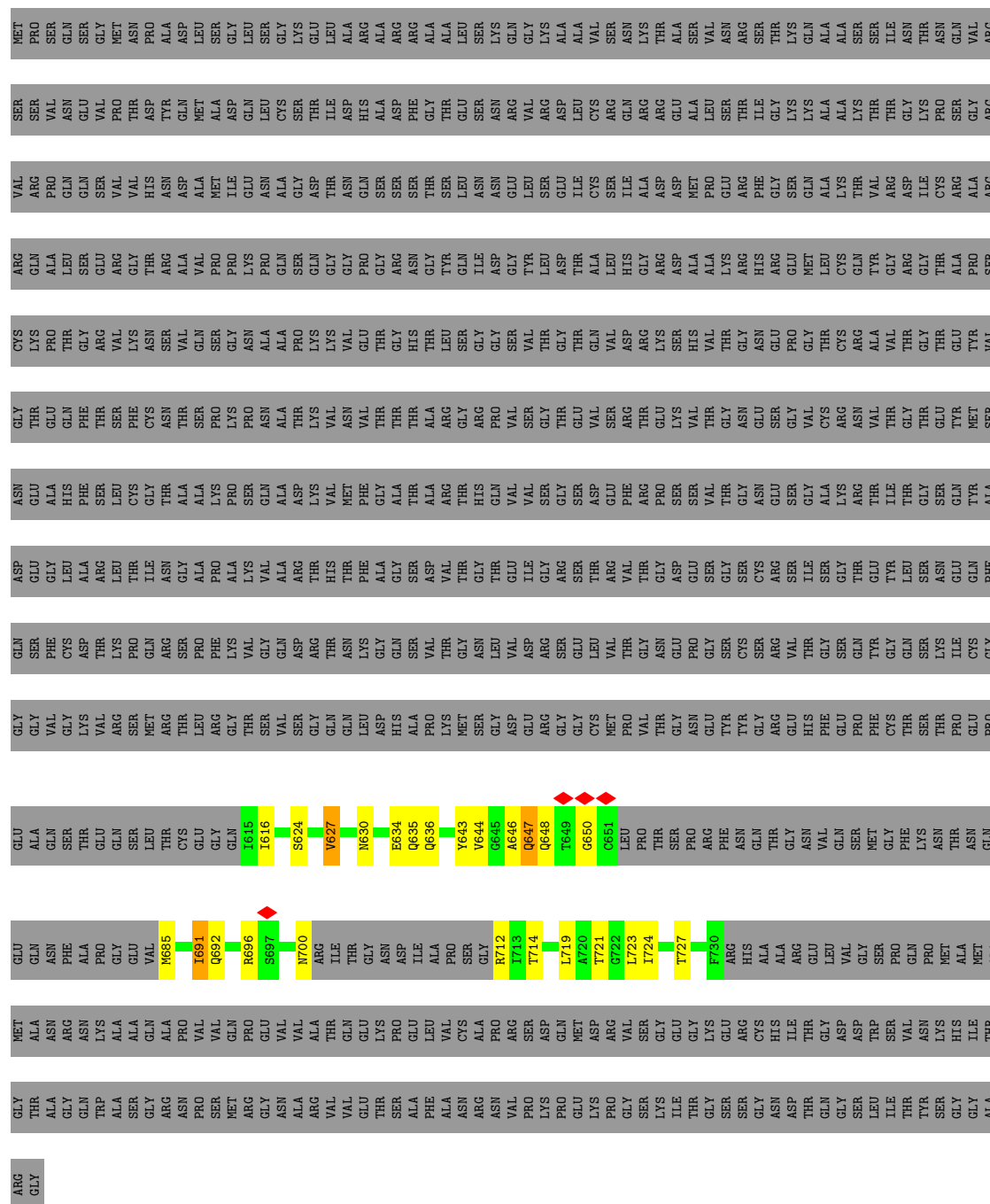
Chain Yx: 





• Molecule 3: Carboxysome assembly protein CsoS2B

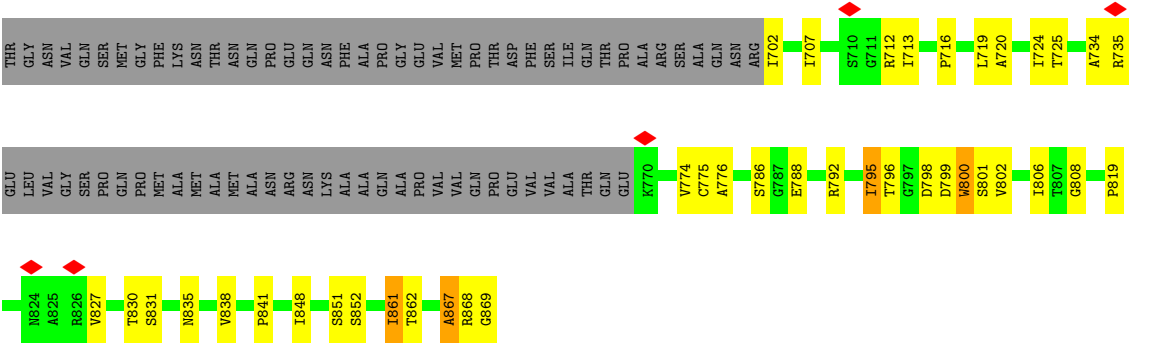
Chain Xk: 5% . 92%



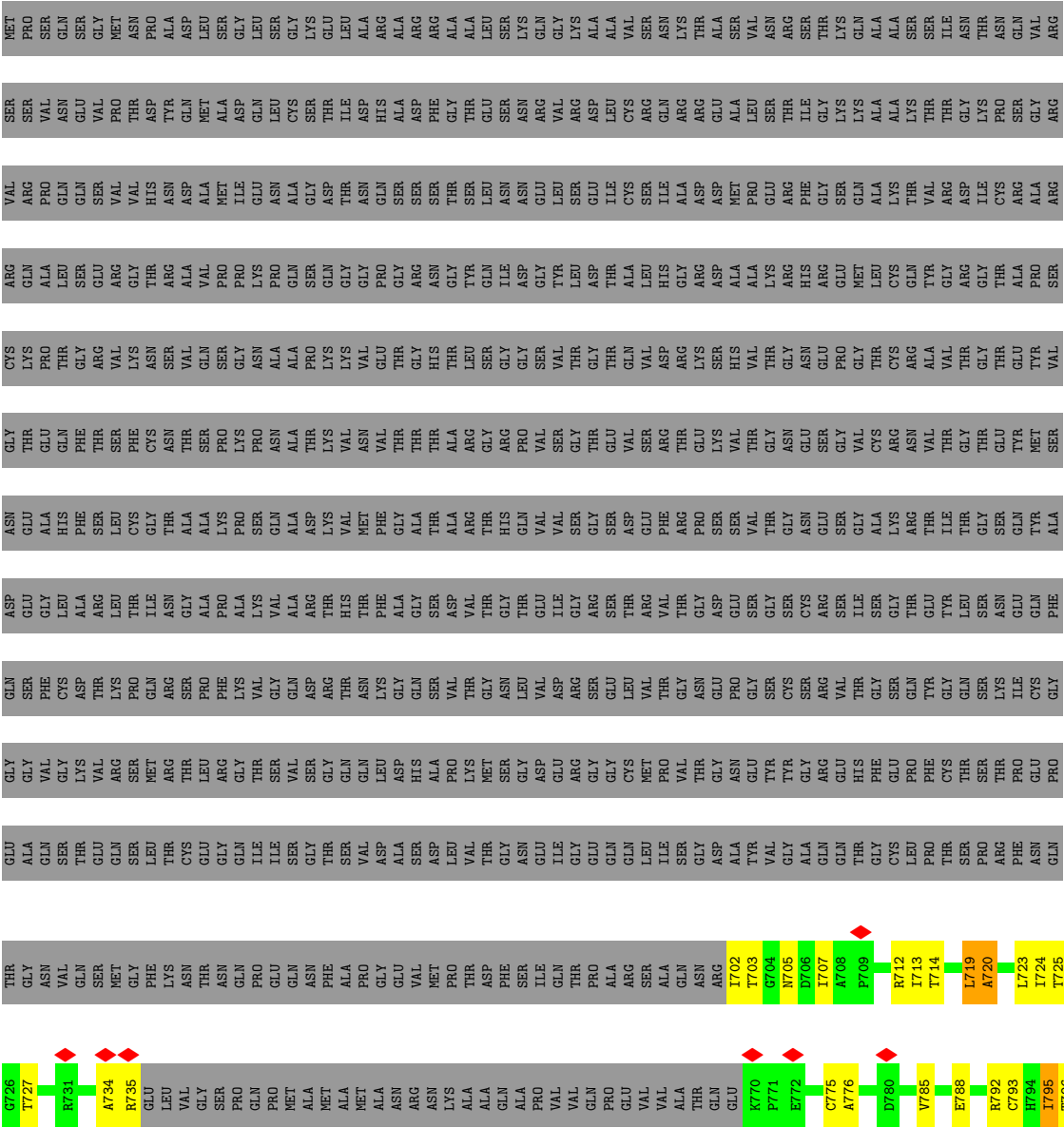
• Molecule 3: Carboxysome assembly protein CsoS2B

Chain XI: 6% .. 92%





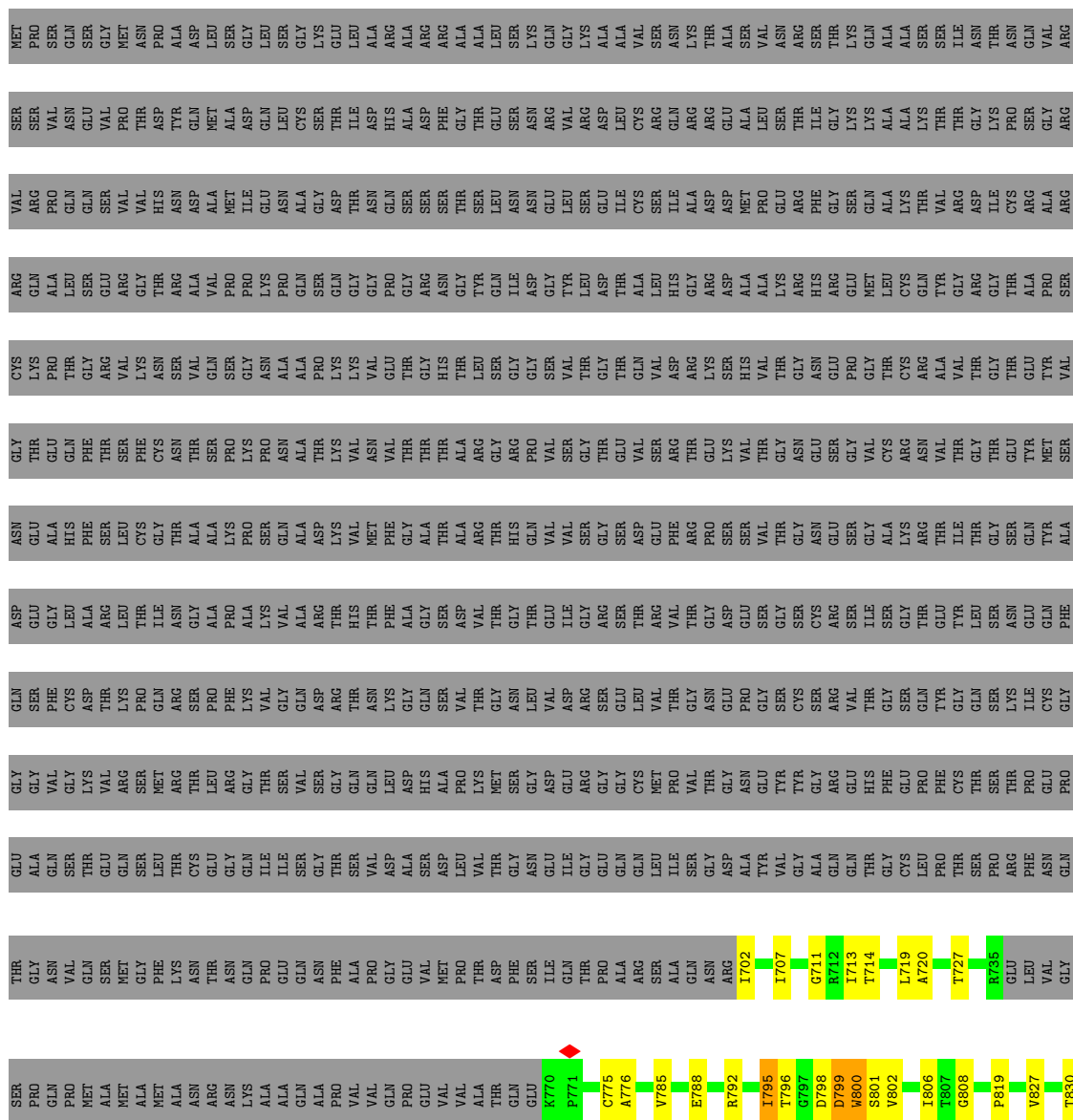
● Molecule 3: Carboxysome assembly protein CsoS2B







- Molecule 3: Carboxysome assembly protein CsoS2B



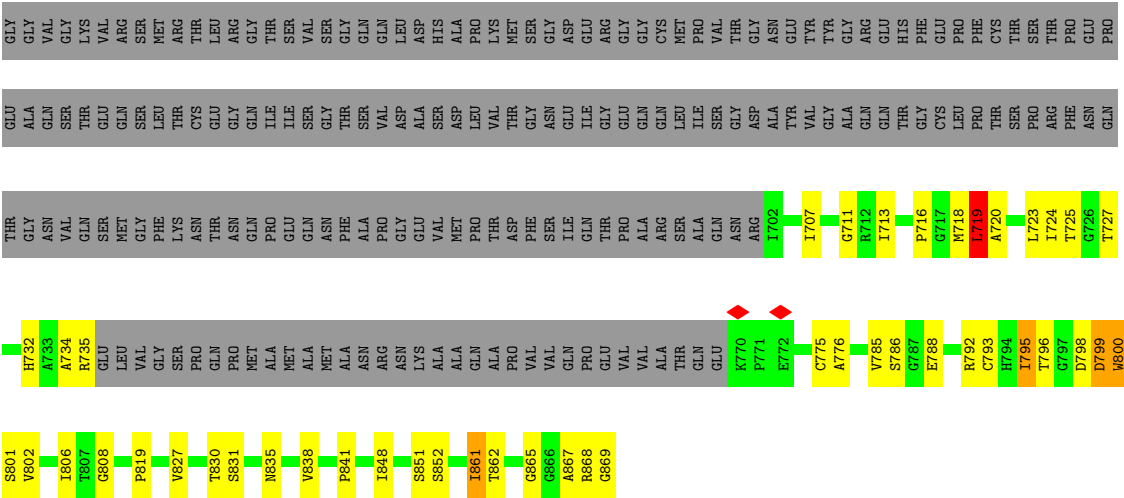



```

graph LR
    S831[S831] --- N835[N835]
    N835 --- V838[V838]
    V838 --- P841[P841]
    P841 --- I848[I848]
    I848 --- S851[S851]
    S851 --- S852[S852]
    S852 --- I861[I861]
    I861 --- T862[T862]
    T862 --- A867[A867]
    A867 --- R868[R868]
    R868 --- G869[G869]
  
```

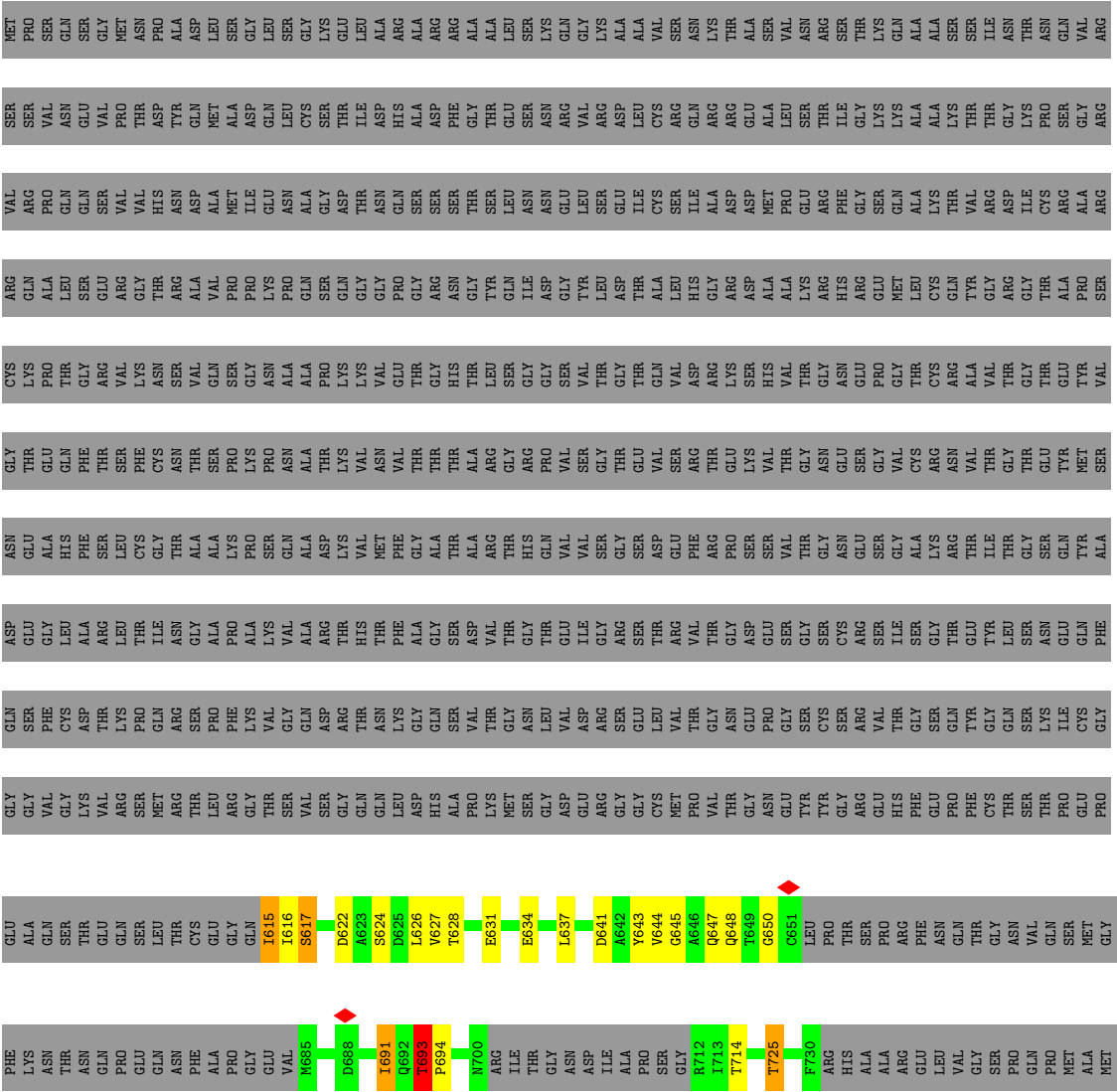
- Molecule 3: Carboxysome assembly protein CsoS2B

Chain Yj: 10% 5% 85%

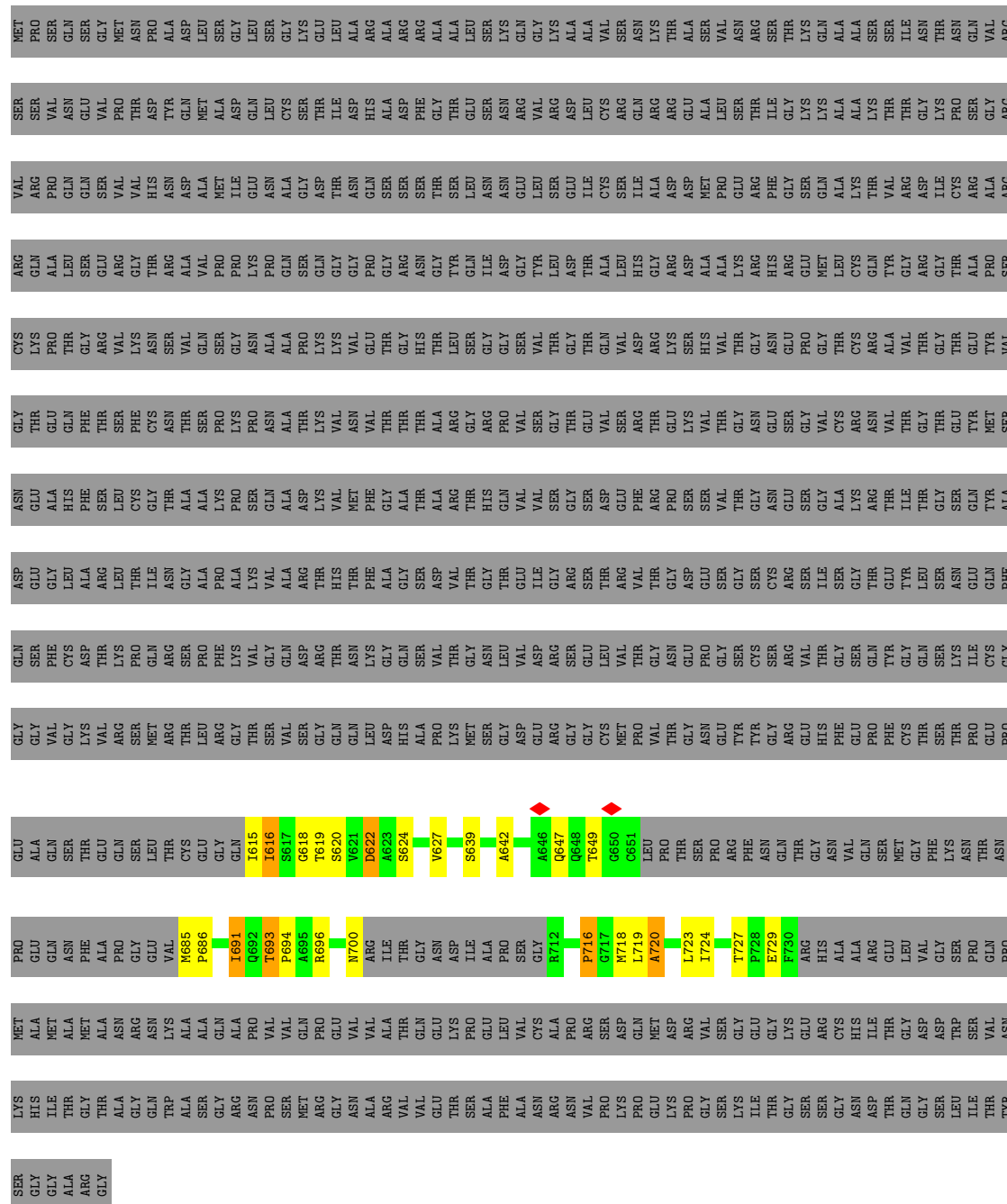


● Molecule 3: Carboxysome assembly protein CsoS2B

Chain XD: 6% 92%



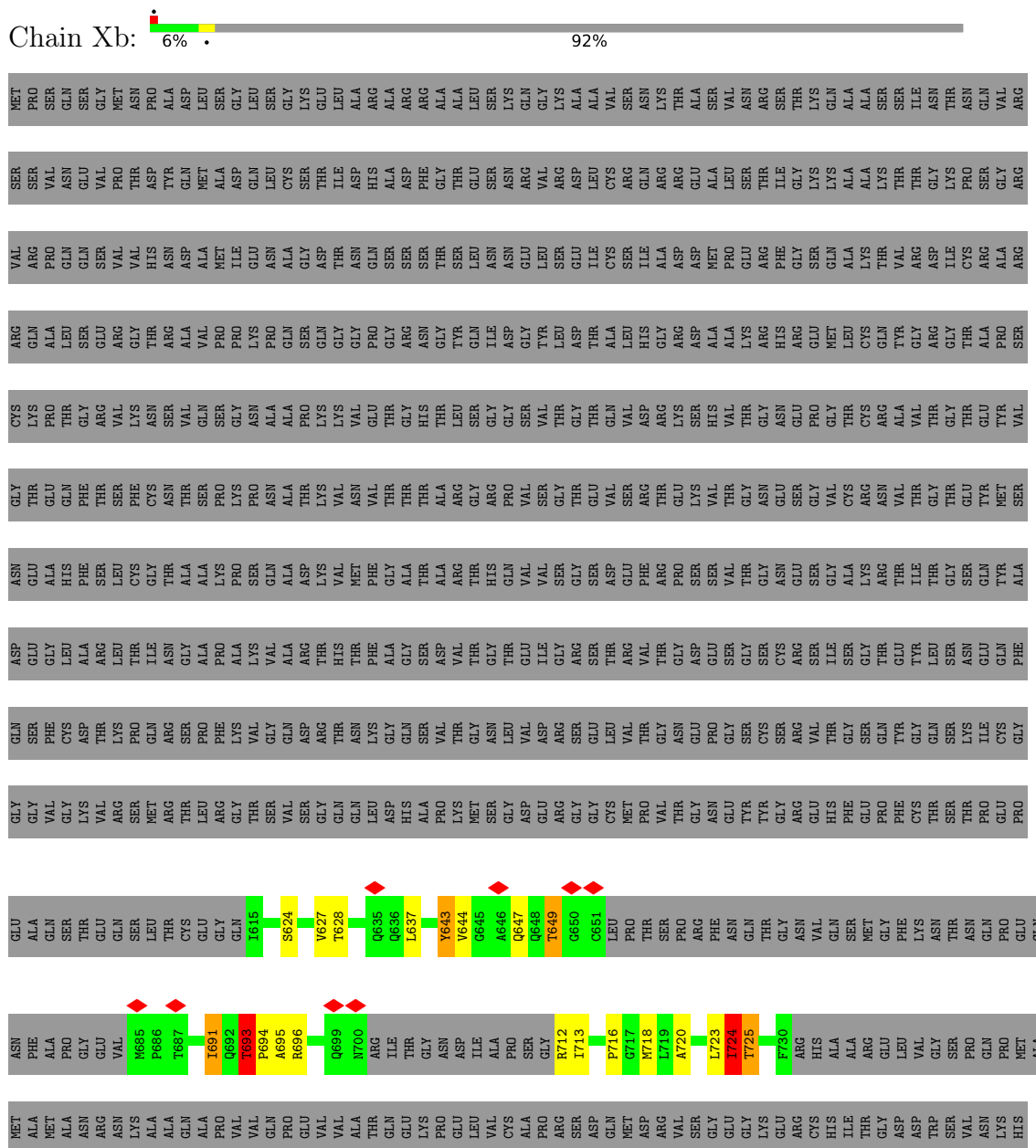
- Molecule 3: Carboxysome assembly protein CsoS2B







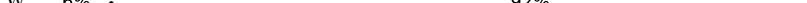
- Molecule 3: Carboxysome assembly protein CsoS2B



- Molecule 3: Carboxysome assembly protein CsoS2B



- Molecule 3: Carboxysome assembly protein CsoS2B

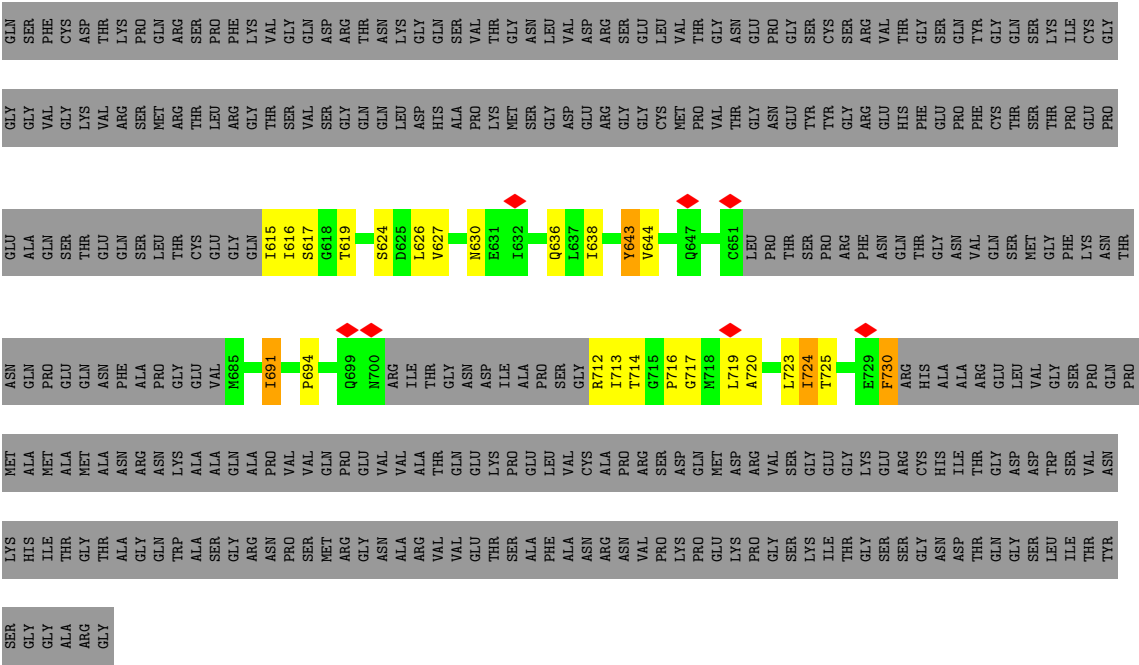
Chain Xw:  6% 92%

- Molecule 3: Carboxysome assembly protein CsoS2B

Chain Xn: 5% .. 92%

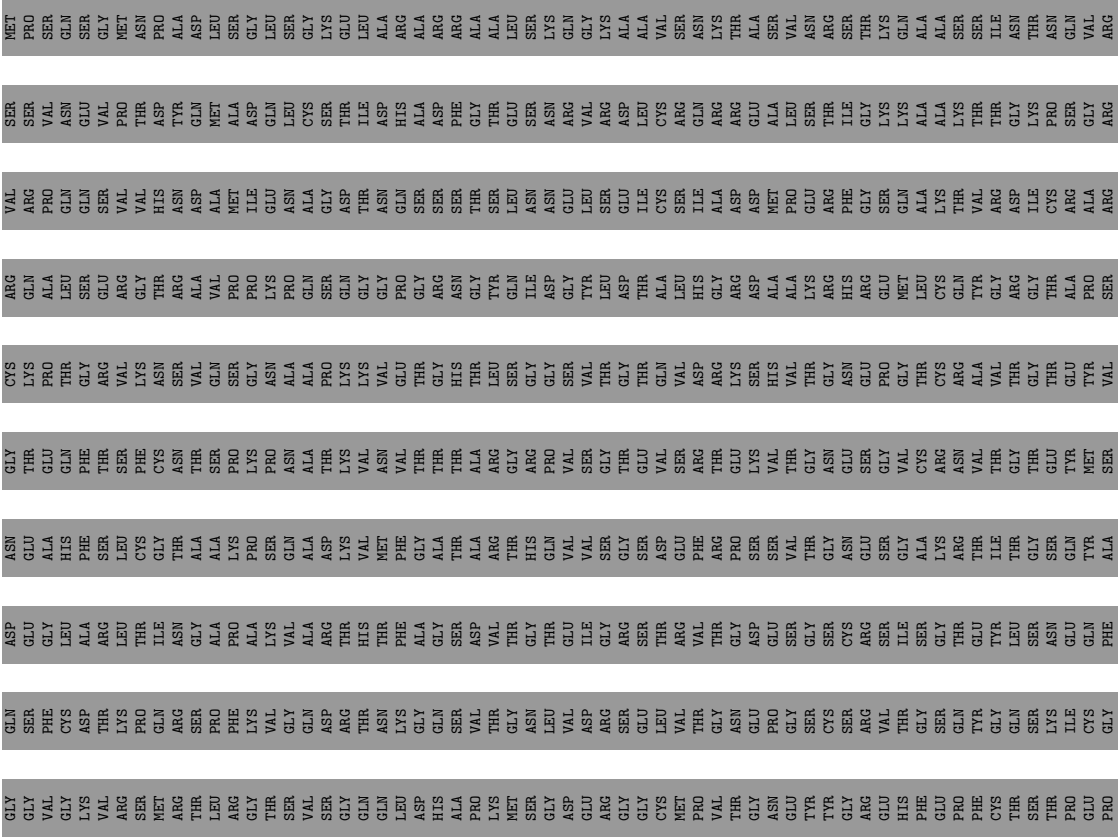
PRO	VAL	ASN	GLN	GLY	MET	ASN	PRO	ALA	ASP	SER	LEU	SER	GLY	LYS	GLU	LEU	ALA	ALA	ARG	ARG	ALA	ALA	LEU	SER	LYS	GLN	GLY	LYS	VAL	SER	ASN	LYS	THR	THR	ALA	ALA	ALA	SER	SER	THR	ILE	ASN	ASN	GLN	GLY	ARG
SER	VAL	ASN	GLU	VAL	PRO	THR	ASP	GLN	MET	ALA	GLN	LEU	CYS	THR	SER	ILE	HIS	ALA	ASP	PRO	GLY	THR	GLU	SER	ASN	ARG	VAL	ARG	ASP	LEU	CYS	ARG	GLN	ARG	ILE	THR	GLY	LYS	ALA	ALA	LYS	THR	PRO	SER	GLY	ARG

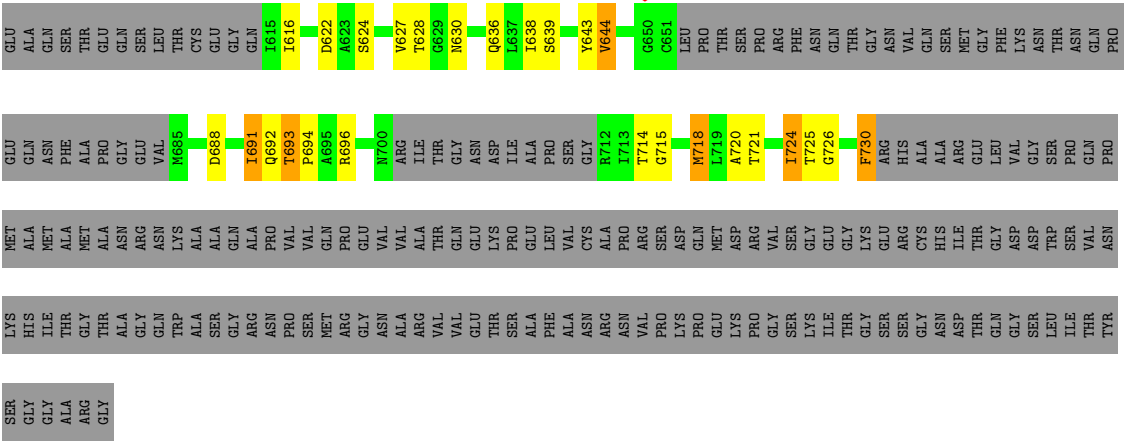




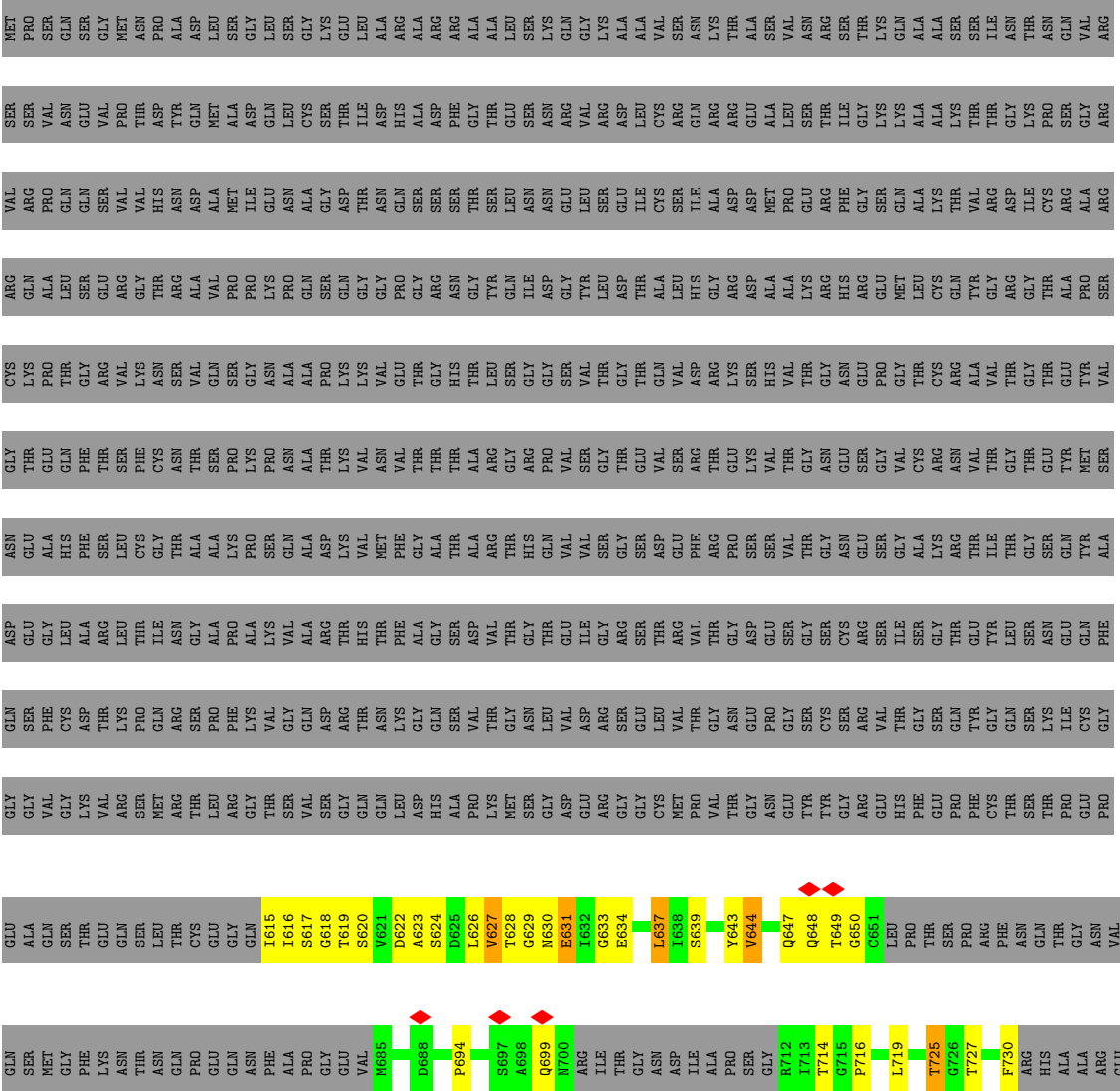
● Molecule 3: Carboxysome assembly protein CsoS2B

Chain X5: 5% .. 92%



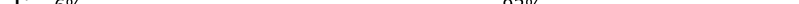


● Molecule 3: Carboxysome assembly protein CsoS2B



GLN
GLY
SER
LEU
ILE
THR
TYR
SER
GLY
GLY
ALA
ARG
GLY

- Molecule 3: Carboxysome assembly protein CsoS2B

Chain XJ:  6% 92%

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

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

GLY

Chain XM: 5% 92%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.902	Depositor
Minimum map value	-0.344	Depositor
Average map value	0.034	Depositor
Map value standard deviation	0.129	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	456.61533, 456.61533, 456.61533	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3046153, 1.3046153, 1.3046153	Depositor

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	A0	1.64	19/662 (2.9%)	1.88	12/897 (1.3%)
1	A1	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	A2	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	A3	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	A4	1.63	19/662 (2.9%)	1.88	12/897 (1.3%)
1	A5	1.63	19/662 (2.9%)	1.88	12/897 (1.3%)
1	A6	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	A7	1.62	18/662 (2.7%)	1.85	11/897 (1.2%)
1	A8	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	A9	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	AA	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	AB	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	AC	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	AD	1.64	19/662 (2.9%)	1.87	12/897 (1.3%)
1	AE	1.63	19/662 (2.9%)	1.88	12/897 (1.3%)
1	AF	1.63	19/662 (2.9%)	1.88	12/897 (1.3%)
1	AG	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	AH	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	AI	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	AJ	1.64	19/662 (2.9%)	1.88	12/897 (1.3%)
1	AK	1.63	19/662 (2.9%)	1.88	12/897 (1.3%)
1	AL	1.57	17/662 (2.6%)	1.77	9/897 (1.0%)
1	AM	1.64	19/662 (2.9%)	1.87	12/897 (1.3%)
1	AN	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	AO	1.64	19/662 (2.9%)	1.88	12/897 (1.3%)
1	AP	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	AQ	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	AR	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	AS	1.64	19/662 (2.9%)	1.87	12/897 (1.3%)
1	AT	1.63	19/662 (2.9%)	1.88	12/897 (1.3%)
1	AU	1.64	19/662 (2.9%)	1.88	12/897 (1.3%)
1	AV	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	AW	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	AX	1.58	17/662 (2.6%)	1.78	11/897 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AY	1.63	19/662 (2.9%)	1.87	12/897 (1.3%)
1	AZ	1.63	19/662 (2.9%)	1.88	12/897 (1.3%)
1	Aa	1.62	17/662 (2.6%)	1.86	11/897 (1.2%)
1	Ab	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	Ac	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	Ad	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	Ae	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	Af	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	Ag	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	Ah	1.64	19/662 (2.9%)	1.87	12/897 (1.3%)
1	Ai	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	Aj	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	Ak	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	Al	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	Am	1.59	17/662 (2.6%)	1.78	9/897 (1.0%)
1	An	1.64	19/662 (2.9%)	1.88	12/897 (1.3%)
1	Ao	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	Ap	1.59	16/662 (2.4%)	1.79	10/897 (1.1%)
1	Aq	1.62	18/662 (2.7%)	1.85	11/897 (1.2%)
1	Ar	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	As	1.63	18/662 (2.7%)	1.86	11/897 (1.2%)
1	At	1.63	19/662 (2.9%)	1.87	12/897 (1.3%)
1	Au	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	Av	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	Aw	1.64	19/662 (2.9%)	1.87	12/897 (1.3%)
1	Ax	1.62	18/662 (2.7%)	1.86	11/897 (1.2%)
1	B0	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	B1	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	B2	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	B3	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	B4	1.43	9/662 (1.4%)	1.72	8/897 (0.9%)
1	B5	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	B6	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	B7	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	B8	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	B9	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BA	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BB	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BC	1.42	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BD	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BE	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BF	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BG	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BH	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BI	1.43	9/662 (1.4%)	1.72	8/897 (0.9%)
1	BJ	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BK	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BL	1.47	8/662 (1.2%)	1.77	9/897 (1.0%)
1	BM	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BN	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BO	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BP	1.42	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BQ	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BR	1.42	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BS	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BT	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BU	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BV	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BW	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BX	1.48	8/640 (1.2%)	1.78	8/866 (0.9%)
1	BY	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	BZ	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Ba	1.45	8/662 (1.2%)	1.76	8/897 (0.9%)
1	Bb	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Bc	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Bd	1.43	8/662 (1.2%)	1.72	7/897 (0.8%)
1	Be	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Bf	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Bg	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Bh	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Bi	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Bj	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Bk	1.43	9/662 (1.4%)	1.72	8/897 (0.9%)
1	Bl	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Bm	1.45	8/662 (1.2%)	1.74	8/897 (0.9%)
1	Bn	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Bo	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Bp	1.44	8/662 (1.2%)	1.75	8/897 (0.9%)
1	Bq	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Br	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Bs	1.43	9/662 (1.4%)	1.72	8/897 (0.9%)
1	Bt	1.42	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Bu	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Bv	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)
1	Bw	1.43	9/662 (1.4%)	1.72	8/897 (0.9%)
1	Bx	1.43	8/662 (1.2%)	1.72	8/897 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C0	1.29	12/662 (1.8%)	1.46	6/897 (0.7%)
1	C1	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	C2	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	C3	1.30	12/662 (1.8%)	1.46	6/897 (0.7%)
1	C4	1.30	12/662 (1.8%)	1.46	6/897 (0.7%)
1	C5	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	C6	1.29	11/662 (1.7%)	1.46	6/897 (0.7%)
1	C7	1.30	12/662 (1.8%)	1.46	6/897 (0.7%)
1	C8	1.29	11/662 (1.7%)	1.46	6/897 (0.7%)
1	C9	1.29	12/662 (1.8%)	1.46	6/897 (0.7%)
1	CA	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	CB	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	CC	1.29	11/662 (1.7%)	1.46	6/897 (0.7%)
1	CD	1.29	11/662 (1.7%)	1.46	6/897 (0.7%)
1	CE	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	CF	1.29	12/662 (1.8%)	1.46	6/897 (0.7%)
1	CG	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	CH	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	CI	1.30	12/662 (1.8%)	1.46	6/897 (0.7%)
1	CJ	1.30	12/662 (1.8%)	1.46	6/897 (0.7%)
1	CK	1.30	12/662 (1.8%)	1.46	6/897 (0.7%)
1	CL	1.29	11/662 (1.7%)	1.46	6/897 (0.7%)
1	CM	1.29	12/662 (1.8%)	1.46	6/897 (0.7%)
1	CN	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	CO	1.30	12/662 (1.8%)	1.46	6/897 (0.7%)
1	CP	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	CQ	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	CR	1.29	11/662 (1.7%)	1.46	6/897 (0.7%)
1	CS	1.30	11/662 (1.7%)	1.45	6/897 (0.7%)
1	CT	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	CU	1.29	12/662 (1.8%)	1.46	6/897 (0.7%)
1	CV	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	CW	1.29	12/662 (1.8%)	1.46	6/897 (0.7%)
1	CX	1.30	12/662 (1.8%)	1.46	6/897 (0.7%)
1	CY	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	CZ	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	Ca	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	Cb	1.30	12/662 (1.8%)	1.46	6/897 (0.7%)
1	Cc	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	Cd	1.30	12/662 (1.8%)	1.46	6/897 (0.7%)
1	Ce	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	Cf	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	Cg	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Ch	1.30	12/662 (1.8%)	1.46	6/897 (0.7%)
1	Ci	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	Cj	1.29	11/662 (1.7%)	1.46	6/897 (0.7%)
1	Ck	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	Cl	1.29	11/662 (1.7%)	1.46	6/897 (0.7%)
1	Cm	1.30	12/662 (1.8%)	1.45	6/897 (0.7%)
1	Cn	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	Co	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	Cp	1.30	12/662 (1.8%)	1.46	6/897 (0.7%)
1	Cq	1.30	12/662 (1.8%)	1.46	6/897 (0.7%)
1	Cr	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	Cs	1.29	12/662 (1.8%)	1.46	6/897 (0.7%)
1	Ct	1.30	12/662 (1.8%)	1.46	6/897 (0.7%)
1	Cu	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	Cv	1.29	11/662 (1.7%)	1.46	6/897 (0.7%)
1	Cw	1.30	12/662 (1.8%)	1.45	6/897 (0.7%)
1	Cx	1.30	11/662 (1.7%)	1.46	6/897 (0.7%)
1	D0	1.39	11/662 (1.7%)	1.60	7/897 (0.8%)
1	D1	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	D2	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	D3	1.39	11/662 (1.7%)	1.60	7/897 (0.8%)
1	D4	0.99	0/662	1.35	11/897 (1.2%)
1	D5	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	D6	1.38	10/662 (1.5%)	1.56	8/897 (0.9%)
1	D7	1.04	0/662	1.39	8/897 (0.9%)
1	D8	1.39	11/662 (1.7%)	1.60	7/897 (0.8%)
1	D9	1.39	11/662 (1.7%)	1.60	7/897 (0.8%)
1	DA	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	DB	1.01	0/662	1.34	13/897 (1.4%)
1	DC	1.39	11/662 (1.7%)	1.60	7/897 (0.8%)
1	DD	1.07	1/662 (0.2%)	1.31	9/897 (1.0%)
1	DE	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	DF	0.96	0/640	1.28	8/866 (0.9%)
1	DG	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	DH	0.98	0/662	1.30	8/897 (0.9%)
1	DI	1.27	10/662 (1.5%)	1.47	9/897 (1.0%)
1	DJ	0.91	0/662	1.31	11/897 (1.2%)
1	DK	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	DL	1.39	11/662 (1.7%)	1.60	7/897 (0.8%)
1	DM	1.32	7/662 (1.1%)	1.57	8/897 (0.9%)
1	DN	1.39	11/662 (1.7%)	1.60	7/897 (0.8%)
1	DO	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	DP	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	DQ	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	DR	1.39	11/662 (1.7%)	1.60	7/897 (0.8%)
1	DS	1.15	3/662 (0.5%)	1.49	17/897 (1.9%)
1	DT	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	DU	1.22	6/662 (0.9%)	1.44	11/897 (1.2%)
1	DV	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	DW	1.31	10/640 (1.6%)	1.45	5/866 (0.6%)
1	DX	1.39	11/662 (1.7%)	1.60	7/897 (0.8%)
1	DY	0.96	0/662	1.38	10/897 (1.1%)
1	DZ	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	Da	1.39	11/662 (1.7%)	1.60	7/897 (0.8%)
1	Db	0.95	0/662	1.21	7/897 (0.8%)
1	Dc	1.39	11/662 (1.7%)	1.60	7/897 (0.8%)
1	Dd	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	De	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	Df	1.47	13/662 (2.0%)	1.74	15/897 (1.7%)
1	Dg	1.39	11/662 (1.7%)	1.60	7/897 (0.8%)
1	Dh	1.10	2/662 (0.3%)	1.39	16/897 (1.8%)
1	Di	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	Dj	1.29	9/640 (1.4%)	1.40	6/866 (0.7%)
1	Dk	1.39	11/662 (1.7%)	1.60	7/897 (0.8%)
1	Dl	1.32	11/640 (1.7%)	1.47	7/866 (0.8%)
1	Dm	1.39	11/662 (1.7%)	1.60	7/897 (0.8%)
1	Dn	0.93	0/662	1.28	10/897 (1.1%)
1	Do	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	Dp	1.39	11/662 (1.7%)	1.60	7/897 (0.8%)
1	Dq	1.03	1/662 (0.2%)	1.30	8/897 (0.9%)
1	Dr	1.39	11/662 (1.7%)	1.59	7/897 (0.8%)
1	Ds	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	Dt	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	Du	1.30	10/640 (1.6%)	1.46	5/866 (0.6%)
1	Dv	1.39	11/662 (1.7%)	1.60	7/897 (0.8%)
1	Dw	1.03	0/662	1.37	13/897 (1.4%)
1	Dx	1.39	11/662 (1.7%)	1.60	6/897 (0.7%)
1	E0	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	E1	1.36	7/662 (1.1%)	1.70	6/897 (0.7%)
1	E2	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	E3	1.33	7/662 (1.1%)	1.68	6/897 (0.7%)
1	E4	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	E5	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	E6	1.36	5/662 (0.8%)	1.70	6/897 (0.7%)
1	E7	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	E8	1.36	5/662 (0.8%)	1.70	6/897 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E9	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	EA	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	EB	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	EC	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	ED	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	EE	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	EF	1.00	0/640	1.25	7/866 (0.8%)
1	EG	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	EH	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	EI	1.32	6/662 (0.9%)	1.65	7/897 (0.8%)
1	EJ	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	EK	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	EL	1.01	0/662	1.27	4/897 (0.4%)
1	EM	1.36	5/662 (0.8%)	1.70	6/897 (0.7%)
1	EN	1.36	6/662 (0.9%)	1.70	5/897 (0.6%)
1	EO	1.37	6/662 (0.9%)	1.70	6/897 (0.7%)
1	EP	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	EQ	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	ER	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	ES	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	ET	1.36	5/662 (0.8%)	1.70	6/897 (0.7%)
1	EU	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	EV	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	EW	1.33	6/640 (0.9%)	1.64	6/866 (0.7%)
1	EX	1.36	6/662 (0.9%)	1.70	5/897 (0.6%)
1	EY	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	EZ	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	Ea	1.36	5/662 (0.8%)	1.70	6/897 (0.7%)
1	Eb	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	Ec	1.36	5/662 (0.8%)	1.70	6/897 (0.7%)
1	Ed	1.37	6/662 (0.9%)	1.70	6/897 (0.7%)
1	Ee	1.36	4/662 (0.6%)	1.70	6/897 (0.7%)
1	Ef	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	Eg	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	EH	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	Ei	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	Ej	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	Ek	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	El	1.31	6/640 (0.9%)	1.63	5/866 (0.6%)
1	Em	1.32	6/662 (0.9%)	1.67	5/897 (0.6%)
1	En	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	Eo	1.36	6/662 (0.9%)	1.70	5/897 (0.6%)
1	Ep	1.36	5/662 (0.8%)	1.70	6/897 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Eq	1.36	5/662 (0.8%)	1.70	6/897 (0.7%)
1	Er	1.36	5/662 (0.8%)	1.70	6/897 (0.7%)
1	Es	1.37	7/662 (1.1%)	1.70	6/897 (0.7%)
1	Et	1.36	4/662 (0.6%)	1.70	6/897 (0.7%)
1	Eu	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	Ev	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	Ew	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	Ex	1.36	6/662 (0.9%)	1.70	6/897 (0.7%)
1	F0	1.50	11/662 (1.7%)	1.75	10/897 (1.1%)
1	F1	1.50	10/662 (1.5%)	1.75	10/897 (1.1%)
1	F2	1.50	10/662 (1.5%)	1.75	9/897 (1.0%)
1	F3	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	F4	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	F5	1.50	11/662 (1.7%)	1.75	10/897 (1.1%)
1	F6	1.50	10/662 (1.5%)	1.75	10/897 (1.1%)
1	F7	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	F8	1.50	11/662 (1.7%)	1.75	10/897 (1.1%)
1	F9	1.50	11/662 (1.7%)	1.75	8/897 (0.9%)
1	FA	1.50	10/662 (1.5%)	1.75	10/897 (1.1%)
1	FB	1.49	11/662 (1.7%)	1.72	8/897 (0.9%)
1	FC	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	FD	1.50	11/662 (1.7%)	1.75	8/897 (0.9%)
1	FE	1.50	11/662 (1.7%)	1.75	10/897 (1.1%)
1	FF	1.26	6/640 (0.9%)	1.44	12/866 (1.4%)
1	FG	1.50	10/662 (1.5%)	1.75	10/897 (1.1%)
1	FH	1.48	10/662 (1.5%)	1.71	8/897 (0.9%)
1	FI	1.47	11/662 (1.7%)	1.68	9/897 (1.0%)
1	FJ	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	FK	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	FL	1.46	10/662 (1.5%)	1.73	9/897 (1.0%)
1	FM	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	FN	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	FO	1.50	11/662 (1.7%)	1.75	8/897 (0.9%)
1	FP	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	FQ	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	FR	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	FS	1.50	11/662 (1.7%)	1.75	8/897 (0.9%)
1	FT	1.50	11/662 (1.7%)	1.75	10/897 (1.1%)
1	FU	1.48	11/662 (1.7%)	1.74	12/897 (1.3%)
1	FV	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	FW	1.49	10/640 (1.6%)	1.71	9/866 (1.0%)
1	FX	1.50	10/662 (1.5%)	1.75	10/897 (1.1%)
1	FY	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	FZ	1.50	10/662 (1.5%)	1.75	10/897 (1.1%)
1	Fa	1.50	10/662 (1.5%)	1.75	9/897 (1.0%)
1	Fb	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	Fc	1.50	11/662 (1.7%)	1.75	8/897 (0.9%)
1	Fd	1.50	11/662 (1.7%)	1.75	8/897 (0.9%)
1	Fe	1.50	10/662 (1.5%)	1.75	10/897 (1.1%)
1	Ff	1.50	11/662 (1.7%)	1.75	10/897 (1.1%)
1	Fg	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	Fh	1.46	10/662 (1.5%)	1.71	9/897 (1.0%)
1	Fi	1.50	11/662 (1.7%)	1.75	10/897 (1.1%)
1	Fj	1.50	11/640 (1.7%)	1.73	10/866 (1.2%)
1	Fk	1.50	11/662 (1.7%)	1.75	10/897 (1.1%)
1	Fl	1.51	11/662 (1.7%)	1.73	8/897 (0.9%)
1	Fm	1.50	10/662 (1.5%)	1.75	9/897 (1.0%)
1	Fn	1.50	11/662 (1.7%)	1.75	8/897 (0.9%)
1	Fo	1.50	10/662 (1.5%)	1.75	10/897 (1.1%)
1	Fp	1.50	10/662 (1.5%)	1.75	9/897 (1.0%)
1	Fq	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	Fr	1.50	10/662 (1.5%)	1.75	8/897 (0.9%)
1	Fs	1.50	11/662 (1.7%)	1.75	8/897 (0.9%)
1	Ft	1.50	10/662 (1.5%)	1.75	10/897 (1.1%)
1	Fu	1.50	11/662 (1.7%)	1.75	10/897 (1.1%)
1	Fv	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	Fw	1.50	11/662 (1.7%)	1.75	8/897 (0.9%)
1	Fx	1.50	11/662 (1.7%)	1.75	9/897 (1.0%)
1	G0	0.99	0/662	1.33	5/897 (0.6%)
1	G1	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	G2	1.05	0/662	1.32	7/897 (0.8%)
1	G3	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	G4	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	G5	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	G6	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	G7	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	G8	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	G9	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GA	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GB	1.05	0/662	1.31	7/897 (0.8%)
1	GC	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GD	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GE	1.59	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GF	1.00	0/662	1.36	6/897 (0.7%)
1	GG	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GH	1.05	0/662	1.32	7/897 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	GI	1.59	15/662 (2.3%)	1.81	12/897 (1.3%)
1	GJ	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GK	1.59	14/662 (2.1%)	1.86	13/897 (1.4%)
1	GL	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GM	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GN	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GO	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GP	1.60	16/662 (2.4%)	1.86	13/897 (1.4%)
1	GQ	1.05	0/662	1.32	7/897 (0.8%)
1	GR	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GS	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GT	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GU	0.99	0/662	1.33	5/897 (0.6%)
1	GV	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GW	1.03	0/662	1.29	5/897 (0.6%)
1	GX	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GY	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	GZ	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	Ga	1.60	16/662 (2.4%)	1.86	14/897 (1.6%)
1	Gb	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	Gc	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	Gd	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	Ge	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	Gf	1.05	0/662	1.32	7/897 (0.8%)
1	Gg	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	Gh	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	Gi	1.59	15/662 (2.3%)	1.86	13/897 (1.4%)
1	Gj	1.00	0/640	1.34	5/866 (0.6%)
1	Gk	1.60	16/662 (2.4%)	1.86	13/897 (1.4%)
1	Gl	1.05	0/640	1.28	5/866 (0.6%)
1	Gm	1.60	15/662 (2.3%)	1.86	14/897 (1.6%)
1	Gn	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	Go	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	Gp	1.60	16/662 (2.4%)	1.86	13/897 (1.4%)
1	Gq	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	Gr	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	Gs	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	Gt	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	Gu	1.05	0/662	1.31	7/897 (0.8%)
1	Gv	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	Gw	1.60	15/662 (2.3%)	1.86	13/897 (1.4%)
1	Gx	1.59	15/662 (2.3%)	1.86	13/897 (1.4%)
1	H0	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	H1	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)
1	H2	1.56	15/662 (2.3%)	1.77	9/897 (1.0%)
1	H3	1.56	15/662 (2.3%)	1.77	9/897 (1.0%)
1	H4	1.57	15/662 (2.3%)	1.77	9/897 (1.0%)
1	H5	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)
1	H6	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)
1	H7	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	H8	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)
1	H9	1.56	15/662 (2.3%)	1.77	9/897 (1.0%)
1	HA	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	HB	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)
1	HC	1.56	15/662 (2.3%)	1.77	9/897 (1.0%)
1	HD	1.56	15/662 (2.3%)	1.77	9/897 (1.0%)
1	HE	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	HF	1.57	15/662 (2.3%)	1.77	9/897 (1.0%)
1	HG	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)
1	HH	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	HI	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)
1	HJ	1.56	15/662 (2.3%)	1.77	9/897 (1.0%)
1	HK	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)
1	HL	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)
1	HM	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	HN	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)
1	HO	1.57	14/662 (2.1%)	1.77	10/897 (1.1%)
1	HP	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)
1	HQ	1.57	15/662 (2.3%)	1.77	9/897 (1.0%)
1	HR	1.57	15/662 (2.3%)	1.77	9/897 (1.0%)
1	HS	1.56	15/662 (2.3%)	1.77	9/897 (1.0%)
1	HT	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	HU	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)
1	HV	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	HW	1.56	15/662 (2.3%)	1.77	9/897 (1.0%)
1	HX	1.57	15/662 (2.3%)	1.77	9/897 (1.0%)
1	HY	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)
1	HZ	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	Ha	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	Hb	1.56	15/662 (2.3%)	1.77	9/897 (1.0%)
1	Hc	1.57	15/662 (2.3%)	1.77	9/897 (1.0%)
1	Hd	1.57	15/662 (2.3%)	1.77	9/897 (1.0%)
1	He	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	Hf	1.57	15/662 (2.3%)	1.77	9/897 (1.0%)
1	Hg	1.56	15/662 (2.3%)	1.77	9/897 (1.0%)
1	Hh	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Hi	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	Hj	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)
1	Hk	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	Hl	1.56	15/662 (2.3%)	1.77	9/897 (1.0%)
1	Hm	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	Hn	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	Ho	1.56	15/662 (2.3%)	1.77	11/897 (1.2%)
1	Hp	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	Hq	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)
1	Hr	1.57	15/662 (2.3%)	1.77	9/897 (1.0%)
1	Hs	1.57	14/662 (2.1%)	1.77	11/897 (1.2%)
1	Ht	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	Hu	1.57	15/662 (2.3%)	1.77	10/897 (1.1%)
1	Hv	1.56	15/662 (2.3%)	1.77	9/897 (1.0%)
1	Hw	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	Hx	1.56	15/662 (2.3%)	1.77	10/897 (1.1%)
1	I0	1.37	11/662 (1.7%)	1.56	3/897 (0.3%)
1	I1	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)
1	I2	1.37	10/662 (1.5%)	1.56	2/897 (0.2%)
1	I3	1.37	11/662 (1.7%)	1.56	4/897 (0.4%)
1	I4	1.37	10/662 (1.5%)	1.56	2/897 (0.2%)
1	I5	1.37	10/662 (1.5%)	1.56	2/897 (0.2%)
1	I6	1.37	10/662 (1.5%)	1.56	4/897 (0.4%)
1	I7	1.37	10/662 (1.5%)	1.56	2/897 (0.2%)
1	I8	1.37	11/662 (1.7%)	1.56	4/897 (0.4%)
1	I9	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)
1	IA	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)
1	IB	1.37	11/662 (1.7%)	1.56	3/897 (0.3%)
1	IC	1.37	11/662 (1.7%)	1.56	4/897 (0.4%)
1	ID	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)
1	IE	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)
1	IF	1.37	11/662 (1.7%)	1.56	3/897 (0.3%)
1	IG	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)
1	IH	1.37	10/662 (1.5%)	1.56	2/897 (0.2%)
1	II	1.37	11/662 (1.7%)	1.56	3/897 (0.3%)
1	IJ	1.37	10/662 (1.5%)	1.56	2/897 (0.2%)
1	IK	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)
1	IL	1.37	10/662 (1.5%)	1.56	4/897 (0.4%)
1	IM	1.37	11/662 (1.7%)	1.56	2/897 (0.2%)
1	IN	1.37	11/662 (1.7%)	1.56	4/897 (0.4%)
1	IO	1.37	10/662 (1.5%)	1.56	2/897 (0.2%)
1	IP	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)
1	IQ	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	IR	1.37	11/662 (1.7%)	1.56	4/897 (0.4%)
1	IS	1.37	13/662 (2.0%)	1.56	3/897 (0.3%)
1	IT	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)
1	IU	1.37	11/662 (1.7%)	1.56	3/897 (0.3%)
1	IV	1.37	10/662 (1.5%)	1.56	4/897 (0.4%)
1	IW	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)
1	IX	1.37	11/662 (1.7%)	1.56	3/897 (0.3%)
1	IY	1.37	12/662 (1.8%)	1.56	2/897 (0.2%)
1	IZ	1.37	11/662 (1.7%)	1.56	3/897 (0.3%)
1	Ia	1.37	10/662 (1.5%)	1.56	2/897 (0.2%)
1	Ib	1.37	10/662 (1.5%)	1.56	2/897 (0.2%)
1	Ic	1.37	11/662 (1.7%)	1.56	4/897 (0.4%)
1	Id	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)
1	Ie	1.37	10/662 (1.5%)	1.56	4/897 (0.4%)
1	If	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)
1	Ig	1.37	11/662 (1.7%)	1.56	3/897 (0.3%)
1	Ih	1.37	9/662 (1.4%)	1.56	3/897 (0.3%)
1	Ii	1.37	10/662 (1.5%)	1.57	3/897 (0.3%)
1	Ij	1.37	11/662 (1.7%)	1.56	3/897 (0.3%)
1	Ik	1.37	10/662 (1.5%)	1.57	3/897 (0.3%)
1	Il	1.37	10/662 (1.5%)	1.56	2/897 (0.2%)
1	Im	1.37	10/662 (1.5%)	1.57	3/897 (0.3%)
1	In	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)
1	Io	1.38	11/662 (1.7%)	1.57	3/897 (0.3%)
1	Ip	1.37	10/662 (1.5%)	1.56	4/897 (0.4%)
1	Iq	1.37	10/662 (1.5%)	1.56	2/897 (0.2%)
1	Ir	1.37	12/662 (1.8%)	1.56	4/897 (0.4%)
1	Is	1.37	10/662 (1.5%)	1.56	2/897 (0.2%)
1	It	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)
1	Iu	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)
1	Iv	1.37	10/662 (1.5%)	1.56	3/897 (0.3%)
1	Iw	1.38	10/662 (1.5%)	1.57	3/897 (0.3%)
1	Ix	1.37	10/662 (1.5%)	1.57	3/897 (0.3%)
1	J0	1.42	6/662 (0.9%)	1.70	2/897 (0.2%)
1	J1	1.42	6/662 (0.9%)	1.70	2/897 (0.2%)
1	J2	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	J3	1.33	6/662 (0.9%)	1.59	4/897 (0.4%)
1	J4	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	J5	1.42	6/662 (0.9%)	1.70	2/897 (0.2%)
1	J6	1.35	6/662 (0.9%)	1.61	5/897 (0.6%)
1	J7	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	J8	1.42	6/662 (0.9%)	1.71	2/897 (0.2%)
1	J9	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	JA	1.42	6/662 (0.9%)	1.70	2/897 (0.2%)
1	JB	1.42	6/662 (0.9%)	1.71	3/897 (0.3%)
1	JC	1.37	6/662 (0.9%)	1.65	5/897 (0.6%)
1	JD	1.42	6/662 (0.9%)	1.71	2/897 (0.2%)
1	JE	1.42	6/662 (0.9%)	1.70	2/897 (0.2%)
1	JF	1.42	6/662 (0.9%)	1.70	2/897 (0.2%)
1	JG	1.42	6/662 (0.9%)	1.71	2/897 (0.2%)
1	JH	1.42	6/662 (0.9%)	1.71	3/897 (0.3%)
1	JI	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	JJ	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	JK	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	JL	1.42	6/662 (0.9%)	1.71	2/897 (0.2%)
1	JM	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	JN	1.42	5/662 (0.8%)	1.71	2/897 (0.2%)
1	JO	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	JP	1.42	6/662 (0.9%)	1.70	2/897 (0.2%)
1	JQ	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	JR	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	JS	1.42	6/662 (0.9%)	1.71	2/897 (0.2%)
1	JT	1.42	6/662 (0.9%)	1.70	2/897 (0.2%)
1	JU	1.45	7/662 (1.1%)	1.72	4/897 (0.4%)
1	JV	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	JW	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	JX	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	JY	1.41	6/662 (0.9%)	1.66	3/897 (0.3%)
1	JZ	1.42	6/662 (0.9%)	1.70	2/897 (0.2%)
1	Ja	1.42	6/662 (0.9%)	1.71	3/897 (0.3%)
1	Jb	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	Jc	1.42	6/662 (0.9%)	1.71	2/897 (0.2%)
1	Jd	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	Je	1.42	5/662 (0.8%)	1.70	2/897 (0.2%)
1	Jf	1.42	6/662 (0.9%)	1.71	3/897 (0.3%)
1	Jg	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	Jh	1.42	6/662 (0.9%)	1.71	3/897 (0.3%)
1	Ji	1.42	6/662 (0.9%)	1.70	2/897 (0.2%)
1	Jj	1.42	6/662 (0.9%)	1.70	2/897 (0.2%)
1	Jk	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	Jl	1.42	6/662 (0.9%)	1.71	3/897 (0.3%)
1	Jm	1.42	5/662 (0.8%)	1.71	3/897 (0.3%)
1	Jn	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	Jo	1.42	6/662 (0.9%)	1.70	2/897 (0.2%)
1	Jp	1.42	6/662 (0.9%)	1.71	3/897 (0.3%)
1	Jq	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Jr	1.42	5/662 (0.8%)	1.71	2/897 (0.2%)
1	Js	1.42	6/662 (0.9%)	1.70	3/897 (0.3%)
1	Jt	1.42	5/662 (0.8%)	1.71	2/897 (0.2%)
1	Ju	1.42	6/662 (0.9%)	1.71	3/897 (0.3%)
1	Jv	0.98	1/662 (0.2%)	1.33	5/897 (0.6%)
1	Jw	1.42	6/662 (0.9%)	1.71	2/897 (0.2%)
1	Jx	1.42	6/662 (0.9%)	1.71	2/897 (0.2%)
1	K0	1.34	9/662 (1.4%)	1.53	8/897 (0.9%)
1	K1	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	K2	1.34	9/662 (1.4%)	1.53	9/897 (1.0%)
1	K3	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	K4	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	K5	1.34	9/662 (1.4%)	1.53	9/897 (1.0%)
1	K6	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	K7	1.33	8/662 (1.2%)	1.53	9/897 (1.0%)
1	K8	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	K9	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	KA	1.33	8/662 (1.2%)	1.53	9/897 (1.0%)
1	KB	1.34	9/662 (1.4%)	1.53	9/897 (1.0%)
1	KC	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	KD	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	KE	1.33	9/662 (1.4%)	1.53	8/897 (0.9%)
1	KF	1.34	9/662 (1.4%)	1.53	8/897 (0.9%)
1	KG	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	KH	1.33	9/662 (1.4%)	1.53	9/897 (1.0%)
1	KI	1.33	8/662 (1.2%)	1.53	9/897 (1.0%)
1	KJ	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	KK	1.34	8/662 (1.2%)	1.53	8/897 (0.9%)
1	KL	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	KM	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	KN	1.34	8/662 (1.2%)	1.53	8/897 (0.9%)
1	KO	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	KP	1.33	8/662 (1.2%)	1.53	9/897 (1.0%)
1	KQ	1.34	9/662 (1.4%)	1.53	9/897 (1.0%)
1	KR	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	KS	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	KT	1.33	9/662 (1.4%)	1.53	8/897 (0.9%)
1	KU	1.34	9/662 (1.4%)	1.53	9/897 (1.0%)
1	KV	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	KW	1.34	9/662 (1.4%)	1.53	9/897 (1.0%)
1	KX	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	KY	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	KZ	1.34	9/662 (1.4%)	1.53	9/897 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Ka	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	Kb	1.34	9/662 (1.4%)	1.53	9/897 (1.0%)
1	Kc	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	Kd	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	Ke	1.33	8/662 (1.2%)	1.53	9/897 (1.0%)
1	Kf	1.34	9/662 (1.4%)	1.53	9/897 (1.0%)
1	Kg	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	Kh	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	Ki	1.33	9/662 (1.4%)	1.53	9/897 (1.0%)
1	Kj	1.34	9/662 (1.4%)	1.53	8/897 (0.9%)
1	Kk	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	Kl	1.34	9/662 (1.4%)	1.53	9/897 (1.0%)
1	Km	1.33	8/662 (1.2%)	1.53	9/897 (1.0%)
1	Kn	1.33	8/662 (1.2%)	1.53	9/897 (1.0%)
1	Ko	1.34	9/662 (1.4%)	1.53	9/897 (1.0%)
1	Kp	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	Kq	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	Kr	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	Ks	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	Kt	1.33	8/662 (1.2%)	1.53	9/897 (1.0%)
1	Ku	1.34	9/662 (1.4%)	1.53	9/897 (1.0%)
1	Kv	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	Kw	1.34	8/662 (1.2%)	1.53	9/897 (1.0%)
1	Kx	1.33	9/662 (1.4%)	1.53	8/897 (0.9%)
1	L0	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	L1	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	L2	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	L3	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	L4	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	L5	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	L6	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	L7	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	L8	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	L9	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	LA	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	LB	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	LC	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	LD	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	LE	1.23	6/662 (0.9%)	1.56	10/897 (1.1%)
1	LF	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	LG	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	LH	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	LI	1.23	6/662 (0.9%)	1.54	11/897 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	LJ	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	LK	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	LL	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	LM	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	LN	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	LO	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	LP	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	LQ	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	LR	1.23	5/662 (0.8%)	1.57	11/897 (1.2%)
1	LS	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	LT	1.23	6/662 (0.9%)	1.56	10/897 (1.1%)
1	LU	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	LV	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	LW	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	LX	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	LY	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	LZ	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	La	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	Lb	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	Lc	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	Ld	1.23	6/662 (0.9%)	1.57	10/897 (1.1%)
1	Le	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	Lf	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	Lg	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	Lh	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	Li	1.24	6/662 (0.9%)	1.56	11/897 (1.2%)
1	Lj	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	Lk	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	Ll	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	Lm	0.98	1/662 (0.2%)	1.25	10/897 (1.1%)
1	Ln	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	Lo	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	Lp	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	Lq	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	Lr	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	Ls	1.23	6/662 (0.9%)	1.57	10/897 (1.1%)
1	Lt	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	Lu	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	Lv	1.23	6/662 (0.9%)	1.57	11/897 (1.2%)
1	Lw	1.23	6/662 (0.9%)	1.56	11/897 (1.2%)
1	Lx	1.24	6/662 (0.9%)	1.56	11/897 (1.2%)
1	M0	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	M1	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	M2	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	M3	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	M4	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	M5	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	M6	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	M7	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	M8	1.07	6/662 (0.9%)	1.23	3/897 (0.3%)
1	M9	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	MA	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	MB	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	MC	1.07	6/662 (0.9%)	1.23	3/897 (0.3%)
1	MD	1.07	6/662 (0.9%)	1.21	2/897 (0.2%)
1	ME	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	MF	1.07	4/662 (0.6%)	1.24	6/897 (0.7%)
1	MG	1.07	6/662 (0.9%)	1.21	2/897 (0.2%)
1	MH	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	MI	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	MJ	1.07	6/662 (0.9%)	1.23	3/897 (0.3%)
1	MK	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	ML	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	MM	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	MN	1.07	6/662 (0.9%)	1.21	2/897 (0.2%)
1	MO	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	MP	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	MQ	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	MR	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	MS	1.07	6/662 (0.9%)	1.21	2/897 (0.2%)
1	MT	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	MU	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	MV	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	MW	1.07	6/662 (0.9%)	1.23	3/897 (0.3%)
1	MX	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	MY	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	MZ	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	Ma	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	Mb	1.07	6/662 (0.9%)	1.23	3/897 (0.3%)
1	Mc	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	Md	1.07	6/662 (0.9%)	1.23	3/897 (0.3%)
1	Me	1.07	6/662 (0.9%)	1.23	3/897 (0.3%)
1	Mf	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	Mg	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	Mh	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	Mi	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Mj	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	Mk	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	MI	1.07	6/662 (0.9%)	1.23	3/897 (0.3%)
1	Mm	1.09	5/662 (0.8%)	1.26	6/897 (0.7%)
1	Mn	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	Mo	1.08	6/662 (0.9%)	1.21	3/897 (0.3%)
1	Mp	1.08	6/662 (0.9%)	1.21	3/897 (0.3%)
1	Mq	1.07	6/662 (0.9%)	1.23	3/897 (0.3%)
1	Mr	1.07	6/662 (0.9%)	1.21	2/897 (0.2%)
1	Ms	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	Mt	1.07	6/662 (0.9%)	1.23	3/897 (0.3%)
1	Mu	1.07	6/662 (0.9%)	1.21	3/897 (0.3%)
1	Mv	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	Mw	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	Mx	1.07	6/662 (0.9%)	1.23	4/897 (0.4%)
1	N0	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	N1	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	N2	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	N3	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	N4	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	N5	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	N6	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	N7	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	N8	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	N9	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	NA	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	NB	1.35	6/662 (0.9%)	1.67	6/897 (0.7%)
1	NC	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	ND	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	NE	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	NF	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	NG	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	NH	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	NI	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	NJ	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	NK	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	NL	1.36	5/662 (0.8%)	1.65	6/897 (0.7%)
1	NM	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	NN	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	NO	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	NP	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	NQ	1.35	6/662 (0.9%)	1.67	6/897 (0.7%)
1	NR	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	NS	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	NT	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	NU	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	NV	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	NW	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	NX	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	NY	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	NZ	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	Na	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	Nb	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	Nc	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	Nd	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	Ne	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	Nf	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	Ng	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	Nh	1.35	5/662 (0.8%)	1.67	7/897 (0.8%)
1	Ni	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	Nj	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	Nk	1.35	5/662 (0.8%)	1.67	7/897 (0.8%)
1	Nl	1.35	4/662 (0.6%)	1.67	7/897 (0.8%)
1	Nm	1.35	4/662 (0.6%)	1.67	7/897 (0.8%)
1	Nn	1.35	4/662 (0.6%)	1.66	6/897 (0.7%)
1	No	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	Np	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	Nq	1.35	5/662 (0.8%)	1.67	7/897 (0.8%)
1	Nr	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	Ns	1.35	5/662 (0.8%)	1.67	7/897 (0.8%)
1	Nt	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	Nu	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	Nv	1.35	6/662 (0.9%)	1.67	7/897 (0.8%)
1	Nw	1.35	5/662 (0.8%)	1.67	6/897 (0.7%)
1	Nx	1.35	4/662 (0.6%)	1.67	6/897 (0.7%)
1	O0	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	O1	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	O2	1.17	5/662 (0.8%)	1.41	7/897 (0.8%)
1	O3	1.16	5/662 (0.8%)	1.40	7/897 (0.8%)
1	O4	1.17	5/662 (0.8%)	1.41	7/897 (0.8%)
1	O5	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	O6	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	O7	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	O8	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	O9	1.17	5/662 (0.8%)	1.41	7/897 (0.8%)
1	OA	1.16	5/662 (0.8%)	1.40	7/897 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	OB	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	OC	1.16	6/662 (0.9%)	1.40	7/897 (0.8%)
1	OD	1.17	5/662 (0.8%)	1.41	7/897 (0.8%)
1	OE	1.17	6/662 (0.9%)	1.40	7/897 (0.8%)
1	OF	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	OG	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	OH	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	OI	1.16	5/662 (0.8%)	1.40	7/897 (0.8%)
1	OJ	1.17	5/662 (0.8%)	1.41	7/897 (0.8%)
1	OK	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	OL	1.16	5/662 (0.8%)	1.40	7/897 (0.8%)
1	OM	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	ON	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	OO	1.17	5/662 (0.8%)	1.41	7/897 (0.8%)
1	OP	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	OQ	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	OR	1.16	5/662 (0.8%)	1.41	7/897 (0.8%)
1	OS	1.17	5/662 (0.8%)	1.41	7/897 (0.8%)
1	OT	1.17	6/662 (0.9%)	1.40	7/897 (0.8%)
1	OU	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	OV	1.16	5/662 (0.8%)	1.40	7/897 (0.8%)
1	OW	1.17	5/662 (0.8%)	1.41	7/897 (0.8%)
1	OX	1.17	5/662 (0.8%)	1.41	7/897 (0.8%)
1	OY	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	OZ	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	Oa	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	Ob	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	Oc	1.16	5/662 (0.8%)	1.40	7/897 (0.8%)
1	Od	1.17	5/662 (0.8%)	1.41	7/897 (0.8%)
1	Oe	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	Of	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	Og	1.16	6/662 (0.9%)	1.41	7/897 (0.8%)
1	Oh	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	Oi	1.17	5/662 (0.8%)	1.41	7/897 (0.8%)
1	Oj	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	Ok	1.16	5/662 (0.8%)	1.40	7/897 (0.8%)
1	Ol	1.17	5/662 (0.8%)	1.41	7/897 (0.8%)
1	Om	1.17	5/662 (0.8%)	1.41	7/897 (0.8%)
1	On	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	Oo	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	Op	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	Oq	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	Or	1.16	5/662 (0.8%)	1.40	7/897 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Os	1.17	5/662 (0.8%)	1.41	7/897 (0.8%)
1	Ot	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	Ou	1.17	5/662 (0.8%)	1.41	7/897 (0.8%)
1	Ov	1.17	6/662 (0.9%)	1.41	7/897 (0.8%)
1	Ow	1.17	5/662 (0.8%)	1.40	7/897 (0.8%)
1	Ox	1.17	5/662 (0.8%)	1.41	7/897 (0.8%)
2	P0	1.05	2/620 (0.3%)	1.52	8/843 (0.9%)
2	P1	1.02	2/620 (0.3%)	1.45	6/843 (0.7%)
2	P2	1.04	2/620 (0.3%)	1.46	6/843 (0.7%)
2	P3	1.05	2/620 (0.3%)	1.44	5/843 (0.6%)
2	P4	1.03	2/620 (0.3%)	1.46	6/843 (0.7%)
2	P5	1.04	2/620 (0.3%)	1.45	6/843 (0.7%)
2	P6	1.02	2/620 (0.3%)	1.47	6/843 (0.7%)
2	P7	1.02	2/620 (0.3%)	1.45	5/843 (0.6%)
2	P8	1.02	2/620 (0.3%)	1.51	8/843 (0.9%)
2	P9	1.01	2/620 (0.3%)	1.55	9/843 (1.1%)
2	PA	1.05	2/620 (0.3%)	1.46	7/843 (0.8%)
2	PB	1.01	2/620 (0.3%)	1.49	6/843 (0.7%)
2	PC	1.03	2/620 (0.3%)	1.46	7/843 (0.8%)
2	PD	0.74	0/620	1.21	5/843 (0.6%)
2	PE	1.05	2/620 (0.3%)	1.48	7/843 (0.8%)
2	PF	1.05	2/620 (0.3%)	1.52	8/843 (0.9%)
2	PG	1.02	2/620 (0.3%)	1.44	6/843 (0.7%)
2	PH	1.03	2/620 (0.3%)	1.46	6/843 (0.7%)
2	PI	1.05	2/620 (0.3%)	1.44	5/843 (0.6%)
2	PJ	1.03	2/620 (0.3%)	1.46	5/843 (0.6%)
2	PK	1.04	2/620 (0.3%)	1.45	6/843 (0.7%)
2	PL	1.02	2/620 (0.3%)	1.47	6/843 (0.7%)
2	PM	1.02	2/620 (0.3%)	1.45	5/843 (0.6%)
2	PN	1.02	2/620 (0.3%)	1.51	8/843 (0.9%)
2	PO	1.01	2/620 (0.3%)	1.55	9/843 (1.1%)
2	PP	1.05	2/620 (0.3%)	1.46	6/843 (0.7%)
2	PQ	1.01	2/620 (0.3%)	1.48	6/843 (0.7%)
2	PR	1.02	2/620 (0.3%)	1.46	7/843 (0.8%)
2	PS	0.74	0/620	1.21	5/843 (0.6%)
2	PT	1.05	2/620 (0.3%)	1.48	7/843 (0.8%)
2	PU	1.05	2/620 (0.3%)	1.52	8/843 (0.9%)
2	PV	1.03	2/620 (0.3%)	1.45	6/843 (0.7%)
2	PW	1.03	2/620 (0.3%)	1.46	6/843 (0.7%)
2	PX	1.05	2/620 (0.3%)	1.43	5/843 (0.6%)
2	PY	1.03	2/620 (0.3%)	1.46	5/843 (0.6%)
2	PZ	1.04	2/620 (0.3%)	1.45	6/843 (0.7%)
2	Pa	1.02	2/620 (0.3%)	1.47	6/843 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Pb	1.02	2/620 (0.3%)	1.45	5/843 (0.6%)
2	Pc	1.01	2/620 (0.3%)	1.51	8/843 (0.9%)
2	Pd	1.01	2/620 (0.3%)	1.55	10/843 (1.2%)
2	Pe	1.05	2/620 (0.3%)	1.46	7/843 (0.8%)
2	Pf	1.01	2/620 (0.3%)	1.49	6/843 (0.7%)
2	Pg	1.03	2/620 (0.3%)	1.46	7/843 (0.8%)
2	Ph	0.74	0/620	1.21	4/843 (0.5%)
2	Pi	1.05	2/620 (0.3%)	1.48	7/843 (0.8%)
2	Pj	1.05	2/620 (0.3%)	1.52	8/843 (0.9%)
2	Pk	1.03	2/620 (0.3%)	1.45	6/843 (0.7%)
2	Pl	1.04	2/620 (0.3%)	1.46	6/843 (0.7%)
2	Pm	1.05	2/620 (0.3%)	1.44	5/843 (0.6%)
2	Pn	1.03	2/620 (0.3%)	1.46	5/843 (0.6%)
2	Po	1.04	2/620 (0.3%)	1.45	6/843 (0.7%)
2	Pp	1.02	2/620 (0.3%)	1.47	6/843 (0.7%)
2	Pq	1.02	2/620 (0.3%)	1.45	5/843 (0.6%)
2	Pr	1.01	2/620 (0.3%)	1.51	8/843 (0.9%)
2	Ps	1.01	2/620 (0.3%)	1.55	9/843 (1.1%)
2	Pt	1.05	2/620 (0.3%)	1.46	7/843 (0.8%)
2	Pu	1.01	2/620 (0.3%)	1.49	6/843 (0.7%)
2	Pv	1.03	2/620 (0.3%)	1.46	7/843 (0.8%)
2	Pw	0.74	0/620	1.21	4/843 (0.5%)
2	Px	1.05	2/620 (0.3%)	1.48	7/843 (0.8%)
3	X0	0.65	0/517	1.16	6/700 (0.9%)
3	X1	0.66	0/517	1.21	7/700 (1.0%)
3	X2	0.63	0/517	1.22	7/700 (1.0%)
3	X3	0.65	0/517	1.22	6/700 (0.9%)
3	X4	0.62	0/517	1.15	4/700 (0.6%)
3	X5	0.64	0/517	1.12	5/700 (0.7%)
3	X6	0.60	0/517	1.27	7/700 (1.0%)
3	X7	0.62	0/517	1.11	4/700 (0.6%)
3	X8	0.64	0/517	1.26	5/700 (0.7%)
3	X9	0.66	0/517	1.24	7/700 (1.0%)
3	XA	0.63	0/517	1.09	4/700 (0.6%)
3	XB	0.89	0/517	1.47	8/700 (1.1%)
3	XC	0.86	0/517	1.49	6/700 (0.9%)
3	XD	0.84	0/517	1.49	8/700 (1.1%)
3	XE	0.92	0/517	1.61	9/700 (1.3%)
3	XF	0.65	0/517	1.16	6/700 (0.9%)
3	XG	0.66	0/517	1.21	7/700 (1.0%)
3	XH	0.63	0/517	1.22	7/700 (1.0%)
3	XI	0.76	1/517 (0.2%)	1.33	11/700 (1.6%)
3	XJ	0.61	0/517	1.13	4/700 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	XK	0.65	0/517	1.09	5/700 (0.7%)
3	XL	0.60	0/517	1.27	7/700 (1.0%)
3	XM	0.60	0/517	1.19	6/700 (0.9%)
3	XN	0.63	0/517	1.22	6/700 (0.9%)
3	XO	0.66	0/517	1.24	6/700 (0.9%)
3	XP	0.63	0/517	1.09	4/700 (0.6%)
3	XQ	0.88	0/517	1.47	8/700 (1.1%)
3	XR	0.86	0/517	1.49	6/700 (0.9%)
3	XS	0.84	0/517	1.51	6/700 (0.9%)
3	XT	0.92	0/517	1.62	9/700 (1.3%)
3	XU	0.65	0/517	1.16	6/700 (0.9%)
3	XV	0.66	0/517	1.21	7/700 (1.0%)
3	XW	0.63	0/517	1.22	7/700 (1.0%)
3	XX	0.64	0/517	1.32	7/700 (1.0%)
3	XY	0.61	0/517	1.20	5/700 (0.7%)
3	XZ	0.65	0/517	1.09	5/700 (0.7%)
3	Xa	0.58	0/517	1.27	7/700 (1.0%)
3	Xb	0.62	0/517	1.12	4/700 (0.6%)
3	Xc	0.64	0/517	1.28	6/700 (0.9%)
3	Xd	0.66	0/517	1.24	6/700 (0.9%)
3	Xe	0.63	0/517	1.09	4/700 (0.6%)
3	Xf	0.88	0/517	1.47	8/700 (1.1%)
3	Xg	0.86	0/517	1.49	6/700 (0.9%)
3	Xh	0.84	0/517	1.47	8/700 (1.1%)
3	Xi	0.92	0/517	1.62	9/700 (1.3%)
3	Xj	0.65	0/517	1.16	6/700 (0.9%)
3	Xk	0.66	0/517	1.21	7/700 (1.0%)
3	Xl	0.63	0/517	1.22	7/700 (1.0%)
3	Xm	0.70	1/517 (0.2%)	1.31	9/700 (1.3%)
3	Xn	0.64	0/517	1.19	7/700 (1.0%)
3	Xo	0.65	0/517	1.09	5/700 (0.7%)
3	Xp	0.60	0/517	1.27	7/700 (1.0%)
3	Xq	0.65	0/517	1.17	5/700 (0.7%)
3	Xr	0.65	0/517	1.20	5/700 (0.7%)
3	Xs	0.67	0/517	1.24	6/700 (0.9%)
3	Xt	0.63	0/517	1.09	4/700 (0.6%)
3	Xu	0.89	0/517	1.47	8/700 (1.1%)
3	Xv	0.86	0/517	1.49	6/700 (0.9%)
3	Xw	0.86	0/517	1.49	8/700 (1.1%)
3	Xx	0.92	0/517	1.62	9/700 (1.3%)
3	Y0	1.17	4/997 (0.4%)	1.60	12/1345 (0.9%)
3	Y1	1.15	5/997 (0.5%)	1.61	14/1345 (1.0%)
3	Y2	1.17	5/997 (0.5%)	1.59	10/1345 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	Y3	1.16	5/997 (0.5%)	1.68	15/1345 (1.1%)
3	Y4	1.17	5/997 (0.5%)	1.60	14/1345 (1.0%)
3	Y5	1.17	4/997 (0.4%)	1.61	12/1345 (0.9%)
3	Y6	1.16	5/997 (0.5%)	1.60	13/1345 (1.0%)
3	Y7	1.16	5/997 (0.5%)	1.58	12/1345 (0.9%)
3	Y8	1.16	5/997 (0.5%)	1.58	12/1345 (0.9%)
3	Y9	1.15	5/997 (0.5%)	1.59	13/1345 (1.0%)
3	YA	1.16	5/997 (0.5%)	1.62	13/1345 (1.0%)
3	YB	1.16	5/997 (0.5%)	1.58	11/1345 (0.8%)
3	YC	1.16	5/997 (0.5%)	1.59	12/1345 (0.9%)
3	YD	1.16	5/997 (0.5%)	1.57	12/1345 (0.9%)
3	YE	1.16	4/997 (0.4%)	1.59	12/1345 (0.9%)
3	YF	1.17	4/997 (0.4%)	1.60	12/1345 (0.9%)
3	YG	1.15	5/997 (0.5%)	1.60	14/1345 (1.0%)
3	YH	1.17	5/997 (0.5%)	1.59	10/1345 (0.7%)
3	YI	1.16	5/997 (0.5%)	1.60	12/1345 (0.9%)
3	YJ	1.17	5/997 (0.5%)	1.60	14/1345 (1.0%)
3	YK	1.17	4/997 (0.4%)	1.61	12/1345 (0.9%)
3	YL	1.16	5/997 (0.5%)	1.60	13/1345 (1.0%)
3	YM	1.16	5/997 (0.5%)	1.58	12/1345 (0.9%)
3	YN	1.16	5/997 (0.5%)	1.58	12/1345 (0.9%)
3	YO	1.15	5/997 (0.5%)	1.59	13/1345 (1.0%)
3	YP	1.16	5/997 (0.5%)	1.62	13/1345 (1.0%)
3	YQ	1.16	5/997 (0.5%)	1.58	11/1345 (0.8%)
3	YR	1.16	5/997 (0.5%)	1.59	12/1345 (0.9%)
3	YS	1.16	5/997 (0.5%)	1.57	12/1345 (0.9%)
3	YT	1.16	4/997 (0.4%)	1.58	12/1345 (0.9%)
3	YU	1.17	4/997 (0.4%)	1.60	12/1345 (0.9%)
3	YV	1.15	5/997 (0.5%)	1.60	14/1345 (1.0%)
3	YW	1.17	5/997 (0.5%)	1.59	10/1345 (0.7%)
3	YX	1.15	5/997 (0.5%)	1.59	12/1345 (0.9%)
3	YY	1.17	5/997 (0.5%)	1.60	14/1345 (1.0%)
3	YZ	1.17	4/997 (0.4%)	1.61	12/1345 (0.9%)
3	Ya	1.16	5/997 (0.5%)	1.60	13/1345 (1.0%)
3	Yb	1.16	5/997 (0.5%)	1.58	12/1345 (0.9%)
3	Yc	1.16	5/997 (0.5%)	1.58	12/1345 (0.9%)
3	Yd	1.15	5/997 (0.5%)	1.60	13/1345 (1.0%)
3	Ye	1.16	5/997 (0.5%)	1.62	13/1345 (1.0%)
3	Yf	1.16	5/997 (0.5%)	1.58	11/1345 (0.8%)
3	Yg	1.16	5/997 (0.5%)	1.59	12/1345 (0.9%)
3	Yh	1.16	5/997 (0.5%)	1.57	12/1345 (0.9%)
3	Yi	1.16	4/997 (0.4%)	1.59	12/1345 (0.9%)
3	Yj	1.17	4/997 (0.4%)	1.60	12/1345 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	Yk	1.15	5/997 (0.5%)	1.61	14/1345 (1.0%)
3	Yl	1.17	5/997 (0.5%)	1.59	10/1345 (0.7%)
3	Ym	1.16	5/997 (0.5%)	1.59	12/1345 (0.9%)
3	Yn	1.17	5/997 (0.5%)	1.60	14/1345 (1.0%)
3	Yo	1.17	4/997 (0.4%)	1.61	12/1345 (0.9%)
3	Yp	1.16	5/997 (0.5%)	1.60	13/1345 (1.0%)
3	Yq	1.16	5/997 (0.5%)	1.58	12/1345 (0.9%)
3	Yr	1.17	5/997 (0.5%)	1.58	12/1345 (0.9%)
3	Ys	1.15	5/997 (0.5%)	1.60	13/1345 (1.0%)
3	Yt	1.16	5/997 (0.5%)	1.61	13/1345 (1.0%)
3	Yu	1.16	5/997 (0.5%)	1.58	11/1345 (0.8%)
3	Yv	1.16	5/997 (0.5%)	1.59	12/1345 (0.9%)
3	Yw	1.16	5/997 (0.5%)	1.57	12/1345 (0.9%)
3	Yx	1.16	4/997 (0.4%)	1.59	12/1345 (0.9%)
All	All	1.32	8529/723532 (1.2%)	1.60	8186/980146 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P0	0	1
2	PF	0	1
2	PU	0	1
2	Pj	0	1
All	All	0	4

The worst 5 of 8529 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Di	93	PRO	C-O	-9.91	1.16	1.24
1	DE	93	PRO	C-O	-9.91	1.16	1.24
1	DK	93	PRO	C-O	-9.91	1.16	1.24
1	DT	93	PRO	C-O	-9.91	1.16	1.24
1	DA	93	PRO	C-O	-9.90	1.16	1.24

The worst 5 of 8186 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y3	707	ILE	N-CA-C	-14.32	98.56	112.17
1	Df	59	ALA	N-CA-C	-14.19	95.81	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Jv	43	GLY	N-CA-C	-13.77	97.43	115.47
2	Ps	55	SER	N-CA-C	13.75	125.78	111.07
2	P9	55	SER	N-CA-C	13.72	125.75	111.07

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P0	68	PRO	Mainchain
2	PF	68	PRO	Mainchain
2	PU	68	PRO	Mainchain
2	Pj	68	PRO	Mainchain

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	A0	656	0	677	15	0
1	A1	656	0	677	14	0
1	A2	656	0	677	16	0
1	A3	656	0	677	17	0
1	A4	656	0	677	14	0
1	A5	656	0	677	15	0
1	A6	656	0	677	14	0
1	A7	656	0	677	15	0
1	A8	656	0	677	16	0
1	A9	656	0	677	15	0
1	AA	656	0	677	14	0
1	AB	656	0	677	16	0
1	AC	656	0	677	18	0
1	AD	656	0	677	17	0
1	AE	656	0	677	15	0
1	AF	656	0	677	15	0
1	AG	656	0	677	14	0
1	AH	656	0	677	16	0
1	AI	656	0	677	17	0
1	AJ	656	0	677	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AK	656	0	677	15	0
1	AL	656	0	677	15	0
1	AM	656	0	677	15	0
1	AN	656	0	677	16	0
1	AO	656	0	677	15	0
1	AP	656	0	677	15	0
1	AQ	656	0	677	16	0
1	AR	656	0	677	16	0
1	AS	656	0	677	14	0
1	AT	656	0	677	15	0
1	AU	656	0	677	16	0
1	AV	656	0	677	15	0
1	AW	656	0	677	16	0
1	AX	656	0	677	17	0
1	AY	656	0	677	15	0
1	AZ	656	0	677	15	0
1	Aa	656	0	677	14	0
1	Ab	656	0	677	15	0
1	Ac	656	0	677	17	0
1	Ad	656	0	677	15	0
1	Ae	656	0	677	14	0
1	Af	656	0	677	16	0
1	Ag	656	0	677	17	0
1	Ah	656	0	677	15	0
1	Ai	656	0	677	15	0
1	Aj	656	0	677	15	0
1	Ak	656	0	677	14	0
1	Al	656	0	677	16	0
1	Am	656	0	677	19	0
1	An	656	0	677	14	0
1	Ao	656	0	677	15	0
1	Ap	656	0	677	20	0
1	Aq	656	0	677	15	0
1	Ar	656	0	677	15	0
1	As	656	0	677	15	0
1	At	656	0	677	14	0
1	Au	656	0	677	17	0
1	Av	656	0	677	15	0
1	Aw	656	0	677	15	0
1	Ax	656	0	677	15	0
1	B0	656	0	677	22	0
1	B1	656	0	677	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B2	656	0	677	22	0
1	B3	656	0	677	24	0
1	B4	656	0	677	24	0
1	B5	656	0	677	22	0
1	B6	656	0	677	23	0
1	B7	656	0	677	19	0
1	B8	656	0	677	24	0
1	B9	656	0	677	22	0
1	BA	656	0	677	22	0
1	BB	656	0	677	22	0
1	BC	656	0	677	21	0
1	BD	656	0	677	23	0
1	BE	656	0	677	21	0
1	BF	656	0	677	22	0
1	BG	656	0	677	21	0
1	BH	656	0	677	22	0
1	BI	656	0	677	24	0
1	BJ	656	0	677	25	0
1	BK	656	0	677	20	0
1	BL	656	0	677	27	0
1	BM	656	0	677	18	0
1	BN	656	0	677	24	0
1	BO	656	0	677	21	0
1	BP	656	0	677	22	0
1	BQ	656	0	677	22	0
1	BR	656	0	677	24	0
1	BS	656	0	677	22	0
1	BT	656	0	677	23	0
1	BU	656	0	677	20	0
1	BV	656	0	677	23	0
1	BW	656	0	677	21	0
1	BX	635	0	657	26	0
1	BY	656	0	677	24	0
1	BZ	656	0	677	21	0
1	Ba	656	0	677	24	0
1	Bb	656	0	677	20	0
1	Bc	656	0	677	23	0
1	Bd	656	0	677	22	0
1	Be	656	0	677	22	0
1	Bf	656	0	677	21	0
1	Bg	656	0	677	23	0
1	Bh	656	0	677	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Bi	656	0	677	24	0
1	Bj	656	0	677	21	0
1	Bk	656	0	677	21	0
1	Bl	656	0	677	22	0
1	Bm	656	0	677	23	0
1	Bn	656	0	677	24	0
1	Bo	656	0	677	23	0
1	Bp	656	0	677	23	0
1	Bq	656	0	677	19	0
1	Br	656	0	677	22	0
1	Bs	656	0	677	22	0
1	Bt	656	0	677	21	0
1	Bu	656	0	677	23	0
1	Bv	656	0	677	23	0
1	Bw	656	0	677	23	0
1	Bx	656	0	677	22	0
1	C0	656	0	677	16	0
1	C1	656	0	677	21	0
1	C2	656	0	677	19	0
1	C3	656	0	677	19	0
1	C4	656	0	677	20	0
1	C5	656	0	677	17	0
1	C6	656	0	677	21	0
1	C7	656	0	677	19	0
1	C8	656	0	677	18	0
1	C9	656	0	677	20	0
1	CA	656	0	677	18	0
1	CB	656	0	677	18	0
1	CC	656	0	677	18	0
1	CD	656	0	677	19	0
1	CE	656	0	677	15	0
1	CF	656	0	677	17	0
1	CG	656	0	677	18	0
1	CH	656	0	677	19	0
1	CI	656	0	677	19	0
1	CJ	656	0	677	19	0
1	CK	656	0	677	16	0
1	CL	656	0	677	20	0
1	CM	656	0	677	18	0
1	CN	656	0	677	18	0
1	CO	656	0	677	20	0
1	CP	656	0	677	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CQ	656	0	677	18	0
1	CR	656	0	677	19	0
1	CS	656	0	677	19	0
1	CT	656	0	677	16	0
1	CU	656	0	677	18	0
1	CV	656	0	677	20	0
1	CW	656	0	677	19	0
1	CX	656	0	677	16	0
1	CY	656	0	677	19	0
1	CZ	656	0	677	16	0
1	Ca	656	0	677	22	0
1	Cb	656	0	677	18	0
1	Cc	656	0	677	20	0
1	Cd	656	0	677	19	0
1	Ce	656	0	677	21	0
1	Cf	656	0	677	19	0
1	Cg	656	0	677	19	0
1	Ch	656	0	677	19	0
1	Ci	656	0	677	15	0
1	Cj	656	0	677	16	0
1	Ck	656	0	677	21	0
1	Cl	656	0	677	19	0
1	Cm	656	0	677	19	0
1	Cn	656	0	677	19	0
1	Co	656	0	677	16	0
1	Cp	656	0	677	21	0
1	Cq	656	0	677	18	0
1	Cr	656	0	677	18	0
1	Cs	656	0	677	19	0
1	Ct	656	0	677	21	0
1	Cu	656	0	677	19	0
1	Cv	656	0	677	20	0
1	Cw	656	0	677	19	0
1	Cx	656	0	677	15	0
1	D0	656	0	677	61	0
1	D1	656	0	677	18	0
1	D2	656	0	677	54	0
1	D3	656	0	677	45	0
1	D4	656	0	677	111	0
1	D5	656	0	677	19	0
1	D6	656	0	677	21	0
1	D7	656	0	676	101	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D8	656	0	677	30	0
1	D9	656	0	677	18	0
1	DA	656	0	677	17	0
1	DB	656	0	677	65	0
1	DC	656	0	677	41	0
1	DD	656	0	677	68	0
1	DE	656	0	677	26	0
1	DF	635	0	657	25	0
1	DG	656	0	677	17	0
1	DH	656	0	677	60	0
1	DI	656	0	677	40	0
1	DJ	656	0	677	68	0
1	DK	656	0	677	19	0
1	DL	656	0	677	32	0
1	DM	656	0	677	46	0
1	DN	656	0	677	31	0
1	DO	656	0	677	17	0
1	DP	656	0	677	18	0
1	DQ	656	0	677	37	0
1	DR	656	0	677	16	0
1	DS	656	0	677	84	0
1	DT	656	0	677	27	0
1	DU	656	0	677	23	0
1	DV	656	0	677	19	0
1	DW	635	0	657	49	0
1	DX	656	0	677	48	0
1	DY	656	0	677	30	0
1	DZ	656	0	677	18	0
1	Da	656	0	677	26	0
1	Db	656	0	675	84	0
1	Dc	656	0	677	30	0
1	Dd	656	0	677	19	0
1	De	656	0	677	18	0
1	Df	656	0	677	32	0
1	Dg	656	0	677	31	0
1	Dh	656	0	677	88	0
1	Di	656	0	677	25	0
1	Dj	635	0	657	37	0
1	Dk	656	0	677	18	0
1	Dl	635	0	657	33	0
1	Dm	656	0	677	43	0
1	Dn	656	0	677	73	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Do	656	0	677	18	0
1	Dp	656	0	677	33	0
1	Dq	656	0	676	70	0
1	Dr	656	0	677	33	0
1	Ds	656	0	677	19	0
1	Dt	656	0	677	18	0
1	Du	635	0	657	48	0
1	Dv	656	0	677	55	0
1	Dw	656	0	676	69	0
1	Dx	656	0	677	31	0
1	E0	656	0	677	16	0
1	E1	656	0	677	26	0
1	E2	656	0	677	19	0
1	E3	656	0	677	31	0
1	E4	656	0	677	20	0
1	E5	656	0	677	20	0
1	E6	656	0	677	21	0
1	E7	656	0	677	27	0
1	E8	656	0	677	18	0
1	E9	656	0	677	22	0
1	EA	656	0	677	31	0
1	EB	656	0	677	20	0
1	EC	656	0	677	49	0
1	ED	656	0	677	23	0
1	EE	656	0	677	20	0
1	EF	635	0	657	19	0
1	EG	656	0	677	28	0
1	EH	656	0	677	21	0
1	EI	656	0	677	14	0
1	EJ	656	0	677	25	0
1	EK	656	0	677	21	0
1	EL	656	0	677	33	0
1	EM	656	0	677	26	0
1	EN	656	0	677	18	0
1	EO	656	0	677	22	0
1	EP	656	0	677	30	0
1	EQ	656	0	677	35	0
1	ER	656	0	677	46	0
1	ES	656	0	677	24	0
1	ET	656	0	677	18	0
1	EU	656	0	676	25	0
1	EV	656	0	677	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EW	635	0	657	31	0
1	EX	656	0	677	33	0
1	EY	656	0	677	20	0
1	EZ	656	0	677	21	0
1	Ea	656	0	677	31	0
1	Eb	656	0	677	25	0
1	Ec	656	0	677	18	0
1	Ed	656	0	677	21	0
1	Ee	656	0	677	29	0
1	Ef	656	0	677	28	0
1	Eg	656	0	677	31	0
1	Eh	656	0	677	24	0
1	Ei	656	0	677	20	0
1	Ej	656	0	677	28	0
1	Ek	656	0	677	29	0
1	El	635	0	657	9	0
1	Em	656	0	676	49	0
1	En	656	0	677	23	0
1	Eo	656	0	677	21	0
1	Ep	656	0	677	40	0
1	Eq	656	0	677	23	0
1	Er	656	0	677	18	0
1	Es	656	0	677	21	0
1	Et	656	0	677	33	0
1	Eu	656	0	677	33	0
1	Ev	656	0	677	62	0
1	Ew	656	0	677	28	0
1	Ex	656	0	677	19	0
1	F0	656	0	677	15	0
1	F1	656	0	677	12	0
1	F2	656	0	677	17	0
1	F3	656	0	677	13	0
1	F4	656	0	677	57	0
1	F5	656	0	677	14	0
1	F6	656	0	677	15	0
1	F7	656	0	677	33	0
1	F8	656	0	677	15	0
1	F9	656	0	677	14	0
1	FA	656	0	677	12	0
1	FB	656	0	677	11	0
1	FC	656	0	677	13	0
1	FD	656	0	676	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FE	656	0	677	11	0
1	FF	635	0	657	22	0
1	FG	656	0	677	11	0
1	FH	656	0	677	15	0
1	FI	656	0	677	17	0
1	FJ	656	0	676	38	0
1	FK	656	0	677	14	0
1	FL	656	0	677	27	0
1	FM	656	0	677	13	0
1	FN	656	0	677	15	0
1	FO	656	0	677	13	0
1	FP	656	0	677	12	0
1	FQ	656	0	677	12	0
1	FR	656	0	677	13	0
1	FS	656	0	677	28	0
1	FT	656	0	677	12	0
1	FU	656	0	677	16	0
1	FV	656	0	677	11	0
1	FW	635	0	657	13	0
1	FX	656	0	677	13	0
1	FY	656	0	677	18	0
1	FZ	656	0	677	16	0
1	Fa	656	0	677	14	0
1	Fb	656	0	676	50	0
1	Fc	656	0	677	15	0
1	Fd	656	0	677	15	0
1	Fe	656	0	677	12	0
1	Ff	656	0	677	12	0
1	Fg	656	0	677	12	0
1	Fh	656	0	677	34	0
1	Fi	656	0	677	13	0
1	Fj	635	0	657	14	0
1	Fk	656	0	677	11	0
1	Fl	656	0	677	15	0
1	Fm	656	0	677	14	0
1	Fn	656	0	677	49	0
1	Fo	656	0	677	14	0
1	Fp	656	0	677	15	0
1	Fq	656	0	677	18	0
1	Fr	656	0	677	16	0
1	Fs	656	0	677	13	0
1	Ft	656	0	677	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Fu	656	0	677	12	0
1	Fv	656	0	677	12	0
1	Fw	656	0	677	34	0
1	Fx	656	0	677	12	0
1	G0	656	0	677	20	0
1	G1	656	0	677	7	0
1	G2	656	0	677	17	0
1	G3	656	0	677	7	0
1	G4	656	0	677	6	0
1	G5	656	0	677	6	0
1	G6	656	0	677	7	0
1	G7	656	0	677	6	0
1	G8	656	0	677	6	0
1	G9	656	0	677	7	0
1	GA	656	0	677	7	0
1	GB	656	0	677	17	0
1	GC	656	0	677	6	0
1	GD	656	0	677	7	0
1	GE	656	0	677	6	0
1	GF	656	0	677	19	0
1	GG	656	0	677	7	0
1	GH	656	0	677	17	0
1	GI	656	0	677	10	0
1	GJ	656	0	677	7	0
1	GK	656	0	677	6	0
1	GL	656	0	677	8	0
1	GM	656	0	677	7	0
1	GN	656	0	677	6	0
1	GO	656	0	677	7	0
1	GP	656	0	677	8	0
1	GQ	656	0	677	19	0
1	GR	656	0	677	6	0
1	GS	656	0	677	6	0
1	GT	656	0	677	6	0
1	GU	656	0	677	18	0
1	GV	656	0	677	7	0
1	GW	656	0	677	16	0
1	GX	656	0	677	6	0
1	GY	656	0	677	6	0
1	GZ	656	0	677	7	0
1	Ga	656	0	677	8	0
1	Gb	656	0	677	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Gc	656	0	677	7	0
1	Gd	656	0	677	6	0
1	Ge	656	0	677	6	0
1	Gf	656	0	677	19	0
1	Gg	656	0	677	6	0
1	Gh	656	0	677	7	0
1	Gi	656	0	677	7	0
1	Gj	635	0	657	17	0
1	Gk	656	0	677	7	0
1	Gl	635	0	657	17	0
1	Gm	656	0	677	6	0
1	Gn	656	0	677	7	0
1	Go	656	0	677	7	0
1	Gp	656	0	677	8	0
1	Gq	656	0	677	6	0
1	Gr	656	0	677	7	0
1	Gs	656	0	677	7	0
1	Gt	656	0	677	7	0
1	Gu	656	0	677	17	0
1	Gv	656	0	677	7	0
1	Gw	656	0	677	6	0
1	Gx	656	0	677	7	0
1	H0	656	0	677	33	0
1	H1	656	0	677	30	0
1	H2	656	0	677	31	0
1	H3	656	0	677	31	0
1	H4	656	0	677	30	0
1	H5	656	0	677	30	0
1	H6	656	0	677	28	0
1	H7	656	0	677	31	0
1	H8	656	0	677	29	0
1	H9	656	0	677	29	0
1	HA	656	0	677	29	0
1	HB	656	0	677	30	0
1	HC	656	0	677	29	0
1	HD	656	0	677	27	0
1	HE	656	0	677	27	0
1	HF	656	0	677	32	0
1	HG	656	0	677	29	0
1	HH	656	0	677	31	0
1	HI	656	0	677	29	0
1	HJ	656	0	677	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	HK	656	0	677	28	0
1	HL	656	0	677	29	0
1	HM	656	0	677	31	0
1	HN	656	0	677	29	0
1	HO	656	0	677	30	0
1	HP	656	0	677	29	0
1	HQ	656	0	677	32	0
1	HR	656	0	677	28	0
1	HS	656	0	677	30	0
1	HT	656	0	677	29	0
1	HU	656	0	677	33	0
1	HV	656	0	677	28	0
1	HW	656	0	677	28	0
1	HX	656	0	677	28	0
1	HY	656	0	677	29	0
1	HZ	656	0	677	32	0
1	Ha	656	0	677	28	0
1	Hb	656	0	677	33	0
1	Hc	656	0	677	29	0
1	Hd	656	0	677	29	0
1	He	656	0	677	29	0
1	Hf	656	0	677	32	0
1	Hg	656	0	677	29	0
1	Hh	656	0	677	27	0
1	Hi	656	0	677	30	0
1	Hj	656	0	677	33	0
1	Hk	656	0	677	29	0
1	Hl	656	0	677	32	0
1	Hm	656	0	677	29	0
1	Hn	656	0	677	27	0
1	Ho	656	0	677	30	0
1	Hp	656	0	677	28	0
1	Hq	656	0	677	31	0
1	Hr	656	0	677	29	0
1	Hs	656	0	677	29	0
1	Ht	656	0	677	27	0
1	Hu	656	0	677	32	0
1	Hv	656	0	677	29	0
1	Hw	656	0	677	29	0
1	Hx	656	0	677	30	0
1	I0	656	0	677	16	0
1	I1	656	0	677	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I2	656	0	677	17	0
1	I3	656	0	677	17	0
1	I4	656	0	677	15	0
1	I5	656	0	677	16	0
1	I6	656	0	677	17	0
1	I7	656	0	677	15	0
1	I8	656	0	677	17	0
1	I9	656	0	677	16	0
1	IA	656	0	677	16	0
1	IB	656	0	677	18	0
1	IC	656	0	677	16	0
1	ID	656	0	677	14	0
1	IE	656	0	677	15	0
1	IF	656	0	677	15	0
1	IG	656	0	677	16	0
1	IH	656	0	677	18	0
1	II	656	0	677	17	0
1	IJ	656	0	677	14	0
1	IK	656	0	677	16	0
1	IL	656	0	677	17	0
1	IM	656	0	677	15	0
1	IN	656	0	677	17	0
1	IO	656	0	677	16	0
1	IP	656	0	677	16	0
1	IQ	656	0	677	19	0
1	IR	656	0	677	17	0
1	IS	656	0	677	16	0
1	IT	656	0	677	14	0
1	IU	656	0	677	16	0
1	IV	656	0	677	16	0
1	IW	656	0	677	15	0
1	IX	656	0	677	17	0
1	IY	656	0	677	15	0
1	IZ	656	0	677	17	0
1	Ia	656	0	677	17	0
1	Ib	656	0	677	16	0
1	Ic	656	0	677	18	0
1	Id	656	0	677	15	0
1	Ie	656	0	677	17	0
1	If	656	0	677	19	0
1	Ig	656	0	677	17	0
1	Ih	656	0	677	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ii	656	0	677	15	0
1	Ij	656	0	677	15	0
1	Ik	656	0	677	17	0
1	Il	656	0	677	14	0
1	Im	656	0	677	17	0
1	In	656	0	677	16	0
1	Io	656	0	677	16	0
1	Ip	656	0	677	17	0
1	Iq	656	0	677	15	0
1	Ir	656	0	677	18	0
1	Is	656	0	677	16	0
1	It	656	0	677	17	0
1	Iu	656	0	677	19	0
1	Iv	656	0	677	16	0
1	Iw	656	0	677	16	0
1	Ix	656	0	677	15	0
1	J0	656	0	676	17	0
1	J1	656	0	677	8	0
1	J2	656	0	676	21	0
1	J3	656	0	677	22	0
1	J4	656	0	676	19	0
1	J5	656	0	677	11	0
1	J6	656	0	677	44	0
1	J7	656	0	677	30	0
1	J8	656	0	677	12	0
1	J9	656	0	677	9	0
1	JA	656	0	677	8	0
1	JB	656	0	676	19	0
1	JC	656	0	677	10	0
1	JD	656	0	677	19	0
1	JE	656	0	677	13	0
1	JF	656	0	677	32	0
1	JG	656	0	677	8	0
1	JH	656	0	677	20	0
1	JI	656	0	677	20	0
1	JJ	656	0	676	28	0
1	JK	656	0	677	10	0
1	JL	656	0	677	36	0
1	JM	656	0	677	17	0
1	JN	656	0	677	11	0
1	JO	656	0	677	9	0
1	JP	656	0	677	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	JQ	656	0	677	23	0
1	JR	656	0	677	21	0
1	JS	656	0	677	31	0
1	JT	656	0	677	13	0
1	JU	656	0	677	11	0
1	JV	656	0	677	8	0
1	JW	656	0	677	18	0
1	JX	656	0	677	21	0
1	JY	656	0	677	15	0
1	JZ	656	0	677	10	0
1	Ja	656	0	677	36	0
1	Jb	656	0	677	19	0
1	Jc	656	0	677	12	0
1	Jd	656	0	677	9	0
1	Je	656	0	677	9	0
1	Jf	656	0	677	20	0
1	Jg	656	0	677	43	0
1	Jh	656	0	677	17	0
1	Ji	656	0	677	12	0
1	Jj	656	0	677	25	0
1	Jk	656	0	677	8	0
1	Jl	656	0	677	22	0
1	Jm	656	0	676	22	0
1	Jn	656	0	677	33	0
1	Jo	656	0	677	10	0
1	Jp	656	0	677	47	0
1	Jq	656	0	677	22	0
1	Jr	656	0	677	12	0
1	Js	656	0	677	9	0
1	Jt	656	0	677	8	0
1	Ju	656	0	677	22	0
1	Jv	656	0	677	75	0
1	Jw	656	0	677	34	0
1	Jx	656	0	677	13	0
1	K0	656	0	677	11	0
1	K1	656	0	677	11	0
1	K2	656	0	677	10	0
1	K3	656	0	677	12	0
1	K4	656	0	677	10	0
1	K5	656	0	677	10	0
1	K6	656	0	677	13	0
1	K7	656	0	677	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K8	656	0	677	12	0
1	K9	656	0	677	11	0
1	KA	656	0	677	14	0
1	KB	656	0	677	12	0
1	KC	656	0	677	11	0
1	KD	656	0	677	9	0
1	KE	656	0	677	11	0
1	KF	656	0	677	12	0
1	KG	656	0	677	13	0
1	KH	656	0	677	13	0
1	KI	656	0	677	11	0
1	KJ	656	0	677	9	0
1	KK	656	0	677	11	0
1	KL	656	0	677	12	0
1	KM	656	0	677	10	0
1	KN	656	0	677	10	0
1	KO	656	0	677	9	0
1	KP	656	0	677	14	0
1	KQ	656	0	677	9	0
1	KR	656	0	677	11	0
1	KS	656	0	677	10	0
1	KT	656	0	677	13	0
1	KU	656	0	677	10	0
1	KV	656	0	677	11	0
1	KW	656	0	677	9	0
1	KX	656	0	677	15	0
1	KY	656	0	677	11	0
1	KZ	656	0	677	11	0
1	Ka	656	0	677	10	0
1	Kb	656	0	677	10	0
1	Kc	656	0	677	11	0
1	Kd	656	0	677	11	0
1	Ke	656	0	677	13	0
1	Kf	656	0	677	10	0
1	Kg	656	0	677	11	0
1	Kh	656	0	677	11	0
1	Ki	656	0	677	12	0
1	Kj	656	0	677	10	0
1	Kk	656	0	677	11	0
1	Kl	656	0	677	10	0
1	Km	656	0	677	12	0
1	Kn	656	0	677	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ko	656	0	677	12	0
1	Kp	656	0	677	16	0
1	Kq	656	0	677	10	0
1	Kr	656	0	677	11	0
1	Ks	656	0	677	10	0
1	Kt	656	0	677	12	0
1	Ku	656	0	677	10	0
1	Kv	656	0	677	10	0
1	Kw	656	0	677	10	0
1	Kx	656	0	677	12	0
1	L0	656	0	677	5	0
1	L1	656	0	677	3	0
1	L2	656	0	677	6	0
1	L3	656	0	676	6	0
1	L4	656	0	677	3	0
1	L5	656	0	677	27	0
1	L6	656	0	677	4	0
1	L7	656	0	677	18	0
1	L8	656	0	677	33	0
1	L9	656	0	677	2	0
1	LA	656	0	677	4	0
1	LB	656	0	677	11	0
1	LC	656	0	677	6	0
1	LD	656	0	677	6	0
1	LE	656	0	677	5	0
1	LF	656	0	677	5	0
1	LG	656	0	677	2	0
1	LH	656	0	677	6	0
1	LI	656	0	677	10	0
1	LJ	656	0	677	2	0
1	LK	656	0	677	4	0
1	LL	656	0	677	6	0
1	LM	656	0	677	10	0
1	LN	656	0	677	37	0
1	LO	656	0	677	3	0
1	LP	656	0	677	4	0
1	LQ	656	0	677	11	0
1	LR	656	0	677	6	0
1	LS	656	0	677	15	0
1	LT	656	0	677	5	0
1	LU	656	0	677	5	0
1	LV	656	0	677	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	LW	656	0	677	6	0
1	LX	656	0	677	8	0
1	LY	656	0	677	5	0
1	LZ	656	0	677	4	0
1	La	656	0	676	25	0
1	Lb	656	0	677	3	0
1	Lc	656	0	675	19	0
1	Ld	656	0	677	3	0
1	Le	656	0	677	4	0
1	Lf	656	0	677	11	0
1	Lg	656	0	677	7	0
1	Lh	656	0	677	5	0
1	Li	656	0	677	7	0
1	Lj	656	0	677	4	0
1	Lk	656	0	677	2	0
1	Ll	656	0	677	6	0
1	Lm	656	0	677	24	0
1	Ln	656	0	677	8	0
1	Lo	656	0	677	4	0
1	Lp	656	0	677	5	0
1	Lq	656	0	677	7	0
1	Lr	656	0	677	7	0
1	Ls	656	0	677	3	0
1	Lt	656	0	677	3	0
1	Lu	656	0	677	11	0
1	Lv	656	0	677	11	0
1	Lw	656	0	677	8	0
1	Lx	656	0	677	6	0
1	M0	656	0	677	7	0
1	M1	656	0	677	7	0
1	M2	656	0	677	7	0
1	M3	656	0	677	12	0
1	M4	656	0	677	5	0
1	M5	656	0	677	7	0
1	M6	656	0	677	10	0
1	M7	656	0	677	6	0
1	M8	656	0	677	7	0
1	M9	656	0	677	7	0
1	MA	656	0	677	6	0
1	MB	656	0	677	9	0
1	MC	656	0	677	9	0
1	MD	656	0	677	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	ME	656	0	677	6	0
1	MF	656	0	677	13	0
1	MG	656	0	677	7	0
1	MH	656	0	677	7	0
1	MI	656	0	677	6	0
1	MJ	656	0	677	7	0
1	MK	656	0	677	7	0
1	ML	656	0	677	7	0
1	MM	656	0	677	5	0
1	MN	656	0	677	7	0
1	MO	656	0	677	6	0
1	MP	656	0	677	6	0
1	MQ	656	0	677	7	0
1	MR	656	0	677	8	0
1	MS	656	0	677	6	0
1	MT	656	0	677	6	0
1	MU	656	0	677	6	0
1	MV	656	0	677	7	0
1	MW	656	0	677	6	0
1	MX	656	0	677	7	0
1	MY	656	0	677	5	0
1	MZ	656	0	677	7	0
1	Ma	656	0	677	5	0
1	Mb	656	0	677	5	0
1	Mc	656	0	677	7	0
1	Md	656	0	677	6	0
1	Me	656	0	677	6	0
1	Mf	656	0	677	6	0
1	Mg	656	0	677	6	0
1	Mh	656	0	677	6	0
1	Mi	656	0	677	7	0
1	Mj	656	0	677	6	0
1	Mk	656	0	677	6	0
1	Ml	656	0	677	7	0
1	Mm	656	0	677	11	0
1	Mn	656	0	677	5	0
1	Mo	656	0	677	7	0
1	Mp	656	0	677	7	0
1	Mq	656	0	677	6	0
1	Mr	656	0	677	7	0
1	Ms	656	0	677	6	0
1	Mt	656	0	677	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Mu	656	0	677	7	0
1	Mv	656	0	677	19	0
1	Mw	656	0	677	8	0
1	Mx	656	0	677	7	0
1	N0	656	0	677	11	0
1	N1	656	0	677	10	0
1	N2	656	0	677	9	0
1	N3	656	0	677	13	0
1	N4	656	0	677	20	0
1	N5	656	0	677	12	0
1	N6	656	0	677	11	0
1	N7	656	0	677	10	0
1	N8	656	0	677	13	0
1	N9	656	0	677	12	0
1	NA	656	0	677	11	0
1	NB	656	0	677	12	0
1	NC	656	0	677	10	0
1	ND	656	0	677	9	0
1	NE	656	0	677	11	0
1	NF	656	0	677	11	0
1	NG	656	0	677	11	0
1	NH	656	0	677	9	0
1	NI	656	0	677	12	0
1	NJ	656	0	677	13	0
1	NK	656	0	677	11	0
1	NL	656	0	677	7	0
1	NM	656	0	677	11	0
1	NN	656	0	677	12	0
1	NO	656	0	677	11	0
1	NP	656	0	677	11	0
1	NQ	656	0	677	12	0
1	NR	656	0	677	12	0
1	NS	656	0	677	9	0
1	NT	656	0	677	12	0
1	NU	656	0	677	11	0
1	NV	656	0	677	10	0
1	NW	656	0	677	9	0
1	NX	656	0	677	14	0
1	NY	656	0	677	13	0
1	NZ	656	0	677	10	0
1	Na	656	0	677	10	0
1	Nb	656	0	677	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Nc	656	0	677	12	0
1	Nd	656	0	677	11	0
1	Ne	656	0	677	11	0
1	Nf	656	0	677	12	0
1	Ng	656	0	677	11	0
1	Nh	656	0	677	9	0
1	Ni	656	0	677	11	0
1	Nj	656	0	677	11	0
1	Nk	656	0	677	11	0
1	Nl	656	0	677	9	0
1	Nm	656	0	677	15	0
1	Nn	656	0	677	29	0
1	No	656	0	677	11	0
1	Np	656	0	677	12	0
1	Nq	656	0	677	10	0
1	Nr	656	0	677	11	0
1	Ns	656	0	677	11	0
1	Nt	656	0	677	11	0
1	Nu	656	0	677	12	0
1	Nv	656	0	677	11	0
1	Nw	656	0	677	9	0
1	Nx	656	0	677	11	0
1	O0	656	0	677	9	0
1	O1	656	0	677	8	0
1	O2	656	0	677	8	0
1	O3	656	0	677	9	0
1	O4	656	0	677	9	0
1	O5	656	0	677	7	0
1	O6	656	0	677	7	0
1	O7	656	0	677	9	0
1	O8	656	0	677	10	0
1	O9	656	0	677	9	0
1	OA	656	0	677	8	0
1	OB	656	0	677	7	0
1	OC	656	0	677	7	0
1	OD	656	0	677	10	0
1	OE	656	0	677	7	0
1	OF	656	0	677	12	0
1	OG	656	0	677	8	0
1	OH	656	0	677	8	0
1	OI	656	0	677	10	0
1	OJ	656	0	677	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	OK	656	0	677	8	0
1	OL	656	0	677	9	0
1	OM	656	0	677	9	0
1	ON	656	0	677	10	0
1	OO	656	0	677	9	0
1	OP	656	0	677	8	0
1	OQ	656	0	677	7	0
1	OR	656	0	677	7	0
1	OS	656	0	677	9	0
1	OT	656	0	677	7	0
1	OU	656	0	677	10	0
1	OV	656	0	677	8	0
1	OW	656	0	677	9	0
1	OX	656	0	677	9	0
1	OY	656	0	677	8	0
1	OZ	656	0	677	7	0
1	Oa	656	0	677	9	0
1	Ob	656	0	677	9	0
1	Oc	656	0	677	10	0
1	Od	656	0	677	8	0
1	Oe	656	0	677	8	0
1	Of	656	0	677	7	0
1	Og	656	0	677	7	0
1	Oh	656	0	677	8	0
1	Oi	656	0	677	7	0
1	Oj	656	0	677	10	0
1	Ok	656	0	677	8	0
1	Ol	656	0	677	8	0
1	Om	656	0	677	9	0
1	On	656	0	677	8	0
1	Oo	656	0	677	7	0
1	Op	656	0	677	10	0
1	Oq	656	0	677	9	0
1	Or	656	0	677	10	0
1	Os	656	0	677	9	0
1	Ot	656	0	677	8	0
1	Ou	656	0	677	7	0
1	Ov	656	0	677	26	0
1	Ow	656	0	677	9	0
1	Ox	656	0	677	7	0
2	P0	608	0	625	46	0
2	P1	608	0	625	42	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P2	608	0	625	41	0
2	P3	608	0	625	46	0
2	P4	608	0	625	36	0
2	P5	608	0	625	42	0
2	P6	608	0	625	42	0
2	P7	608	0	625	38	0
2	P8	608	0	625	42	0
2	P9	608	0	625	37	0
2	PA	608	0	625	40	0
2	PB	608	0	625	43	0
2	PC	608	0	625	45	0
2	PD	608	0	625	29	0
2	PE	608	0	625	34	0
2	PF	608	0	625	48	0
2	PG	608	0	625	43	0
2	PH	608	0	625	40	0
2	PI	608	0	625	44	0
2	PJ	608	0	625	37	0
2	PK	608	0	625	41	0
2	PL	608	0	625	43	0
2	PM	608	0	625	36	0
2	PN	608	0	625	40	0
2	PO	608	0	625	40	0
2	PP	608	0	625	42	0
2	PQ	608	0	625	42	0
2	PR	608	0	625	43	0
2	PS	608	0	625	27	0
2	PT	608	0	625	34	0
2	PU	608	0	625	47	0
2	PV	608	0	625	43	0
2	PW	608	0	625	38	0
2	PX	608	0	625	43	0
2	PY	608	0	625	37	0
2	PZ	608	0	625	42	0
2	Pa	608	0	625	43	0
2	Pb	608	0	625	36	0
2	Pc	608	0	625	41	0
2	Pd	608	0	625	40	0
2	Pe	608	0	625	43	0
2	Pf	608	0	625	43	0
2	Pg	608	0	625	44	0
2	Ph	608	0	625	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Pi	608	0	625	34	0
2	Pj	608	0	625	46	0
2	Pk	608	0	625	43	0
2	Pl	608	0	625	39	0
2	Pm	608	0	625	44	0
2	Pn	608	0	625	37	0
2	Po	608	0	625	42	0
2	Pp	608	0	625	43	0
2	Pq	608	0	625	37	0
2	Pr	608	0	625	42	0
2	Ps	608	0	625	39	0
2	Pt	608	0	625	41	0
2	Pu	608	0	625	41	0
2	Pv	608	0	625	43	0
2	Pw	608	0	625	29	0
2	Px	608	0	625	35	0
3	X0	513	0	496	16	0
3	X1	513	0	496	11	0
3	X2	513	0	496	13	0
3	X3	513	0	496	26	0
3	X4	513	0	496	23	0
3	X5	513	0	496	41	0
3	X6	513	0	495	49	0
3	X7	513	0	496	47	0
3	X8	513	0	495	67	0
3	X9	513	0	496	12	0
3	XA	513	0	496	9	0
3	XB	513	0	496	19	0
3	XC	513	0	495	55	0
3	XD	513	0	496	26	0
3	XE	513	0	496	53	0
3	XF	513	0	496	14	0
3	XG	513	0	496	11	0
3	XH	513	0	496	14	0
3	XI	513	0	496	16	0
3	XJ	513	0	496	10	0
3	XK	513	0	495	42	0
3	XL	513	0	495	44	0
3	XM	513	0	496	34	0
3	XN	513	0	496	75	0
3	XO	513	0	496	12	0
3	XP	513	0	496	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	XQ	513	0	496	18	0
3	XR	513	0	496	49	0
3	XS	513	0	496	18	0
3	XT	513	0	496	42	0
3	XU	513	0	496	14	0
3	XV	513	0	496	12	0
3	XW	513	0	496	14	0
3	XX	513	0	496	56	0
3	XY	513	0	496	41	0
3	XZ	513	0	495	39	0
3	Xa	513	0	496	49	0
3	Xb	513	0	496	25	0
3	Xc	513	0	495	56	0
3	Xd	513	0	496	12	0
3	Xe	513	0	496	9	0
3	Xf	513	0	496	20	0
3	Xg	513	0	496	50	0
3	Xh	513	0	496	19	0
3	Xi	513	0	496	60	0
3	Xj	513	0	496	14	0
3	Xk	513	0	496	10	0
3	Xl	513	0	496	15	0
3	Xm	513	0	496	18	0
3	Xn	513	0	496	29	0
3	Xo	513	0	496	49	0
3	Xp	513	0	496	40	0
3	Xq	513	0	496	27	0
3	Xr	513	0	495	42	0
3	Xs	513	0	496	10	0
3	Xt	513	0	496	9	0
3	Xu	513	0	496	19	0
3	Xv	513	0	495	53	0
3	Xw	513	0	496	19	0
3	Xx	513	0	496	42	0
3	Y0	980	0	956	44	0
3	Y1	980	0	956	37	0
3	Y2	980	0	956	46	0
3	Y3	980	0	956	42	0
3	Y4	980	0	956	38	0
3	Y5	980	0	956	41	0
3	Y6	980	0	956	36	0
3	Y7	980	0	956	47	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Y8	980	0	956	38	0
3	Y9	980	0	956	39	0
3	YA	980	0	956	43	0
3	YB	980	0	956	42	0
3	YC	980	0	956	39	0
3	YD	980	0	956	41	0
3	YE	980	0	956	43	0
3	YF	980	0	956	46	0
3	YG	980	0	956	40	0
3	YH	980	0	956	44	0
3	YI	980	0	956	44	0
3	YJ	980	0	956	40	0
3	YK	980	0	956	43	0
3	YL	980	0	956	47	0
3	YM	980	0	956	48	0
3	YN	980	0	956	37	0
3	YO	980	0	956	39	0
3	YP	980	0	956	42	0
3	YQ	980	0	956	42	0
3	YR	980	0	956	43	0
3	YS	980	0	956	41	0
3	YT	980	0	956	43	0
3	YU	980	0	956	45	0
3	YV	980	0	956	36	0
3	YW	980	0	956	47	0
3	YX	980	0	956	45	0
3	YY	980	0	956	37	0
3	YZ	980	0	956	40	0
3	Ya	980	0	956	37	0
3	Yb	980	0	956	47	0
3	Yc	980	0	956	37	0
3	Yd	980	0	956	37	0
3	Ye	980	0	956	43	0
3	Yf	980	0	956	41	0
3	Yg	980	0	956	41	0
3	Yh	980	0	956	41	0
3	Yi	980	0	956	42	0
3	Yj	980	0	956	45	0
3	Yk	980	0	956	39	0
3	Yl	980	0	956	45	0
3	Ym	980	0	954	58	0
3	Yn	980	0	956	39	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Yo	980	0	956	42	0
3	Yp	980	0	956	35	0
3	Yq	980	0	956	48	0
3	Yr	980	0	956	37	0
3	Ys	980	0	956	38	0
3	Yt	980	0	956	40	0
3	Yu	980	0	956	43	0
3	Yv	980	0	956	37	0
3	Yw	980	0	956	40	0
3	Yx	980	0	956	39	0
All	All	716166	0	733609	13143	0

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 9.

The worst 5 of 13143 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)
1:Dv:58:ASN:HB3	3:X8:643:TYR:CE1	1.26	1.70
1:FD:28:THR:HG22	1:DD:85:HIS:CE1	1.21	1.70
3:Xv:694:PRO:HG3	1:Jv:45:TYR:CZ	1.29	1.63
1:LN:62:ARG:CZ	3:XN:644:VAL:HG11	1.23	1.62
1:F4:29:LYS:HG3	1:D4:85:HIS:CD2	1.23	1.61

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	90/98 (92%)	90 (100%)	0	0	100	100
1	A1	90/98 (92%)	90 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A2	90/98 (92%)	90 (100%)	0	0	100	100
1	A3	90/98 (92%)	90 (100%)	0	0	100	100
1	A4	90/98 (92%)	90 (100%)	0	0	100	100
1	A5	90/98 (92%)	90 (100%)	0	0	100	100
1	A6	90/98 (92%)	90 (100%)	0	0	100	100
1	A7	90/98 (92%)	90 (100%)	0	0	100	100
1	A8	90/98 (92%)	90 (100%)	0	0	100	100
1	A9	90/98 (92%)	90 (100%)	0	0	100	100
1	AA	90/98 (92%)	90 (100%)	0	0	100	100
1	AB	90/98 (92%)	90 (100%)	0	0	100	100
1	AC	90/98 (92%)	90 (100%)	0	0	100	100
1	AD	90/98 (92%)	90 (100%)	0	0	100	100
1	AE	90/98 (92%)	90 (100%)	0	0	100	100
1	AF	90/98 (92%)	90 (100%)	0	0	100	100
1	AG	90/98 (92%)	90 (100%)	0	0	100	100
1	AH	90/98 (92%)	90 (100%)	0	0	100	100
1	AI	90/98 (92%)	90 (100%)	0	0	100	100
1	AJ	90/98 (92%)	90 (100%)	0	0	100	100
1	AK	90/98 (92%)	90 (100%)	0	0	100	100
1	AL	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	AM	90/98 (92%)	90 (100%)	0	0	100	100
1	AN	90/98 (92%)	90 (100%)	0	0	100	100
1	AO	90/98 (92%)	90 (100%)	0	0	100	100
1	AP	90/98 (92%)	90 (100%)	0	0	100	100
1	AQ	90/98 (92%)	90 (100%)	0	0	100	100
1	AR	90/98 (92%)	90 (100%)	0	0	100	100
1	AS	90/98 (92%)	90 (100%)	0	0	100	100
1	AT	90/98 (92%)	90 (100%)	0	0	100	100
1	AU	90/98 (92%)	90 (100%)	0	0	100	100
1	AV	90/98 (92%)	90 (100%)	0	0	100	100
1	AW	90/98 (92%)	90 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AX	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	AY	90/98 (92%)	90 (100%)	0	0	100	100
1	AZ	90/98 (92%)	90 (100%)	0	0	100	100
1	Aa	90/98 (92%)	90 (100%)	0	0	100	100
1	Ab	90/98 (92%)	90 (100%)	0	0	100	100
1	Ac	90/98 (92%)	90 (100%)	0	0	100	100
1	Ad	90/98 (92%)	90 (100%)	0	0	100	100
1	Ae	90/98 (92%)	90 (100%)	0	0	100	100
1	Af	90/98 (92%)	90 (100%)	0	0	100	100
1	Ag	90/98 (92%)	90 (100%)	0	0	100	100
1	Ah	90/98 (92%)	90 (100%)	0	0	100	100
1	Ai	90/98 (92%)	90 (100%)	0	0	100	100
1	Aj	90/98 (92%)	90 (100%)	0	0	100	100
1	Ak	90/98 (92%)	90 (100%)	0	0	100	100
1	Al	90/98 (92%)	90 (100%)	0	0	100	100
1	Am	90/98 (92%)	90 (100%)	0	0	100	100
1	An	90/98 (92%)	90 (100%)	0	0	100	100
1	Ao	90/98 (92%)	90 (100%)	0	0	100	100
1	Ap	90/98 (92%)	90 (100%)	0	0	100	100
1	Aq	90/98 (92%)	90 (100%)	0	0	100	100
1	Ar	90/98 (92%)	90 (100%)	0	0	100	100
1	As	90/98 (92%)	90 (100%)	0	0	100	100
1	At	90/98 (92%)	90 (100%)	0	0	100	100
1	Au	90/98 (92%)	90 (100%)	0	0	100	100
1	Av	90/98 (92%)	90 (100%)	0	0	100	100
1	Aw	90/98 (92%)	90 (100%)	0	0	100	100
1	Ax	90/98 (92%)	90 (100%)	0	0	100	100
1	B0	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	B1	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	B2	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	B3	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B4	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	B5	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	B6	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	B7	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	B8	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	B9	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BA	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BB	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BC	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BD	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BE	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BF	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BG	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BH	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BI	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BJ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BK	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BL	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BM	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BN	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BO	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BP	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BQ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BR	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BS	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BT	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BU	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BV	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BW	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	BX	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
1	BY	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BZ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ba	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bb	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bc	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bd	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Be	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bf	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bg	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bh	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bi	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bj	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bk	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bl	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bm	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bn	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bo	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bp	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bq	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Br	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bs	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bt	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bu	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bv	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bw	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Bx	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	C0	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	C1	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	C2	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	C3	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	C4	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	C5	90/98 (92%)	88 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C6	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	C7	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	C8	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	C9	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	CA	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CB	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CC	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CD	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CE	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	CF	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	CG	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CH	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CI	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CJ	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CK	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	CL	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CM	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CN	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CO	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CP	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CQ	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CR	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CS	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CT	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	CU	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	CV	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CW	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CX	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CY	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	CZ	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Ca	90/98 (92%)	87 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Cb	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Cc	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Cd	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Ce	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Cf	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Cg	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Ch	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Ci	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Cj	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Ck	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Cl	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Cm	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Cn	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Co	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Cp	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Cq	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Cr	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Cs	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Ct	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Cu	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Cv	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Cw	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	Cx	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	D0	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	D1	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	D2	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	D3	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	D4	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	D5	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	D6	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	D7	90/98 (92%)	88 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D8	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	D9	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DA	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DB	90/98 (92%)	90 (100%)	0	0	100	100
1	DC	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DD	90/98 (92%)	90 (100%)	0	0	100	100
1	DE	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DF	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
1	DG	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DH	90/98 (92%)	90 (100%)	0	0	100	100
1	DI	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DJ	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	DK	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DL	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DM	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DN	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DO	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DP	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DQ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DR	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DS	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	DT	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DU	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	DV	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DW	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
1	DX	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DY	90/98 (92%)	90 (100%)	0	0	100	100
1	DZ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Da	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Db	90/98 (92%)	90 (100%)	0	0	100	100
1	Dc	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Dd	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	De	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Df	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Dg	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Dh	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Di	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Dj	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
1	Dk	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Dl	87/98 (89%)	85 (98%)	2 (2%)	0	100	100
1	Dm	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Dn	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Do	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Dp	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Dq	90/98 (92%)	90 (100%)	0	0	100	100
1	Dr	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ds	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Dt	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Du	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
1	Dv	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Dw	90/98 (92%)	90 (100%)	0	0	100	100
1	Dx	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	E0	90/98 (92%)	90 (100%)	0	0	100	100
1	E1	90/98 (92%)	90 (100%)	0	0	100	100
1	E2	90/98 (92%)	90 (100%)	0	0	100	100
1	E3	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	E4	90/98 (92%)	90 (100%)	0	0	100	100
1	E5	90/98 (92%)	90 (100%)	0	0	100	100
1	E6	90/98 (92%)	90 (100%)	0	0	100	100
1	E7	90/98 (92%)	90 (100%)	0	0	100	100
1	E8	90/98 (92%)	90 (100%)	0	0	100	100
1	E9	90/98 (92%)	90 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EA	90/98 (92%)	90 (100%)	0	0	100	100
1	EB	90/98 (92%)	90 (100%)	0	0	100	100
1	EC	90/98 (92%)	90 (100%)	0	0	100	100
1	ED	90/98 (92%)	90 (100%)	0	0	100	100
1	EE	90/98 (92%)	90 (100%)	0	0	100	100
1	EF	87/98 (89%)	87 (100%)	0	0	100	100
1	EG	90/98 (92%)	90 (100%)	0	0	100	100
1	EH	90/98 (92%)	90 (100%)	0	0	100	100
1	EI	90/98 (92%)	90 (100%)	0	0	100	100
1	EJ	90/98 (92%)	90 (100%)	0	0	100	100
1	EK	90/98 (92%)	90 (100%)	0	0	100	100
1	EL	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	EM	90/98 (92%)	90 (100%)	0	0	100	100
1	EN	90/98 (92%)	90 (100%)	0	0	100	100
1	EO	90/98 (92%)	90 (100%)	0	0	100	100
1	EP	90/98 (92%)	90 (100%)	0	0	100	100
1	EQ	90/98 (92%)	90 (100%)	0	0	100	100
1	ER	90/98 (92%)	90 (100%)	0	0	100	100
1	ES	90/98 (92%)	90 (100%)	0	0	100	100
1	ET	90/98 (92%)	90 (100%)	0	0	100	100
1	EU	90/98 (92%)	90 (100%)	0	0	100	100
1	EV	90/98 (92%)	90 (100%)	0	0	100	100
1	EW	87/98 (89%)	87 (100%)	0	0	100	100
1	EX	90/98 (92%)	90 (100%)	0	0	100	100
1	EY	90/98 (92%)	90 (100%)	0	0	100	100
1	EZ	90/98 (92%)	90 (100%)	0	0	100	100
1	Ea	90/98 (92%)	90 (100%)	0	0	100	100
1	Eb	90/98 (92%)	90 (100%)	0	0	100	100
1	Ec	90/98 (92%)	90 (100%)	0	0	100	100
1	Ed	90/98 (92%)	90 (100%)	0	0	100	100
1	Ee	90/98 (92%)	90 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ef	90/98 (92%)	90 (100%)	0	0	100	100
1	Eg	90/98 (92%)	90 (100%)	0	0	100	100
1	Eh	90/98 (92%)	90 (100%)	0	0	100	100
1	Ei	90/98 (92%)	90 (100%)	0	0	100	100
1	Ej	90/98 (92%)	90 (100%)	0	0	100	100
1	Ek	90/98 (92%)	90 (100%)	0	0	100	100
1	El	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
1	Em	90/98 (92%)	90 (100%)	0	0	100	100
1	En	90/98 (92%)	90 (100%)	0	0	100	100
1	Eo	90/98 (92%)	90 (100%)	0	0	100	100
1	Ep	90/98 (92%)	90 (100%)	0	0	100	100
1	Eq	90/98 (92%)	90 (100%)	0	0	100	100
1	Er	90/98 (92%)	90 (100%)	0	0	100	100
1	Es	90/98 (92%)	90 (100%)	0	0	100	100
1	Et	90/98 (92%)	90 (100%)	0	0	100	100
1	Eu	90/98 (92%)	90 (100%)	0	0	100	100
1	Ev	90/98 (92%)	90 (100%)	0	0	100	100
1	Ew	90/98 (92%)	90 (100%)	0	0	100	100
1	Ex	90/98 (92%)	90 (100%)	0	0	100	100
1	F0	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	F1	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	F2	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	F3	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	F4	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	F5	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	F6	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	F7	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	F8	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	F9	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FA	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FB	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	FC	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FD	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FE	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FF	87/98 (89%)	85 (98%)	2 (2%)	0	100	100
1	FG	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FH	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FI	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	FJ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FK	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FL	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FM	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FN	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FO	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FP	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FQ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FR	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FS	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FT	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FU	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FV	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FW	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
1	FX	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FY	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	FZ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fa	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fb	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fc	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fd	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fe	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ff	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fg	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Fh	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fi	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fj	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
1	Fk	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fl	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fm	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fn	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fo	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fp	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fq	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fr	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fs	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ft	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fu	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fv	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fw	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Fx	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	G0	90/98 (92%)	90 (100%)	0	0	100	100
1	G1	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	G2	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	G3	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	G4	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	G5	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	G6	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	G7	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	G8	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	G9	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GA	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GB	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GC	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GD	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GE	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GF	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GG	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GH	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GI	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GJ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GK	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GL	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GM	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GN	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GO	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GP	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GQ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GR	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GS	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GT	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GU	90/98 (92%)	90 (100%)	0	0	100	100
1	GV	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GW	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GX	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GY	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	GZ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ga	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gb	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gc	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gd	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ge	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gf	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gg	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gh	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gi	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Gj	87/98 (89%)	87 (100%)	0	0	100	100
1	Gk	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gl	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
1	Gm	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gn	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Go	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gp	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gq	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gr	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gs	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gt	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gu	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gv	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Gw	90/98 (92%)	90 (100%)	0	0	100	100
1	Gx	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	H0	90/98 (92%)	90 (100%)	0	0	100	100
1	H1	90/98 (92%)	90 (100%)	0	0	100	100
1	H2	90/98 (92%)	90 (100%)	0	0	100	100
1	H3	90/98 (92%)	90 (100%)	0	0	100	100
1	H4	90/98 (92%)	90 (100%)	0	0	100	100
1	H5	90/98 (92%)	90 (100%)	0	0	100	100
1	H6	90/98 (92%)	90 (100%)	0	0	100	100
1	H7	90/98 (92%)	90 (100%)	0	0	100	100
1	H8	90/98 (92%)	90 (100%)	0	0	100	100
1	H9	90/98 (92%)	90 (100%)	0	0	100	100
1	HA	90/98 (92%)	90 (100%)	0	0	100	100
1	HB	90/98 (92%)	90 (100%)	0	0	100	100
1	HC	90/98 (92%)	90 (100%)	0	0	100	100
1	HD	90/98 (92%)	90 (100%)	0	0	100	100
1	HE	90/98 (92%)	90 (100%)	0	0	100	100
1	HF	90/98 (92%)	90 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	HG	90/98 (92%)	90 (100%)	0	0	100	100
1	HH	90/98 (92%)	90 (100%)	0	0	100	100
1	HI	90/98 (92%)	90 (100%)	0	0	100	100
1	HJ	90/98 (92%)	90 (100%)	0	0	100	100
1	HK	90/98 (92%)	90 (100%)	0	0	100	100
1	HL	90/98 (92%)	90 (100%)	0	0	100	100
1	HM	90/98 (92%)	90 (100%)	0	0	100	100
1	HN	90/98 (92%)	90 (100%)	0	0	100	100
1	HO	90/98 (92%)	90 (100%)	0	0	100	100
1	HP	90/98 (92%)	90 (100%)	0	0	100	100
1	HQ	90/98 (92%)	90 (100%)	0	0	100	100
1	HR	90/98 (92%)	90 (100%)	0	0	100	100
1	HS	90/98 (92%)	90 (100%)	0	0	100	100
1	HT	90/98 (92%)	90 (100%)	0	0	100	100
1	HU	90/98 (92%)	90 (100%)	0	0	100	100
1	HV	90/98 (92%)	90 (100%)	0	0	100	100
1	HW	90/98 (92%)	90 (100%)	0	0	100	100
1	HX	90/98 (92%)	90 (100%)	0	0	100	100
1	HY	90/98 (92%)	90 (100%)	0	0	100	100
1	HZ	90/98 (92%)	90 (100%)	0	0	100	100
1	Ha	90/98 (92%)	90 (100%)	0	0	100	100
1	Hb	90/98 (92%)	90 (100%)	0	0	100	100
1	Hc	90/98 (92%)	90 (100%)	0	0	100	100
1	Hd	90/98 (92%)	90 (100%)	0	0	100	100
1	He	90/98 (92%)	90 (100%)	0	0	100	100
1	Hf	90/98 (92%)	90 (100%)	0	0	100	100
1	Hg	90/98 (92%)	90 (100%)	0	0	100	100
1	Hh	90/98 (92%)	90 (100%)	0	0	100	100
1	Hi	90/98 (92%)	90 (100%)	0	0	100	100
1	Hj	90/98 (92%)	90 (100%)	0	0	100	100
1	Hk	90/98 (92%)	90 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Hl	90/98 (92%)	90 (100%)	0	0	100	100
1	Hm	90/98 (92%)	90 (100%)	0	0	100	100
1	Hn	90/98 (92%)	90 (100%)	0	0	100	100
1	Ho	90/98 (92%)	90 (100%)	0	0	100	100
1	Hp	90/98 (92%)	90 (100%)	0	0	100	100
1	Hq	90/98 (92%)	90 (100%)	0	0	100	100
1	Hr	90/98 (92%)	90 (100%)	0	0	100	100
1	Hs	90/98 (92%)	90 (100%)	0	0	100	100
1	Ht	90/98 (92%)	90 (100%)	0	0	100	100
1	Hu	90/98 (92%)	90 (100%)	0	0	100	100
1	Hv	90/98 (92%)	90 (100%)	0	0	100	100
1	Hw	90/98 (92%)	90 (100%)	0	0	100	100
1	Hx	90/98 (92%)	90 (100%)	0	0	100	100
1	I0	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	I1	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	I2	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	I3	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	I4	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	I5	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	I6	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	I7	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	I8	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	I9	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IA	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IB	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IC	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	ID	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IE	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IF	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IG	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IH	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	II	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IJ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IK	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IL	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IM	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IN	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IO	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IP	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IQ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IR	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IS	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IT	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IU	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IV	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IW	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IX	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IY	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	IZ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ia	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ib	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ic	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Id	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ie	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	If	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ig	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ih	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ii	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ij	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ik	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Il	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Im	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	In	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Io	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ip	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Iq	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ir	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Is	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	It	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Iu	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Iv	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Iw	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ix	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	J0	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	J1	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	J2	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	J3	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	J4	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	J5	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	J6	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	J7	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	J8	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	J9	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JA	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JB	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JC	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JD	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JE	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JF	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JG	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JH	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JI	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JJ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	JK	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JL	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JM	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JN	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JO	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JP	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JQ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JR	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JS	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JT	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JU	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JV	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JW	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JX	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JY	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	JZ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ja	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jb	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jc	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jd	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Je	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jf	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jg	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jh	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ji	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jj	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jk	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jl	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jm	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jn	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jo	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Jp	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jq	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jr	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Js	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jt	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ju	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jv	90/98 (92%)	90 (100%)	0	0	100	100
1	Jw	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Jx	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	K0	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	K1	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	K2	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	K3	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	K4	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	K5	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	K6	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	K7	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	K8	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	K9	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KA	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KB	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KC	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KD	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KE	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KF	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KG	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KH	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KI	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KJ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KK	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KL	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	KM	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KN	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KO	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KP	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KQ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KR	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KS	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KT	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KU	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KV	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KW	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KX	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KY	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	KZ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ka	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Kb	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Kc	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Kd	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ke	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Kf	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Kg	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Kh	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ki	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Kj	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Kk	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Kl	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Km	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Kn	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ko	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Kp	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Kq	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Kr	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ks	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Kt	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ku	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Kv	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Kw	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Kx	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	L0	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	L1	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	L2	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	L3	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	L4	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	L5	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	L6	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	L7	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	L8	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	L9	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LA	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LB	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LC	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LD	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LE	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LF	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LG	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LH	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LI	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LJ	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LK	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LL	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LM	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LN	90/98 (92%)	88 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	LO	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LP	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LQ	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LR	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LS	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LT	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LU	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LV	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LW	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LX	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LY	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	LZ	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	La	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Lb	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Lc	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Ld	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Le	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Lf	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Lg	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Lh	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Li	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Lj	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Lk	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Ll	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Lm	90/98 (92%)	90 (100%)	0	0	100	100
1	Ln	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Lo	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Lp	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Lq	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Lr	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Ls	90/98 (92%)	88 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Lt	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Lu	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Lv	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Lw	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Lx	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	M0	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	M1	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	M2	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	M3	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	M4	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	M5	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	M6	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	M7	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	M8	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	M9	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MA	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MB	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MC	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MD	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	ME	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MF	90/98 (92%)	90 (100%)	0	0	100	100
1	MG	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MH	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MI	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MJ	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MK	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	ML	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MM	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MN	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MO	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MP	90/98 (92%)	88 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	MQ	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MR	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MS	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MT	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MU	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MV	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MW	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MX	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MY	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	MZ	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Ma	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mb	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mc	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Md	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Me	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mf	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mg	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mh	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mi	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mj	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mk	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Ml	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mm	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mn	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mo	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mp	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mq	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mr	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Ms	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mt	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mu	90/98 (92%)	88 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Mv	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mw	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	Mx	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	N0	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	N1	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	N2	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	N3	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	N4	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	N5	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	N6	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	N7	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	N8	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	N9	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NA	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NB	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NC	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	ND	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NE	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NF	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NG	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NH	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NI	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NJ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NK	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NL	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NM	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NN	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NO	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NP	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NQ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NR	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	NS	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NT	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NU	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NV	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NW	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NX	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NY	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	NZ	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Na	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Nb	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Nc	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Nd	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ne	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Nf	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ng	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Nh	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ni	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Nj	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Nk	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Nl	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Nm	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Nn	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	No	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Np	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Nq	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Nr	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ns	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Nt	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Nu	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Nv	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Nw	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Nx	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	O0	90/98 (92%)	90 (100%)	0	0	100	100
1	O1	90/98 (92%)	90 (100%)	0	0	100	100
1	O2	90/98 (92%)	90 (100%)	0	0	100	100
1	O3	90/98 (92%)	90 (100%)	0	0	100	100
1	O4	90/98 (92%)	90 (100%)	0	0	100	100
1	O5	90/98 (92%)	90 (100%)	0	0	100	100
1	O6	90/98 (92%)	90 (100%)	0	0	100	100
1	O7	90/98 (92%)	90 (100%)	0	0	100	100
1	O8	90/98 (92%)	90 (100%)	0	0	100	100
1	O9	90/98 (92%)	90 (100%)	0	0	100	100
1	OA	90/98 (92%)	90 (100%)	0	0	100	100
1	OB	90/98 (92%)	90 (100%)	0	0	100	100
1	OC	90/98 (92%)	90 (100%)	0	0	100	100
1	OD	90/98 (92%)	90 (100%)	0	0	100	100
1	OE	90/98 (92%)	90 (100%)	0	0	100	100
1	OF	90/98 (92%)	90 (100%)	0	0	100	100
1	OG	90/98 (92%)	90 (100%)	0	0	100	100
1	OH	90/98 (92%)	90 (100%)	0	0	100	100
1	OI	90/98 (92%)	90 (100%)	0	0	100	100
1	OJ	90/98 (92%)	90 (100%)	0	0	100	100
1	OK	90/98 (92%)	90 (100%)	0	0	100	100
1	OL	90/98 (92%)	90 (100%)	0	0	100	100
1	OM	90/98 (92%)	90 (100%)	0	0	100	100
1	ON	90/98 (92%)	90 (100%)	0	0	100	100
1	OO	90/98 (92%)	90 (100%)	0	0	100	100
1	OP	90/98 (92%)	90 (100%)	0	0	100	100
1	OQ	90/98 (92%)	90 (100%)	0	0	100	100
1	OR	90/98 (92%)	90 (100%)	0	0	100	100
1	OS	90/98 (92%)	90 (100%)	0	0	100	100
1	OT	90/98 (92%)	90 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	OU	90/98 (92%)	90 (100%)	0	0	100	100
1	OV	90/98 (92%)	90 (100%)	0	0	100	100
1	OW	90/98 (92%)	90 (100%)	0	0	100	100
1	OX	90/98 (92%)	90 (100%)	0	0	100	100
1	OY	90/98 (92%)	90 (100%)	0	0	100	100
1	OZ	90/98 (92%)	90 (100%)	0	0	100	100
1	Oa	90/98 (92%)	90 (100%)	0	0	100	100
1	Ob	90/98 (92%)	90 (100%)	0	0	100	100
1	Oc	90/98 (92%)	90 (100%)	0	0	100	100
1	Od	90/98 (92%)	90 (100%)	0	0	100	100
1	Oe	90/98 (92%)	90 (100%)	0	0	100	100
1	Of	90/98 (92%)	90 (100%)	0	0	100	100
1	Og	90/98 (92%)	90 (100%)	0	0	100	100
1	Oh	90/98 (92%)	90 (100%)	0	0	100	100
1	Oi	90/98 (92%)	90 (100%)	0	0	100	100
1	Oj	90/98 (92%)	90 (100%)	0	0	100	100
1	Ok	90/98 (92%)	90 (100%)	0	0	100	100
1	Ol	90/98 (92%)	90 (100%)	0	0	100	100
1	Om	90/98 (92%)	90 (100%)	0	0	100	100
1	On	90/98 (92%)	90 (100%)	0	0	100	100
1	Oo	90/98 (92%)	90 (100%)	0	0	100	100
1	Op	90/98 (92%)	90 (100%)	0	0	100	100
1	Oq	90/98 (92%)	90 (100%)	0	0	100	100
1	Or	90/98 (92%)	90 (100%)	0	0	100	100
1	Os	90/98 (92%)	90 (100%)	0	0	100	100
1	Ot	90/98 (92%)	90 (100%)	0	0	100	100
1	Ou	90/98 (92%)	90 (100%)	0	0	100	100
1	Ov	90/98 (92%)	90 (100%)	0	0	100	100
1	Ow	90/98 (92%)	90 (100%)	0	0	100	100
1	Ox	90/98 (92%)	90 (100%)	0	0	100	100
2	P0	79/83 (95%)	75 (95%)	4 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P1	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	P2	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	P3	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	P4	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	P5	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	P6	79/83 (95%)	74 (94%)	5 (6%)	0	100	100
2	P7	79/83 (95%)	74 (94%)	4 (5%)	1 (1%)	9	38
2	P8	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	P9	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	PA	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	PB	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	PC	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	PD	79/83 (95%)	74 (94%)	5 (6%)	0	100	100
2	PE	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	PF	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	PG	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	PH	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	PI	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	PJ	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	PK	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	PL	79/83 (95%)	74 (94%)	5 (6%)	0	100	100
2	PM	79/83 (95%)	74 (94%)	4 (5%)	1 (1%)	9	38
2	PN	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	PO	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	PP	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	PQ	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	PR	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	PS	79/83 (95%)	74 (94%)	5 (6%)	0	100	100
2	PT	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	PU	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	PV	79/83 (95%)	75 (95%)	4 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	PW	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	PX	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	PY	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	PZ	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	Pa	79/83 (95%)	74 (94%)	5 (6%)	0	100	100
2	Pb	79/83 (95%)	74 (94%)	4 (5%)	1 (1%)	9	38
2	Pc	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	Pd	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	Pe	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	Pf	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	Pg	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	Ph	79/83 (95%)	74 (94%)	5 (6%)	0	100	100
2	Pi	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	Pj	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	Pk	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	Pl	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	Pm	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	Pn	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	Po	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	Pp	79/83 (95%)	74 (94%)	5 (6%)	0	100	100
2	Pq	79/83 (95%)	74 (94%)	4 (5%)	1 (1%)	9	38
2	Pr	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	Ps	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	Pt	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	Pu	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	Pv	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	Pw	79/83 (95%)	74 (94%)	5 (6%)	0	100	100
2	Px	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
3	X0	66/869 (8%)	65 (98%)	0	1 (2%)	8	36
3	X1	66/869 (8%)	64 (97%)	2 (3%)	0	100	100
3	X2	66/869 (8%)	66 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	X3	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	X4	66/869 (8%)	64 (97%)	2 (3%)	0	100	100
3	X5	66/869 (8%)	66 (100%)	0	0	100	100
3	X6	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	X7	66/869 (8%)	66 (100%)	0	0	100	100
3	X8	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	X9	66/869 (8%)	66 (100%)	0	0	100	100
3	XA	66/869 (8%)	64 (97%)	2 (3%)	0	100	100
3	XB	66/869 (8%)	64 (97%)	2 (3%)	0	100	100
3	XC	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	XD	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	XE	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	XF	66/869 (8%)	65 (98%)	0	1 (2%)	8	36
3	XG	66/869 (8%)	64 (97%)	2 (3%)	0	100	100
3	XH	66/869 (8%)	66 (100%)	0	0	100	100
3	XI	66/869 (8%)	66 (100%)	0	0	100	100
3	XJ	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	XK	66/869 (8%)	66 (100%)	0	0	100	100
3	XL	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	XM	66/869 (8%)	64 (97%)	2 (3%)	0	100	100
3	XN	66/869 (8%)	66 (100%)	0	0	100	100
3	XO	66/869 (8%)	66 (100%)	0	0	100	100
3	XP	66/869 (8%)	64 (97%)	2 (3%)	0	100	100
3	XQ	66/869 (8%)	64 (97%)	2 (3%)	0	100	100
3	XR	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	XS	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	XT	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	XU	66/869 (8%)	65 (98%)	0	1 (2%)	8	36
3	XV	66/869 (8%)	64 (97%)	2 (3%)	0	100	100
3	XW	66/869 (8%)	66 (100%)	0	0	100	100
3	XX	66/869 (8%)	66 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	XY	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	XZ	66/869 (8%)	66 (100%)	0	0	100	100
3	Xa	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	Xb	66/869 (8%)	66 (100%)	0	0	100	100
3	Xc	66/869 (8%)	66 (100%)	0	0	100	100
3	Xd	66/869 (8%)	66 (100%)	0	0	100	100
3	Xe	66/869 (8%)	64 (97%)	2 (3%)	0	100	100
3	Xf	66/869 (8%)	64 (97%)	2 (3%)	0	100	100
3	Xg	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	Xh	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	Xi	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	Xj	66/869 (8%)	65 (98%)	0	1 (2%)	8	36
3	Xk	66/869 (8%)	64 (97%)	2 (3%)	0	100	100
3	Xl	66/869 (8%)	66 (100%)	0	0	100	100
3	Xm	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	Xn	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	Xo	66/869 (8%)	66 (100%)	0	0	100	100
3	Xp	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	Xq	66/869 (8%)	66 (100%)	0	0	100	100
3	Xr	66/869 (8%)	66 (100%)	0	0	100	100
3	Xs	66/869 (8%)	66 (100%)	0	0	100	100
3	Xt	66/869 (8%)	64 (97%)	2 (3%)	0	100	100
3	Xu	66/869 (8%)	64 (97%)	2 (3%)	0	100	100
3	Xv	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	Xw	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	Xx	66/869 (8%)	65 (98%)	1 (2%)	0	100	100
3	Y0	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Y1	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Y2	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Y3	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Y4	130/869 (15%)	125 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Y5	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Y6	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Y7	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Y8	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Y9	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YA	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YB	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YC	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YD	130/869 (15%)	125 (96%)	5 (4%)	0	100	100
3	YE	130/869 (15%)	125 (96%)	5 (4%)	0	100	100
3	YF	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YG	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YH	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YI	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YJ	130/869 (15%)	125 (96%)	5 (4%)	0	100	100
3	YK	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YL	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YM	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YN	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YO	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YP	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YQ	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YR	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YS	130/869 (15%)	125 (96%)	5 (4%)	0	100	100
3	YT	130/869 (15%)	125 (96%)	5 (4%)	0	100	100
3	YU	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YV	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YW	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YX	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	YY	130/869 (15%)	125 (96%)	5 (4%)	0	100	100
3	YZ	130/869 (15%)	126 (97%)	4 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Ya	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Yb	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Yc	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Yd	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Ye	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Yf	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Yg	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Yh	130/869 (15%)	125 (96%)	5 (4%)	0	100	100
3	Yi	130/869 (15%)	125 (96%)	5 (4%)	0	100	100
3	Yj	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Yk	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Yl	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Ym	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Yn	130/869 (15%)	125 (96%)	5 (4%)	0	100	100
3	Yo	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Yp	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Yq	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Yr	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Ys	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Yt	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Yu	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Yv	130/869 (15%)	126 (97%)	4 (3%)	0	100	100
3	Yw	130/869 (15%)	125 (96%)	5 (4%)	0	100	100
3	Yx	130/869 (15%)	125 (96%)	5 (4%)	0	100	100
All	All	97458/197460 (49%)	96041 (98%)	1409 (1%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P7	68	PRO
3	X0	728	PRO
2	PM	68	PRO
3	XF	728	PRO
2	Pb	68	PRO

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	A1	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	A2	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	A3	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	A4	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	A5	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	A6	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	A7	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	A8	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	A9	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AA	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AB	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AC	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AD	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AE	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AF	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AG	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AH	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AI	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AJ	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AK	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AL	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AM	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AN	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AO	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AP	63/67 (94%)	61 (97%)	2 (3%)	34	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AQ	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AR	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AS	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AT	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AU	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AV	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AW	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AX	63/67 (94%)	60 (95%)	3 (5%)	23	48
1	AY	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	AZ	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Aa	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ab	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ac	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ad	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ae	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Af	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ag	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ah	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ai	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Aj	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ak	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Al	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Am	63/67 (94%)	59 (94%)	4 (6%)	16	43
1	An	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ao	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ap	63/67 (94%)	59 (94%)	4 (6%)	16	43
1	Aq	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ar	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	As	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	At	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Au	63/67 (94%)	61 (97%)	2 (3%)	34	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Av	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Aw	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ax	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	B0	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	B1	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	B2	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	B3	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	B4	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	B5	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	B6	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	B7	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	B8	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	B9	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BA	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BB	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BC	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BD	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BE	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BF	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BG	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BH	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BI	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BJ	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BK	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BL	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BM	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BN	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BO	63/67 (94%)	63 (100%)	0	100	100
1	BP	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BQ	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BR	63/67 (94%)	62 (98%)	1 (2%)	55	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BS	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BT	63/67 (94%)	63 (100%)	0	100	100
1	BU	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BV	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BW	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BX	61/67 (91%)	60 (98%)	1 (2%)	55	68
1	BY	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	BZ	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Ba	63/67 (94%)	63 (100%)	0	100	100
1	Bb	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bc	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bd	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Be	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bf	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bg	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bh	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bi	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bj	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bk	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bl	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bm	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Bn	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bo	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bp	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bq	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Br	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bs	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bt	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bu	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Bv	63/67 (94%)	63 (100%)	0	100	100
1	Bw	63/67 (94%)	62 (98%)	1 (2%)	55	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bx	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	C0	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	C1	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	C2	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	C3	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	C4	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	C5	63/67 (94%)	63 (100%)	0	100	100
1	C6	63/67 (94%)	63 (100%)	0	100	100
1	C7	63/67 (94%)	63 (100%)	0	100	100
1	C8	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	C9	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CA	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CB	63/67 (94%)	63 (100%)	0	100	100
1	CC	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CD	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CE	63/67 (94%)	63 (100%)	0	100	100
1	CF	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CG	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CH	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CI	63/67 (94%)	63 (100%)	0	100	100
1	CJ	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CK	63/67 (94%)	63 (100%)	0	100	100
1	CL	63/67 (94%)	63 (100%)	0	100	100
1	CM	63/67 (94%)	63 (100%)	0	100	100
1	CN	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CO	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CP	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CQ	63/67 (94%)	63 (100%)	0	100	100
1	CR	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CS	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CT	63/67 (94%)	63 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CU	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CV	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CW	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CX	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CY	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	CZ	63/67 (94%)	63 (100%)	0	100	100
1	Ca	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Cb	63/67 (94%)	63 (100%)	0	100	100
1	Cc	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Cd	63/67 (94%)	63 (100%)	0	100	100
1	Ce	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Cf	63/67 (94%)	63 (100%)	0	100	100
1	Cg	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Ch	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Ci	63/67 (94%)	63 (100%)	0	100	100
1	Cj	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Ck	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Cl	63/67 (94%)	63 (100%)	0	100	100
1	Cm	63/67 (94%)	63 (100%)	0	100	100
1	Cn	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Co	63/67 (94%)	63 (100%)	0	100	100
1	Cp	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Cq	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Cr	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Cs	63/67 (94%)	63 (100%)	0	100	100
1	Ct	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Cu	63/67 (94%)	63 (100%)	0	100	100
1	Cv	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Cw	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Cx	63/67 (94%)	63 (100%)	0	100	100
1	D0	63/67 (94%)	57 (90%)	6 (10%)	8	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D1	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	D2	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	D3	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	D4	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	D5	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	D6	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	D7	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	D8	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	D9	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DA	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DB	63/67 (94%)	54 (86%)	9 (14%)	3	18
1	DC	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DD	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DE	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DF	61/67 (91%)	53 (87%)	8 (13%)	4	20
1	DG	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DH	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	DI	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DJ	63/67 (94%)	53 (84%)	10 (16%)	2	15
1	DK	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DL	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DM	63/67 (94%)	56 (89%)	7 (11%)	6	25
1	DN	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DO	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DP	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DQ	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DR	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DS	63/67 (94%)	56 (89%)	7 (11%)	6	25
1	DT	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DU	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DV	63/67 (94%)	57 (90%)	6 (10%)	8	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DW	61/67 (91%)	55 (90%)	6 (10%)	7	30
1	DX	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	DY	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	DZ	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Da	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Db	63/67 (94%)	55 (87%)	8 (13%)	4	21
1	Dc	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Dd	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	De	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Df	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Dg	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Dh	63/67 (94%)	55 (87%)	8 (13%)	4	21
1	Di	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Dj	61/67 (91%)	56 (92%)	5 (8%)	10	35
1	Dk	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Dl	61/67 (91%)	54 (88%)	7 (12%)	5	24
1	Dm	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Dn	63/67 (94%)	59 (94%)	4 (6%)	16	43
1	Do	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Dp	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Dq	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Dr	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Ds	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Dt	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Du	61/67 (91%)	56 (92%)	5 (8%)	10	35
1	Dv	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Dw	63/67 (94%)	55 (87%)	8 (13%)	4	21
1	Dx	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	E0	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	E1	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	E2	63/67 (94%)	61 (97%)	2 (3%)	34	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E3	63/67 (94%)	60 (95%)	3 (5%)	23	48
1	E4	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	E5	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	E6	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	E7	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	E8	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	E9	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EA	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EB	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EC	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	ED	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EE	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EF	61/67 (91%)	56 (92%)	5 (8%)	10	35
1	EG	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EH	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EI	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EJ	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EK	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EL	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	EM	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EN	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EO	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EP	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EQ	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	ER	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	ES	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	ET	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EU	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EV	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EW	61/67 (91%)	59 (97%)	2 (3%)	33	55
1	EX	63/67 (94%)	61 (97%)	2 (3%)	34	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EY	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	EZ	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ea	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Eb	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ec	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ed	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ee	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ef	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Eg	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Eh	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ei	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ej	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ek	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	El	61/67 (91%)	59 (97%)	2 (3%)	33	55
1	Em	63/67 (94%)	59 (94%)	4 (6%)	16	43
1	En	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Eo	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ep	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Eq	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Er	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Es	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Et	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Eu	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ev	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ew	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ex	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	F0	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	F1	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	F2	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	F3	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	F4	63/67 (94%)	62 (98%)	1 (2%)	55	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F5	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	F6	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	F7	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	F8	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	F9	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FA	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FB	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FC	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FD	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FE	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FF	61/67 (91%)	55 (90%)	6 (10%)	7	30
1	FG	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FH	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	FI	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	FJ	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FK	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FL	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FM	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FN	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FO	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FP	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FQ	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FR	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FS	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FT	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FU	63/67 (94%)	59 (94%)	4 (6%)	16	43
1	FV	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FW	61/67 (91%)	59 (97%)	2 (3%)	33	55
1	FX	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FY	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	FZ	63/67 (94%)	62 (98%)	1 (2%)	55	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Fa	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fb	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fc	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fd	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fe	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Ff	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fg	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fh	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Fi	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fj	61/67 (91%)	59 (97%)	2 (3%)	33	55
1	Fk	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fl	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Fm	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fn	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fo	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fp	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fq	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fr	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fs	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Ft	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fu	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fv	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fw	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Fx	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	G0	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	G1	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	G2	63/67 (94%)	59 (94%)	4 (6%)	16	43
1	G3	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	G4	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	G5	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	G6	63/67 (94%)	62 (98%)	1 (2%)	55	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G7	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	G8	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	G9	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GA	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GB	63/67 (94%)	59 (94%)	4 (6%)	16	43
1	GC	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GD	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GE	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GF	63/67 (94%)	59 (94%)	4 (6%)	16	43
1	GG	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GH	63/67 (94%)	59 (94%)	4 (6%)	16	43
1	GI	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GJ	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GK	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GL	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GM	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GN	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GO	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GP	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GQ	63/67 (94%)	59 (94%)	4 (6%)	16	43
1	GR	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GS	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GT	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GU	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	GV	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GW	63/67 (94%)	59 (94%)	4 (6%)	16	43
1	GX	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GY	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	GZ	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Ga	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Gb	63/67 (94%)	62 (98%)	1 (2%)	55	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Gc	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Gd	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Ge	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Gf	63/67 (94%)	59 (94%)	4 (6%)	16	43
1	Gg	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Gh	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Gi	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Gj	61/67 (91%)	56 (92%)	5 (8%)	10	35
1	Gk	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Gl	61/67 (91%)	57 (93%)	4 (7%)	15	42
1	Gm	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Gn	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Go	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Gp	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Gq	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Gr	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Gs	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Gt	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Gu	63/67 (94%)	59 (94%)	4 (6%)	16	43
1	Gv	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Gw	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Gx	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	H0	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	H1	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	H2	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	H3	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	H4	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	H5	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	H6	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	H7	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	H8	63/67 (94%)	62 (98%)	1 (2%)	55	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H9	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HA	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HB	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HC	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HD	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HE	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HF	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HG	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HH	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HI	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HJ	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HK	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HL	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HM	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HN	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HO	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HP	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HQ	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HR	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HS	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HT	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HU	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HV	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HW	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HX	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HY	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	HZ	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Ha	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hb	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hc	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hd	63/67 (94%)	62 (98%)	1 (2%)	55	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	He	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hf	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hg	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hh	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hi	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hj	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hk	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hl	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hm	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hn	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Ho	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hp	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hq	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hr	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hs	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Ht	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hu	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hv	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hw	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Hx	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	I0	63/67 (94%)	63 (100%)	0	100	100
1	I1	63/67 (94%)	63 (100%)	0	100	100
1	I2	63/67 (94%)	63 (100%)	0	100	100
1	I3	63/67 (94%)	63 (100%)	0	100	100
1	I4	63/67 (94%)	63 (100%)	0	100	100
1	I5	63/67 (94%)	63 (100%)	0	100	100
1	I6	63/67 (94%)	63 (100%)	0	100	100
1	I7	63/67 (94%)	63 (100%)	0	100	100
1	I8	63/67 (94%)	63 (100%)	0	100	100
1	I9	63/67 (94%)	63 (100%)	0	100	100
1	IA	63/67 (94%)	63 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	IB	63/67 (94%)	63 (100%)	0	100	100
1	IC	63/67 (94%)	63 (100%)	0	100	100
1	ID	63/67 (94%)	63 (100%)	0	100	100
1	IE	63/67 (94%)	63 (100%)	0	100	100
1	IF	63/67 (94%)	63 (100%)	0	100	100
1	IG	63/67 (94%)	63 (100%)	0	100	100
1	IH	63/67 (94%)	63 (100%)	0	100	100
1	II	63/67 (94%)	63 (100%)	0	100	100
1	IJ	63/67 (94%)	63 (100%)	0	100	100
1	IK	63/67 (94%)	63 (100%)	0	100	100
1	IL	63/67 (94%)	63 (100%)	0	100	100
1	IM	63/67 (94%)	63 (100%)	0	100	100
1	IN	63/67 (94%)	63 (100%)	0	100	100
1	IO	63/67 (94%)	63 (100%)	0	100	100
1	IP	63/67 (94%)	63 (100%)	0	100	100
1	IQ	63/67 (94%)	63 (100%)	0	100	100
1	IR	63/67 (94%)	63 (100%)	0	100	100
1	IS	63/67 (94%)	63 (100%)	0	100	100
1	IT	63/67 (94%)	63 (100%)	0	100	100
1	IU	63/67 (94%)	63 (100%)	0	100	100
1	IV	63/67 (94%)	63 (100%)	0	100	100
1	IW	63/67 (94%)	63 (100%)	0	100	100
1	IX	63/67 (94%)	63 (100%)	0	100	100
1	IY	63/67 (94%)	63 (100%)	0	100	100
1	IZ	63/67 (94%)	63 (100%)	0	100	100
1	Ia	63/67 (94%)	63 (100%)	0	100	100
1	Ib	63/67 (94%)	63 (100%)	0	100	100
1	Ic	63/67 (94%)	63 (100%)	0	100	100
1	Id	63/67 (94%)	63 (100%)	0	100	100
1	Ie	63/67 (94%)	63 (100%)	0	100	100
1	If	63/67 (94%)	63 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ig	63/67 (94%)	63 (100%)	0	100	100
1	Ih	63/67 (94%)	63 (100%)	0	100	100
1	Ii	63/67 (94%)	63 (100%)	0	100	100
1	Ij	63/67 (94%)	63 (100%)	0	100	100
1	Ik	63/67 (94%)	63 (100%)	0	100	100
1	Il	63/67 (94%)	63 (100%)	0	100	100
1	Im	63/67 (94%)	63 (100%)	0	100	100
1	In	63/67 (94%)	63 (100%)	0	100	100
1	Io	63/67 (94%)	63 (100%)	0	100	100
1	Ip	63/67 (94%)	63 (100%)	0	100	100
1	Iq	63/67 (94%)	63 (100%)	0	100	100
1	Ir	63/67 (94%)	63 (100%)	0	100	100
1	Is	63/67 (94%)	63 (100%)	0	100	100
1	It	63/67 (94%)	63 (100%)	0	100	100
1	Iu	63/67 (94%)	63 (100%)	0	100	100
1	Iv	63/67 (94%)	63 (100%)	0	100	100
1	Iw	63/67 (94%)	63 (100%)	0	100	100
1	Ix	63/67 (94%)	63 (100%)	0	100	100
1	J0	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	J1	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	J2	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	J3	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	J4	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	J5	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	J6	63/67 (94%)	60 (95%)	3 (5%)	23	48
1	J7	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	J8	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	J9	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	JA	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	JB	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	JC	63/67 (94%)	57 (90%)	6 (10%)	8	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	JD	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	JE	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	JF	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	JG	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	JH	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	JI	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	JJ	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	JK	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	JL	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	JM	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	JN	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	JO	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	JP	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	JQ	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	JR	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	JS	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	JT	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	JU	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	JV	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	JW	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	JX	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	JY	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	JZ	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Ja	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	Jb	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Jc	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	Jd	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Je	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	Jf	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Jg	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	Jh	63/67 (94%)	58 (92%)	5 (8%)	11	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ji	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	Jj	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	Jk	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	Jl	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Jm	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	Jn	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	Jo	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Jp	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	Jq	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Jr	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	Js	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	Jt	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	Ju	63/67 (94%)	57 (90%)	6 (10%)	8	31
1	Jv	63/67 (94%)	56 (89%)	7 (11%)	6	25
1	Jw	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	Jx	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	K0	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	K1	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	K2	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	K3	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	K4	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	K5	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	K6	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	K7	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	K8	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	K9	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KA	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KB	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KC	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KD	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KE	63/67 (94%)	61 (97%)	2 (3%)	34	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	KF	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KG	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KH	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KI	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KJ	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KK	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KL	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KM	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KN	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KO	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KP	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KQ	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KR	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KS	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KT	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KU	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KV	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KW	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KX	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KY	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	KZ	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ka	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Kb	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Kc	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Kd	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ke	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Kf	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Kg	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Kh	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ki	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Kj	63/67 (94%)	61 (97%)	2 (3%)	34	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Kk	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Kl	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Km	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Kn	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ko	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Kp	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Kq	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Kr	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ks	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Kt	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ku	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Kv	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Kw	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Kx	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	L0	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	L1	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	L2	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	L3	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	L4	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	L5	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	L6	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	L7	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	L8	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	L9	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LA	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LB	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LC	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LD	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LE	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LF	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LG	63/67 (94%)	61 (97%)	2 (3%)	34	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	LH	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LI	63/67 (94%)	60 (95%)	3 (5%)	23	48
1	LJ	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LK	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LL	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LM	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LN	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LO	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LP	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LQ	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LR	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LS	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LT	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LU	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LV	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LW	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LX	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LY	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	LZ	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	La	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Lb	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Lc	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ld	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Le	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Lf	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Lg	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Lh	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Li	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Lj	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Lk	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ll	63/67 (94%)	61 (97%)	2 (3%)	34	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Lm	63/67 (94%)	58 (92%)	5 (8%)	11	37
1	Ln	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Lo	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Lp	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Lq	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Lr	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ls	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Lt	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Lu	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Lv	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Lw	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Lx	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	M0	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	M1	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	M2	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	M3	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	M4	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	M5	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	M6	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	M7	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	M8	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	M9	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MA	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MB	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MC	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MD	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	ME	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MF	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	MG	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MH	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MI	63/67 (94%)	62 (98%)	1 (2%)	55	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	MJ	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MK	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	ML	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MM	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MN	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MO	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MP	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MQ	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MR	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MS	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MT	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MU	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MV	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MW	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MX	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MY	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	MZ	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Ma	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mb	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mc	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Md	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Me	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mf	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mg	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mh	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mi	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mj	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mk	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Ml	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mm	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Mn	63/67 (94%)	62 (98%)	1 (2%)	55	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Mo	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mp	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mq	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mr	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Ms	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mt	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mu	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mv	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mw	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	Mx	63/67 (94%)	62 (98%)	1 (2%)	55	68
1	N0	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	N1	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	N2	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	N3	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	N4	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	N5	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	N6	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	N7	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	N8	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	N9	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NA	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NB	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NC	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	ND	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NE	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NF	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NG	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NH	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NI	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NJ	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NK	63/67 (94%)	61 (97%)	2 (3%)	34	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	NL	63/67 (94%)	60 (95%)	3 (5%)	23	48
1	NM	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NN	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NO	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NP	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NQ	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NR	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NS	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NT	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NU	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NV	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NW	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NX	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NY	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	NZ	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Na	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Nb	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Nc	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Nd	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ne	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Nf	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ng	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Nh	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ni	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Nj	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Nk	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Nl	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Nm	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Nn	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	No	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Np	63/67 (94%)	61 (97%)	2 (3%)	34	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Nq	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Nr	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Ns	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Nt	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Nu	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Nv	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Nw	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	Nx	63/67 (94%)	61 (97%)	2 (3%)	34	55
1	O0	63/67 (94%)	63 (100%)	0	100	100
1	O1	63/67 (94%)	63 (100%)	0	100	100
1	O2	63/67 (94%)	63 (100%)	0	100	100
1	O3	63/67 (94%)	63 (100%)	0	100	100
1	O4	63/67 (94%)	63 (100%)	0	100	100
1	O5	63/67 (94%)	63 (100%)	0	100	100
1	O6	63/67 (94%)	63 (100%)	0	100	100
1	O7	63/67 (94%)	63 (100%)	0	100	100
1	O8	63/67 (94%)	63 (100%)	0	100	100
1	O9	63/67 (94%)	63 (100%)	0	100	100
1	OA	63/67 (94%)	63 (100%)	0	100	100
1	OB	63/67 (94%)	63 (100%)	0	100	100
1	OC	63/67 (94%)	63 (100%)	0	100	100
1	OD	63/67 (94%)	63 (100%)	0	100	100
1	OE	63/67 (94%)	63 (100%)	0	100	100
1	OF	63/67 (94%)	63 (100%)	0	100	100
1	OG	63/67 (94%)	63 (100%)	0	100	100
1	OH	63/67 (94%)	63 (100%)	0	100	100
1	OI	63/67 (94%)	63 (100%)	0	100	100
1	OJ	63/67 (94%)	63 (100%)	0	100	100
1	OK	63/67 (94%)	63 (100%)	0	100	100
1	OL	63/67 (94%)	63 (100%)	0	100	100
1	OM	63/67 (94%)	63 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	ON	63/67 (94%)	63 (100%)	0	100	100
1	OO	63/67 (94%)	63 (100%)	0	100	100
1	OP	63/67 (94%)	63 (100%)	0	100	100
1	OQ	63/67 (94%)	63 (100%)	0	100	100
1	OR	63/67 (94%)	63 (100%)	0	100	100
1	OS	63/67 (94%)	63 (100%)	0	100	100
1	OT	63/67 (94%)	63 (100%)	0	100	100
1	OU	63/67 (94%)	63 (100%)	0	100	100
1	OV	63/67 (94%)	63 (100%)	0	100	100
1	OW	63/67 (94%)	63 (100%)	0	100	100
1	OX	63/67 (94%)	63 (100%)	0	100	100
1	OY	63/67 (94%)	63 (100%)	0	100	100
1	OZ	63/67 (94%)	63 (100%)	0	100	100
1	Oa	63/67 (94%)	63 (100%)	0	100	100
1	Ob	63/67 (94%)	63 (100%)	0	100	100
1	Oc	63/67 (94%)	63 (100%)	0	100	100
1	Od	63/67 (94%)	63 (100%)	0	100	100
1	Oe	63/67 (94%)	63 (100%)	0	100	100
1	Of	63/67 (94%)	63 (100%)	0	100	100
1	Og	63/67 (94%)	63 (100%)	0	100	100
1	Oh	63/67 (94%)	63 (100%)	0	100	100
1	Oi	63/67 (94%)	63 (100%)	0	100	100
1	Oj	63/67 (94%)	63 (100%)	0	100	100
1	Ok	63/67 (94%)	63 (100%)	0	100	100
1	Ol	63/67 (94%)	63 (100%)	0	100	100
1	Om	63/67 (94%)	63 (100%)	0	100	100
1	On	63/67 (94%)	63 (100%)	0	100	100
1	Oo	63/67 (94%)	63 (100%)	0	100	100
1	Op	63/67 (94%)	63 (100%)	0	100	100
1	Oq	63/67 (94%)	63 (100%)	0	100	100
1	Or	63/67 (94%)	63 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Os	63/67 (94%)	63 (100%)	0	100	100
1	Ot	63/67 (94%)	63 (100%)	0	100	100
1	Ou	63/67 (94%)	63 (100%)	0	100	100
1	Ov	63/67 (94%)	63 (100%)	0	100	100
1	Ow	63/67 (94%)	63 (100%)	0	100	100
1	Ox	63/67 (94%)	63 (100%)	0	100	100
2	P0	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	P1	66/67 (98%)	60 (91%)	6 (9%)	9	32
2	P2	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	P3	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	P4	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	P5	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	P6	66/67 (98%)	60 (91%)	6 (9%)	9	32
2	P7	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	P8	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	P9	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	PA	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	PB	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	PC	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	PD	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	PE	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	PF	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	PG	66/67 (98%)	60 (91%)	6 (9%)	9	32
2	PH	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	PI	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	PJ	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	PK	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	PL	66/67 (98%)	60 (91%)	6 (9%)	9	32
2	PM	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	PN	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	PO	66/67 (98%)	62 (94%)	4 (6%)	17	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	PP	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	PQ	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	PR	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	PS	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	PT	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	PU	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	PV	66/67 (98%)	60 (91%)	6 (9%)	9	32
2	PW	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	PX	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	PY	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	PZ	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	Pa	66/67 (98%)	60 (91%)	6 (9%)	9	32
2	Pb	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	Pc	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	Pd	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	Pe	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	Pf	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	Pg	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	Ph	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	Pi	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	Pj	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	Pk	66/67 (98%)	60 (91%)	6 (9%)	9	32
2	Pl	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	Pm	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	Pn	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	Po	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	Pp	66/67 (98%)	60 (91%)	6 (9%)	9	32
2	Pq	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	Pr	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	Ps	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	Pt	66/67 (98%)	61 (92%)	5 (8%)	12	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Pu	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	Pv	66/67 (98%)	61 (92%)	5 (8%)	12	38
2	Pw	66/67 (98%)	62 (94%)	4 (6%)	17	44
2	Px	66/67 (98%)	61 (92%)	5 (8%)	12	38
3	X0	56/702 (8%)	47 (84%)	9 (16%)	2	14
3	X1	56/702 (8%)	45 (80%)	11 (20%)	1	9
3	X2	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	X3	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	X4	56/702 (8%)	46 (82%)	10 (18%)	2	12
3	X5	56/702 (8%)	49 (88%)	7 (12%)	4	21
3	X6	56/702 (8%)	52 (93%)	4 (7%)	13	40
3	X7	56/702 (8%)	50 (89%)	6 (11%)	6	27
3	X8	56/702 (8%)	49 (88%)	7 (12%)	4	21
3	X9	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	XA	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	XB	56/702 (8%)	51 (91%)	5 (9%)	9	33
3	XC	56/702 (8%)	49 (88%)	7 (12%)	4	21
3	XD	56/702 (8%)	47 (84%)	9 (16%)	2	14
3	XE	56/702 (8%)	47 (84%)	9 (16%)	2	14
3	XF	56/702 (8%)	47 (84%)	9 (16%)	2	14
3	XG	56/702 (8%)	45 (80%)	11 (20%)	1	9
3	XH	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	XI	56/702 (8%)	51 (91%)	5 (9%)	9	33
3	XJ	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	XK	56/702 (8%)	49 (88%)	7 (12%)	4	21
3	XL	56/702 (8%)	52 (93%)	4 (7%)	13	40
3	XM	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	XN	56/702 (8%)	50 (89%)	6 (11%)	6	27
3	XO	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	XP	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	XQ	56/702 (8%)	51 (91%)	5 (9%)	9	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	XR	56/702 (8%)	49 (88%)	7 (12%)	4	21
3	XS	56/702 (8%)	49 (88%)	7 (12%)	4	21
3	XT	56/702 (8%)	47 (84%)	9 (16%)	2	14
3	XU	56/702 (8%)	47 (84%)	9 (16%)	2	14
3	XV	56/702 (8%)	45 (80%)	11 (20%)	1	9
3	XW	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	XX	56/702 (8%)	49 (88%)	7 (12%)	4	21
3	XY	56/702 (8%)	47 (84%)	9 (16%)	2	14
3	XZ	56/702 (8%)	49 (88%)	7 (12%)	4	21
3	Xa	56/702 (8%)	51 (91%)	5 (9%)	9	33
3	Xb	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	Xc	56/702 (8%)	50 (89%)	6 (11%)	6	27
3	Xd	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	Xe	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	Xf	56/702 (8%)	51 (91%)	5 (9%)	9	33
3	Xg	56/702 (8%)	49 (88%)	7 (12%)	4	21
3	Xh	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	Xi	56/702 (8%)	47 (84%)	9 (16%)	2	14
3	Xj	56/702 (8%)	47 (84%)	9 (16%)	2	14
3	Xk	56/702 (8%)	45 (80%)	11 (20%)	1	9
3	Xl	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	Xm	56/702 (8%)	51 (91%)	5 (9%)	9	33
3	Xn	56/702 (8%)	47 (84%)	9 (16%)	2	14
3	Xo	56/702 (8%)	49 (88%)	7 (12%)	4	21
3	Xp	56/702 (8%)	52 (93%)	4 (7%)	13	40
3	Xq	56/702 (8%)	47 (84%)	9 (16%)	2	14
3	Xr	56/702 (8%)	49 (88%)	7 (12%)	4	21
3	Xs	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	Xt	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	Xu	56/702 (8%)	51 (91%)	5 (9%)	9	33
3	Xv	56/702 (8%)	49 (88%)	7 (12%)	4	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Xw	56/702 (8%)	48 (86%)	8 (14%)	3	18
3	Xx	56/702 (8%)	47 (84%)	9 (16%)	2	14
3	Y0	103/702 (15%)	95 (92%)	8 (8%)	11	37
3	Y1	103/702 (15%)	98 (95%)	5 (5%)	22	48
3	Y2	103/702 (15%)	97 (94%)	6 (6%)	18	45
3	Y3	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	Y4	103/702 (15%)	95 (92%)	8 (8%)	11	37
3	Y5	103/702 (15%)	95 (92%)	8 (8%)	11	37
3	Y6	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	Y7	103/702 (15%)	98 (95%)	5 (5%)	22	48
3	Y8	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	Y9	103/702 (15%)	99 (96%)	4 (4%)	28	52
3	YA	103/702 (15%)	97 (94%)	6 (6%)	18	45
3	YB	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	YC	103/702 (15%)	97 (94%)	6 (6%)	18	45
3	YD	103/702 (15%)	95 (92%)	8 (8%)	11	37
3	YE	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	YF	103/702 (15%)	95 (92%)	8 (8%)	11	37
3	YG	103/702 (15%)	98 (95%)	5 (5%)	22	48
3	YH	103/702 (15%)	97 (94%)	6 (6%)	18	45
3	YI	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	YJ	103/702 (15%)	95 (92%)	8 (8%)	11	37
3	YK	103/702 (15%)	95 (92%)	8 (8%)	11	37
3	YL	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	YM	103/702 (15%)	98 (95%)	5 (5%)	22	48
3	YN	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	YO	103/702 (15%)	99 (96%)	4 (4%)	28	52
3	YP	103/702 (15%)	97 (94%)	6 (6%)	18	45
3	YQ	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	YR	103/702 (15%)	97 (94%)	6 (6%)	18	45
3	YS	103/702 (15%)	95 (92%)	8 (8%)	11	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	YT	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	YU	103/702 (15%)	95 (92%)	8 (8%)	11	37
3	YV	103/702 (15%)	98 (95%)	5 (5%)	22	48
3	YW	103/702 (15%)	97 (94%)	6 (6%)	18	45
3	YX	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	YY	103/702 (15%)	95 (92%)	8 (8%)	11	37
3	YZ	103/702 (15%)	95 (92%)	8 (8%)	11	37
3	Ya	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	Yb	103/702 (15%)	98 (95%)	5 (5%)	22	48
3	Yc	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	Yd	103/702 (15%)	99 (96%)	4 (4%)	28	52
3	Ye	103/702 (15%)	97 (94%)	6 (6%)	18	45
3	Yf	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	Yg	103/702 (15%)	97 (94%)	6 (6%)	18	45
3	Yh	103/702 (15%)	95 (92%)	8 (8%)	11	37
3	Yi	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	Yj	103/702 (15%)	95 (92%)	8 (8%)	11	37
3	Yk	103/702 (15%)	98 (95%)	5 (5%)	22	48
3	Yl	103/702 (15%)	97 (94%)	6 (6%)	18	45
3	Ym	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	Yn	103/702 (15%)	95 (92%)	8 (8%)	11	37
3	Yo	103/702 (15%)	95 (92%)	8 (8%)	11	37
3	Yp	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	Yq	103/702 (15%)	98 (95%)	5 (5%)	22	48
3	Yr	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	Ys	103/702 (15%)	99 (96%)	4 (4%)	28	52
3	Yt	103/702 (15%)	97 (94%)	6 (6%)	18	45
3	Yu	103/702 (15%)	96 (93%)	7 (7%)	14	41
3	Yv	103/702 (15%)	97 (94%)	6 (6%)	18	45
3	Yw	103/702 (15%)	95 (92%)	8 (8%)	11	37
3	Yx	103/702 (15%)	96 (93%)	7 (7%)	14	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	70172/148560 (47%)	67333 (96%)	2839 (4%)	29	52

5 of 2839 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Dx	97	GLN
1	JP	28	THR
1	Kv	94	LYS
1	Dx	48	VAL
1	Hk	48	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 846 such sidechains are listed below:

Mol	Chain	Res	Type
1	IX	85	HIS
1	Dv	79	HIS
3	XM	700	ASN
1	KY	39	GLN
1	IX	58	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

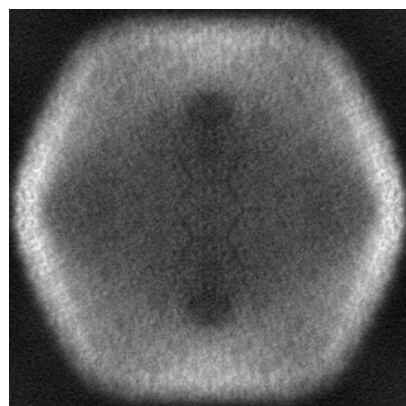
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62529. These allow visual inspection of the internal detail of the map and identification of artifacts.

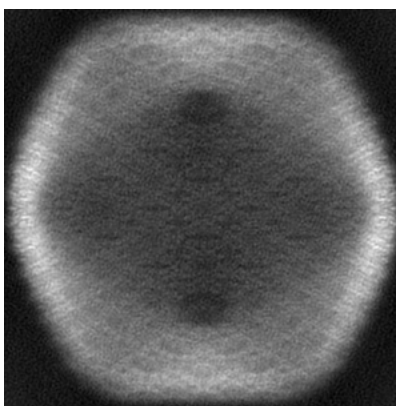
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

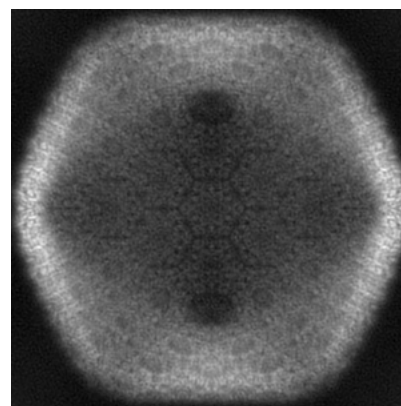
6.1.1 Primary map



X

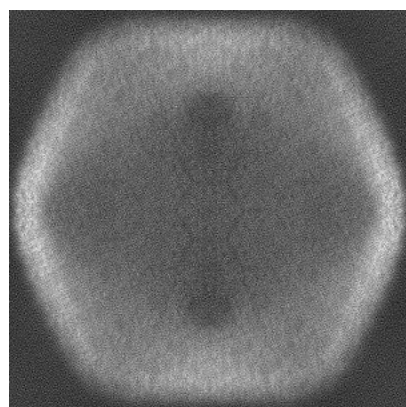


Y

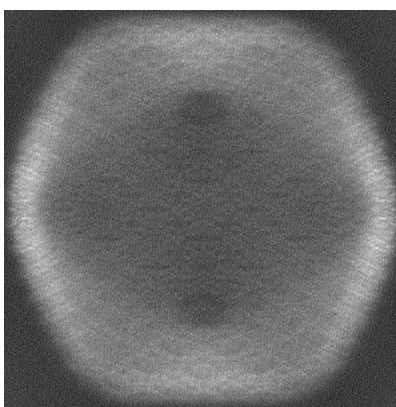


Z

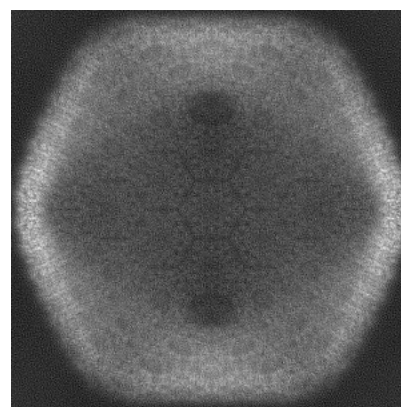
6.1.2 Raw map



X



Y

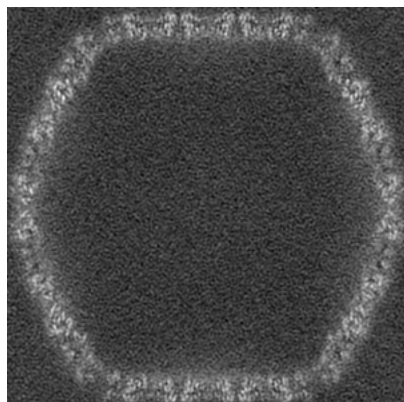


Z

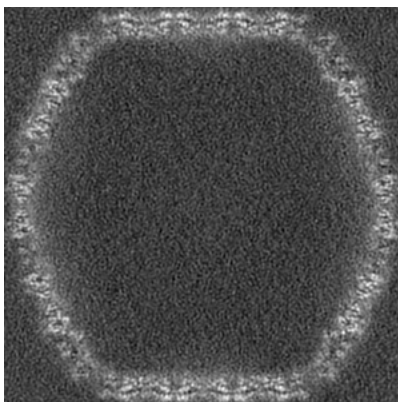
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

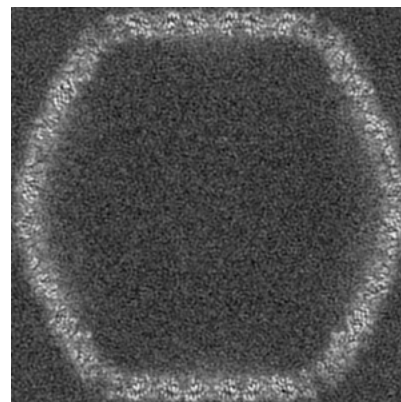
6.2.1 Primary map



X Index: 175

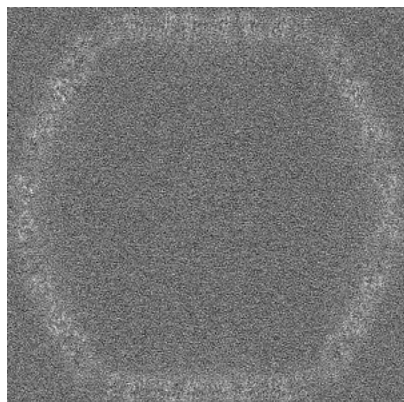


Y Index: 175

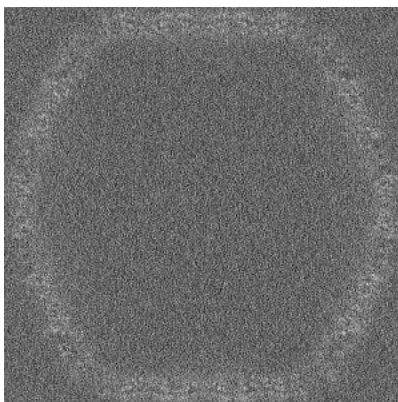


Z Index: 175

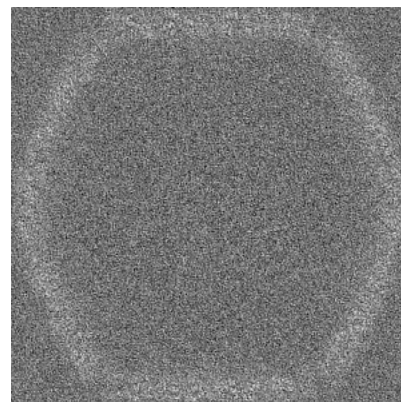
6.2.2 Raw map



X Index: 175



Y Index: 175

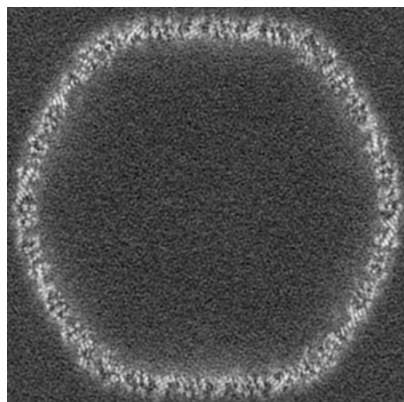


Z Index: 175

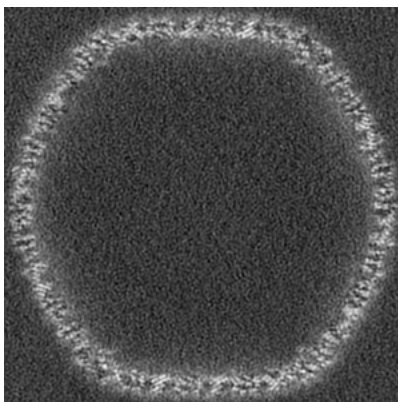
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

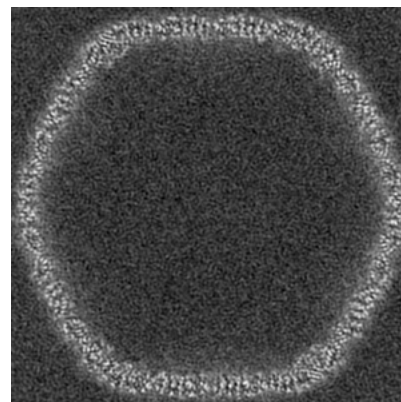
6.3.1 Primary map



X Index: 141

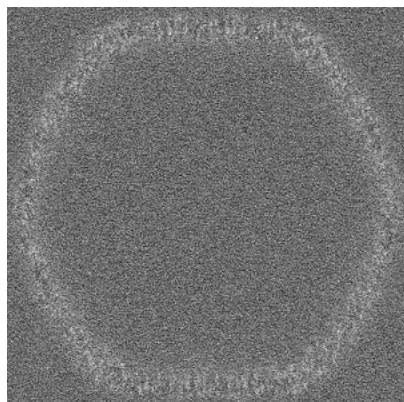


Y Index: 141

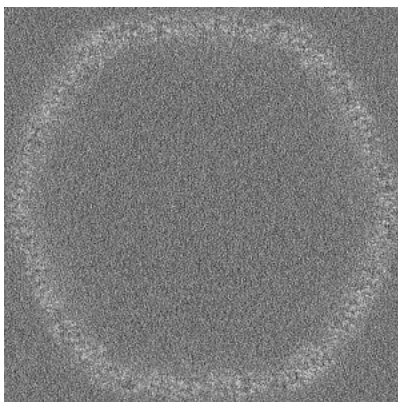


Z Index: 204

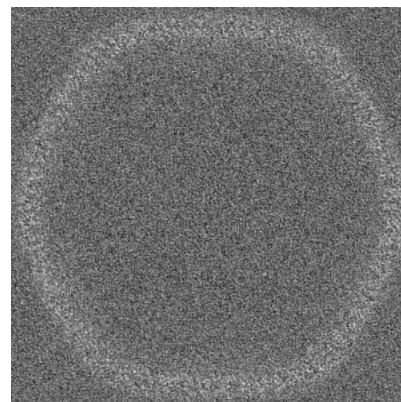
6.3.2 Raw map



X Index: 144



Y Index: 205

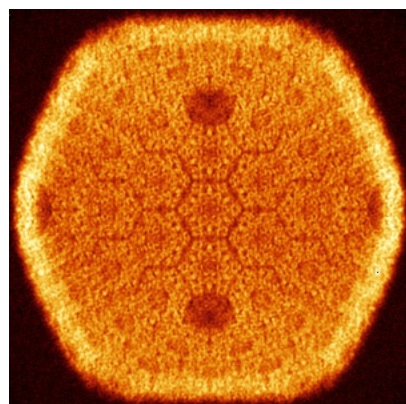


Z Index: 140

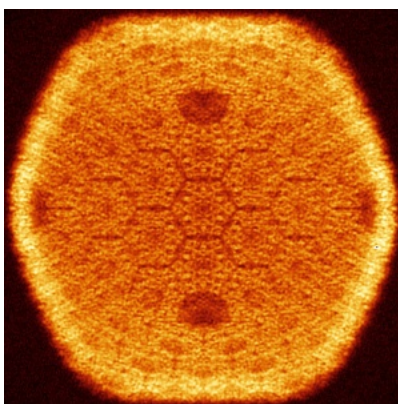
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

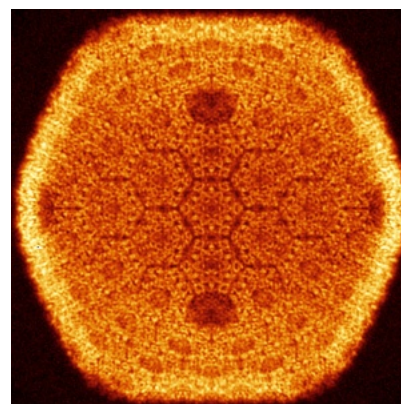
6.4.1 Primary map



X

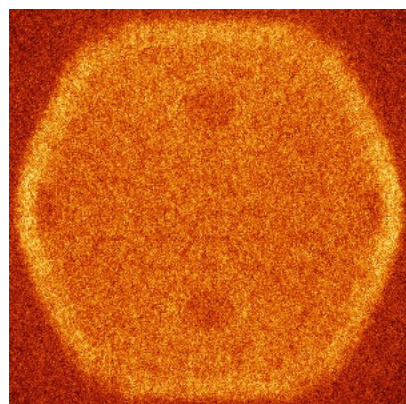


Y

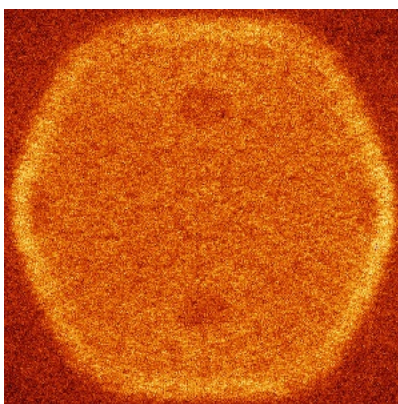


Z

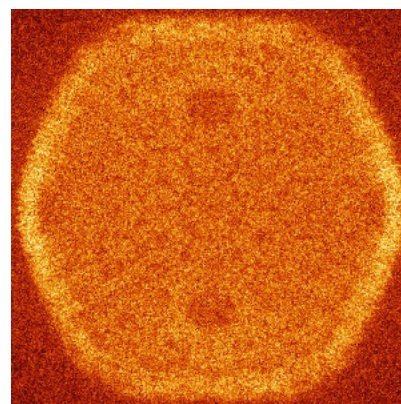
6.4.2 Raw map



X



Y

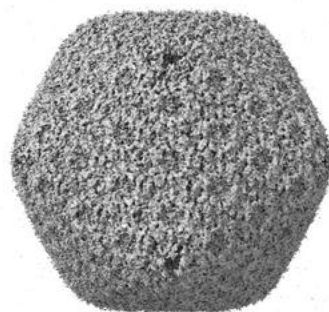


Z

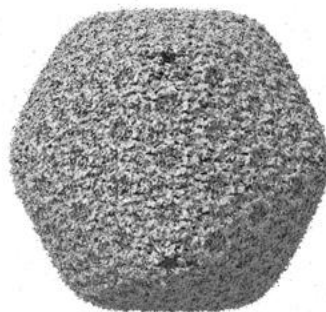
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

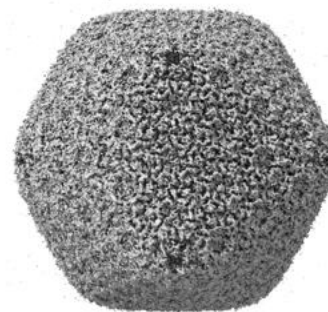
6.5.1 Primary map



X



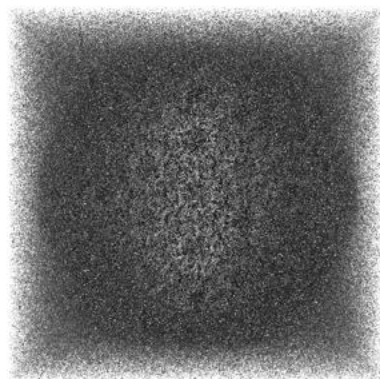
Y



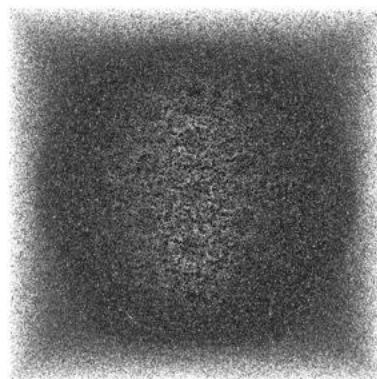
Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

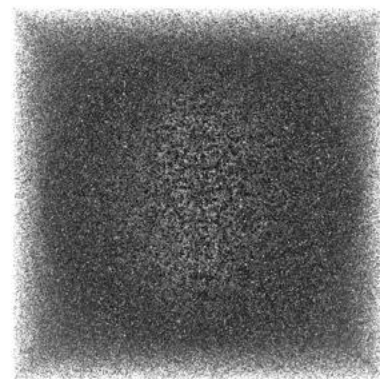
6.5.2 Raw map



X



Y



Z

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

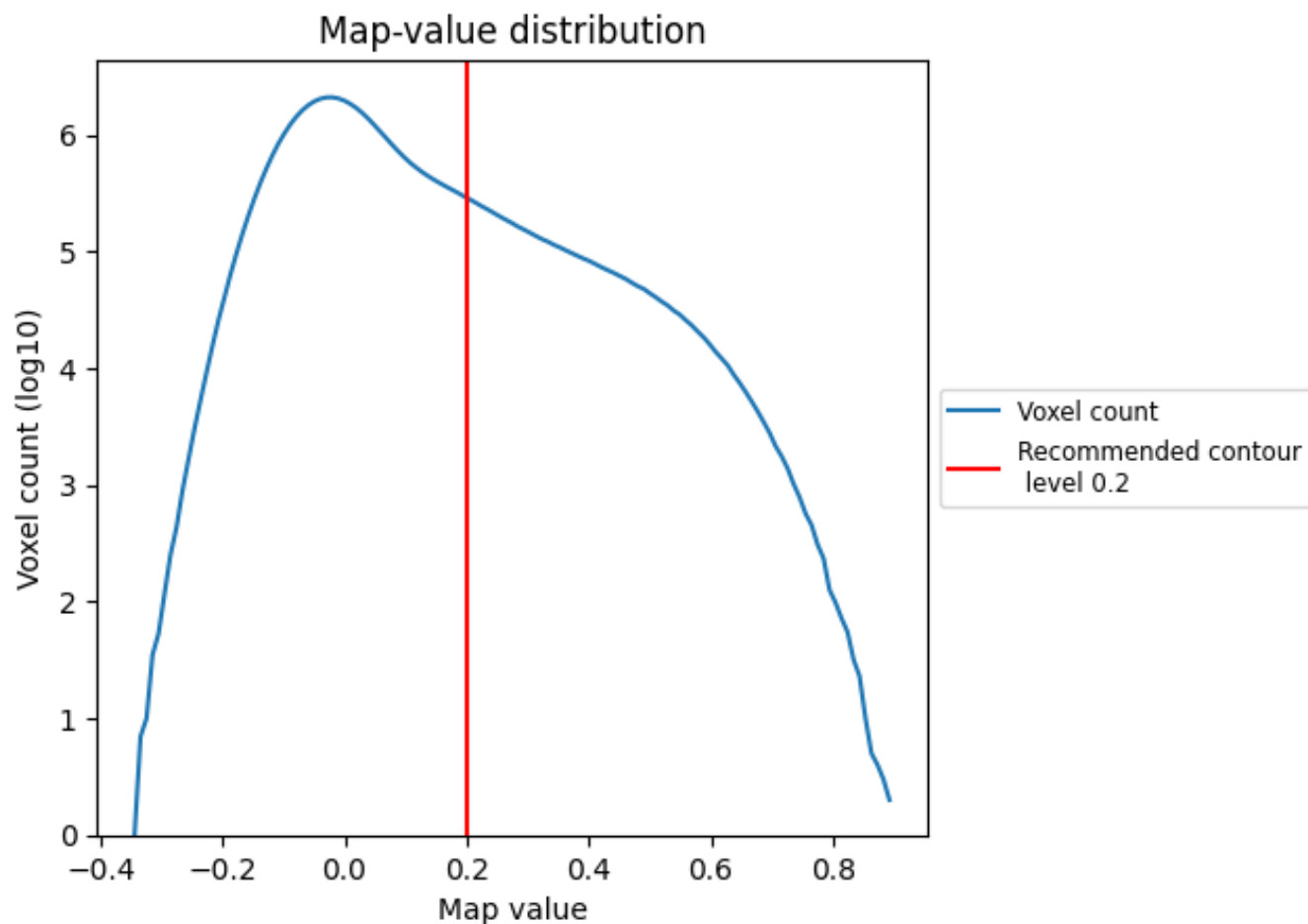
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

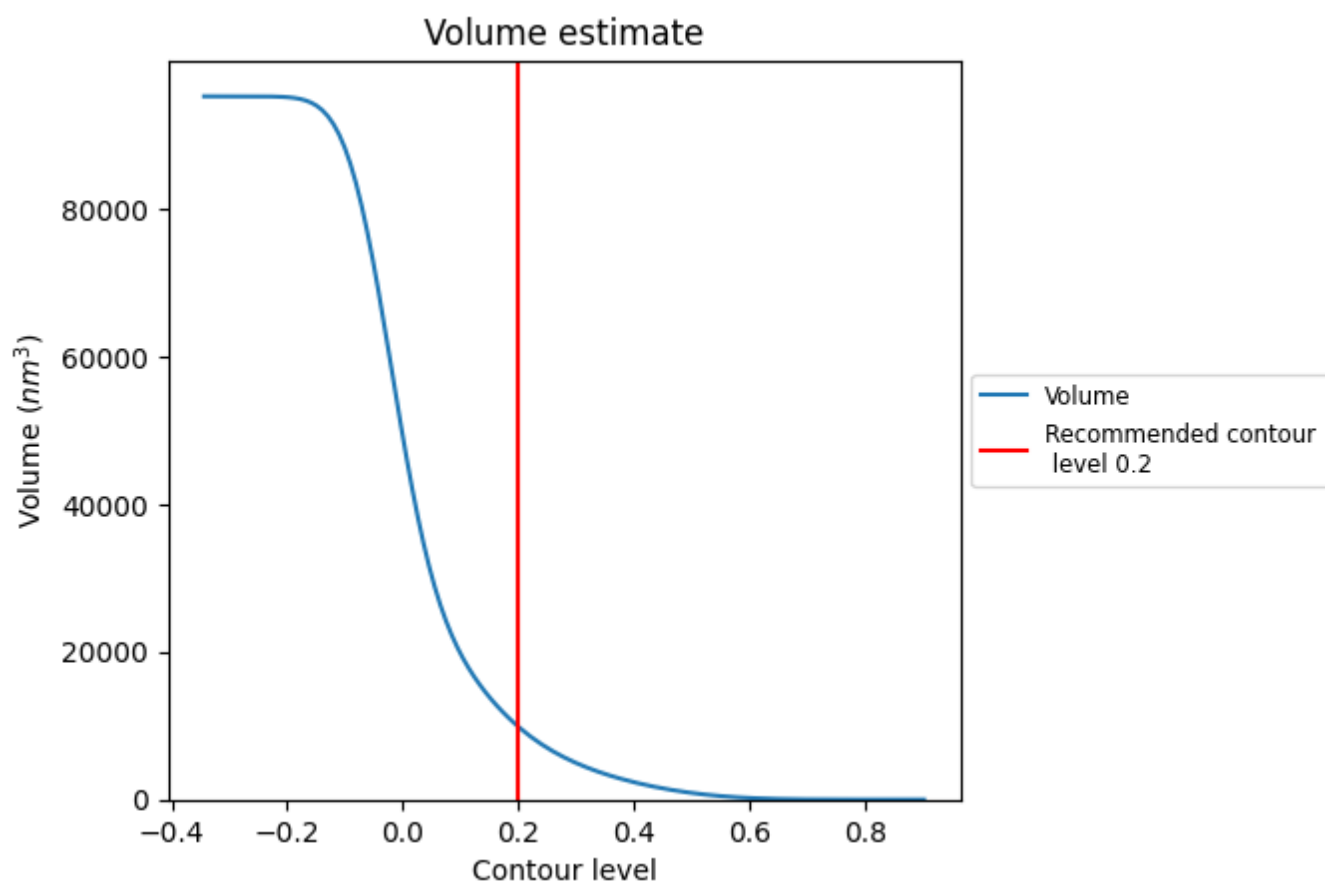
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

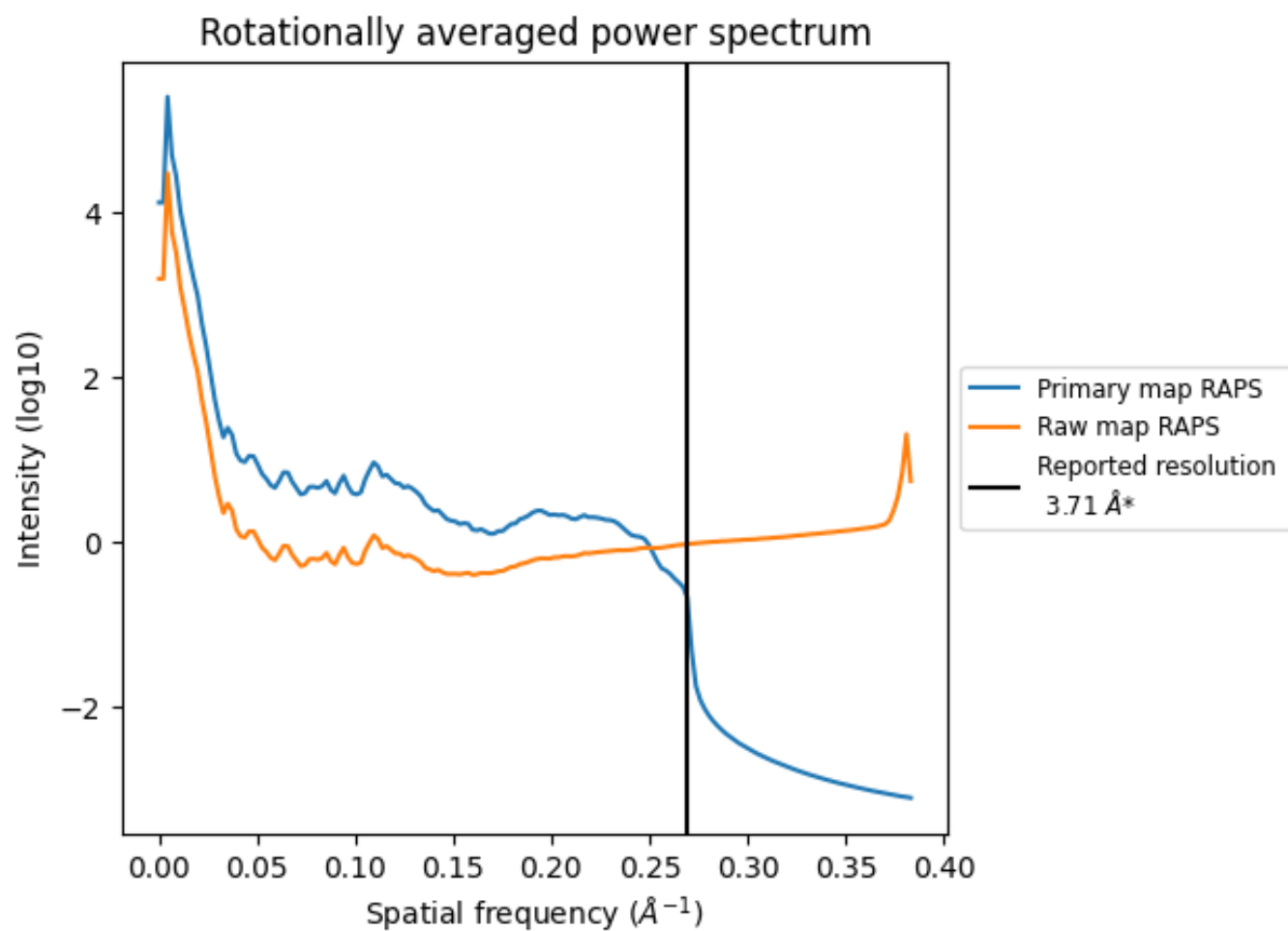
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 9866 nm³; this corresponds to an approximate mass of 8912 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

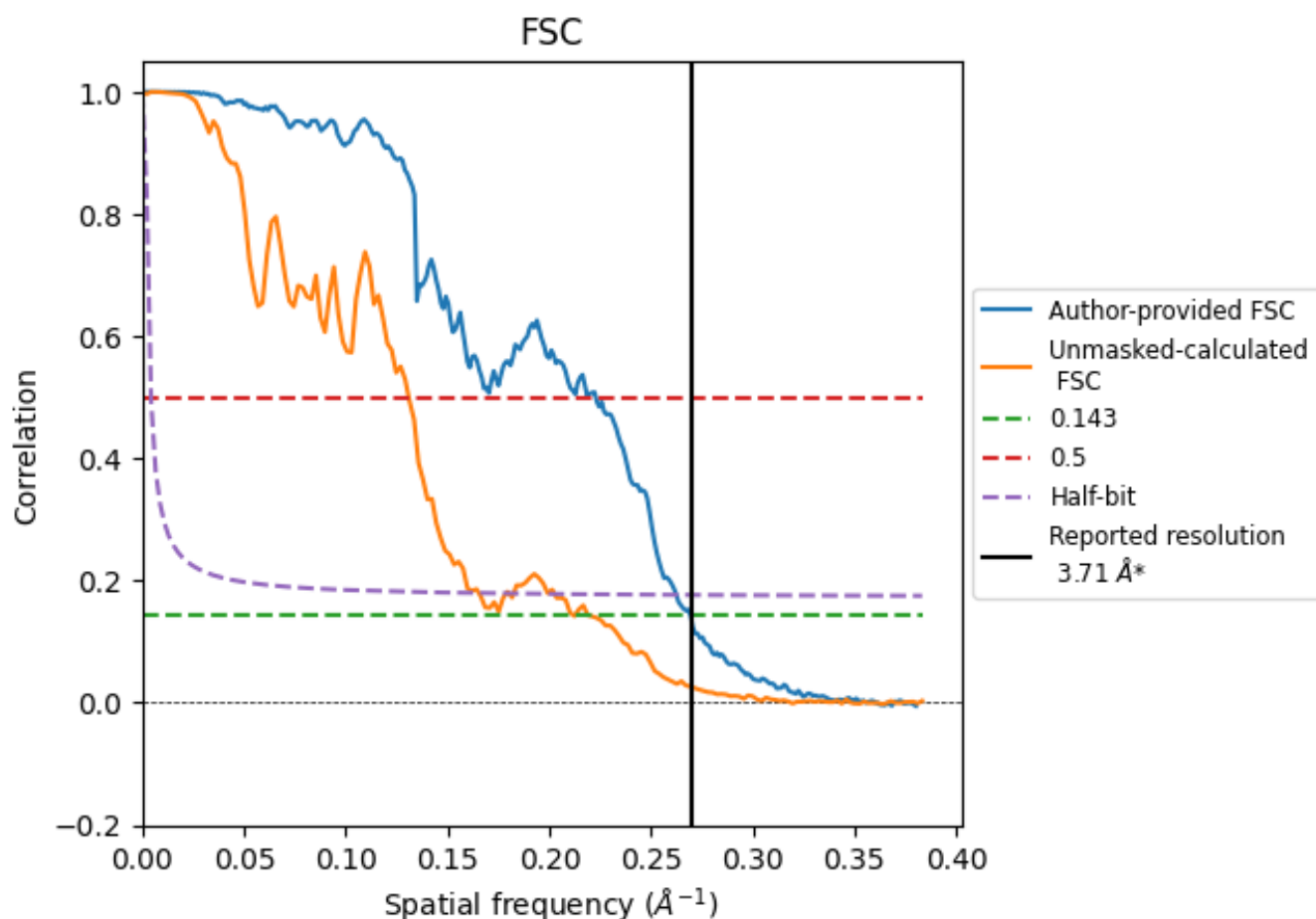


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.71	-	-
Author-provided FSC curve	3.71	4.49	3.81
Unmasked-calculated*	4.72	7.63	6.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.72 differs from the reported value 3.71 by more than 10 %

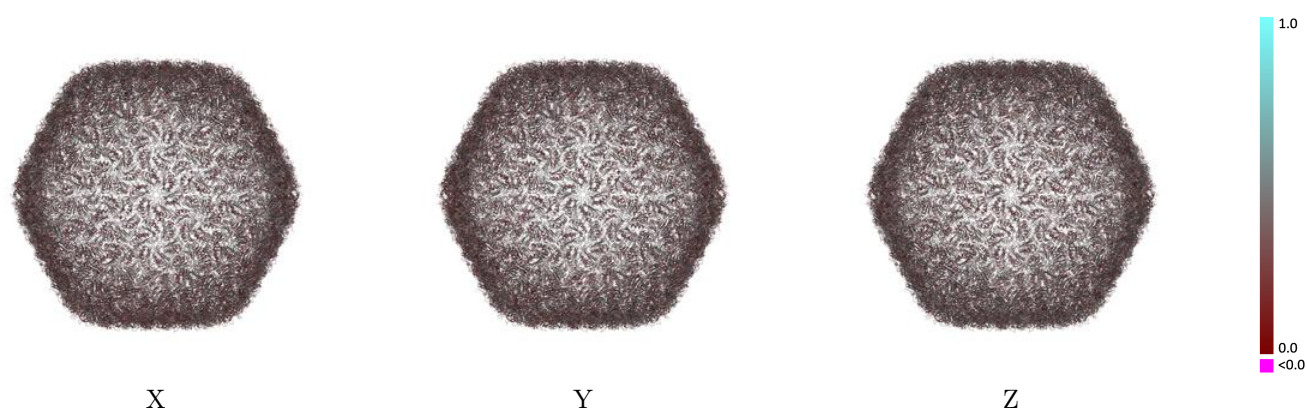
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62529 and PDB model 9LY9. Per-residue inclusion information can be found in section 3 on page 99.

9.1 Map-model overlay [i](#)

This section was not generated.

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

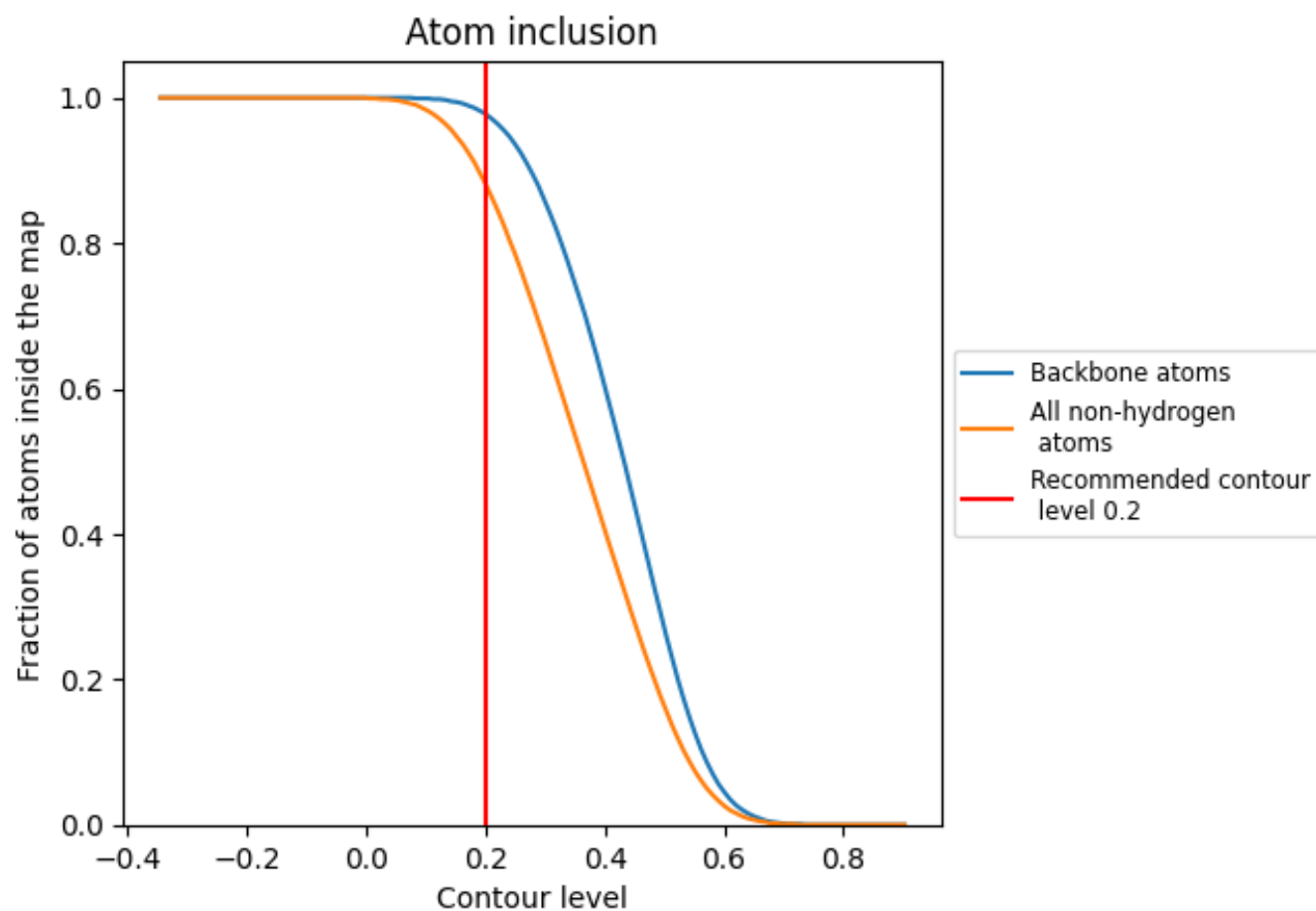


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8820	 0.3610
A0	 0.9060	 0.3710
A1	 0.9300	 0.3930
A2	 0.9360	 0.3980
A3	 0.8990	 0.3820
A4	 0.9170	 0.4000
A5	 0.9200	 0.3730
A6	 0.9270	 0.3890
A7	 0.9080	 0.3790
A8	 0.9080	 0.3860
A9	 0.9240	 0.3800
AA	 0.9450	 0.3810
AB	 0.9190	 0.3660
AC	 0.8130	 0.3730
AD	 0.8720	 0.3520
AE	 0.9410	 0.3940
AF	 0.9220	 0.3860
AG	 0.9330	 0.3830
AH	 0.8240	 0.3590
AI	 0.8270	 0.3560
AJ	 0.9270	 0.3630
AK	 0.9190	 0.3700
AL	 0.8990	 0.3890
AM	 0.9170	 0.3750
AN	 0.9080	 0.3800
AO	 0.9020	 0.3610
AP	 0.9050	 0.3660
AQ	 0.9050	 0.3710
AR	 0.9310	 0.3840
AS	 0.9140	 0.3730
AT	 0.8500	 0.3590
AU	 0.8530	 0.3480
AV	 0.8990	 0.3660
AW	 0.8880	 0.3690
AX	 0.9470	 0.4000



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
AY	 0.9220	 0.3830
AZ	 0.9080	 0.3550
Aa	 0.7830	 0.3570
Ab	 0.8880	 0.3560
Ac	 0.9200	 0.3770
Ad	 0.9280	 0.3690
Ae	 0.9050	 0.3750
Af	 0.9140	 0.3880
Ag	 0.9110	 0.3840
Ah	 0.9240	 0.3800
Ai	 0.9170	 0.3860
Aj	 0.8990	 0.3900
Ak	 0.9060	 0.3800
Al	 0.9280	 0.4010
Am	 0.9020	 0.3980
An	 0.9090	 0.3770
Ao	 0.9140	 0.3910
Ap	 0.9440	 0.4020
Aq	 0.9000	 0.3830
Ar	 0.8360	 0.3700
As	 0.8940	 0.3740
At	 0.9220	 0.3860
Au	 0.8580	 0.3770
Av	 0.8460	 0.3580
Aw	 0.8770	 0.3760
Ax	 0.9170	 0.3700
B0	 0.9310	 0.3850
B1	 0.8880	 0.3880
B2	 0.9310	 0.3970
B3	 0.9130	 0.3990
B4	 0.9130	 0.3870
B5	 0.9310	 0.3820
B6	 0.9050	 0.3790
B7	 0.9060	 0.3830
B8	 0.9060	 0.3780
B9	 0.9190	 0.3790
BA	 0.9200	 0.3800
BB	 0.9130	 0.3680
BC	 0.8330	 0.3720
BD	 0.8670	 0.3790
BE	 0.9240	 0.3750
BF	 0.9030	 0.3650

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BG	 0.9110	 0.3550
BH	 0.8940	 0.3830
BI	 0.8420	 0.3780
BJ	 0.9160	 0.3760
BK	 0.9200	 0.3680
BL	 0.9170	 0.4020
BM	 0.8880	 0.3710
BN	 0.9200	 0.3990
BO	 0.9300	 0.3910
BP	 0.8950	 0.3870
BQ	 0.9140	 0.3720
BR	 0.9000	 0.3650
BS	 0.9250	 0.3880
BT	 0.9030	 0.3610
BU	 0.8740	 0.3720
BV	 0.8770	 0.3690
BW	 0.9130	 0.3870
BX	 0.9310	 0.3920
BY	 0.9060	 0.3850
BZ	 0.8940	 0.3580
Ba	 0.8180	 0.3660
Bb	 0.8780	 0.3540
Bc	 0.9170	 0.3610
Bd	 0.8920	 0.3740
Be	 0.8880	 0.3770
Bf	 0.8860	 0.3750
Bg	 0.9160	 0.3910
Bh	 0.9110	 0.3800
Bi	 0.9130	 0.3790
Bj	 0.9190	 0.3970
Bk	 0.9090	 0.3800
Bl	 0.9060	 0.3680
Bm	 0.9250	 0.3830
Bn	 0.9000	 0.3740
Bo	 0.9060	 0.3770
Bp	 0.9220	 0.3900
Bq	 0.9130	 0.3850
Br	 0.8570	 0.3840
Bs	 0.8880	 0.3750
Bt	 0.9160	 0.3780
Bu	 0.8570	 0.3660
Bv	 0.8110	 0.3620

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Bw	 0.8710	 0.3600
Bx	 0.8990	 0.3700
C0	 0.9240	 0.3780
C1	 0.9280	 0.3740
C2	 0.9030	 0.3710
C3	 0.9170	 0.3880
C4	 0.9060	 0.3790
C5	 0.9190	 0.3770
C6	 0.9170	 0.3840
C7	 0.9160	 0.3710
C8	 0.9000	 0.3670
C9	 0.9300	 0.3820
CA	 0.9360	 0.3740
CB	 0.9090	 0.3820
CC	 0.8300	 0.3720
CD	 0.8910	 0.3830
CE	 0.9450	 0.3930
CF	 0.9110	 0.3710
CG	 0.9190	 0.3590
CH	 0.8740	 0.3600
CI	 0.8440	 0.3480
CJ	 0.9380	 0.3660
CK	 0.9340	 0.3840
CL	 0.9060	 0.3810
CM	 0.8850	 0.3740
CN	 0.8950	 0.3780
CO	 0.9340	 0.3850
CP	 0.8860	 0.3660
CQ	 0.9200	 0.3870
CR	 0.9060	 0.3710
CS	 0.9050	 0.3560
CT	 0.8690	 0.3740
CU	 0.8710	 0.3550
CV	 0.8830	 0.3610
CW	 0.9080	 0.3700
CX	 0.9190	 0.3750
CY	 0.9200	 0.3650
CZ	 0.9080	 0.3630
Ca	 0.8300	 0.3690
Cb	 0.8940	 0.3590
Cc	 0.9250	 0.3650
Cd	 0.8970	 0.3530

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Ce	 0.9090	 0.3830
Cf	 0.8810	 0.3680
Cg	 0.9110	 0.3790
Ch	 0.9080	 0.3680
Ci	 0.8920	 0.3630
Cj	 0.9250	 0.3820
Ck	 0.9220	 0.3860
Cl	 0.9020	 0.3760
Cm	 0.9140	 0.3810
Cn	 0.9090	 0.3860
Co	 0.9030	 0.3680
Cp	 0.8990	 0.3860
Cq	 0.8860	 0.3630
Cr	 0.8720	 0.3880
Cs	 0.8670	 0.3830
Ct	 0.9110	 0.3760
Cu	 0.8490	 0.3730
Cv	 0.8300	 0.3680
Cw	 0.9160	 0.3700
Cx	 0.9030	 0.3750
D0	 0.9360	 0.3810
D1	 0.9090	 0.3810
D2	 0.8830	 0.3560
D3	 0.8940	 0.3480
D4	 0.9440	 0.4130
D5	 0.9000	 0.3510
D6	 0.8970	 0.3630
D7	 0.9240	 0.4060
D8	 0.9060	 0.3690
D9	 0.9160	 0.3760
DA	 0.9360	 0.3710
DB	 0.8940	 0.4150
DC	 0.8460	 0.3670
DD	 0.9310	 0.4010
DE	 0.9190	 0.3660
DF	 0.9390	 0.4100
DG	 0.8910	 0.3430
DH	 0.8580	 0.3820
DI	 0.8920	 0.3670
DJ	 0.9330	 0.3990
DK	 0.9190	 0.3800
DL	 0.9110	 0.3520

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
DM	 0.9060	 0.3770
DN	 0.8880	 0.3470
DO	 0.9130	 0.3600
DP	 0.9090	 0.3630
DQ	 0.9420	 0.3800
DR	 0.9190	 0.3720
DS	 0.9390	 0.3950
DT	 0.8600	 0.3550
DU	 0.8570	 0.3690
DV	 0.8990	 0.3610
DW	 0.9320	 0.3850
DX	 0.9030	 0.3570
DY	 0.9300	 0.4060
DZ	 0.8630	 0.3350
Da	 0.8640	 0.3530
Db	 0.9440	 0.4140
Dc	 0.9020	 0.3620
Dd	 0.8750	 0.3590
De	 0.9030	 0.3520
Df	 0.8770	 0.3500
Dg	 0.9280	 0.3700
Dh	 0.9520	 0.4170
Di	 0.9110	 0.3640
Dj	 0.9290	 0.3890
Dk	 0.9130	 0.3780
Dl	 0.9230	 0.3850
Dm	 0.9200	 0.3620
Dn	 0.9390	 0.4060
Do	 0.9190	 0.3680
Dp	 0.9160	 0.3600
Dq	 0.9170	 0.4020
Dr	 0.8550	 0.3650
Ds	 0.9050	 0.3670
Dt	 0.9060	 0.3730
Du	 0.8530	 0.3760
Dv	 0.8950	 0.3630
Dw	 0.9470	 0.4150
Dx	 0.9170	 0.3810
E0	 0.9200	 0.3640
E1	 0.9160	 0.3630
E2	 0.8890	 0.3590
E3	 0.9330	 0.3880

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
E4	 0.9240	 0.3700
E5	 0.9090	 0.3760
E6	 0.9060	 0.3680
E7	 0.8920	 0.3680
E8	 0.9190	 0.3500
E9	 0.9310	 0.3800
EA	 0.9050	 0.3580
EB	 0.8280	 0.3470
EC	 0.8860	 0.3650
ED	 0.9240	 0.3600
EE	 0.9330	 0.3610
EF	 0.9500	 0.4190
EG	 0.8600	 0.3520
EH	 0.8520	 0.3490
EI	 0.8950	 0.3490
EJ	 0.9090	 0.3500
EK	 0.9340	 0.3620
EL	 0.9410	 0.4200
EM	 0.8850	 0.3610
EN	 0.9250	 0.3650
EO	 0.9280	 0.3690
EP	 0.9220	 0.3730
EQ	 0.9280	 0.3660
ER	 0.9270	 0.3690
ES	 0.8880	 0.3550
ET	 0.8800	 0.3520
EU	 0.8210	 0.3450
EV	 0.8940	 0.3730
EW	 0.9230	 0.3790
EX	 0.9160	 0.3570
EY	 0.8940	 0.3610
EZ	 0.8750	 0.3400
Ea	 0.8990	 0.3460
Eb	 0.9110	 0.3460
Ec	 0.9080	 0.3560
Ed	 0.8660	 0.3480
Ee	 0.8950	 0.3520
Ef	 0.9050	 0.3610
Eg	 0.9220	 0.3660
Eh	 0.9190	 0.3650
Ei	 0.9240	 0.3810
Ej	 0.9110	 0.3740

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Ek	 0.9000	 0.3650
El	 0.9100	 0.3850
Em	 0.9000	 0.3740
En	 0.9020	 0.3540
Eo	 0.9190	 0.3780
Ep	 0.9130	 0.3730
Eq	 0.8670	 0.3740
Er	 0.8920	 0.3570
Es	 0.9090	 0.3710
Et	 0.8720	 0.3630
Eu	 0.8380	 0.3510
Ev	 0.8940	 0.3750
Ew	 0.9160	 0.3650
Ex	 0.9200	 0.3620
F0	 0.9280	 0.3660
F1	 0.9130	 0.3820
F2	 0.8990	 0.3720
F3	 0.8990	 0.3660
F4	 0.9270	 0.3750
F5	 0.9030	 0.3660
F6	 0.9280	 0.3810
F7	 0.9280	 0.3800
F8	 0.9130	 0.3420
F9	 0.9110	 0.3650
FA	 0.9250	 0.3590
FB	 0.8460	 0.3710
FC	 0.8600	 0.3610
FD	 0.9050	 0.3660
FE	 0.9190	 0.3690
FF	 0.9370	 0.4040
FG	 0.8970	 0.3550
FH	 0.8110	 0.3430
FI	 0.8950	 0.3650
FJ	 0.8950	 0.3650
FK	 0.9110	 0.3580
FL	 0.9000	 0.3760
FM	 0.9140	 0.3710
FN	 0.9140	 0.3650
FO	 0.9020	 0.3510
FP	 0.9200	 0.3560
FQ	 0.8970	 0.3600
FR	 0.9490	 0.3680

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
FS	 0.8940	 0.3500
FT	 0.8850	 0.3550
FU	 0.8250	 0.3640
FV	 0.9000	 0.3820
FW	 0.9110	 0.3660
FX	 0.9090	 0.3720
FY	 0.8880	 0.3520
FZ	 0.8780	 0.3470
Fa	 0.8580	 0.3530
Fb	 0.9110	 0.3680
Fc	 0.8990	 0.3520
Fd	 0.8770	 0.3510
Fe	 0.8830	 0.3550
Ff	 0.9110	 0.3860
Fg	 0.9030	 0.3610
Fh	 0.9390	 0.3750
Fi	 0.8920	 0.3560
Fj	 0.9130	 0.3820
Fk	 0.8970	 0.3560
Fl	 0.9030	 0.3810
Fm	 0.8890	 0.3610
Fn	 0.9140	 0.3570
Fo	 0.9190	 0.3790
Fp	 0.9390	 0.3800
Fq	 0.8890	 0.3760
Fr	 0.8710	 0.3740
Fs	 0.9300	 0.3900
Ft	 0.9060	 0.3810
Fu	 0.8240	 0.3550
Fv	 0.8940	 0.3620
Fw	 0.9060	 0.3620
Fx	 0.9090	 0.3560
G0	 0.9520	 0.4280
G1	 0.9050	 0.3760
G2	 0.9250	 0.4090
G3	 0.8810	 0.3810
G4	 0.9030	 0.3780
G5	 0.8850	 0.3670
G6	 0.9170	 0.3870
G7	 0.8950	 0.3780
G8	 0.9050	 0.3870
G9	 0.9340	 0.3830

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
GA	 0.9440	 0.3910
GB	 0.8690	 0.3790
GC	 0.8520	 0.3720
GD	 0.9270	 0.3870
GE	 0.9380	 0.3860
GF	 0.9080	 0.3880
GG	 0.9130	 0.3720
GH	 0.8240	 0.3690
GI	 0.9170	 0.3960
GJ	 0.9200	 0.3550
GK	 0.9280	 0.3780
GL	 0.8890	 0.3760
GM	 0.8860	 0.3730
GN	 0.8890	 0.3710
GO	 0.9030	 0.3780
GP	 0.8990	 0.3690
GQ	 0.9090	 0.3910
GR	 0.9080	 0.3760
GS	 0.8860	 0.3410
GT	 0.8640	 0.3670
GU	 0.8320	 0.3590
GV	 0.8830	 0.3720
GW	 0.9360	 0.3930
GX	 0.9130	 0.3850
GY	 0.8950	 0.3670
GZ	 0.8800	 0.3650
Ga	 0.8390	 0.3600
Gb	 0.9220	 0.3800
Gc	 0.9080	 0.3720
Gd	 0.8850	 0.3640
Ge	 0.8890	 0.3750
Gf	 0.8910	 0.3890
Gg	 0.8970	 0.3830
Gh	 0.9060	 0.3770
Gi	 0.9000	 0.3740
Gj	 0.9350	 0.4160
Gk	 0.8890	 0.3720
Gl	 0.9260	 0.4010
Gm	 0.9000	 0.3780
Gn	 0.9050	 0.3700
Go	 0.8860	 0.3670
Gp	 0.9110	 0.3860

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Gq	 0.8580	 0.3790
Gr	 0.8720	 0.3800
Gs	 0.8970	 0.3820
Gt	 0.8880	 0.3820
Gu	 0.8320	 0.3710
Gv	 0.8860	 0.3820
Gw	 0.9160	 0.3780
Gx	 0.9130	 0.3840
H0	 0.9000	 0.3760
H1	 0.8950	 0.3870
H2	 0.9330	 0.3780
H3	 0.8940	 0.3840
H4	 0.9390	 0.3920
H5	 0.9310	 0.3900
H6	 0.9410	 0.3940
H7	 0.9280	 0.3800
H8	 0.9090	 0.3810
H9	 0.9440	 0.3720
HA	 0.9410	 0.3830
HB	 0.8780	 0.3750
HC	 0.8520	 0.3720
HD	 0.9050	 0.3530
HE	 0.9610	 0.3980
HF	 0.9310	 0.3910
HG	 0.9130	 0.3690
HH	 0.8270	 0.3590
HI	 0.8950	 0.3600
HJ	 0.9250	 0.3760
HK	 0.9340	 0.3780
HL	 0.9020	 0.3760
HM	 0.9240	 0.3920
HN	 0.9360	 0.3820
HO	 0.9130	 0.3760
HP	 0.9170	 0.3700
HQ	 0.8910	 0.3630
HR	 0.9380	 0.3890
HS	 0.8800	 0.3650
HT	 0.8830	 0.3680
HU	 0.8380	 0.3720
HV	 0.9110	 0.3800
HW	 0.8950	 0.3630
HX	 0.9310	 0.3810

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
HY	 0.9300	 0.3710
HZ	 0.8990	 0.3800
Ha	 0.8580	 0.3560
Hb	 0.9280	 0.3620
Hc	 0.9060	 0.3580
Hd	 0.9020	 0.3590
He	 0.8920	 0.3800
Hf	 0.9140	 0.3930
Hg	 0.9000	 0.3660
Hh	 0.9360	 0.3900
Hi	 0.9090	 0.3830
Hj	 0.9160	 0.3770
Hk	 0.8990	 0.3660
Hl	 0.9390	 0.3950
Hm	 0.9080	 0.3880
Hz	 0.9300	 0.3930
Ho	 0.9360	 0.3970
Hp	 0.9390	 0.4050
Hq	 0.8890	 0.3840
Hr	 0.8520	 0.3760
Hs	 0.9390	 0.3950
Ht	 0.8890	 0.3810
Hu	 0.8280	 0.3740
Hv	 0.8890	 0.3660
Hw	 0.8950	 0.3630
Hx	 0.9250	 0.3760
I0	 0.9110	 0.3750
I1	 0.9140	 0.3750
I2	 0.8950	 0.3900
I3	 0.9060	 0.3760
I4	 0.9200	 0.3760
I5	 0.9190	 0.3800
I6	 0.8890	 0.3600
I7	 0.9060	 0.3720
I8	 0.9110	 0.3700
I9	 0.9470	 0.3990
IA	 0.9200	 0.3720
IB	 0.8440	 0.3570
IC	 0.8780	 0.3820
ID	 0.9450	 0.3880
IE	 0.9410	 0.3840
IF	 0.9200	 0.3850

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
IG	 0.9080	 0.3700
IH	 0.8330	 0.3420
II	 0.9000	 0.3860
IJ	 0.9170	 0.3820
IK	 0.9270	 0.3800
IL	 0.9190	 0.3820
IM	 0.8990	 0.3770
IN	 0.9310	 0.3770
IO	 0.9080	 0.3560
IP	 0.9410	 0.3900
IQ	 0.9170	 0.3730
IR	 0.9200	 0.3790
IS	 0.8970	 0.3860
IT	 0.8710	 0.3690
IU	 0.8470	 0.3540
IV	 0.8990	 0.3690
IW	 0.9130	 0.3670
IX	 0.8950	 0.3630
IY	 0.9000	 0.3600
IZ	 0.8740	 0.3520
Ia	 0.8720	 0.3640
Ib	 0.9270	 0.3820
Ic	 0.9000	 0.3590
Id	 0.8740	 0.3630
Ie	 0.8690	 0.3640
If	 0.9000	 0.3790
Ig	 0.9190	 0.3620
Ih	 0.9030	 0.3710
Ii	 0.9000	 0.3710
Ij	 0.9330	 0.3900
Ik	 0.9000	 0.3720
Il	 0.8970	 0.3760
Im	 0.8920	 0.3780
In	 0.8990	 0.3760
Io	 0.9200	 0.3690
Ip	 0.9190	 0.3800
Iq	 0.8710	 0.3770
Ir	 0.8610	 0.3750
Is	 0.9420	 0.3930
It	 0.8890	 0.3720
Iu	 0.8080	 0.3590
Iv	 0.8780	 0.3680

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Iw	 0.9240	 0.3900
Ix	 0.9200	 0.3770
J0	 0.9160	 0.3520
J1	 0.9170	 0.3730
J2	 0.8990	 0.3690
J3	 0.9130	 0.3850
J4	 0.9280	 0.3720
J5	 0.9000	 0.3640
J6	 0.9160	 0.3850
J7	 0.8990	 0.3620
J8	 0.9090	 0.3680
J9	 0.9110	 0.3760
JA	 0.9270	 0.3650
JB	 0.8740	 0.3580
JC	 0.8330	 0.3740
JD	 0.9190	 0.3660
JE	 0.9330	 0.3700
JF	 0.9130	 0.3650
JG	 0.9140	 0.3730
JH	 0.8070	 0.3390
JI	 0.8740	 0.3420
JJ	 0.8890	 0.3620
JK	 0.9060	 0.3520
JL	 0.8950	 0.3570
JM	 0.9030	 0.3610
JN	 0.9190	 0.3580
JO	 0.9130	 0.3590
JP	 0.9130	 0.3440
JQ	 0.8940	 0.3480
JR	 0.9050	 0.3610
JS	 0.9190	 0.3510
JT	 0.8630	 0.3500
JU	 0.8660	 0.3460
JV	 0.8830	 0.3680
JW	 0.9020	 0.3600
JX	 0.9160	 0.3700
JY	 0.9000	 0.3470
JZ	 0.8810	 0.3600
Ja	 0.8350	 0.3430
Jb	 0.9300	 0.3520
Jc	 0.8950	 0.3500
Jd	 0.8990	 0.3520

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Je	 0.8950	 0.3530
Jf	 0.9080	 0.3700
Jg	 0.9110	 0.3580
Jh	 0.9080	 0.3540
Ji	 0.9280	 0.3710
Jj	 0.9060	 0.3580
Jk	 0.9080	 0.3670
Jl	 0.9000	 0.3730
Jm	 0.9030	 0.3490
Jn	 0.8970	 0.3440
Jo	 0.9200	 0.3660
Jp	 0.9310	 0.3740
Jq	 0.9060	 0.3530
Jr	 0.8460	 0.3480
Js	 0.9160	 0.3680
Jt	 0.9110	 0.3750
Ju	 0.8100	 0.3570
Jv	 0.9200	 0.3980
Jw	 0.9080	 0.3630
Jx	 0.9110	 0.3590
K0	 0.9030	 0.3810
K1	 0.9130	 0.3810
K2	 0.8950	 0.3690
K3	 0.9030	 0.3760
K4	 0.9000	 0.3740
K5	 0.9110	 0.3890
K6	 0.8920	 0.3700
K7	 0.9000	 0.3750
K8	 0.9060	 0.3670
K9	 0.9300	 0.3840
KA	 0.9170	 0.3520
KB	 0.8750	 0.3610
KC	 0.8460	 0.3800
KD	 0.9130	 0.3640
KE	 0.9160	 0.3530
KF	 0.9080	 0.3750
KG	 0.9060	 0.3780
KH	 0.8570	 0.3590
KI	 0.8690	 0.3590
KJ	 0.9250	 0.3770
KK	 0.9080	 0.3670
KL	 0.9050	 0.3760

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
KM	 0.8800	 0.3600
KN	 0.9170	 0.3740
KO	 0.9250	 0.3730
KP	 0.9360	 0.3850
KQ	 0.9080	 0.3700
KR	 0.9030	 0.3590
KS	 0.9190	 0.3780
KT	 0.8570	 0.3600
KU	 0.8520	 0.3520
KV	 0.8970	 0.3790
KW	 0.9130	 0.3850
KX	 0.9080	 0.3690
KY	 0.8940	 0.3600
KZ	 0.8710	 0.3600
Ka	 0.8190	 0.3540
Kb	 0.9380	 0.3750
Kc	 0.8830	 0.3590
Kd	 0.9000	 0.3750
Ke	 0.9030	 0.3730
Kf	 0.8950	 0.3750
Kg	 0.9250	 0.3760
Kh	 0.8850	 0.3510
Ki	 0.9140	 0.3890
Kj	 0.9140	 0.3860
Kk	 0.9270	 0.3910
Kl	 0.9130	 0.3610
Km	 0.9020	 0.3730
Kn	 0.9220	 0.3790
Ko	 0.9250	 0.3890
Kp	 0.9030	 0.3620
Kq	 0.9140	 0.3920
Kr	 0.8390	 0.3690
Ks	 0.9270	 0.3770
Kt	 0.9060	 0.3610
Ku	 0.8210	 0.3650
Kv	 0.8800	 0.3650
Kw	 0.9060	 0.3630
Kx	 0.9020	 0.3660
L0	 0.9310	 0.3740
L1	 0.9030	 0.3670
L2	 0.9170	 0.3770
L3	 0.8990	 0.3630

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
L4	 0.9200	 0.3750
L5	 0.9170	 0.3750
L6	 0.9170	 0.3610
L7	 0.9000	 0.3700
L8	 0.9110	 0.3590
L9	 0.9190	 0.3540
LA	 0.9220	 0.3640
LB	 0.9090	 0.3700
LC	 0.8380	 0.3670
LD	 0.9190	 0.3570
LE	 0.9390	 0.3870
LF	 0.9170	 0.3530
LG	 0.9160	 0.3630
LH	 0.8320	 0.3330
LI	 0.8720	 0.3540
LJ	 0.9060	 0.3550
LK	 0.9110	 0.3640
LL	 0.8830	 0.3590
LM	 0.9200	 0.3760
LN	 0.8920	 0.3550
LO	 0.9420	 0.3700
LP	 0.9000	 0.3600
LQ	 0.9360	 0.3770
LR	 0.9080	 0.3600
LS	 0.8970	 0.3390
LT	 0.8530	 0.3450
LU	 0.8780	 0.3460
LV	 0.8830	 0.3490
LW	 0.9360	 0.3660
LX	 0.9130	 0.3730
LY	 0.9020	 0.3540
LZ	 0.9090	 0.3490
La	 0.8300	 0.3510
Lb	 0.9250	 0.3500
Lc	 0.9390	 0.3580
Ld	 0.9000	 0.3640
Le	 0.9140	 0.3620
Lf	 0.8810	 0.3480
Lg	 0.9250	 0.3800
Lh	 0.9200	 0.3650
Li	 0.9000	 0.3560
Lj	 0.9410	 0.3880

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Lk	 0.9270	 0.3760
Ll	 0.8920	 0.3570
Lm	 0.9590	 0.4170
Ln	 0.9200	 0.3590
Lo	 0.9160	 0.3570
Lp	 0.9190	 0.3810
Lq	 0.9060	 0.3500
Lr	 0.8470	 0.3580
Ls	 0.9050	 0.3680
Lt	 0.9050	 0.3690
Lu	 0.8320	 0.3630
Lv	 0.8890	 0.3550
Lw	 0.9050	 0.3480
Lx	 0.9250	 0.3800
M0	 0.9160	 0.3740
M1	 0.9280	 0.3860
M2	 0.9050	 0.3760
M3	 0.9110	 0.3760
M4	 0.9110	 0.3500
M5	 0.9190	 0.3880
M6	 0.8890	 0.3540
M7	 0.8990	 0.3650
M8	 0.9060	 0.3690
M9	 0.9140	 0.3770
MA	 0.9090	 0.3630
MB	 0.9080	 0.3550
MC	 0.8280	 0.3570
MD	 0.9170	 0.3660
ME	 0.9030	 0.3660
MF	 0.9130	 0.3680
MG	 0.9110	 0.3650
MH	 0.8270	 0.3410
MI	 0.8810	 0.3440
MJ	 0.9170	 0.3700
MK	 0.9160	 0.3640
ML	 0.9240	 0.3710
MM	 0.9030	 0.3700
MN	 0.9200	 0.3710
MO	 0.9200	 0.3810
MP	 0.9270	 0.3640
MQ	 0.8920	 0.3620
MR	 0.9090	 0.3720

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
MS	 0.9130	 0.3460
MT	 0.8410	 0.3490
MU	 0.8780	 0.3390
MV	 0.8990	 0.3750
MW	 0.9170	 0.3710
MX	 0.9170	 0.3620
MY	 0.9270	 0.3850
MZ	 0.8910	 0.3540
Ma	 0.8210	 0.3440
Mb	 0.9200	 0.3470
Mc	 0.9080	 0.3610
Md	 0.8890	 0.3630
Me	 0.9020	 0.3730
Mf	 0.8970	 0.3650
Mg	 0.9140	 0.3710
Mh	 0.8970	 0.3630
Mi	 0.9330	 0.3840
Mj	 0.9170	 0.3660
Mk	 0.9110	 0.3600
ML	 0.9060	 0.3620
Mm	 0.9160	 0.3750
Mn	 0.9030	 0.3740
Mo	 0.9200	 0.3820
Mp	 0.9200	 0.3750
Mq	 0.9280	 0.3650
Mr	 0.8350	 0.3670
Ms	 0.9240	 0.3730
Mt	 0.9190	 0.3670
Mu	 0.8110	 0.3470
Mv	 0.8770	 0.3440
Mw	 0.9030	 0.3630
Mx	 0.9020	 0.3710
N0	 0.9060	 0.3700
N1	 0.9080	 0.3720
N2	 0.9020	 0.3670
N3	 0.8860	 0.3670
N4	 0.9170	 0.3640
N5	 0.9140	 0.3780
N6	 0.9050	 0.3720
N7	 0.8970	 0.3660
N8	 0.8950	 0.3390
N9	 0.9240	 0.3620

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
NA	 0.9250	 0.3700
NB	 0.9060	 0.3710
NC	 0.8220	 0.3620
ND	 0.9050	 0.3650
NE	 0.9140	 0.3650
NF	 0.9110	 0.3660
NG	 0.9310	 0.3720
NH	 0.8160	 0.3310
NI	 0.8270	 0.3350
NJ	 0.9050	 0.3590
NK	 0.8920	 0.3500
NL	 0.8830	 0.3710
NM	 0.9170	 0.3600
NN	 0.9020	 0.3670
NO	 0.8880	 0.3400
NP	 0.9280	 0.3810
NQ	 0.8990	 0.3500
NR	 0.9060	 0.3600
NS	 0.9190	 0.3720
NT	 0.8610	 0.3540
NU	 0.8580	 0.3450
NV	 0.8830	 0.3690
NW	 0.8910	 0.3550
NX	 0.9160	 0.3550
NY	 0.9200	 0.3780
NZ	 0.8810	 0.3460
Na	 0.8030	 0.3470
Nb	 0.9090	 0.3540
Nc	 0.8990	 0.3550
Nd	 0.8990	 0.3630
Ne	 0.9060	 0.3600
Nf	 0.8970	 0.3620
Ng	 0.8970	 0.3640
Nh	 0.8950	 0.3570
Ni	 0.9050	 0.3580
Nj	 0.9030	 0.3560
Nk	 0.9030	 0.3650
Nl	 0.9060	 0.3610
Nm	 0.8920	 0.3610
Nn	 0.9080	 0.3540
No	 0.9060	 0.3660
Np	 0.9360	 0.3780

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Nq	 0.9050	 0.3600
Nr	 0.8410	 0.3710
Ns	 0.9190	 0.3790
Nt	 0.9130	 0.3690
Nu	 0.8460	 0.3730
Nv	 0.8640	 0.3550
Nw	 0.8890	 0.3520
Nx	 0.8970	 0.3580
O0	 0.9340	 0.3740
O1	 0.9190	 0.3930
O2	 0.9020	 0.3690
O3	 0.8880	 0.3730
O4	 0.9130	 0.3680
O5	 0.8940	 0.3700
O6	 0.9050	 0.3760
O7	 0.8940	 0.3680
O8	 0.9140	 0.3650
O9	 0.9030	 0.3680
OA	 0.9280	 0.3670
OB	 0.8470	 0.3530
OC	 0.8460	 0.3710
OD	 0.9390	 0.3670
OE	 0.9270	 0.3820
OF	 0.8950	 0.3620
OG	 0.8850	 0.3580
OH	 0.8080	 0.3580
OI	 0.8910	 0.3610
OJ	 0.9160	 0.3740
OK	 0.9160	 0.3620
OL	 0.9220	 0.3820
OM	 0.9130	 0.3830
ON	 0.8990	 0.3620
OO	 0.9160	 0.3730
OP	 0.8920	 0.3440
OQ	 0.9280	 0.3780
OR	 0.9270	 0.3780
OS	 0.9130	 0.3640
OT	 0.8470	 0.3470
OU	 0.8460	 0.3550
OV	 0.8860	 0.3620
OW	 0.9220	 0.3670
OX	 0.9060	 0.3740

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
OY	 0.9110	 0.3710
OZ	 0.8570	 0.3570
Oa	 0.8460	 0.3580
Ob	 0.9220	 0.3640
Oc	 0.9170	 0.3630
Od	 0.9030	 0.3680
Oe	 0.9200	 0.3860
Of	 0.9000	 0.3740
Og	 0.9280	 0.3770
Oh	 0.9310	 0.3810
Oi	 0.8940	 0.3650
Oj	 0.9270	 0.3870
Ok	 0.9190	 0.3710
Ol	 0.8890	 0.3660
Om	 0.9190	 0.3780
On	 0.9060	 0.3680
Oo	 0.8860	 0.3610
Op	 0.9310	 0.3830
Oq	 0.8970	 0.3770
Or	 0.8630	 0.3640
Os	 0.9160	 0.3720
Ot	 0.8940	 0.3700
Ou	 0.8070	 0.3610
Ov	 0.8750	 0.3670
Ow	 0.9240	 0.3630
Ox	 0.9140	 0.3590
P0	 0.7810	 0.3380
P1	 0.7480	 0.3550
P2	 0.7930	 0.3450
P3	 0.7520	 0.3360
P4	 0.7790	 0.3430
P5	 0.7490	 0.3420
P6	 0.8010	 0.3680
P7	 0.7510	 0.3520
P8	 0.7860	 0.3610
P9	 0.8030	 0.3460
PA	 0.7880	 0.3430
PB	 0.6770	 0.3520
PC	 0.7070	 0.3550
PD	 0.8110	 0.3750
PE	 0.8040	 0.3350
PF	 0.7690	 0.3340

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
PG	 0.7060	 0.3330
PH	 0.6350	 0.3370
PI	 0.7410	 0.3230
PJ	 0.7830	 0.3180
PK	 0.7490	 0.3090
PL	 0.7380	 0.3580
PM	 0.7560	 0.3530
PN	 0.7860	 0.3250
PO	 0.7620	 0.3390
PP	 0.7510	 0.3320
PQ	 0.7490	 0.3380
PR	 0.7440	 0.3260
PS	 0.7220	 0.3270
PT	 0.7160	 0.3480
PU	 0.6400	 0.3520
PV	 0.7680	 0.3550
PW	 0.7560	 0.3420
PX	 0.7540	 0.3220
PY	 0.7520	 0.3440
PZ	 0.7430	 0.3470
Pa	 0.6870	 0.3270
Pb	 0.7410	 0.3440
Pc	 0.7380	 0.3310
Pd	 0.6940	 0.3270
Pe	 0.7120	 0.3390
Pf	 0.7430	 0.3360
Pg	 0.7320	 0.3320
Ph	 0.7760	 0.3610
Pi	 0.7170	 0.3450
Pj	 0.7410	 0.3410
Pk	 0.7560	 0.3430
Pl	 0.7560	 0.3350
Pm	 0.7810	 0.3460
Pn	 0.7730	 0.3480
Po	 0.7960	 0.3580
Pp	 0.7070	 0.3430
Pq	 0.6550	 0.3420
Pr	 0.6820	 0.3460
Ps	 0.7440	 0.3470
Pt	 0.6840	 0.3400
Pu	 0.6190	 0.3420
Pv	 0.6640	 0.3390

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Pw	 0.7490	 0.3630
Px	 0.7480	 0.3400
X0	 0.8760	 0.3620
X1	 0.7700	 0.3480
X2	 0.8390	 0.3380
X3	 0.8560	 0.3490
X4	 0.8600	 0.3500
X5	 0.8720	 0.3470
X6	 0.8580	 0.3610
X7	 0.8070	 0.3460
X8	 0.8270	 0.3550
X9	 0.7870	 0.3540
XA	 0.7930	 0.3470
XB	 0.7560	 0.2800
XC	 0.8450	 0.3010
XD	 0.8520	 0.2910
XE	 0.7950	 0.2930
XF	 0.7400	 0.2260
XG	 0.7680	 0.2330
XH	 0.8470	 0.2210
XI	 0.7890	 0.2850
XJ	 0.6670	 0.2610
XK	 0.7790	 0.2680
XL	 0.7620	 0.2530
XM	 0.7280	 0.2820
XN	 0.8540	 0.3150
XO	 0.7460	 0.2410
XP	 0.7990	 0.2330
XQ	 0.7850	 0.2340
XR	 0.8010	 0.2590
XS	 0.8010	 0.2810
XT	 0.8600	 0.2590
XU	 0.7030	 0.2270
XV	 0.6160	 0.2430
XW	 0.7680	 0.2220
XX	 0.7740	 0.2670
XY	 0.6810	 0.2370
XZ	 0.6420	 0.2530
Xa	 0.8350	 0.2540
Xb	 0.7320	 0.1970
Xc	 0.7600	 0.2330
Xd	 0.6500	 0.2520

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Xe	 0.6530	 0.2410
Xf	 0.7640	 0.2370
Xg	 0.7950	 0.2790
Xh	 0.7600	 0.2270
Xi	 0.8130	 0.2680
Xj	 0.7970	 0.2590
Xk	 0.8190	 0.2630
Xl	 0.7700	 0.2260
Xm	 0.8560	 0.3170
Xn	 0.7440	 0.2550
Xo	 0.7700	 0.2310
Xp	 0.8230	 0.2660
Xq	 0.8210	 0.2630
Xr	 0.7910	 0.2890
Xs	 0.8190	 0.2690
Xt	 0.8050	 0.2390
Xu	 0.8050	 0.2650
Xv	 0.7830	 0.2600
Xw	 0.6480	 0.2140
Xx	 0.7560	 0.2490
Y0	 0.8520	 0.3470
Y1	 0.8230	 0.3290
Y2	 0.8310	 0.3390
Y3	 0.8390	 0.3400
Y4	 0.8260	 0.3240
Y5	 0.8110	 0.3390
Y6	 0.8110	 0.3280
Y7	 0.8290	 0.3490
Y8	 0.8490	 0.3610
Y9	 0.8550	 0.3450
YA	 0.8460	 0.3330
YB	 0.8650	 0.3430
YC	 0.8940	 0.3500
YD	 0.8710	 0.3480
YE	 0.8530	 0.3370
YF	 0.7960	 0.3090
YG	 0.8600	 0.3050
YH	 0.8360	 0.3180
YI	 0.7780	 0.3170
YJ	 0.8270	 0.3350
YK	 0.8510	 0.3200
YL	 0.8070	 0.3210

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
YM	 0.8190	 0.3060
YN	 0.8300	 0.3220
YO	 0.8290	 0.3200
YP	 0.8500	 0.3160
YQ	 0.8630	 0.3260
YR	 0.8690	 0.3290
YS	 0.8560	 0.3160
YT	 0.8550	 0.3230
YU	 0.8600	 0.3010
YV	 0.8460	 0.3260
YW	 0.8200	 0.3030
YX	 0.7820	 0.3140
YY	 0.7510	 0.3190
YZ	 0.7530	 0.3120
Ya	 0.8640	 0.3150
Yb	 0.8110	 0.3150
Yc	 0.7870	 0.3130
Yd	 0.8280	 0.3210
Ye	 0.8140	 0.3220
Yf	 0.8430	 0.3250
Yg	 0.8370	 0.3140
Yh	 0.8280	 0.3260
Yi	 0.7810	 0.3030
Yj	 0.8570	 0.3270
Yk	 0.8580	 0.3270
Yl	 0.8340	 0.3170
Ym	 0.8130	 0.3240
Yn	 0.8280	 0.3230
Yo	 0.8250	 0.3180
Yp	 0.8590	 0.3370
Yq	 0.8280	 0.3180
Yr	 0.8430	 0.3190
Ys	 0.8530	 0.3400
Yt	 0.8400	 0.3180
Yu	 0.8290	 0.3210
Yv	 0.8030	 0.3260
Yw	 0.8480	 0.3270
Yx	 0.8530	 0.3270