



## wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 09:27 PM UTC

PDB ID : 9LY8 / pdb\_00009ly8  
EMDB ID : EMD-62530  
Title : Cryo-EM structure of carboxysomal midi-shell: T=9 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 : 2.77 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](mailto: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>.

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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

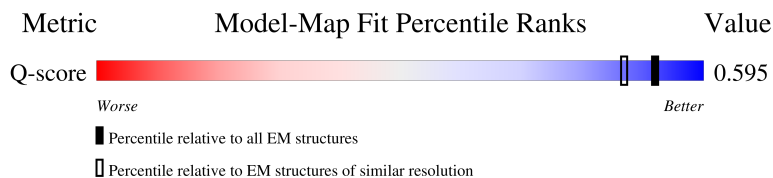
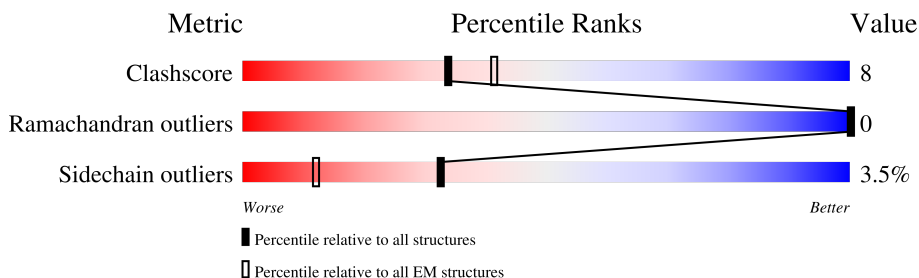
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.77 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.









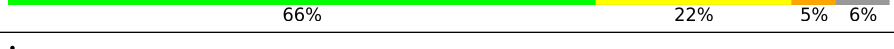
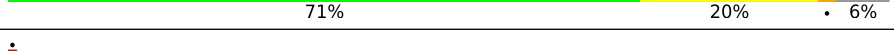
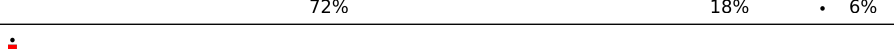
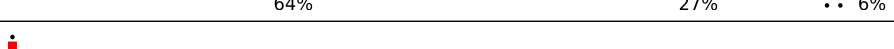
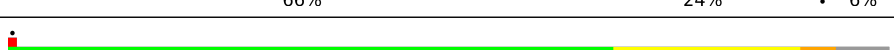

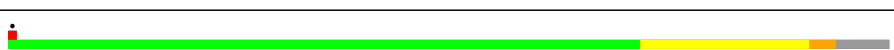

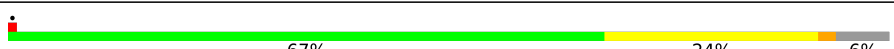





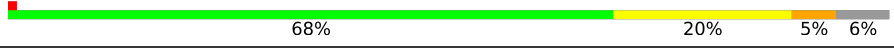
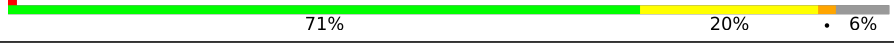



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10695 ( 2.27 - 3.27 )

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  $\geq 3$ , 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	 64% 26% • • 6%
1	A1	98	 65% 26% • 6%
1	A2	98	 67% 21% 5% 6% 6%
1	A3	98	 72% 19% • 6%







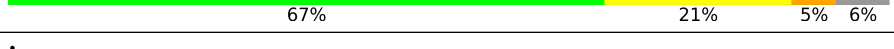
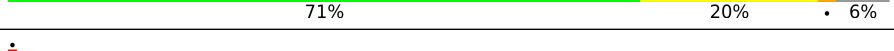
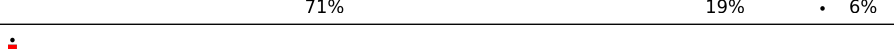
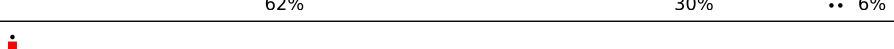
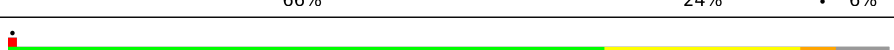

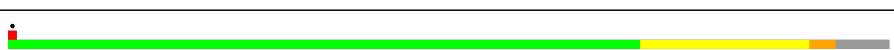

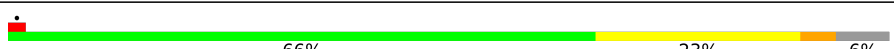





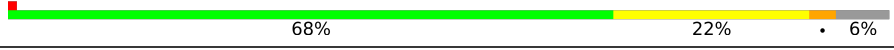
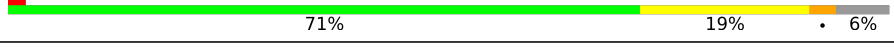



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Mol	Chain	Length	Quality of chain
1	A4	98	
1	A5	98	
1	A6	98	
1	A7	98	
1	A8	98	
1	A9	98	
1	AA	98	
1	AB	98	
1	AC	98	
1	AD	98	
1	AE	98	
1	AF	98	
1	AG	98	
1	AH	98	
1	AI	98	
1	AJ	98	
1	AK	98	
1	AL	98	
1	AM	98	
1	AN	98	
1	AO	98	
1	AP	98	
1	AQ	98	
1	AR	98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







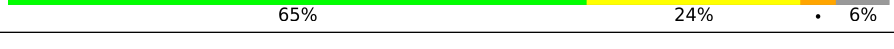
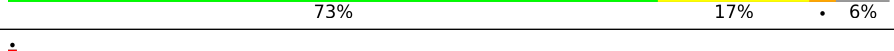
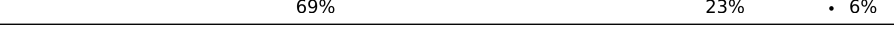
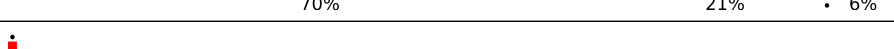
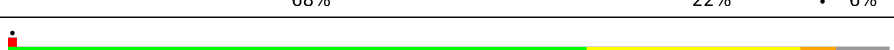

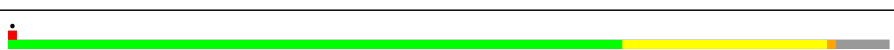

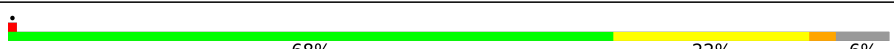





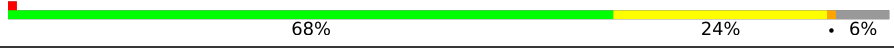
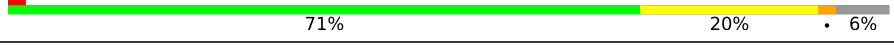



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Mol	Chain	Length	Quality of chain
1	AT	98	
1	AU	98	
1	AV	98	
1	AW	98	
1	AX	98	
1	Aa	98	
1	Ab	98	
1	Ac	98	
1	Ad	98	
1	Ae	98	
1	Af	98	
1	Ag	98	
1	Ah	98	
1	Ai	98	
1	Aj	98	
1	Ak	98	
1	Al	98	
1	Am	98	
1	An	98	
1	Ao	98	
1	Ap	98	
1	Aq	98	
1	Ar	98	
1	As	98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







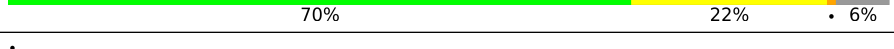
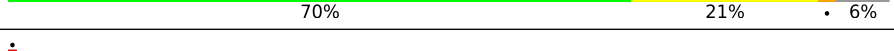
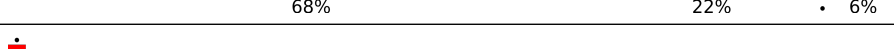
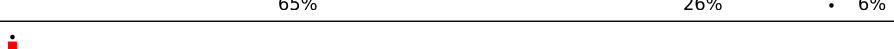
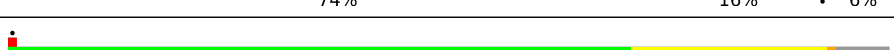

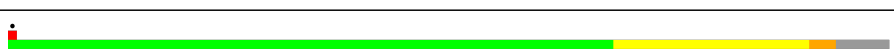

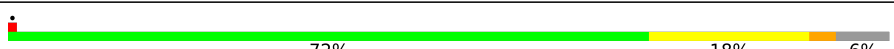





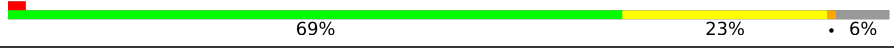
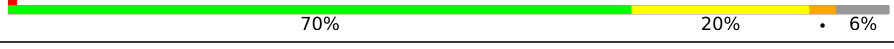



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Mol	Chain	Length	Quality of chain
1	Au	98	
1	Av	98	
1	Aw	98	
1	Ax	98	
1	Ay	98	
1	Az	98	
1	B0	98	
1	B1	98	
1	B2	98	
1	B3	98	
1	B4	98	
1	B5	98	
1	B6	98	
1	B7	98	
1	B8	98	
1	B9	98	
1	BA	98	
1	BB	98	
1	BC	98	
1	BD	98	
1	BE	98	
1	BF	98	
1	BG	98	
1	BH	98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







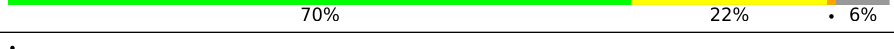
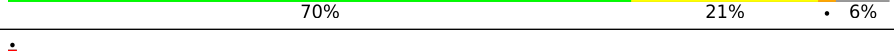
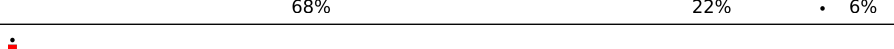
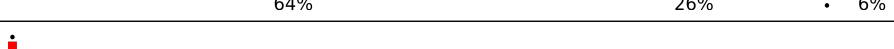
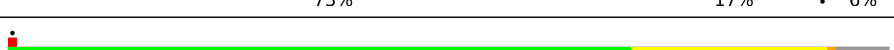

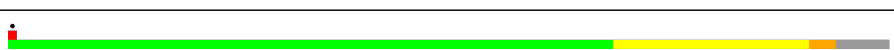

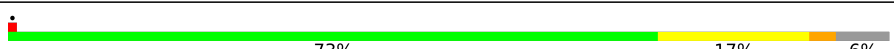





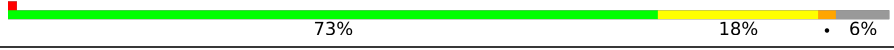
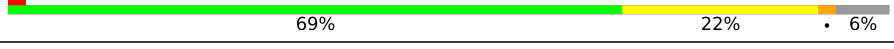



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Mol	Chain	Length	Quality of chain
1	BJ	98	
1	BK	98	
1	BL	98	
1	BM	98	
1	BN	98	
1	BO	98	
1	BP	98	
1	BQ	98	
1	BR	98	
1	BS	98	
1	BT	98	
1	BU	98	
1	BV	98	
1	BW	98	
1	BX	98	
1	Ba	98	
1	Bb	98	
1	Bc	98	
1	Bd	98	
1	Be	98	
1	Bf	98	
1	Bg	98	
1	Bh	98	
1	Bi	98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







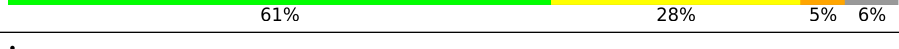
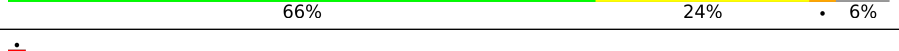
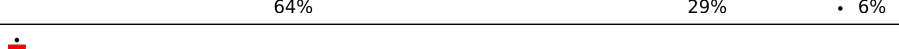
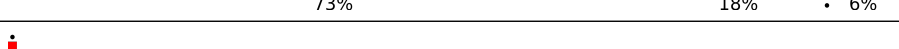
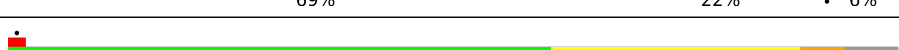

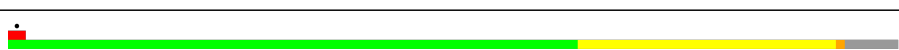

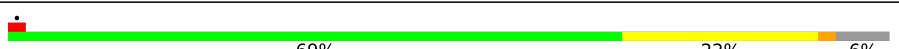





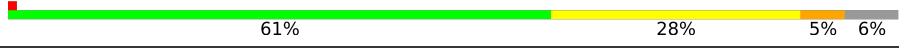
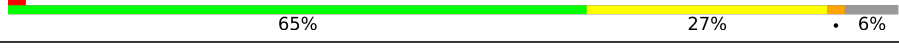



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Mol	Chain	Length	Quality of chain
1	Bk	98	
1	Bl	98	
1	Bm	98	
1	Bn	98	
1	Bo	98	
1	Bp	98	
1	Bq	98	
1	Br	98	
1	Bs	98	
1	Bt	98	
1	Bu	98	
1	Bv	98	
1	Bw	98	
1	Bx	98	
1	By	98	
1	Bz	98	
1	C0	98	
1	C1	98	
1	C2	98	
1	C3	98	
1	C4	98	
1	C5	98	
1	C6	98	
1	C7	98	
1	C8	98	







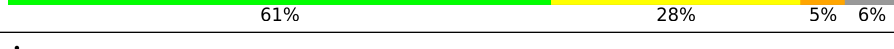
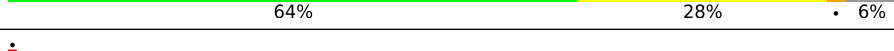
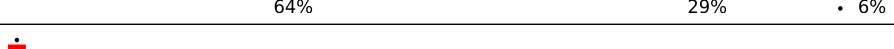
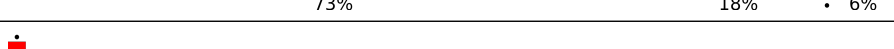
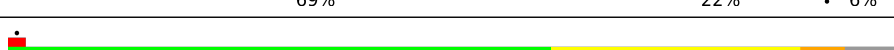

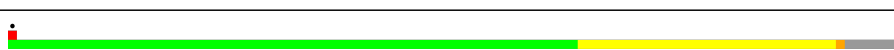

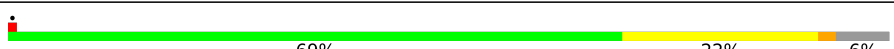





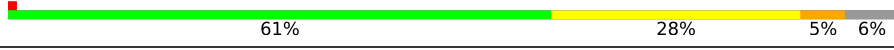
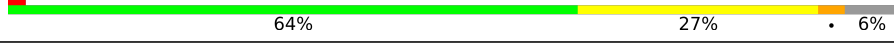



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Mol	Chain	Length	Quality of chain
1	C9	98	
1	CA	98	
1	CB	98	
1	CC	98	
1	CD	98	
1	CE	98	
1	CF	98	
1	CG	98	
1	CH	98	
1	CI	98	
1	CJ	98	
1	CK	98	
1	CL	98	
1	CM	98	
1	CN	98	
1	CO	98	
1	CP	98	
1	CQ	98	
1	CR	98	
1	CS	98	
1	CT	98	
1	CU	98	
1	CV	98	
1	CW	98	
1	CX	98	







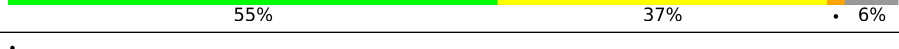
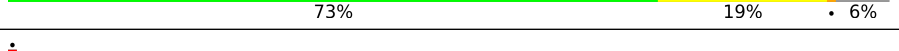
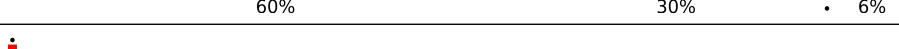
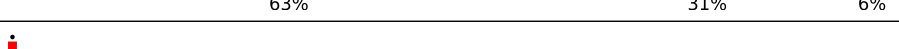
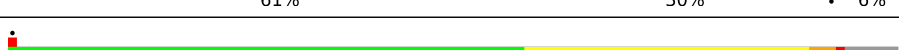

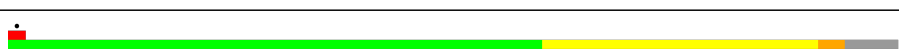

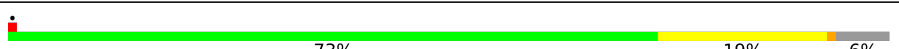





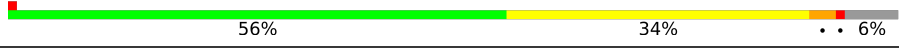
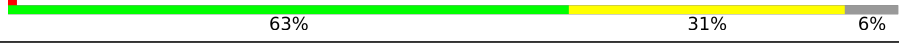



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Mol	Chain	Length	Quality of chain
1	Ca	98	
1	Cb	98	
1	Cc	98	
1	Cd	98	
1	Ce	98	
1	Cf	98	
1	Cg	98	
1	Ch	98	
1	Ci	98	
1	Cj	98	
1	Ck	98	
1	Cl	98	
1	Cm	98	
1	Cn	98	
1	Co	98	
1	Cp	98	
1	Cq	98	
1	Cr	98	
1	Cs	98	
1	Ct	98	
1	Cu	98	
1	Cv	98	
1	Cw	98	
1	Cx	98	
1	Cy	98	







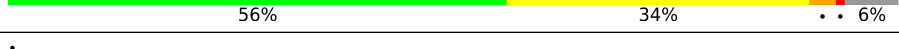
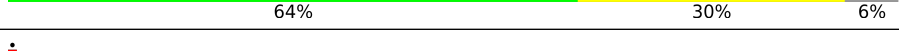
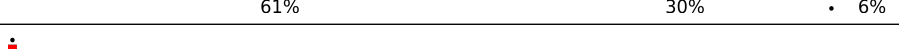
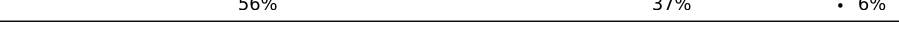
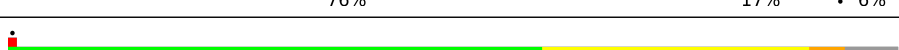

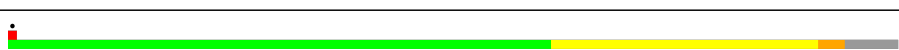

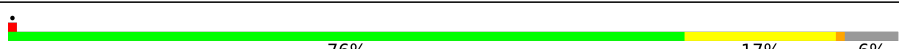





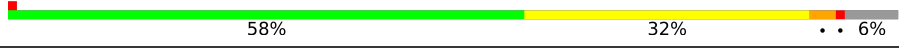
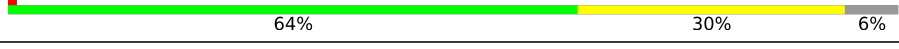



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Mol	Chain	Length	Quality of chain
1	Cz	98	
1	D0	98	
1	D1	98	
1	D2	98	
1	D3	98	
1	D4	98	
1	D5	98	
1	D6	98	
1	D7	98	
1	D8	98	
1	D9	98	
1	DA	98	
1	DB	98	
1	DC	98	
1	DD	98	
1	DE	98	
1	DF	98	
1	DG	98	
1	DH	98	
1	DI	98	
1	DJ	98	
1	DK	98	
1	DL	98	
1	DM	98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







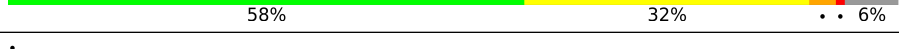
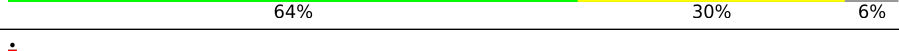
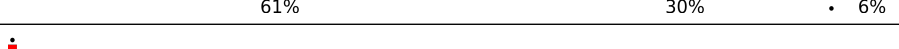
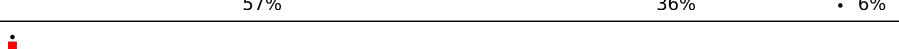
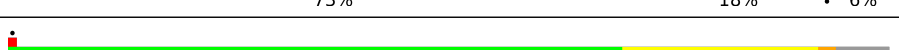

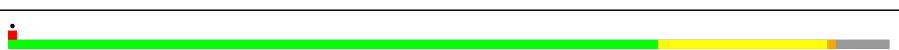

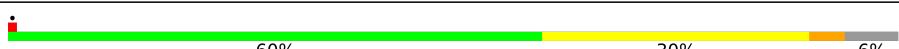





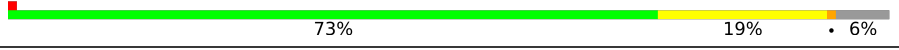
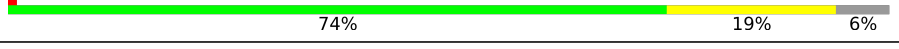



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Mol	Chain	Length	Quality of chain
1	DO	98	
1	DP	98	
1	DQ	98	
1	DR	98	
1	DS	98	
1	DT	98	
1	DU	98	
1	DV	98	
1	DW	98	
1	DX	98	
1	Da	98	
1	Db	98	
1	Dc	98	
1	Dd	98	
1	De	98	
1	Df	98	
1	Dg	98	
1	Dh	98	
1	Di	98	
1	Dj	98	
1	Dk	98	
1	Dl	98	
1	Dm	98	
1	Dn	98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







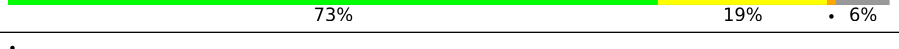
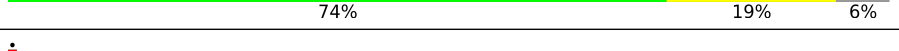
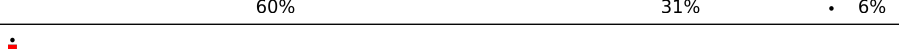
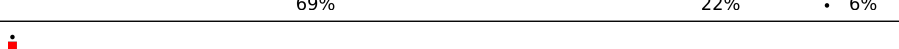
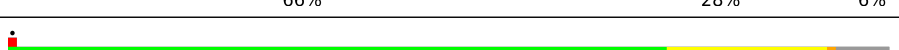

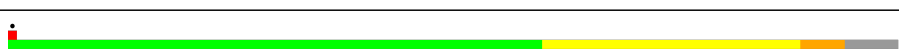

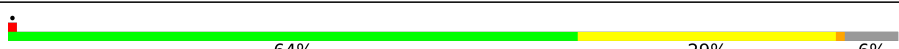





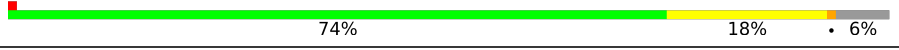
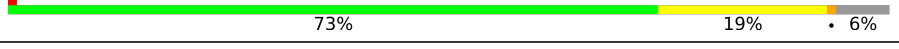



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Mol	Chain	Length	Quality of chain
1	Dp	98	
1	Dq	98	
1	Dr	98	
1	Ds	98	
1	Dt	98	
1	Du	98	
1	Dv	98	
1	Dw	98	
1	Dx	98	
1	Dy	98	
1	Dz	98	
1	E0	98	
1	E1	98	
1	E2	98	
1	E3	98	
1	E4	98	
1	E5	98	
1	E6	98	
1	E7	98	
1	E8	98	
1	E9	98	
1	EA	98	
1	EB	98	
1	EC	98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







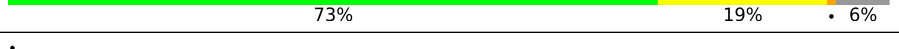
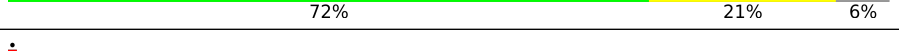
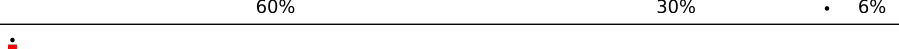
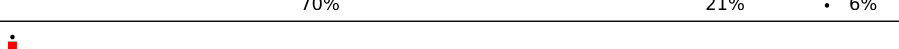
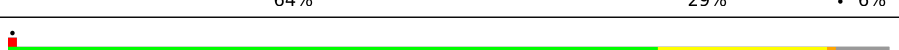

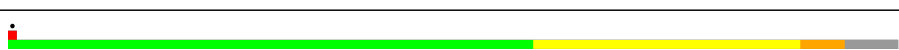

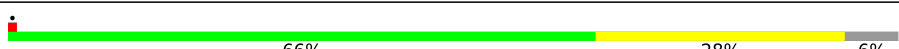





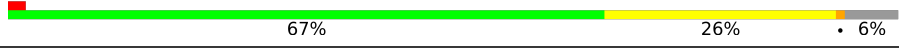
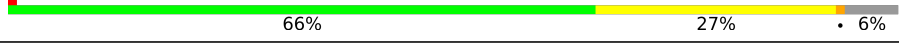



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Mol	Chain	Length	Quality of chain
1	EE	98	
1	EF	98	
1	EG	98	
1	EH	98	
1	EI	98	
1	EJ	98	
1	EK	98	
1	EL	98	
1	EM	98	
1	EN	98	
1	EO	98	
1	EP	98	
1	EQ	98	
1	ER	98	
1	ES	98	
1	ET	98	
1	EU	98	
1	EV	98	
1	EW	98	
1	EX	98	
1	Ea	98	
1	Eb	98	
1	Ec	98	
1	Ed	98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







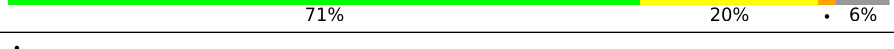
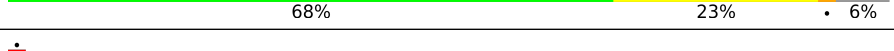
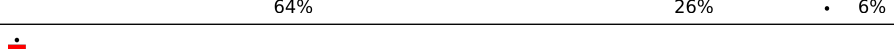
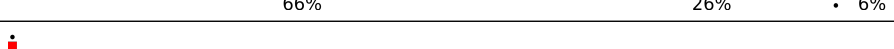
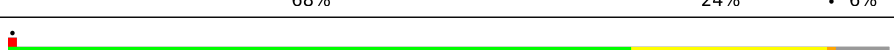

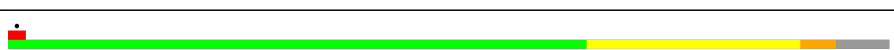

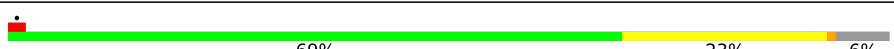





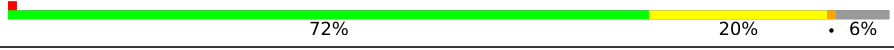
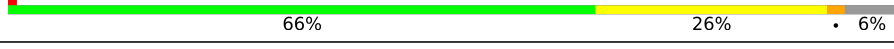



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Mol	Chain	Length	Quality of chain
1	Ef	98	
1	Eg	98	
1	Eh	98	
1	Ei	98	
1	Ej	98	
1	Ek	98	
1	El	98	
1	Em	98	
1	En	98	
1	Eo	98	
1	Ep	98	
1	Eq	98	
1	Er	98	
1	Es	98	
1	Et	98	
1	Eu	98	
1	Ev	98	
1	Ew	98	
1	Ex	98	
1	Ey	98	
1	Ez	98	
1	F0	98	
1	F1	98	
1	F2	98	
1	F3	98	







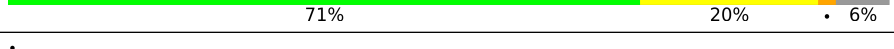
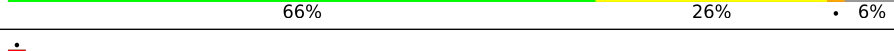
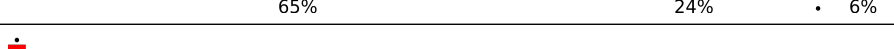
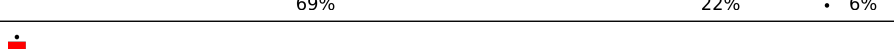
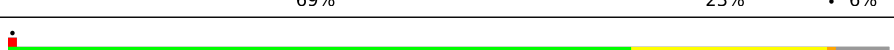

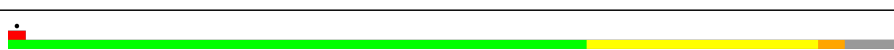

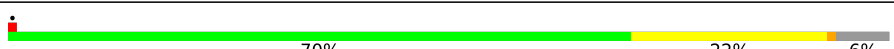





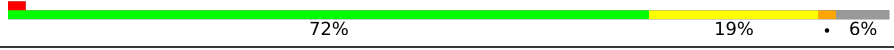
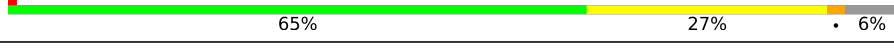



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Mol	Chain	Length	Quality of chain
1	F4	98	
1	F5	98	
1	F6	98	
1	F7	98	
1	F8	98	
1	F9	98	
1	FA	98	
1	FB	98	
1	FC	98	
1	FD	98	
1	FE	98	
1	FF	98	
1	FG	98	
1	FH	98	
1	FI	98	
1	FJ	98	
1	FK	98	
1	FL	98	
1	FM	98	
1	FN	98	
1	FO	98	
1	FP	98	
1	FQ	98	
1	FR	98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







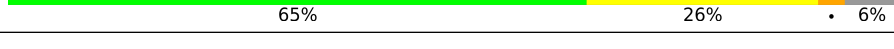
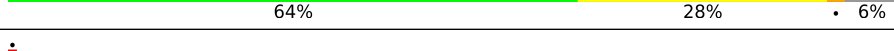
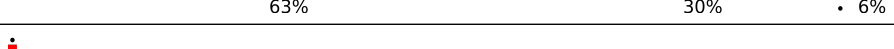
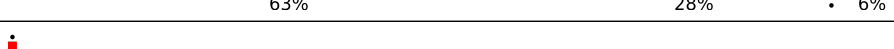
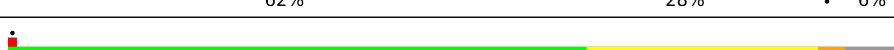

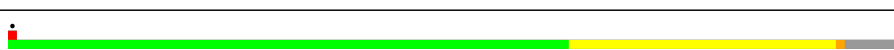

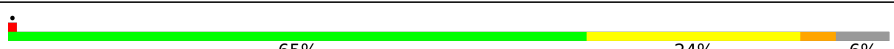





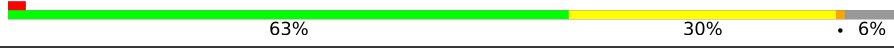
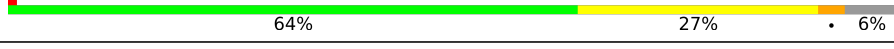



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Mol	Chain	Length	Quality of chain
1	FT	98	
1	FU	98	
1	FV	98	
1	FW	98	
1	FX	98	
1	Fa	98	
1	Fb	98	
1	Fc	98	
1	Fd	98	
1	Fe	98	
1	Ff	98	
1	Fg	98	
1	Fh	98	
1	Fi	98	
1	Fj	98	
1	Fk	98	
1	Fl	98	
1	Fm	98	
1	Fn	98	
1	Fo	98	
1	Fp	98	
1	Fq	98	
1	Fr	98	
1	Fs	98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







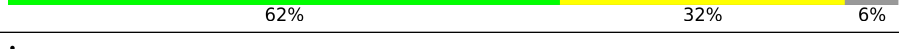
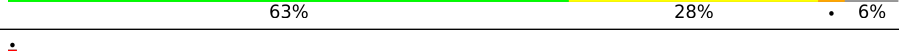
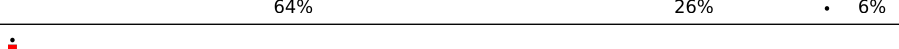
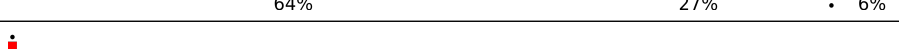
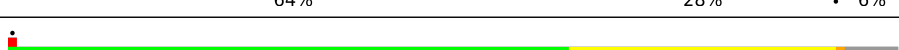

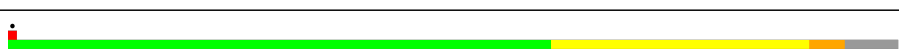

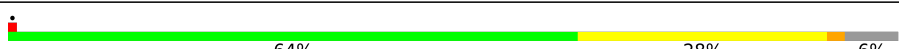





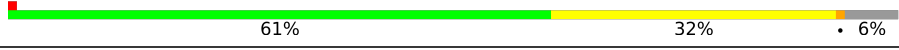
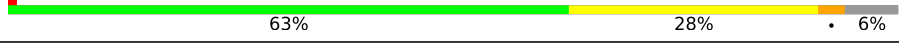



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Mol	Chain	Length	Quality of chain
1	Fu	98	
1	Fv	98	
1	Fw	98	
1	Fx	98	
1	Fy	98	
1	Fz	98	
1	G0	98	
1	G1	98	
1	G2	98	
1	G3	98	
1	G4	98	
1	G5	98	
1	G6	98	
1	G7	98	
1	G8	98	
1	G9	98	
1	GA	98	
1	GB	98	
1	GC	98	
1	GD	98	
1	GE	98	
1	GF	98	
1	GG	98	
1	GH	98	
1	GI	98	







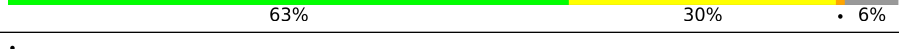
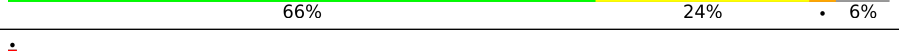
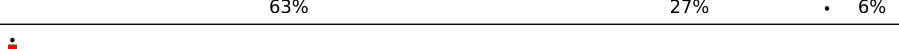
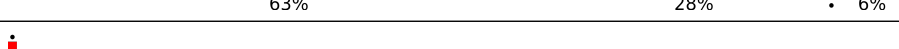
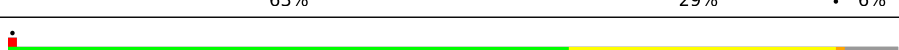

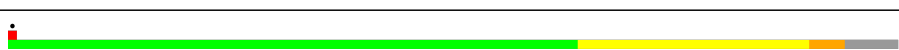

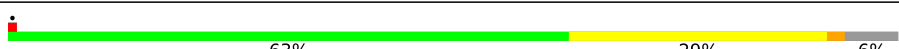





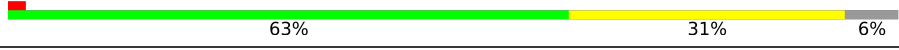
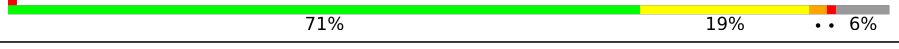



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Mol	Chain	Length	Quality of chain
1	GJ	98	
1	GK	98	
1	GL	98	
1	GM	98	
1	GN	98	
1	GO	98	
1	GP	98	
1	GQ	98	
1	GR	98	
1	GS	98	
1	GT	98	
1	GU	98	
1	GV	98	
1	GW	98	
1	GX	98	
1	Ga	98	
1	Gb	98	
1	Gc	98	
1	Gd	98	
1	Ge	98	
1	Gf	98	
1	Gg	98	
1	Gh	98	
1	Gi	98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







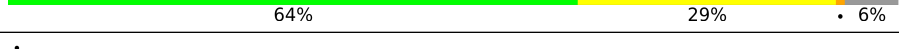
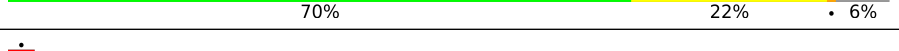
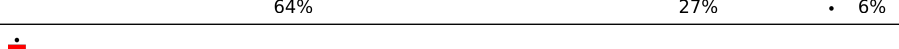
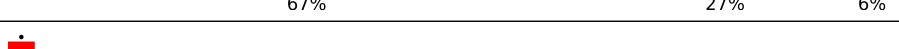
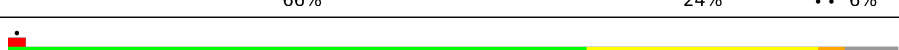

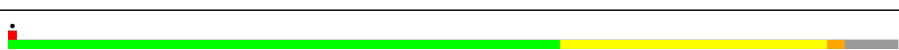

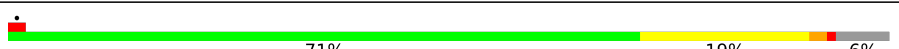





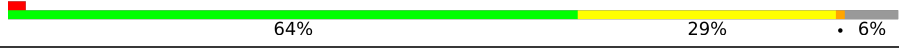
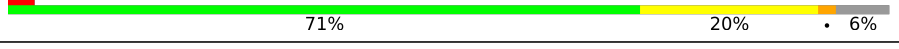



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Mol	Chain	Length	Quality of chain
1	Gk	98	
1	Gl	98	
1	Gm	98	
1	Gn	98	
1	Go	98	
1	Gp	98	
1	Gq	98	
1	Gr	98	
1	Gs	98	
1	Gt	98	
1	Gu	98	
1	Gv	98	
1	Gw	98	
1	Gx	98	
1	Gy	98	
1	Gz	98	
1	H0	98	
1	H1	98	
1	H2	98	
1	H3	98	
1	H4	98	
1	H5	98	
1	H6	98	
1	H7	98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







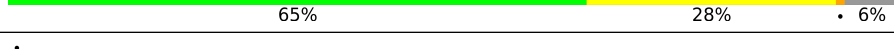
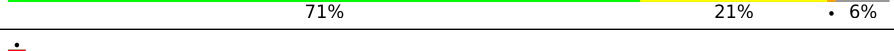
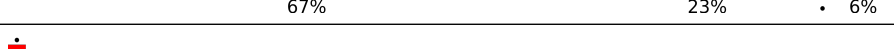
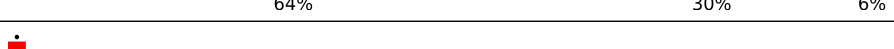
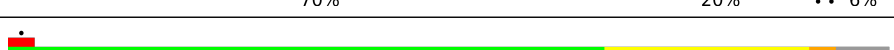

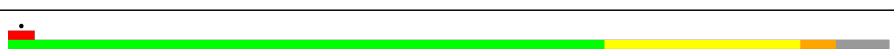

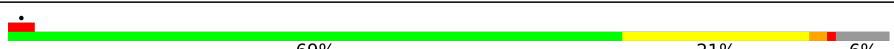





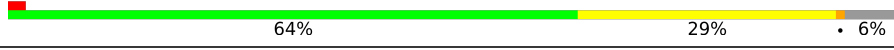
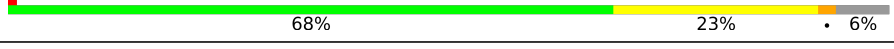



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Mol	Chain	Length	Quality of chain
1	H9	98	
1	HA	98	
1	HB	98	
1	HC	98	
1	HD	98	
1	HE	98	
1	HF	98	
1	HG	98	
1	HH	98	
1	HI	98	
1	HJ	98	
1	HK	98	
1	HL	98	
1	HM	98	
1	HN	98	
1	HO	98	
1	HP	98	
1	HQ	98	
1	HR	98	
1	HS	98	
1	HT	98	
1	HU	98	
1	HV	98	
1	HW	98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














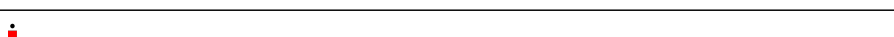
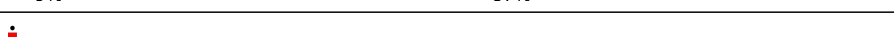
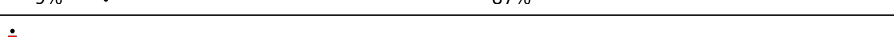



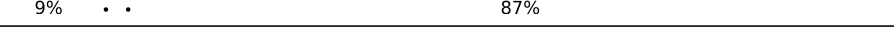





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Mol	Chain	Length	Quality of chain
1	Ha	98	
1	Hb	98	
1	Hc	98	
1	Hd	98	
1	He	98	
1	Hf	98	
1	Hg	98	
1	Hh	98	
1	Hi	98	
1	Hj	98	
1	Hk	98	
1	Hl	98	
1	Hm	98	
1	Hn	98	
1	Ho	98	
1	Hp	98	
1	Hq	98	
1	Hr	98	
1	Hs	98	
1	Ht	98	
1	Hu	98	
1	Hv	98	
1	Hw	98	
1	Hx	98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






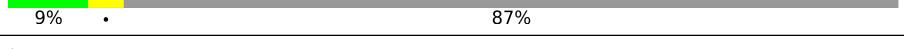

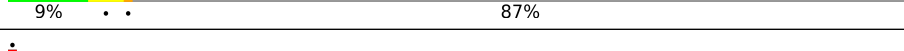
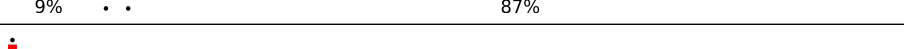
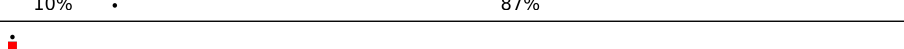















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Mol	Chain	Length	Quality of chain
1	Hz	98	 69%21%6%
2	X0	869	 9%87%
2	X1	869	 9%87%
2	X2	869	 10%87%
2	X3	869	 9%87%
2	X4	869	 9%87%
2	X5	869	 9%87%
2	X6	869	 9%87%
2	X7	869	 10%87%
2	X8	869	 9%87%
2	X9	869	 9%87%
2	XA	869	 10%87%
2	XB	869	 9%87%
2	XC	869	 9%87%
2	XD	869	 9%87%
2	XE	869	 9%87%
2	XF	869	 10%87%
2	XG	869	 9%87%
2	XH	869	 9%87%
2	XI	869	 10%87%
2	XJ	869	 9%87%
2	XK	869	 10%87%
2	XL	869	 9%87%
2	XM	869	 9%87%
2	XN	869	 10%87%






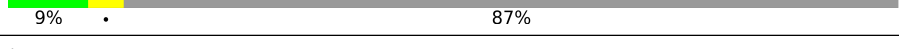

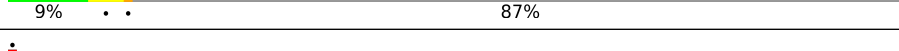
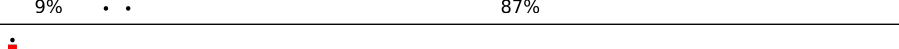
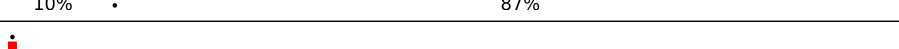
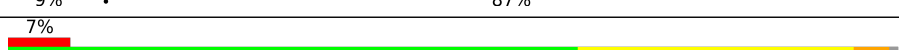

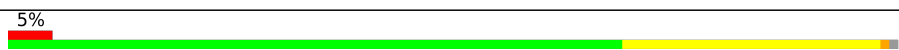

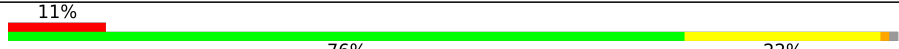





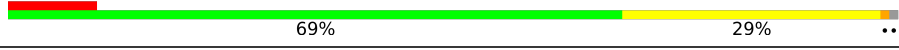
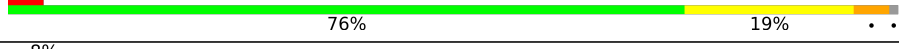



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Mol	Chain	Length	Quality of chain
2	XO	869	 9% 87%
2	XP	869	 10% 87%
2	XQ	869	 9% 87%
2	XR	869	 9% 87%
2	XS	869	 10% 87%
2	XT	869	 9% 87%
2	XU	869	 10% 87%
2	XV	869	 9% 87%
2	XW	869	 9% 87%
2	XX	869	 10% 87%
2	Xa	869	 9% 87%
2	Xb	869	 10% 87%
2	Xc	869	 9% 87%
2	Xd	869	 9% 87%
2	Xe	869	 10% 87%
2	Xf	869	 9% 87%
2	Xg	869	 10% 87%
2	Xh	869	 9% 87%
2	Xi	869	 9% 87%
2	Xj	869	 9% 87%
2	Xk	869	 10% 87%
2	Xl	869	 10% 87%
2	Xm	869	 9% 87%
2	Xn	869	 9% 87%
2	Xo	869	 10% 87%

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Mol	Chain	Length	Quality of chain
2	Xp	869	
2	Xq	869	
2	Xr	869	
2	Xs	869	
2	Xt	869	
2	Xu	869	
2	Xv	869	
2	Xw	869	
2	Xx	869	
2	Xy	869	
2	Xz	869	
3	P0	83	
3	P1	83	
3	P2	83	
3	P3	83	
3	P4	83	
3	P5	83	
3	P6	83	
3	P7	83	
3	P8	83	
3	P9	83	
3	PA	83	
3	PB	83	
3	PC	83	
3	PD	83	

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Mol	Chain	Length	Quality of chain
3	PE	83	
3	PF	83	
3	PG	83	
3	PH	83	
3	PI	83	
3	PJ	83	
3	PK	83	
3	PL	83	
3	PM	83	
3	PN	83	
3	PO	83	
3	PP	83	
3	PQ	83	
3	PR	83	
3	PS	83	
3	PT	83	
3	PU	83	
3	PV	83	
3	PW	83	
3	PX	83	
3	Pa	83	
3	Pb	83	
3	Pc	83	
3	Pd	83	
3	Pe	83	

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Mol	Chain	Length	Quality of chain
3	Pf	83	
3	Pg	83	
3	Ph	83	
3	Pi	83	
3	Pj	83	
3	Pk	83	
3	Pl	83	
3	Pm	83	
3	Pn	83	
3	Po	83	
3	Pp	83	
3	Pq	83	
3	Pr	83	
3	Ps	83	
3	Pt	83	
3	Pu	83	
3	Pv	83	
3	Pw	83	
3	Px	83	
3	Py	83	
3	Pz	83	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 403140 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	A2	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
1	C2	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	E2	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	G2	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	A1	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	C1	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	E1	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	G1	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	B5	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	C5	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	E5	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
1	G5	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	A3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	B3	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	D3	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	F3	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	H3	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	B4	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	D4	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	F4	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

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	H4	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	B7	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	D7	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	E7	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	G7	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	A6	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	C6	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	E6	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	G6	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	B0	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	D0	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

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	F0	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	H0	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	B8	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	D8	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	F8	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	H8	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	B9	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	D9	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	F9	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	H9	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	Bb	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Cb	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	Eb	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	Gb	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	Aa	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	Ca	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	Ea	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	Ga	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	Ae	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	Ce	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	Ee	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	Ge	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	He	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	Bc	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	Dc	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	Fc	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	Hc	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	Bd	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	Dd	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	Fd	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	Hd	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	Bg	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	Dg	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Eg	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	Gg	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	Af	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	Cf	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	Ef	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	Gf	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	Bj	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	Dj	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	Fj	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	Hj	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	Bh	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ch	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	Eh	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	Gh	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	Ai	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	Ci	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	Ei	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	Gi	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	Al	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	Cl	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	El	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	Gl	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Hl	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	Bk	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	Dk	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	Fk	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	Ao	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	Co	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	Eo	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	Go	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	Am	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	Cm	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	Em	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Fm	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	Hm	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	Bn	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	Dn	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	Fn	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	Hn	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	Bq	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	Dq	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	Fq	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	Hq	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	Bp	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Cp	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	Ep	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	Gp	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	At	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	Ct	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	Et	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	Gt	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	Ar	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	Cr	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	Er	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	Gr	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Hr	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	Bs	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	Ds	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	Fs	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	Hs	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	Bv	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	Dv	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	Fv	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	Hv	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	Bu	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	Du	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Eu	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	Gu	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	By	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	Dy	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	Fy	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
1	Hy	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	Bw	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
1	Dw	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	Fw	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	Hw	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	Bx	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Cx	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	Ex	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	Gx	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	AA	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	CA	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	EA	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	GA	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	Az	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	Cz	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	Ez	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	Gz	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AD	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	CD	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	ED	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	GD	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	AB	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	CB	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	EB	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	GB	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	AC	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	CC	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	EC	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	FC	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	HC	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	BF	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	DF	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
1	FF	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	HF	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	BE	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	DE	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	FE	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	HE	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	BI	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CI	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	EI	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	GI	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	AG	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	CG	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	EG	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	GG	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	AH	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	CH	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	EH	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	GH	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	HH	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	BK	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	DK	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	FK	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	HK	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	BJ	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	DJ	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	FJ	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	HJ	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	BN	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	DN	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	EN	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	GN	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	AL	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	CL	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	EL	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	GL	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	AM	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	CM	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	EM	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	GM	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	AP	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BP	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	DP	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	FP	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	HP	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	BO	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	DO	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	FO	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	AS	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	CS	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	ES	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	GS	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	HS	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	BQ	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	DQ	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	FQ	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	HQ	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	BR	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	DR	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	FR	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	HR	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	BU	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	DU	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	EU	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	GU	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	AT	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	CT	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	ET	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	GT	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	AX	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	CX	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	EX	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	GX	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	AV	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BV	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	DV	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	FV	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	HV	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	BW	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
1	DW	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	FW	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	HW	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	H6	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	Hk	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	Hz	92	Total 656	C 408	N 123	O 122	S 3	0	0

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

- Molecule 2 is a protein called Carboxysome assembly protein CsoS2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X2	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	X1	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	X5	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	X3	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	X4	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	X7	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	X6	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	X0	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	X9	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xb	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xa	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xe	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xd	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xg	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xf	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xj	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xh	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xi	117	Total	C	N	O	S	0	0
			859	518	167	169	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Xl	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xk	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xo	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xn	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xq	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xp	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xt	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xs	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xv	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xu	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xy	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xw	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xx	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XA	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xz	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XD	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XC	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XF	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XE	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XI	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XH	117	Total	C	N	O	S	0	0
			859	518	167	169	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	XK	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XJ	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XN	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XL	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XM	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XP	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XO	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XS	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XQ	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XR	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XU	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XT	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XX	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XW	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	X8	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xc	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xm	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	Xr	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XB	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XG	117	Total	C	N	O	S	0	0
			859	518	167	169	5		
2	XV	117	Total	C	N	O	S	0	0
			859	518	167	169	5		

- Molecule 3 is a protein called Carboxysome shell vertex protein CsoS4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P2	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	P1	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	P5	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	P3	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	P4	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	P7	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	P6	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	P0	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	P8	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	P9	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	Pb	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	Pa	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	Pe	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	Pc	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	Pd	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	Pg	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	Pf	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	Pj	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	Ph	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	Pi	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
3	Pl	82	Total	C	N	O	S	0	0
			612	388	106	113	5		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Pk	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	Po	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	Pm	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	Pn	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	Pq	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	Pp	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	Pt	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	Pr	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	Ps	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	Pv	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	Pu	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	Py	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	Pw	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	Px	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PA	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	Pz	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PD	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PB	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PC	82	Total 612	C 388	N 106	O 113	S 5	0	0
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*Continued on next page...*

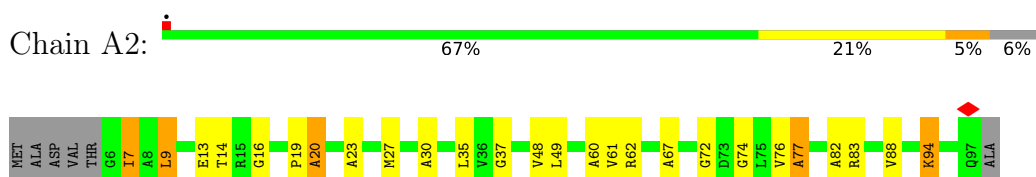
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Mol	Chain	Residues	Atoms					AltConf	Trace
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3	PG	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PH	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PK	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PJ	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PN	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PL	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PM	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PP	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PO	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PS	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PQ	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PR	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PU	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PT	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PX	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PV	82	Total 612	C 388	N 106	O 113	S 5	0	0
3	PW	82	Total 612	C 388	N 106	O 113	S 5	0	0

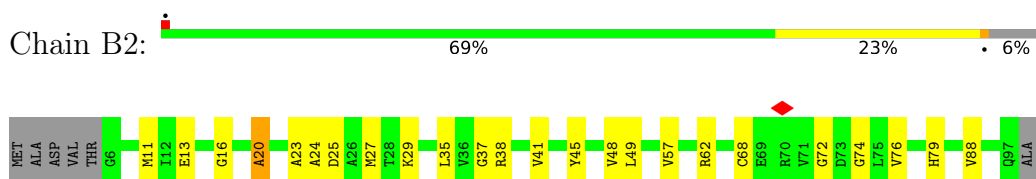
### 3 Residue-property plots [i](#)

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

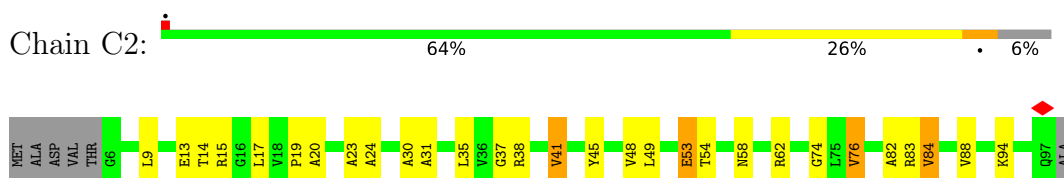
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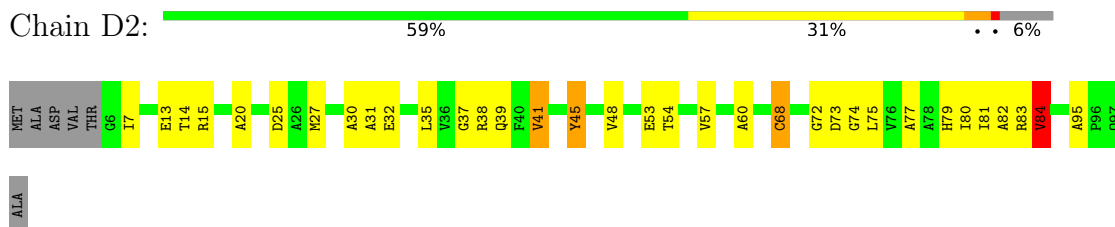
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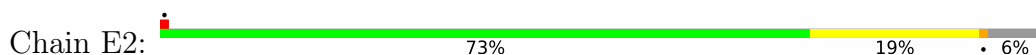
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

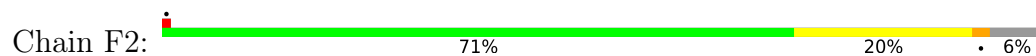


- Molecule 1: Major carboxysome shell protein CsoS1A

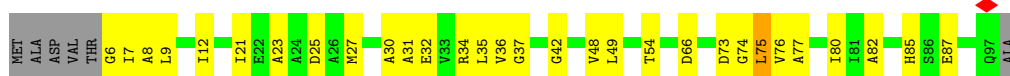




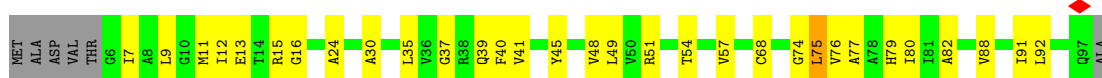
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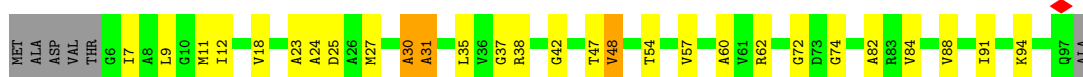
- Molecule 1: Major carboxysome shell protein CsoS1A



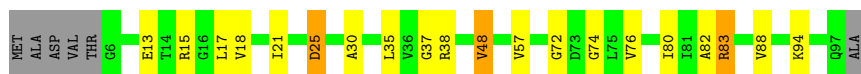
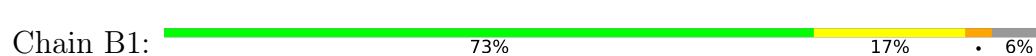
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A




- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



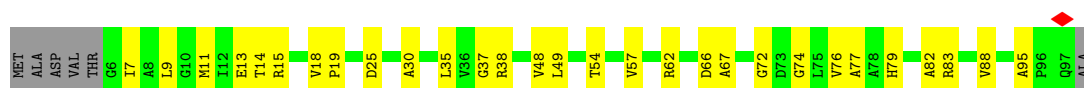
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain D1:  73% 19% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain E1:  64% 30% 6%



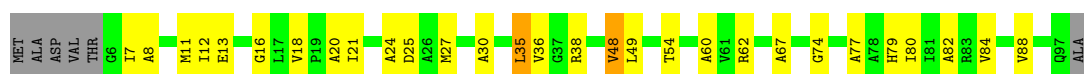
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain F1:  66% 27% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain G1:  64% 28% • 6%



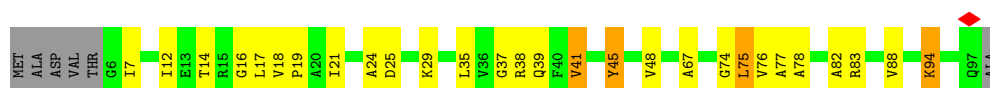
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain A5:  64% 27% • • 6%




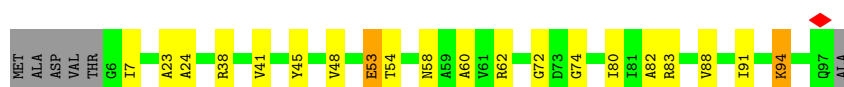
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain B5:  65% 24% • 6%



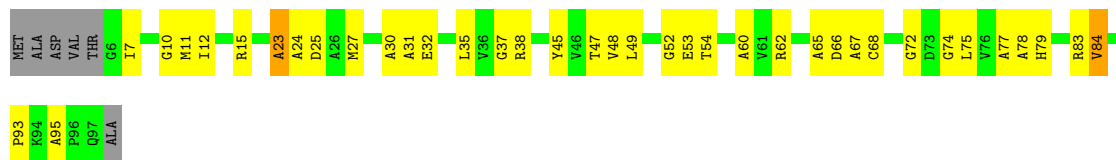
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain C5:  73% 18% • 6%



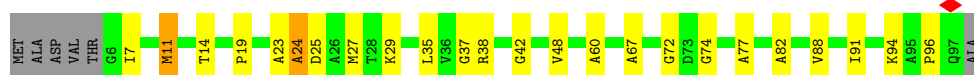
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain D5:  55% 37% 6%



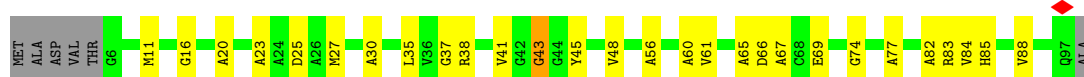
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain E5:  69% 22% 6%



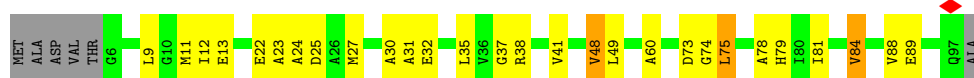
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain F5:  65% 28% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain G5:  65% 26% 6%




- Molecule 1: Major carboxysome shell protein CsoS1A

Chain H5:  63% 31% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain A3:  72% 19% 6%



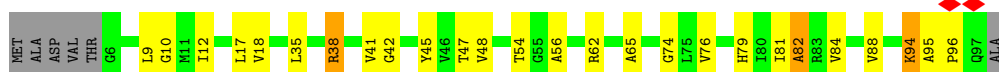
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain B3:  70% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain C3:  67% 23% 6%




- Molecule 1: Major carboxysome shell protein CsoS1A

Chain D3:  63% 31% 6%



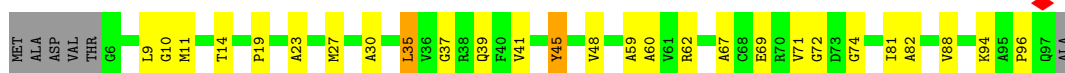
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain E3:  73% 20% 6%



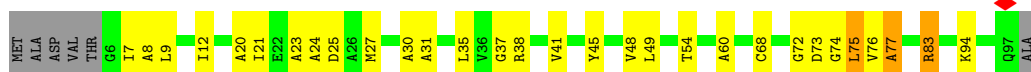
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain F3:  66% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain G3:  63% 28% 6%

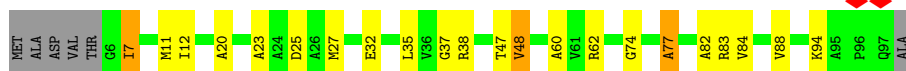
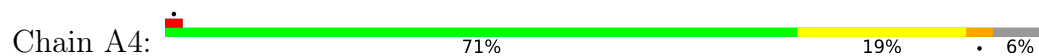


- Molecule 1: Major carboxysome shell protein CsoS1A

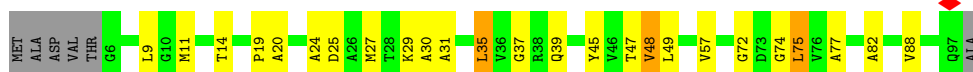
Chain H3:  70% 21% 6%



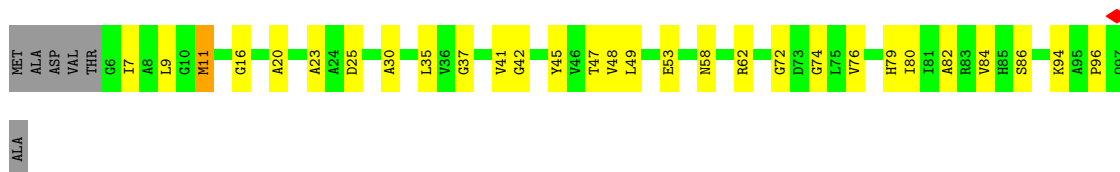
- Molecule 1: Major carboxysome shell protein CsoS1A



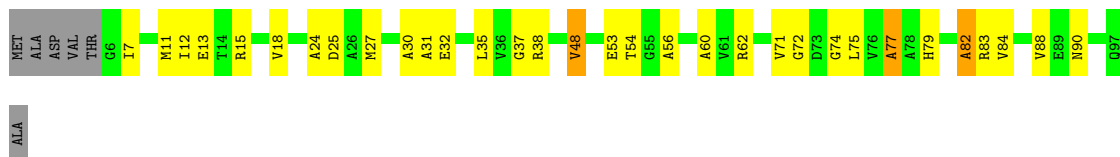
- Molecule 1: Major carboxysome shell protein CsoS1A



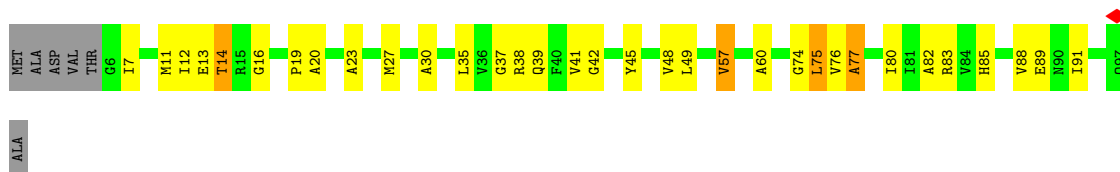
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

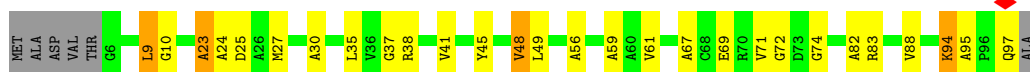


- Molecule 1: Major carboxysome shell protein CsoS1A



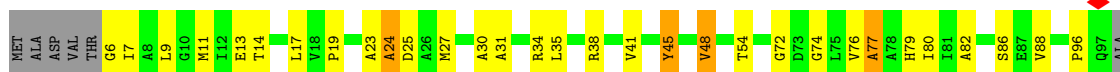
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain F4: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain G4: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain H4: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain A7: 



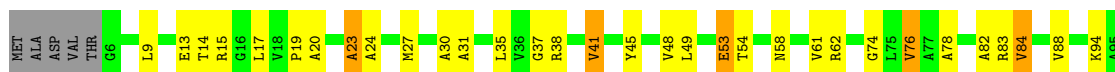
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Chain B7: 



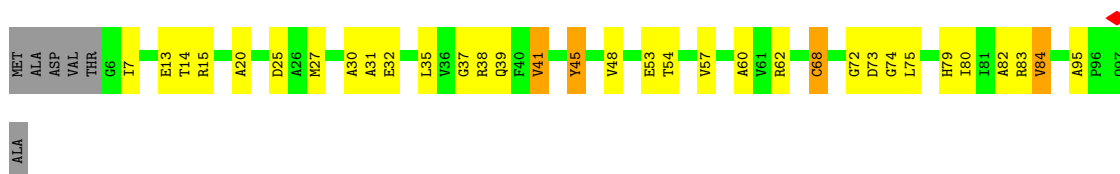
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain C7: 

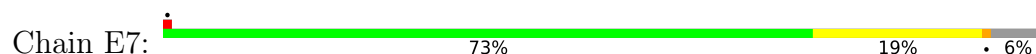


- Molecule 1: Major carboxysome shell protein CsoS1A

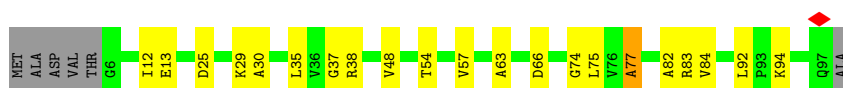
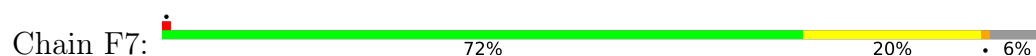
Chain D7: 



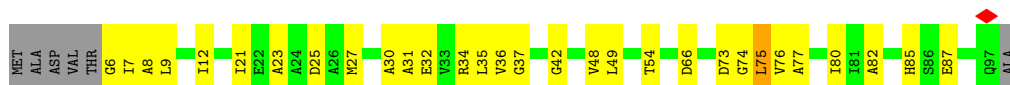
- Molecule 1: Major carboxysome shell protein CsoS1A



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- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

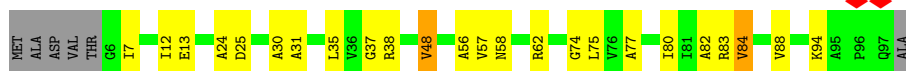


- Molecule 1: Major carboxysome shell protein CsoS1A

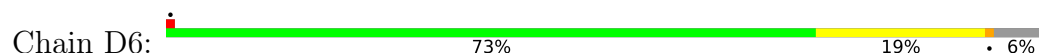




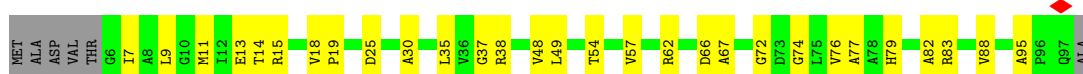
- Molecule 1: Major carboxysome shell protein CsoS1A



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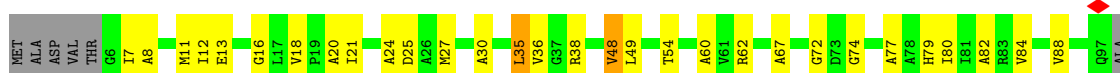
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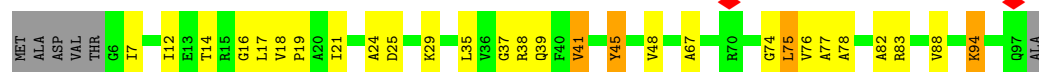
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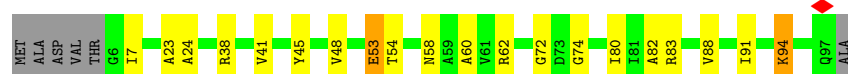
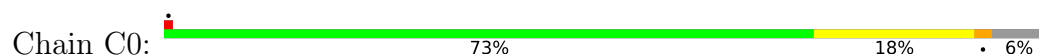
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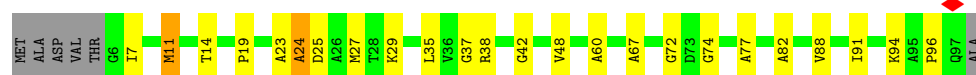
- Molecule 1: Major carboxysome shell protein CsoS1A



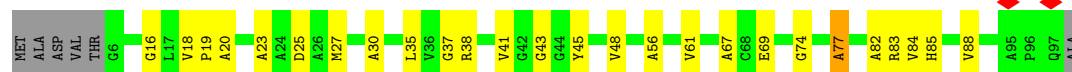
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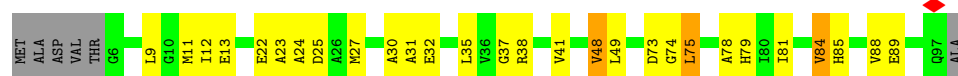
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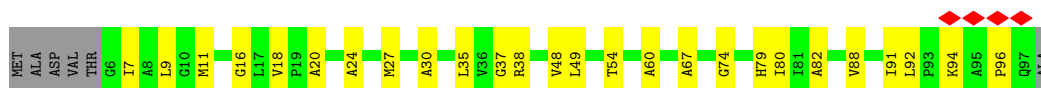


- Molecule 1: Major carboxysome shell protein CsoS1A



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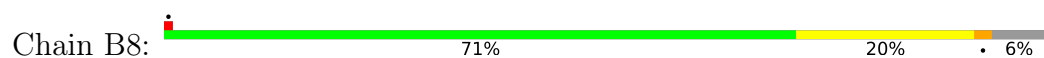




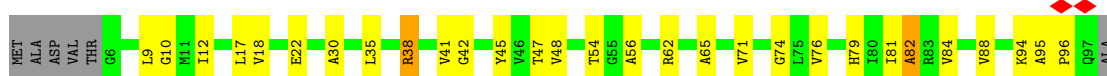
- Molecule 1: Major carboxysome shell protein CsoS1A



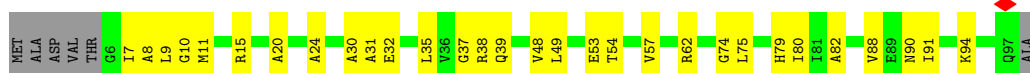
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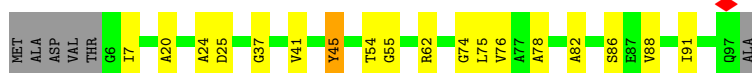
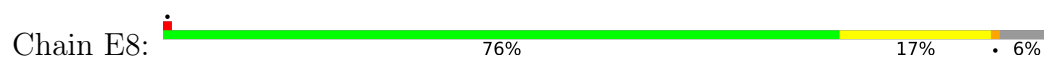
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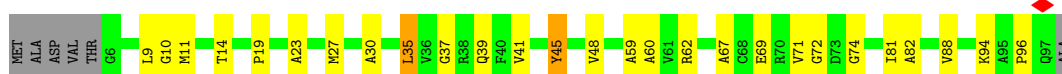
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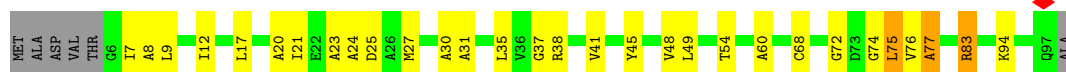
- Molecule 1: Major carboxysome shell protein CsoS1A



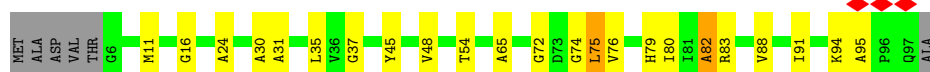
- Molecule 1: Major carboxysome shell protein CsoS1A



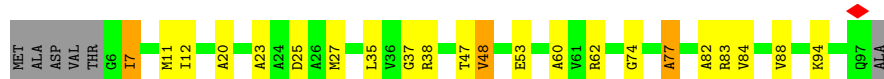
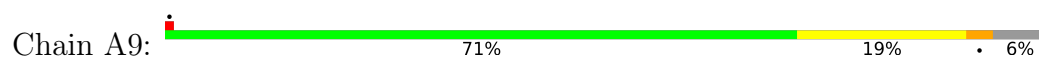
- Molecule 1: Major carboxysome shell protein CsoS1A



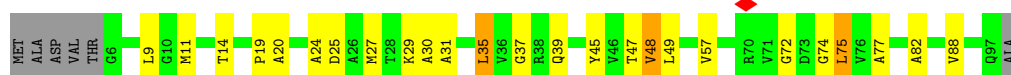
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

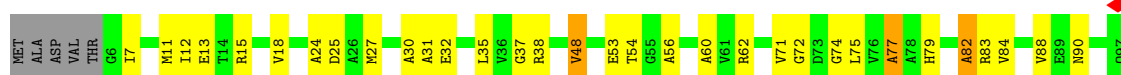


- Molecule 1: Major carboxysome shell protein CsoS1A



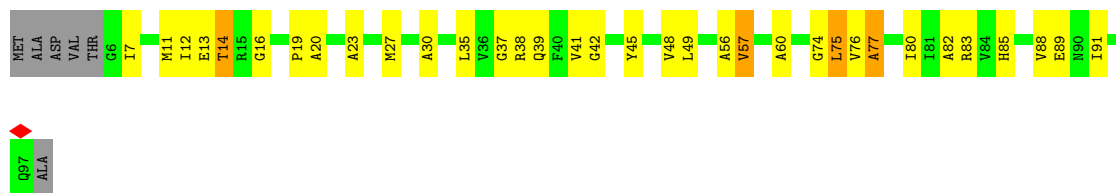
ALA

- Molecule 1: Major carboxysome shell protein CsoS1A



ALA

- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



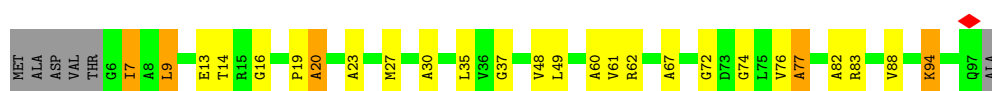
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

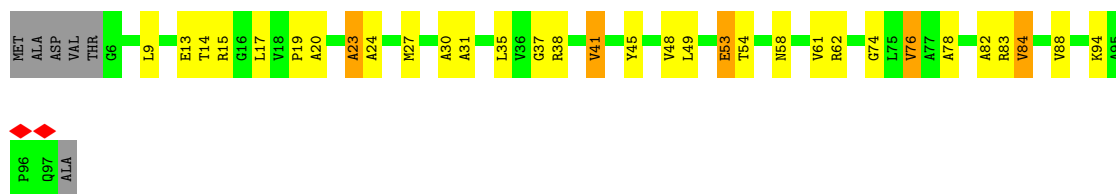


- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

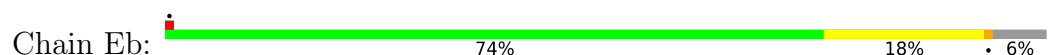




- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

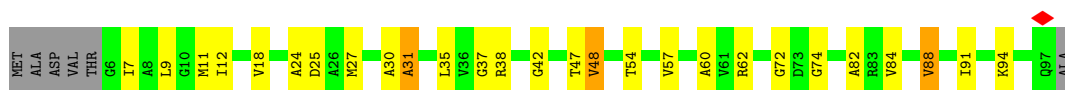


- Molecule 1: Major carboxysome shell protein CsoS1A

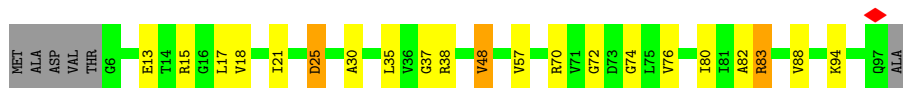
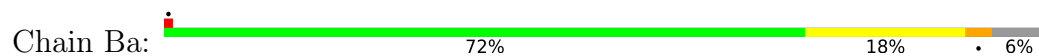


- Molecule 1: Major carboxysome shell protein CsoS1A





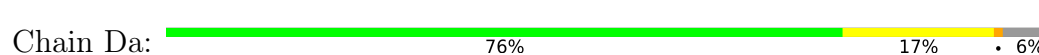
- Molecule 1: Major carboxysome shell protein CsoS1A



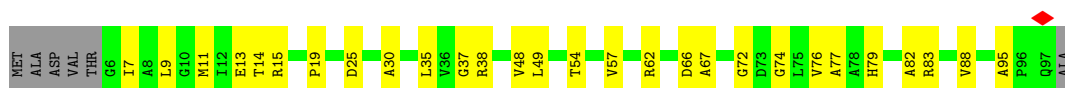
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- Molecule 1: Major carboxysome shell protein CsoS1A



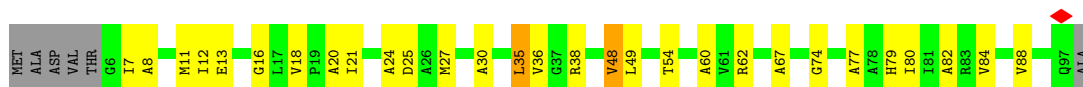
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- Molecule 1: Major carboxysome shell protein CsoS1A



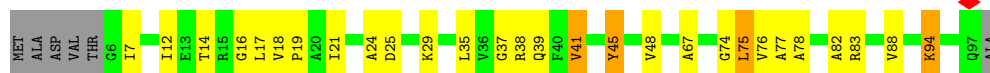
- Molecule 1: Major carboxysome shell protein CsoS1A



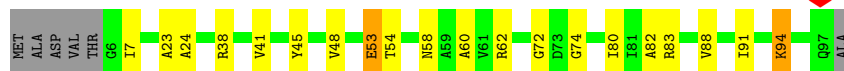
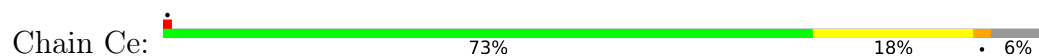
- Molecule 1: Major carboxysome shell protein CsoS1A



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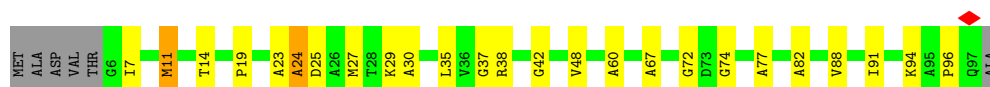
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

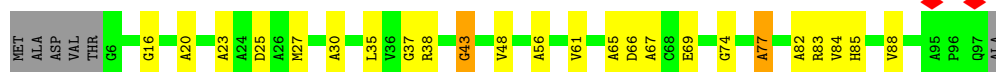


- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fe:  69% 22% 6%



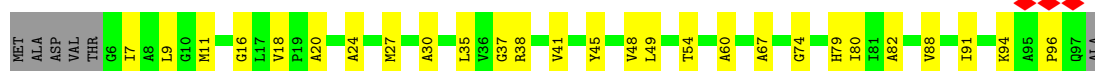
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ge:  63% 28% 6%




- Molecule 1: Major carboxysome shell protein CsoS1A

Chain He:  66% 28% 6%



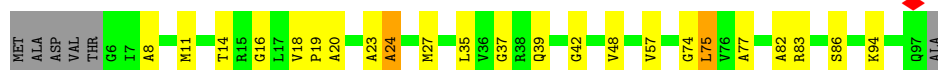
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ac:  71% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bc:  70% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cc:  67% 23% 6%




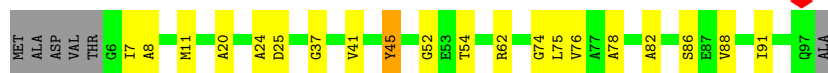
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dc:  66% 28% 6%



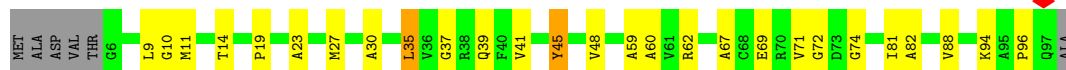
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ec:  73% 19% 6%



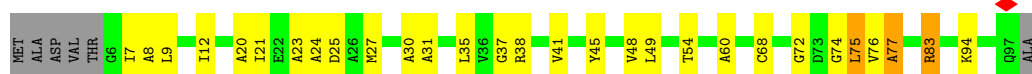
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fc:  66% 26% 6%




- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Gc:  64% 27% 6%




- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Hc:  71% 20% 6%



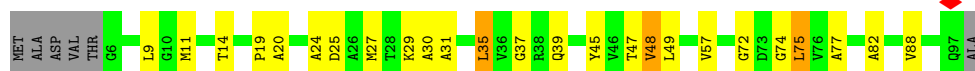
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ad:  71% 19% 6%



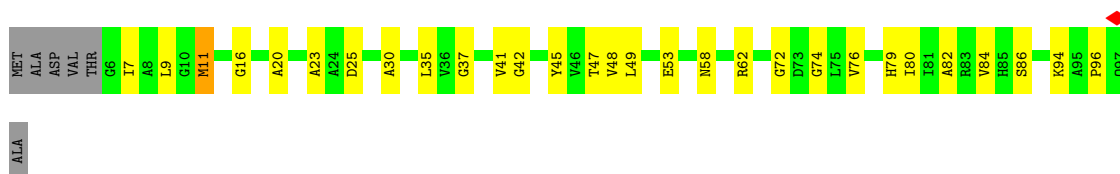
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bd:  68% 22% 6%



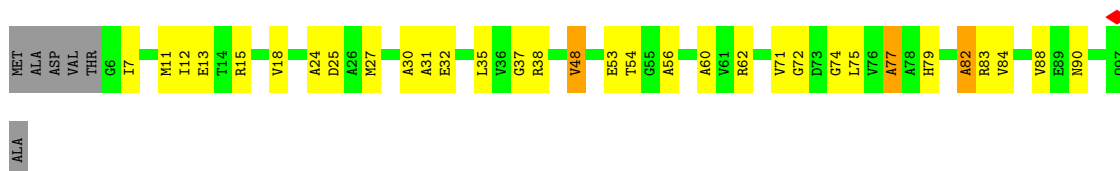
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cd:  64% 29% 6%



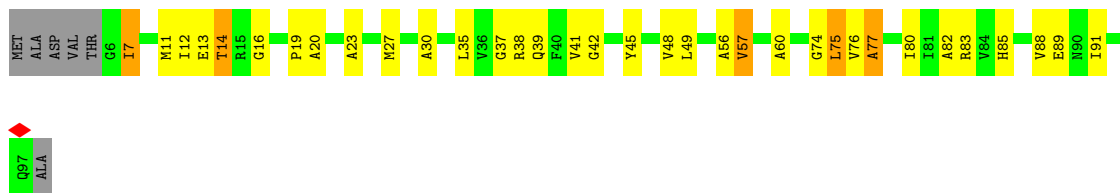
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dd: 61% 30% 6%



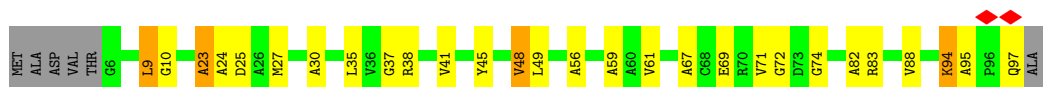
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ed: 59% 30% 5% 6%



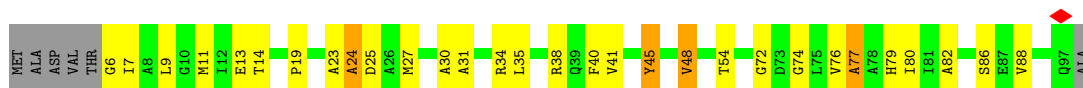
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fd: 65% 24% 6%



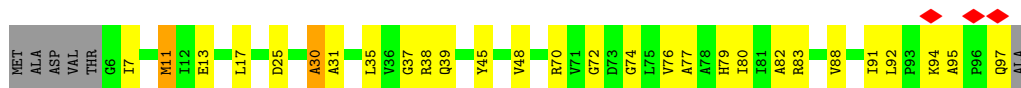
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Gd: 63% 27% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Hd: 65% 27% 6%



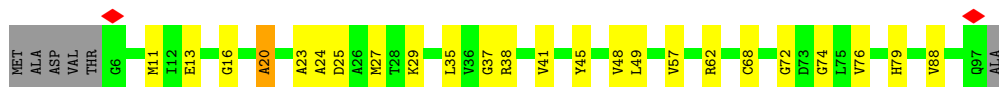
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ag:  67% 22% 6%



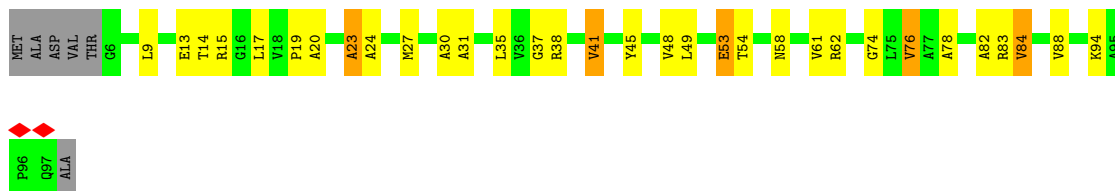
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bg:  69% 23% 6%



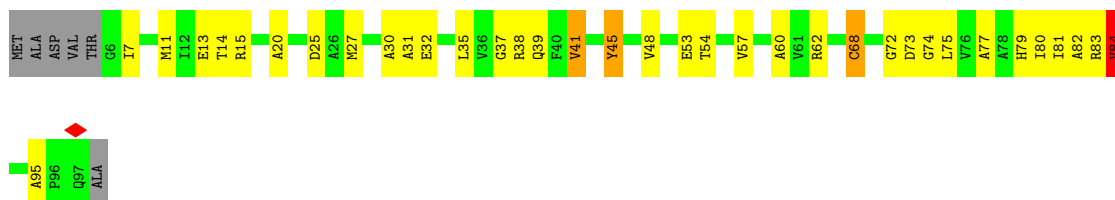
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cg:  61% 28% 5% 6%




- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dg:  57% 33% 6%



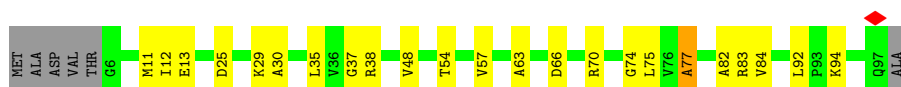
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Eg:  73% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fg:  70% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Gg:  61% 32% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Hg:  65% 28% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Af:  66% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bf:  72% 18% 6%




- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cf:  69% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Df:  76% 17% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ef:  64% 30% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



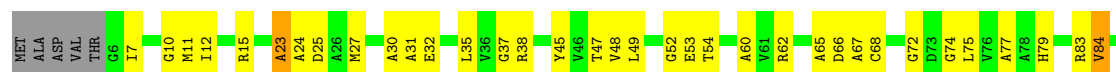
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

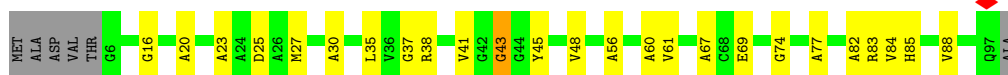




- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



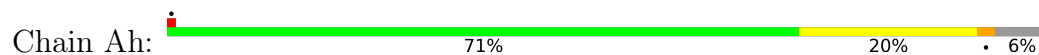
- Molecule 1: Major carboxysome shell protein CsoS1A



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- Molecule 1: Major carboxysome shell protein CsoS1A



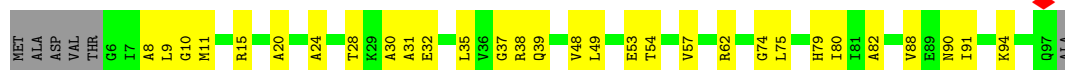
- Molecule 1: Major carboxysome shell protein CsoS1A



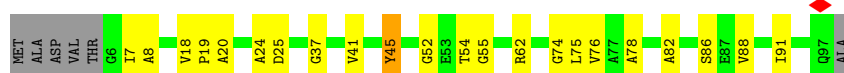
- Molecule 1: Major carboxysome shell protein CsoS1A



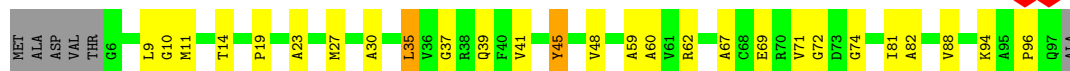
- Molecule 1: Major carboxysome shell protein CsoS1A



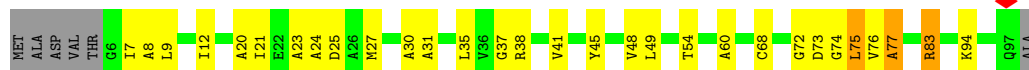
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



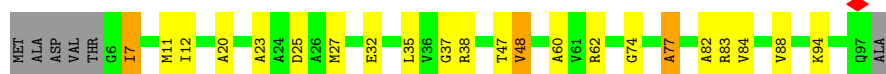
- Molecule 1: Major carboxysome shell protein CsoS1A



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- Molecule 1: Major carboxysome shell protein CsoS1A



- | Met | ASP | VAL | THR | G6 | A7 | A8 | L9 | G10 | M11 | I12 | E13 | T14 | A23 | A24 | D25 | A26 | M27 | A30 | A31 | R34 | L35 | R38 | V41 | Y45 | V48 | T54 | G72 | D73 | G74 | L75 | V76 | A77 | A78 | H79 | L80 | I81 | A82 | S86 | E87 | V88 | A95 | P96 | Q97 |
|-----|-----|-----|-----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Met | ASP | VAL | THR | G6 | A7 | A8 | L9 | G10 | M11 | I12 | E13 | T14 | A23 | A24 | D25 | A26 | M27 | A30 | A31 | R34 | L35 | R38 | V41 | Y45 | V48 | T54 | G72 | D73 | G74 | L75 | V76 | A77 | A78 | H79 | L80 | I81 | A82 | S86 | E87 | V88 | A95 | P96 | Q97 |

ALA

- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Hi:  67% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ai:  69% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bi:  68% 24% 6%



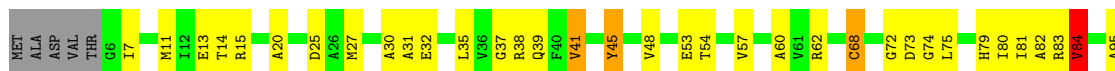
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ci:  61% 28% 5% 6%




- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Di:  58% 32% 6%

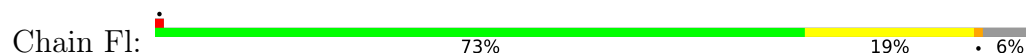


- Molecule 1: Major carboxysome shell protein CsoS1A

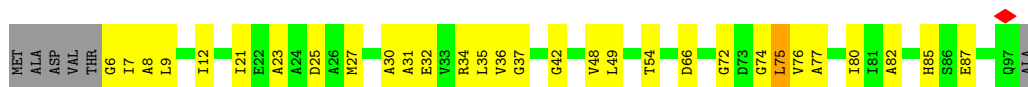
Chain Ei:  73% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



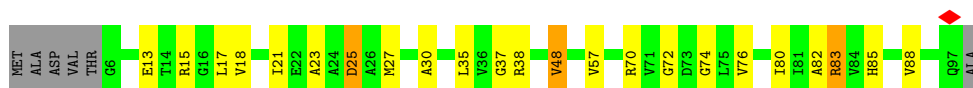
- Molecule 1: Major carboxysome shell protein CsoS1A



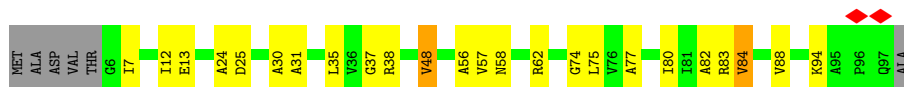
- Molecule 1: Major carboxysome shell protein CsoS1A




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- Molecule 1: Major carboxysome shell protein CsoS1A



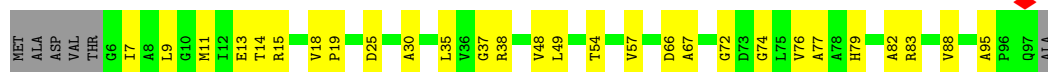
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dk:  73% 19% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ek:  65% 29% 6%



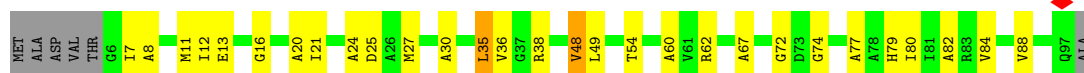
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fk:  70% 22% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Gk:  64% 28% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ao:  64% 27% • • 6%




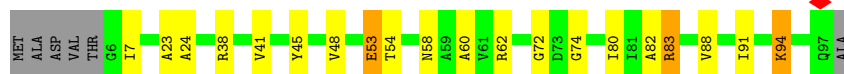
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bo:  65% 24% • 6%

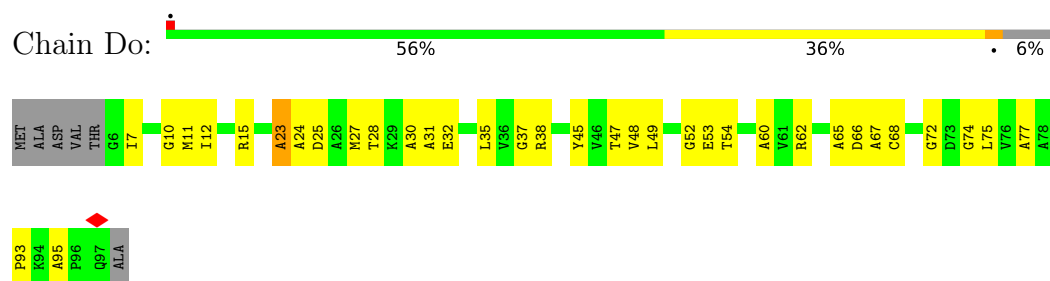


- Molecule 1: Major carboxysome shell protein CsoS1A

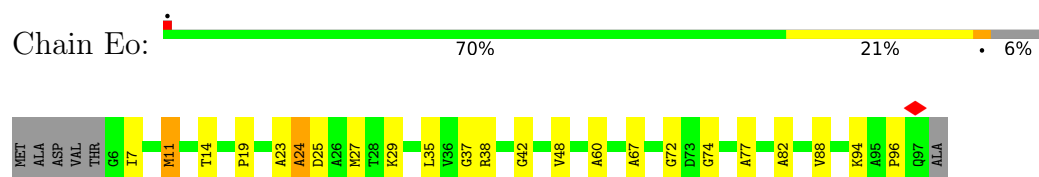
Chain Co:  73% 17% • 6%



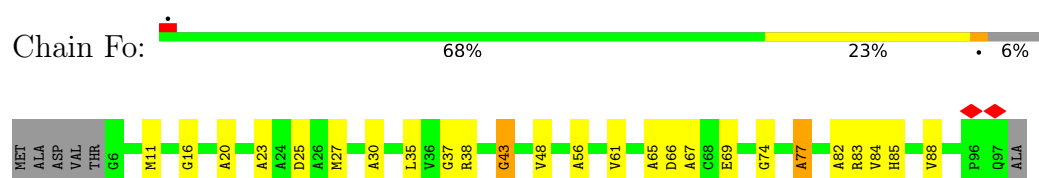
- Molecule 1: Major carboxysome shell protein CsoS1A



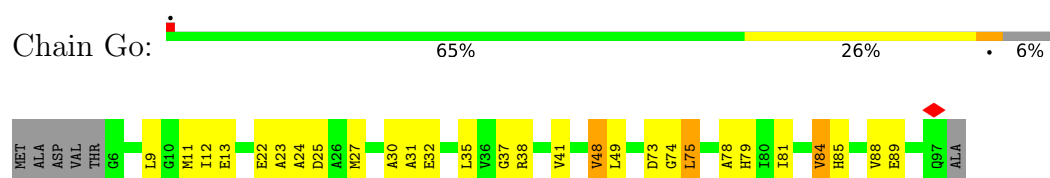
- Molecule 1: Major carboxysome shell protein CsoS1A



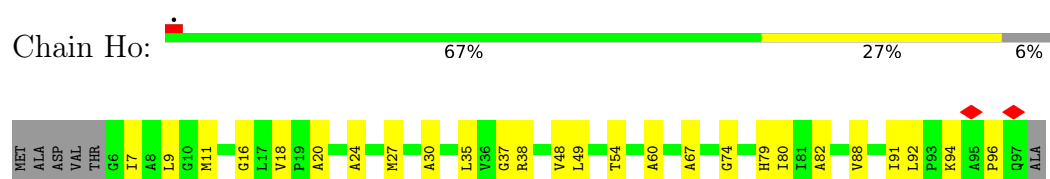
- Molecule 1: Major carboxysome shell protein CsoS1A



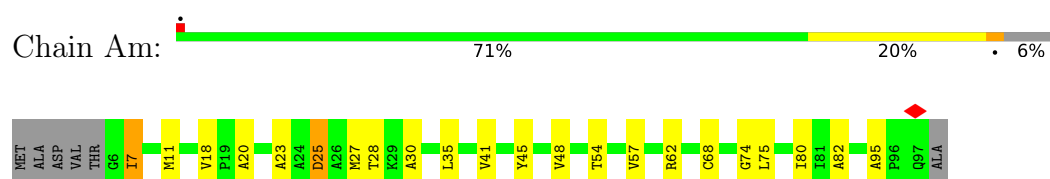
- Molecule 1: Major carboxysome shell protein CsoS1A




- Molecule 1: Major carboxysome shell protein CsoS1A

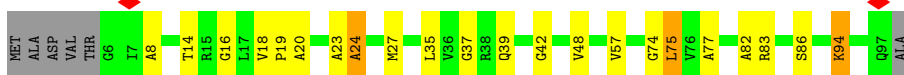


- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bm:  71% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cm:  64% 28% 6%




- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dm:  64% 30% 6%



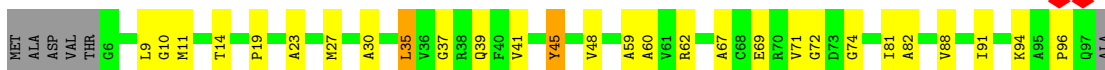
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Em:  72% 21% 6%



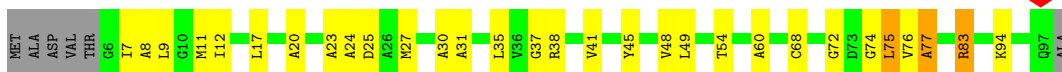
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fm:  65% 27% 6%




- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Gm:  63% 28% 6%




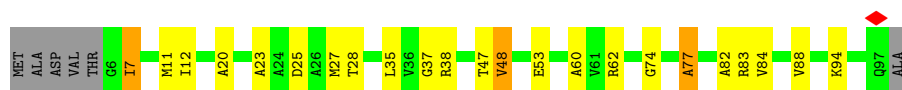
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Hm:  71% 20% 6%



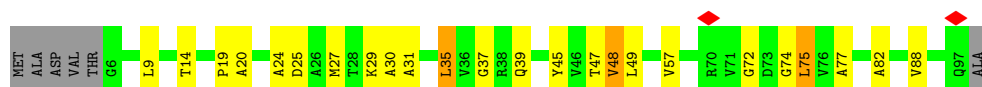
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain An:  70% 20% 6%



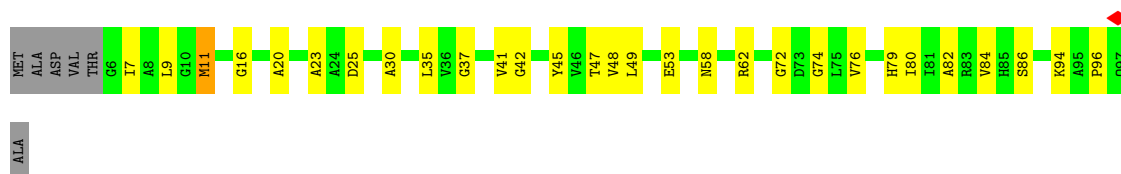
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bn:  69% 21% 6%



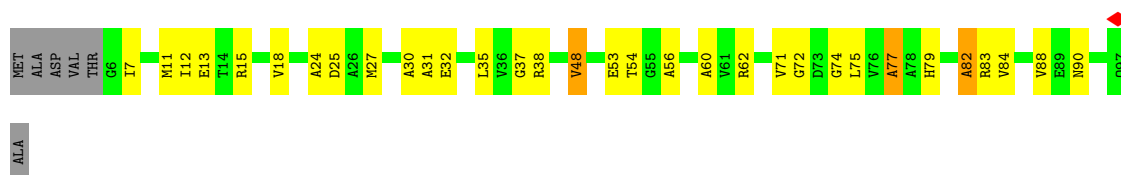
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cn:  64% 29% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dn:  61% 30% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain En:  60% 30% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fn:  64% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A



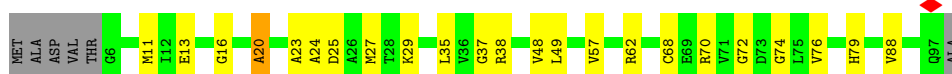
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



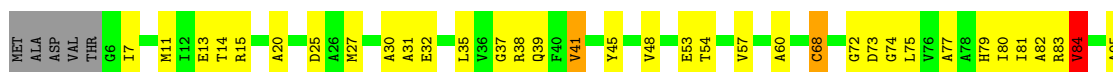
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

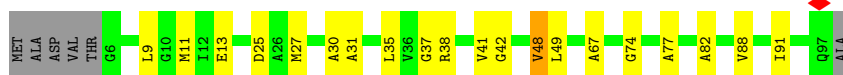
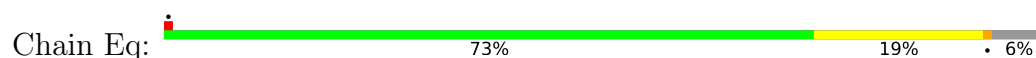


- Molecule 1: Major carboxysome shell protein CsoS1A

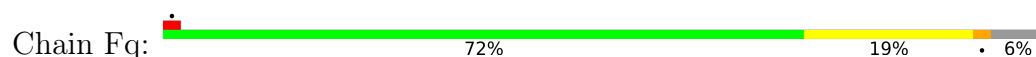




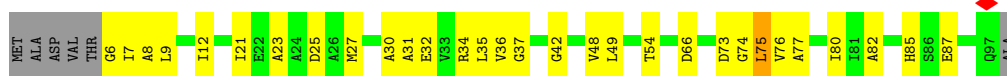
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



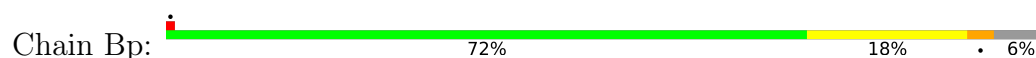
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



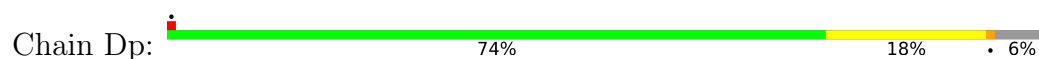
- Molecule 1: Major carboxysome shell protein CsoS1A



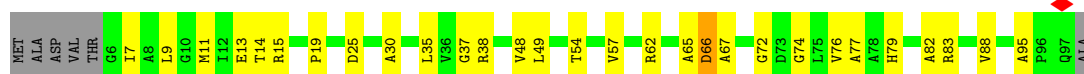
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



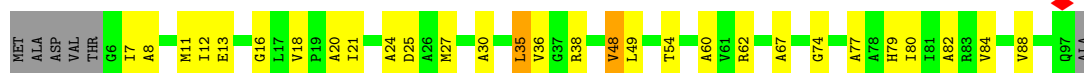
- Molecule 1: Major carboxysome shell protein CsoS1A



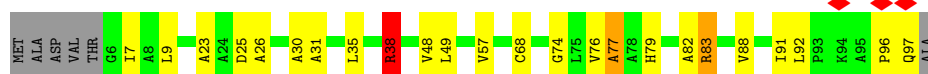
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- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

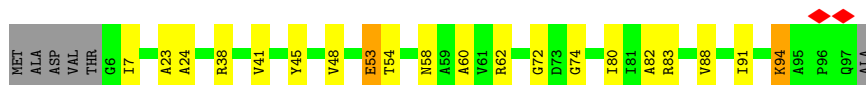
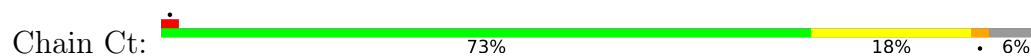




- Molecule 1: Major carboxysome shell protein CsoS1A



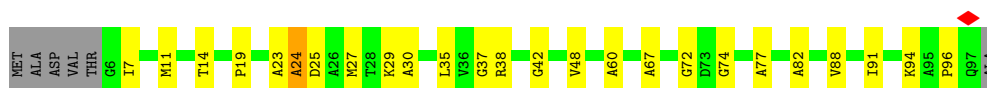
- Molecule 1: Major carboxysome shell protein CsoS1A



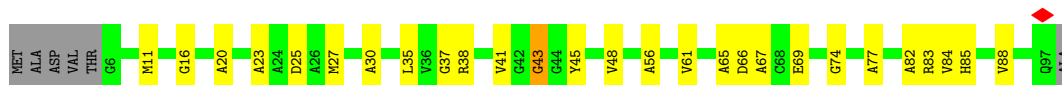
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

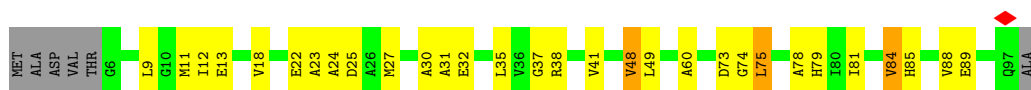


- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A





- Molecule 1: Major carboxysome shell protein CsoS1A



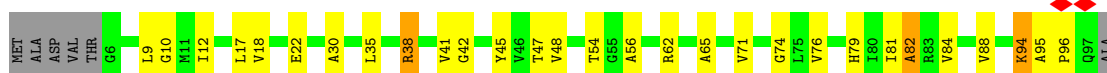
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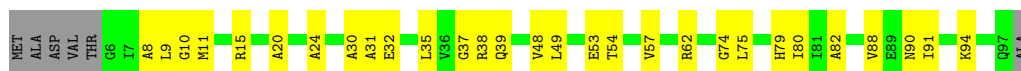
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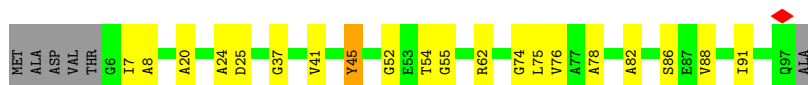
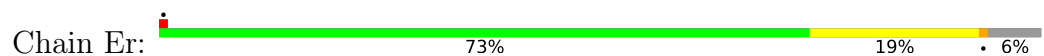
- Molecule 1: Major carboxysome shell protein CsoS1A



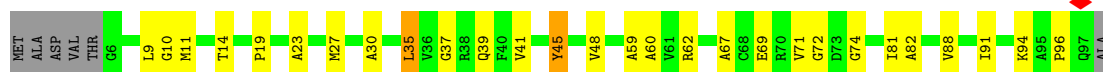
- Molecule 1: Major carboxysome shell protein CsoS1A



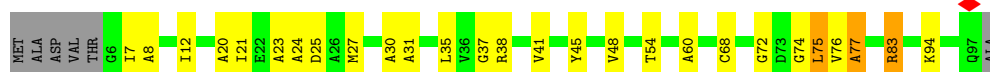
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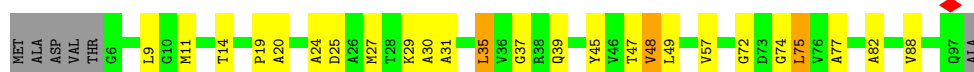
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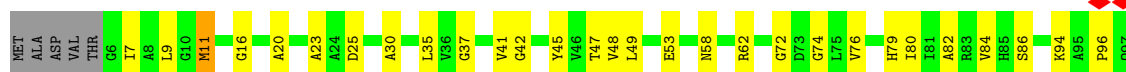
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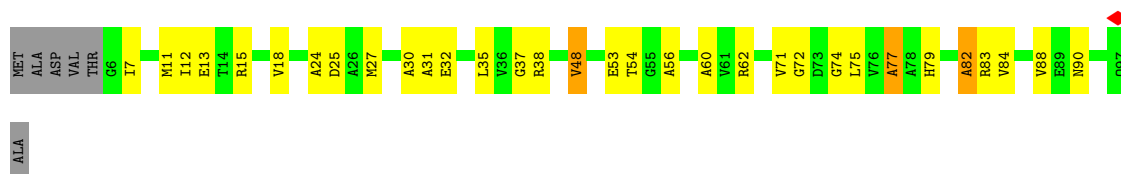
- Molecule 1: Major carboxysome shell protein CsoS1A



ALA

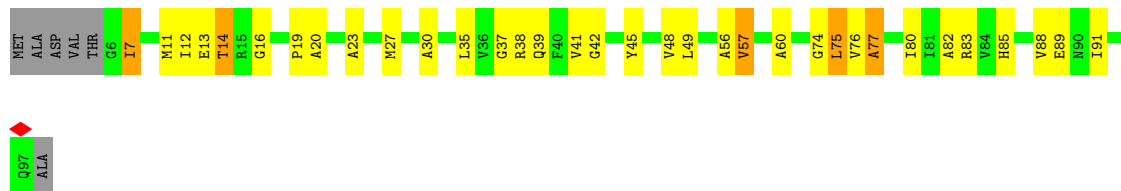
- Molecule 1: Major carboxysome shell protein CsoS1A





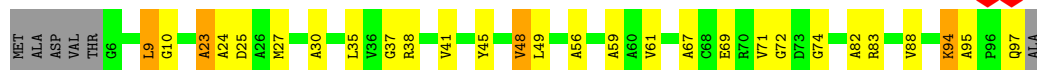
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Es: 59% 30% 5% 6%



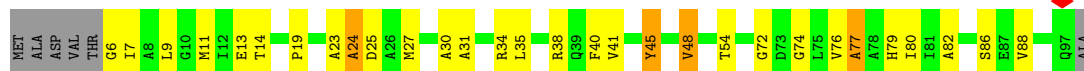
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fs: 65% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Gs: 63% 27% 6%



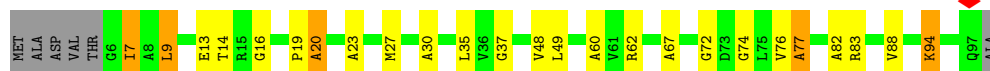
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Hs: 64% 28% 6%



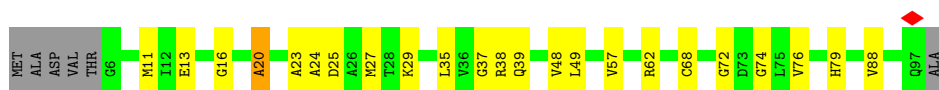
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Av: 68% 20% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

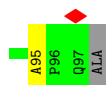
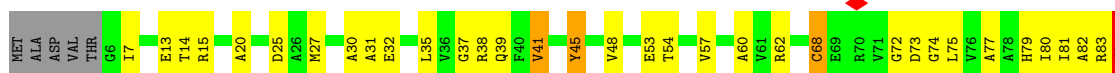
Chain Bv: 70% 22% 6%



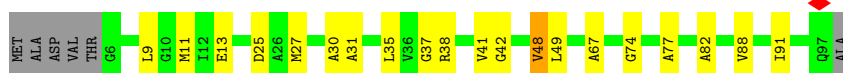
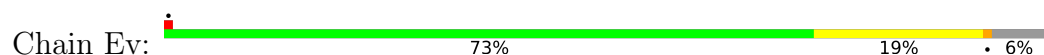
- Molecule 1: Major carboxysome shell protein CsoS1A



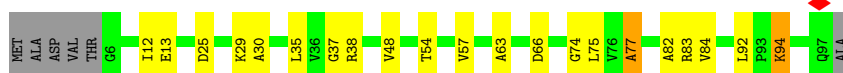
- Molecule 1: Major carboxysome shell protein CsoS1A



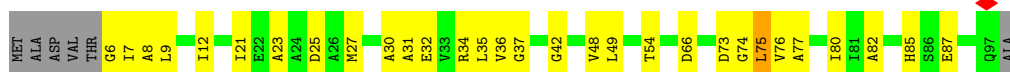
- Molecule 1: Major carboxysome shell protein CsoS1A



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- Molecule 1: Major carboxysome shell protein CsoS1A



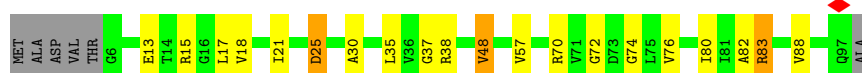
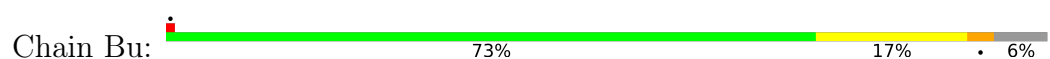
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



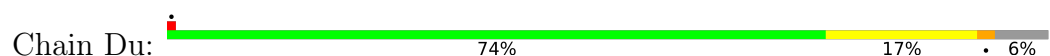
- Molecule 1: Major carboxysome shell protein CsoS1A



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- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

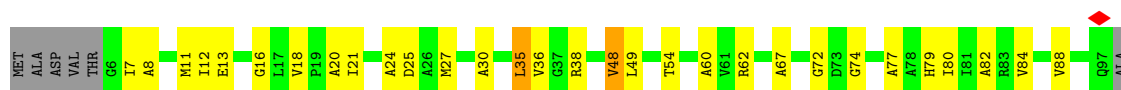


- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Gu: 



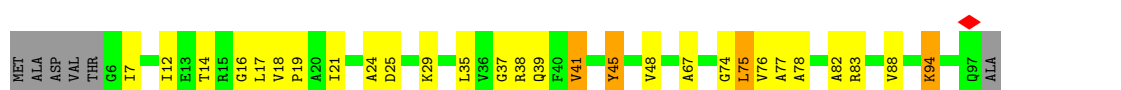
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ay: 




- Molecule 1: Major carboxysome shell protein CsoS1A

Chain By: 



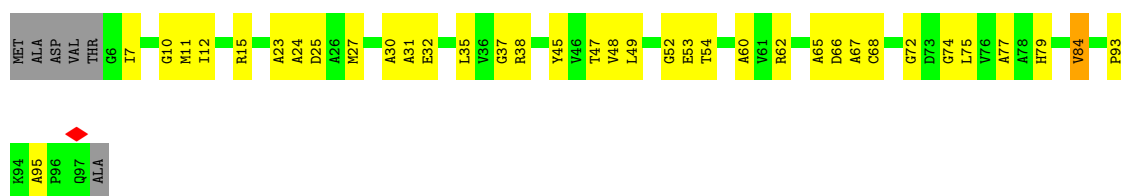
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cy: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dy: 

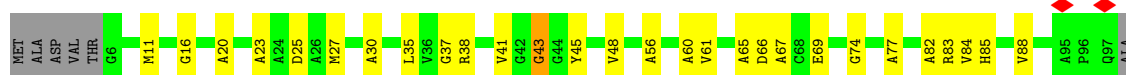


- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Ey: 



- Molecule 1: Major carboxysome shell protein CsoS1A



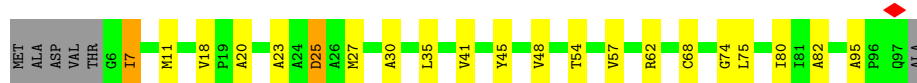
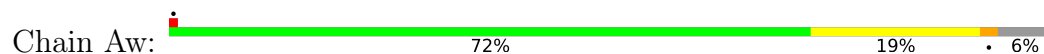
- Molecule 1: Major carboxysome shell protein CsoS1A



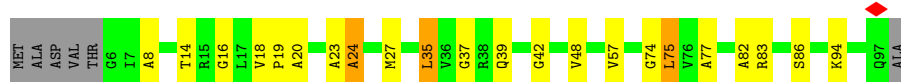
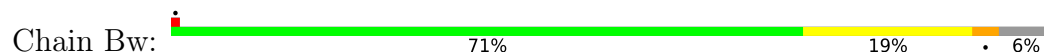
- Molecule 1: Major carboxysome shell protein CsoS1A



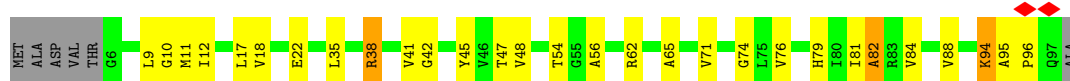
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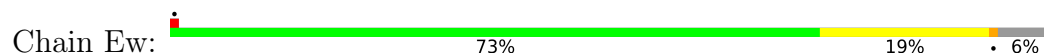


- Molecule 1: Major carboxysome shell protein CsoS1A

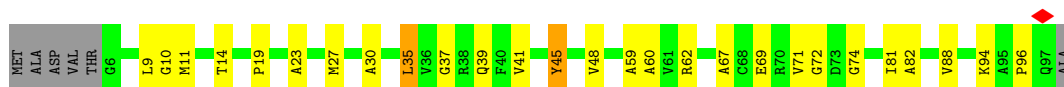




- Molecule 1: Major carboxysome shell protein CsoS1A



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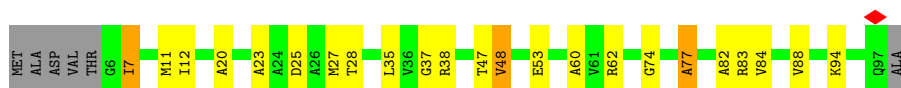
- Molecule 1: Major carboxysome shell protein CsoS1A



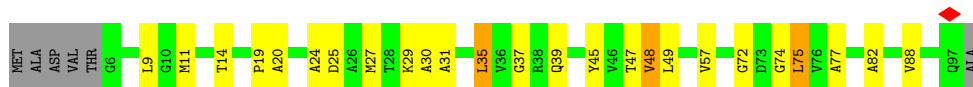
- Molecule 1: Major carboxysome shell protein CsoS1A



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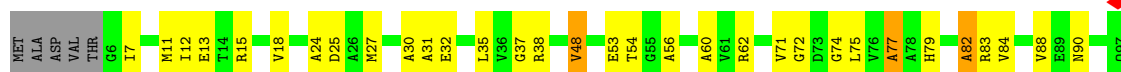
Chain Cx:  64% 29% 6%



ALA

- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dx:  61% 30% 6%



ALA

- Molecule 1: Major carboxysome shell protein CsoS1A

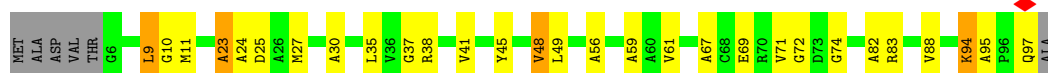
Chain Ex:  60% 29% 5% 6%



ALA

- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Fx:  64% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Gx:  64% 26% 6%



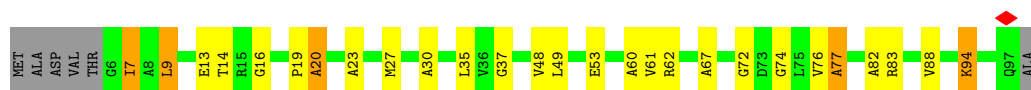
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Hx:  63% 30% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AA:  66% 22% 5% 6%



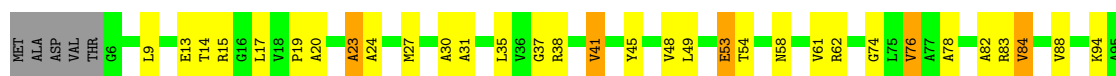
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BA:  67% 26% 6%



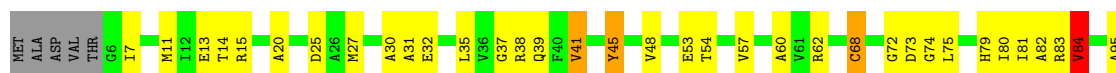
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CA:  61% 28% 5% 6%




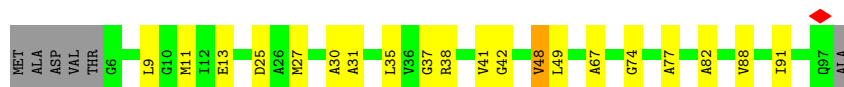
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DA:  58% 32% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EA:  73% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FA:  71% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GA: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HA: 




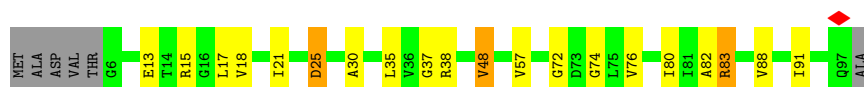
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Az: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Bz: 




- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Cz: 



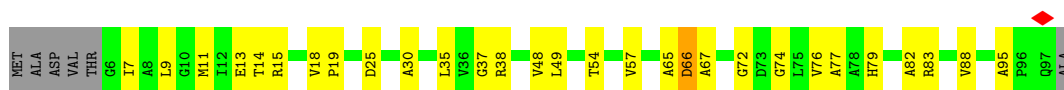
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Dz: 



- Molecule 1: Major carboxysome shell protein CsoS1A

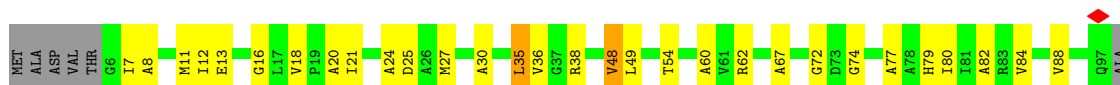
Chain Ez: 



- Molecule 1: Major carboxysome shell protein CsoS1A



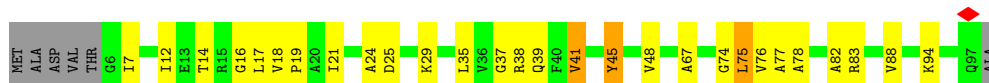
- Molecule 1: Major carboxysome shell protein CsoS1A



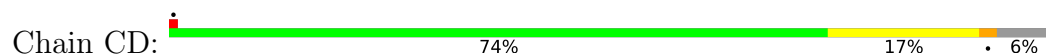
- Molecule 1: Major carboxysome shell protein CsoS1A



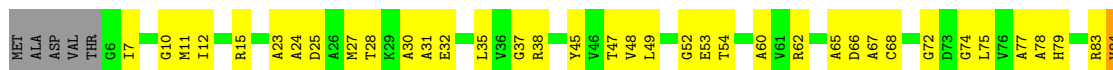
- Molecule 1: Major carboxysome shell protein CsoS1A

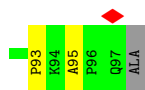


- Molecule 1: Major carboxysome shell protein CsoS1A

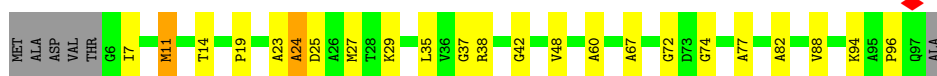
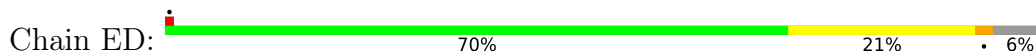


- Molecule 1: Major carboxysome shell protein CsoS1A

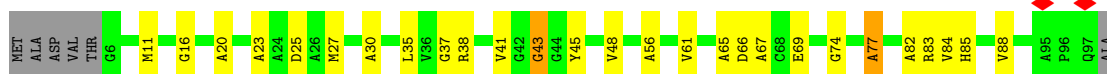




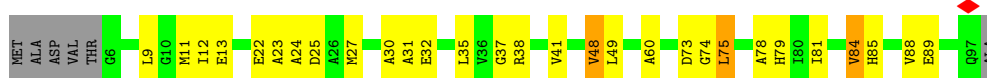
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



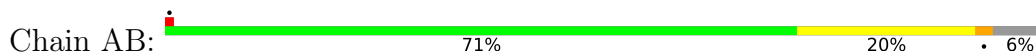
- Molecule 1: Major carboxysome shell protein CsoS1A



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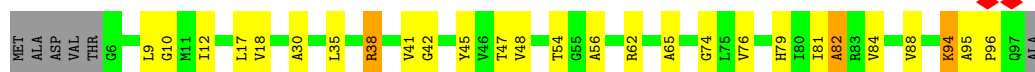


- Molecule 1: Major carboxysome shell protein CsoS1A



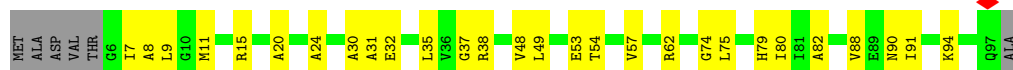
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CB:  66% 24% 6%




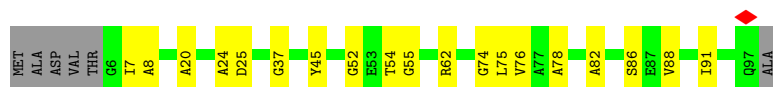
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DB:  65% 29% 6%



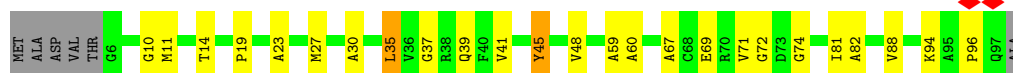
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EB:  74% 19% 6%



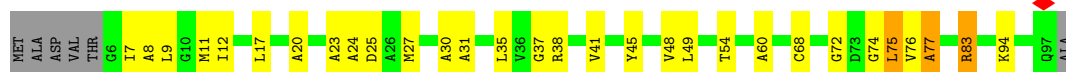
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FB:  68% 23% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GB:  63% 28% 6%




- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HB:  70% 21% 6%



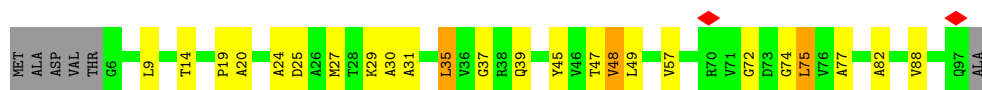
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AC:  72% 18% 6%



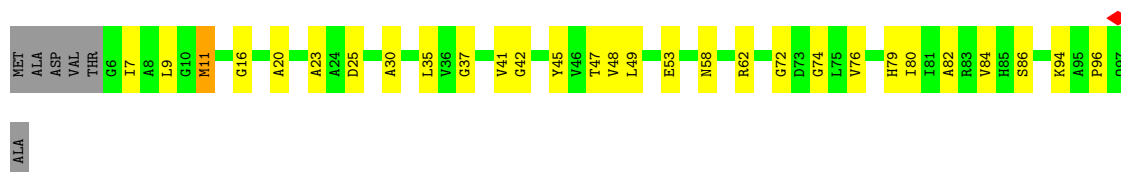
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BC:  69% 21% 6%



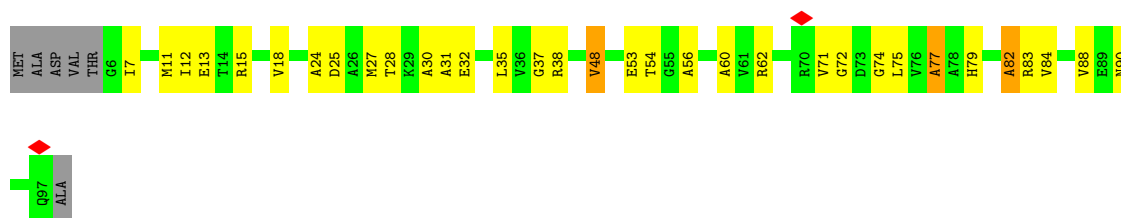
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CC:  64% 29% 6%



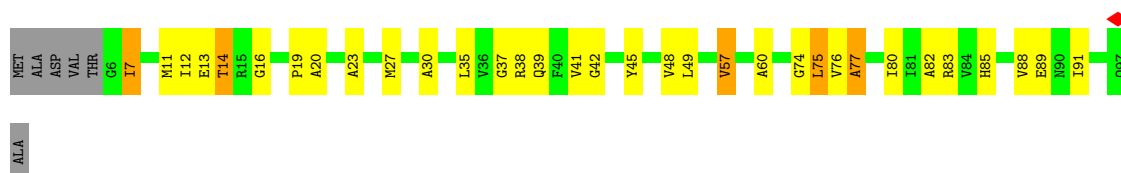
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DC:  60% 31% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EC:  60% 29% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FC:  64% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GC:  63% 27% 6%

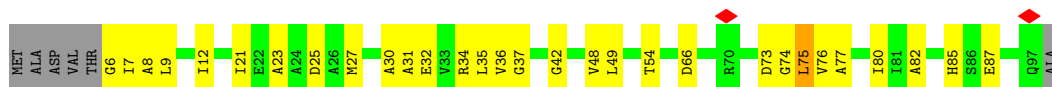




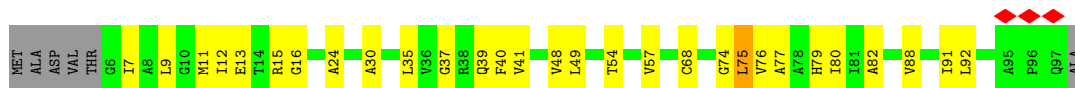
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



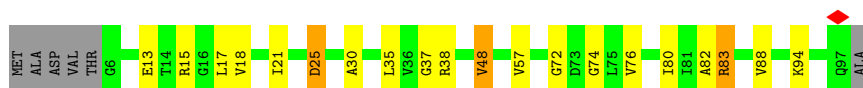
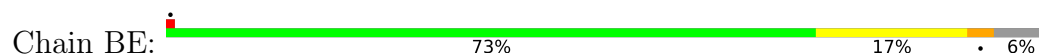
- Molecule 1: Major carboxysome shell protein CsoS1A



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- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



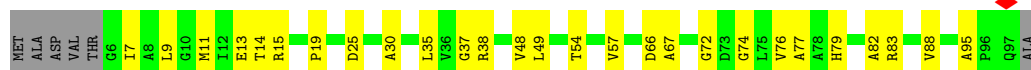
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DE:  73% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EE:  66% 28% 6%



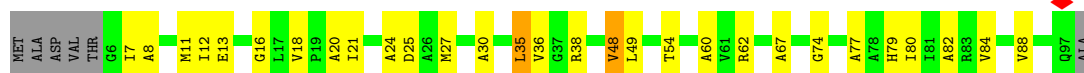
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FE:  68% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GE:  64% 28% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HE:  68% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AI:  63% 29% 6%




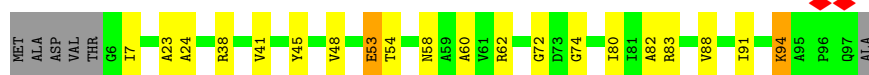
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BI:  64% 26% 6%



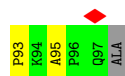
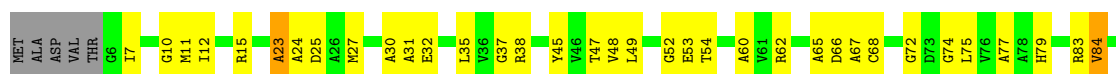
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CI:  73% 18% • 6%



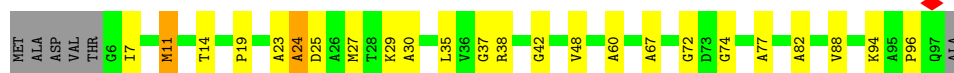
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DI:  56% 36% • 6%



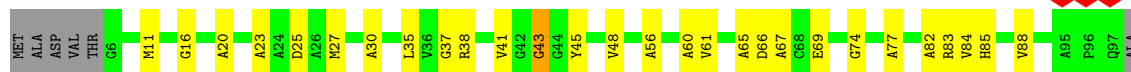
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EI:  69% 22% • 6%



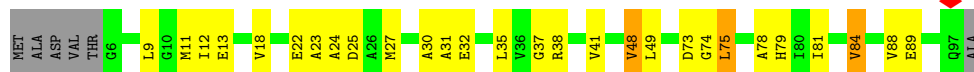
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FI:  65% 28% • 6%



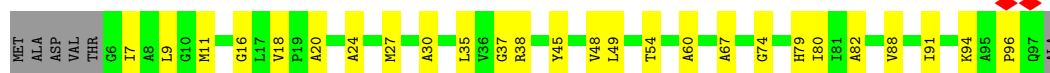
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GI:  65% 26% • 6%




- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HI:  67% 27% • 6%




- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AG:  71% 20% 6%



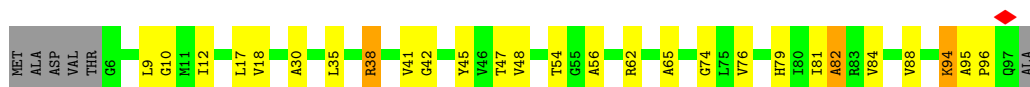
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BG:  71% 20% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CG:  66% 24% 6%




- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DG:  64% 30% 6%



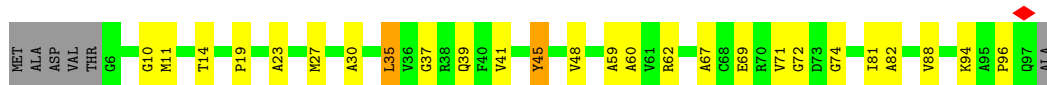
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EG:  76% 18% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FG:  67% 24% 6%




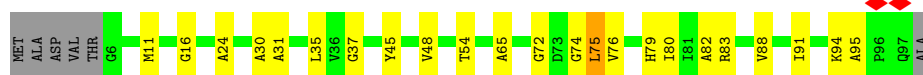
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GG:  64% 27% 6%




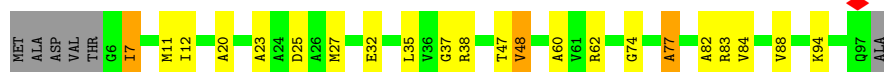
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HG:  70% 22% 6%



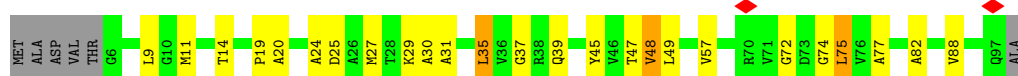
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AH:  71% 19% 6%



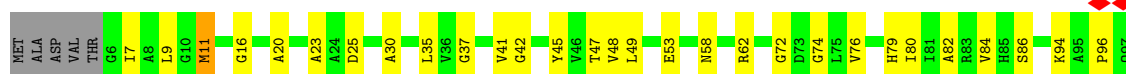
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BH:  68% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CH:  64% 29% 6%



ALA

- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DH:  61% 30% 6%



ALA

- Molecule 1: Major carboxysome shell protein CsoS1A

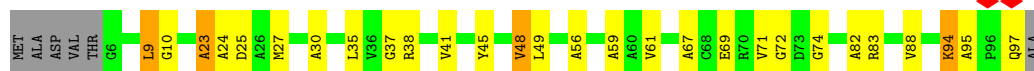
Chain EH:  59% 30% 5% 6%





- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FH: 65% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GH: 64% 26% 6%



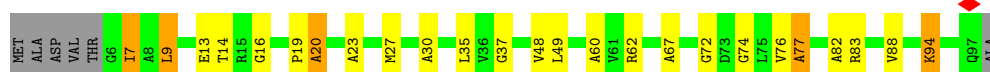
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HH: 64% 27% 6%



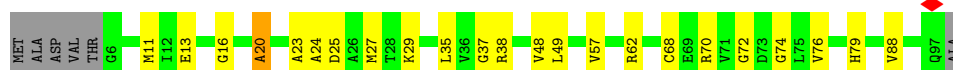
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AK: 68% 20% 5% 6%



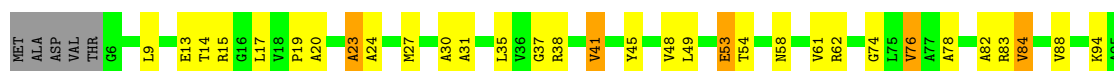
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BK: 70% 22% 6%

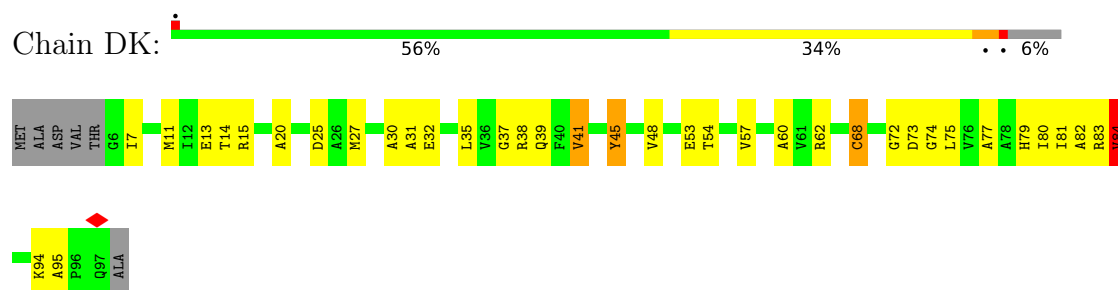


- Molecule 1: Major carboxysome shell protein CsoS1A

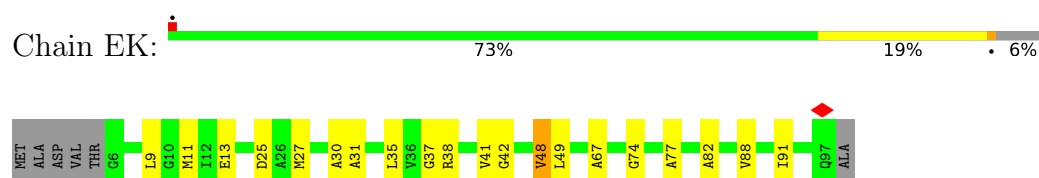
Chain CK: 61% 28% 5% 6%



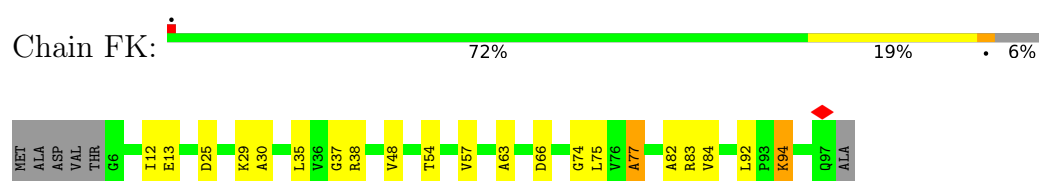
- Molecule 1: Major carboxysome shell protein CsoS1A



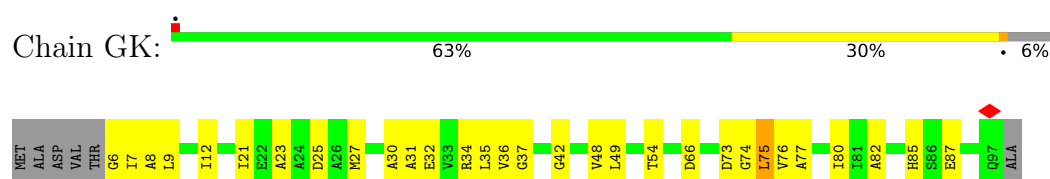
- Molecule 1: Major carboxysome shell protein CsoS1A



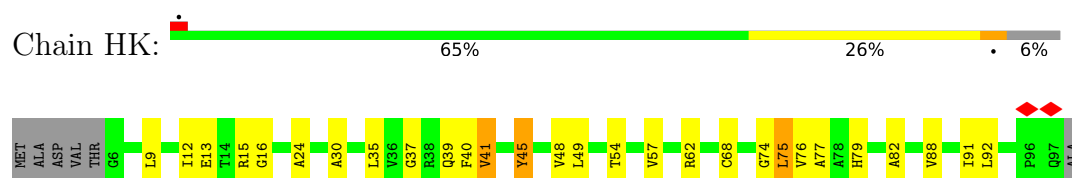
- Molecule 1: Major carboxysome shell protein CsoS1A



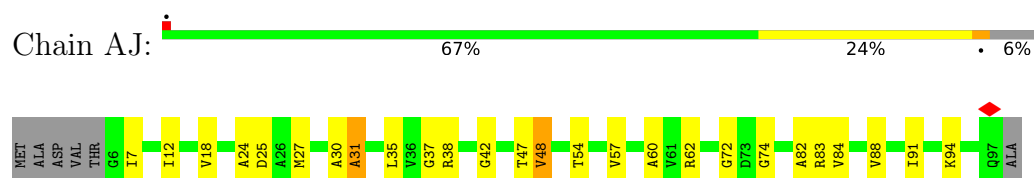
- Molecule 1: Major carboxysome shell protein CsoS1A



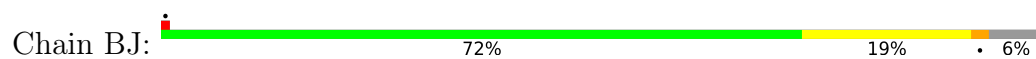
- Molecule 1: Major carboxysome shell protein CsoS1A



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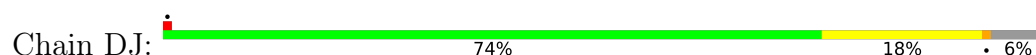
- Molecule 1: Major carboxysome shell protein CsoS1A



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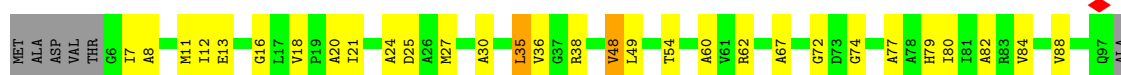
- Molecule 1: Major carboxysome shell protein CsoS1A



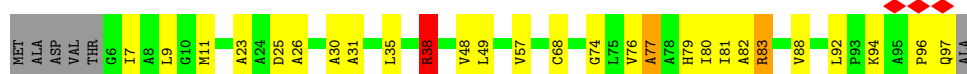
- Molecule 1: Major carboxysome shell protein CsoS1A



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- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AN: 




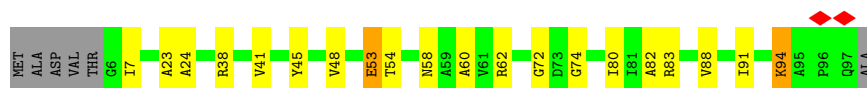
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BN: 



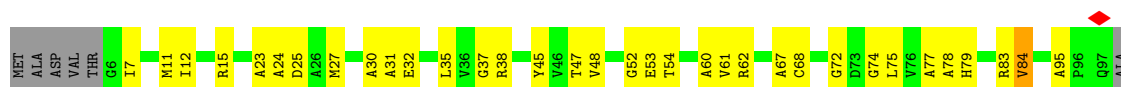
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CN: 



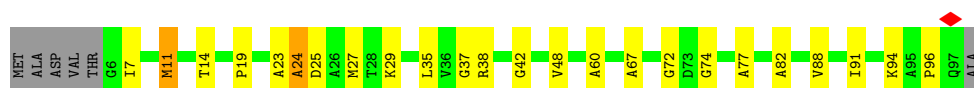
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DN: 



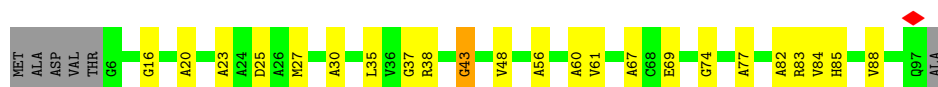
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EN: 



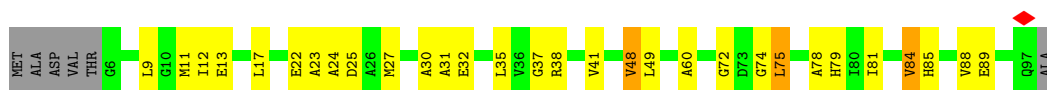
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FN: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GN: 



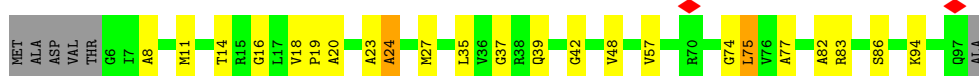
- Molecule 1: Major carboxysome shell protein CsoS1A



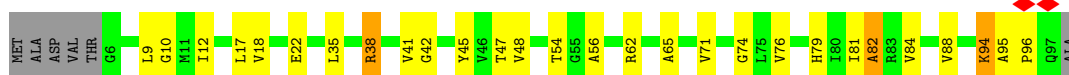
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



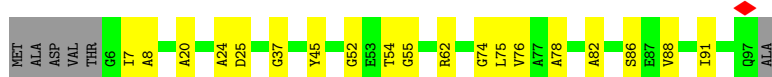
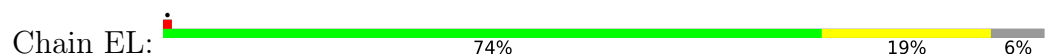
- Molecule 1: Major carboxysome shell protein CsoS1A



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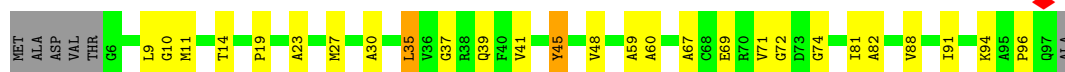


- Molecule 1: Major carboxysome shell protein CsoS1A



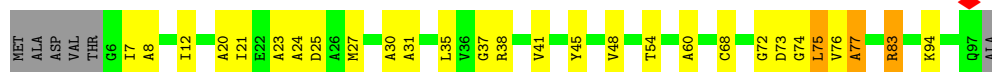
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FL:  66% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GL:  65% 26% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HL:  68% 24% 6%



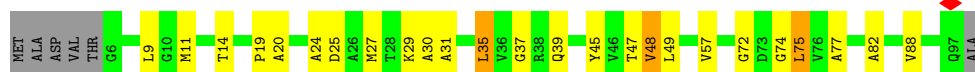
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AM:  68% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BM:  68% 22% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

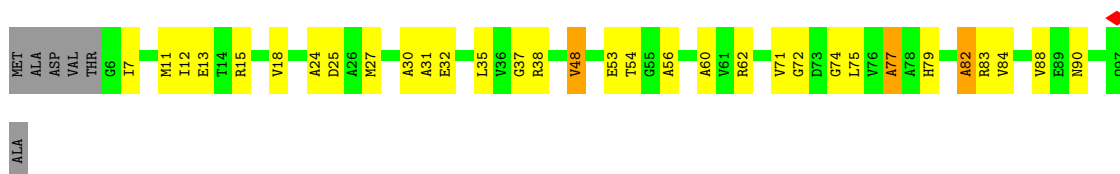
Chain CM:  64% 29% 6%



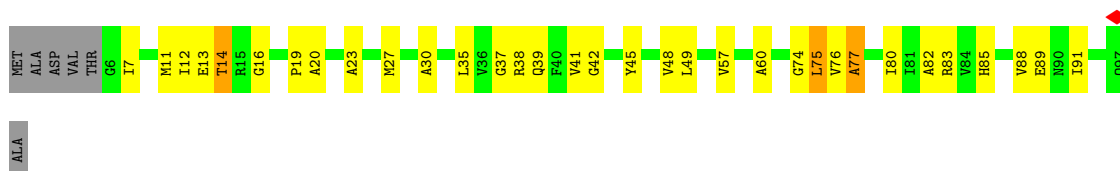
ALA

- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DM:  61% 30% 6%



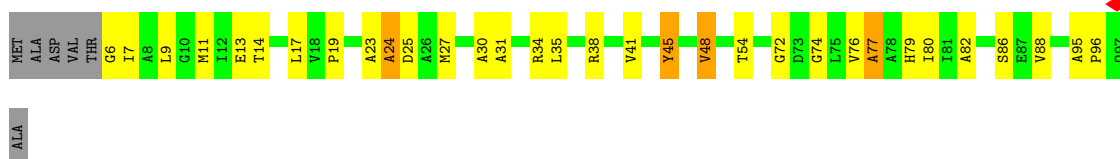
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



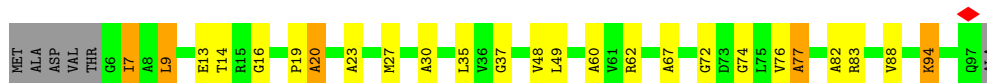
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



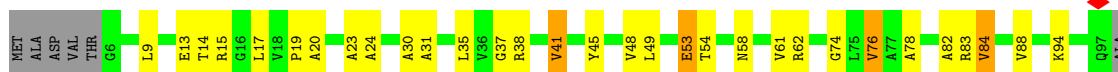
- Molecule 1: Major carboxysome shell protein CsoS1A



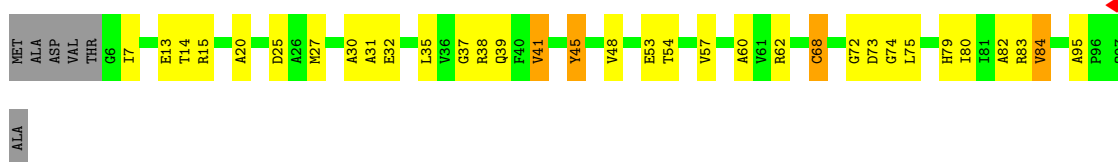
- Molecule 1: Major carboxysome shell protein CsoS1A



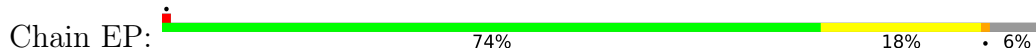
- Molecule 1: Major carboxysome shell protein CsoS1A



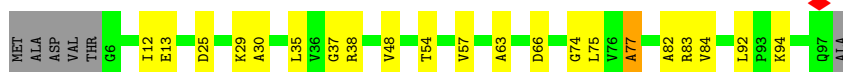
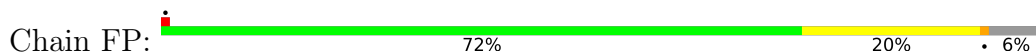
- Molecule 1: Major carboxysome shell protein CsoS1A



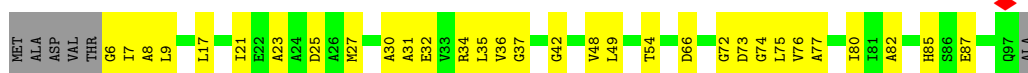
- Molecule 1: Major carboxysome shell protein CsoS1A



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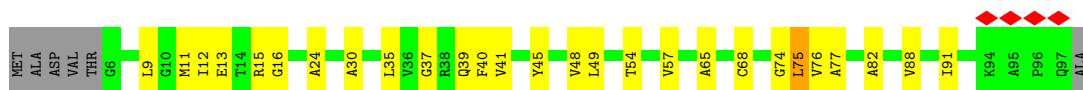


- Molecule 1: Major carboxysome shell protein CsoS1A

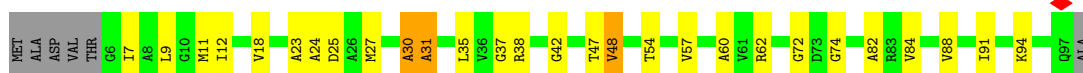


- Molecule 1: Major carboxysome shell protein CsoS1A

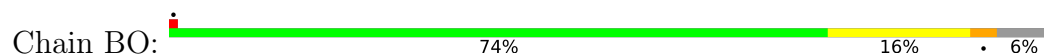




- Molecule 1: Major carboxysome shell protein CsoS1A



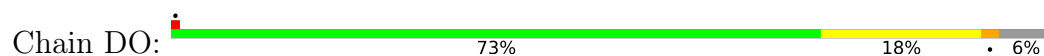
- Molecule 1: Major carboxysome shell protein CsoS1A



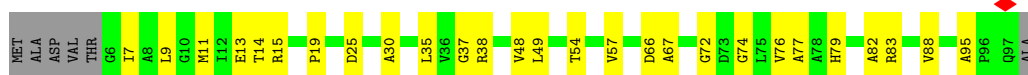
- Molecule 1: Major carboxysome shell protein CsoS1A



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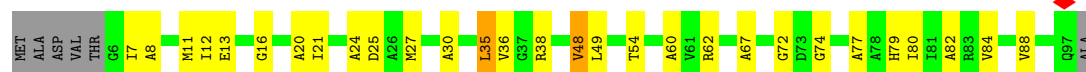
- Molecule 1: Major carboxysome shell protein CsoS1A



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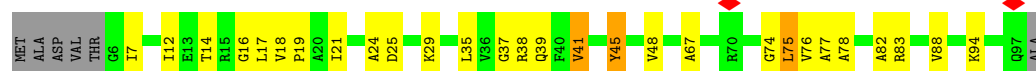
- Molecule 1: Major carboxysome shell protein CsoS1A



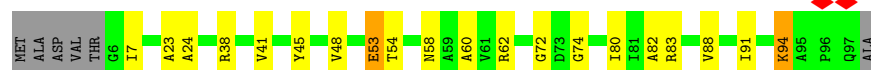
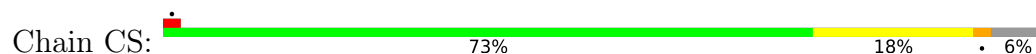
- Molecule 1: Major carboxysome shell protein CsoS1A



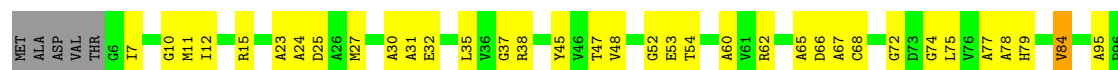
- Molecule 1: Major carboxysome shell protein CsoS1A



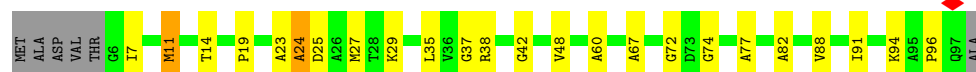
- Molecule 1: Major carboxysome shell protein CsoS1A



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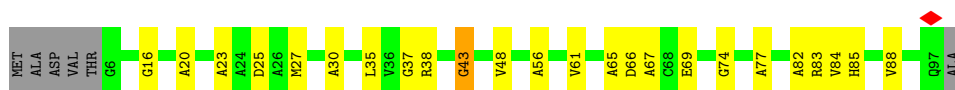


- Molecule 1: Major carboxysome shell protein CsoS1A



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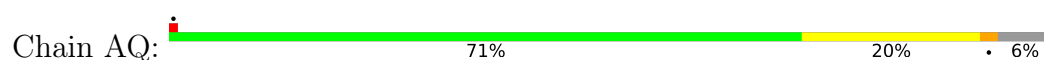
- Molecule 1: Major carboxysome shell protein CsoS1A



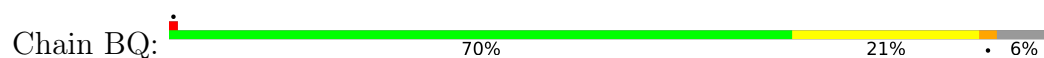
- Molecule 1: Major carboxysome shell protein CsoS1A



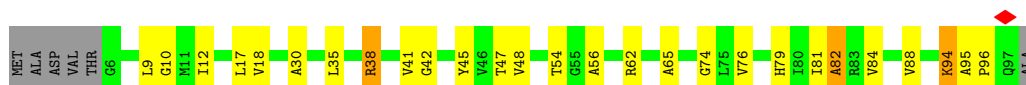
- Molecule 1: Major carboxysome shell protein CsoS1A



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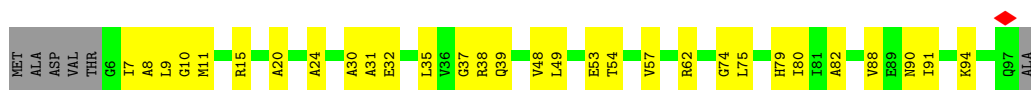


- Molecule 1: Major carboxysome shell protein CsoS1A

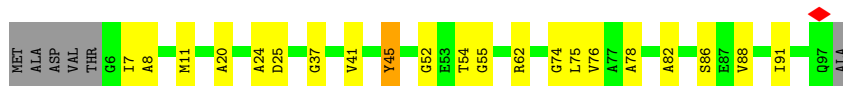
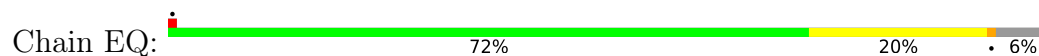


- Molecule 1: Major carboxysome shell protein CsoS1A





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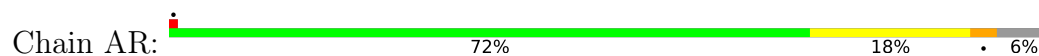
- Molecule 1: Major carboxysome shell protein CsoS1A



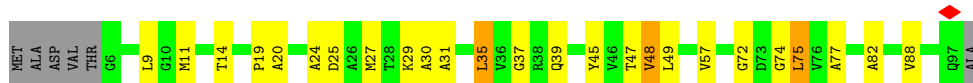
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A

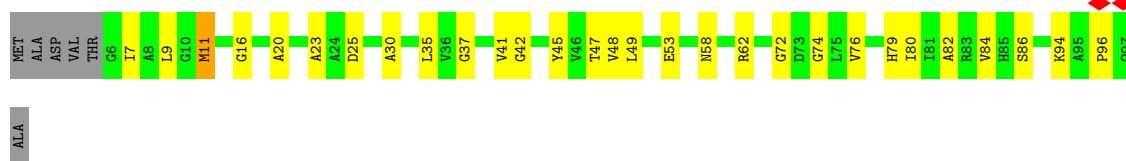


- Molecule 1: Major carboxysome shell protein CsoS1A



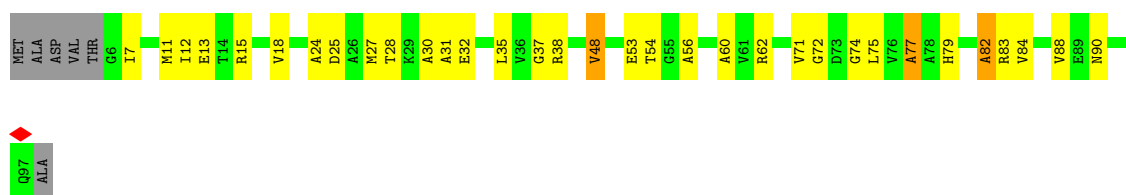
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CR: 



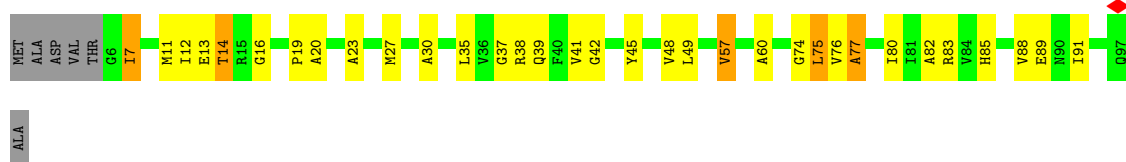
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DR: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain ER: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FR: 



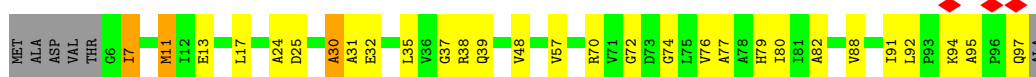
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GR: 



- Molecule 1: Major carboxysome shell protein CsoS1A

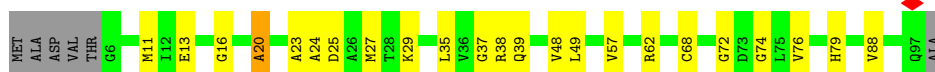
Chain HR: 



- Molecule 1: Major carboxysome shell protein CsoS1A



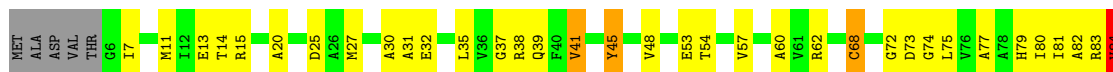
- Molecule 1: Major carboxysome shell protein CsoS1A



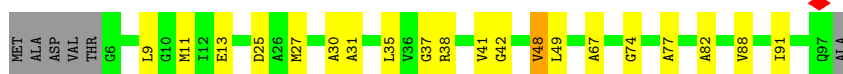
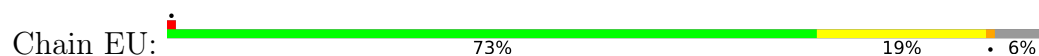
- Molecule 1: Major carboxysome shell protein CsoS1A



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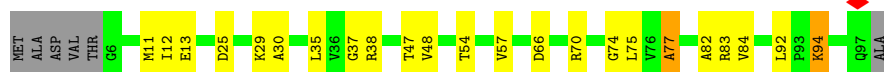


- Molecule 1: Major carboxysome shell protein CsoS1A



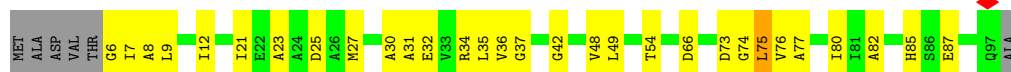
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FU:  70% 21% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GU:  63% 30% 6%



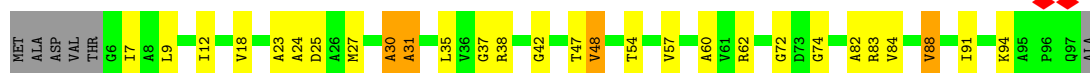
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HU:  64% 29% 6%




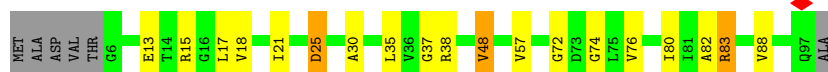
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AT:  65% 24% 6%



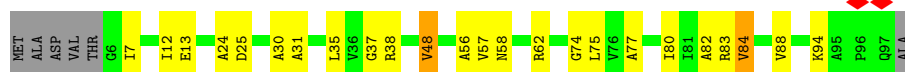
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BT:  74% 16% 6%




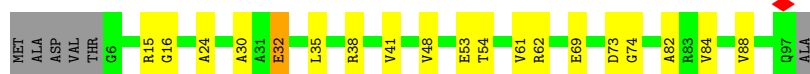
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CT:  69% 22% 6%



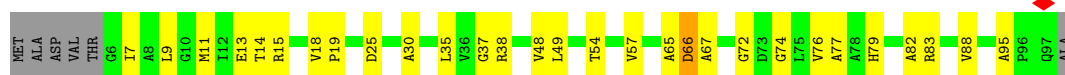
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DT:  74% 18% 6%



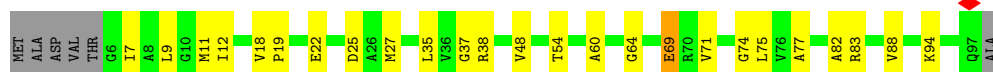
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain ET:  64% 29% • 6%



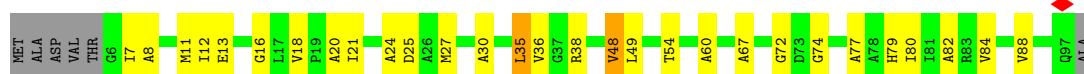
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FT:  68% 24% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GT:  64% 28% • 6%



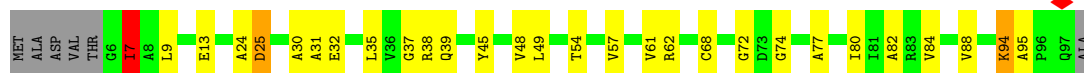
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HT:  66% 24% • • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AX:  64% 27% • • 6%




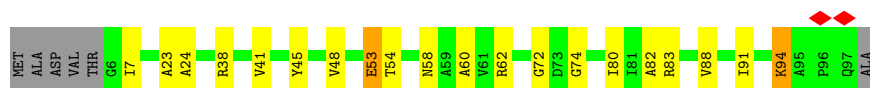
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BX:  63% 28% • 6%

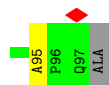


- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CX:  73% 18% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A



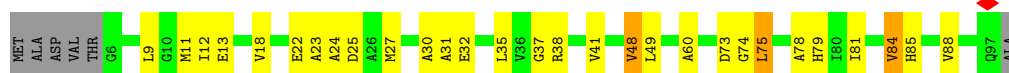
- Molecule 1: Major carboxysome shell protein CsoS1A



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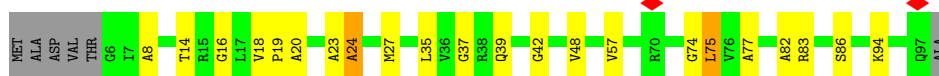
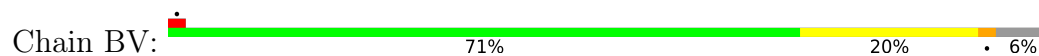


- Molecule 1: Major carboxysome shell protein CsoS1A

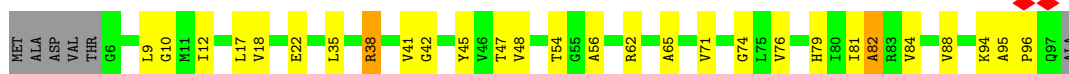




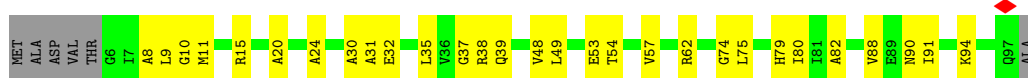
- Molecule 1: Major carboxysome shell protein CsoS1A



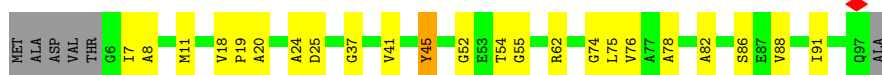
- Molecule 1: Major carboxysome shell protein CsoS1A



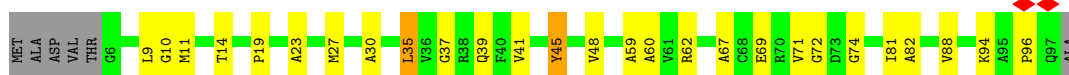
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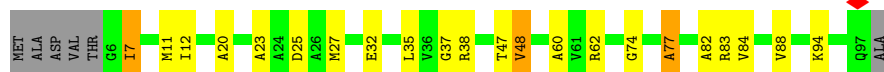
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HV:  71% 20% 6%



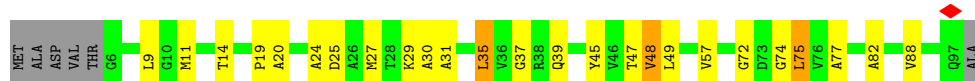
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain AW:  71% 19% 6%



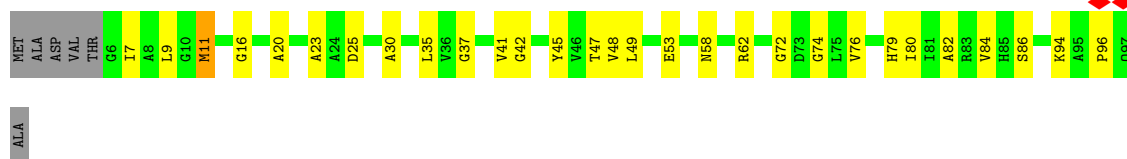
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain BW:  68% 22% 6%



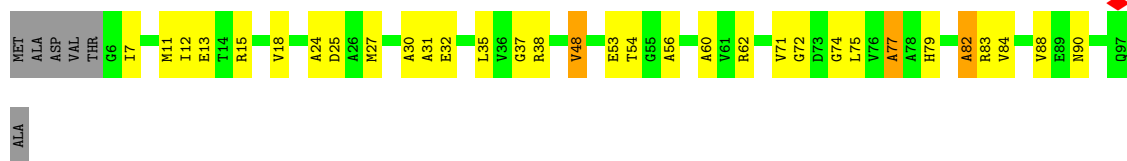
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain CW:  64% 29% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain DW:  61% 30% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain EW:  59% 30% 5% 6%





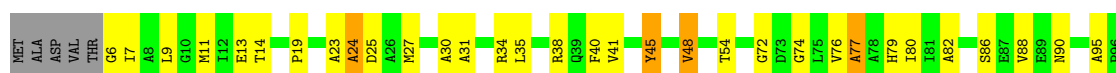
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain FW: 65% 24% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain GW: 61% 29% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain HW: 63% 28% 6%



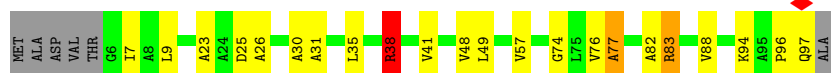
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain H1: 71% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain H6: 71% 19% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Hf: 68% 22% 6%









Chain X4:  9% 87%

[illegible]

- Molecule 2: Carboxysome assembly protein CsoS2B

Chain X7:  10% 87%

[illegible]

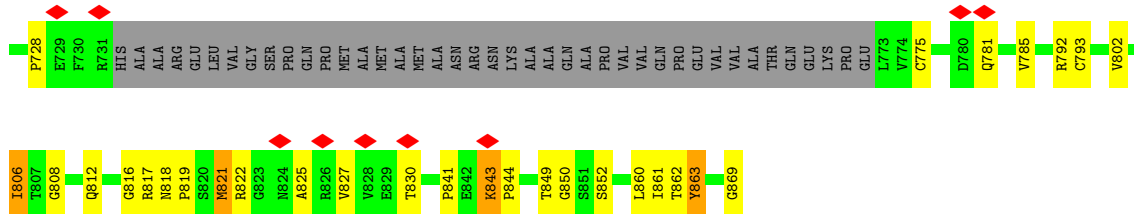








Chain Xa:  9% 87%

[illegible]

- Molecule 2: Carboxysome assembly protein CsoS2B

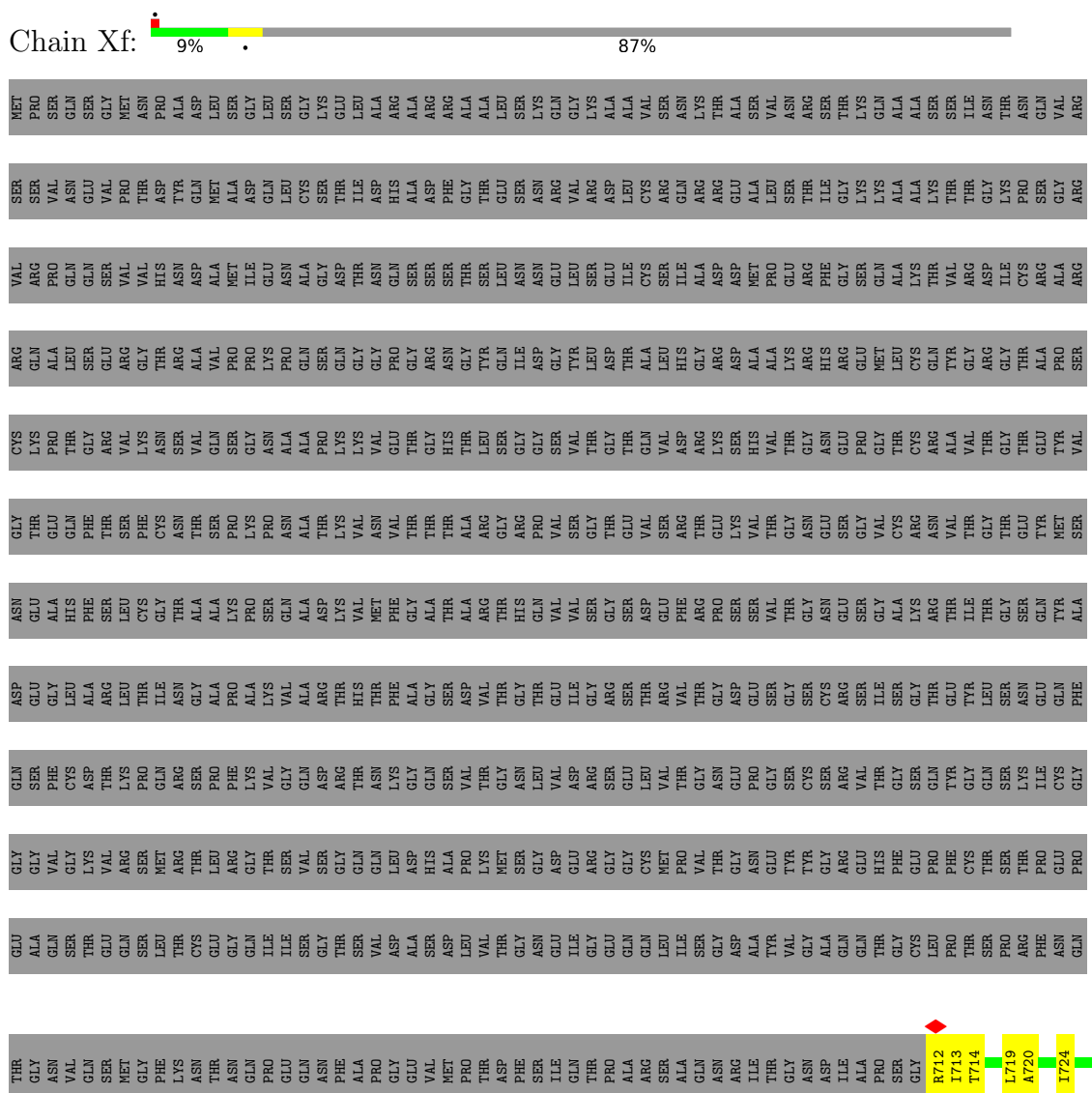
Chain Xe:  10% 87%

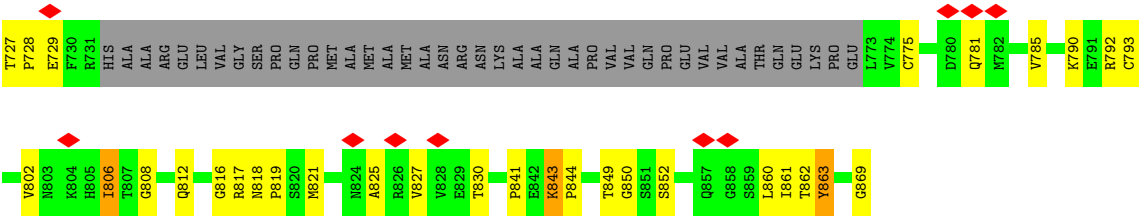
[illegible]



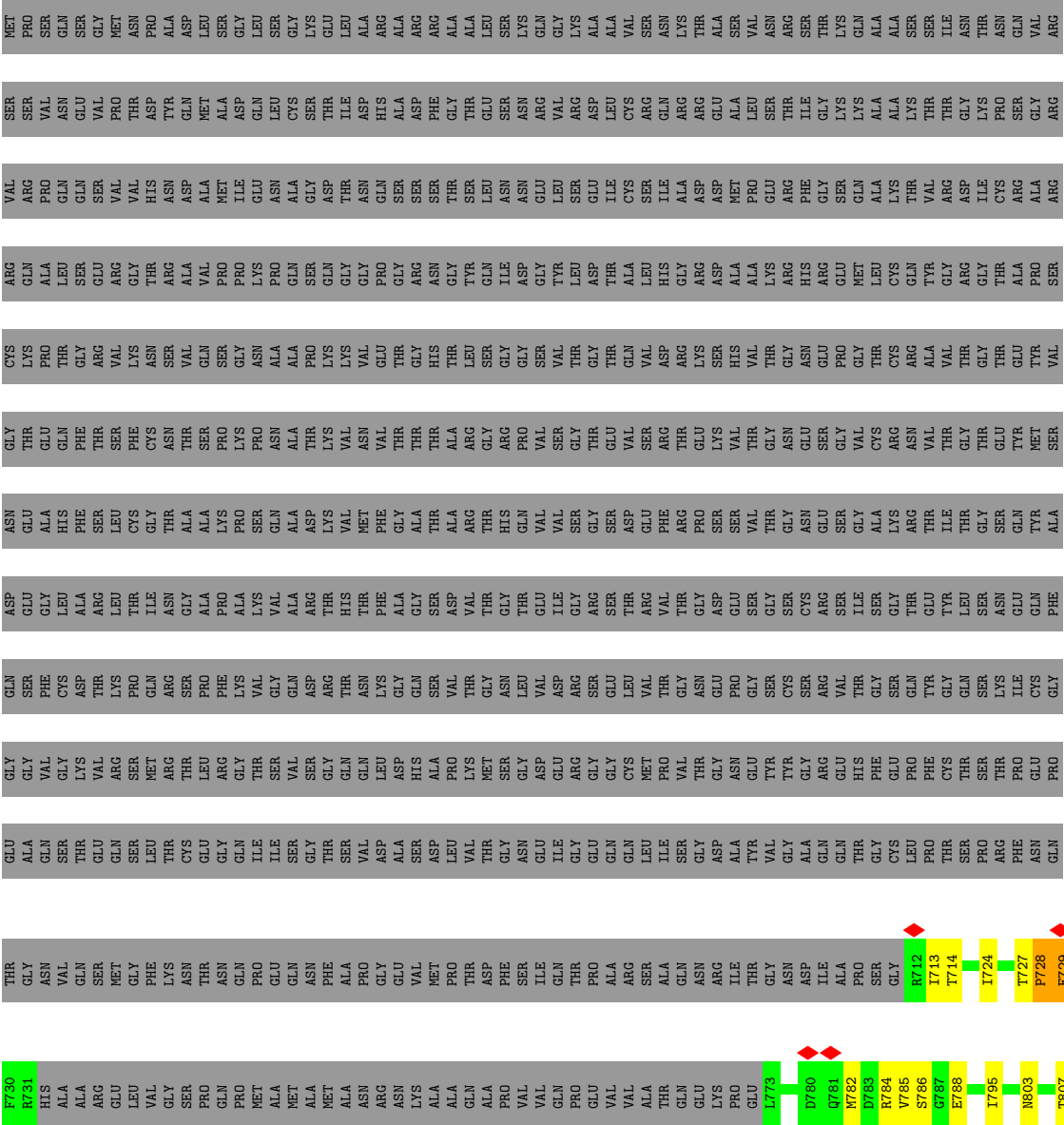


- Molecule 2: Carboxysome assembly protein CsoS2B





• Molecule 2: Carboxysome assembly protein CsoS2B



• Molecule 2: Carboxysome assembly protein CsoS2B

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

[illegible]





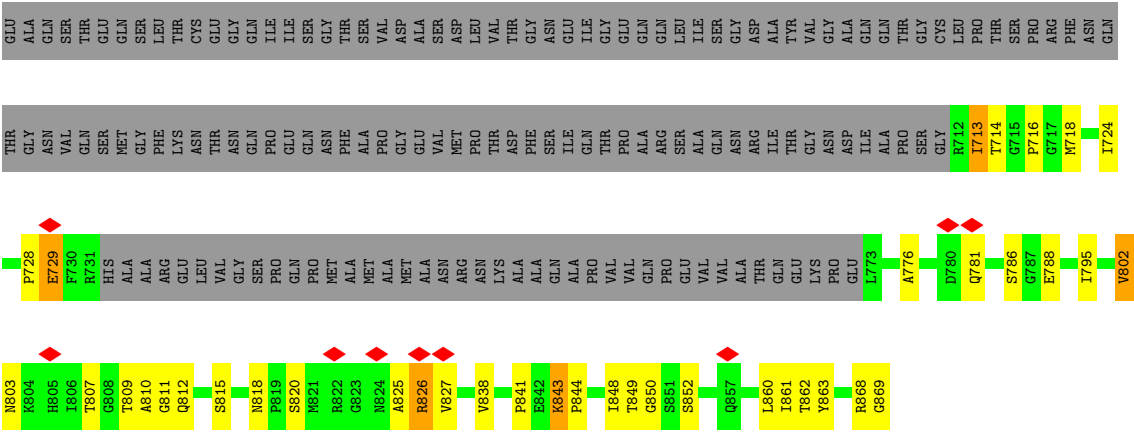




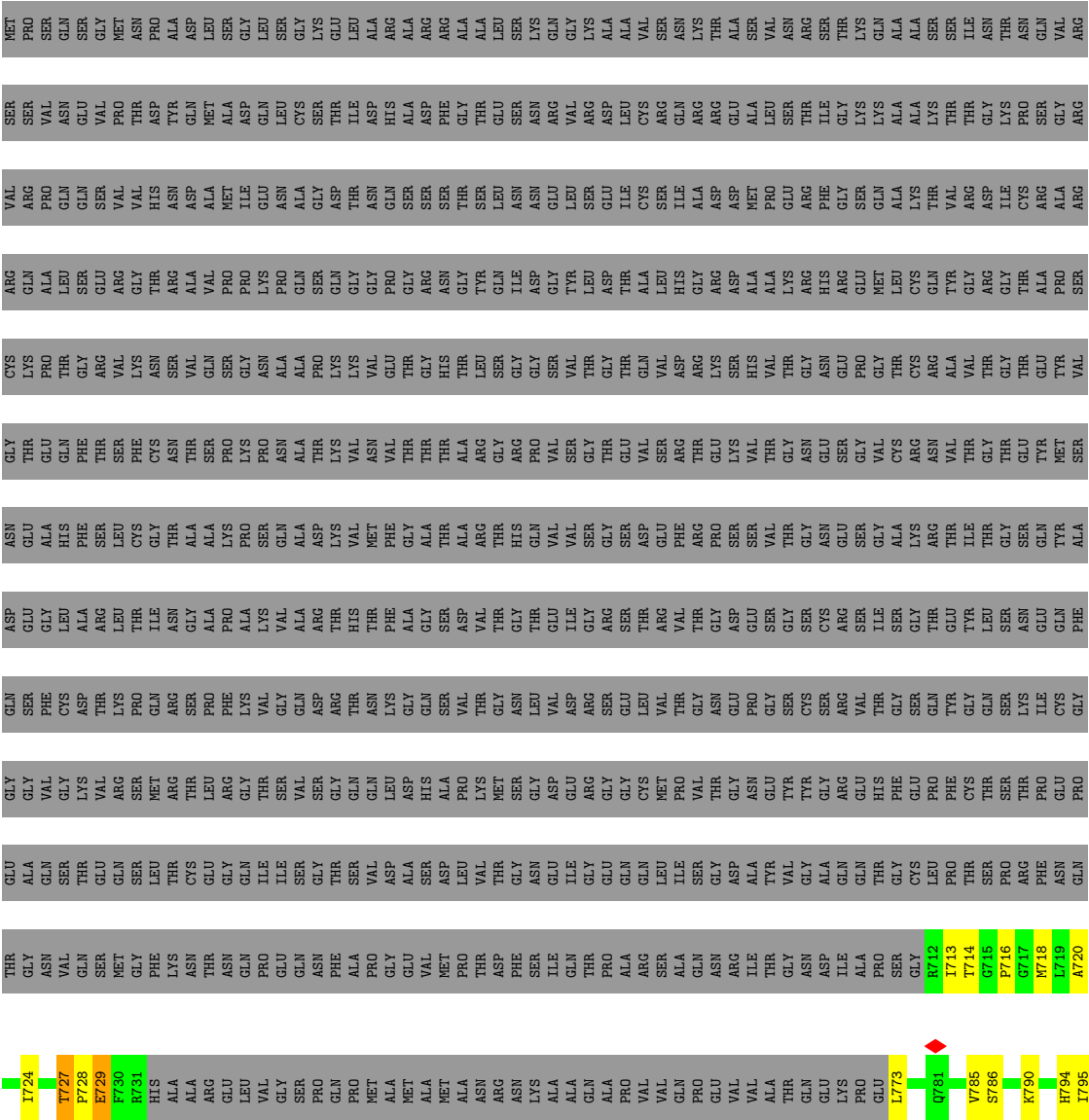








● Molecule 2: Carboxysome assembly protein CsoS2B



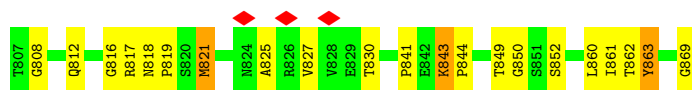






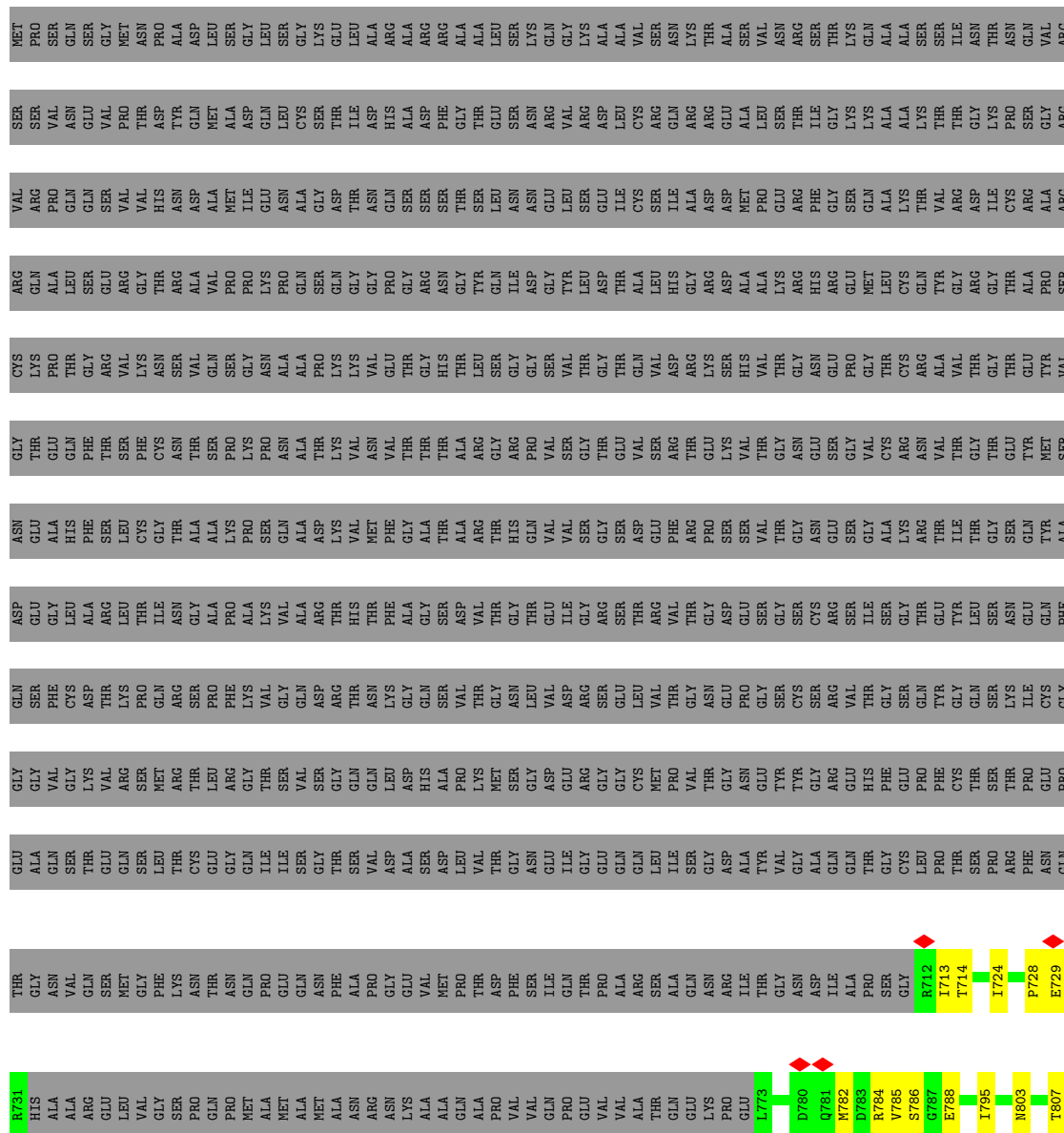






• Molecule 2: Carboxysome assembly protein CsoS2B

Chain XD: 9% 87%



• Molecule 2: Carboxysome assembly protein CsoS2B

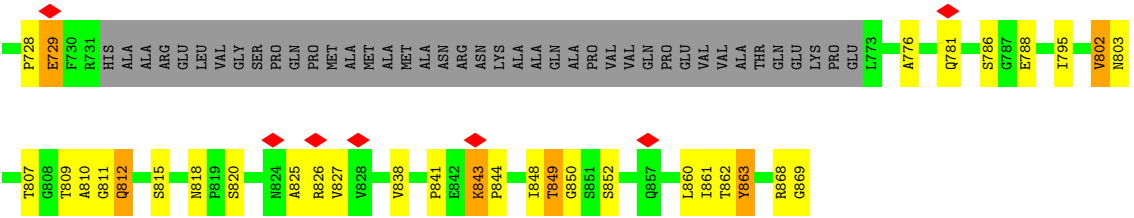
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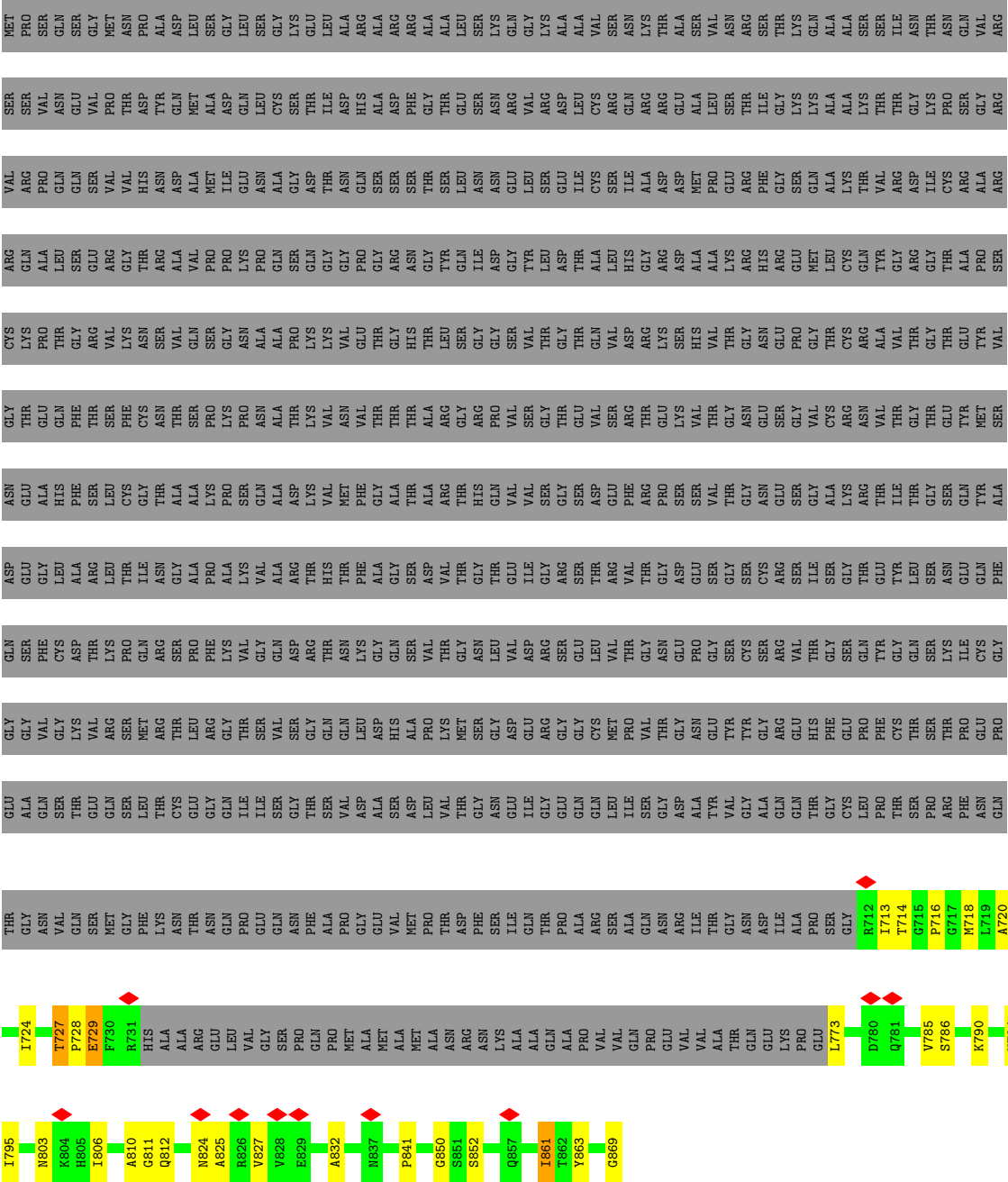








• Molecule 2: Carboxysome assembly protein CsoS2B



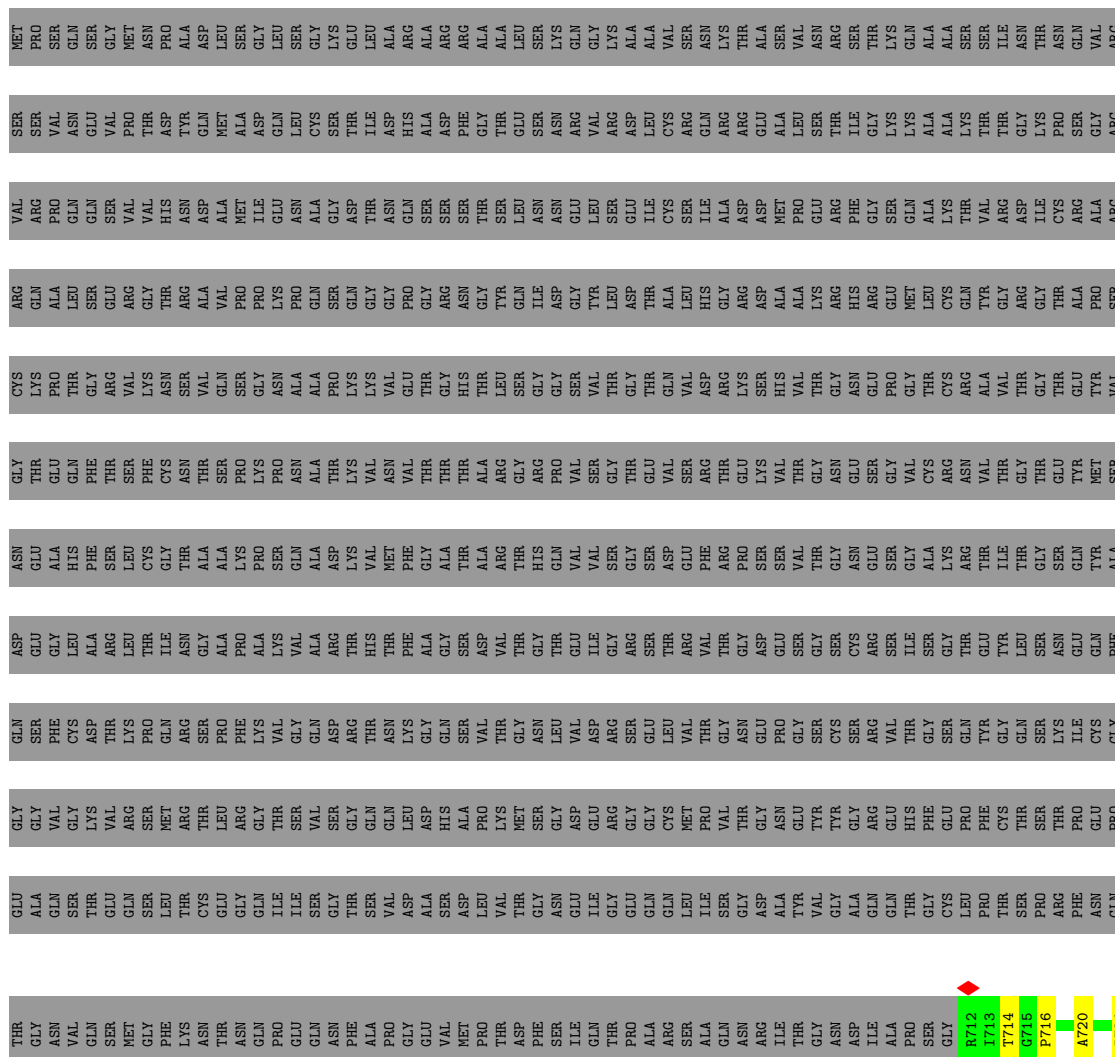
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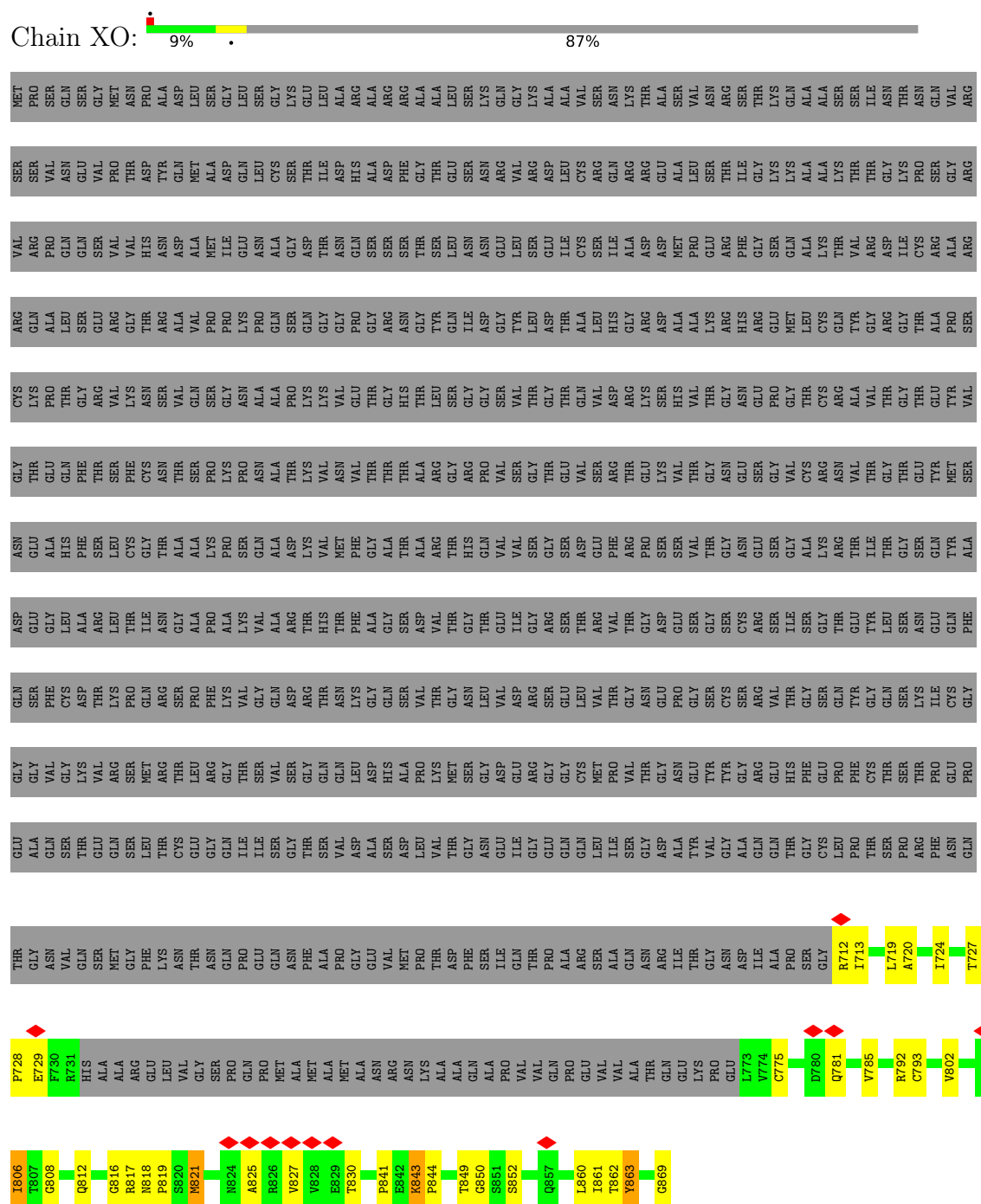




- Molecule 2: Carboxysome assembly protein CsoS2B



- Molecule 2: Carboxysome assembly protein CsoS2B



- Molecule 2: Carboxysome assembly protein CsoS2B



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

- Molecule 2: Carboxysome assembly protein CsoS2B

[illegible]







- Molecule 2: Carboxysome assembly protein CsoS2B

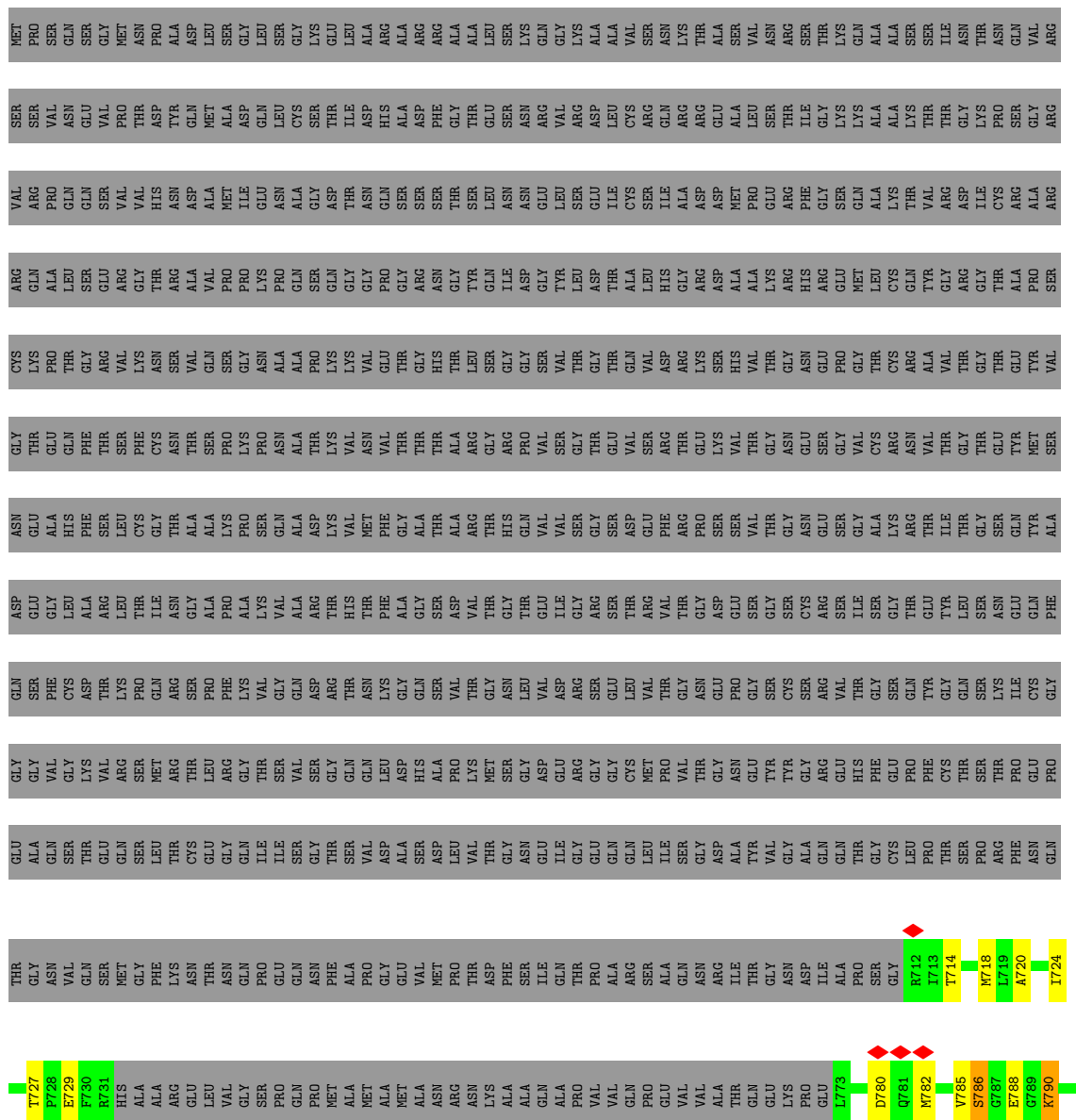






- Molecule 2: Carboxysome assembly protein CsoS2B

Chain Xr:  9% 87%

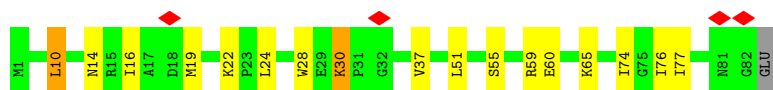
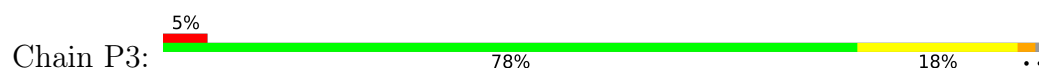




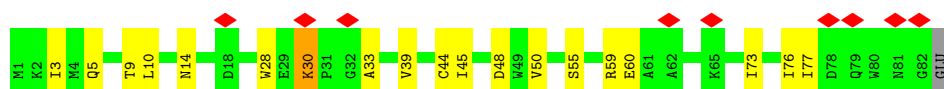
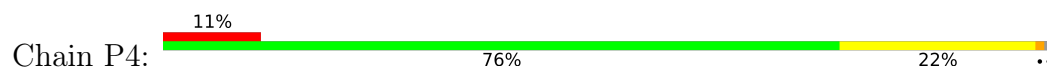




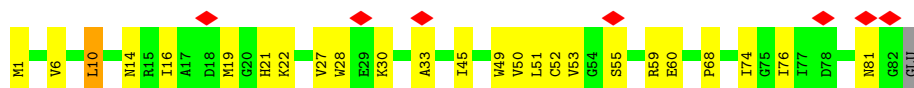
- Molecule 3: Carboxysome shell vertex protein CsoS4A



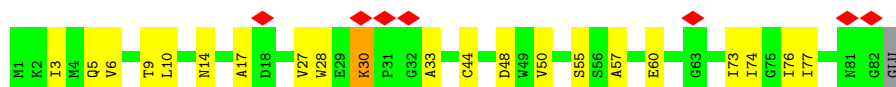
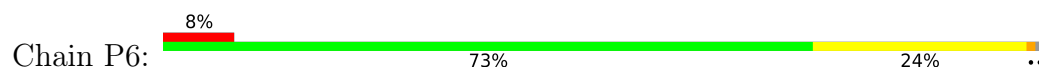
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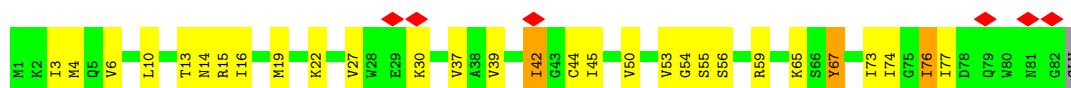
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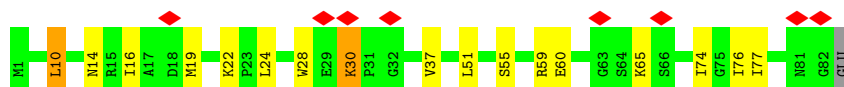
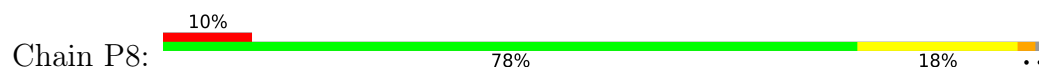
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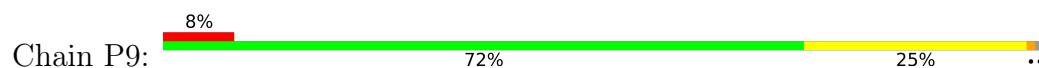
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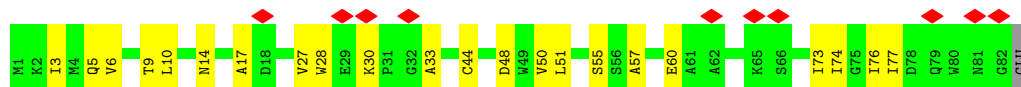
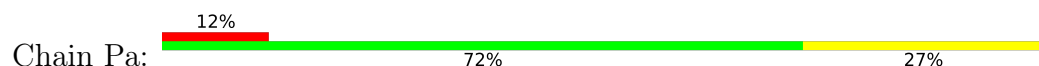




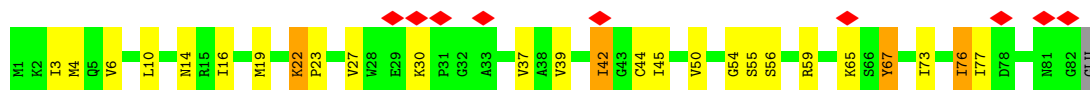
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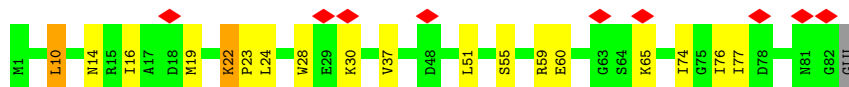
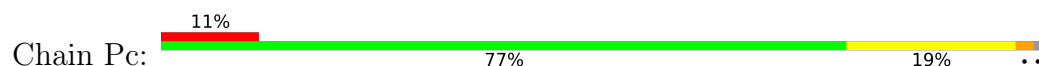
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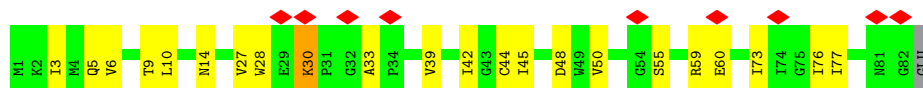
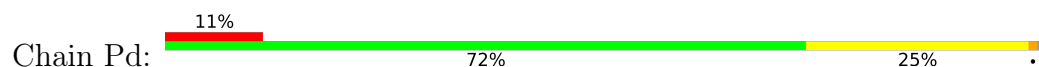
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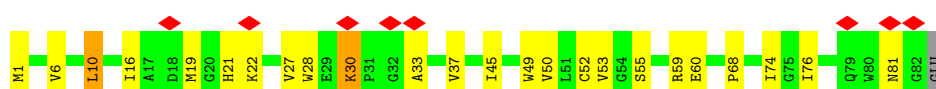
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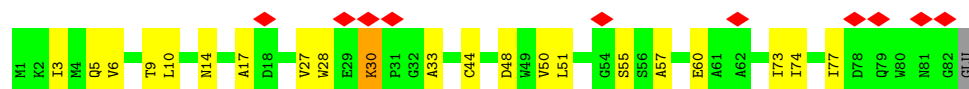
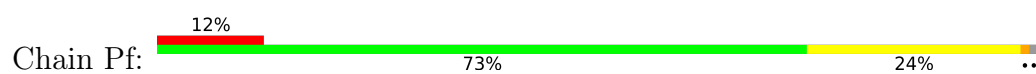
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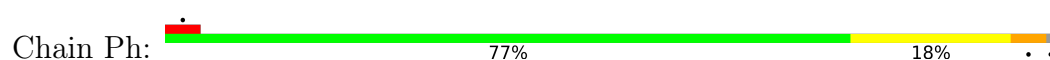
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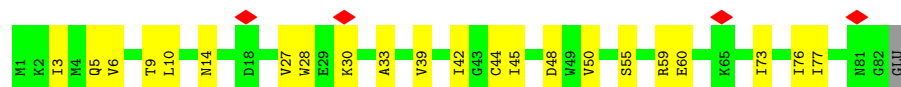
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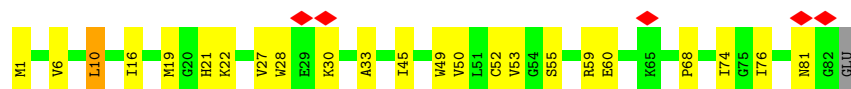
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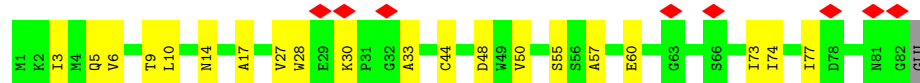
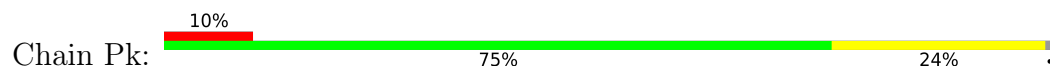
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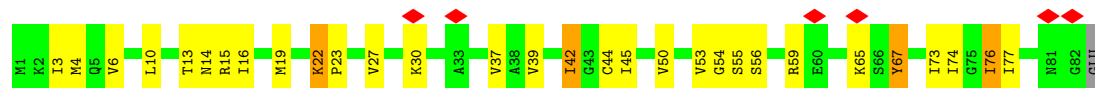
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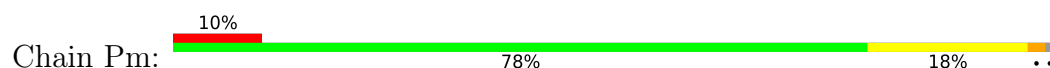
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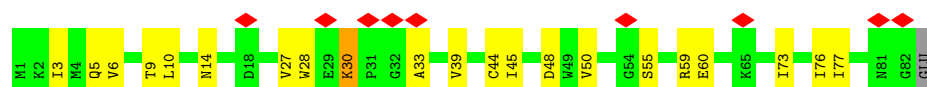
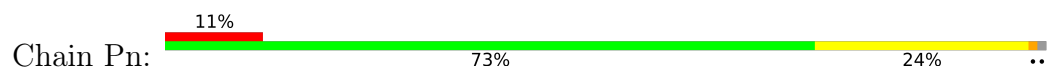
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## ● Molecule 3: Carboxysome shell vertex protein CsoS4A



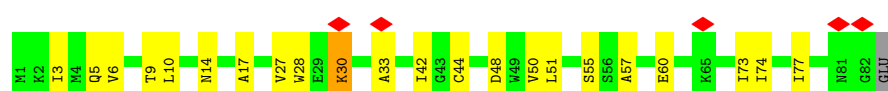
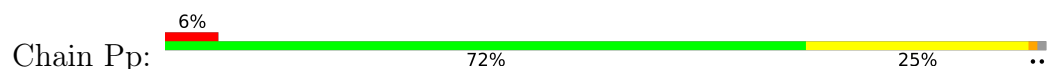
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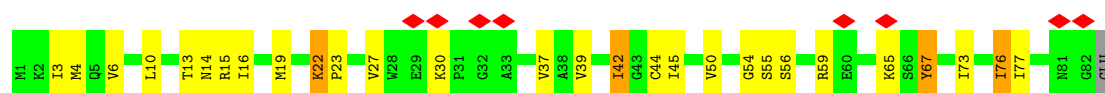
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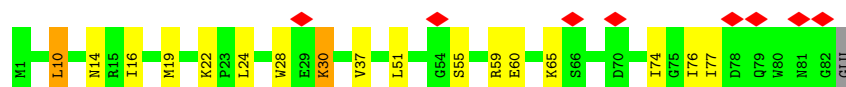
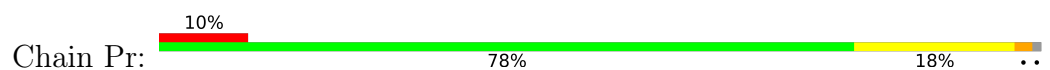
## ● Molecule 3: Carboxysome shell vertex protein CsoS4A



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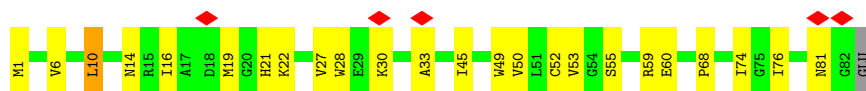


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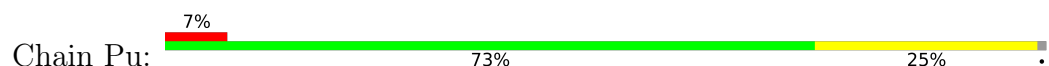




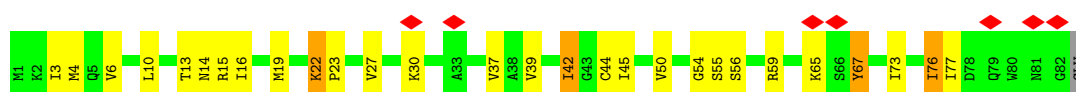
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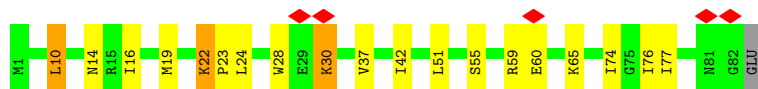
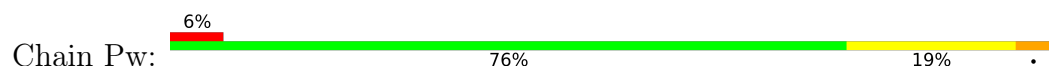
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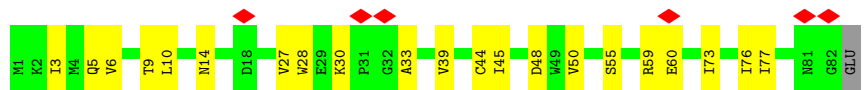
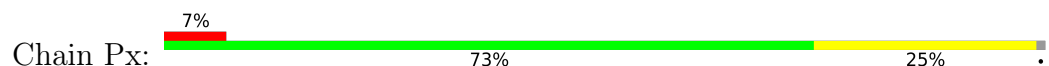
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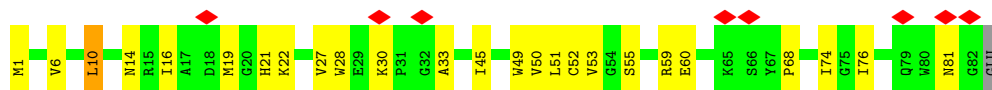
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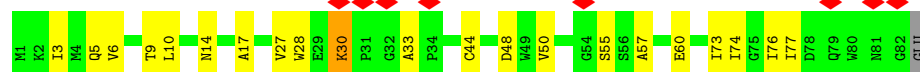
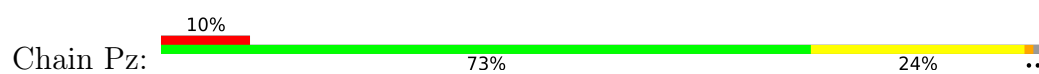
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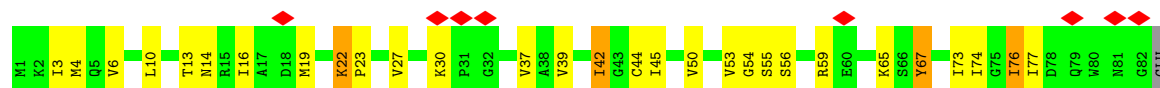
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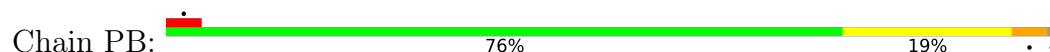
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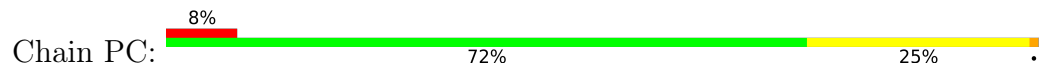
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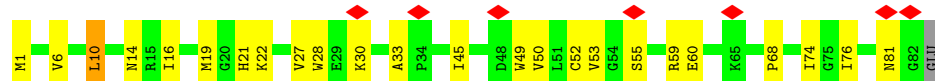
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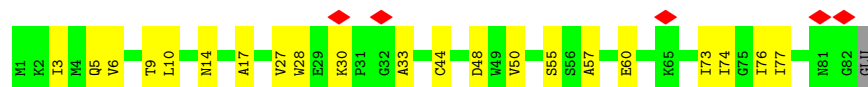
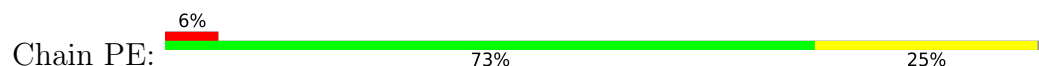
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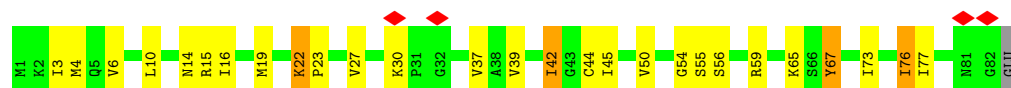
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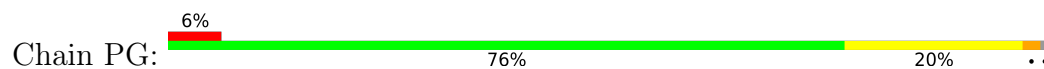
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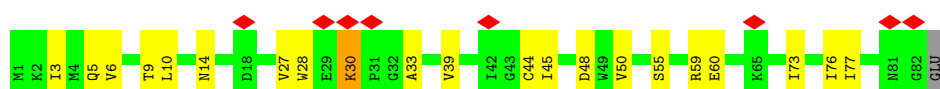
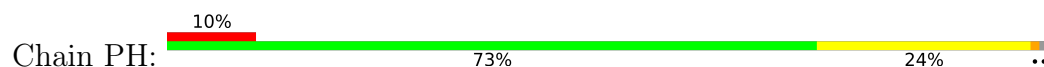
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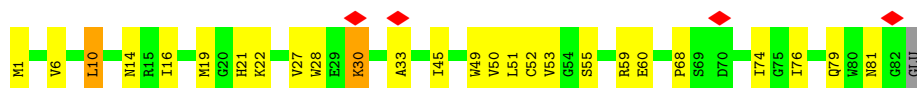
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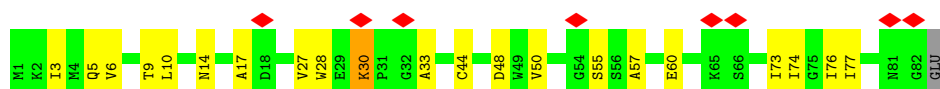
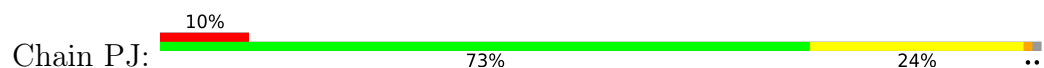
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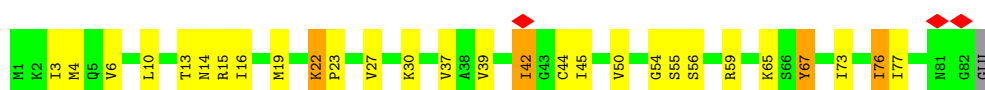
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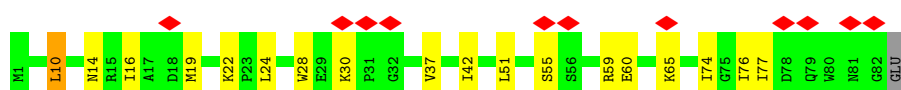
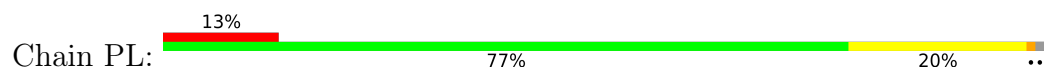
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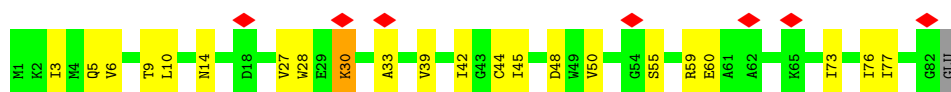


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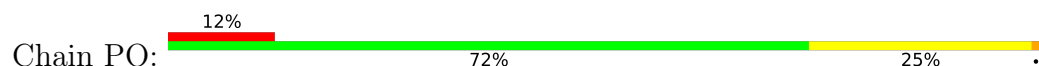




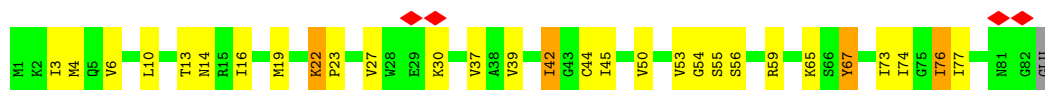
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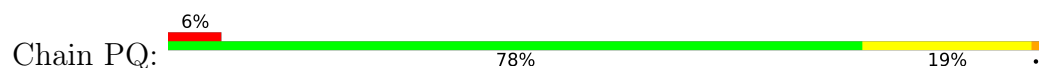
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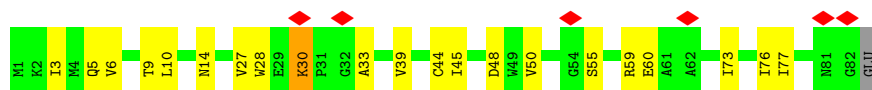
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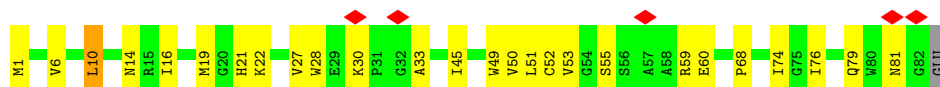
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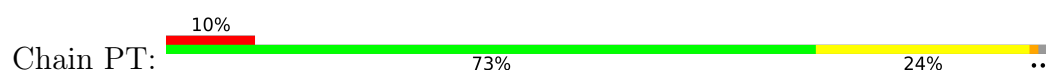
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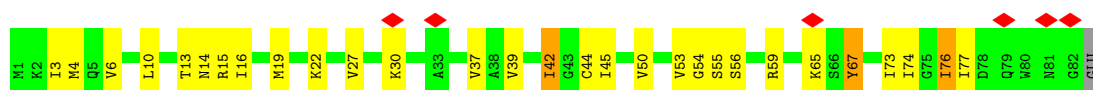
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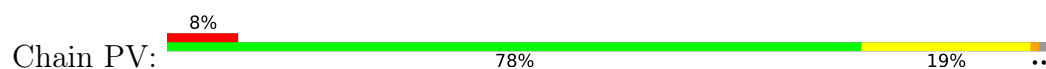
- Molecule 3: Carboxysome shell vertex protein CsoS4A



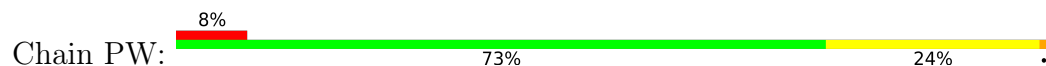
- Molecule 3: Carboxysome shell vertex protein CsoS4A



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- Molecule 3: Carboxysome shell vertex protein CsoS4A



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40177	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	1.813	Depositor
Minimum map value	-0.956	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.3	Depositor
Map size ( $\text{\AA}$ )	530.0, 530.0, 530.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	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	1.85	6/662 (0.9%)	1.41	13/897 (1.4%)
1	A1	1.84	3/662 (0.5%)	1.38	9/897 (1.0%)
1	A2	1.82	3/662 (0.5%)	1.30	9/897 (1.0%)
1	A3	1.70	3/662 (0.5%)	1.37	5/897 (0.6%)
1	A4	1.80	5/662 (0.8%)	1.39	8/897 (0.9%)
1	A5	1.85	6/662 (0.9%)	1.41	13/897 (1.4%)
1	A6	1.84	3/662 (0.5%)	1.38	9/897 (1.0%)
1	A7	1.82	3/662 (0.5%)	1.30	9/897 (1.0%)
1	A8	1.70	3/662 (0.5%)	1.37	5/897 (0.6%)
1	A9	1.80	5/662 (0.8%)	1.39	8/897 (0.9%)
1	AA	1.82	3/662 (0.5%)	1.30	9/897 (1.0%)
1	AB	1.69	2/662 (0.3%)	1.37	7/897 (0.8%)
1	AC	1.80	5/662 (0.8%)	1.40	8/897 (0.9%)
1	AD	1.85	6/662 (0.9%)	1.41	13/897 (1.4%)
1	AE	1.84	4/662 (0.6%)	1.38	9/897 (1.0%)
1	AF	1.82	3/662 (0.5%)	1.30	8/897 (0.9%)
1	AG	1.70	3/662 (0.5%)	1.37	5/897 (0.6%)
1	AH	1.80	5/662 (0.8%)	1.39	8/897 (0.9%)
1	AI	1.85	6/662 (0.9%)	1.41	13/897 (1.4%)
1	AJ	1.84	2/662 (0.3%)	1.38	9/897 (1.0%)
1	AK	1.82	3/662 (0.5%)	1.30	9/897 (1.0%)
1	AL	1.70	3/662 (0.5%)	1.37	5/897 (0.6%)
1	AM	1.80	5/662 (0.8%)	1.39	8/897 (0.9%)
1	AN	1.85	6/662 (0.9%)	1.41	13/897 (1.4%)
1	AO	1.84	3/662 (0.5%)	1.38	9/897 (1.0%)
1	AP	1.82	3/662 (0.5%)	1.30	9/897 (1.0%)
1	AQ	1.69	3/662 (0.5%)	1.37	7/897 (0.8%)
1	AR	1.80	5/662 (0.8%)	1.39	8/897 (0.9%)
1	AS	1.85	6/662 (0.9%)	1.41	13/897 (1.4%)
1	AT	1.84	4/662 (0.6%)	1.38	9/897 (1.0%)
1	AU	1.82	3/662 (0.5%)	1.30	9/897 (1.0%)
1	AV	1.70	2/662 (0.3%)	1.37	5/897 (0.6%)
1	AW	1.80	5/662 (0.8%)	1.40	8/897 (0.9%)
1	AX	1.85	6/662 (0.9%)	1.41	13/897 (1.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	Aa	1.84	4/662 (0.6%)	1.38	9/897 (1.0%)
1	Ab	1.82	3/662 (0.5%)	1.30	9/897 (1.0%)
1	Ac	1.70	2/662 (0.3%)	1.37	5/897 (0.6%)
1	Ad	1.80	5/662 (0.8%)	1.39	8/897 (0.9%)
1	Ae	1.85	6/662 (0.9%)	1.41	13/897 (1.4%)
1	Af	1.84	3/662 (0.5%)	1.38	9/897 (1.0%)
1	Ag	1.82	3/662 (0.5%)	1.30	9/897 (1.0%)
1	Ah	1.69	3/662 (0.5%)	1.37	7/897 (0.8%)
1	Ai	1.80	5/662 (0.8%)	1.40	8/897 (0.9%)
1	Aj	1.85	6/662 (0.9%)	1.41	13/897 (1.4%)
1	Ak	1.84	4/662 (0.6%)	1.38	9/897 (1.0%)
1	Al	1.82	2/662 (0.3%)	1.30	9/897 (1.0%)
1	Am	1.70	3/662 (0.5%)	1.37	5/897 (0.6%)
1	An	1.80	5/662 (0.8%)	1.40	8/897 (0.9%)
1	Ao	1.85	6/662 (0.9%)	1.41	13/897 (1.4%)
1	Ap	1.84	4/662 (0.6%)	1.38	9/897 (1.0%)
1	Aq	1.82	2/662 (0.3%)	1.30	9/897 (1.0%)
1	Ar	1.70	3/662 (0.5%)	1.37	5/897 (0.6%)
1	As	1.80	5/662 (0.8%)	1.39	8/897 (0.9%)
1	At	1.85	6/662 (0.9%)	1.41	13/897 (1.4%)
1	Au	1.84	4/662 (0.6%)	1.38	9/897 (1.0%)
1	Av	1.82	3/662 (0.5%)	1.30	9/897 (1.0%)
1	Aw	1.69	3/662 (0.5%)	1.37	5/897 (0.6%)
1	Ax	1.80	5/662 (0.8%)	1.39	8/897 (0.9%)
1	Ay	1.85	6/662 (0.9%)	1.41	13/897 (1.4%)
1	Az	1.84	3/662 (0.5%)	1.38	9/897 (1.0%)
1	B0	1.74	2/662 (0.3%)	1.37	11/897 (1.2%)
1	B1	1.73	1/662 (0.2%)	1.32	9/897 (1.0%)
1	B2	1.81	3/662 (0.5%)	1.32	6/897 (0.7%)
1	B3	1.82	3/662 (0.5%)	1.42	12/897 (1.3%)
1	B4	1.80	7/662 (1.1%)	1.35	5/897 (0.6%)
1	B5	1.74	2/662 (0.3%)	1.37	11/897 (1.2%)
1	B6	1.73	1/662 (0.2%)	1.32	9/897 (1.0%)
1	B7	1.81	4/662 (0.6%)	1.33	6/897 (0.7%)
1	B8	1.82	3/662 (0.5%)	1.42	12/897 (1.3%)
1	B9	1.80	7/662 (1.1%)	1.35	5/897 (0.6%)
1	BA	1.81	4/662 (0.6%)	1.32	6/897 (0.7%)
1	BB	1.82	3/662 (0.5%)	1.43	12/897 (1.3%)
1	BC	1.80	7/662 (1.1%)	1.35	5/897 (0.6%)
1	BD	1.74	2/662 (0.3%)	1.36	11/897 (1.2%)
1	BE	1.73	1/662 (0.2%)	1.32	9/897 (1.0%)
1	BF	1.81	4/662 (0.6%)	1.33	6/897 (0.7%)
1	BG	1.82	3/662 (0.5%)	1.42	12/897 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	BH	1.80	7/662 (1.1%)	1.35	5/897 (0.6%)
1	BI	1.74	3/662 (0.5%)	1.37	11/897 (1.2%)
1	BJ	1.73	1/662 (0.2%)	1.32	8/897 (0.9%)
1	BK	1.81	3/662 (0.5%)	1.32	6/897 (0.7%)
1	BL	1.82	3/662 (0.5%)	1.43	12/897 (1.3%)
1	BM	1.80	7/662 (1.1%)	1.35	5/897 (0.6%)
1	BN	1.74	3/662 (0.5%)	1.37	11/897 (1.2%)
1	BO	1.74	1/662 (0.2%)	1.32	9/897 (1.0%)
1	BP	1.81	4/662 (0.6%)	1.33	5/897 (0.6%)
1	BQ	1.82	3/662 (0.5%)	1.42	12/897 (1.3%)
1	BR	1.79	7/662 (1.1%)	1.35	5/897 (0.6%)
1	BS	1.74	2/662 (0.3%)	1.36	11/897 (1.2%)
1	BT	1.73	1/662 (0.2%)	1.32	9/897 (1.0%)
1	BU	1.81	4/662 (0.6%)	1.33	6/897 (0.7%)
1	BV	1.82	3/662 (0.5%)	1.42	12/897 (1.3%)
1	BW	1.80	7/662 (1.1%)	1.35	5/897 (0.6%)
1	BX	1.74	2/662 (0.3%)	1.37	11/897 (1.2%)
1	Ba	1.73	1/662 (0.2%)	1.32	9/897 (1.0%)
1	Bb	1.81	4/662 (0.6%)	1.33	6/897 (0.7%)
1	Bc	1.82	3/662 (0.5%)	1.42	12/897 (1.3%)
1	Bd	1.80	7/662 (1.1%)	1.35	5/897 (0.6%)
1	Be	1.74	2/662 (0.3%)	1.37	11/897 (1.2%)
1	Bf	1.73	1/662 (0.2%)	1.32	9/897 (1.0%)
1	Bg	1.81	3/662 (0.5%)	1.33	6/897 (0.7%)
1	Bh	1.82	3/662 (0.5%)	1.42	12/897 (1.3%)
1	Bi	1.80	7/662 (1.1%)	1.35	5/897 (0.6%)
1	Bj	1.74	3/662 (0.5%)	1.37	11/897 (1.2%)
1	Bk	1.73	1/662 (0.2%)	1.32	9/897 (1.0%)
1	Bl	1.81	3/662 (0.5%)	1.33	6/897 (0.7%)
1	Bm	1.83	3/662 (0.5%)	1.43	12/897 (1.3%)
1	Bn	1.80	7/662 (1.1%)	1.35	5/897 (0.6%)
1	Bo	1.74	2/662 (0.3%)	1.37	11/897 (1.2%)
1	Bp	1.73	1/662 (0.2%)	1.32	9/897 (1.0%)
1	Bq	1.81	3/662 (0.5%)	1.32	6/897 (0.7%)
1	Br	1.82	3/662 (0.5%)	1.42	12/897 (1.3%)
1	Bs	1.80	7/662 (1.1%)	1.35	5/897 (0.6%)
1	Bt	1.74	2/662 (0.3%)	1.37	11/897 (1.2%)
1	Bu	1.73	1/662 (0.2%)	1.32	9/897 (1.0%)
1	Bv	1.81	4/662 (0.6%)	1.33	6/897 (0.7%)
1	Bw	1.82	4/662 (0.6%)	1.42	12/897 (1.3%)
1	Bx	1.80	7/662 (1.1%)	1.35	5/897 (0.6%)
1	By	1.74	2/662 (0.3%)	1.37	11/897 (1.2%)
1	Bz	1.73	1/662 (0.2%)	1.32	9/897 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	C0	1.80	2/662 (0.3%)	1.31	4/897 (0.4%)
1	C1	1.83	3/662 (0.5%)	1.34	7/897 (0.8%)
1	C2	1.80	5/662 (0.8%)	1.40	10/897 (1.1%)
1	C3	1.83	5/662 (0.8%)	1.43	10/897 (1.1%)
1	C4	1.80	4/662 (0.6%)	1.32	10/897 (1.1%)
1	C5	1.80	2/662 (0.3%)	1.31	4/897 (0.4%)
1	C6	1.83	3/662 (0.5%)	1.34	7/897 (0.8%)
1	C7	1.80	5/662 (0.8%)	1.40	10/897 (1.1%)
1	C8	1.83	6/662 (0.9%)	1.43	10/897 (1.1%)
1	C9	1.80	4/662 (0.6%)	1.32	10/897 (1.1%)
1	CA	1.80	5/662 (0.8%)	1.39	10/897 (1.1%)
1	CB	1.83	6/662 (0.9%)	1.43	10/897 (1.1%)
1	CC	1.80	4/662 (0.6%)	1.32	10/897 (1.1%)
1	CD	1.80	1/662 (0.2%)	1.31	4/897 (0.4%)
1	CE	1.83	3/662 (0.5%)	1.34	7/897 (0.8%)
1	CF	1.80	5/662 (0.8%)	1.40	10/897 (1.1%)
1	CG	1.83	6/662 (0.9%)	1.43	10/897 (1.1%)
1	CH	1.80	4/662 (0.6%)	1.32	10/897 (1.1%)
1	CI	1.80	2/662 (0.3%)	1.31	4/897 (0.4%)
1	CJ	1.83	3/662 (0.5%)	1.35	7/897 (0.8%)
1	CK	1.80	5/662 (0.8%)	1.40	10/897 (1.1%)
1	CL	1.83	5/662 (0.8%)	1.43	10/897 (1.1%)
1	CM	1.80	4/662 (0.6%)	1.32	10/897 (1.1%)
1	CN	1.80	2/662 (0.3%)	1.31	4/897 (0.4%)
1	CO	1.83	3/662 (0.5%)	1.35	7/897 (0.8%)
1	CP	1.80	5/662 (0.8%)	1.39	10/897 (1.1%)
1	CQ	1.83	6/662 (0.9%)	1.43	10/897 (1.1%)
1	CR	1.80	4/662 (0.6%)	1.32	10/897 (1.1%)
1	CS	1.80	2/662 (0.3%)	1.31	4/897 (0.4%)
1	CT	1.83	3/662 (0.5%)	1.34	7/897 (0.8%)
1	CU	1.80	5/662 (0.8%)	1.40	10/897 (1.1%)
1	CV	1.83	5/662 (0.8%)	1.43	10/897 (1.1%)
1	CW	1.80	4/662 (0.6%)	1.32	10/897 (1.1%)
1	CX	1.80	2/662 (0.3%)	1.31	4/897 (0.4%)
1	Ca	1.83	3/662 (0.5%)	1.34	7/897 (0.8%)
1	Cb	1.80	5/662 (0.8%)	1.40	10/897 (1.1%)
1	Cc	1.83	5/662 (0.8%)	1.43	10/897 (1.1%)
1	Cd	1.80	4/662 (0.6%)	1.32	10/897 (1.1%)
1	Ce	1.80	2/662 (0.3%)	1.31	4/897 (0.4%)
1	Cf	1.83	3/662 (0.5%)	1.34	7/897 (0.8%)
1	Cg	1.80	5/662 (0.8%)	1.40	10/897 (1.1%)
1	Ch	1.83	6/662 (0.9%)	1.43	10/897 (1.1%)
1	Ci	1.80	4/662 (0.6%)	1.32	10/897 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	Cj	1.80	2/662 (0.3%)	1.31	4/897 (0.4%)
1	Ck	1.83	3/662 (0.5%)	1.34	7/897 (0.8%)
1	Cl	1.80	5/662 (0.8%)	1.39	10/897 (1.1%)
1	Cm	1.83	6/662 (0.9%)	1.43	10/897 (1.1%)
1	Cn	1.80	4/662 (0.6%)	1.32	10/897 (1.1%)
1	Co	1.80	2/662 (0.3%)	1.31	4/897 (0.4%)
1	Cp	1.83	3/662 (0.5%)	1.34	7/897 (0.8%)
1	Cq	1.80	5/662 (0.8%)	1.40	10/897 (1.1%)
1	Cr	1.83	6/662 (0.9%)	1.43	10/897 (1.1%)
1	Cs	1.80	4/662 (0.6%)	1.32	10/897 (1.1%)
1	Ct	1.80	2/662 (0.3%)	1.31	4/897 (0.4%)
1	Cu	1.83	3/662 (0.5%)	1.35	7/897 (0.8%)
1	Cv	1.80	5/662 (0.8%)	1.39	10/897 (1.1%)
1	Cw	1.83	6/662 (0.9%)	1.43	10/897 (1.1%)
1	Cx	1.80	4/662 (0.6%)	1.32	10/897 (1.1%)
1	Cy	1.80	1/662 (0.2%)	1.31	4/897 (0.4%)
1	Cz	1.83	3/662 (0.5%)	1.34	7/897 (0.8%)
1	D0	1.81	6/662 (0.9%)	1.40	10/897 (1.1%)
1	D1	1.74	2/662 (0.3%)	1.29	8/897 (0.9%)
1	D2	1.87	8/662 (1.2%)	1.43	15/897 (1.7%)
1	D3	1.81	5/662 (0.8%)	1.39	10/897 (1.1%)
1	D4	1.79	5/662 (0.8%)	1.35	8/897 (0.9%)
1	D5	1.81	7/662 (1.1%)	1.40	10/897 (1.1%)
1	D6	1.75	2/662 (0.3%)	1.29	8/897 (0.9%)
1	D7	1.87	8/662 (1.2%)	1.44	14/897 (1.6%)
1	D8	1.81	5/662 (0.8%)	1.39	11/897 (1.2%)
1	D9	1.79	5/662 (0.8%)	1.35	8/897 (0.9%)
1	DA	1.87	8/662 (1.2%)	1.44	14/897 (1.6%)
1	DB	1.81	3/662 (0.5%)	1.39	11/897 (1.2%)
1	DC	1.79	5/662 (0.8%)	1.35	8/897 (0.9%)
1	DD	1.82	7/662 (1.1%)	1.39	10/897 (1.1%)
1	DE	1.75	2/662 (0.3%)	1.29	8/897 (0.9%)
1	DF	1.87	8/662 (1.2%)	1.44	14/897 (1.6%)
1	DG	1.81	5/662 (0.8%)	1.39	10/897 (1.1%)
1	DH	1.80	5/662 (0.8%)	1.35	8/897 (0.9%)
1	DI	1.81	7/662 (1.1%)	1.40	10/897 (1.1%)
1	DJ	1.75	1/662 (0.2%)	1.29	8/897 (0.9%)
1	DK	1.87	8/662 (1.2%)	1.44	15/897 (1.7%)
1	DL	1.81	5/662 (0.8%)	1.39	10/897 (1.1%)
1	DM	1.79	5/662 (0.8%)	1.35	8/897 (0.9%)
1	DN	1.81	6/662 (0.9%)	1.40	10/897 (1.1%)
1	DO	1.75	2/662 (0.3%)	1.29	9/897 (1.0%)
1	DP	1.87	8/662 (1.2%)	1.44	14/897 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	DQ	1.81	5/662 (0.8%)	1.39	11/897 (1.2%)
1	DR	1.79	5/662 (0.8%)	1.35	8/897 (0.9%)
1	DS	1.81	6/662 (0.9%)	1.39	10/897 (1.1%)
1	DT	1.75	1/662 (0.2%)	1.29	8/897 (0.9%)
1	DU	1.87	8/662 (1.2%)	1.44	15/897 (1.7%)
1	DV	1.81	5/662 (0.8%)	1.39	10/897 (1.1%)
1	DW	1.79	5/662 (0.8%)	1.35	8/897 (0.9%)
1	DX	1.81	7/662 (1.1%)	1.39	11/897 (1.2%)
1	Da	1.75	1/662 (0.2%)	1.29	8/897 (0.9%)
1	Db	1.87	8/662 (1.2%)	1.44	15/897 (1.7%)
1	Dc	1.81	5/662 (0.8%)	1.39	10/897 (1.1%)
1	Dd	1.79	5/662 (0.8%)	1.35	8/897 (0.9%)
1	De	1.81	7/662 (1.1%)	1.39	11/897 (1.2%)
1	Df	1.74	1/662 (0.2%)	1.29	8/897 (0.9%)
1	Dg	1.87	8/662 (1.2%)	1.43	15/897 (1.7%)
1	Dh	1.81	5/662 (0.8%)	1.39	10/897 (1.1%)
1	Di	1.79	5/662 (0.8%)	1.35	8/897 (0.9%)
1	Dj	1.81	7/662 (1.1%)	1.39	10/897 (1.1%)
1	Dk	1.75	2/662 (0.3%)	1.29	8/897 (0.9%)
1	Dl	1.87	8/662 (1.2%)	1.44	14/897 (1.6%)
1	Dm	1.81	4/662 (0.6%)	1.39	11/897 (1.2%)
1	Dn	1.80	5/662 (0.8%)	1.35	8/897 (0.9%)
1	Do	1.82	6/662 (0.9%)	1.40	10/897 (1.1%)
1	Dp	1.75	2/662 (0.3%)	1.29	8/897 (0.9%)
1	Dq	1.86	7/662 (1.1%)	1.44	15/897 (1.7%)
1	Dr	1.81	4/662 (0.6%)	1.39	10/897 (1.1%)
1	Ds	1.79	5/662 (0.8%)	1.35	8/897 (0.9%)
1	Dt	1.81	7/662 (1.1%)	1.40	11/897 (1.2%)
1	Du	1.75	1/662 (0.2%)	1.29	9/897 (1.0%)
1	Dv	1.87	8/662 (1.2%)	1.43	15/897 (1.7%)
1	Dw	1.81	4/662 (0.6%)	1.38	10/897 (1.1%)
1	Dx	1.79	5/662 (0.8%)	1.35	8/897 (0.9%)
1	Dy	1.81	6/662 (0.9%)	1.39	10/897 (1.1%)
1	Dz	1.75	2/662 (0.3%)	1.29	9/897 (1.0%)
1	E0	1.80	3/662 (0.5%)	1.35	10/897 (1.1%)
1	E1	1.78	3/662 (0.5%)	1.35	9/897 (1.0%)
1	E2	1.77	2/662 (0.3%)	1.29	8/897 (0.9%)
1	E3	1.74	3/662 (0.5%)	1.32	7/897 (0.8%)
1	E4	1.82	7/662 (1.1%)	1.29	8/897 (0.9%)
1	E5	1.80	3/662 (0.5%)	1.35	10/897 (1.1%)
1	E6	1.78	3/662 (0.5%)	1.35	9/897 (1.0%)
1	E7	1.77	2/662 (0.3%)	1.29	8/897 (0.9%)
1	E8	1.74	3/662 (0.5%)	1.32	7/897 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	E9	1.82	8/662 (1.2%)	1.29	8/897 (0.9%)
1	EA	1.77	2/662 (0.3%)	1.29	8/897 (0.9%)
1	EB	1.74	3/662 (0.5%)	1.32	7/897 (0.8%)
1	EC	1.82	7/662 (1.1%)	1.29	9/897 (1.0%)
1	ED	1.80	3/662 (0.5%)	1.35	10/897 (1.1%)
1	EE	1.78	3/662 (0.5%)	1.35	9/897 (1.0%)
1	EF	1.77	2/662 (0.3%)	1.29	8/897 (0.9%)
1	EG	1.74	3/662 (0.5%)	1.32	7/897 (0.8%)
1	EH	1.82	8/662 (1.2%)	1.29	9/897 (1.0%)
1	EI	1.80	4/662 (0.6%)	1.35	10/897 (1.1%)
1	EJ	1.78	3/662 (0.5%)	1.35	9/897 (1.0%)
1	EK	1.77	2/662 (0.3%)	1.29	8/897 (0.9%)
1	EL	1.74	3/662 (0.5%)	1.32	7/897 (0.8%)
1	EM	1.82	6/662 (0.9%)	1.29	8/897 (0.9%)
1	EN	1.80	3/662 (0.5%)	1.35	10/897 (1.1%)
1	EO	1.78	3/662 (0.5%)	1.35	9/897 (1.0%)
1	EP	1.77	2/662 (0.3%)	1.29	8/897 (0.9%)
1	EQ	1.74	3/662 (0.5%)	1.32	7/897 (0.8%)
1	ER	1.82	7/662 (1.1%)	1.29	9/897 (1.0%)
1	ES	1.80	3/662 (0.5%)	1.35	10/897 (1.1%)
1	ET	1.78	3/662 (0.5%)	1.35	9/897 (1.0%)
1	EU	1.77	2/662 (0.3%)	1.29	8/897 (0.9%)
1	EV	1.74	3/662 (0.5%)	1.32	7/897 (0.8%)
1	EW	1.82	8/662 (1.2%)	1.29	9/897 (1.0%)
1	EX	1.80	4/662 (0.6%)	1.35	10/897 (1.1%)
1	Ea	1.78	3/662 (0.5%)	1.35	9/897 (1.0%)
1	Eb	1.77	2/662 (0.3%)	1.29	8/897 (0.9%)
1	Ec	1.74	3/662 (0.5%)	1.32	7/897 (0.8%)
1	Ed	1.82	8/662 (1.2%)	1.29	9/897 (1.0%)
1	Ee	1.80	4/662 (0.6%)	1.35	10/897 (1.1%)
1	Ef	1.78	3/662 (0.5%)	1.35	9/897 (1.0%)
1	Eg	1.77	2/662 (0.3%)	1.29	8/897 (0.9%)
1	Eh	1.74	3/662 (0.5%)	1.32	7/897 (0.8%)
1	Ei	1.82	7/662 (1.1%)	1.29	8/897 (0.9%)
1	Ej	1.80	3/662 (0.5%)	1.35	10/897 (1.1%)
1	Ek	1.77	3/662 (0.5%)	1.36	9/897 (1.0%)
1	El	1.77	2/662 (0.3%)	1.29	8/897 (0.9%)
1	Em	1.74	3/662 (0.5%)	1.32	7/897 (0.8%)
1	En	1.82	7/662 (1.1%)	1.29	8/897 (0.9%)
1	Eo	1.80	3/662 (0.5%)	1.35	10/897 (1.1%)
1	Ep	1.78	3/662 (0.5%)	1.36	9/897 (1.0%)
1	Eq	1.77	2/662 (0.3%)	1.29	8/897 (0.9%)
1	Er	1.74	3/662 (0.5%)	1.32	7/897 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	Es	1.82	8/662 (1.2%)	1.29	9/897 (1.0%)
1	Et	1.80	4/662 (0.6%)	1.35	10/897 (1.1%)
1	Eu	1.78	3/662 (0.5%)	1.36	9/897 (1.0%)
1	Ev	1.77	2/662 (0.3%)	1.29	8/897 (0.9%)
1	Ew	1.74	3/662 (0.5%)	1.32	7/897 (0.8%)
1	Ex	1.82	7/662 (1.1%)	1.29	9/897 (1.0%)
1	Ey	1.80	3/662 (0.5%)	1.35	10/897 (1.1%)
1	Ez	1.78	3/662 (0.5%)	1.35	9/897 (1.0%)
1	F0	1.78	3/662 (0.5%)	1.34	9/897 (1.0%)
1	F1	1.77	2/662 (0.3%)	1.32	8/897 (0.9%)
1	F2	1.77	3/662 (0.5%)	1.41	10/897 (1.1%)
1	F3	1.88	7/662 (1.1%)	1.43	7/897 (0.8%)
1	F4	1.82	3/662 (0.5%)	1.42	11/897 (1.2%)
1	F5	1.78	3/662 (0.5%)	1.34	9/897 (1.0%)
1	F6	1.77	2/662 (0.3%)	1.32	8/897 (0.9%)
1	F7	1.77	3/662 (0.5%)	1.41	10/897 (1.1%)
1	F8	1.88	7/662 (1.1%)	1.43	7/897 (0.8%)
1	F9	1.81	3/662 (0.5%)	1.42	11/897 (1.2%)
1	FA	1.77	2/662 (0.3%)	1.41	10/897 (1.1%)
1	FB	1.88	7/662 (1.1%)	1.43	7/897 (0.8%)
1	FC	1.82	3/662 (0.5%)	1.42	11/897 (1.2%)
1	FD	1.78	3/662 (0.5%)	1.34	9/897 (1.0%)
1	FE	1.77	2/662 (0.3%)	1.32	8/897 (0.9%)
1	FF	1.78	3/662 (0.5%)	1.41	10/897 (1.1%)
1	FG	1.88	7/662 (1.1%)	1.43	7/897 (0.8%)
1	FH	1.81	2/662 (0.3%)	1.43	11/897 (1.2%)
1	FI	1.78	3/662 (0.5%)	1.34	9/897 (1.0%)
1	FJ	1.77	1/662 (0.2%)	1.32	8/897 (0.9%)
1	FK	1.77	3/662 (0.5%)	1.41	10/897 (1.1%)
1	FL	1.88	7/662 (1.1%)	1.43	7/897 (0.8%)
1	FM	1.82	3/662 (0.5%)	1.42	11/897 (1.2%)
1	FN	1.78	3/662 (0.5%)	1.34	9/897 (1.0%)
1	FO	1.77	1/662 (0.2%)	1.32	8/897 (0.9%)
1	FP	1.77	3/662 (0.5%)	1.41	10/897 (1.1%)
1	FQ	1.88	7/662 (1.1%)	1.43	7/897 (0.8%)
1	FR	1.81	3/662 (0.5%)	1.42	11/897 (1.2%)
1	FS	1.78	2/662 (0.3%)	1.34	9/897 (1.0%)
1	FT	1.77	2/662 (0.3%)	1.32	8/897 (0.9%)
1	FU	1.78	3/662 (0.5%)	1.41	10/897 (1.1%)
1	FV	1.88	7/662 (1.1%)	1.43	7/897 (0.8%)
1	FW	1.81	2/662 (0.3%)	1.43	11/897 (1.2%)
1	FX	1.78	3/662 (0.5%)	1.34	9/897 (1.0%)
1	Fa	1.77	2/662 (0.3%)	1.32	8/897 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	Fb	1.78	4/662 (0.6%)	1.41	10/897 (1.1%)
1	Fc	1.88	7/662 (1.1%)	1.43	7/897 (0.8%)
1	Fd	1.81	2/662 (0.3%)	1.43	11/897 (1.2%)
1	Fe	1.78	3/662 (0.5%)	1.34	9/897 (1.0%)
1	Ff	1.77	1/662 (0.2%)	1.32	8/897 (0.9%)
1	Fg	1.77	3/662 (0.5%)	1.41	10/897 (1.1%)
1	Fh	1.89	7/662 (1.1%)	1.43	7/897 (0.8%)
1	Fi	1.82	2/662 (0.3%)	1.42	11/897 (1.2%)
1	Fj	1.78	3/662 (0.5%)	1.34	9/897 (1.0%)
1	Fk	1.77	2/662 (0.3%)	1.32	8/897 (0.9%)
1	Fl	1.77	2/662 (0.3%)	1.41	10/897 (1.1%)
1	Fm	1.88	7/662 (1.1%)	1.43	7/897 (0.8%)
1	Fn	1.82	2/662 (0.3%)	1.42	11/897 (1.2%)
1	Fo	1.78	3/662 (0.5%)	1.34	9/897 (1.0%)
1	Fp	1.77	1/662 (0.2%)	1.32	8/897 (0.9%)
1	Fq	1.78	3/662 (0.5%)	1.41	10/897 (1.1%)
1	Fr	1.89	7/662 (1.1%)	1.43	7/897 (0.8%)
1	Fs	1.81	2/662 (0.3%)	1.42	11/897 (1.2%)
1	Ft	1.78	2/662 (0.3%)	1.34	9/897 (1.0%)
1	Fu	1.77	2/662 (0.3%)	1.32	8/897 (0.9%)
1	Fv	1.78	3/662 (0.5%)	1.41	10/897 (1.1%)
1	Fw	1.89	7/662 (1.1%)	1.43	7/897 (0.8%)
1	Fx	1.81	2/662 (0.3%)	1.43	11/897 (1.2%)
1	Fy	1.78	3/662 (0.5%)	1.33	9/897 (1.0%)
1	Fz	1.77	3/662 (0.5%)	1.32	8/897 (0.9%)
1	G0	1.83	2/662 (0.3%)	1.33	7/897 (0.8%)
1	G1	1.75	4/662 (0.6%)	1.33	11/897 (1.2%)
1	G2	1.79	3/662 (0.5%)	1.37	10/897 (1.1%)
1	G3	1.82	2/662 (0.3%)	1.34	10/897 (1.1%)
1	G4	1.86	5/662 (0.8%)	1.40	8/897 (0.9%)
1	G5	1.83	2/662 (0.3%)	1.33	7/897 (0.8%)
1	G6	1.75	4/662 (0.6%)	1.33	11/897 (1.2%)
1	G7	1.79	3/662 (0.5%)	1.37	10/897 (1.1%)
1	G8	1.82	2/662 (0.3%)	1.34	10/897 (1.1%)
1	G9	1.86	5/662 (0.8%)	1.40	10/897 (1.1%)
1	GA	1.79	3/662 (0.5%)	1.37	10/897 (1.1%)
1	GB	1.82	2/662 (0.3%)	1.34	10/897 (1.1%)
1	GC	1.86	5/662 (0.8%)	1.40	10/897 (1.1%)
1	GD	1.83	2/662 (0.3%)	1.33	7/897 (0.8%)
1	GE	1.75	4/662 (0.6%)	1.33	11/897 (1.2%)
1	GF	1.80	3/662 (0.5%)	1.37	10/897 (1.1%)
1	GG	1.82	2/662 (0.3%)	1.34	10/897 (1.1%)
1	GH	1.85	5/662 (0.8%)	1.40	10/897 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	GI	1.83	2/662 (0.3%)	1.33	7/897 (0.8%)
1	GJ	1.75	4/662 (0.6%)	1.33	11/897 (1.2%)
1	GK	1.79	3/662 (0.5%)	1.37	10/897 (1.1%)
1	GL	1.81	2/662 (0.3%)	1.34	10/897 (1.1%)
1	GM	1.85	5/662 (0.8%)	1.40	10/897 (1.1%)
1	GN	1.83	2/662 (0.3%)	1.33	7/897 (0.8%)
1	GO	1.75	4/662 (0.6%)	1.33	11/897 (1.2%)
1	GP	1.79	3/662 (0.5%)	1.37	10/897 (1.1%)
1	GQ	1.82	2/662 (0.3%)	1.34	10/897 (1.1%)
1	GR	1.86	5/662 (0.8%)	1.40	8/897 (0.9%)
1	GS	1.83	2/662 (0.3%)	1.33	7/897 (0.8%)
1	GT	1.75	4/662 (0.6%)	1.32	11/897 (1.2%)
1	GU	1.79	3/662 (0.5%)	1.37	10/897 (1.1%)
1	GV	1.82	2/662 (0.3%)	1.34	10/897 (1.1%)
1	GW	1.86	5/662 (0.8%)	1.40	10/897 (1.1%)
1	GX	1.83	2/662 (0.3%)	1.33	7/897 (0.8%)
1	Ga	1.75	4/662 (0.6%)	1.33	11/897 (1.2%)
1	Gb	1.79	3/662 (0.5%)	1.37	10/897 (1.1%)
1	Gc	1.82	2/662 (0.3%)	1.34	10/897 (1.1%)
1	Gd	1.86	5/662 (0.8%)	1.40	8/897 (0.9%)
1	Ge	1.83	2/662 (0.3%)	1.33	7/897 (0.8%)
1	Gf	1.75	4/662 (0.6%)	1.33	11/897 (1.2%)
1	Gg	1.79	3/662 (0.5%)	1.37	10/897 (1.1%)
1	Gh	1.81	2/662 (0.3%)	1.34	10/897 (1.1%)
1	Gi	1.85	5/662 (0.8%)	1.40	10/897 (1.1%)
1	Gj	1.83	2/662 (0.3%)	1.33	7/897 (0.8%)
1	Gk	1.75	4/662 (0.6%)	1.33	11/897 (1.2%)
1	Gl	1.79	3/662 (0.5%)	1.37	10/897 (1.1%)
1	Gm	1.82	2/662 (0.3%)	1.34	10/897 (1.1%)
1	Gn	1.86	5/662 (0.8%)	1.40	10/897 (1.1%)
1	Go	1.83	2/662 (0.3%)	1.33	7/897 (0.8%)
1	Gp	1.75	4/662 (0.6%)	1.33	11/897 (1.2%)
1	Gq	1.79	3/662 (0.5%)	1.37	10/897 (1.1%)
1	Gr	1.82	2/662 (0.3%)	1.34	10/897 (1.1%)
1	Gs	1.86	5/662 (0.8%)	1.40	8/897 (0.9%)
1	Gt	1.83	2/662 (0.3%)	1.33	7/897 (0.8%)
1	Gu	1.75	4/662 (0.6%)	1.33	11/897 (1.2%)
1	Gv	1.79	3/662 (0.5%)	1.37	10/897 (1.1%)
1	Gw	1.82	2/662 (0.3%)	1.34	10/897 (1.1%)
1	Gx	1.86	5/662 (0.8%)	1.39	8/897 (0.9%)
1	Gy	1.83	2/662 (0.3%)	1.33	7/897 (0.8%)
1	Gz	1.75	4/662 (0.6%)	1.33	11/897 (1.2%)
1	H0	1.73	0/662	1.36	11/897 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	H1	1.82	4/662 (0.6%)	1.23	8/897 (0.9%)
1	H2	1.75	3/662 (0.5%)	1.32	8/897 (0.9%)
1	H3	1.76	2/662 (0.3%)	1.39	11/897 (1.2%)
1	H4	1.76	4/662 (0.6%)	1.32	8/897 (0.9%)
1	H5	1.73	0/662	1.36	11/897 (1.2%)
1	H6	1.83	4/662 (0.6%)	1.21	7/897 (0.8%)
1	H7	1.75	3/662 (0.5%)	1.32	8/897 (0.9%)
1	H8	1.76	3/662 (0.5%)	1.39	11/897 (1.2%)
1	H9	1.76	5/662 (0.8%)	1.32	8/897 (0.9%)
1	HA	1.75	3/662 (0.5%)	1.32	8/897 (0.9%)
1	HB	1.76	3/662 (0.5%)	1.39	11/897 (1.2%)
1	HC	1.76	4/662 (0.6%)	1.32	8/897 (0.9%)
1	HD	1.74	0/662	1.36	11/897 (1.2%)
1	HE	1.83	5/662 (0.8%)	1.24	8/897 (0.9%)
1	HF	1.75	2/662 (0.3%)	1.32	8/897 (0.9%)
1	HG	1.76	3/662 (0.5%)	1.39	11/897 (1.2%)
1	HH	1.75	3/662 (0.5%)	1.32	8/897 (0.9%)
1	HI	1.73	0/662	1.36	11/897 (1.2%)
1	HJ	1.83	4/662 (0.6%)	1.23	8/897 (0.9%)
1	HK	1.75	3/662 (0.5%)	1.32	8/897 (0.9%)
1	HL	1.76	3/662 (0.5%)	1.39	11/897 (1.2%)
1	HM	1.76	4/662 (0.6%)	1.32	8/897 (0.9%)
1	HN	1.74	0/662	1.36	11/897 (1.2%)
1	HO	1.83	4/662 (0.6%)	1.22	7/897 (0.8%)
1	HP	1.75	3/662 (0.5%)	1.32	8/897 (0.9%)
1	HQ	1.76	3/662 (0.5%)	1.39	11/897 (1.2%)
1	HR	1.76	5/662 (0.8%)	1.32	8/897 (0.9%)
1	HS	1.74	0/662	1.36	11/897 (1.2%)
1	HT	1.83	4/662 (0.6%)	1.23	8/897 (0.9%)
1	HU	1.75	2/662 (0.3%)	1.32	8/897 (0.9%)
1	HV	1.76	2/662 (0.3%)	1.39	11/897 (1.2%)
1	HW	1.76	3/662 (0.5%)	1.32	8/897 (0.9%)
1	HX	1.73	0/662	1.35	11/897 (1.2%)
1	Ha	1.83	4/662 (0.6%)	1.23	8/897 (0.9%)
1	Hb	1.75	2/662 (0.3%)	1.32	8/897 (0.9%)
1	Hc	1.76	2/662 (0.3%)	1.39	11/897 (1.2%)
1	Hd	1.76	3/662 (0.5%)	1.32	8/897 (0.9%)
1	He	1.73	0/662	1.36	11/897 (1.2%)
1	Hf	1.83	4/662 (0.6%)	1.23	8/897 (0.9%)
1	Hg	1.75	3/662 (0.5%)	1.32	8/897 (0.9%)
1	Hh	1.76	2/662 (0.3%)	1.39	11/897 (1.2%)
1	Hi	1.76	4/662 (0.6%)	1.32	8/897 (0.9%)
1	Hj	1.74	0/662	1.36	11/897 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	Hk	1.83	4/662 (0.6%)	1.23	8/897 (0.9%)
1	Hl	1.75	3/662 (0.5%)	1.32	8/897 (0.9%)
1	Hm	1.76	2/662 (0.3%)	1.39	11/897 (1.2%)
1	Hn	1.75	4/662 (0.6%)	1.32	8/897 (0.9%)
1	Ho	1.73	0/662	1.36	11/897 (1.2%)
1	Hp	1.83	4/662 (0.6%)	1.23	8/897 (0.9%)
1	Hq	1.75	2/662 (0.3%)	1.32	8/897 (0.9%)
1	Hr	1.76	3/662 (0.5%)	1.39	11/897 (1.2%)
1	Hs	1.76	3/662 (0.5%)	1.32	8/897 (0.9%)
1	Ht	1.73	0/662	1.35	11/897 (1.2%)
1	Hu	1.83	4/662 (0.6%)	1.22	7/897 (0.8%)
1	Hv	1.75	2/662 (0.3%)	1.32	8/897 (0.9%)
1	Hw	1.76	3/662 (0.5%)	1.39	11/897 (1.2%)
1	Hx	1.76	4/662 (0.6%)	1.32	8/897 (0.9%)
1	Hy	1.73	0/662	1.36	11/897 (1.2%)
1	Hz	1.83	4/662 (0.6%)	1.23	8/897 (0.9%)
2	X0	1.38	0/873	1.38	15/1176 (1.3%)
2	X1	1.38	2/873 (0.2%)	1.33	9/1176 (0.8%)
2	X2	1.41	1/873 (0.1%)	1.39	11/1176 (0.9%)
2	X3	1.37	2/873 (0.2%)	1.61	13/1176 (1.1%)
2	X4	1.42	2/873 (0.2%)	1.41	15/1176 (1.3%)
2	X5	1.38	0/873	1.38	15/1176 (1.3%)
2	X6	1.38	2/873 (0.2%)	1.33	9/1176 (0.8%)
2	X7	1.41	1/873 (0.1%)	1.39	9/1176 (0.8%)
2	X8	1.37	2/873 (0.2%)	1.61	13/1176 (1.1%)
2	X9	1.42	2/873 (0.2%)	1.41	16/1176 (1.4%)
2	XA	1.41	1/873 (0.1%)	1.39	11/1176 (0.9%)
2	XB	1.38	2/873 (0.2%)	1.61	13/1176 (1.1%)
2	XC	1.42	2/873 (0.2%)	1.41	15/1176 (1.3%)
2	XD	1.38	0/873	1.38	15/1176 (1.3%)
2	XE	1.38	2/873 (0.2%)	1.32	9/1176 (0.8%)
2	XF	1.41	1/873 (0.1%)	1.39	11/1176 (0.9%)
2	XG	1.36	2/873 (0.2%)	1.61	13/1176 (1.1%)
2	XH	1.42	2/873 (0.2%)	1.41	17/1176 (1.4%)
2	XI	1.38	0/873	1.38	14/1176 (1.2%)
2	XJ	1.38	2/873 (0.2%)	1.32	9/1176 (0.8%)
2	XK	1.41	1/873 (0.1%)	1.39	11/1176 (0.9%)
2	XL	1.37	2/873 (0.2%)	1.61	13/1176 (1.1%)
2	XM	1.42	2/873 (0.2%)	1.41	15/1176 (1.3%)
2	XN	1.38	0/873	1.38	15/1176 (1.3%)
2	XO	1.38	2/873 (0.2%)	1.32	9/1176 (0.8%)
2	XP	1.41	1/873 (0.1%)	1.39	9/1176 (0.8%)
2	XQ	1.37	2/873 (0.2%)	1.61	13/1176 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	XR	1.42	2/873 (0.2%)	1.41	17/1176 (1.4%)
2	XS	1.38	0/873	1.38	15/1176 (1.3%)
2	XT	1.38	2/873 (0.2%)	1.33	9/1176 (0.8%)
2	XU	1.41	1/873 (0.1%)	1.39	9/1176 (0.8%)
2	XV	1.37	2/873 (0.2%)	1.62	13/1176 (1.1%)
2	XW	1.42	2/873 (0.2%)	1.41	17/1176 (1.4%)
2	XX	1.38	0/873	1.38	14/1176 (1.2%)
2	Xa	1.38	2/873 (0.2%)	1.32	9/1176 (0.8%)
2	Xb	1.41	1/873 (0.1%)	1.39	9/1176 (0.8%)
2	Xc	1.37	2/873 (0.2%)	1.61	13/1176 (1.1%)
2	Xd	1.42	2/873 (0.2%)	1.41	16/1176 (1.4%)
2	Xe	1.38	0/873	1.38	14/1176 (1.2%)
2	Xf	1.38	2/873 (0.2%)	1.33	9/1176 (0.8%)
2	Xg	1.41	1/873 (0.1%)	1.39	11/1176 (0.9%)
2	Xh	1.37	2/873 (0.2%)	1.61	13/1176 (1.1%)
2	Xi	1.42	2/873 (0.2%)	1.41	15/1176 (1.3%)
2	Xj	1.38	0/873	1.38	14/1176 (1.2%)
2	Xk	1.38	2/873 (0.2%)	1.32	9/1176 (0.8%)
2	Xl	1.41	1/873 (0.1%)	1.39	9/1176 (0.8%)
2	Xm	1.37	2/873 (0.2%)	1.61	13/1176 (1.1%)
2	Xn	1.42	2/873 (0.2%)	1.41	17/1176 (1.4%)
2	Xo	1.38	0/873	1.38	14/1176 (1.2%)
2	Xp	1.38	2/873 (0.2%)	1.33	9/1176 (0.8%)
2	Xq	1.41	1/873 (0.1%)	1.39	9/1176 (0.8%)
2	Xr	1.38	2/873 (0.2%)	1.62	13/1176 (1.1%)
2	Xs	1.42	2/873 (0.2%)	1.41	16/1176 (1.4%)
2	Xt	1.38	0/873	1.38	14/1176 (1.2%)
2	Xu	1.38	2/873 (0.2%)	1.32	9/1176 (0.8%)
2	Xv	1.41	1/873 (0.1%)	1.39	11/1176 (0.9%)
2	Xw	1.38	2/873 (0.2%)	1.62	13/1176 (1.1%)
2	Xx	1.42	2/873 (0.2%)	1.41	16/1176 (1.4%)
2	Xy	1.38	0/873	1.38	14/1176 (1.2%)
2	Xz	1.38	2/873 (0.2%)	1.33	9/1176 (0.8%)
3	P0	1.29	0/624	1.43	11/848 (1.3%)
3	P1	1.20	1/624 (0.2%)	1.33	5/848 (0.6%)
3	P2	1.28	1/624 (0.2%)	1.32	9/848 (1.1%)
3	P3	1.26	0/624	1.35	5/848 (0.6%)
3	P4	1.20	0/624	1.35	5/848 (0.6%)
3	P5	1.29	0/624	1.43	11/848 (1.3%)
3	P6	1.20	1/624 (0.2%)	1.33	5/848 (0.6%)
3	P7	1.28	0/624	1.32	9/848 (1.1%)
3	P8	1.26	0/624	1.35	5/848 (0.6%)
3	P9	1.20	0/624	1.35	5/848 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	PA	1.28	0/624	1.32	9/848 (1.1%)
3	PB	1.26	0/624	1.35	5/848 (0.6%)
3	PC	1.20	0/624	1.35	5/848 (0.6%)
3	PD	1.30	0/624	1.43	11/848 (1.3%)
3	PE	1.20	1/624 (0.2%)	1.33	5/848 (0.6%)
3	PF	1.28	0/624	1.32	9/848 (1.1%)
3	PG	1.26	0/624	1.35	5/848 (0.6%)
3	PH	1.20	0/624	1.35	5/848 (0.6%)
3	PI	1.30	0/624	1.43	11/848 (1.3%)
3	PJ	1.20	1/624 (0.2%)	1.33	5/848 (0.6%)
3	PK	1.28	1/624 (0.2%)	1.32	9/848 (1.1%)
3	PL	1.26	0/624	1.35	5/848 (0.6%)
3	PM	1.20	0/624	1.35	5/848 (0.6%)
3	PN	1.29	0/624	1.42	11/848 (1.3%)
3	PO	1.20	1/624 (0.2%)	1.33	5/848 (0.6%)
3	PP	1.28	1/624 (0.2%)	1.32	9/848 (1.1%)
3	PQ	1.26	0/624	1.35	5/848 (0.6%)
3	PR	1.20	0/624	1.35	5/848 (0.6%)
3	PS	1.29	0/624	1.42	11/848 (1.3%)
3	PT	1.20	1/624 (0.2%)	1.33	5/848 (0.6%)
3	PU	1.28	1/624 (0.2%)	1.32	9/848 (1.1%)
3	PV	1.26	0/624	1.35	5/848 (0.6%)
3	PW	1.20	0/624	1.35	5/848 (0.6%)
3	PX	1.30	0/624	1.42	11/848 (1.3%)
3	Pa	1.20	1/624 (0.2%)	1.33	5/848 (0.6%)
3	Pb	1.28	0/624	1.32	9/848 (1.1%)
3	Pc	1.26	0/624	1.35	5/848 (0.6%)
3	Pd	1.20	0/624	1.35	5/848 (0.6%)
3	Pe	1.30	0/624	1.43	11/848 (1.3%)
3	Pf	1.20	1/624 (0.2%)	1.33	5/848 (0.6%)
3	Pg	1.28	0/624	1.32	9/848 (1.1%)
3	Ph	1.26	0/624	1.35	5/848 (0.6%)
3	Pi	1.20	0/624	1.35	5/848 (0.6%)
3	Pj	1.29	0/624	1.42	11/848 (1.3%)
3	Pk	1.20	1/624 (0.2%)	1.33	5/848 (0.6%)
3	Pl	1.28	0/624	1.31	9/848 (1.1%)
3	Pm	1.26	0/624	1.35	5/848 (0.6%)
3	Pn	1.20	0/624	1.35	5/848 (0.6%)
3	Po	1.29	0/624	1.43	11/848 (1.3%)
3	Pp	1.20	1/624 (0.2%)	1.33	5/848 (0.6%)
3	Pq	1.28	1/624 (0.2%)	1.32	9/848 (1.1%)
3	Pr	1.26	0/624	1.35	5/848 (0.6%)
3	Ps	1.20	0/624	1.35	5/848 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	Pt	1.30	0/624	1.42	11/848 (1.3%)
3	Pu	1.20	1/624 (0.2%)	1.33	5/848 (0.6%)
3	Pv	1.28	0/624	1.32	9/848 (1.1%)
3	Pw	1.26	0/624	1.35	5/848 (0.6%)
3	Px	1.20	0/624	1.35	5/848 (0.6%)
3	Py	1.29	0/624	1.43	11/848 (1.3%)
3	Pz	1.20	1/624 (0.2%)	1.33	5/848 (0.6%)
All	All	1.70	1862/407580 (0.5%)	1.37	5491/552000 (1.0%)

The worst 5 of 1862 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Bl	13	GLU	CA-C	-7.26	1.44	1.52
1	Bv	13	GLU	CA-C	-7.26	1.44	1.52
1	B7	13	GLU	CA-C	-7.26	1.44	1.52
1	BP	13	GLU	CA-C	-7.26	1.44	1.52
1	GW	24	ALA	CA-C	-7.25	1.43	1.52

The worst 5 of 5491 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Xw	808	GLY	N-CA-C	29.61	148.31	112.49
2	Xr	808	GLY	N-CA-C	29.61	148.31	112.49
2	Xc	808	GLY	N-CA-C	29.60	148.31	112.49
2	XL	808	GLY	N-CA-C	29.60	148.31	112.49
2	X3	808	GLY	N-CA-C	29.60	148.30	112.49

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	656	0	677	15	0
1	A1	656	0	677	22	0
1	A2	656	0	677	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A3	656	0	677	13	0
1	A4	656	0	677	13	0
1	A5	656	0	677	13	0
1	A6	656	0	677	20	0
1	A7	656	0	677	18	0
1	A8	656	0	677	15	0
1	A9	656	0	677	13	0
1	AA	656	0	677	19	0
1	AB	656	0	677	14	0
1	AC	656	0	677	11	0
1	AD	656	0	677	14	0
1	AE	656	0	677	18	0
1	AF	656	0	677	16	0
1	AG	656	0	677	14	0
1	AH	656	0	677	12	0
1	AI	656	0	677	13	0
1	AJ	656	0	677	20	0
1	AK	656	0	677	14	0
1	AL	656	0	677	15	0
1	AM	656	0	677	13	0
1	AN	656	0	677	13	0
1	AO	656	0	677	22	0
1	AP	656	0	677	16	0
1	AQ	656	0	677	14	0
1	AR	656	0	677	11	0
1	AS	656	0	677	14	0
1	AT	656	0	677	22	0
1	AU	656	0	677	14	0
1	AV	656	0	677	15	0
1	AW	656	0	677	13	0
1	AX	656	0	677	14	0
1	Aa	656	0	677	18	0
1	Ab	656	0	677	17	0
1	Ac	656	0	677	15	0
1	Ad	656	0	677	13	0
1	Ae	656	0	677	15	0
1	Af	656	0	677	21	0
1	Ag	656	0	677	15	0
1	Ah	656	0	677	13	0
1	Ai	656	0	677	12	0
1	Aj	656	0	677	14	0
1	Ak	656	0	677	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Al	656	0	677	17	0
1	Am	656	0	677	15	0
1	An	656	0	677	12	0
1	Ao	656	0	677	14	0
1	Ap	656	0	677	17	0
1	Aq	656	0	677	15	0
1	Ar	656	0	677	16	0
1	As	656	0	677	13	0
1	At	656	0	677	15	0
1	Au	656	0	677	21	0
1	Av	656	0	677	14	0
1	Aw	656	0	677	13	0
1	Ax	656	0	677	11	0
1	Ay	656	0	677	13	0
1	Az	656	0	677	19	0
1	B0	656	0	677	14	0
1	B1	656	0	677	13	0
1	B2	656	0	677	12	0
1	B3	656	0	677	10	0
1	B4	656	0	677	13	0
1	B5	656	0	677	14	0
1	B6	656	0	677	15	0
1	B7	656	0	677	12	0
1	B8	656	0	677	9	0
1	B9	656	0	677	13	0
1	BA	656	0	677	13	0
1	BB	656	0	677	10	0
1	BC	656	0	677	12	0
1	BD	656	0	677	12	0
1	BE	656	0	677	13	0
1	BF	656	0	677	12	0
1	BG	656	0	677	9	0
1	BH	656	0	677	13	0
1	BI	656	0	677	13	0
1	BJ	656	0	677	14	0
1	BK	656	0	677	12	0
1	BL	656	0	677	10	0
1	BM	656	0	677	13	0
1	BN	656	0	677	15	0
1	BO	656	0	677	12	0
1	BP	656	0	677	11	0
1	BQ	656	0	677	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BR	656	0	677	13	0
1	BS	656	0	677	13	0
1	BT	656	0	677	12	0
1	BU	656	0	677	11	0
1	BV	656	0	677	9	0
1	BW	656	0	677	13	0
1	BX	656	0	677	13	0
1	Ba	656	0	677	14	0
1	Bb	656	0	677	11	0
1	Bc	656	0	677	10	0
1	Bd	656	0	677	13	0
1	Be	656	0	677	14	0
1	Bf	656	0	677	14	0
1	Bg	656	0	677	12	0
1	Bh	656	0	677	11	0
1	Bi	656	0	677	13	0
1	Bj	656	0	677	14	0
1	Bk	656	0	677	15	0
1	Bl	656	0	677	13	0
1	Bm	656	0	677	10	0
1	Bn	656	0	677	12	0
1	Bo	656	0	677	13	0
1	Bp	656	0	677	14	0
1	Bq	656	0	677	12	0
1	Br	656	0	677	10	0
1	Bs	656	0	677	13	0
1	Bt	656	0	677	14	0
1	Bu	656	0	677	13	0
1	Bv	656	0	677	12	0
1	Bw	656	0	677	9	0
1	Bx	656	0	677	13	0
1	By	656	0	677	13	0
1	Bz	656	0	677	13	0
1	C0	656	0	677	11	0
1	C1	656	0	677	11	0
1	C2	656	0	677	10	0
1	C3	656	0	677	11	0
1	C4	656	0	677	12	0
1	C5	656	0	677	11	0
1	C6	656	0	677	11	0
1	C7	656	0	677	12	0
1	C8	656	0	677	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C9	656	0	677	11	0
1	CA	656	0	677	12	0
1	CB	656	0	677	11	0
1	CC	656	0	677	12	0
1	CD	656	0	677	11	0
1	CE	656	0	677	11	0
1	CF	656	0	677	12	0
1	CG	656	0	677	11	0
1	CH	656	0	677	11	0
1	CI	656	0	677	11	0
1	CJ	656	0	677	11	0
1	CK	656	0	677	12	0
1	CL	656	0	677	12	0
1	CM	656	0	677	11	0
1	CN	656	0	677	11	0
1	CO	656	0	677	11	0
1	CP	656	0	677	11	0
1	CQ	656	0	677	11	0
1	CR	656	0	677	11	0
1	CS	656	0	677	11	0
1	CT	656	0	677	11	0
1	CU	656	0	677	12	0
1	CV	656	0	677	11	0
1	CW	656	0	677	11	0
1	CX	656	0	677	11	0
1	Ca	656	0	677	11	0
1	Cb	656	0	677	12	0
1	Cc	656	0	677	11	0
1	Cd	656	0	677	11	0
1	Ce	656	0	677	11	0
1	Cf	656	0	677	11	0
1	Cg	656	0	677	12	0
1	Ch	656	0	677	11	0
1	Ci	656	0	677	11	0
1	Cj	656	0	677	11	0
1	Ck	656	0	677	11	0
1	Cl	656	0	677	12	0
1	Cm	656	0	677	11	0
1	Cn	656	0	677	12	0
1	Co	656	0	677	12	0
1	Cp	656	0	677	11	0
1	Cq	656	0	677	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Cr	656	0	677	12	0
1	Cs	656	0	677	12	0
1	Ct	656	0	677	11	0
1	Cu	656	0	677	11	0
1	Cv	656	0	677	12	0
1	Cw	656	0	677	12	0
1	Cx	656	0	677	11	0
1	Cy	656	0	677	10	0
1	Cz	656	0	677	11	0
1	D0	656	0	677	18	0
1	D1	656	0	677	13	0
1	D2	656	0	677	16	0
1	D3	656	0	677	19	0
1	D4	656	0	677	18	0
1	D5	656	0	677	20	0
1	D6	656	0	677	14	0
1	D7	656	0	677	20	0
1	D8	656	0	677	22	0
1	D9	656	0	677	24	0
1	DA	656	0	677	22	0
1	DB	656	0	677	22	0
1	DC	656	0	677	21	0
1	DD	656	0	677	20	0
1	DE	656	0	677	11	0
1	DF	656	0	677	16	0
1	DG	656	0	677	23	0
1	DH	656	0	677	18	0
1	DI	656	0	677	22	0
1	DJ	656	0	677	11	0
1	DK	656	0	677	21	0
1	DL	656	0	677	18	0
1	DM	656	0	677	20	0
1	DN	656	0	677	18	0
1	DO	656	0	677	14	0
1	DP	656	0	677	20	0
1	DQ	656	0	677	17	0
1	DR	656	0	677	21	0
1	DS	656	0	677	18	0
1	DT	656	0	677	11	0
1	DU	656	0	677	21	0
1	DV	656	0	677	23	0
1	DW	656	0	677	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DX	656	0	677	18	0
1	Da	656	0	677	10	0
1	Db	656	0	677	15	0
1	Dc	656	0	677	21	0
1	Dd	656	0	677	18	0
1	De	656	0	677	23	0
1	Df	656	0	677	13	0
1	Dg	656	0	677	26	0
1	Dh	656	0	677	19	0
1	Di	656	0	677	21	0
1	Dj	656	0	677	19	0
1	Dk	656	0	677	13	0
1	Dl	656	0	677	22	0
1	Dm	656	0	677	23	0
1	Dn	656	0	677	28	0
1	Do	656	0	677	20	0
1	Dp	656	0	677	9	0
1	Dq	656	0	677	17	0
1	Dr	656	0	677	22	0
1	Ds	656	0	677	18	0
1	Dt	656	0	677	23	0
1	Du	656	0	677	15	0
1	Dv	656	0	677	19	0
1	Dw	656	0	677	19	0
1	Dx	656	0	677	20	0
1	Dy	656	0	677	18	0
1	Dz	656	0	677	14	0
1	E0	656	0	677	13	0
1	E1	656	0	677	14	0
1	E2	656	0	677	10	0
1	E3	656	0	677	6	0
1	E4	656	0	677	12	0
1	E5	656	0	677	13	0
1	E6	656	0	677	14	0
1	E7	656	0	677	9	0
1	E8	656	0	677	5	0
1	E9	656	0	677	12	0
1	EA	656	0	677	10	0
1	EB	656	0	677	5	0
1	EC	656	0	677	12	0
1	ED	656	0	677	12	0
1	EE	656	0	677	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EF	656	0	677	9	0
1	EG	656	0	677	4	0
1	EH	656	0	677	12	0
1	EI	656	0	677	12	0
1	EJ	656	0	677	13	0
1	EK	656	0	677	10	0
1	EL	656	0	677	5	0
1	EM	656	0	677	12	0
1	EN	656	0	677	13	0
1	EO	656	0	677	11	0
1	EP	656	0	677	9	0
1	EQ	656	0	677	7	0
1	ER	656	0	677	12	0
1	ES	656	0	677	13	0
1	ET	656	0	677	13	0
1	EU	656	0	677	9	0
1	EV	656	0	677	8	0
1	EW	656	0	677	12	0
1	EX	656	0	677	12	0
1	Ea	656	0	677	13	0
1	Eb	656	0	677	9	0
1	Ec	656	0	677	6	0
1	Ed	656	0	677	12	0
1	Ee	656	0	677	13	0
1	Ef	656	0	677	14	0
1	Eg	656	0	677	10	0
1	Eh	656	0	677	7	0
1	Ei	656	0	677	11	0
1	Ej	656	0	677	13	0
1	Ek	656	0	677	14	0
1	El	656	0	677	10	0
1	Em	656	0	677	6	0
1	En	656	0	677	12	0
1	Eo	656	0	677	12	0
1	Ep	656	0	677	13	0
1	Eq	656	0	677	9	0
1	Er	656	0	677	6	0
1	Es	656	0	677	12	0
1	Et	656	0	677	12	0
1	Eu	656	0	677	12	0
1	Ev	656	0	677	10	0
1	Ew	656	0	677	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ex	656	0	677	12	0
1	Ey	656	0	677	12	0
1	Ez	656	0	677	14	0
1	F0	656	0	677	11	0
1	F1	656	0	677	13	0
1	F2	656	0	677	7	0
1	F3	656	0	677	14	0
1	F4	656	0	677	13	0
1	F5	656	0	677	13	0
1	F6	656	0	677	12	0
1	F7	656	0	677	5	0
1	F8	656	0	677	14	0
1	F9	656	0	677	13	0
1	FA	656	0	677	8	0
1	FB	656	0	677	13	0
1	FC	656	0	677	14	0
1	FD	656	0	677	13	0
1	FE	656	0	677	11	0
1	FF	656	0	677	7	0
1	FG	656	0	677	13	0
1	FH	656	0	677	13	0
1	FI	656	0	677	13	0
1	FJ	656	0	677	11	0
1	FK	656	0	677	6	0
1	FL	656	0	677	14	0
1	FM	656	0	677	13	0
1	FN	656	0	677	10	0
1	FO	656	0	677	11	0
1	FP	656	0	677	5	0
1	FQ	656	0	677	14	0
1	FR	656	0	677	14	0
1	FS	656	0	677	11	0
1	FT	656	0	677	11	0
1	FU	656	0	677	8	0
1	FV	656	0	677	13	0
1	FW	656	0	677	13	0
1	FX	656	0	677	13	0
1	Fa	656	0	677	11	0
1	Fb	656	0	677	6	0
1	Fc	656	0	677	14	0
1	Fd	656	0	677	13	0
1	Fe	656	0	677	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ff	656	0	677	11	0
1	Fg	656	0	677	7	0
1	Fh	656	0	677	14	0
1	Fi	656	0	677	13	0
1	Fj	656	0	677	11	0
1	Fk	656	0	677	10	0
1	Fl	656	0	677	5	0
1	Fm	656	0	677	15	0
1	Fn	656	0	677	14	0
1	Fo	656	0	677	12	0
1	Fp	656	0	677	11	0
1	Fq	656	0	677	6	0
1	Fr	656	0	677	16	0
1	Fs	656	0	677	13	0
1	Ft	656	0	677	13	0
1	Fu	656	0	677	10	0
1	Fv	656	0	677	6	0
1	Fw	656	0	677	14	0
1	Fx	656	0	677	14	0
1	Fy	656	0	677	13	0
1	Fz	656	0	677	12	0
1	G0	656	0	677	19	0
1	G1	656	0	677	15	0
1	G2	656	0	677	18	0
1	G3	656	0	677	19	0
1	G4	656	0	677	20	0
1	G5	656	0	677	20	0
1	G6	656	0	677	21	0
1	G7	656	0	677	19	0
1	G8	656	0	677	21	0
1	G9	656	0	677	17	0
1	GA	656	0	677	25	0
1	GB	656	0	677	22	0
1	GC	656	0	677	19	0
1	GD	656	0	677	21	0
1	GE	656	0	677	15	0
1	GF	656	0	677	21	0
1	GG	656	0	677	18	0
1	GH	656	0	677	18	0
1	GI	656	0	677	21	0
1	GJ	656	0	677	19	0
1	GK	656	0	677	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GL	656	0	677	18	0
1	GM	656	0	677	21	0
1	GN	656	0	677	27	0
1	GO	656	0	677	19	0
1	GP	656	0	677	23	0
1	GQ	656	0	677	19	0
1	GR	656	0	677	18	0
1	GS	656	0	677	21	0
1	GT	656	0	677	19	0
1	GU	656	0	677	17	0
1	GV	656	0	677	22	0
1	GW	656	0	677	20	0
1	GX	656	0	677	23	0
1	Ga	656	0	677	17	0
1	Gb	656	0	677	19	0
1	Gc	656	0	677	19	0
1	Gd	656	0	677	19	0
1	Ge	656	0	677	23	0
1	Gf	656	0	677	15	0
1	Gg	656	0	677	23	0
1	Gh	656	0	677	19	0
1	Gi	656	0	677	21	0
1	Gj	656	0	677	19	0
1	Gk	656	0	677	19	0
1	Gl	656	0	677	17	0
1	Gm	656	0	677	20	0
1	Gn	656	0	677	18	0
1	Go	656	0	677	19	0
1	Gp	656	0	677	18	0
1	Gq	656	0	677	20	0
1	Gr	656	0	677	18	0
1	Gs	656	0	677	19	0
1	Gt	656	0	677	24	0
1	Gu	656	0	677	19	0
1	Gv	656	0	677	19	0
1	Gw	656	0	677	19	0
1	Gx	656	0	677	19	0
1	Gy	656	0	677	20	0
1	Gz	656	0	677	20	0
1	H0	656	0	677	17	0
1	H1	656	0	677	13	0
1	H2	656	0	677	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H3	656	0	677	17	0
1	H4	656	0	677	23	0
1	H5	656	0	677	25	0
1	H6	656	0	677	15	0
1	H7	656	0	677	20	0
1	H8	656	0	677	18	0
1	H9	656	0	677	21	0
1	HA	656	0	677	20	0
1	HB	656	0	677	18	0
1	HC	656	0	677	21	0
1	HD	656	0	677	18	0
1	HE	656	0	677	17	0
1	HF	656	0	677	22	0
1	HG	656	0	677	17	0
1	HH	656	0	677	25	0
1	HI	656	0	677	25	0
1	HJ	656	0	677	18	0
1	HK	656	0	677	28	0
1	HL	656	0	677	16	0
1	HM	656	0	677	29	0
1	HN	656	0	677	25	0
1	HO	656	0	677	15	0
1	HP	656	0	677	19	0
1	HQ	656	0	677	22	0
1	HR	656	0	677	22	0
1	HS	656	0	677	25	0
1	HT	656	0	677	20	0
1	HU	656	0	677	25	0
1	HV	656	0	677	17	0
1	HW	656	0	677	26	0
1	HX	656	0	677	19	0
1	Ha	656	0	677	17	0
1	Hb	656	0	677	19	0
1	Hc	656	0	677	18	0
1	Hd	656	0	677	22	0
1	He	656	0	677	25	0
1	Hf	656	0	677	17	0
1	Hg	656	0	677	26	0
1	Hh	656	0	677	15	0
1	Hi	656	0	677	22	0
1	Hj	656	0	677	25	0
1	Hk	656	0	677	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Hl	656	0	677	20	0
1	Hm	656	0	677	18	0
1	Hn	656	0	677	26	0
1	Ho	656	0	677	19	0
1	Hp	656	0	677	15	0
1	Hq	656	0	677	21	0
1	Hr	656	0	677	18	0
1	Hs	656	0	677	23	0
1	Ht	656	0	677	23	0
1	Hu	656	0	677	17	0
1	Hv	656	0	677	27	0
1	Hw	656	0	677	18	0
1	Hx	656	0	677	25	0
1	Hy	656	0	677	26	0
1	Hz	656	0	677	16	0
2	X0	859	0	838	25	0
2	X1	859	0	837	27	0
2	X2	859	0	838	27	0
2	X3	859	0	836	27	0
2	X4	859	0	838	24	0
2	X5	859	0	838	29	0
2	X6	859	0	837	26	0
2	X7	859	0	838	23	0
2	X8	859	0	838	25	0
2	X9	859	0	838	26	0
2	XA	859	0	838	23	0
2	XB	859	0	838	24	0
2	XC	859	0	838	22	0
2	XD	859	0	838	24	0
2	XE	859	0	837	29	0
2	XF	859	0	838	25	0
2	XG	859	0	838	23	0
2	XH	859	0	838	25	0
2	XI	859	0	838	22	0
2	XJ	859	0	838	26	0
2	XK	859	0	838	25	0
2	XL	859	0	836	26	0
2	XM	859	0	838	29	0
2	XN	859	0	838	27	0
2	XO	859	0	837	26	0
2	XP	859	0	838	22	0
2	XQ	859	0	836	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	XR	859	0	838	22	0
2	XS	859	0	838	27	0
2	XT	859	0	837	28	0
2	XU	859	0	838	23	0
2	XV	859	0	838	22	0
2	XW	859	0	838	26	0
2	XX	859	0	838	24	0
2	Xa	859	0	837	28	0
2	Xb	859	0	838	29	0
2	Xc	859	0	838	22	0
2	Xd	859	0	838	25	0
2	Xe	859	0	838	21	0
2	Xf	859	0	837	27	0
2	Xg	859	0	838	25	0
2	Xh	859	0	836	27	0
2	Xi	859	0	838	23	0
2	Xj	859	0	838	28	0
2	Xk	859	0	837	24	0
2	Xl	859	0	838	23	0
2	Xm	859	0	838	24	0
2	Xn	859	0	838	22	0
2	Xo	859	0	838	23	0
2	Xp	859	0	837	28	0
2	Xq	859	0	838	25	0
2	Xr	859	0	838	23	0
2	Xs	859	0	838	24	0
2	Xt	859	0	838	21	0
2	Xu	859	0	837	27	0
2	Xv	859	0	838	24	0
2	Xw	859	0	836	27	0
2	Xx	859	0	838	28	0
2	Xy	859	0	838	28	0
2	Xz	859	0	837	27	0
3	P0	612	0	628	19	0
3	P1	612	0	628	12	0
3	P2	612	0	628	15	0
3	P3	612	0	628	15	0
3	P4	612	0	628	14	0
3	P5	612	0	628	20	0
3	P6	612	0	628	13	0
3	P7	612	0	628	16	0
3	P8	612	0	628	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P9	612	0	628	16	0
3	PA	612	0	628	16	0
3	PB	612	0	628	18	0
3	PC	612	0	628	16	0
3	PD	612	0	628	19	0
3	PE	612	0	628	12	0
3	PF	612	0	628	15	0
3	PG	612	0	628	16	0
3	PH	612	0	628	15	0
3	PI	612	0	628	18	0
3	PJ	612	0	628	13	0
3	PK	612	0	628	17	0
3	PL	612	0	628	16	0
3	PM	612	0	628	16	0
3	PN	612	0	628	19	0
3	PO	612	0	628	14	0
3	PP	612	0	628	17	0
3	PQ	612	0	628	14	0
3	PR	612	0	628	15	0
3	PS	612	0	628	19	0
3	PT	612	0	628	13	0
3	PU	612	0	628	16	0
3	PV	612	0	628	14	0
3	PW	612	0	628	15	0
3	PX	612	0	628	19	0
3	Pa	612	0	628	13	0
3	Pb	612	0	628	18	0
3	Pc	612	0	628	16	0
3	Pd	612	0	628	16	0
3	Pe	612	0	628	17	0
3	Pf	612	0	628	13	0
3	Pg	612	0	628	16	0
3	Ph	612	0	628	17	0
3	Pi	612	0	628	15	0
3	Pj	612	0	628	20	0
3	Pk	612	0	628	11	0
3	Pl	612	0	628	14	0
3	Pm	612	0	628	15	0
3	Pn	612	0	628	15	0
3	Po	612	0	628	20	0
3	Pp	612	0	628	14	0
3	Pq	612	0	628	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Pr	612	0	628	16	0
3	Ps	612	0	628	16	0
3	Pt	612	0	628	19	0
3	Pu	612	0	628	12	0
3	Pv	612	0	628	15	0
3	Pw	612	0	628	17	0
3	Px	612	0	628	14	0
3	Py	612	0	628	19	0
3	Pz	612	0	628	13	0
All	All	403140	0	412899	6677	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 8.

The worst 5 of 6677 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Xp:714:THR:OG1	1:Hi:79:HIS:ND1	1.56	1.38
2:X9:714:THR:HG23	1:Hq:79:HIS:ND1	1.38	1.38
1:Hn:79:HIS:ND1	2:XT:714:THR:OG1	1.58	1.35
1:He:79:HIS:ND1	2:XE:714:THR:OG1	1.59	1.34
2:Xf:714:THR:OG1	1:HB:79:HIS:ND1	1.58	1.33

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%)	89 (99%)	1 (1%)	0	100	100
1	A1	90/98 (92%)	90 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A2	90/98 (92%)	90 (100%)	0	0	100	100
1	A3	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	A4	90/98 (92%)	90 (100%)	0	0	100	100
1	A5	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	AC	90/98 (92%)	90 (100%)	0	0	100	100
1	AD	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	AH	90/98 (92%)	90 (100%)	0	0	100	100
1	AI	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	AR	90/98 (92%)	90 (100%)	0	0	100	100
1	AS	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	AW	90/98 (92%)	90 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AX	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	Ad	90/98 (92%)	90 (100%)	0	0	100	100
1	Ae	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	Ai	90/98 (92%)	90 (100%)	0	0	100	100
1	Aj	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	An	90/98 (92%)	90 (100%)	0	0	100	100
1	Ao	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	As	90/98 (92%)	90 (100%)	0	0	100	100
1	At	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	Ax	90/98 (92%)	90 (100%)	0	0	100	100
1	Ay	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Az	90/98 (92%)	90 (100%)	0	0	100	100
1	B0	90/98 (92%)	90 (100%)	0	0	100	100
1	B1	90/98 (92%)	90 (100%)	0	0	100	100
1	B2	90/98 (92%)	90 (100%)	0	0	100	100
1	B3	90/98 (92%)	90 (100%)	0	0	100	100

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

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D8	90/98 (92%)	90 (100%)	0	0	100	100
1	D9	90/98 (92%)	90 (100%)	0	0	100	100
1	DA	90/98 (92%)	90 (100%)	0	0	100	100
1	DB	90/98 (92%)	90 (100%)	0	0	100	100
1	DC	90/98 (92%)	90 (100%)	0	0	100	100
1	DD	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DE	90/98 (92%)	90 (100%)	0	0	100	100
1	DF	90/98 (92%)	90 (100%)	0	0	100	100
1	DG	90/98 (92%)	90 (100%)	0	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%)	90 (100%)	0	0	100	100
1	DK	90/98 (92%)	90 (100%)	0	0	100	100
1	DL	90/98 (92%)	90 (100%)	0	0	100	100
1	DM	90/98 (92%)	90 (100%)	0	0	100	100
1	DN	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DO	90/98 (92%)	90 (100%)	0	0	100	100
1	DP	90/98 (92%)	90 (100%)	0	0	100	100
1	DQ	90/98 (92%)	90 (100%)	0	0	100	100
1	DR	90/98 (92%)	90 (100%)	0	0	100	100
1	DS	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	DT	90/98 (92%)	90 (100%)	0	0	100	100
1	DU	90/98 (92%)	90 (100%)	0	0	100	100
1	DV	90/98 (92%)	90 (100%)	0	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	Da	90/98 (92%)	90 (100%)	0	0	100	100
1	Db	90/98 (92%)	90 (100%)	0	0	100	100
1	Dc	90/98 (92%)	90 (100%)	0	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Df	90/98 (92%)	90 (100%)	0	0	100	100
1	Dg	90/98 (92%)	90 (100%)	0	0	100	100
1	Dh	90/98 (92%)	90 (100%)	0	0	100	100
1	Di	90/98 (92%)	90 (100%)	0	0	100	100
1	Dj	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Dk	90/98 (92%)	90 (100%)	0	0	100	100
1	Dl	90/98 (92%)	90 (100%)	0	0	100	100
1	Dm	90/98 (92%)	90 (100%)	0	0	100	100
1	Dn	90/98 (92%)	90 (100%)	0	0	100	100
1	Do	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Dp	90/98 (92%)	90 (100%)	0	0	100	100
1	Dq	90/98 (92%)	90 (100%)	0	0	100	100
1	Dr	90/98 (92%)	90 (100%)	0	0	100	100
1	Ds	90/98 (92%)	90 (100%)	0	0	100	100
1	Dt	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Du	90/98 (92%)	90 (100%)	0	0	100	100
1	Dv	90/98 (92%)	90 (100%)	0	0	100	100
1	Dw	90/98 (92%)	90 (100%)	0	0	100	100
1	Dx	90/98 (92%)	90 (100%)	0	0	100	100
1	Dy	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Dz	90/98 (92%)	90 (100%)	0	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%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	E9	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EA	90/98 (92%)	90 (100%)	0	0	100	100
1	EB	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	EC	90/98 (92%)	89 (99%)	1 (1%)	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	90/98 (92%)	90 (100%)	0	0	100	100
1	EG	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	EH	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	ER	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	EW	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	EX	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%)	89 (99%)	1 (1%)	0	100	100
1	Ed	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ee	90/98 (92%)	90 (100%)	0	0	100	100
1	Ef	90/98 (92%)	90 (100%)	0	0	100	100
1	Eg	90/98 (92%)	90 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Eh	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Ei	90/98 (92%)	89 (99%)	1 (1%)	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%)	90 (100%)	0	0	100	100
1	Em	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	En	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	Es	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	Ex	90/98 (92%)	89 (99%)	1 (1%)	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	F0	90/98 (92%)	90 (100%)	0	0	100	100
1	F1	90/98 (92%)	90 (100%)	0	0	100	100
1	F2	90/98 (92%)	90 (100%)	0	0	100	100
1	F3	90/98 (92%)	90 (100%)	0	0	100	100
1	F4	90/98 (92%)	90 (100%)	0	0	100	100
1	F5	90/98 (92%)	90 (100%)	0	0	100	100
1	F6	90/98 (92%)	90 (100%)	0	0	100	100
1	F7	90/98 (92%)	90 (100%)	0	0	100	100
1	F8	90/98 (92%)	90 (100%)	0	0	100	100
1	F9	90/98 (92%)	90 (100%)	0	0	100	100
1	FA	90/98 (92%)	90 (100%)	0	0	100	100
1	FB	90/98 (92%)	90 (100%)	0	0	100	100

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Gl	90/98 (92%)	90 (100%)	0	0	100	100
1	Gm	90/98 (92%)	90 (100%)	0	0	100	100
1	Gn	90/98 (92%)	90 (100%)	0	0	100	100
1	Go	90/98 (92%)	90 (100%)	0	0	100	100
1	Gp	90/98 (92%)	90 (100%)	0	0	100	100
1	Gq	90/98 (92%)	90 (100%)	0	0	100	100
1	Gr	90/98 (92%)	90 (100%)	0	0	100	100
1	Gs	90/98 (92%)	90 (100%)	0	0	100	100
1	Gt	90/98 (92%)	90 (100%)	0	0	100	100
1	Gu	90/98 (92%)	90 (100%)	0	0	100	100
1	Gv	90/98 (92%)	90 (100%)	0	0	100	100
1	Gw	90/98 (92%)	90 (100%)	0	0	100	100
1	Gx	90/98 (92%)	90 (100%)	0	0	100	100
1	Gy	90/98 (92%)	90 (100%)	0	0	100	100
1	Gz	90/98 (92%)	90 (100%)	0	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%)	89 (99%)	1 (1%)	0	100	100
1	H3	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	H8	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	H9	90/98 (92%)	90 (100%)	0	0	100	100
1	HA	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	HB	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	HG	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	HL	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	HQ	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	HV	90/98 (92%)	89 (99%)	1 (1%)	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	Ha	90/98 (92%)	90 (100%)	0	0	100	100
1	Hb	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Hc	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	Hh	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	Hm	90/98 (92%)	89 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	89 (99%)	1 (1%)	0	100	100
1	Hr	90/98 (92%)	89 (99%)	1 (1%)	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%)	89 (99%)	1 (1%)	0	100	100
1	Hw	90/98 (92%)	89 (99%)	1 (1%)	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
2	X0	113/869 (13%)	109 (96%)	4 (4%)	0	100	100
2	X1	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	X2	113/869 (13%)	110 (97%)	3 (3%)	0	100	100
2	X3	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	X4	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	X5	113/869 (13%)	109 (96%)	4 (4%)	0	100	100
2	X6	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	X7	113/869 (13%)	110 (97%)	3 (3%)	0	100	100
2	X8	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	X9	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	XA	113/869 (13%)	110 (97%)	3 (3%)	0	100	100
2	XB	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	XC	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	XD	113/869 (13%)	109 (96%)	4 (4%)	0	100	100
2	XE	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	XF	113/869 (13%)	110 (97%)	3 (3%)	0	100	100
2	XG	113/869 (13%)	110 (97%)	3 (3%)	0	100	100
2	XH	113/869 (13%)	111 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	XI	113/869 (13%)	109 (96%)	4 (4%)	0	100	100
2	XJ	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	XK	113/869 (13%)	110 (97%)	3 (3%)	0	100	100
2	XL	113/869 (13%)	110 (97%)	3 (3%)	0	100	100
2	XM	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	XN	113/869 (13%)	109 (96%)	4 (4%)	0	100	100
2	XO	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	XP	113/869 (13%)	110 (97%)	3 (3%)	0	100	100
2	XQ	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	XR	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	XS	113/869 (13%)	109 (96%)	4 (4%)	0	100	100
2	XT	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	XU	113/869 (13%)	110 (97%)	3 (3%)	0	100	100
2	XV	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	XW	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	XX	113/869 (13%)	109 (96%)	4 (4%)	0	100	100
2	Xa	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	Xb	113/869 (13%)	110 (97%)	3 (3%)	0	100	100
2	Xc	113/869 (13%)	110 (97%)	3 (3%)	0	100	100
2	Xd	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	Xe	113/869 (13%)	109 (96%)	4 (4%)	0	100	100
2	Xf	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	Xg	113/869 (13%)	110 (97%)	3 (3%)	0	100	100
2	Xh	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	Xi	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	Xj	113/869 (13%)	109 (96%)	4 (4%)	0	100	100
2	Xk	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	Xl	113/869 (13%)	110 (97%)	3 (3%)	0	100	100
2	Xm	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	Xn	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	Xo	113/869 (13%)	109 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Xp	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	Xq	113/869 (13%)	110 (97%)	3 (3%)	0	100	100
2	Xr	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	Xs	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	Xt	113/869 (13%)	109 (96%)	4 (4%)	0	100	100
2	Xu	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	Xv	113/869 (13%)	110 (97%)	3 (3%)	0	100	100
2	Xw	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	Xx	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
2	Xy	113/869 (13%)	109 (96%)	4 (4%)	0	100	100
2	Xz	113/869 (13%)	111 (98%)	2 (2%)	0	100	100
3	P0	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
3	P1	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	P2	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
3	P3	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	P4	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	P5	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
3	P6	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	P7	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
3	P8	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	P9	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	PA	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
3	PB	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	PC	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	PD	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
3	PE	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	PF	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
3	PG	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	PH	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	PI	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
3	PJ	80/83 (96%)	79 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	PK	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
3	PL	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	PM	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	PN	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
3	PO	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	PP	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
3	PQ	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	PR	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	PS	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
3	PT	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	PU	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
3	PV	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	PW	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	PX	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
3	Pa	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	Pb	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
3	Pc	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	Pd	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	Pe	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
3	Pf	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	Pg	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
3	Ph	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	Pi	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	Pj	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
3	Pk	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	Pl	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
3	Pm	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	Pn	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	Po	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
3	Pp	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	Pq	80/83 (96%)	76 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Pr	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	Ps	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	Pt	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
3	Pu	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	Pv	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
3	Pw	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	Px	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
3	Py	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
3	Pz	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
All	All	54780/104160 (53%)	54428 (99%)	352 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	67
1	A1	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	A2	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	A3	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	A4	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	A5	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	A6	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	A7	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	A8	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	A9	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	AA	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	AB	63/67 (94%)	62 (98%)	1 (2%)	55	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AC	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	AD	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	AE	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	AF	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	AG	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	AH	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	AI	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	AJ	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	AK	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	AL	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	AM	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	AN	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	AO	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	AP	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	AQ	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	AR	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	AS	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	AT	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	AU	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	AV	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	AW	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	AX	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Aa	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ab	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Ac	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Ad	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ae	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Af	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ag	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Ah	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Ai	63/67 (94%)	61 (97%)	2 (3%)	34	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aj	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ak	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Al	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Am	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	An	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ao	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ap	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Aq	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Ar	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	As	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	At	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Au	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Av	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Aw	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Ax	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ay	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Az	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	B0	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	B1	63/67 (94%)	63 (100%)	0	100	100
1	B2	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	B3	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	B4	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	B5	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	B6	63/67 (94%)	63 (100%)	0	100	100
1	B7	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	B8	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	B9	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	BA	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	BB	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	BC	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	BD	63/67 (94%)	61 (97%)	2 (3%)	34	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BE	63/67 (94%)	63 (100%)	0	100	100
1	BF	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	BG	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	BH	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	BI	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	BJ	63/67 (94%)	63 (100%)	0	100	100
1	BK	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	BL	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	BM	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	BN	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	BO	63/67 (94%)	63 (100%)	0	100	100
1	BP	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	BQ	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	BR	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	BS	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	BT	63/67 (94%)	63 (100%)	0	100	100
1	BU	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	BV	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	BW	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	BX	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ba	63/67 (94%)	63 (100%)	0	100	100
1	Bb	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Bc	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Bd	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Be	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Bf	63/67 (94%)	63 (100%)	0	100	100
1	Bg	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Bh	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Bi	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Bj	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Bk	63/67 (94%)	63 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bl	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Bm	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Bn	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Bo	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Bp	63/67 (94%)	63 (100%)	0	100	100
1	Bq	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Br	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Bs	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Bt	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Bu	63/67 (94%)	63 (100%)	0	100	100
1	Bv	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Bw	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Bx	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	By	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Bz	63/67 (94%)	63 (100%)	0	100	100
1	C0	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	C1	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	C2	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	C3	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	C4	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	C5	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	C6	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	C7	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	C8	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	C9	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	CA	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	CB	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	CC	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	CD	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	CE	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	CF	63/67 (94%)	61 (97%)	2 (3%)	34	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CG	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	CH	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	CI	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	CJ	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	CK	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	CL	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	CM	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	CN	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	CO	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	CP	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	CQ	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	CR	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	CS	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	CT	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	CU	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	CV	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	CW	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	CX	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Ca	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Cb	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Cc	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Cd	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ce	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Cf	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Cg	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ch	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ci	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Cj	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Ck	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Cl	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Cm	63/67 (94%)	61 (97%)	2 (3%)	34	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Cn	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Co	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Cp	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Cq	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Cr	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Cs	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ct	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Cu	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Cv	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Cw	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Cx	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Cy	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Cz	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	D0	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	D1	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	D2	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	D3	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	D4	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	D5	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	D6	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	D7	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	D8	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	D9	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	DA	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	DB	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	DC	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	DD	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	DE	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	DF	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	DG	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	DH	63/67 (94%)	60 (95%)	3 (5%)	23	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DI	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	DJ	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	DK	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	DL	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	DM	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	DN	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	DO	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	DP	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	DQ	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	DR	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	DS	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	DT	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	DU	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	DV	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	DW	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	DX	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Da	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Db	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Dc	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Dd	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	De	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Df	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Dg	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Dh	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Di	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Dj	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Dk	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	DL	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Dm	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Dn	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Do	63/67 (94%)	60 (95%)	3 (5%)	23	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Dp	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Dq	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Dr	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Ds	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Dt	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Du	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Dv	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Dw	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Dx	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Dy	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Dz	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	E0	63/67 (94%)	63 (100%)	0	100	100
1	E1	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	E2	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	E3	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	E4	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	E5	63/67 (94%)	63 (100%)	0	100	100
1	E6	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	E7	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	E8	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	E9	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	EA	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	EB	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	EC	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	ED	63/67 (94%)	63 (100%)	0	100	100
1	EE	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	EF	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	EG	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	EH	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	EI	63/67 (94%)	63 (100%)	0	100	100
1	EJ	63/67 (94%)	61 (97%)	2 (3%)	34	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EK	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	EL	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	EM	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	EN	63/67 (94%)	63 (100%)	0	100	100
1	EO	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	EP	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	EQ	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	ER	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	ES	63/67 (94%)	63 (100%)	0	100	100
1	ET	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	EU	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	EV	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	EW	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	EX	63/67 (94%)	63 (100%)	0	100	100
1	Ea	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Eb	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Ec	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Ed	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ee	63/67 (94%)	63 (100%)	0	100	100
1	Ef	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Eg	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Eh	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Ei	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ej	63/67 (94%)	63 (100%)	0	100	100
1	Ek	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	El	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Em	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	En	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Eo	63/67 (94%)	63 (100%)	0	100	100
1	Ep	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Eq	63/67 (94%)	62 (98%)	1 (2%)	55	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Er	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Es	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Et	63/67 (94%)	63 (100%)	0	100	100
1	Eu	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ev	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Ew	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Ex	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ey	63/67 (94%)	63 (100%)	0	100	100
1	Ez	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	F0	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	F1	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	F2	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	F3	63/67 (94%)	63 (100%)	0	100	100
1	F4	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	F5	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	F6	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	F7	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	F8	63/67 (94%)	63 (100%)	0	100	100
1	F9	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	FA	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	FB	63/67 (94%)	63 (100%)	0	100	100
1	FC	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	FD	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	FE	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	FF	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	FG	63/67 (94%)	63 (100%)	0	100	100
1	FH	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	FI	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	FJ	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	FK	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	FL	63/67 (94%)	63 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FM	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	FN	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	FO	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	FP	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	FQ	63/67 (94%)	63 (100%)	0	100	100
1	FR	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	FS	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	FT	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	FU	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	FV	63/67 (94%)	63 (100%)	0	100	100
1	FW	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	FX	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Fa	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Fb	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Fc	63/67 (94%)	63 (100%)	0	100	100
1	Fd	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Fe	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Ff	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Fg	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Fh	63/67 (94%)	63 (100%)	0	100	100
1	Fi	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Fj	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Fk	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Fl	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Fm	63/67 (94%)	63 (100%)	0	100	100
1	Fn	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Fo	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Fp	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Fq	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Fr	63/67 (94%)	63 (100%)	0	100	100
1	Fs	63/67 (94%)	60 (95%)	3 (5%)	23	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ft	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Fu	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Fv	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Fw	63/67 (94%)	63 (100%)	0	100	100
1	Fx	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Fy	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Fz	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	G0	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	G1	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	G2	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	G3	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	G4	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	G5	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	G6	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	G7	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	G8	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	G9	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	GA	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	GB	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	GC	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	GD	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	GE	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	GF	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	GG	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	GH	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	GI	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	GJ	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	GK	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	GL	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	GM	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	GN	63/67 (94%)	60 (95%)	3 (5%)	23	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GO	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	GP	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	GQ	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	GR	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	GS	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	GT	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	GU	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	GV	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	GW	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	GX	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Ga	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Gb	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Gc	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Gd	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ge	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Gf	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Gg	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Gh	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Gi	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Gj	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Gk	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Gl	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Gm	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Gn	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Go	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Gp	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Gq	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Gr	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Gs	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Gt	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Gu	63/67 (94%)	60 (95%)	3 (5%)	23	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Gv	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Gw	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Gx	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Gy	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	Gz	63/67 (94%)	60 (95%)	3 (5%)	23	53
1	H0	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	H1	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	H2	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	H3	63/67 (94%)	63 (100%)	0	100	100
1	H4	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	H5	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	H6	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	H7	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	H8	63/67 (94%)	63 (100%)	0	100	100
1	H9	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	HA	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	HB	63/67 (94%)	63 (100%)	0	100	100
1	HC	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	HD	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	HE	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	HF	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	HG	63/67 (94%)	63 (100%)	0	100	100
1	HH	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	HI	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	HJ	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	HK	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	HL	63/67 (94%)	63 (100%)	0	100	100
1	HM	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	HN	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	HO	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	HP	63/67 (94%)	62 (98%)	1 (2%)	55	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	HQ	63/67 (94%)	63 (100%)	0	100	100
1	HR	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	HS	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	HT	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	HU	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	HV	63/67 (94%)	63 (100%)	0	100	100
1	HW	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	HX	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Ha	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Hb	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Hc	63/67 (94%)	63 (100%)	0	100	100
1	Hd	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	He	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Hf	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Hg	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Hh	63/67 (94%)	63 (100%)	0	100	100
1	Hi	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Hj	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Hk	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Hl	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Hm	63/67 (94%)	63 (100%)	0	100	100
1	Hn	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ho	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Hp	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Hq	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Hr	63/67 (94%)	63 (100%)	0	100	100
1	Hs	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Ht	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Hu	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Hv	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	Hw	63/67 (94%)	63 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Hx	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	Hy	63/67 (94%)	62 (98%)	1 (2%)	55	81
1	H <sub>z</sub>	63/67 (94%)	61 (97%)	2 (3%)	34	67
2	X0	91/702 (13%)	87 (96%)	4 (4%)	25	56
2	X1	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	X2	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	X3	91/702 (13%)	83 (91%)	8 (9%)	9	27
2	X4	91/702 (13%)	81 (89%)	10 (11%)	6	18
2	X5	91/702 (13%)	87 (96%)	4 (4%)	25	56
2	X6	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	X7	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	X8	91/702 (13%)	82 (90%)	9 (10%)	7	22
2	X9	91/702 (13%)	81 (89%)	10 (11%)	6	18
2	XA	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	XB	91/702 (13%)	81 (89%)	10 (11%)	6	18
2	XC	91/702 (13%)	81 (89%)	10 (11%)	6	18
2	XD	91/702 (13%)	87 (96%)	4 (4%)	25	56
2	XE	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	XF	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	XG	91/702 (13%)	81 (89%)	10 (11%)	6	18
2	XH	91/702 (13%)	81 (89%)	10 (11%)	6	18
2	XI	91/702 (13%)	87 (96%)	4 (4%)	25	56
2	XJ	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	XK	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	XL	91/702 (13%)	83 (91%)	8 (9%)	9	27
2	XM	91/702 (13%)	81 (89%)	10 (11%)	6	18
2	XN	91/702 (13%)	87 (96%)	4 (4%)	25	56
2	XO	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	XP	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	XQ	91/702 (13%)	83 (91%)	8 (9%)	9	27
2	XR	91/702 (13%)	81 (89%)	10 (11%)	6	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	XS	91/702 (13%)	87 (96%)	4 (4%)	25	56
2	XT	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	XU	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	XV	91/702 (13%)	83 (91%)	8 (9%)	9	27
2	XW	91/702 (13%)	81 (89%)	10 (11%)	6	18
2	XX	91/702 (13%)	87 (96%)	4 (4%)	25	56
2	Xa	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	Xb	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	Xc	91/702 (13%)	82 (90%)	9 (10%)	7	22
2	Xd	91/702 (13%)	81 (89%)	10 (11%)	6	18
2	Xe	91/702 (13%)	87 (96%)	4 (4%)	25	56
2	Xf	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	Xg	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	Xh	91/702 (13%)	83 (91%)	8 (9%)	9	27
2	Xi	91/702 (13%)	81 (89%)	10 (11%)	6	18
2	Xj	91/702 (13%)	87 (96%)	4 (4%)	25	56
2	Xk	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	Xl	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	Xm	91/702 (13%)	83 (91%)	8 (9%)	9	27
2	Xn	91/702 (13%)	81 (89%)	10 (11%)	6	18
2	Xo	91/702 (13%)	87 (96%)	4 (4%)	25	56
2	Xp	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	Xq	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	Xr	91/702 (13%)	83 (91%)	8 (9%)	9	27
2	Xs	91/702 (13%)	81 (89%)	10 (11%)	6	18
2	Xt	91/702 (13%)	87 (96%)	4 (4%)	25	56
2	Xu	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	Xv	91/702 (13%)	86 (94%)	5 (6%)	19	47
2	Xw	91/702 (13%)	83 (91%)	8 (9%)	9	27
2	Xx	91/702 (13%)	81 (89%)	10 (11%)	6	18
2	Xy	91/702 (13%)	87 (96%)	4 (4%)	25	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Xz	91/702 (13%)	86 (94%)	5 (6%)	19	47
3	P0	66/67 (98%)	65 (98%)	1 (2%)	57	81
3	P1	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	P2	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	P3	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	P4	66/67 (98%)	63 (96%)	3 (4%)	24	55
3	P5	66/67 (98%)	65 (98%)	1 (2%)	57	81
3	P6	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	P7	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	P8	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	P9	66/67 (98%)	63 (96%)	3 (4%)	24	55
3	PA	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	PB	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	PC	66/67 (98%)	63 (96%)	3 (4%)	24	55
3	PD	66/67 (98%)	65 (98%)	1 (2%)	57	81
3	PE	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	PF	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	PG	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	PH	66/67 (98%)	63 (96%)	3 (4%)	24	55
3	PI	66/67 (98%)	65 (98%)	1 (2%)	57	81
3	PJ	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	PK	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	PL	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	PM	66/67 (98%)	63 (96%)	3 (4%)	24	55
3	PN	66/67 (98%)	65 (98%)	1 (2%)	57	81
3	PO	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	PP	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	PQ	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	PR	66/67 (98%)	63 (96%)	3 (4%)	24	55
3	PS	66/67 (98%)	65 (98%)	1 (2%)	57	81
3	PT	66/67 (98%)	64 (97%)	2 (3%)	36	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	PU	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	PV	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	PW	66/67 (98%)	63 (96%)	3 (4%)	24	55
3	PX	66/67 (98%)	65 (98%)	1 (2%)	57	81
3	Pa	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	Pb	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	Pc	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	Pd	66/67 (98%)	63 (96%)	3 (4%)	24	55
3	Pe	66/67 (98%)	65 (98%)	1 (2%)	57	81
3	Pf	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	Pg	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	Ph	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	Pi	66/67 (98%)	63 (96%)	3 (4%)	24	55
3	Pj	66/67 (98%)	65 (98%)	1 (2%)	57	81
3	Pk	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	Pl	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	Pm	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	Pn	66/67 (98%)	63 (96%)	3 (4%)	24	55
3	Po	66/67 (98%)	65 (98%)	1 (2%)	57	81
3	Pp	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	Pq	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	Pr	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	Ps	66/67 (98%)	63 (96%)	3 (4%)	24	55
3	Pt	66/67 (98%)	65 (98%)	1 (2%)	57	81
3	Pu	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	Pv	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	Pw	66/67 (98%)	64 (97%)	2 (3%)	36	69
3	Px	66/67 (98%)	63 (96%)	3 (4%)	24	55
3	Py	66/67 (98%)	65 (98%)	1 (2%)	57	81
3	Pz	66/67 (98%)	64 (97%)	2 (3%)	36	69
All	All	39660/78300 (51%)	38286 (96%)	1374 (4%)	32	64

5 of 1374 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CG	12	ILE
1	DQ	53	GLU
2	XH	729	GLU
1	BG	86	SER
2	XL	786	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 439 such sidechains are listed below:

Mol	Chain	Res	Type
3	Pw	36	GLN
1	BI	85	HIS
2	XV	812	GLN
1	DX	79	HIS
1	Gx	90	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

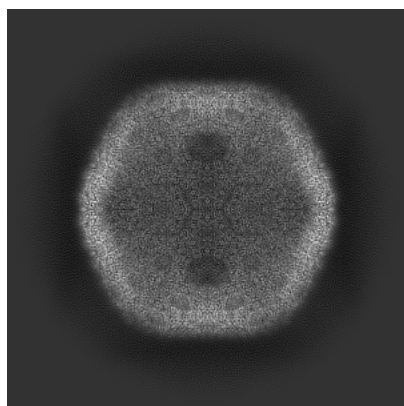
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62530. These allow visual inspection of the internal detail of the map and identification of artifacts.

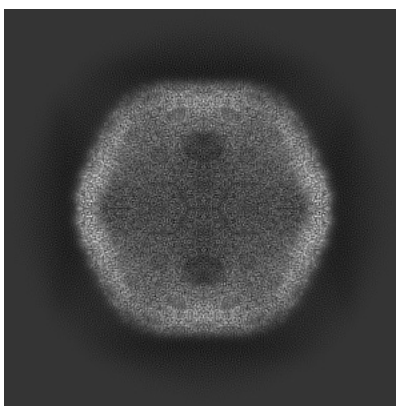
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

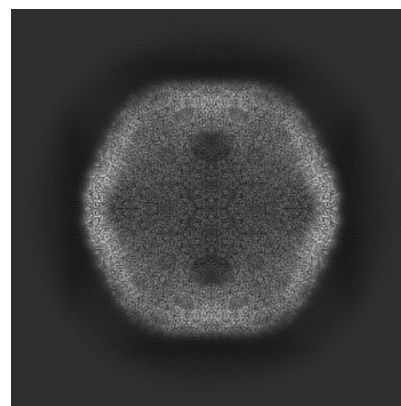
#### 6.1.1 Primary map



X

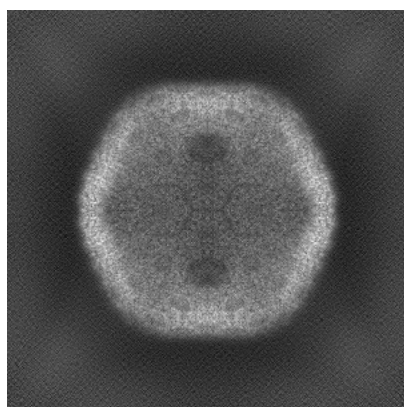


Y

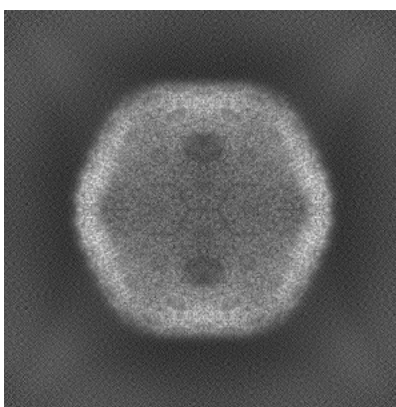


Z

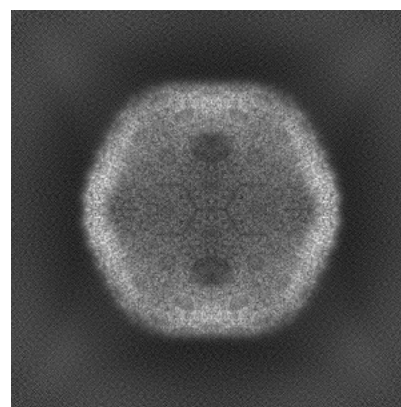
#### 6.1.2 Raw map



X



Y

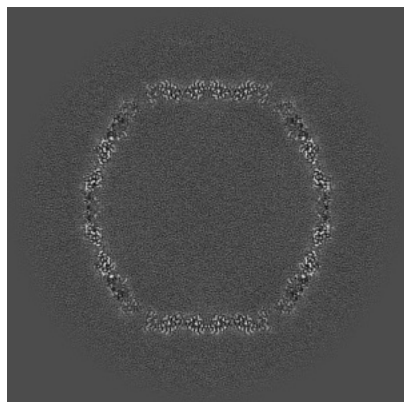


Z

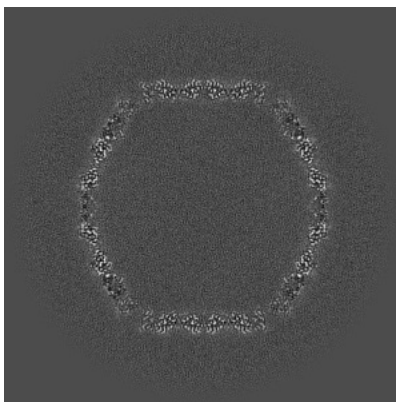
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

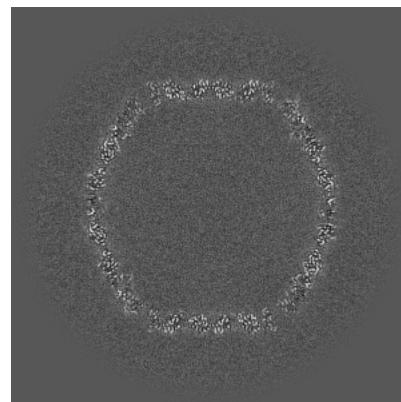
### 6.2.1 Primary map



X Index: 250

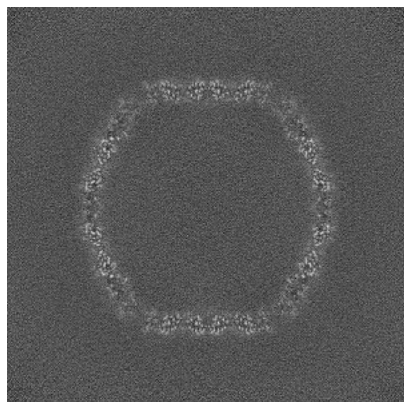


Y Index: 250

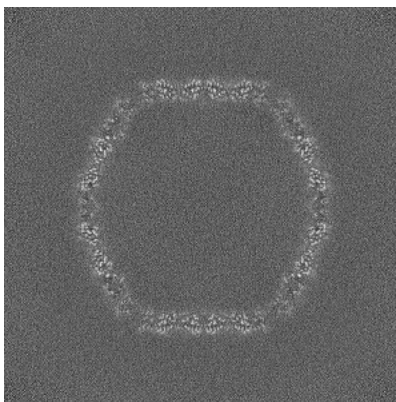


Z Index: 250

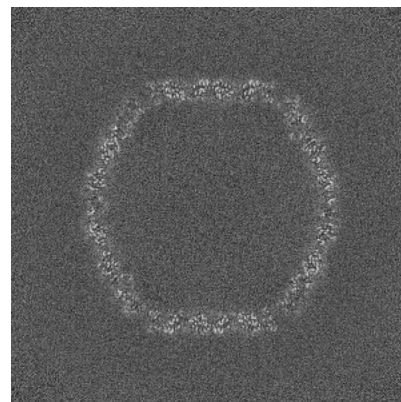
### 6.2.2 Raw map



X Index: 250



Y Index: 250

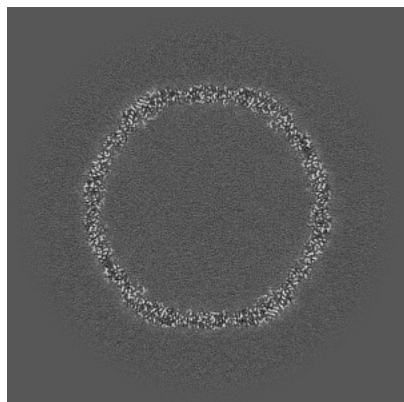


Z Index: 250

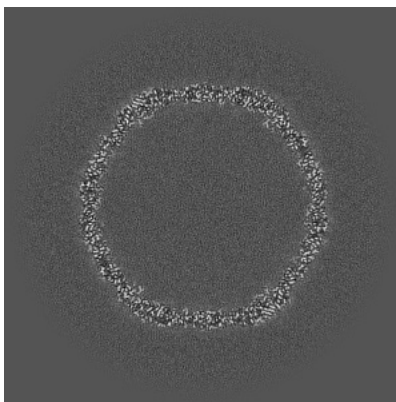
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

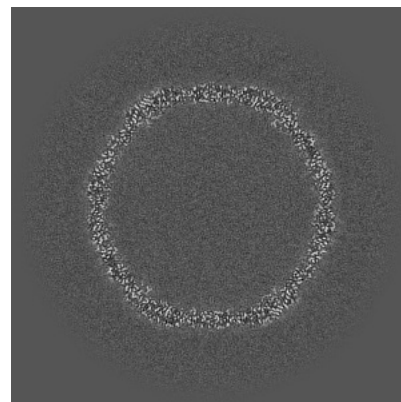
### 6.3.1 Primary map



X Index: 287

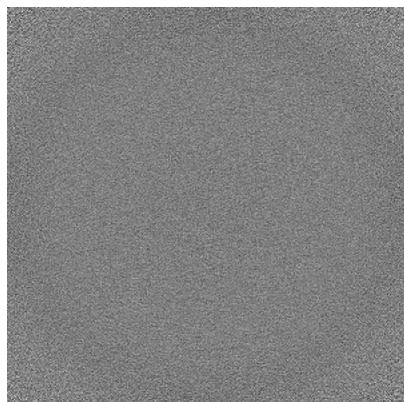


Y Index: 287

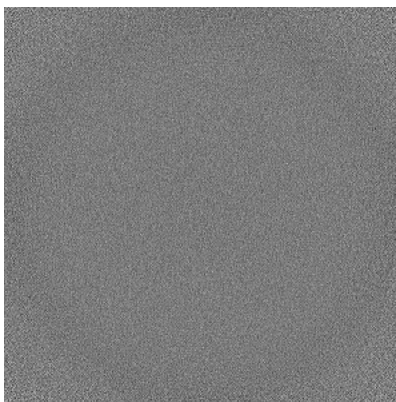


Z Index: 286

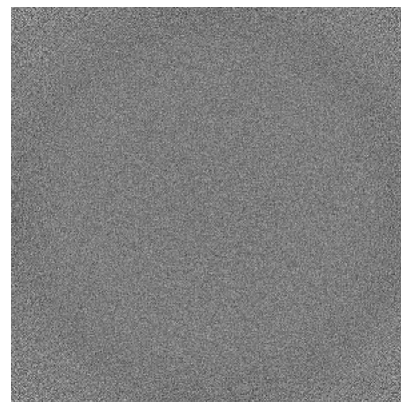
### 6.3.2 Raw map



X Index: 0



Y Index: 0

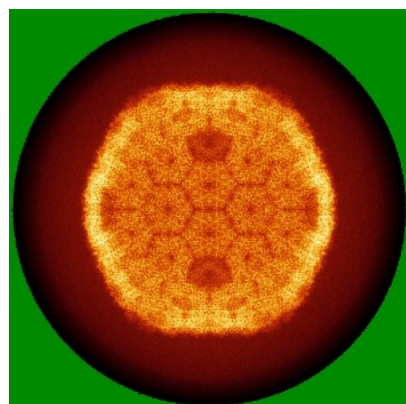


Z Index: 499

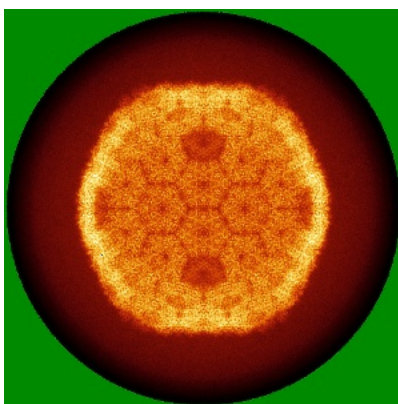
The images above show the largest variance slices of the map in three orthogonal directions.

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

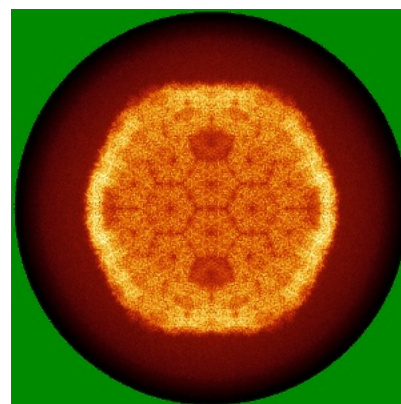
### 6.4.1 Primary map



X

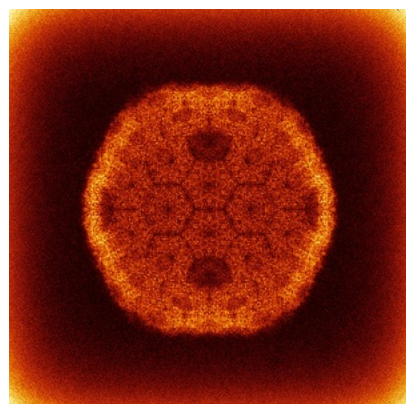


Y

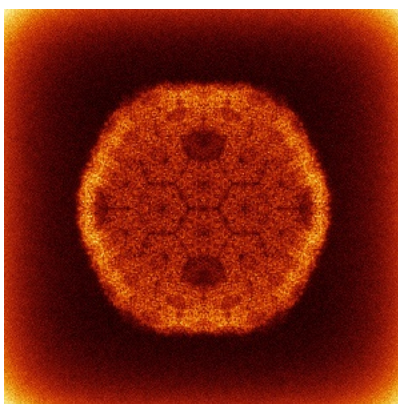


Z

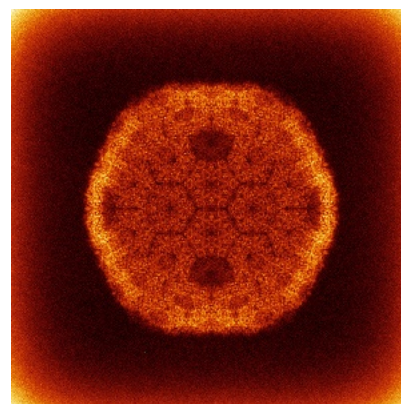
### 6.4.2 Raw map



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



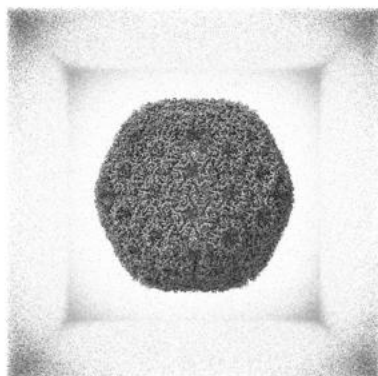
Y



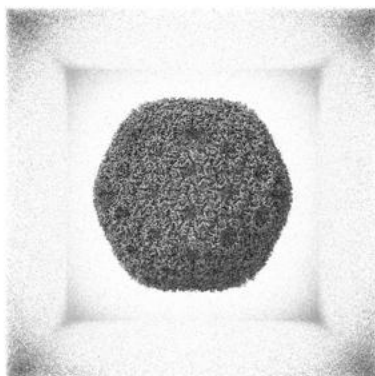
Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

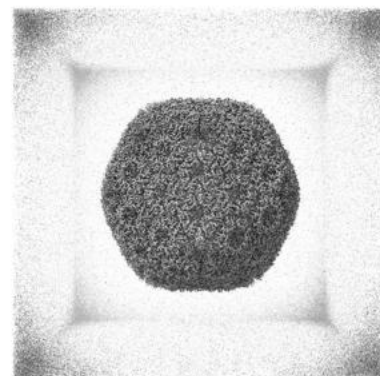
### 6.5.2 Raw map



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.

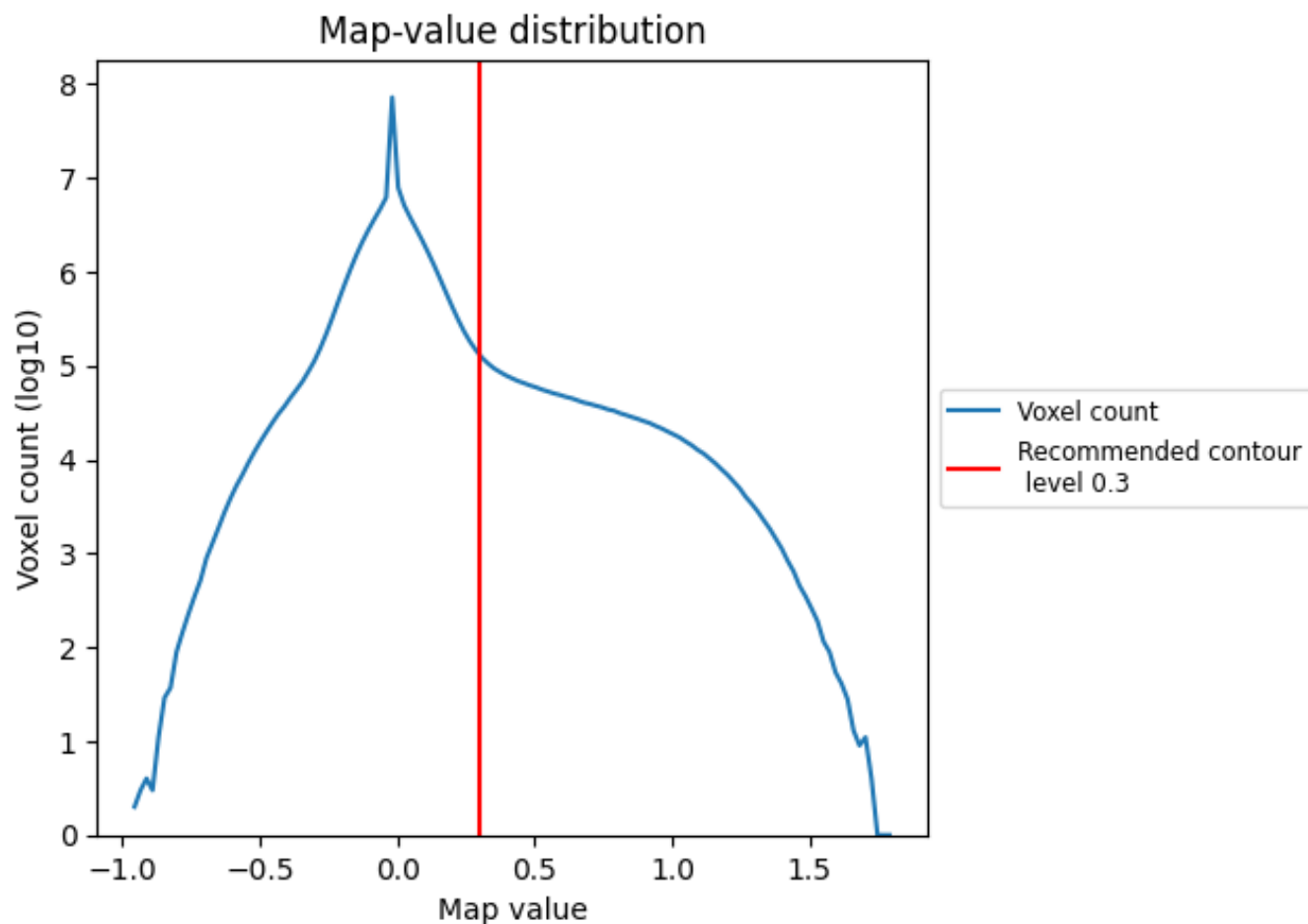
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

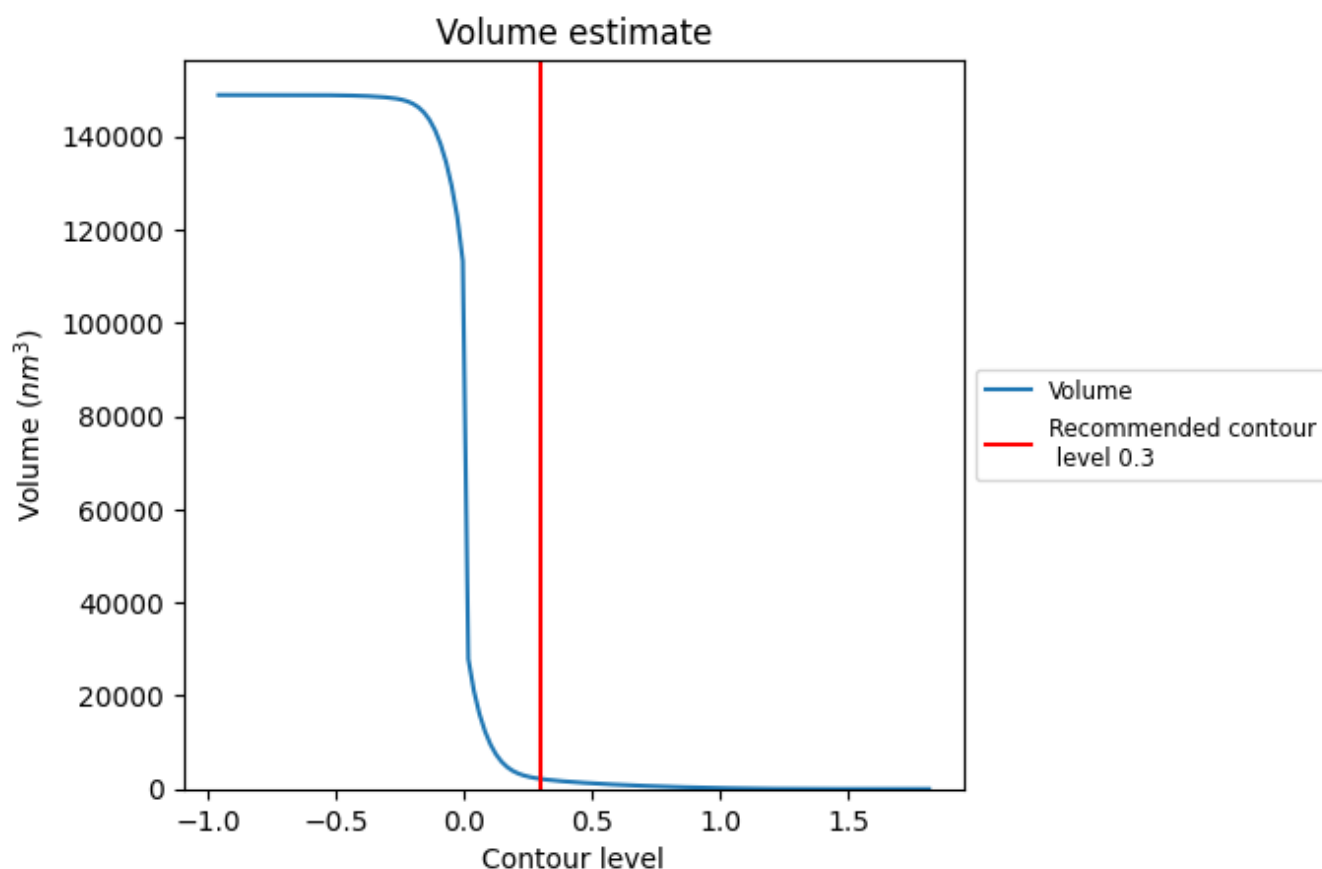
This section contains the results of statistical analysis of the map.

### 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.

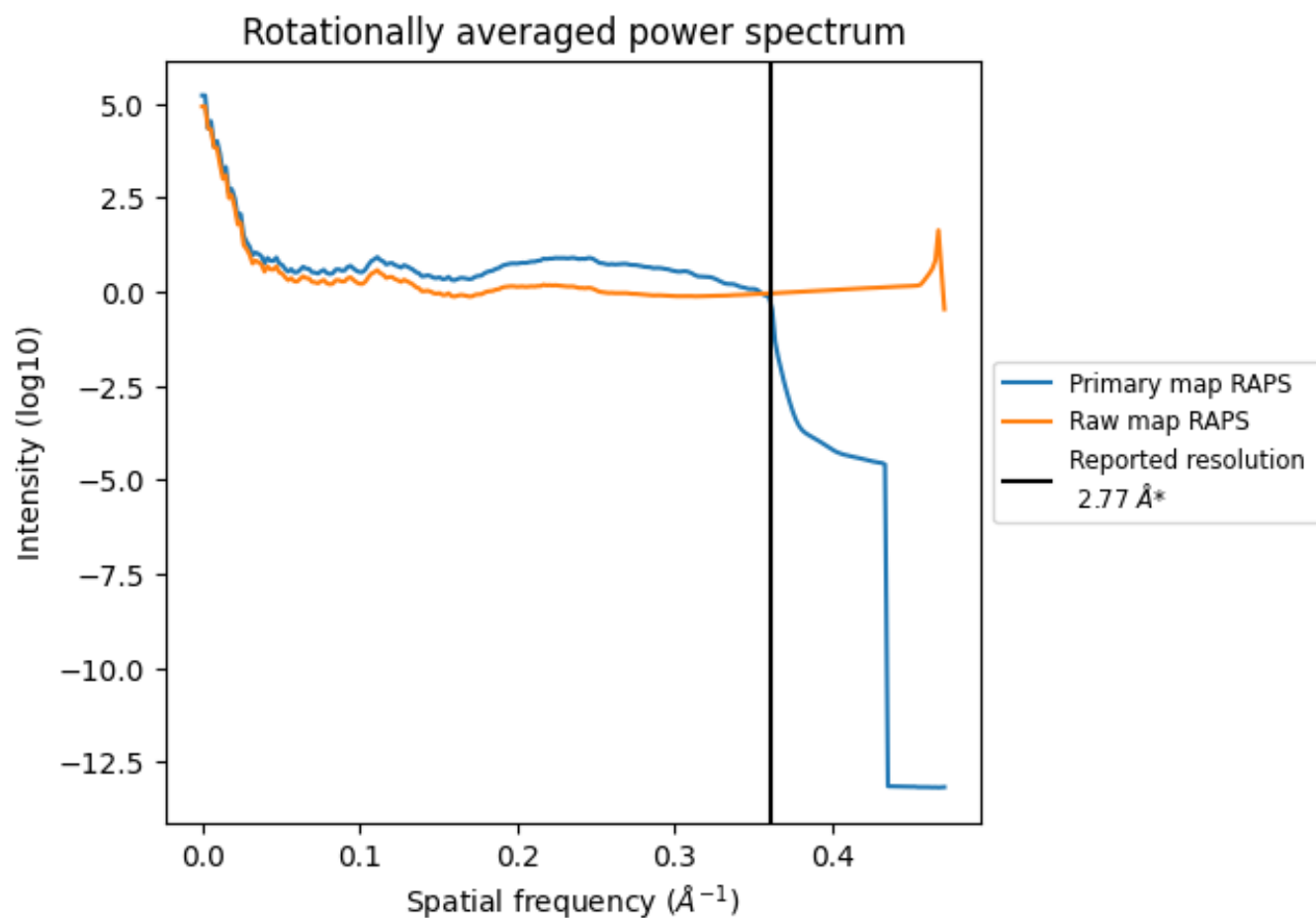
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2152 nm<sup>3</sup>; this corresponds to an approximate mass of 1944 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 ⓘ

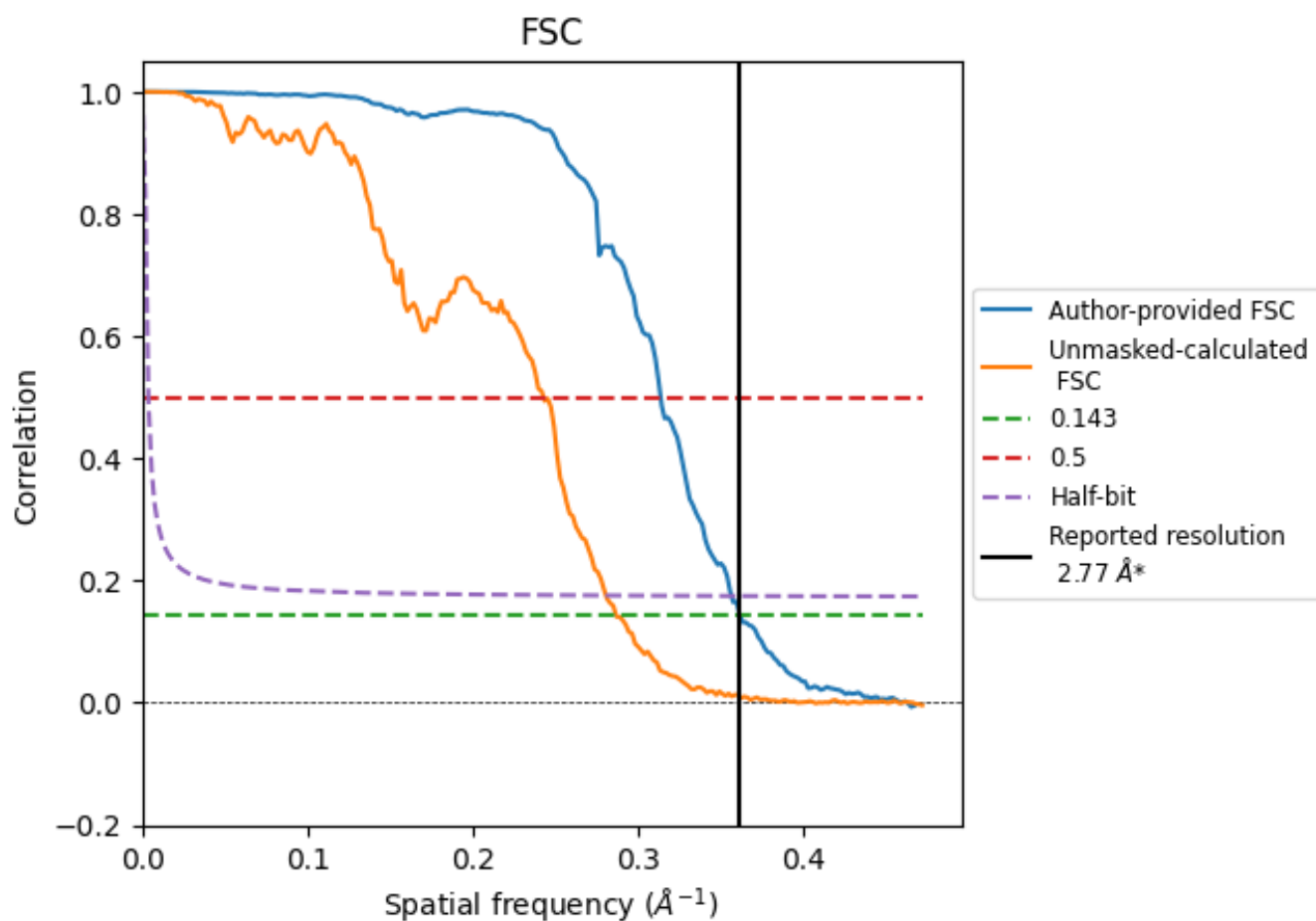


\*Reported resolution corresponds to spatial frequency of 0.361  $\text{\AA}^{-1}$

## 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 0.361 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

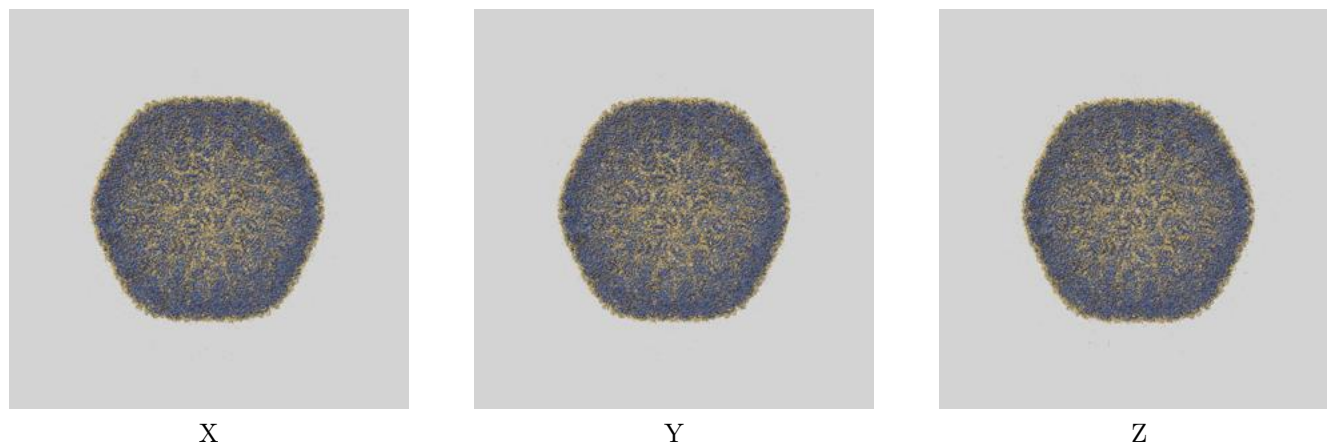
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	2.77	3.19	2.81
Unmasked-calculated*	3.49	4.12	3.57

\*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 3.49 differs from the reported value 2.77 by more than 10 %

## 9 Map-model fit [i](#)

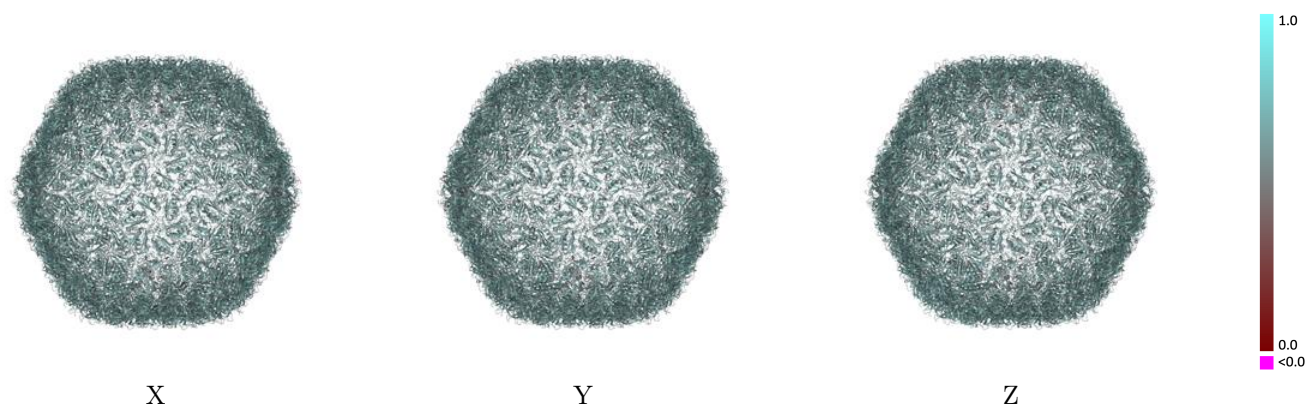
This section contains information regarding the fit between EMDB map EMD-62530 and PDB model 9LY8. Per-residue inclusion information can be found in [section 3](#) on [page 56](#).

### 9.1 Map-model overlay [i](#)



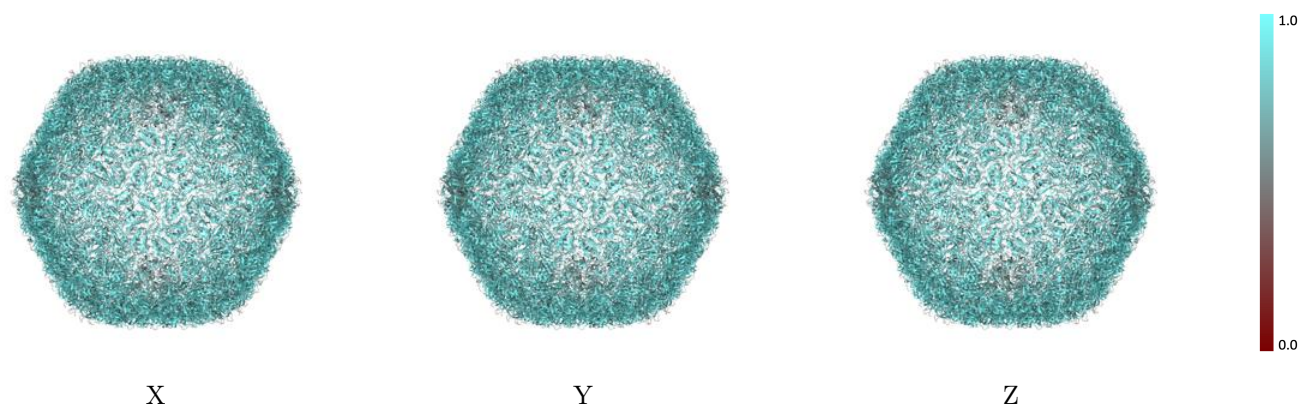
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



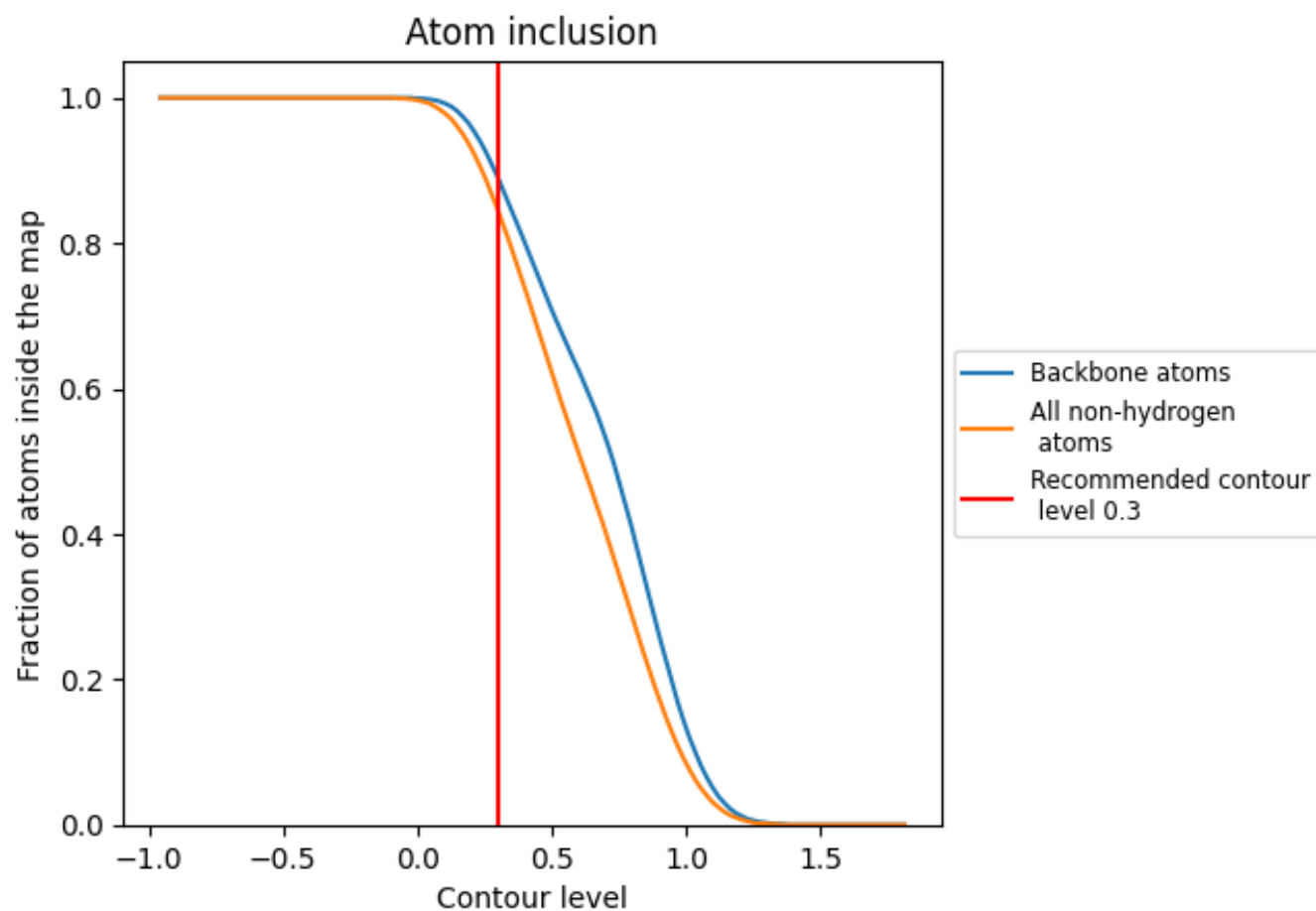
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8450	 0.5950
A0	 0.8830	 0.6030
A1	 0.9030	 0.6320
A2	 0.9000	 0.6330
A3	 0.8910	 0.6280
A4	 0.8860	 0.6270
A5	 0.9000	 0.6260
A6	 0.8810	 0.6050
A7	 0.8640	 0.5980
A8	 0.8810	 0.6100
A9	 0.8910	 0.6040
AA	 0.8810	 0.6130
AB	 0.8880	 0.6060
AC	 0.8920	 0.6090
AD	 0.8830	 0.6060
AE	 0.8810	 0.6020
AF	 0.8890	 0.6110
AG	 0.8810	 0.6080
AH	 0.8880	 0.6060
AI	 0.8890	 0.6130
AJ	 0.8890	 0.6030
AK	 0.8860	 0.6140
AL	 0.8740	 0.6070
AM	 0.8800	 0.6050
AN	 0.8880	 0.6090
AO	 0.8860	 0.6050
AP	 0.8800	 0.6010
AQ	 0.8970	 0.6090
AR	 0.8780	 0.6040
AS	 0.8850	 0.6070
AT	 0.8740	 0.5970
AU	 0.8850	 0.6010
AV	 0.8800	 0.5980
AW	 0.8810	 0.6030
AX	 0.8850	 0.6020























































































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Chain	Atom inclusion	Q-score
Aa	 0.8720	 0.6010
Ab	 0.8850	 0.6050
Ac	 0.8800	 0.6100
Ad	 0.8860	 0.5990
Ae	 0.8770	 0.6070
Af	 0.8850	 0.6060
Ag	 0.8860	 0.6010
Ah	 0.8810	 0.6090
Ai	 0.8880	 0.6060
Aj	 0.8830	 0.6040
Ak	 0.8750	 0.5970
Al	 0.8800	 0.6010
Am	 0.8750	 0.6030
An	 0.8850	 0.6040
Ao	 0.8880	 0.6100
Ap	 0.8750	 0.6000
Aq	 0.8750	 0.6030
Ar	 0.8810	 0.6030
As	 0.8780	 0.6070
At	 0.8720	 0.5970
Au	 0.8860	 0.6030
Av	 0.8830	 0.6090
Aw	 0.8910	 0.6090
Ax	 0.8890	 0.6020
Ay	 0.8920	 0.6020
Az	 0.8910	 0.6150
B0	 0.8750	 0.5950
B1	 0.9050	 0.6260
B2	 0.8880	 0.6260
B3	 0.8860	 0.6250
B4	 0.8950	 0.6280
B5	 0.8940	 0.6260
B6	 0.8640	 0.6000
B7	 0.8800	 0.6020
B8	 0.8770	 0.6020
B9	 0.8610	 0.5950
BA	 0.8890	 0.6010
BB	 0.8800	 0.6030
BC	 0.8830	 0.6030
BD	 0.8810	 0.6090
BE	 0.8800	 0.5940
BF	 0.8580	 0.5980





















































































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Chain	Atom inclusion	Q-score
BG	 0.8550	 0.5930
BH	 0.8720	 0.5970
BI	 0.8770	 0.5970
BJ	 0.8750	 0.5910
BK	 0.8780	 0.5920
BL	 0.8720	 0.5990
BM	 0.8720	 0.6020
BN	 0.8880	 0.5940
BO	 0.8800	 0.6050
BP	 0.8640	 0.5980
BQ	 0.8830	 0.5950
BR	 0.8640	 0.5970
BS	 0.8720	 0.5950
BT	 0.8630	 0.5940
BU	 0.8690	 0.5990
BV	 0.8710	 0.6000
BW	 0.8690	 0.5970
BX	 0.8810	 0.5930
Ba	 0.8600	 0.5940
Bb	 0.8750	 0.5950
Bc	 0.8890	 0.5880
Bd	 0.8690	 0.5990
Be	 0.8780	 0.5980
Bf	 0.8720	 0.5910
Bg	 0.8600	 0.5920
Bh	 0.8800	 0.6020
Bi	 0.8850	 0.5970
Bj	 0.8740	 0.5970
Bk	 0.8850	 0.5990
Bl	 0.8880	 0.6080
Bm	 0.8860	 0.6030
Bn	 0.8710	 0.6030
Bo	 0.8670	 0.5990
Bp	 0.8800	 0.5980
Bq	 0.8670	 0.5920
Br	 0.8800	 0.5990
Bs	 0.8690	 0.5990
Bt	 0.8720	 0.5990
Bu	 0.8780	 0.6020
Bv	 0.8780	 0.6020
Bw	 0.8890	 0.6020
Bx	 0.8810	 0.5980





















































































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Chain	Atom inclusion	Q-score
By	 0.8600	 0.5990
Bz	 0.8880	 0.6000
C0	 0.8880	 0.6000
C1	 0.9020	 0.6270
C2	 0.9080	 0.6300
C3	 0.9020	 0.6220
C4	 0.9020	 0.6270
C5	 0.9170	 0.6310
C6	 0.8720	 0.6040
C7	 0.8770	 0.6040
C8	 0.8970	 0.6070
C9	 0.8890	 0.6050
CA	 0.8890	 0.6110
CB	 0.9000	 0.6110
CC	 0.8950	 0.6130
CD	 0.9060	 0.6110
CE	 0.8720	 0.6080
CF	 0.8860	 0.6090
CG	 0.8860	 0.6070
CH	 0.8660	 0.6060
CI	 0.8770	 0.5960
CJ	 0.8800	 0.6070
CK	 0.8810	 0.6030
CL	 0.8800	 0.6060
CM	 0.8690	 0.6040
CN	 0.8970	 0.6080
CO	 0.8810	 0.6020
CP	 0.8670	 0.5970
CQ	 0.9060	 0.6080
CR	 0.8830	 0.6030
CS	 0.8880	 0.6040
CT	 0.8750	 0.6040
CU	 0.8940	 0.6080
CV	 0.8850	 0.5990
CW	 0.8830	 0.6030
CX	 0.8880	 0.6070
Ca	 0.8660	 0.6040
Cb	 0.8810	 0.6080
Cc	 0.8750	 0.6000
Cd	 0.8880	 0.6050
Ce	 0.8890	 0.6070
Cf	 0.8770	 0.6100







































































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Chain	Atom inclusion	Q-score
Cg	 0.8950	 0.6120
Ch	 0.8880	 0.6040
Ci	 0.8920	 0.6090
Cj	 0.8890	 0.5990
Ck	 0.8710	 0.6020
Cl	 0.8920	 0.6090
Cm	 0.8890	 0.6050
Cn	 0.8910	 0.6110
Co	 0.8740	 0.6020
Cp	 0.8750	 0.6030
Cq	 0.8970	 0.6030
Cr	 0.8720	 0.5970
Cs	 0.8860	 0.6090
Ct	 0.8860	 0.6000
Cu	 0.8860	 0.6100
Cv	 0.8750	 0.6000
Cw	 0.9020	 0.6060
Cx	 0.8910	 0.6100
Cy	 0.8860	 0.5980
Cz	 0.8880	 0.6160
D0	 0.8810	 0.6030
D1	 0.8940	 0.6300
D2	 0.8990	 0.6260
D3	 0.8950	 0.6280
D4	 0.8950	 0.6240
D5	 0.8950	 0.6280
D6	 0.8850	 0.5990
D7	 0.8800	 0.6050
D8	 0.8740	 0.5990
D9	 0.8770	 0.6000
DA	 0.8950	 0.6120
DB	 0.8940	 0.6140
DC	 0.8630	 0.5980
DD	 0.8740	 0.6050
DE	 0.8880	 0.6120
DF	 0.8950	 0.6070
DG	 0.8880	 0.6100
DH	 0.8880	 0.6010
DI	 0.8780	 0.6000
DJ	 0.8750	 0.6020
DK	 0.8850	 0.6120
DL	 0.8800	 0.6100





















































































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Chain	Atom inclusion	Q-score
DM	 0.8640	 0.6050
DN	 0.8780	 0.6030
DO	 0.8750	 0.6080
DP	 0.8610	 0.6010
DQ	 0.8860	 0.6030
DR	 0.8800	 0.6050
DS	 0.8850	 0.6030
DT	 0.8750	 0.6100
DU	 0.8800	 0.6010
DV	 0.8720	 0.5960
DW	 0.8780	 0.6030
DX	 0.8890	 0.6090
Da	 0.8770	 0.6070
Db	 0.8830	 0.6100
Dc	 0.8720	 0.5980
Dd	 0.8810	 0.5960
De	 0.8670	 0.6050
Df	 0.8750	 0.6030
Dg	 0.8780	 0.6060
Dh	 0.8890	 0.6020
Di	 0.8800	 0.6050
Dj	 0.8740	 0.6010
Dk	 0.8720	 0.6100
Dl	 0.9000	 0.6070
Dm	 0.8710	 0.6060
Dn	 0.8850	 0.6000
Do	 0.8770	 0.6040
Dp	 0.8830	 0.6020
Dq	 0.8780	 0.6050
Dr	 0.8950	 0.6060
Ds	 0.8890	 0.6020
Dt	 0.8710	 0.5950
Du	 0.8860	 0.6060
Dv	 0.8750	 0.6040
Dw	 0.8880	 0.6060
Dx	 0.8850	 0.5980
Dy	 0.8810	 0.6050
Dz	 0.8850	 0.6120
E0	 0.8890	 0.6010
E1	 0.9080	 0.6310
E2	 0.9020	 0.6260
E3	 0.8990	 0.6260





















































































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Chain	Atom inclusion	Q-score
E4	 0.9020	 0.6270
E5	 0.8970	 0.6250
E6	 0.8860	 0.6030
E7	 0.8800	 0.5960
E8	 0.8920	 0.5970
E9	 0.8810	 0.5990
EA	 0.8910	 0.6130
EB	 0.8810	 0.6010
EC	 0.8890	 0.6080
ED	 0.8880	 0.6120
EE	 0.8890	 0.6030
EF	 0.8880	 0.6000
EG	 0.8750	 0.5980
EH	 0.9050	 0.6050
EI	 0.8860	 0.6080
EJ	 0.8970	 0.6010
EK	 0.8950	 0.6030
EL	 0.8800	 0.5990
EM	 0.8800	 0.6030
EN	 0.8940	 0.6030
EO	 0.8800	 0.5950
EP	 0.8920	 0.5950
EQ	 0.8850	 0.6010
ER	 0.8810	 0.5960
ES	 0.9020	 0.6070
ET	 0.8910	 0.6070
EU	 0.8690	 0.5990
EV	 0.8910	 0.6040
EW	 0.8910	 0.6020
EX	 0.8810	 0.6050
Ea	 0.8740	 0.6000
Eb	 0.8720	 0.6040
Ec	 0.8810	 0.5950
Ed	 0.8780	 0.5920
Ee	 0.8780	 0.6010
Ef	 0.8750	 0.5970
Eg	 0.8570	 0.5960
Eh	 0.8750	 0.6050
Ei	 0.8770	 0.5940
Ej	 0.8800	 0.6050
Ek	 0.8800	 0.5940
El	 0.8800	 0.6080





















































































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Chain	Atom inclusion	Q-score
Em	 0.8990	 0.6070
En	 0.8850	 0.6000
Eo	 0.8780	 0.6080
Ep	 0.8780	 0.6050
Eq	 0.8810	 0.5930
Er	 0.8710	 0.5940
Es	 0.8910	 0.6010
Et	 0.8830	 0.6020
Eu	 0.8690	 0.6000
Ev	 0.8860	 0.5990
Ew	 0.8800	 0.6060
Ex	 0.8830	 0.6060
Ey	 0.8770	 0.6050
Ez	 0.8860	 0.6100
F0	 0.8880	 0.6040
F1	 0.9130	 0.6320
F2	 0.9030	 0.6290
F3	 0.9030	 0.6280
F4	 0.9020	 0.6270
F5	 0.9020	 0.6280
F6	 0.8810	 0.6030
F7	 0.8850	 0.6090
F8	 0.9030	 0.6110
F9	 0.8800	 0.6090
FA	 0.8910	 0.6140
FB	 0.8940	 0.6090
FC	 0.8830	 0.6100
FD	 0.8890	 0.6100
FE	 0.8970	 0.6130
FF	 0.8850	 0.5970
FG	 0.8850	 0.6110
FH	 0.8920	 0.6100
FI	 0.8810	 0.6090
FJ	 0.8910	 0.6090
FK	 0.8950	 0.6070
FL	 0.8850	 0.6050
FM	 0.8810	 0.6150
FN	 0.8950	 0.6130
FO	 0.8950	 0.6050
FP	 0.8750	 0.6050
FQ	 0.8880	 0.6060
FR	 0.8780	 0.6090





















































































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Chain	Atom inclusion	Q-score
FS	 0.8890	 0.6040
FT	 0.8920	 0.6170
FU	 0.8950	 0.6100
FV	 0.8850	 0.6000
FW	 0.8920	 0.6070
FX	 0.8860	 0.6120
Fa	 0.8740	 0.6060
Fb	 0.8740	 0.6010
Fc	 0.8780	 0.6040
Fd	 0.8880	 0.6050
Fe	 0.8800	 0.6060
Ff	 0.8920	 0.6110
Fg	 0.9020	 0.6110
Fh	 0.8810	 0.6030
Fi	 0.8770	 0.6030
Fj	 0.8910	 0.6110
Fk	 0.8910	 0.6090
Fl	 0.8860	 0.6120
Fm	 0.8910	 0.6070
Fn	 0.8780	 0.6110
Fo	 0.8780	 0.6040
Fp	 0.8810	 0.6020
Fq	 0.9000	 0.6130
Fr	 0.8940	 0.6040
Fs	 0.8830	 0.6050
Ft	 0.8800	 0.6120
Fu	 0.8810	 0.6080
Fv	 0.8950	 0.6110
Fw	 0.8970	 0.6060
Fx	 0.8850	 0.6010
Fy	 0.8800	 0.6140
Fz	 0.8830	 0.6070
G0	 0.8920	 0.6060
G1	 0.9060	 0.6300
G2	 0.8970	 0.6220
G3	 0.8830	 0.6260
G4	 0.9030	 0.6310
G5	 0.9030	 0.6270
G6	 0.8890	 0.6050
G7	 0.8800	 0.5990
G8	 0.8800	 0.6070
G9	 0.8950	 0.6020





















































































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Chain	Atom inclusion	Q-score
GA	 0.9020	 0.6100
GB	 0.8830	 0.6030
GC	 0.8740	 0.6080
GD	 0.8850	 0.6050
GE	 0.8830	 0.5960
GF	 0.8740	 0.6020
GG	 0.8890	 0.6000
GH	 0.8990	 0.6080
GI	 0.8830	 0.6040
GJ	 0.8720	 0.6060
GK	 0.8810	 0.6020
GL	 0.8690	 0.5990
GM	 0.8860	 0.6050
GN	 0.8920	 0.6050
GO	 0.8910	 0.5990
GP	 0.8770	 0.6000
GQ	 0.8860	 0.6020
GR	 0.8990	 0.6010
GS	 0.8780	 0.6080
GT	 0.8690	 0.6010
GU	 0.8890	 0.5980
GV	 0.8750	 0.6000
GW	 0.8780	 0.6010
GX	 0.8830	 0.6040
Ga	 0.8670	 0.5960
Gb	 0.8770	 0.6040
Gc	 0.8800	 0.6010
Gd	 0.9000	 0.6010
Ge	 0.8830	 0.5980
Gf	 0.8740	 0.5960
Gg	 0.8860	 0.5990
Gh	 0.8810	 0.6030
Gi	 0.8780	 0.6020
Gj	 0.8850	 0.6070
Gk	 0.8890	 0.6070
Gl	 0.8800	 0.6030
Gm	 0.9020	 0.6000
Gn	 0.8880	 0.6070
Go	 0.8920	 0.6010
Gp	 0.8950	 0.5960
Gq	 0.8780	 0.5950
Gr	 0.8610	 0.6000





















































































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Chain	Atom inclusion	Q-score
Gs	 0.8940	 0.6100
Gt	 0.8770	 0.5960
Gu	 0.8860	 0.6050
Gv	 0.8800	 0.6040
Gw	 0.8740	 0.5930
Gx	 0.8810	 0.6020
Gy	 0.8800	 0.6040
Gz	 0.9030	 0.6110
H0	 0.8550	 0.5970
H1	 0.8890	 0.6280
H2	 0.8880	 0.6250
H3	 0.8830	 0.6220
H4	 0.8910	 0.6240
H5	 0.8910	 0.6250
H6	 0.8800	 0.6060
H7	 0.8690	 0.5980
H8	 0.8770	 0.6070
H9	 0.8770	 0.6060
HA	 0.8750	 0.6070
HB	 0.8770	 0.6110
HC	 0.8750	 0.6060
HD	 0.8740	 0.6060
HE	 0.8740	 0.6050
HF	 0.8710	 0.6050
HG	 0.8750	 0.6100
HH	 0.8690	 0.6040
HI	 0.8570	 0.5970
HJ	 0.8660	 0.6030
HK	 0.8630	 0.6070
HL	 0.8640	 0.6080
HM	 0.8720	 0.6090
HN	 0.8670	 0.6010
HO	 0.8710	 0.6060
HP	 0.8720	 0.5970
HQ	 0.8800	 0.6050
HR	 0.8640	 0.6000
HS	 0.8770	 0.5970
HT	 0.8780	 0.6100
HU	 0.8580	 0.5950
HV	 0.8570	 0.6010
HW	 0.8580	 0.6100
HX	 0.8690	 0.5910





















































































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Chain	Atom inclusion	Q-score
Ha	 0.8530	 0.6030
Hb	 0.8720	 0.6020
Hc	 0.8880	 0.6090
Hd	 0.8550	 0.6000
He	 0.8640	 0.6020
Hf	 0.8670	 0.6030
Hg	 0.8910	 0.6010
Hh	 0.8710	 0.6040
Hi	 0.8710	 0.6010
Hj	 0.8690	 0.6040
Hk	 0.8670	 0.6080
Hl	 0.8830	 0.6070
Hm	 0.8810	 0.6030
Hz	 0.8660	 0.6080
Ho	 0.8810	 0.6000
Hp	 0.8690	 0.6030
Hq	 0.8550	 0.5960
Hr	 0.8740	 0.6070
Hs	 0.8630	 0.6010
Ht	 0.8610	 0.6000
Hu	 0.8770	 0.6080
Hv	 0.8660	 0.5950
Hw	 0.8850	 0.6080
Hx	 0.8720	 0.6070
Hy	 0.8710	 0.5950
Hx	 0.8850	 0.6070
P0	 0.6690	 0.5690
P1	 0.7130	 0.6130
P2	 0.7160	 0.6050
P3	 0.6880	 0.6000
P4	 0.6910	 0.5720
P5	 0.7040	 0.6030
P6	 0.6790	 0.5680
P7	 0.6730	 0.5660
P8	 0.6810	 0.5600
P9	 0.6960	 0.5690
PA	 0.6830	 0.5720
PB	 0.7080	 0.5660
PC	 0.6830	 0.5650
PD	 0.6910	 0.5640
PE	 0.6880	 0.5620
PF	 0.6960	 0.5760





















































































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Chain	Atom inclusion	Q-score
PG	 0.6830	 0.5660
PH	 0.6760	 0.5750
PI	 0.6830	 0.5690
PJ	 0.6590	 0.5640
PK	 0.6960	 0.5710
PL	 0.6560	 0.5530
PM	 0.6830	 0.5590
PN	 0.6760	 0.5610
PO	 0.6660	 0.5580
PP	 0.6480	 0.5580
PQ	 0.6810	 0.5560
PR	 0.6790	 0.5580
PS	 0.6860	 0.5700
PT	 0.6640	 0.5670
PU	 0.6990	 0.5600
PV	 0.6840	 0.5540
PW	 0.6940	 0.5670
PX	 0.6930	 0.5680
Pa	 0.6510	 0.5580
Pb	 0.6540	 0.5640
Pc	 0.6630	 0.5540
Pd	 0.6680	 0.5670
Pe	 0.6630	 0.5630
Pf	 0.6730	 0.5660
Pg	 0.6910	 0.5700
Ph	 0.6590	 0.5610
Pi	 0.6960	 0.5780
Pj	 0.6710	 0.5660
Pk	 0.6740	 0.5660
Pl	 0.6840	 0.5550
Pm	 0.6790	 0.5660
Pn	 0.6890	 0.5580
Po	 0.6810	 0.5720
Pp	 0.6630	 0.5690
Pq	 0.6680	 0.5640
Pr	 0.6610	 0.5660
Ps	 0.6610	 0.5570
Pt	 0.6540	 0.5530
Pu	 0.6910	 0.5790
Pv	 0.7130	 0.5710
Pw	 0.6990	 0.5670
Px	 0.7090	 0.5650









































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Chain	Atom inclusion	Q-score
Py	 0.6860	 0.5670
Pz	 0.6840	 0.5700
X0	 0.7260	 0.5480
X1	 0.7640	 0.5970
X2	 0.7750	 0.5890
X3	 0.7540	 0.5890
X4	 0.7610	 0.5970
X5	 0.7760	 0.5930
X6	 0.7240	 0.5530
X7	 0.7480	 0.5430
X8	 0.7370	 0.5420
X9	 0.7460	 0.5510
XA	 0.7540	 0.5610
XB	 0.7270	 0.5550
XC	 0.7370	 0.5540
XD	 0.7300	 0.5520
XE	 0.7260	 0.5500
XF	 0.7250	 0.5350
XG	 0.7400	 0.5520
XH	 0.7380	 0.5490
XI	 0.7300	 0.5460
XJ	 0.7190	 0.5540
XK	 0.7330	 0.5530
XL	 0.7250	 0.5460
XM	 0.7240	 0.5480
XN	 0.7200	 0.5520
XO	 0.7180	 0.5480
XP	 0.7250	 0.5470
XQ	 0.7330	 0.5510
XR	 0.7320	 0.5530
XS	 0.7270	 0.5410
XT	 0.7340	 0.5580
XU	 0.7450	 0.5520
XV	 0.7320	 0.5440
XW	 0.7290	 0.5480
XX	 0.7290	 0.5560
Xa	 0.7310	 0.5480
Xb	 0.7180	 0.5280
Xc	 0.7360	 0.5430
Xd	 0.7330	 0.5560
Xe	 0.7260	 0.5470
Xf	 0.7360	 0.5510

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Chain	Atom inclusion	Q-score
Xg	 0.7450	 0.5440
Xh	 0.7320	 0.5500
Xi	 0.7290	 0.5550
Xj	 0.7400	 0.5490
Xk	 0.7290	 0.5560
Xl	 0.7320	 0.5510
Xm	 0.7550	 0.5450
Xn	 0.7490	 0.5650
Xo	 0.7390	 0.5490
Xp	 0.7300	 0.5470
Xq	 0.7270	 0.5420
Xr	 0.7310	 0.5390
Xs	 0.7290	 0.5420
Xt	 0.7240	 0.5450
Xu	 0.7380	 0.5590
Xv	 0.7440	 0.5540
Xw	 0.7460	 0.5570
Xx	 0.7240	 0.5540
Xy	 0.7420	 0.5450
Xz	 0.7570	 0.5600