



Full wwPDB EM Validation Report ⓘ

May 20, 2024 – 12:03 AM JST

PDB ID : 7CKB
EMDB ID : EMD-30384
Title : Simplified Alpha-Carboxysome, T=3
Authors : Tan, Y.Q.; Ali, S.; Xue, B.; Robinson, R.C.; Narita, A.; Yew, W.S.
Deposited on : 2020-07-16
Resolution : 3.24 Å (reported)
Based on initial models : 2RCF, 2EWH

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

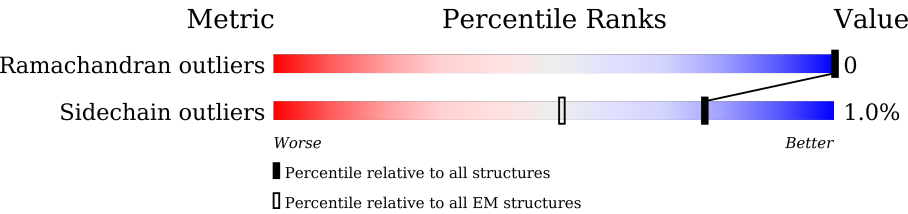
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.24 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A0	94	
1	A1	94	
1	A2	94	
1	A3	94	
1	A4	94	
1	A5	94	
1	A6	94	
1	A7	94	
1	A8	94	









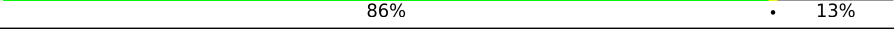

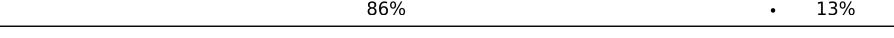
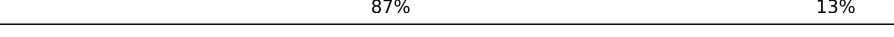

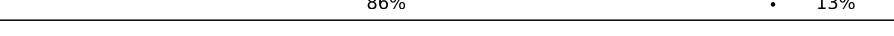


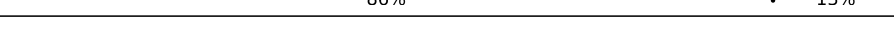

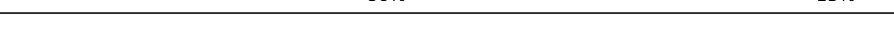






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Mol	Chain	Length	Quality of chain
1	A9	94	 86% • 13%
1	AA	94	 86% • 13%
1	AB	94	 86% • 13%
1	AC	94	 86% • 13%
1	AD	94	 86% • 13%
1	AE	94	 86% • 13%
1	AF	94	 87% 13%
1	AG	94	 86% • 13%
1	AH	94	 86% • 13%
1	AI	94	 86% • 13%
1	AJ	94	 86% • 13%
1	AK	94	 87% 13%
1	AL	94	 87% 13%
1	AM	94	 86% • 13%
1	AN	94	 86% • 13%
1	AO	94	 86% • 13%
1	AP	94	 86% • 13%
1	AQ	94	 86% • 13%
1	AR	94	 86% • 13%
1	AS	94	 86% • 13%
1	AT	94	 86% • 13%
1	AV	94	 86% • 13%
1	AW	94	 86% • 13%
1	AX	94	 86% • 13%
1	AY	94	 86% • 13%
















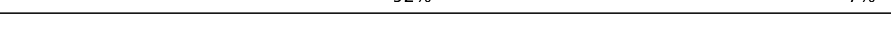
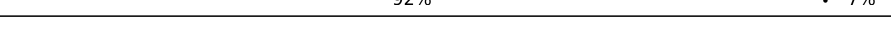
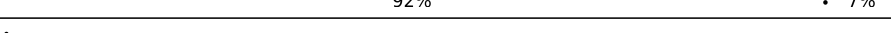
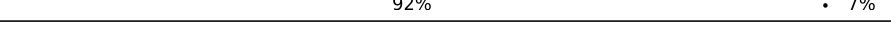
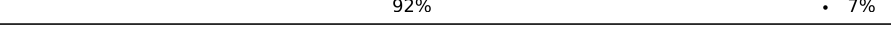
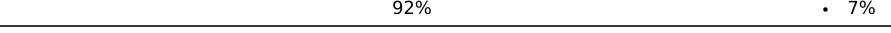
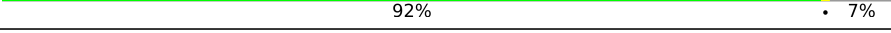



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Mol	Chain	Length	Quality of chain
1	AZ	94	
1	Aa	94	
1	Ab	94	
1	Ac	94	
1	Ad	94	
1	Ae	94	
1	Af	94	
1	Ag	94	
1	Ah	94	
1	Ai	94	
1	Aj	94	
1	Ak	94	
1	Al	94	
1	Am	94	
1	An	94	
1	Ao	94	
1	Ap	94	
1	Aq	94	
1	Ar	94	
1	As	94	
1	At	94	
1	Av	94	
1	Aw	94	
1	Ax	94	
1	Ay	94	

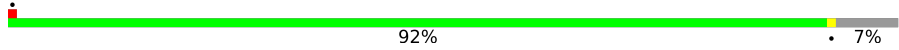
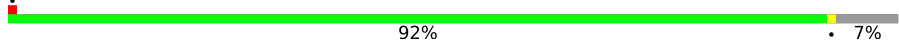
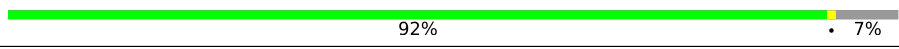
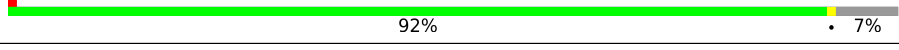
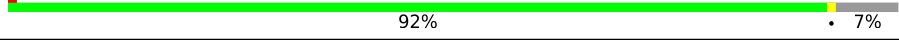
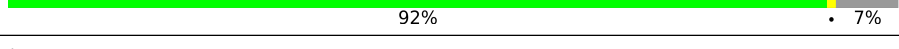
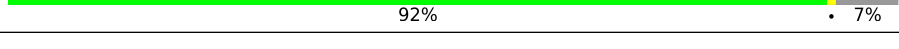
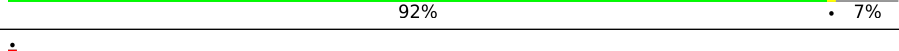
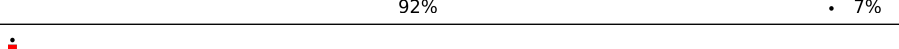
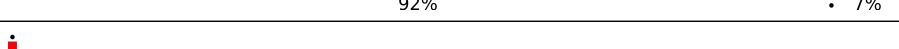
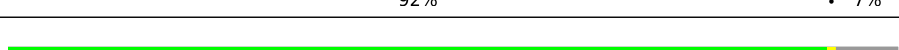
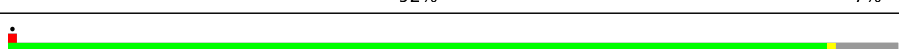
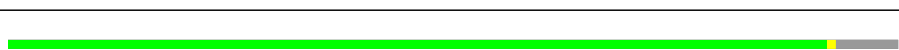
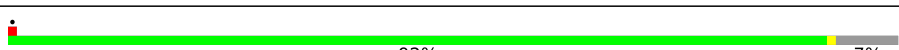
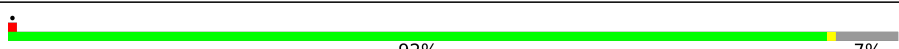


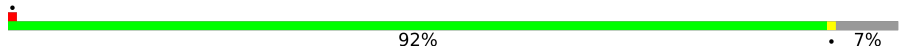
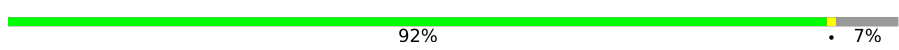
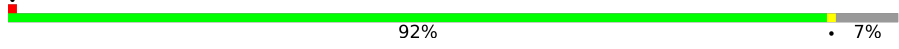
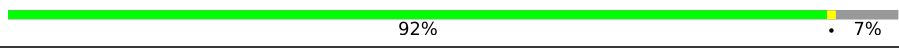
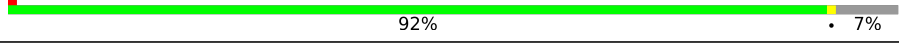
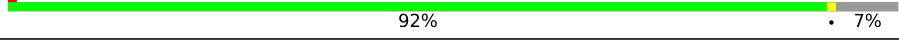


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Mol	Chain	Length	Quality of chain
1	Az	94	 86% • 13%
2	B0	98	 92% • 7%
2	B1	98	 92% • 7%
2	B2	98	 92% • 7%
2	B3	98	 92% • 7%
2	B4	98	 92% • 7%
2	B5	98	 92% • 7%
2	B6	98	 92% • 7%
2	B7	98	 92% • 7%
2	B8	98	 92% • 7%
2	B9	98	 92% • 7%
2	BA	98	 92% • 7%
2	BB	98	 92% • 7%
2	BC	98	 92% • 7%
2	BD	98	 92% • 7%
2	BE	98	 92% • 7%
2	BF	98	 92% • 7%
2	BG	98	 92% • 7%
2	BH	98	 92% • 7%
2	BI	98	 92% • 7%
2	BJ	98	 92% • 7%
2	BK	98	 92% • 7%
2	BL	98	 92% • 7%
2	BM	98	 92% • 7%
2	BN	98	 92% • 7%
















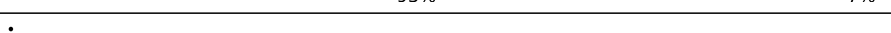
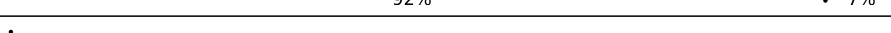
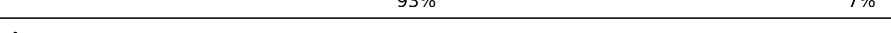
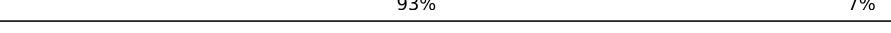
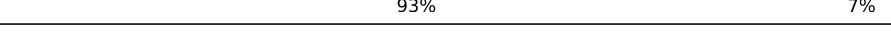
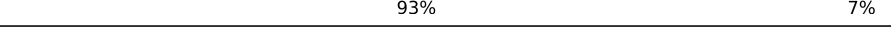
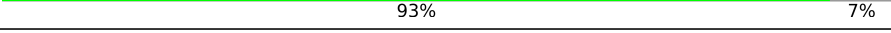

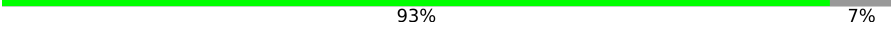
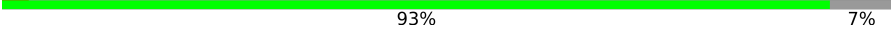
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Mol	Chain	Length	Quality of chain
2	BO	98	
2	BP	98	
2	BQ	98	
2	BR	98	
2	BS	98	
2	BT	98	
2	BV	98	
2	BW	98	
2	BX	98	
2	BY	98	
2	BZ	98	
2	Ba	98	
2	Bb	98	
2	Bc	98	
2	Bd	98	
2	Be	98	
2	Bf	98	
2	Bg	98	
2	Bh	98	
2	Bi	98	
2	Bj	98	
2	Bk	98	
2	Bl	98	
2	Bm	98	
2	Bn	98	

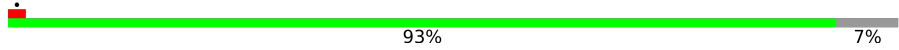
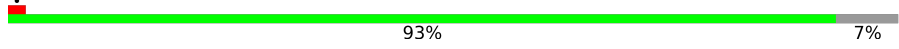
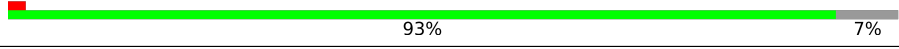
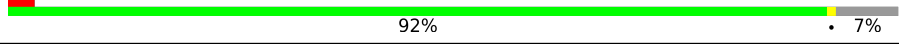
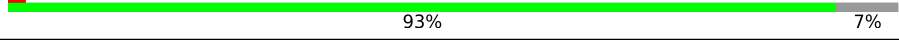
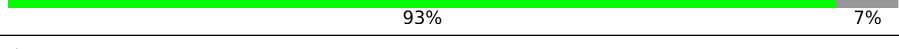
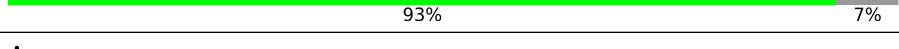
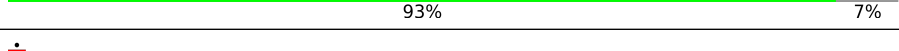
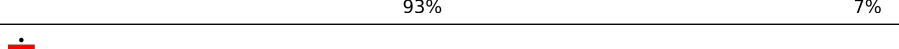
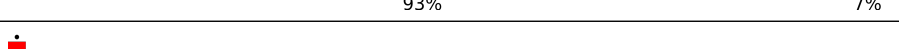
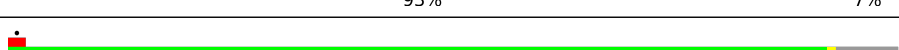
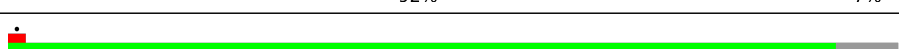
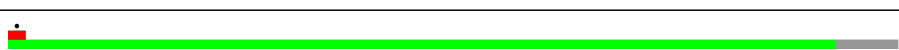
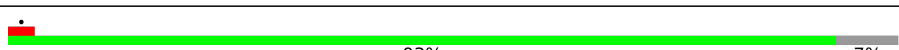
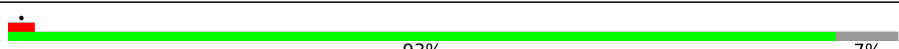
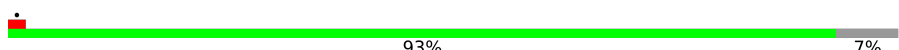
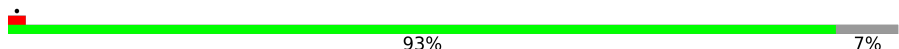
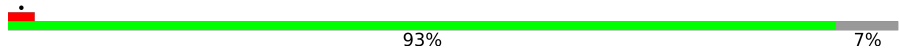
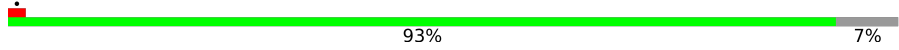
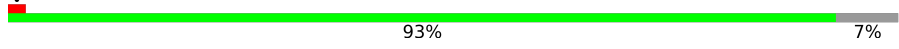
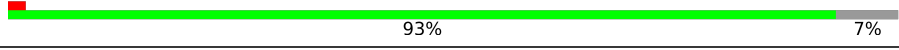
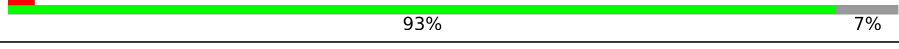
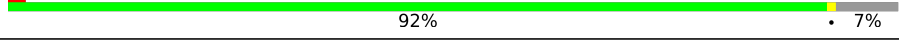


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Mol	Chain	Length	Quality of chain
2	Bo	98	 92% 7%
2	Bp	98	 92% 7%
2	Bq	98	 92% 7%
2	Br	98	 92% 7%
2	Bs	98	 92% 7%
2	Bt	98	 92% 7%
2	Bv	98	 92% 7%
2	Bw	98	 92% 7%
2	Bx	98	 92% 7%
2	By	98	 92% 7%
2	Bz	98	 92% 7%
2	C0	98	 93% 7%
2	C1	98	 93% 7%
2	C2	98	 93% 7%
2	C3	98	 93% 7%
2	C4	98	 92% 7%
2	C5	98	 93% 7%
2	C6	98	 93% 7%
2	C7	98	 93% 7%
2	C8	98	 93% 7%
2	C9	98	 93% 7%
2	CA	98	 92% 7%
2	CB	98	 93% 7%
2	CC	98	 93% 7%
2	CD	98	 93% 7%

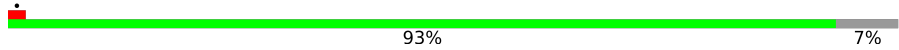
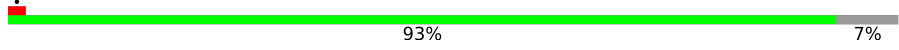
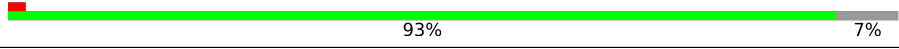
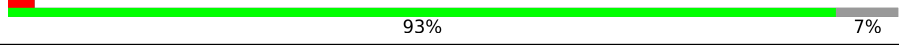
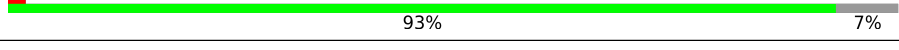
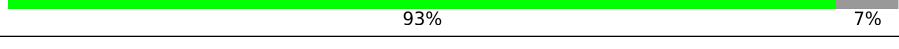
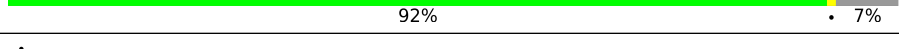
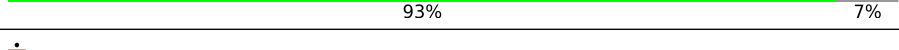
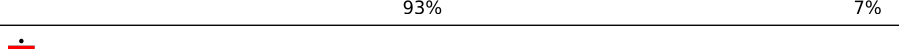
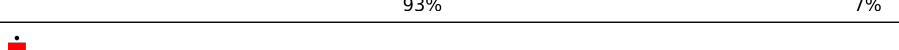
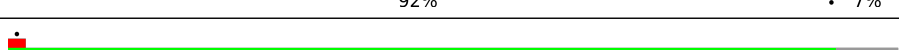
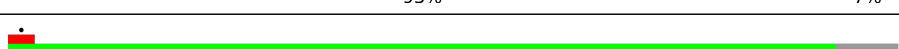

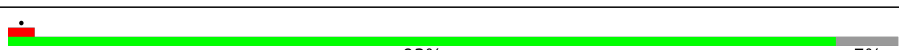
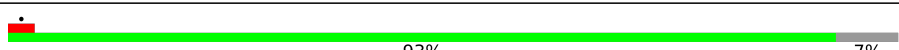
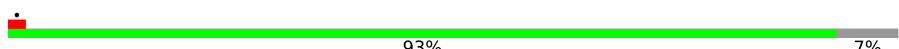
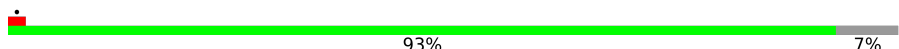
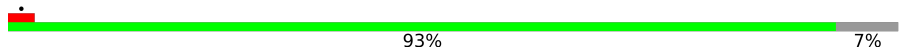
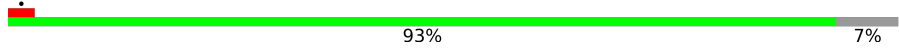
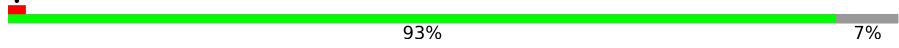

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Mol	Chain	Length	Quality of chain
2	CE	98	
2	CF	98	
2	CG	98	
2	CH	98	
2	CI	98	
2	CJ	98	
2	CK	98	
2	CL	98	
2	CM	98	
2	CN	98	
2	CO	98	
2	CP	98	
2	CQ	98	
2	CR	98	
2	CS	98	
2	CT	98	
2	CV	98	
2	CW	98	
2	CX	98	
2	CY	98	
2	CZ	98	
2	Ca	98	
2	Cb	98	
2	Cc	98	
2	Cd	98	

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Mol	Chain	Length	Quality of chain
2	Ce	98	 93%7%
2	Cf	98	 93%7%
2	Cg	98	 93%7%
2	Ch	98	 93%7%
2	Ci	98	 93%7%
2	Cj	98	 93%7%
2	Ck	98	 92%7%
2	Cl	98	 93%7%
2	Cm	98	 93%7%
2	Cn	98	 93%7%
2	Co	98	 92%7%
2	Cp	98	 93%7%
2	Cq	98	 93%7%
2	Cr	98	 92%7%
2	Cs	98	 93%7%
2	Ct	98	 93%7%
2	Cv	98	 93%7%
2	Cw	98	 93%7%
2	Cx	98	 93%7%
2	Cy	98	 93%7%
2	Cz	98	 93%7%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 114840 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 Unidentified carboxysome polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
1	AB	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
1	AC	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
1	AD	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
1	AE	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
1	AF	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
1	AG	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
1	AH	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
1	AI	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
1	AJ	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
1	AK	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
1	AL	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
1	AM	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
1	AN	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
1	AO	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
1	AP	82	Total	C	N	O	S	0	0
			612	388	106	113	5		
1	AQ	82	Total	C	N	O	S	0	0
			612	388	106	113	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AR	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	AS	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	AT	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	AV	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	AW	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	AX	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	AY	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	AZ	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Aa	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Ab	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Ac	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Ad	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Ae	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Af	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Ag	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Ah	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Ai	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Aj	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Ak	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Al	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Am	82	Total 612	C 388	N 106	O 113	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	An	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Ao	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Ap	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Aq	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Ar	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	As	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	At	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Av	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Aw	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Ax	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Ay	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	Az	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	A0	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	A1	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	A2	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	A3	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	A4	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	A5	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	A6	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	A7	82	Total 612	C 388	N 106	O 113	S 5	0	0
1	A8	82	Total 612	C 388	N 106	O 113	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	A9	82	Total	C	N	O	S	0	0
			612	388	106	113	5		

There are 660 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	84	GLY	-	expression tag	UNP O85043
AA	85	SER	-	expression tag	UNP O85043
AA	86	SER	-	expression tag	UNP O85043
AA	87	TRP	-	expression tag	UNP O85043
AA	88	SER	-	expression tag	UNP O85043
AA	89	HIS	-	expression tag	UNP O85043
AA	90	PRO	-	expression tag	UNP O85043
AA	91	GLN	-	expression tag	UNP O85043
AA	92	PHE	-	expression tag	UNP O85043
AA	93	GLU	-	expression tag	UNP O85043
AA	94	LYS	-	expression tag	UNP O85043
AB	84	GLY	-	expression tag	UNP O85043
AB	85	SER	-	expression tag	UNP O85043
AB	86	SER	-	expression tag	UNP O85043
AB	87	TRP	-	expression tag	UNP O85043
AB	88	SER	-	expression tag	UNP O85043
AB	89	HIS	-	expression tag	UNP O85043
AB	90	PRO	-	expression tag	UNP O85043
AB	91	GLN	-	expression tag	UNP O85043
AB	92	PHE	-	expression tag	UNP O85043
AB	93	GLU	-	expression tag	UNP O85043
AB	94	LYS	-	expression tag	UNP O85043
AC	84	GLY	-	expression tag	UNP O85043
AC	85	SER	-	expression tag	UNP O85043
AC	86	SER	-	expression tag	UNP O85043
AC	87	TRP	-	expression tag	UNP O85043
AC	88	SER	-	expression tag	UNP O85043
AC	89	HIS	-	expression tag	UNP O85043
AC	90	PRO	-	expression tag	UNP O85043
AC	91	GLN	-	expression tag	UNP O85043
AC	92	PHE	-	expression tag	UNP O85043
AC	93	GLU	-	expression tag	UNP O85043
AC	94	LYS	-	expression tag	UNP O85043
AD	84	GLY	-	expression tag	UNP O85043
AD	85	SER	-	expression tag	UNP O85043
AD	86	SER	-	expression tag	UNP O85043

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Chain	Residue	Modelled	Actual	Comment	Reference
AD	87	TRP	-	expression tag	UNP O85043
AD	88	SER	-	expression tag	UNP O85043
AD	89	HIS	-	expression tag	UNP O85043
AD	90	PRO	-	expression tag	UNP O85043
AD	91	GLN	-	expression tag	UNP O85043
AD	92	PHE	-	expression tag	UNP O85043
AD	93	GLU	-	expression tag	UNP O85043
AD	94	LYS	-	expression tag	UNP O85043
AE	84	GLY	-	expression tag	UNP O85043
AE	85	SER	-	expression tag	UNP O85043
AE	86	SER	-	expression tag	UNP O85043
AE	87	TRP	-	expression tag	UNP O85043
AE	88	SER	-	expression tag	UNP O85043
AE	89	HIS	-	expression tag	UNP O85043
AE	90	PRO	-	expression tag	UNP O85043
AE	91	GLN	-	expression tag	UNP O85043
AE	92	PHE	-	expression tag	UNP O85043
AE	93	GLU	-	expression tag	UNP O85043
AE	94	LYS	-	expression tag	UNP O85043
AF	84	GLY	-	expression tag	UNP O85043
AF	85	SER	-	expression tag	UNP O85043
AF	86	SER	-	expression tag	UNP O85043
AF	87	TRP	-	expression tag	UNP O85043
AF	88	SER	-	expression tag	UNP O85043
AF	89	HIS	-	expression tag	UNP O85043
AF	90	PRO	-	expression tag	UNP O85043
AF	91	GLN	-	expression tag	UNP O85043
AF	92	PHE	-	expression tag	UNP O85043
AF	93	GLU	-	expression tag	UNP O85043
AF	94	LYS	-	expression tag	UNP O85043
AG	84	GLY	-	expression tag	UNP O85043
AG	85	SER	-	expression tag	UNP O85043
AG	86	SER	-	expression tag	UNP O85043
AG	87	TRP	-	expression tag	UNP O85043
AG	88	SER	-	expression tag	UNP O85043
AG	89	HIS	-	expression tag	UNP O85043
AG	90	PRO	-	expression tag	UNP O85043
AG	91	GLN	-	expression tag	UNP O85043
AG	92	PHE	-	expression tag	UNP O85043
AG	93	GLU	-	expression tag	UNP O85043
AG	94	LYS	-	expression tag	UNP O85043
AH	84	GLY	-	expression tag	UNP O85043

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Chain	Residue	Modelled	Actual	Comment	Reference
AH	85	SER	-	expression tag	UNP O85043
AH	86	SER	-	expression tag	UNP O85043
AH	87	TRP	-	expression tag	UNP O85043
AH	88	SER	-	expression tag	UNP O85043
AH	89	HIS	-	expression tag	UNP O85043
AH	90	PRO	-	expression tag	UNP O85043
AH	91	GLN	-	expression tag	UNP O85043
AH	92	PHE	-	expression tag	UNP O85043
AH	93	GLU	-	expression tag	UNP O85043
AH	94	LYS	-	expression tag	UNP O85043
AI	84	GLY	-	expression tag	UNP O85043
AI	85	SER	-	expression tag	UNP O85043
AI	86	SER	-	expression tag	UNP O85043
AI	87	TRP	-	expression tag	UNP O85043
AI	88	SER	-	expression tag	UNP O85043
AI	89	HIS	-	expression tag	UNP O85043
AI	90	PRO	-	expression tag	UNP O85043
AI	91	GLN	-	expression tag	UNP O85043
AI	92	PHE	-	expression tag	UNP O85043
AI	93	GLU	-	expression tag	UNP O85043
AI	94	LYS	-	expression tag	UNP O85043
AJ	84	GLY	-	expression tag	UNP O85043
AJ	85	SER	-	expression tag	UNP O85043
AJ	86	SER	-	expression tag	UNP O85043
AJ	87	TRP	-	expression tag	UNP O85043
AJ	88	SER	-	expression tag	UNP O85043
AJ	89	HIS	-	expression tag	UNP O85043
AJ	90	PRO	-	expression tag	UNP O85043
AJ	91	GLN	-	expression tag	UNP O85043
AJ	92	PHE	-	expression tag	UNP O85043
AJ	93	GLU	-	expression tag	UNP O85043
AJ	94	LYS	-	expression tag	UNP O85043
AK	84	GLY	-	expression tag	UNP O85043
AK	85	SER	-	expression tag	UNP O85043
AK	86	SER	-	expression tag	UNP O85043
AK	87	TRP	-	expression tag	UNP O85043
AK	88	SER	-	expression tag	UNP O85043
AK	89	HIS	-	expression tag	UNP O85043
AK	90	PRO	-	expression tag	UNP O85043
AK	91	GLN	-	expression tag	UNP O85043
AK	92	PHE	-	expression tag	UNP O85043
AK	93	GLU	-	expression tag	UNP O85043

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Chain	Residue	Modelled	Actual	Comment	Reference
AK	94	LYS	-	expression tag	UNP O85043
AL	84	GLY	-	expression tag	UNP O85043
AL	85	SER	-	expression tag	UNP O85043
AL	86	SER	-	expression tag	UNP O85043
AL	87	TRP	-	expression tag	UNP O85043
AL	88	SER	-	expression tag	UNP O85043
AL	89	HIS	-	expression tag	UNP O85043
AL	90	PRO	-	expression tag	UNP O85043
AL	91	GLN	-	expression tag	UNP O85043
AL	92	PHE	-	expression tag	UNP O85043
AL	93	GLU	-	expression tag	UNP O85043
AL	94	LYS	-	expression tag	UNP O85043
AM	84	GLY	-	expression tag	UNP O85043
AM	85	SER	-	expression tag	UNP O85043
AM	86	SER	-	expression tag	UNP O85043
AM	87	TRP	-	expression tag	UNP O85043
AM	88	SER	-	expression tag	UNP O85043
AM	89	HIS	-	expression tag	UNP O85043
AM	90	PRO	-	expression tag	UNP O85043
AM	91	GLN	-	expression tag	UNP O85043
AM	92	PHE	-	expression tag	UNP O85043
AM	93	GLU	-	expression tag	UNP O85043
AM	94	LYS	-	expression tag	UNP O85043
AN	84	GLY	-	expression tag	UNP O85043
AN	85	SER	-	expression tag	UNP O85043
AN	86	SER	-	expression tag	UNP O85043
AN	87	TRP	-	expression tag	UNP O85043
AN	88	SER	-	expression tag	UNP O85043
AN	89	HIS	-	expression tag	UNP O85043
AN	90	PRO	-	expression tag	UNP O85043
AN	91	GLN	-	expression tag	UNP O85043
AN	92	PHE	-	expression tag	UNP O85043
AN	93	GLU	-	expression tag	UNP O85043
AN	94	LYS	-	expression tag	UNP O85043
AO	84	GLY	-	expression tag	UNP O85043
AO	85	SER	-	expression tag	UNP O85043
AO	86	SER	-	expression tag	UNP O85043
AO	87	TRP	-	expression tag	UNP O85043
AO	88	SER	-	expression tag	UNP O85043
AO	89	HIS	-	expression tag	UNP O85043
AO	90	PRO	-	expression tag	UNP O85043
AO	91	GLN	-	expression tag	UNP O85043

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Chain	Residue	Modelled	Actual	Comment	Reference
AO	92	PHE	-	expression tag	UNP O85043
AO	93	GLU	-	expression tag	UNP O85043
AO	94	LYS	-	expression tag	UNP O85043
AP	84	GLY	-	expression tag	UNP O85043
AP	85	SER	-	expression tag	UNP O85043
AP	86	SER	-	expression tag	UNP O85043
AP	87	TRP	-	expression tag	UNP O85043
AP	88	SER	-	expression tag	UNP O85043
AP	89	HIS	-	expression tag	UNP O85043
AP	90	PRO	-	expression tag	UNP O85043
AP	91	GLN	-	expression tag	UNP O85043
AP	92	PHE	-	expression tag	UNP O85043
AP	93	GLU	-	expression tag	UNP O85043
AP	94	LYS	-	expression tag	UNP O85043
AQ	84	GLY	-	expression tag	UNP O85043
AQ	85	SER	-	expression tag	UNP O85043
AQ	86	SER	-	expression tag	UNP O85043
AQ	87	TRP	-	expression tag	UNP O85043
AQ	88	SER	-	expression tag	UNP O85043
AQ	89	HIS	-	expression tag	UNP O85043
AQ	90	PRO	-	expression tag	UNP O85043
AQ	91	GLN	-	expression tag	UNP O85043
AQ	92	PHE	-	expression tag	UNP O85043
AQ	93	GLU	-	expression tag	UNP O85043
AQ	94	LYS	-	expression tag	UNP O85043
AR	84	GLY	-	expression tag	UNP O85043
AR	85	SER	-	expression tag	UNP O85043
AR	86	SER	-	expression tag	UNP O85043
AR	87	TRP	-	expression tag	UNP O85043
AR	88	SER	-	expression tag	UNP O85043
AR	89	HIS	-	expression tag	UNP O85043
AR	90	PRO	-	expression tag	UNP O85043
AR	91	GLN	-	expression tag	UNP O85043
AR	92	PHE	-	expression tag	UNP O85043
AR	93	GLU	-	expression tag	UNP O85043
AR	94	LYS	-	expression tag	UNP O85043
AS	84	GLY	-	expression tag	UNP O85043
AS	85	SER	-	expression tag	UNP O85043
AS	86	SER	-	expression tag	UNP O85043
AS	87	TRP	-	expression tag	UNP O85043
AS	88	SER	-	expression tag	UNP O85043
AS	89	HIS	-	expression tag	UNP O85043

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Chain	Residue	Modelled	Actual	Comment	Reference
AS	90	PRO	-	expression tag	UNP O85043
AS	91	GLN	-	expression tag	UNP O85043
AS	92	PHE	-	expression tag	UNP O85043
AS	93	GLU	-	expression tag	UNP O85043
AS	94	LYS	-	expression tag	UNP O85043
AT	84	GLY	-	expression tag	UNP O85043
AT	85	SER	-	expression tag	UNP O85043
AT	86	SER	-	expression tag	UNP O85043
AT	87	TRP	-	expression tag	UNP O85043
AT	88	SER	-	expression tag	UNP O85043
AT	89	HIS	-	expression tag	UNP O85043
AT	90	PRO	-	expression tag	UNP O85043
AT	91	GLN	-	expression tag	UNP O85043
AT	92	PHE	-	expression tag	UNP O85043
AT	93	GLU	-	expression tag	UNP O85043
AT	94	LYS	-	expression tag	UNP O85043
AV	84	GLY	-	expression tag	UNP O85043
AV	85	SER	-	expression tag	UNP O85043
AV	86	SER	-	expression tag	UNP O85043
AV	87	TRP	-	expression tag	UNP O85043
AV	88	SER	-	expression tag	UNP O85043
AV	89	HIS	-	expression tag	UNP O85043
AV	90	PRO	-	expression tag	UNP O85043
AV	91	GLN	-	expression tag	UNP O85043
AV	92	PHE	-	expression tag	UNP O85043
AV	93	GLU	-	expression tag	UNP O85043
AV	94	LYS	-	expression tag	UNP O85043
AW	84	GLY	-	expression tag	UNP O85043
AW	85	SER	-	expression tag	UNP O85043
AW	86	SER	-	expression tag	UNP O85043
AW	87	TRP	-	expression tag	UNP O85043
AW	88	SER	-	expression tag	UNP O85043
AW	89	HIS	-	expression tag	UNP O85043
AW	90	PRO	-	expression tag	UNP O85043
AW	91	GLN	-	expression tag	UNP O85043
AW	92	PHE	-	expression tag	UNP O85043
AW	93	GLU	-	expression tag	UNP O85043
AW	94	LYS	-	expression tag	UNP O85043
AX	84	GLY	-	expression tag	UNP O85043
AX	85	SER	-	expression tag	UNP O85043
AX	86	SER	-	expression tag	UNP O85043
AX	87	TRP	-	expression tag	UNP O85043

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Chain	Residue	Modelled	Actual	Comment	Reference
AX	88	SER	-	expression tag	UNP O85043
AX	89	HIS	-	expression tag	UNP O85043
AX	90	PRO	-	expression tag	UNP O85043
AX	91	GLN	-	expression tag	UNP O85043
AX	92	PHE	-	expression tag	UNP O85043
AX	93	GLU	-	expression tag	UNP O85043
AX	94	LYS	-	expression tag	UNP O85043
AY	84	GLY	-	expression tag	UNP O85043
AY	85	SER	-	expression tag	UNP O85043
AY	86	SER	-	expression tag	UNP O85043
AY	87	TRP	-	expression tag	UNP O85043
AY	88	SER	-	expression tag	UNP O85043
AY	89	HIS	-	expression tag	UNP O85043
AY	90	PRO	-	expression tag	UNP O85043
AY	91	GLN	-	expression tag	UNP O85043
AY	92	PHE	-	expression tag	UNP O85043
AY	93	GLU	-	expression tag	UNP O85043
AY	94	LYS	-	expression tag	UNP O85043
AZ	84	GLY	-	expression tag	UNP O85043
AZ	85	SER	-	expression tag	UNP O85043
AZ	86	SER	-	expression tag	UNP O85043
AZ	87	TRP	-	expression tag	UNP O85043
AZ	88	SER	-	expression tag	UNP O85043
AZ	89	HIS	-	expression tag	UNP O85043
AZ	90	PRO	-	expression tag	UNP O85043
AZ	91	GLN	-	expression tag	UNP O85043
AZ	92	PHE	-	expression tag	UNP O85043
AZ	93	GLU	-	expression tag	UNP O85043
AZ	94	LYS	-	expression tag	UNP O85043
Aa	84	GLY	-	expression tag	UNP O85043
Aa	85	SER	-	expression tag	UNP O85043
Aa	86	SER	-	expression tag	UNP O85043
Aa	87	TRP	-	expression tag	UNP O85043
Aa	88	SER	-	expression tag	UNP O85043
Aa	89	HIS	-	expression tag	UNP O85043
Aa	90	PRO	-	expression tag	UNP O85043
Aa	91	GLN	-	expression tag	UNP O85043
Aa	92	PHE	-	expression tag	UNP O85043
Aa	93	GLU	-	expression tag	UNP O85043
Aa	94	LYS	-	expression tag	UNP O85043
Ab	84	GLY	-	expression tag	UNP O85043
Ab	85	SER	-	expression tag	UNP O85043

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Chain	Residue	Modelled	Actual	Comment	Reference
Ab	86	SER	-	expression tag	UNP O85043
Ab	87	TRP	-	expression tag	UNP O85043
Ab	88	SER	-	expression tag	UNP O85043
Ab	89	HIS	-	expression tag	UNP O85043
Ab	90	PRO	-	expression tag	UNP O85043
Ab	91	GLN	-	expression tag	UNP O85043
Ab	92	PHE	-	expression tag	UNP O85043
Ab	93	GLU	-	expression tag	UNP O85043
Ab	94	LYS	-	expression tag	UNP O85043
Ac	84	GLY	-	expression tag	UNP O85043
Ac	85	SER	-	expression tag	UNP O85043
Ac	86	SER	-	expression tag	UNP O85043
Ac	87	TRP	-	expression tag	UNP O85043
Ac	88	SER	-	expression tag	UNP O85043
Ac	89	HIS	-	expression tag	UNP O85043
Ac	90	PRO	-	expression tag	UNP O85043
Ac	91	GLN	-	expression tag	UNP O85043
Ac	92	PHE	-	expression tag	UNP O85043
Ac	93	GLU	-	expression tag	UNP O85043
Ac	94	LYS	-	expression tag	UNP O85043
Ad	84	GLY	-	expression tag	UNP O85043
Ad	85	SER	-	expression tag	UNP O85043
Ad	86	SER	-	expression tag	UNP O85043
Ad	87	TRP	-	expression tag	UNP O85043
Ad	88	SER	-	expression tag	UNP O85043
Ad	89	HIS	-	expression tag	UNP O85043
Ad	90	PRO	-	expression tag	UNP O85043
Ad	91	GLN	-	expression tag	UNP O85043
Ad	92	PHE	-	expression tag	UNP O85043
Ad	93	GLU	-	expression tag	UNP O85043
Ad	94	LYS	-	expression tag	UNP O85043
Ae	84	GLY	-	expression tag	UNP O85043
Ae	85	SER	-	expression tag	UNP O85043
Ae	86	SER	-	expression tag	UNP O85043
Ae	87	TRP	-	expression tag	UNP O85043
Ae	88	SER	-	expression tag	UNP O85043
Ae	89	HIS	-	expression tag	UNP O85043
Ae	90	PRO	-	expression tag	UNP O85043
Ae	91	GLN	-	expression tag	UNP O85043
Ae	92	PHE	-	expression tag	UNP O85043
Ae	93	GLU	-	expression tag	UNP O85043
Ae	94	LYS	-	expression tag	UNP O85043

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Chain	Residue	Modelled	Actual	Comment	Reference
Af	84	GLY	-	expression tag	UNP O85043
Af	85	SER	-	expression tag	UNP O85043
Af	86	SER	-	expression tag	UNP O85043
Af	87	TRP	-	expression tag	UNP O85043
Af	88	SER	-	expression tag	UNP O85043
Af	89	HIS	-	expression tag	UNP O85043
Af	90	PRO	-	expression tag	UNP O85043
Af	91	GLN	-	expression tag	UNP O85043
Af	92	PHE	-	expression tag	UNP O85043
Af	93	GLU	-	expression tag	UNP O85043
Af	94	LYS	-	expression tag	UNP O85043
Ag	84	GLY	-	expression tag	UNP O85043
Ag	85	SER	-	expression tag	UNP O85043
Ag	86	SER	-	expression tag	UNP O85043
Ag	87	TRP	-	expression tag	UNP O85043
Ag	88	SER	-	expression tag	UNP O85043
Ag	89	HIS	-	expression tag	UNP O85043
Ag	90	PRO	-	expression tag	UNP O85043
Ag	91	GLN	-	expression tag	UNP O85043
Ag	92	PHE	-	expression tag	UNP O85043
Ag	93	GLU	-	expression tag	UNP O85043
Ag	94	LYS	-	expression tag	UNP O85043
Ah	84	GLY	-	expression tag	UNP O85043
Ah	85	SER	-	expression tag	UNP O85043
Ah	86	SER	-	expression tag	UNP O85043
Ah	87	TRP	-	expression tag	UNP O85043
Ah	88	SER	-	expression tag	UNP O85043
Ah	89	HIS	-	expression tag	UNP O85043
Ah	90	PRO	-	expression tag	UNP O85043
Ah	91	GLN	-	expression tag	UNP O85043
Ah	92	PHE	-	expression tag	UNP O85043
Ah	93	GLU	-	expression tag	UNP O85043
Ah	94	LYS	-	expression tag	UNP O85043
Ai	84	GLY	-	expression tag	UNP O85043
Ai	85	SER	-	expression tag	UNP O85043
Ai	86	SER	-	expression tag	UNP O85043
Ai	87	TRP	-	expression tag	UNP O85043
Ai	88	SER	-	expression tag	UNP O85043
Ai	89	HIS	-	expression tag	UNP O85043
Ai	90	PRO	-	expression tag	UNP O85043
Ai	91	GLN	-	expression tag	UNP O85043
Ai	92	PHE	-	expression tag	UNP O85043

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Chain	Residue	Modelled	Actual	Comment	Reference
Ai	93	GLU	-	expression tag	UNP O85043
Ai	94	LYS	-	expression tag	UNP O85043
Aj	84	GLY	-	expression tag	UNP O85043
Aj	85	SER	-	expression tag	UNP O85043
Aj	86	SER	-	expression tag	UNP O85043
Aj	87	TRP	-	expression tag	UNP O85043
Aj	88	SER	-	expression tag	UNP O85043
Aj	89	HIS	-	expression tag	UNP O85043
Aj	90	PRO	-	expression tag	UNP O85043
Aj	91	GLN	-	expression tag	UNP O85043
Aj	92	PHE	-	expression tag	UNP O85043
Aj	93	GLU	-	expression tag	UNP O85043
Aj	94	LYS	-	expression tag	UNP O85043
Ak	84	GLY	-	expression tag	UNP O85043
Ak	85	SER	-	expression tag	UNP O85043
Ak	86	SER	-	expression tag	UNP O85043
Ak	87	TRP	-	expression tag	UNP O85043
Ak	88	SER	-	expression tag	UNP O85043
Ak	89	HIS	-	expression tag	UNP O85043
Ak	90	PRO	-	expression tag	UNP O85043
Ak	91	GLN	-	expression tag	UNP O85043
Ak	92	PHE	-	expression tag	UNP O85043
Ak	93	GLU	-	expression tag	UNP O85043
Ak	94	LYS	-	expression tag	UNP O85043
Al	84	GLY	-	expression tag	UNP O85043
Al	85	SER	-	expression tag	UNP O85043
Al	86	SER	-	expression tag	UNP O85043
Al	87	TRP	-	expression tag	UNP O85043
Al	88	SER	-	expression tag	UNP O85043
Al	89	HIS	-	expression tag	UNP O85043
Al	90	PRO	-	expression tag	UNP O85043
Al	91	GLN	-	expression tag	UNP O85043
Al	92	PHE	-	expression tag	UNP O85043
Al	93	GLU	-	expression tag	UNP O85043
Al	94	LYS	-	expression tag	UNP O85043
Am	84	GLY	-	expression tag	UNP O85043
Am	85	SER	-	expression tag	UNP O85043
Am	86	SER	-	expression tag	UNP O85043
Am	87	TRP	-	expression tag	UNP O85043
Am	88	SER	-	expression tag	UNP O85043
Am	89	HIS	-	expression tag	UNP O85043
Am	90	PRO	-	expression tag	UNP O85043

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Chain	Residue	Modelled	Actual	Comment	Reference
Am	91	GLN	-	expression tag	UNP O85043
Am	92	PHE	-	expression tag	UNP O85043
Am	93	GLU	-	expression tag	UNP O85043
Am	94	LYS	-	expression tag	UNP O85043
An	84	GLY	-	expression tag	UNP O85043
An	85	SER	-	expression tag	UNP O85043
An	86	SER	-	expression tag	UNP O85043
An	87	TRP	-	expression tag	UNP O85043
An	88	SER	-	expression tag	UNP O85043
An	89	HIS	-	expression tag	UNP O85043
An	90	PRO	-	expression tag	UNP O85043
An	91	GLN	-	expression tag	UNP O85043
An	92	PHE	-	expression tag	UNP O85043
An	93	GLU	-	expression tag	UNP O85043
An	94	LYS	-	expression tag	UNP O85043
Ao	84	GLY	-	expression tag	UNP O85043
Ao	85	SER	-	expression tag	UNP O85043
Ao	86	SER	-	expression tag	UNP O85043
Ao	87	TRP	-	expression tag	UNP O85043
Ao	88	SER	-	expression tag	UNP O85043
Ao	89	HIS	-	expression tag	UNP O85043
Ao	90	PRO	-	expression tag	UNP O85043
Ao	91	GLN	-	expression tag	UNP O85043
Ao	92	PHE	-	expression tag	UNP O85043
Ao	93	GLU	-	expression tag	UNP O85043
Ao	94	LYS	-	expression tag	UNP O85043
Ap	84	GLY	-	expression tag	UNP O85043
Ap	85	SER	-	expression tag	UNP O85043
Ap	86	SER	-	expression tag	UNP O85043
Ap	87	TRP	-	expression tag	UNP O85043
Ap	88	SER	-	expression tag	UNP O85043
Ap	89	HIS	-	expression tag	UNP O85043
Ap	90	PRO	-	expression tag	UNP O85043
Ap	91	GLN	-	expression tag	UNP O85043
Ap	92	PHE	-	expression tag	UNP O85043
Ap	93	GLU	-	expression tag	UNP O85043
Ap	94	LYS	-	expression tag	UNP O85043
Aq	84	GLY	-	expression tag	UNP O85043
Aq	85	SER	-	expression tag	UNP O85043
Aq	86	SER	-	expression tag	UNP O85043
Aq	87	TRP	-	expression tag	UNP O85043
Aq	88	SER	-	expression tag	UNP O85043

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Chain	Residue	Modelled	Actual	Comment	Reference
Aq	89	HIS	-	expression tag	UNP O85043
Aq	90	PRO	-	expression tag	UNP O85043
Aq	91	GLN	-	expression tag	UNP O85043
Aq	92	PHE	-	expression tag	UNP O85043
Aq	93	GLU	-	expression tag	UNP O85043
Aq	94	LYS	-	expression tag	UNP O85043
Ar	84	GLY	-	expression tag	UNP O85043
Ar	85	SER	-	expression tag	UNP O85043
Ar	86	SER	-	expression tag	UNP O85043
Ar	87	TRP	-	expression tag	UNP O85043
Ar	88	SER	-	expression tag	UNP O85043
Ar	89	HIS	-	expression tag	UNP O85043
Ar	90	PRO	-	expression tag	UNP O85043
Ar	91	GLN	-	expression tag	UNP O85043
Ar	92	PHE	-	expression tag	UNP O85043
Ar	93	GLU	-	expression tag	UNP O85043
Ar	94	LYS	-	expression tag	UNP O85043
As	84	GLY	-	expression tag	UNP O85043
As	85	SER	-	expression tag	UNP O85043
As	86	SER	-	expression tag	UNP O85043
As	87	TRP	-	expression tag	UNP O85043
As	88	SER	-	expression tag	UNP O85043
As	89	HIS	-	expression tag	UNP O85043
As	90	PRO	-	expression tag	UNP O85043
As	91	GLN	-	expression tag	UNP O85043
As	92	PHE	-	expression tag	UNP O85043
As	93	GLU	-	expression tag	UNP O85043
As	94	LYS	-	expression tag	UNP O85043
At	84	GLY	-	expression tag	UNP O85043
At	85	SER	-	expression tag	UNP O85043
At	86	SER	-	expression tag	UNP O85043
At	87	TRP	-	expression tag	UNP O85043
At	88	SER	-	expression tag	UNP O85043
At	89	HIS	-	expression tag	UNP O85043
At	90	PRO	-	expression tag	UNP O85043
At	91	GLN	-	expression tag	UNP O85043
At	92	PHE	-	expression tag	UNP O85043
At	93	GLU	-	expression tag	UNP O85043
At	94	LYS	-	expression tag	UNP O85043
Av	84	GLY	-	expression tag	UNP O85043
Av	85	SER	-	expression tag	UNP O85043
Av	86	SER	-	expression tag	UNP O85043

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Chain	Residue	Modelled	Actual	Comment	Reference
Av	87	TRP	-	expression tag	UNP O85043
Av	88	SER	-	expression tag	UNP O85043
Av	89	HIS	-	expression tag	UNP O85043
Av	90	PRO	-	expression tag	UNP O85043
Av	91	GLN	-	expression tag	UNP O85043
Av	92	PHE	-	expression tag	UNP O85043
Av	93	GLU	-	expression tag	UNP O85043
Av	94	LYS	-	expression tag	UNP O85043
Aw	84	GLY	-	expression tag	UNP O85043
Aw	85	SER	-	expression tag	UNP O85043
Aw	86	SER	-	expression tag	UNP O85043
Aw	87	TRP	-	expression tag	UNP O85043
Aw	88	SER	-	expression tag	UNP O85043
Aw	89	HIS	-	expression tag	UNP O85043
Aw	90	PRO	-	expression tag	UNP O85043
Aw	91	GLN	-	expression tag	UNP O85043
Aw	92	PHE	-	expression tag	UNP O85043
Aw	93	GLU	-	expression tag	UNP O85043
Aw	94	LYS	-	expression tag	UNP O85043
Ax	84	GLY	-	expression tag	UNP O85043
Ax	85	SER	-	expression tag	UNP O85043
Ax	86	SER	-	expression tag	UNP O85043
Ax	87	TRP	-	expression tag	UNP O85043
Ax	88	SER	-	expression tag	UNP O85043
Ax	89	HIS	-	expression tag	UNP O85043
Ax	90	PRO	-	expression tag	UNP O85043
Ax	91	GLN	-	expression tag	UNP O85043
Ax	92	PHE	-	expression tag	UNP O85043
Ax	93	GLU	-	expression tag	UNP O85043
Ax	94	LYS	-	expression tag	UNP O85043
Ay	84	GLY	-	expression tag	UNP O85043
Ay	85	SER	-	expression tag	UNP O85043
Ay	86	SER	-	expression tag	UNP O85043
Ay	87	TRP	-	expression tag	UNP O85043
Ay	88	SER	-	expression tag	UNP O85043
Ay	89	HIS	-	expression tag	UNP O85043
Ay	90	PRO	-	expression tag	UNP O85043
Ay	91	GLN	-	expression tag	UNP O85043
Ay	92	PHE	-	expression tag	UNP O85043
Ay	93	GLU	-	expression tag	UNP O85043
Ay	94	LYS	-	expression tag	UNP O85043
Az	84	GLY	-	expression tag	UNP O85043

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Chain	Residue	Modelled	Actual	Comment	Reference
Az	85	SER	-	expression tag	UNP O85043
Az	86	SER	-	expression tag	UNP O85043
Az	87	TRP	-	expression tag	UNP O85043
Az	88	SER	-	expression tag	UNP O85043
Az	89	HIS	-	expression tag	UNP O85043
Az	90	PRO	-	expression tag	UNP O85043
Az	91	GLN	-	expression tag	UNP O85043
Az	92	PHE	-	expression tag	UNP O85043
Az	93	GLU	-	expression tag	UNP O85043
Az	94	LYS	-	expression tag	UNP O85043
A0	84	GLY	-	expression tag	UNP O85043
A0	85	SER	-	expression tag	UNP O85043
A0	86	SER	-	expression tag	UNP O85043
A0	87	TRP	-	expression tag	UNP O85043
A0	88	SER	-	expression tag	UNP O85043
A0	89	HIS	-	expression tag	UNP O85043
A0	90	PRO	-	expression tag	UNP O85043
A0	91	GLN	-	expression tag	UNP O85043
A0	92	PHE	-	expression tag	UNP O85043
A0	93	GLU	-	expression tag	UNP O85043
A0	94	LYS	-	expression tag	UNP O85043
A1	84	GLY	-	expression tag	UNP O85043
A1	85	SER	-	expression tag	UNP O85043
A1	86	SER	-	expression tag	UNP O85043
A1	87	TRP	-	expression tag	UNP O85043
A1	88	SER	-	expression tag	UNP O85043
A1	89	HIS	-	expression tag	UNP O85043
A1	90	PRO	-	expression tag	UNP O85043
A1	91	GLN	-	expression tag	UNP O85043
A1	92	PHE	-	expression tag	UNP O85043
A1	93	GLU	-	expression tag	UNP O85043
A1	94	LYS	-	expression tag	UNP O85043
A2	84	GLY	-	expression tag	UNP O85043
A2	85	SER	-	expression tag	UNP O85043
A2	86	SER	-	expression tag	UNP O85043
A2	87	TRP	-	expression tag	UNP O85043
A2	88	SER	-	expression tag	UNP O85043
A2	89	HIS	-	expression tag	UNP O85043
A2	90	PRO	-	expression tag	UNP O85043
A2	91	GLN	-	expression tag	UNP O85043
A2	92	PHE	-	expression tag	UNP O85043
A2	93	GLU	-	expression tag	UNP O85043

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Chain	Residue	Modelled	Actual	Comment	Reference
A2	94	LYS	-	expression tag	UNP O85043
A3	84	GLY	-	expression tag	UNP O85043
A3	85	SER	-	expression tag	UNP O85043
A3	86	SER	-	expression tag	UNP O85043
A3	87	TRP	-	expression tag	UNP O85043
A3	88	SER	-	expression tag	UNP O85043
A3	89	HIS	-	expression tag	UNP O85043
A3	90	PRO	-	expression tag	UNP O85043
A3	91	GLN	-	expression tag	UNP O85043
A3	92	PHE	-	expression tag	UNP O85043
A3	93	GLU	-	expression tag	UNP O85043
A3	94	LYS	-	expression tag	UNP O85043
A4	84	GLY	-	expression tag	UNP O85043
A4	85	SER	-	expression tag	UNP O85043
A4	86	SER	-	expression tag	UNP O85043
A4	87	TRP	-	expression tag	UNP O85043
A4	88	SER	-	expression tag	UNP O85043
A4	89	HIS	-	expression tag	UNP O85043
A4	90	PRO	-	expression tag	UNP O85043
A4	91	GLN	-	expression tag	UNP O85043
A4	92	PHE	-	expression tag	UNP O85043
A4	93	GLU	-	expression tag	UNP O85043
A4	94	LYS	-	expression tag	UNP O85043
A5	84	GLY	-	expression tag	UNP O85043
A5	85	SER	-	expression tag	UNP O85043
A5	86	SER	-	expression tag	UNP O85043
A5	87	TRP	-	expression tag	UNP O85043
A5	88	SER	-	expression tag	UNP O85043
A5	89	HIS	-	expression tag	UNP O85043
A5	90	PRO	-	expression tag	UNP O85043
A5	91	GLN	-	expression tag	UNP O85043
A5	92	PHE	-	expression tag	UNP O85043
A5	93	GLU	-	expression tag	UNP O85043
A5	94	LYS	-	expression tag	UNP O85043
A6	84	GLY	-	expression tag	UNP O85043
A6	85	SER	-	expression tag	UNP O85043
A6	86	SER	-	expression tag	UNP O85043
A6	87	TRP	-	expression tag	UNP O85043
A6	88	SER	-	expression tag	UNP O85043
A6	89	HIS	-	expression tag	UNP O85043
A6	90	PRO	-	expression tag	UNP O85043
A6	91	GLN	-	expression tag	UNP O85043

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Chain	Residue	Modelled	Actual	Comment	Reference
A6	92	PHE	-	expression tag	UNP O85043
A6	93	GLU	-	expression tag	UNP O85043
A6	94	LYS	-	expression tag	UNP O85043
A7	84	GLY	-	expression tag	UNP O85043
A7	85	SER	-	expression tag	UNP O85043
A7	86	SER	-	expression tag	UNP O85043
A7	87	TRP	-	expression tag	UNP O85043
A7	88	SER	-	expression tag	UNP O85043
A7	89	HIS	-	expression tag	UNP O85043
A7	90	PRO	-	expression tag	UNP O85043
A7	91	GLN	-	expression tag	UNP O85043
A7	92	PHE	-	expression tag	UNP O85043
A7	93	GLU	-	expression tag	UNP O85043
A7	94	LYS	-	expression tag	UNP O85043
A8	84	GLY	-	expression tag	UNP O85043
A8	85	SER	-	expression tag	UNP O85043
A8	86	SER	-	expression tag	UNP O85043
A8	87	TRP	-	expression tag	UNP O85043
A8	88	SER	-	expression tag	UNP O85043
A8	89	HIS	-	expression tag	UNP O85043
A8	90	PRO	-	expression tag	UNP O85043
A8	91	GLN	-	expression tag	UNP O85043
A8	92	PHE	-	expression tag	UNP O85043
A8	93	GLU	-	expression tag	UNP O85043
A8	94	LYS	-	expression tag	UNP O85043
A9	84	GLY	-	expression tag	UNP O85043
A9	85	SER	-	expression tag	UNP O85043
A9	86	SER	-	expression tag	UNP O85043
A9	87	TRP	-	expression tag	UNP O85043
A9	88	SER	-	expression tag	UNP O85043
A9	89	HIS	-	expression tag	UNP O85043
A9	90	PRO	-	expression tag	UNP O85043
A9	91	GLN	-	expression tag	UNP O85043
A9	92	PHE	-	expression tag	UNP O85043
A9	93	GLU	-	expression tag	UNP O85043
A9	94	LYS	-	expression tag	UNP O85043

- Molecule 2 is a protein called Major carboxysome shell protein 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	91	Total	C	N	O	S	1	0
			655	408	124	120	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	CA	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BB	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CB	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BC	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CC	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BD	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CD	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BE	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CE	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BF	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CF	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BG	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CG	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BH	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CH	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BI	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CI	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BJ	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CJ	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BK	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CK	91	Total 647	C 403	N 121	O 120	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BL	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CL	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BM	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CM	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BN	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CN	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BO	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CO	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BP	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CP	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BQ	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CQ	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BR	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CR	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BS	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CS	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BT	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CT	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BV	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CV	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BW	91	Total 655	C 408	N 124	O 120	S 3	1	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	CW	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BX	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CX	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BY	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CY	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	BZ	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	CZ	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Ba	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Ca	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bb	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cb	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bc	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cc	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bd	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cd	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Be	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Ce	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bf	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cf	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bg	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cg	91	Total 647	C 403	N 121	O 120	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Bh	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Ch	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bi	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Ci	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bj	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cj	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bk	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Ck	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bl	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cl	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bm	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cm	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bn	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cn	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bo	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Co	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bp	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cp	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bq	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cq	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Br	91	Total 655	C 408	N 124	O 120	S 3	1	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Cr	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bs	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cs	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bt	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Ct	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bv	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cv	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bw	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cw	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bx	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cx	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	By	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cy	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	Bz	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	Cz	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	B0	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	C0	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	B1	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	C1	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	B2	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	C2	91	Total 647	C 403	N 121	O 120	S 3	0	0

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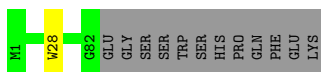
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2	B4	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	C4	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	B5	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	C5	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	B6	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	C6	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	B7	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	C7	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	B8	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	C8	91	Total 647	C 403	N 121	O 120	S 3	0	0
2	B9	91	Total 655	C 408	N 124	O 120	S 3	1	0
2	C9	91	Total 647	C 403	N 121	O 120	S 3	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.

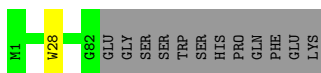
- Molecule 1: Unidentified carboxysome polypeptide

Chain AA:  86% 13%




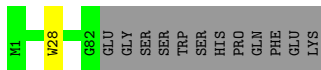
- Molecule 1: Unidentified carboxysome polypeptide

Chain AB:  86% 13%




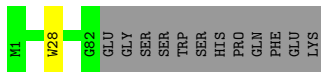
- Molecule 1: Unidentified carboxysome polypeptide

Chain AC:  86% 13%




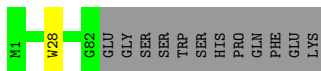
- Molecule 1: Unidentified carboxysome polypeptide

Chain AD:  86% 13%




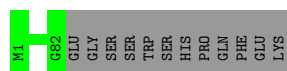
- Molecule 1: Unidentified carboxysome polypeptide

Chain AE:  86% 13%



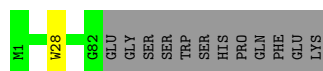
- Molecule 1: Unidentified carboxysome polypeptide

Chain AF:  87% 13%



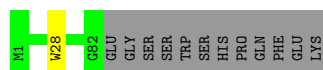
- Molecule 1: Unidentified carboxysome polypeptide

Chain AG:  86% 13%



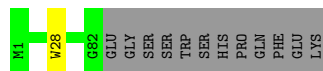
- Molecule 1: Unidentified carboxysome polypeptide

Chain AH:  86% 13%




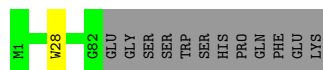
- Molecule 1: Unidentified carboxysome polypeptide

Chain AI:  86% 13%



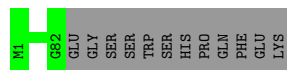
- Molecule 1: Unidentified carboxysome polypeptide

Chain AJ:  86% 13%




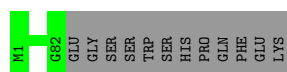
- Molecule 1: Unidentified carboxysome polypeptide

Chain AK:  87% 13%




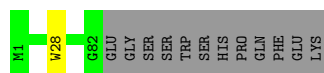
- Molecule 1: Unidentified carboxysome polypeptide

Chain AL:  87% 13%




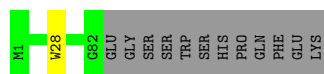
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Chain AM:  86% 13%




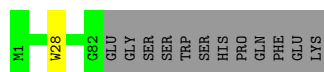
- Molecule 1: Unidentified carboxysome polypeptide

Chain AN:  86% 13%



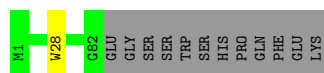
- Molecule 1: Unidentified carboxysome polypeptide

Chain AO:  86% 13%




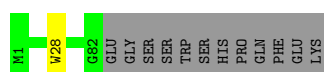
- Molecule 1: Unidentified carboxysome polypeptide

Chain AP:  86% 13%



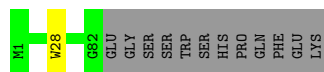
- Molecule 1: Unidentified carboxysome polypeptide

Chain AQ:  86% 13%




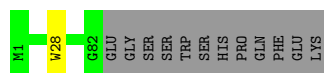
- Molecule 1: Unidentified carboxysome polypeptide

Chain AR:  86% 13%




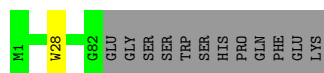
- Molecule 1: Unidentified carboxysome polypeptide

Chain AS:  86% 13%



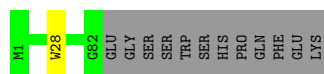
- Molecule 1: Unidentified carboxysome polypeptide

Chain AT:  86% 13%




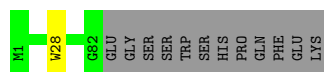
- Molecule 1: Unidentified carboxysome polypeptide

Chain AV:  86% 13%



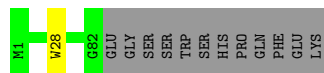
- Molecule 1: Unidentified carboxysome polypeptide

Chain AW:  86% 13%




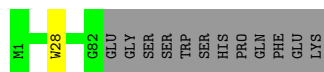
- Molecule 1: Unidentified carboxysome polypeptide

Chain AX:  86% 13%



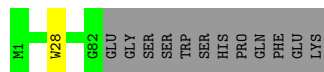
- Molecule 1: Unidentified carboxysome polypeptide

Chain AY:  86% 13%




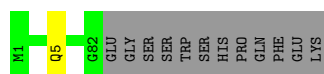
- Molecule 1: Unidentified carboxysome polypeptide

Chain AZ:  86% 13%




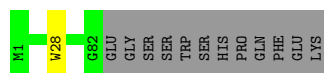
- Molecule 1: Unidentified carboxysome polypeptide

Chain Aa:  86% 13%




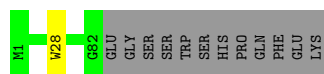
- Molecule 1: Unidentified carboxysome polypeptide

Chain Ab:  86% 13%




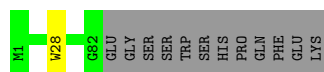
- Molecule 1: Unidentified carboxysome polypeptide

Chain Ac:  86% 13%




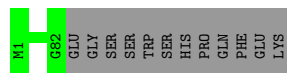
- Molecule 1: Unidentified carboxysome polypeptide

Chain Ad:  86% 13%




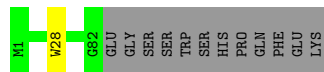
- Molecule 1: Unidentified carboxysome polypeptide

Chain Ae:  87% 13%




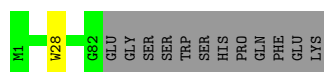
- Molecule 1: Unidentified carboxysome polypeptide

Chain Af:  86% 13%




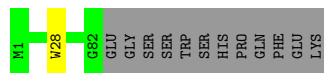
- Molecule 1: Unidentified carboxysome polypeptide

Chain Ag:  86% 13%




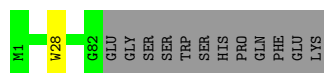
- Molecule 1: Unidentified carboxysome polypeptide

Chain Ah:  86% 13%




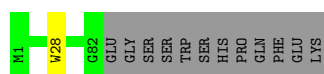
- Molecule 1: Unidentified carboxysome polypeptide

Chain Ai:  86% 13%




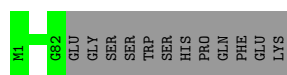
- Molecule 1: Unidentified carboxysome polypeptide

Chain Aj:  86% 13%




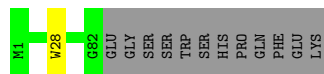
- Molecule 1: Unidentified carboxysome polypeptide

Chain Ak:  87% 13%



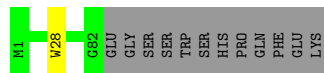
- Molecule 1: Unidentified carboxysome polypeptide

Chain Al:  86% 13%



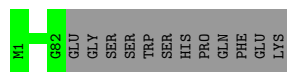
- Molecule 1: Unidentified carboxysome polypeptide

Chain Am:  86% 13%




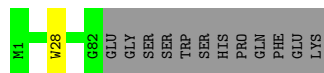
- Molecule 1: Unidentified carboxysome polypeptide

Chain An:  87% 13%




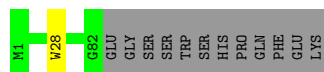
- Molecule 1: Unidentified carboxysome polypeptide

Chain Ao:  86% 13%




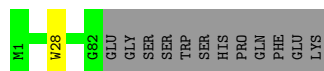
- Molecule 1: Unidentified carboxysome polypeptide

Chain Ap:  86% 13%




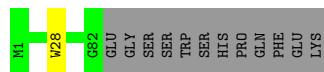
- Molecule 1: Unidentified carboxysome polypeptide

Chain Aq:  86% 13%




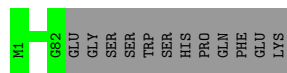
- Molecule 1: Unidentified carboxysome polypeptide

Chain Ar:  86% 13%




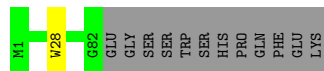
- Molecule 1: Unidentified carboxysome polypeptide

Chain As:  87% 13%



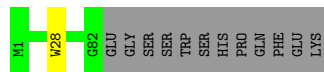
- Molecule 1: Unidentified carboxysome polypeptide

Chain At:  86% 13%



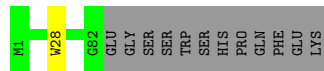
- Molecule 1: Unidentified carboxysome polypeptide

Chain Av:  86% 13%




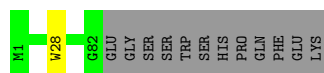
- Molecule 1: Unidentified carboxysome polypeptide

Chain Aw:  86% 13%




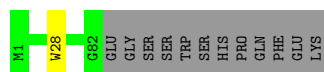
- Molecule 1: Unidentified carboxysome polypeptide

Chain Ax:  86% 13%




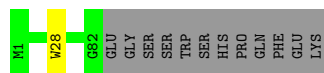
- Molecule 1: Unidentified carboxysome polypeptide

Chain Ay:  86% 13%




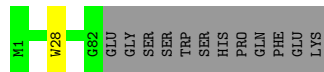
- Molecule 1: Unidentified carboxysome polypeptide

Chain Az:  86% 13%




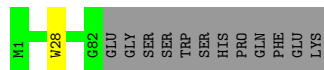
- Molecule 1: Unidentified carboxysome polypeptide

Chain A0:  86% 13%




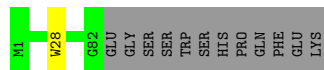
- Molecule 1: Unidentified carboxysome polypeptide

Chain A1:  86% 13%




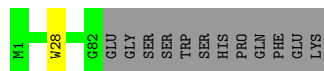
- Molecule 1: Unidentified carboxysome polypeptide

Chain A2:  86% 13%




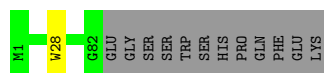
- Molecule 1: Unidentified carboxysome polypeptide

Chain A3:  86% 13%




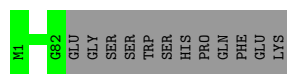
- Molecule 1: Unidentified carboxysome polypeptide

Chain A4:  86% 13%




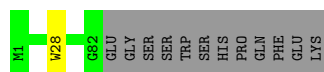
- Molecule 1: Unidentified carboxysome polypeptide

Chain A5:  87% 13%




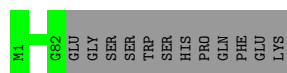
- Molecule 1: Unidentified carboxysome polypeptide

Chain A6:  86% 13%




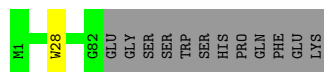
- Molecule 1: Unidentified carboxysome polypeptide

Chain A7:  87% 13%




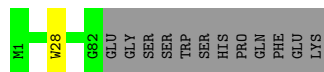
- Molecule 1: Unidentified carboxysome polypeptide

Chain A8:  86% 13%



- Molecule 1: Unidentified carboxysome polypeptide

Chain A9:  86% 13%



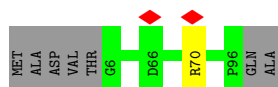
- Molecule 2: Major carboxysome shell protein 1A

Chain BA:  92% 7%



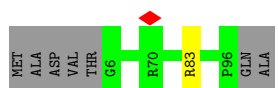
- Molecule 2: Major carboxysome shell protein 1A

Chain CA:  92% 7%



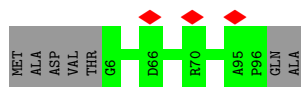
- Molecule 2: Major carboxysome shell protein 1A

Chain BB:  92% 7%



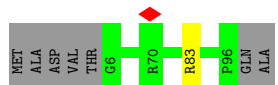
- Molecule 2: Major carboxysome shell protein 1A

Chain CB:  93% 7%



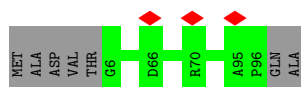
- Molecule 2: Major carboxysome shell protein 1A

Chain BC:  92% 7%



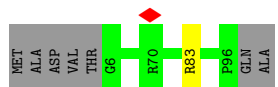
- Molecule 2: Major carboxysome shell protein 1A

Chain CC:  93% 7%



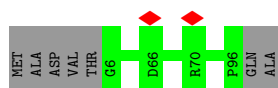
- Molecule 2: Major carboxysome shell protein 1A

Chain BD:  92% 7%



- Molecule 2: Major carboxysome shell protein 1A

Chain CD:  93% 7%



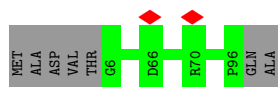
- Molecule 2: Major carboxysome shell protein 1A

Chain BE:  92% 7%



- Molecule 2: Major carboxysome shell protein 1A

Chain CE:  93% 7%



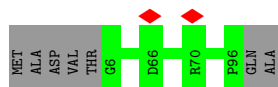
- Molecule 2: Major carboxysome shell protein 1A

Chain BF:  92% 7%



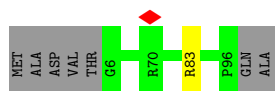
- Molecule 2: Major carboxysome shell protein 1A

Chain CF:  93% 7%



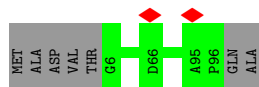
- Molecule 2: Major carboxysome shell protein 1A

Chain BG:  92% 7%



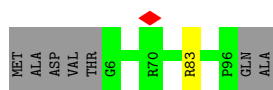
- Molecule 2: Major carboxysome shell protein 1A

Chain CG:  93% 7%

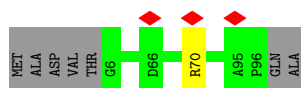


- Molecule 2: Major carboxysome shell protein 1A

Chain BH:  92% 7%



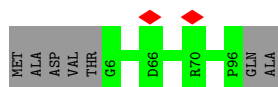
- Molecule 2: Major carboxysome shell protein 1A



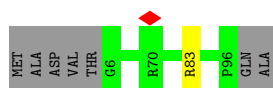
- Molecule 2: Major carboxysome shell protein 1A



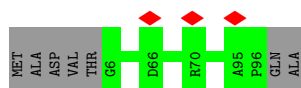
- Molecule 2: Major carboxysome shell protein 1A



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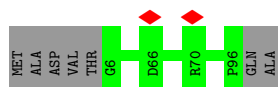


- Molecule 2: Major carboxysome shell protein 1A



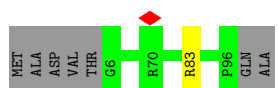
- Molecule 2: Major carboxysome shell protein 1A

Chain CK:  93% 7%



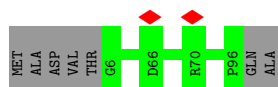
- Molecule 2: Major carboxysome shell protein 1A

Chain BL:  92% 7%



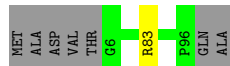
- Molecule 2: Major carboxysome shell protein 1A

Chain CL:  93% 7%



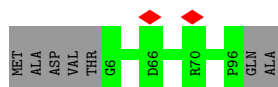
- Molecule 2: Major carboxysome shell protein 1A

Chain BM:  92% 7%



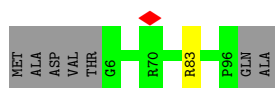
- Molecule 2: Major carboxysome shell protein 1A

Chain CM:  93% 7%



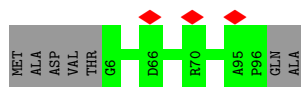
- Molecule 2: Major carboxysome shell protein 1A

Chain BN:  92% 7%



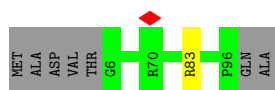
- Molecule 2: Major carboxysome shell protein 1A

Chain CN:  93% 7%



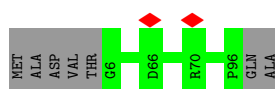
- Molecule 2: Major carboxysome shell protein 1A

Chain BO:  92% 7%



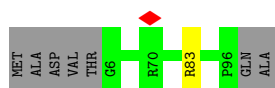
- Molecule 2: Major carboxysome shell protein 1A

Chain CO:  93% 7%



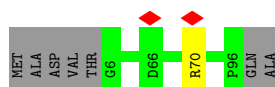
- Molecule 2: Major carboxysome shell protein 1A

Chain BP:  92% 7%



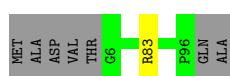
- Molecule 2: Major carboxysome shell protein 1A

Chain CP:  92% 7%



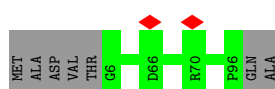
- Molecule 2: Major carboxysome shell protein 1A

Chain BQ:  92% 7%



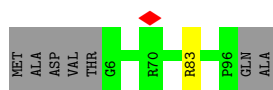
- Molecule 2: Major carboxysome shell protein 1A

Chain CQ:  93% 7%

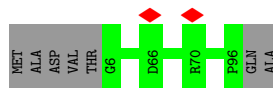


- Molecule 2: Major carboxysome shell protein 1A

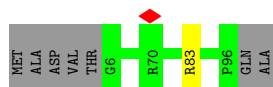
Chain BR:  92% 7%



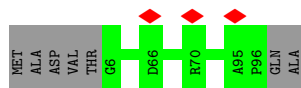
- Molecule 2: Major carboxysome shell protein 1A



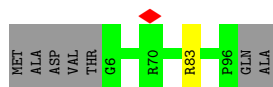
- Molecule 2: Major carboxysome shell protein 1A



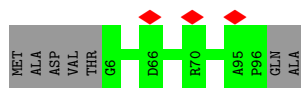
- Molecule 2: Major carboxysome shell protein 1A



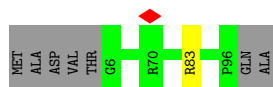
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A

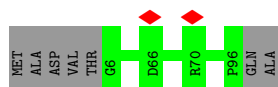


- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A

Chain CV:  93% 7%



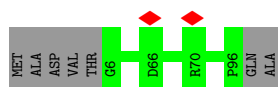
- Molecule 2: Major carboxysome shell protein 1A

Chain BW:  92% 7%



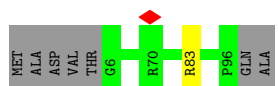
- Molecule 2: Major carboxysome shell protein 1A

Chain CW:  93% 7%



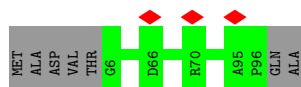
- Molecule 2: Major carboxysome shell protein 1A

Chain BX:  92% 7%



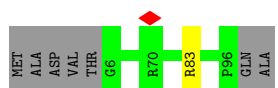
- Molecule 2: Major carboxysome shell protein 1A

Chain CX:  93% 7%



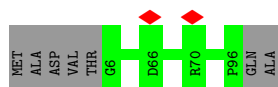
- Molecule 2: Major carboxysome shell protein 1A

Chain BY:  92% 7%



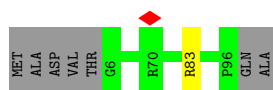
- Molecule 2: Major carboxysome shell protein 1A

Chain CY:  93% 7%



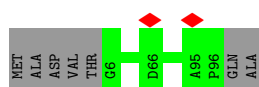
- Molecule 2: Major carboxysome shell protein 1A

Chain BZ:  92% 7%



- Molecule 2: Major carboxysome shell protein 1A

Chain CZ:  93% 7%



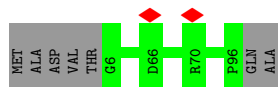
- Molecule 2: Major carboxysome shell protein 1A

Chain Ba:  92% 7%



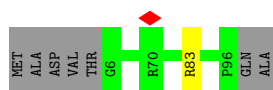
- Molecule 2: Major carboxysome shell protein 1A

Chain Ca:  93% 7%



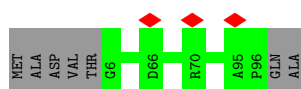
- Molecule 2: Major carboxysome shell protein 1A

Chain Bb:  92% 7%



- Molecule 2: Major carboxysome shell protein 1A

Chain Cb:  93% 7%



- Molecule 2: Major carboxysome shell protein 1A

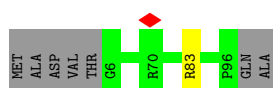
Chain Bc:  92% 7%



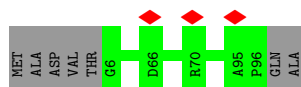
- Molecule 2: Major carboxysome shell protein 1A



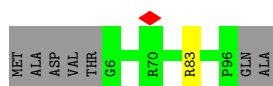
- Molecule 2: Major carboxysome shell protein 1A



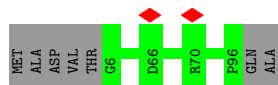
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



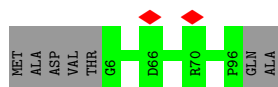
- Molecule 2: Major carboxysome shell protein 1A



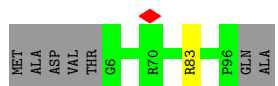
- Molecule 2: Major carboxysome shell protein 1A



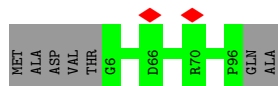
- Molecule 2: Major carboxysome shell protein 1A



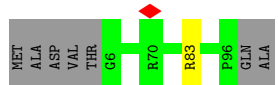
- Molecule 2: Major carboxysome shell protein 1A



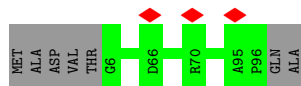
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



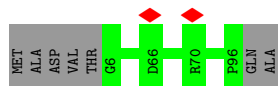
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A

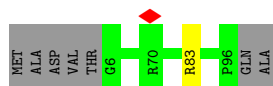


- Molecule 2: Major carboxysome shell protein 1A



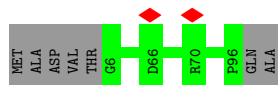
- Molecule 2: Major carboxysome shell protein 1A

Chain Bj:  92% 7%



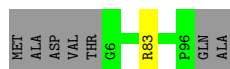
- Molecule 2: Major carboxysome shell protein 1A

Chain Cj:  93% 7%



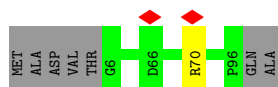
- Molecule 2: Major carboxysome shell protein 1A

Chain Bk:  92% 7%



- Molecule 2: Major carboxysome shell protein 1A

Chain Ck:  92% 7%



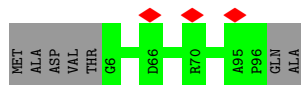
- Molecule 2: Major carboxysome shell protein 1A

Chain Bl:  92% 7%



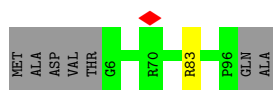
- Molecule 2: Major carboxysome shell protein 1A

Chain Cl:  93% 7%

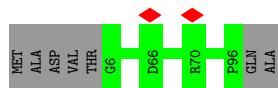


- Molecule 2: Major carboxysome shell protein 1A

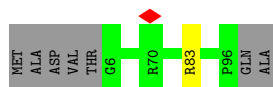
Chain Bm:  92% 7%



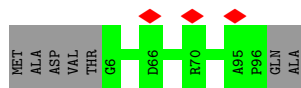
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



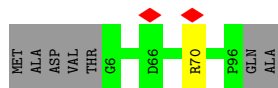
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



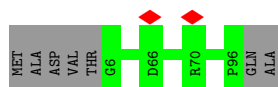
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



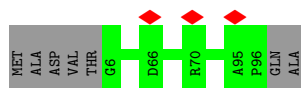
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



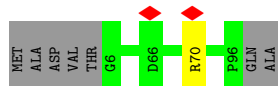
- Molecule 2: Major carboxysome shell protein 1A



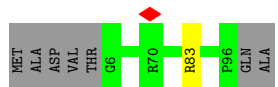
- Molecule 2: Major carboxysome shell protein 1A



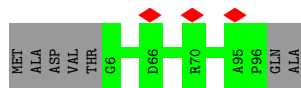
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A

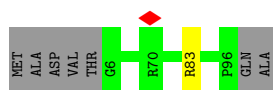


- Molecule 2: Major carboxysome shell protein 1A



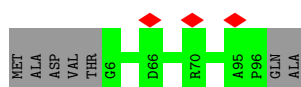
- Molecule 2: Major carboxysome shell protein 1A

Chain Bt:  92% 7%



- Molecule 2: Major carboxysome shell protein 1A

Chain Ct:  93% 7%



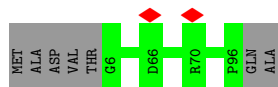
- Molecule 2: Major carboxysome shell protein 1A

Chain Bv:  92% 7%



- Molecule 2: Major carboxysome shell protein 1A

Chain Cv:  93% 7%



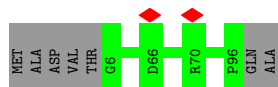
- Molecule 2: Major carboxysome shell protein 1A

Chain Bw:  92% 7%



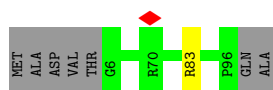
- Molecule 2: Major carboxysome shell protein 1A

Chain Cw:  93% 7%

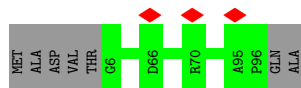


- Molecule 2: Major carboxysome shell protein 1A

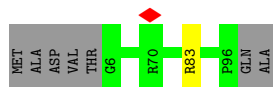
Chain Bx:  92% 7%



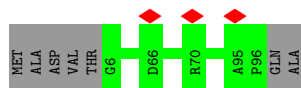
- Molecule 2: Major carboxysome shell protein 1A



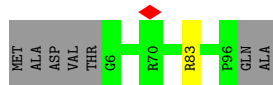
- Molecule 2: Major carboxysome shell protein 1A



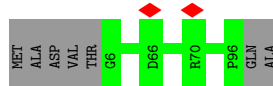
- Molecule 2: Major carboxysome shell protein 1A



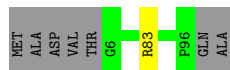
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



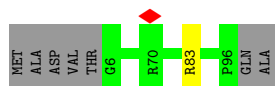
- Molecule 2: Major carboxysome shell protein 1A

Chain C0:  93% 7%



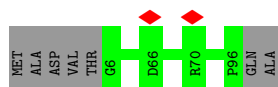
- Molecule 2: Major carboxysome shell protein 1A

Chain B1:  92% 7%



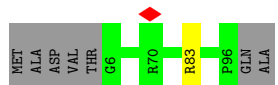
- Molecule 2: Major carboxysome shell protein 1A

Chain C1:  93% 7%



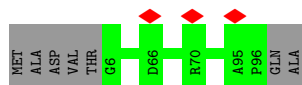
- Molecule 2: Major carboxysome shell protein 1A

Chain B2:  92% 7%



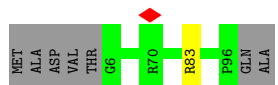
- Molecule 2: Major carboxysome shell protein 1A

Chain C2:  93% 7%



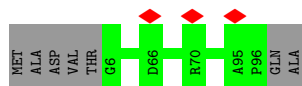
- Molecule 2: Major carboxysome shell protein 1A

Chain B3:  92% 7%



- Molecule 2: Major carboxysome shell protein 1A

Chain C3:  93% 7%



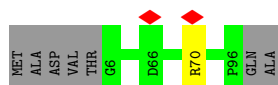
- Molecule 2: Major carboxysome shell protein 1A

Chain B4:  92% 7%



- Molecule 2: Major carboxysome shell protein 1A

Chain C4:  92% 7%



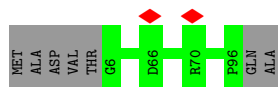
- Molecule 2: Major carboxysome shell protein 1A

Chain B5:  92% 7%



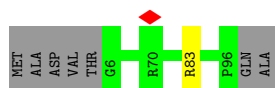
- Molecule 2: Major carboxysome shell protein 1A

Chain C5:  93% 7%



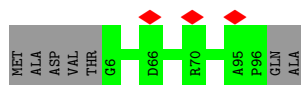
- Molecule 2: Major carboxysome shell protein 1A

Chain B6:  92% 7%



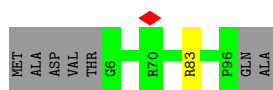
- Molecule 2: Major carboxysome shell protein 1A

Chain C6:  93% 7%

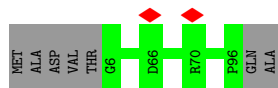


- Molecule 2: Major carboxysome shell protein 1A

Chain B7:  92% 7%



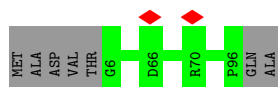
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



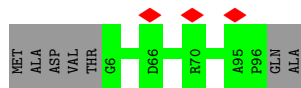
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11468	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64.3	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.122	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	275.2, 275.2, 275.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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	0.39	0/624	0.51	0/848
1	A1	0.39	0/624	0.52	0/848
1	A2	0.39	0/624	0.51	0/848
1	A3	0.40	0/624	0.52	0/848
1	A4	0.39	0/624	0.51	0/848
1	A5	0.39	0/624	0.51	0/848
1	A6	0.39	0/624	0.50	0/848
1	A7	0.39	0/624	0.51	0/848
1	A8	0.38	0/624	0.51	0/848
1	A9	0.39	0/624	0.52	0/848
1	AA	0.39	0/624	0.52	0/848
1	AB	0.39	0/624	0.51	0/848
1	AC	0.39	0/624	0.52	0/848
1	AD	0.39	0/624	0.52	0/848
1	AE	0.39	0/624	0.51	0/848
1	AF	0.39	0/624	0.51	0/848
1	AG	0.40	0/624	0.52	0/848
1	AH	0.39	0/624	0.51	0/848
1	AI	0.39	0/624	0.51	0/848
1	AJ	0.39	0/624	0.52	0/848
1	AK	0.40	0/624	0.51	0/848
1	AL	0.39	0/624	0.51	0/848
1	AM	0.38	0/624	0.51	0/848
1	AN	0.39	0/624	0.51	0/848
1	AO	0.39	0/624	0.52	0/848
1	AP	0.39	0/624	0.51	0/848
1	AQ	0.38	0/624	0.51	0/848
1	AR	0.39	0/624	0.52	0/848
1	AS	0.39	0/624	0.52	0/848
1	AT	0.39	0/624	0.51	0/848
1	AV	0.39	0/624	0.52	0/848
1	AW	0.39	0/624	0.51	0/848
1	AX	0.39	0/624	0.51	0/848
1	AY	0.39	0/624	0.52	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AZ	0.39	0/624	0.51	0/848
1	Aa	0.39	0/624	0.51	0/848
1	Ab	0.39	0/624	0.51	0/848
1	Ac	0.38	0/624	0.51	0/848
1	Ad	0.39	0/624	0.52	0/848
1	Ae	0.39	0/624	0.51	0/848
1	Af	0.39	0/624	0.52	0/848
1	Ag	0.39	0/624	0.52	0/848
1	Ah	0.40	0/624	0.51	0/848
1	Ai	0.38	0/624	0.51	0/848
1	Aj	0.39	0/624	0.51	0/848
1	Ak	0.39	0/624	0.51	0/848
1	Al	0.40	0/624	0.52	0/848
1	Am	0.39	0/624	0.52	0/848
1	An	0.39	0/624	0.50	0/848
1	Ao	0.37	0/624	0.51	0/848
1	Ap	0.39	0/624	0.52	0/848
1	Aq	0.40	0/624	0.52	0/848
1	Ar	0.38	0/624	0.51	0/848
1	As	0.39	0/624	0.51	0/848
1	At	0.39	0/624	0.51	0/848
1	Av	0.39	0/624	0.52	0/848
1	Aw	0.39	0/624	0.51	0/848
1	Ax	0.40	0/624	0.52	0/848
1	Ay	0.39	0/624	0.51	0/848
1	Az	0.39	0/624	0.52	0/848
2	B0	0.37	0/664	0.59	0/899
2	B1	0.37	0/664	0.58	0/899
2	B2	0.38	0/664	0.59	0/899
2	B3	0.38	0/664	0.58	0/899
2	B4	0.38	0/664	0.59	0/899
2	B5	0.37	0/664	0.59	0/899
2	B6	0.37	0/664	0.60	0/899
2	B7	0.37	0/664	0.58	0/899
2	B8	0.38	0/664	0.58	0/899
2	B9	0.38	0/664	0.60	0/899
2	BA	0.37	0/664	0.60	0/899
2	BB	0.37	0/664	0.60	0/899
2	BC	0.38	0/664	0.59	0/899
2	BD	0.38	0/664	0.58	0/899
2	BE	0.38	0/664	0.58	0/899
2	BF	0.37	0/664	0.59	0/899
2	BG	0.38	0/664	0.59	0/899

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	BH	0.37	0/664	0.60	0/899
2	BI	0.37	0/664	0.57	0/899
2	BJ	0.37	0/664	0.59	0/899
2	BK	0.37	0/664	0.59	0/899
2	BL	0.37	0/664	0.59	0/899
2	BM	0.38	0/664	0.59	0/899
2	BN	0.38	0/664	0.60	0/899
2	BO	0.38	0/664	0.59	0/899
2	BP	0.37	0/664	0.59	0/899
2	BQ	0.38	0/664	0.57	0/899
2	BR	0.37	0/664	0.59	0/899
2	BS	0.38	0/664	0.58	0/899
2	BT	0.37	0/664	0.60	0/899
2	BV	0.37	0/664	0.59	0/899
2	BW	0.38	0/664	0.58	0/899
2	BX	0.38	0/664	0.60	0/899
2	BY	0.37	0/664	0.58	0/899
2	BZ	0.38	0/664	0.60	0/899
2	Ba	0.37	0/664	0.59	0/899
2	Bb	0.38	0/664	0.60	0/899
2	Bc	0.38	0/664	0.58	0/899
2	Bd	0.38	0/664	0.59	0/899
2	Be	0.37	0/664	0.58	0/899
2	Bf	0.37	0/664	0.57	0/899
2	Bg	0.37	0/664	0.58	0/899
2	Bh	0.38	0/664	0.59	0/899
2	Bi	0.38	0/664	0.58	0/899
2	Bj	0.38	0/664	0.60	0/899
2	Bk	0.37	0/664	0.60	0/899
2	Bl	0.38	0/664	0.59	0/899
2	Bm	0.37	0/664	0.58	0/899
2	Bn	0.38	0/664	0.61	0/899
2	Bo	0.38	0/664	0.59	0/899
2	Bp	0.37	0/664	0.58	0/899
2	Bq	0.38	0/664	0.59	0/899
2	Br	0.38	0/664	0.58	0/899
2	Bs	0.37	0/664	0.59	0/899
2	Bt	0.37	0/664	0.61	0/899
2	Bv	0.37	0/664	0.59	0/899
2	Bw	0.38	0/664	0.59	0/899
2	Bx	0.38	0/664	0.59	0/899
2	By	0.37	0/664	0.62	0/899
2	Bz	0.37	0/664	0.58	0/899

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	C0	0.38	0/653	0.57	0/885
2	C1	0.38	0/653	0.57	0/885
2	C2	0.38	0/653	0.58	0/885
2	C3	0.38	0/653	0.57	0/885
2	C4	0.39	0/653	0.60	0/885
2	C5	0.39	0/653	0.58	0/885
2	C6	0.38	0/653	0.59	0/885
2	C7	0.38	0/653	0.59	0/885
2	C8	0.39	0/653	0.61	0/885
2	C9	0.38	0/653	0.57	0/885
2	CA	0.39	0/653	0.58	0/885
2	CB	0.38	0/653	0.59	0/885
2	CC	0.38	0/653	0.56	0/885
2	CD	0.38	0/653	0.60	0/885
2	CE	0.39	0/653	0.60	0/885
2	CF	0.39	0/653	0.57	0/885
2	CG	0.38	0/653	0.58	0/885
2	CH	0.39	0/653	0.62	0/885
2	CI	0.39	0/653	0.60	0/885
2	CJ	0.38	0/653	0.58	0/885
2	CK	0.39	0/653	0.58	0/885
2	CL	0.39	0/653	0.59	0/885
2	CM	0.39	0/653	0.60	0/885
2	CN	0.38	0/653	0.59	0/885
2	CO	0.38	0/653	0.58	0/885
2	CP	0.39	0/653	0.58	0/885
2	CQ	0.39	0/653	0.60	0/885
2	CR	0.38	0/653	0.58	0/885
2	CS	0.38	0/653	0.57	0/885
2	CT	0.38	0/653	0.59	0/885
2	CV	0.39	0/653	0.58	0/885
2	CW	0.39	0/653	0.60	0/885
2	CX	0.39	0/653	0.60	0/885
2	CY	0.38	0/653	0.57	0/885
2	CZ	0.38	0/653	0.57	0/885
2	Ca	0.39	0/653	0.58	0/885
2	Cb	0.38	0/653	0.59	0/885
2	Cc	0.39	0/653	0.59	0/885
2	Cd	0.38	0/653	0.57	0/885
2	Ce	0.38	0/653	0.58	0/885
2	Cf	0.39	0/653	0.58	0/885
2	Cg	0.39	0/653	0.59	0/885
2	Ch	0.38	0/653	0.58	0/885

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Ci	0.39	0/653	0.60	0/885
2	Cj	0.38	0/653	0.59	0/885
2	Ck	0.39	0/653	0.58	0/885
2	Cl	0.38	0/653	0.58	0/885
2	Cm	0.38	0/653	0.59	0/885
2	Cn	0.38	0/653	0.59	0/885
2	Co	0.39	0/653	0.62	0/885
2	Cp	0.39	0/653	0.58	0/885
2	Cq	0.38	0/653	0.58	0/885
2	Cr	0.38	0/653	0.60	0/885
2	Cs	0.38	0/653	0.58	0/885
2	Ct	0.38	0/653	0.58	0/885
2	Cv	0.39	0/653	0.58	0/885
2	Cw	0.39	0/653	0.61	0/885
2	Cx	0.38	0/653	0.58	0/885
2	Cy	0.38	0/653	0.59	0/885
2	Cz	0.38	0/653	0.57	0/885
All	All	0.38	0/116460	0.56	0/157920

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	A1	80/94 (85%)	74 (92%)	6 (8%)	0	100	100
1	A2	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	A3	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	A4	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	A5	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
1	A6	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
1	A7	80/94 (85%)	74 (92%)	6 (8%)	0	100	100
1	A8	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	A9	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	AA	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
1	AB	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
1	AC	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	AD	80/94 (85%)	72 (90%)	8 (10%)	0	100	100
1	AE	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	AF	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
1	AG	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	AH	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
1	AI	80/94 (85%)	74 (92%)	6 (8%)	0	100	100
1	AJ	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	AK	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
1	AL	80/94 (85%)	74 (92%)	6 (8%)	0	100	100
1	AM	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	AN	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	AO	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	AP	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
1	AQ	80/94 (85%)	74 (92%)	6 (8%)	0	100	100
1	AR	80/94 (85%)	73 (91%)	7 (9%)	0	100	100
1	AS	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	AT	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
1	AV	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	AW	80/94 (85%)	74 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AX	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	AY	80/94 (85%)	74 (92%)	6 (8%)	0	100	100
1	AZ	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	Aa	80/94 (85%)	74 (92%)	6 (8%)	0	100	100
1	Ab	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	Ac	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	Ad	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	Ae	80/94 (85%)	74 (92%)	6 (8%)	0	100	100
1	Af	80/94 (85%)	74 (92%)	6 (8%)	0	100	100
1	Ag	80/94 (85%)	73 (91%)	7 (9%)	0	100	100
1	Ah	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	Ai	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	Aj	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
1	Ak	80/94 (85%)	74 (92%)	6 (8%)	0	100	100
1	Al	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	Am	80/94 (85%)	74 (92%)	6 (8%)	0	100	100
1	An	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
1	Ao	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	Ap	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
1	Aq	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	Ar	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	As	80/94 (85%)	73 (91%)	7 (9%)	0	100	100
1	At	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
1	Av	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
1	Aw	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	Ax	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
1	Ay	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
1	Az	80/94 (85%)	73 (91%)	7 (9%)	0	100	100
2	B0	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	B1	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	B2	90/98 (92%)	88 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B3	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	B4	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	B5	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	B6	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	B7	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	B8	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	B9	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	BA	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	BB	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	BC	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	BD	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	BE	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	BF	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	BG	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	BH	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	BI	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	BJ	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	BK	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	BL	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	BM	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	BN	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	BO	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	BP	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	BQ	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	BR	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	BS	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	BT	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	BV	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	BW	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	BX	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	BY	90/98 (92%)	87 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BZ	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	Ba	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	Bb	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	Bc	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	Bd	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	Be	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	Bf	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	Bg	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	Bh	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	Bi	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	Bj	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	Bk	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	Bl	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	Bm	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	Bn	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	Bo	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	Bp	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	Bq	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	Br	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	Bs	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	Bt	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	Bv	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	Bw	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	Bx	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
2	By	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	Bz	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
2	C0	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	C1	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	C2	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	C3	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	C4	89/98 (91%)	86 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C5	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	C6	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	C7	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	C8	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	C9	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	CA	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	CB	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	CC	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	CD	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	CE	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	CF	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	CG	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	CH	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	CI	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	CJ	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	CK	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	CL	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	CM	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	CN	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	CO	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	CP	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	CQ	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	CR	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	CS	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	CT	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	CV	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	CW	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	CX	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	CY	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	CZ	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	Ca	89/98 (91%)	86 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Cb	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	Cc	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	Cd	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	Ce	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	Cf	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	Cg	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	Ch	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	Ci	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	Cj	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	Ck	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	Cl	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	Cm	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	Cn	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	Co	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	Cp	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	Cq	89/98 (91%)	87 (98%)	2 (2%)	0	100	100
2	Cr	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	Cs	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	Ct	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	Cv	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	Cw	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	Cx	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	Cy	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
2	Cz	89/98 (91%)	86 (97%)	3 (3%)	0	100	100
All	All	15540/17400 (89%)	14923 (96%)	617 (4%)	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	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	A1	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	A2	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	A3	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	A4	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	A5	66/77 (86%)	66 (100%)	0	100	100
1	A6	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	A7	66/77 (86%)	66 (100%)	0	100	100
1	A8	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	A9	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AA	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AB	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AC	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AD	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AE	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AF	66/77 (86%)	66 (100%)	0	100	100
1	AG	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AH	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AI	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AJ	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AK	66/77 (86%)	66 (100%)	0	100	100
1	AL	66/77 (86%)	66 (100%)	0	100	100
1	AM	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AN	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AO	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AP	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AQ	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AR	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AS	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AT	66/77 (86%)	65 (98%)	1 (2%)	65	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AV	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AW	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AX	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AY	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	AZ	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Aa	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Ab	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Ac	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Ad	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Ae	66/77 (86%)	66 (100%)	0	100	100
1	Af	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Ag	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Ah	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Ai	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Aj	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Ak	66/77 (86%)	66 (100%)	0	100	100
1	Al	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Am	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	An	66/77 (86%)	66 (100%)	0	100	100
1	Ao	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Ap	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Aq	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Ar	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	As	66/77 (86%)	66 (100%)	0	100	100
1	At	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Av	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Aw	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Ax	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Ay	66/77 (86%)	65 (98%)	1 (2%)	65	83
1	Az	66/77 (86%)	65 (98%)	1 (2%)	65	83
2	B0	63/67 (94%)	61 (97%)	2 (3%)	39	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B1	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	B2	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	B3	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	B4	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	B5	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	B6	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	B7	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	B8	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	B9	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BA	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BB	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BC	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BD	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BE	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BF	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BG	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BH	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BI	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BJ	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BK	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BL	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BM	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BN	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BO	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BP	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BQ	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BR	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BS	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BT	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BV	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BW	63/67 (94%)	61 (97%)	2 (3%)	39	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BX	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BY	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	BZ	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Ba	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bb	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bc	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bd	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Be	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bf	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bg	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bh	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bi	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bj	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bk	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bl	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bm	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bn	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bo	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bp	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bq	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Br	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bs	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bt	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bv	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bw	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bx	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	By	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	Bz	63/67 (94%)	61 (97%)	2 (3%)	39	69
2	C0	62/67 (92%)	62 (100%)	0	100	100
2	C1	62/67 (92%)	62 (100%)	0	100	100
2	C2	62/67 (92%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C3	62/67 (92%)	62 (100%)	0	100	100
2	C4	62/67 (92%)	61 (98%)	1 (2%)	62	82
2	C5	62/67 (92%)	62 (100%)	0	100	100
2	C6	62/67 (92%)	62 (100%)	0	100	100
2	C7	62/67 (92%)	62 (100%)	0	100	100
2	C8	62/67 (92%)	62 (100%)	0	100	100
2	C9	62/67 (92%)	62 (100%)	0	100	100
2	CA	62/67 (92%)	61 (98%)	1 (2%)	62	82
2	CB	62/67 (92%)	62 (100%)	0	100	100
2	CC	62/67 (92%)	62 (100%)	0	100	100
2	CD	62/67 (92%)	62 (100%)	0	100	100
2	CE	62/67 (92%)	62 (100%)	0	100	100
2	CF	62/67 (92%)	62 (100%)	0	100	100
2	CG	62/67 (92%)	62 (100%)	0	100	100
2	CH	62/67 (92%)	61 (98%)	1 (2%)	62	82
2	CI	62/67 (92%)	62 (100%)	0	100	100
2	CJ	62/67 (92%)	62 (100%)	0	100	100
2	CK	62/67 (92%)	62 (100%)	0	100	100
2	CL	62/67 (92%)	62 (100%)	0	100	100
2	CM	62/67 (92%)	62 (100%)	0	100	100
2	CN	62/67 (92%)	62 (100%)	0	100	100
2	CO	62/67 (92%)	62 (100%)	0	100	100
2	CP	62/67 (92%)	61 (98%)	1 (2%)	62	82
2	CQ	62/67 (92%)	62 (100%)	0	100	100
2	CR	62/67 (92%)	62 (100%)	0	100	100
2	CS	62/67 (92%)	62 (100%)	0	100	100
2	CT	62/67 (92%)	62 (100%)	0	100	100
2	CV	62/67 (92%)	62 (100%)	0	100	100
2	CW	62/67 (92%)	62 (100%)	0	100	100
2	CX	62/67 (92%)	62 (100%)	0	100	100
2	CY	62/67 (92%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	CZ	62/67 (92%)	62 (100%)	0	100	100
2	Ca	62/67 (92%)	62 (100%)	0	100	100
2	Cb	62/67 (92%)	62 (100%)	0	100	100
2	Cc	62/67 (92%)	61 (98%)	1 (2%)	62	82
2	Cd	62/67 (92%)	62 (100%)	0	100	100
2	Ce	62/67 (92%)	62 (100%)	0	100	100
2	Cf	62/67 (92%)	62 (100%)	0	100	100
2	Cg	62/67 (92%)	62 (100%)	0	100	100
2	Ch	62/67 (92%)	62 (100%)	0	100	100
2	Ci	62/67 (92%)	62 (100%)	0	100	100
2	Cj	62/67 (92%)	62 (100%)	0	100	100
2	Ck	62/67 (92%)	61 (98%)	1 (2%)	62	82
2	Cl	62/67 (92%)	62 (100%)	0	100	100
2	Cm	62/67 (92%)	62 (100%)	0	100	100
2	Cn	62/67 (92%)	62 (100%)	0	100	100
2	Co	62/67 (92%)	61 (98%)	1 (2%)	62	82
2	Cp	62/67 (92%)	62 (100%)	0	100	100
2	Cq	62/67 (92%)	62 (100%)	0	100	100
2	Cr	62/67 (92%)	61 (98%)	1 (2%)	62	82
2	Cs	62/67 (92%)	62 (100%)	0	100	100
2	Ct	62/67 (92%)	62 (100%)	0	100	100
2	Cv	62/67 (92%)	62 (100%)	0	100	100
2	Cw	62/67 (92%)	62 (100%)	0	100	100
2	Cx	62/67 (92%)	62 (100%)	0	100	100
2	Cy	62/67 (92%)	62 (100%)	0	100	100
2	Cz	62/67 (92%)	62 (100%)	0	100	100
All	All	11460/12660 (90%)	11281 (98%)	179 (2%)	77	82

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	28	TRP
2	BA	83[A]	ARG

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Mol	Chain	Res	Type
2	BA	83[B]	ARG
2	CA	70	ARG
1	AB	28	TRP
2	BB	83[A]	ARG
2	BB	83[B]	ARG
1	AC	28	TRP
2	BC	83[A]	ARG
2	BC	83[B]	ARG
1	AD	28	TRP
2	BD	83[A]	ARG
2	BD	83[B]	ARG
1	AE	28	TRP
2	BE	83[A]	ARG
2	BE	83[B]	ARG
2	BF	83[A]	ARG
2	BF	83[B]	ARG
1	AG	28	TRP
2	BG	83[A]	ARG
2	BG	83[B]	ARG
1	AH	28	TRP
2	BH	83[A]	ARG
2	BH	83[B]	ARG
2	CH	70	ARG
1	AI	28	TRP
2	BI	83[A]	ARG
2	BI	83[B]	ARG
1	AJ	28	TRP
2	BJ	83[A]	ARG
2	BJ	83[B]	ARG
2	BK	83[A]	ARG
2	BK	83[B]	ARG
2	BL	83[A]	ARG
2	BL	83[B]	ARG
1	AM	28	TRP
2	BM	83[A]	ARG
2	BM	83[B]	ARG
1	AN	28	TRP
2	BN	83[A]	ARG
2	BN	83[B]	ARG
1	AO	28	TRP
2	BO	83[A]	ARG
2	BO	83[B]	ARG

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Mol	Chain	Res	Type
1	AP	28	TRP
2	BP	83[A]	ARG
2	BP	83[B]	ARG
2	CP	70	ARG
1	AQ	28	TRP
2	BQ	83[A]	ARG
2	BQ	83[B]	ARG
1	AR	28	TRP
2	BR	83[A]	ARG
2	BR	83[B]	ARG
1	AS	28	TRP
2	BS	83[A]	ARG
2	BS	83[B]	ARG
1	AT	28	TRP
2	BT	83[A]	ARG
2	BT	83[B]	ARG
1	AV	28	TRP
2	BV	83[A]	ARG
2	BV	83[B]	ARG
1	AW	28	TRP
2	BW	83[A]	ARG
2	BW	83[B]	ARG
1	AX	28	TRP
2	BX	83[A]	ARG
2	BX	83[B]	ARG
1	AY	28	TRP
2	BY	83[A]	ARG
2	BY	83[B]	ARG
1	AZ	28	TRP
2	BZ	83[A]	ARG
2	BZ	83[B]	ARG
1	Aa	5	GLN
2	Ba	83[A]	ARG
2	Ba	83[B]	ARG
1	Ab	28	TRP
2	Bb	83[A]	ARG
2	Bb	83[B]	ARG
1	Ac	28	TRP
2	Bc	83[A]	ARG
2	Bc	83[B]	ARG
2	Cc	70	ARG
1	Ad	28	TRP

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Mol	Chain	Res	Type
2	Bd	83[A]	ARG
2	Bd	83[B]	ARG
2	Be	83[A]	ARG
2	Be	83[B]	ARG
1	Af	28	TRP
2	Bf	83[A]	ARG
2	Bf	83[B]	ARG
1	Ag	28	TRP
2	Bg	83[A]	ARG
2	Bg	83[B]	ARG
1	Ah	28	TRP
2	Bh	83[A]	ARG
2	Bh	83[B]	ARG
1	Ai	28	TRP
2	Bi	83[A]	ARG
2	Bi	83[B]	ARG
1	Aj	28	TRP
2	Bj	83[A]	ARG
2	Bj	83[B]	ARG
2	Bk	83[A]	ARG
2	Bk	83[B]	ARG
2	Ck	70	ARG
1	Al	28	TRP
2	Bl	83[A]	ARG
2	Bl	83[B]	ARG
1	Am	28	TRP
2	Bm	83[A]	ARG
2	Bm	83[B]	ARG
2	Bn	83[A]	ARG
2	Bn	83[B]	ARG
1	Ao	28	TRP
2	Bo	83[A]	ARG
2	Bo	83[B]	ARG
2	Co	70	ARG
1	Ap	28	TRP
2	Bp	83[A]	ARG
2	Bp	83[B]	ARG
1	Aq	28	TRP
2	Bq	83[A]	ARG
2	Bq	83[B]	ARG
1	Ar	28	TRP
2	Br	83[A]	ARG

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Mol	Chain	Res	Type
2	Br	83[B]	ARG
2	Cr	70	ARG
2	Bs	83[A]	ARG
2	Bs	83[B]	ARG
1	At	28	TRP
2	Bt	83[A]	ARG
2	Bt	83[B]	ARG
1	Av	28	TRP
2	Bv	83[A]	ARG
2	Bv	83[B]	ARG
1	Aw	28	TRP
2	Bw	83[A]	ARG
2	Bw	83[B]	ARG
1	Ax	28	TRP
2	Bx	83[A]	ARG
2	Bx	83[B]	ARG
1	Ay	28	TRP
2	By	83[A]	ARG
2	By	83[B]	ARG
1	Az	28	TRP
2	Bz	83[A]	ARG
2	Bz	83[B]	ARG
1	A0	28	TRP
2	B0	83[A]	ARG
2	B0	83[B]	ARG
1	A1	28	TRP
2	B1	83[A]	ARG
2	B1	83[B]	ARG
1	A2	28	TRP
2	B2	83[A]	ARG
2	B2	83[B]	ARG
1	A3	28	TRP
2	B3	83[A]	ARG
2	B3	83[B]	ARG
1	A4	28	TRP
2	B4	83[A]	ARG
2	B4	83[B]	ARG
2	C4	70	ARG
2	B5	83[A]	ARG
2	B5	83[B]	ARG
1	A6	28	TRP
2	B6	83[A]	ARG

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Mol	Chain	Res	Type
2	B6	83[B]	ARG
2	B7	83[A]	ARG
2	B7	83[B]	ARG
1	A8	28	TRP
2	B8	83[A]	ARG
2	B8	83[B]	ARG
1	A9	28	TRP
2	B9	83[A]	ARG
2	B9	83[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	21	HIS
2	BA	90	ASN
1	AB	21	HIS
1	AC	21	HIS
2	BC	90	ASN
1	AD	21	HIS
1	AE	21	HIS
2	BE	90	ASN
1	AF	21	HIS
2	BF	90	ASN
1	AG	21	HIS
2	BG	90	ASN
1	AH	21	HIS
2	BH	90	ASN
1	AI	21	HIS
2	BI	90	ASN
1	AJ	21	HIS
2	BJ	90	ASN
1	AK	21	HIS
2	BK	90	ASN
1	AL	21	HIS
2	BL	90	ASN
1	AM	21	HIS
1	AN	21	HIS
2	BO	90	ASN
1	AP	21	HIS
2	BP	90	ASN
1	AQ	21	HIS
1	AR	21	HIS

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Mol	Chain	Res	Type
2	BR	90	ASN
1	AS	21	HIS
2	BS	90	ASN
2	BT	90	ASN
1	AV	21	HIS
2	BV	90	ASN
1	AW	21	HIS
2	BW	90	ASN
1	AX	21	HIS
1	AY	21	HIS
2	BY	90	ASN
1	AZ	21	HIS
2	BZ	90	ASN
1	Aa	5	GLN
1	Aa	21	HIS
2	Ba	90	ASN
1	Ab	21	HIS
1	Ac	21	HIS
2	Bc	90	ASN
1	Ad	21	HIS
2	Bd	90	ASN
2	Be	90	ASN
1	Af	21	HIS
2	Bf	90	ASN
1	Ag	21	HIS
2	Bg	90	ASN
1	Ah	21	HIS
2	Bh	90	ASN
1	Ai	21	HIS
2	Bi	90	ASN
1	Aj	21	HIS
2	Bj	90	ASN
1	Ak	21	HIS
2	Bk	90	ASN
1	Al	21	HIS
2	Bl	90	ASN
1	Am	21	HIS
2	Bm	90	ASN
1	An	21	HIS
1	Ao	21	HIS
2	Bo	90	ASN
1	Ap	21	HIS

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Mol	Chain	Res	Type
2	Bp	90	ASN
1	Aq	21	HIS
2	Bq	90	ASN
1	Ar	21	HIS
1	As	21	HIS
2	Bs	90	ASN
1	At	21	HIS
1	Av	21	HIS
2	Bv	90	ASN
1	Aw	21	HIS
2	Bw	90	ASN
1	Ax	21	HIS
2	Bx	90	ASN
1	Az	21	HIS
2	Bz	90	ASN
1	A0	21	HIS
2	B0	90	ASN
1	A1	21	HIS
2	B1	90	ASN
1	A2	21	HIS
1	A3	21	HIS
2	B3	90	ASN
1	A4	21	HIS
2	B4	90	ASN
1	A5	21	HIS
2	B5	90	ASN
1	A6	21	HIS
2	B7	90	ASN
1	A8	21	HIS
2	B9	90	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

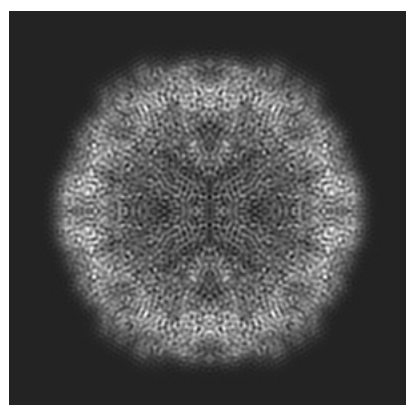
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30384. These allow visual inspection of the internal detail of the map and identification of artifacts.

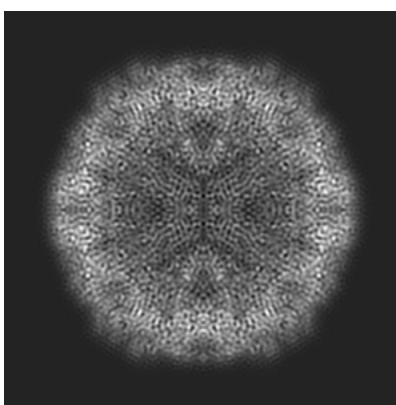
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

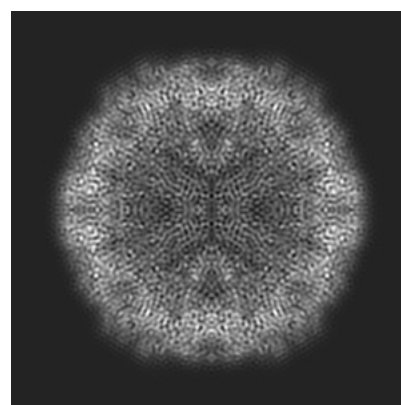
6.1.1 Primary map



X



Y

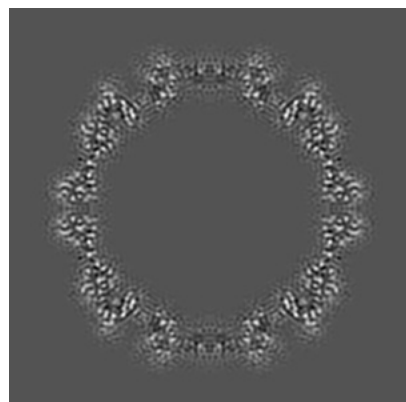


Z

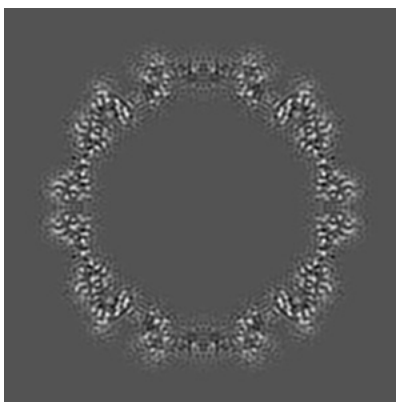
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

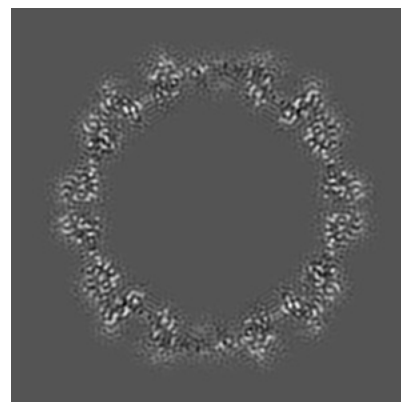
6.2.1 Primary map



X Index: 160



Y Index: 160

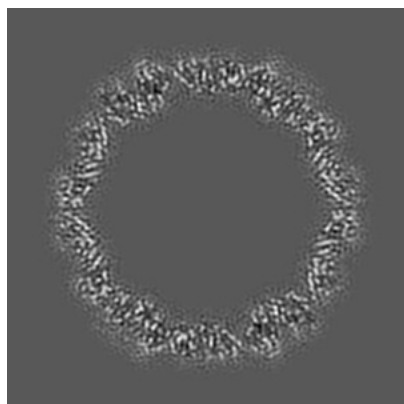


Z Index: 160

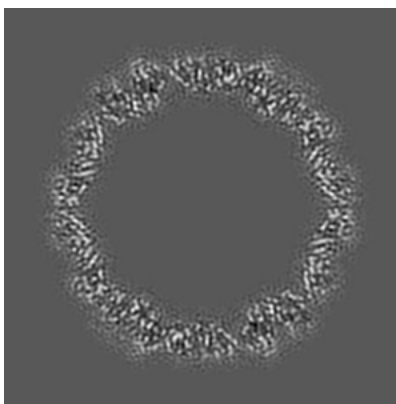
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

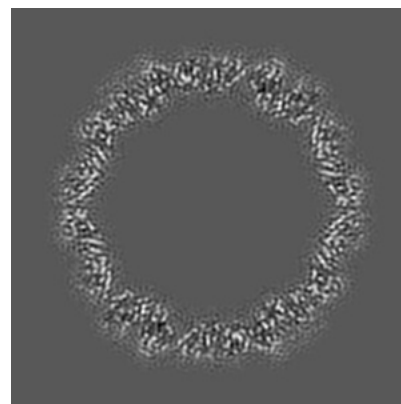
6.3.1 Primary map



X Index: 172



Y Index: 172

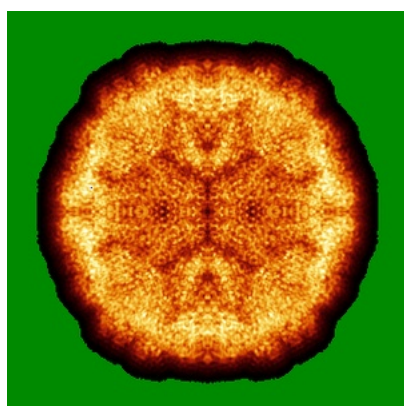


Z Index: 147

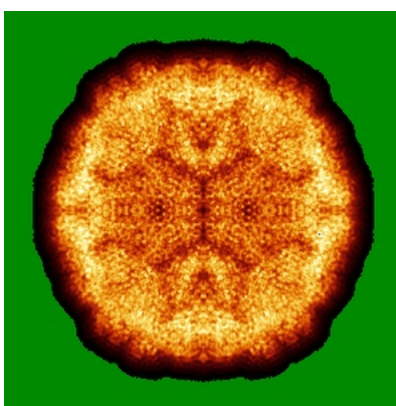
The images above show the largest variance slices of the map in three orthogonal directions.

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

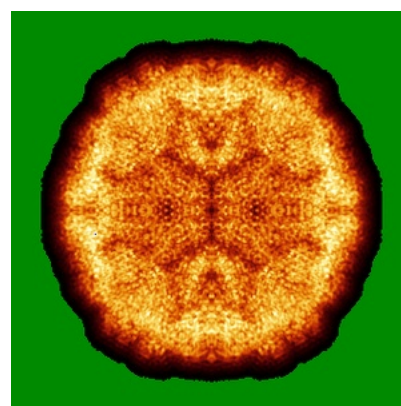
6.4.1 Primary map



X



Y

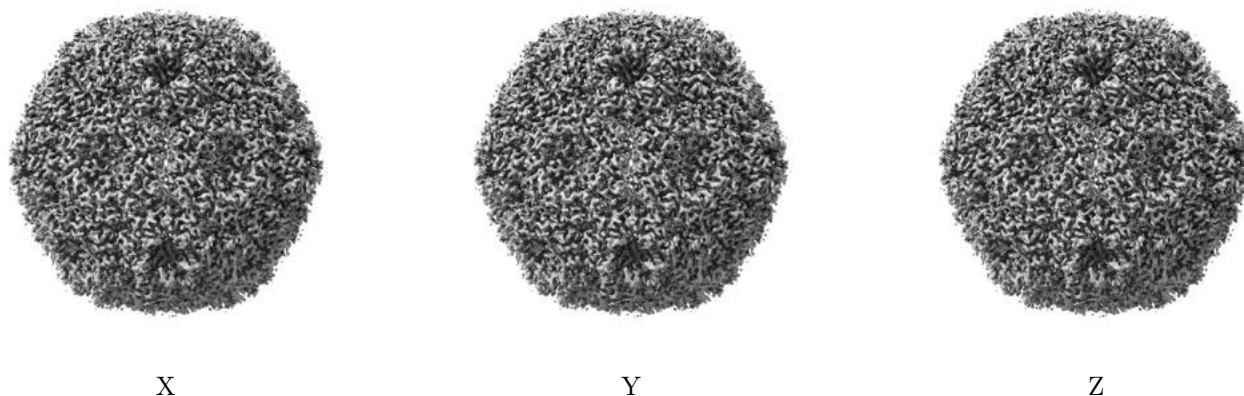


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

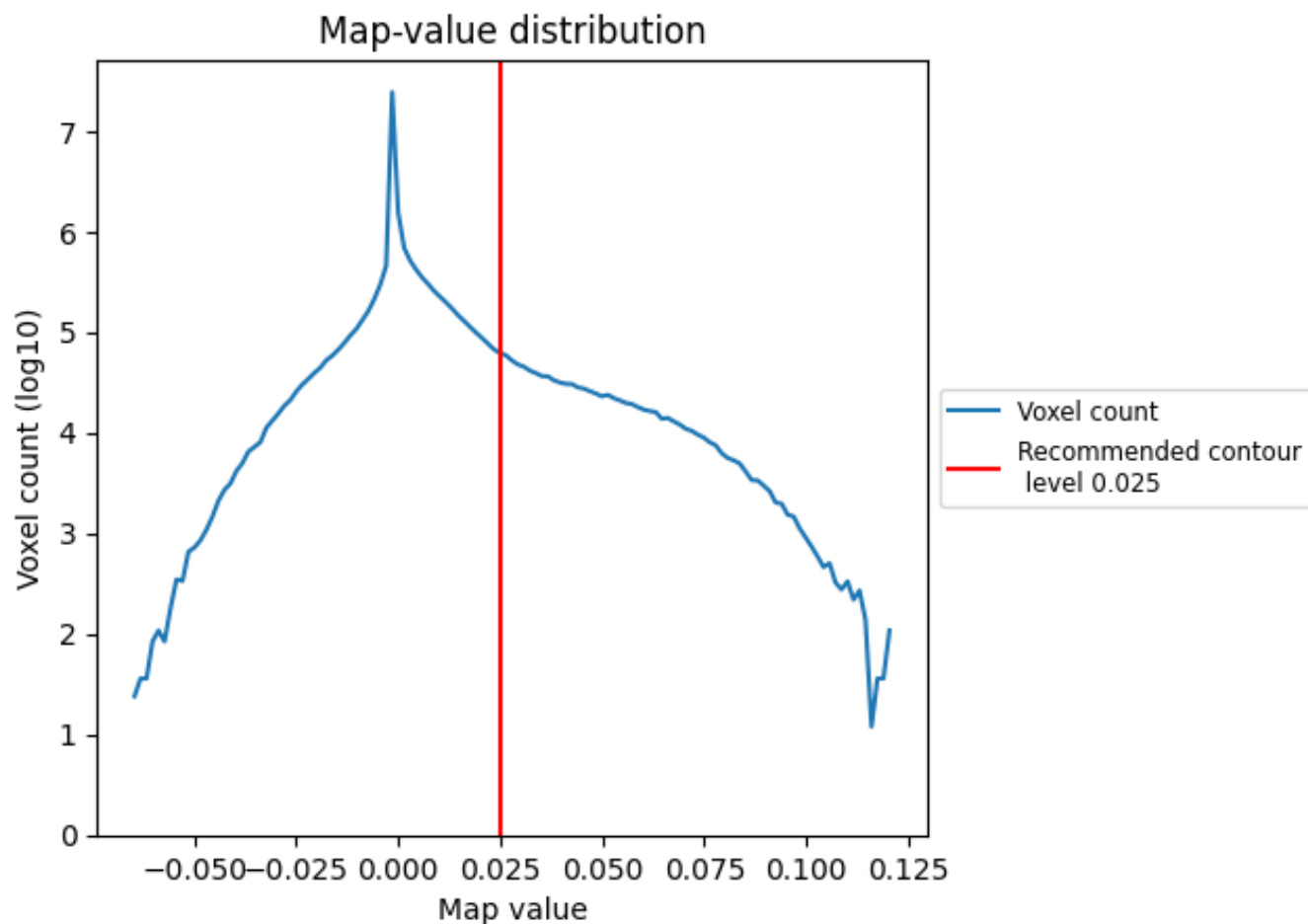
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

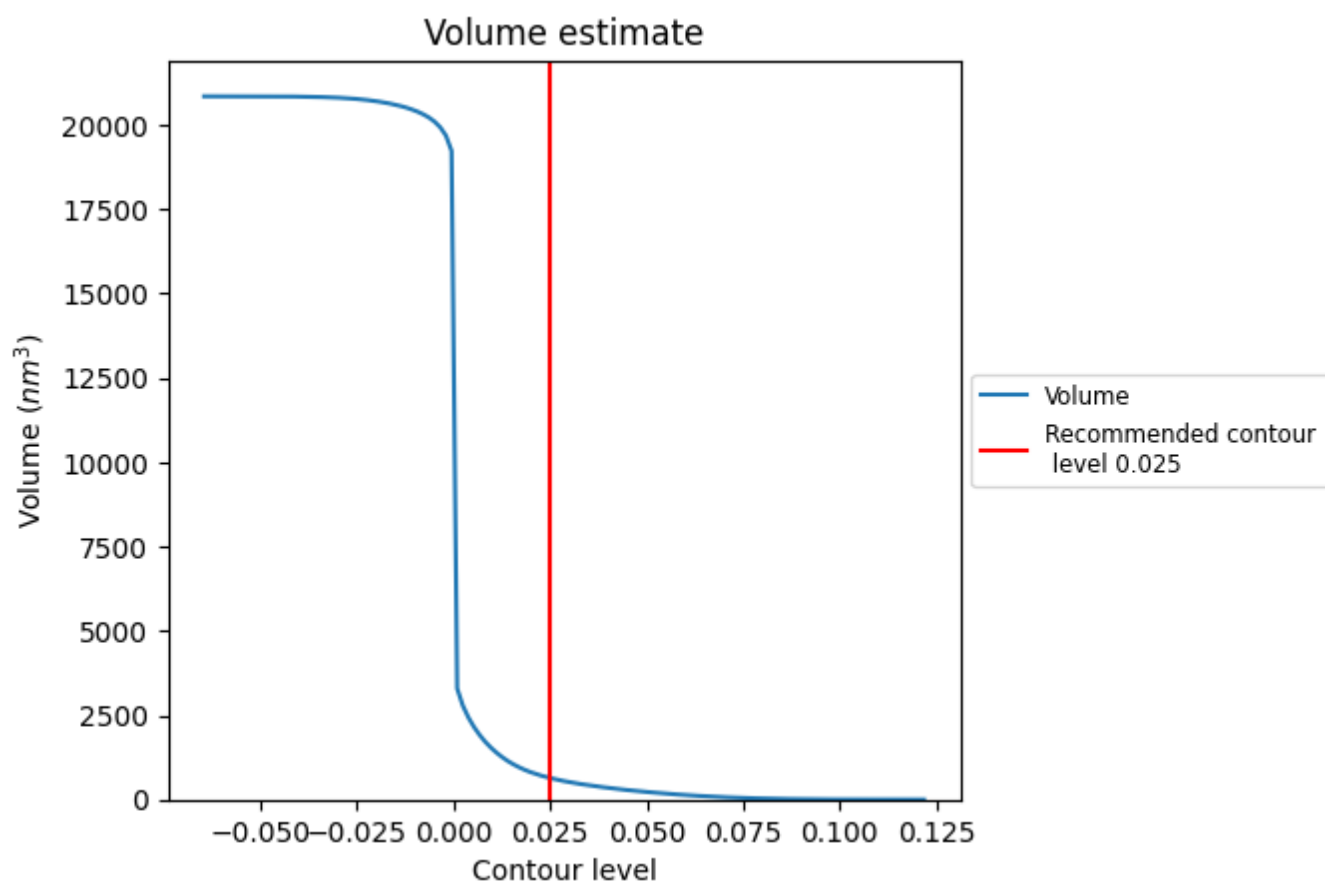
This section contains the results of statistical analysis of the map.

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.

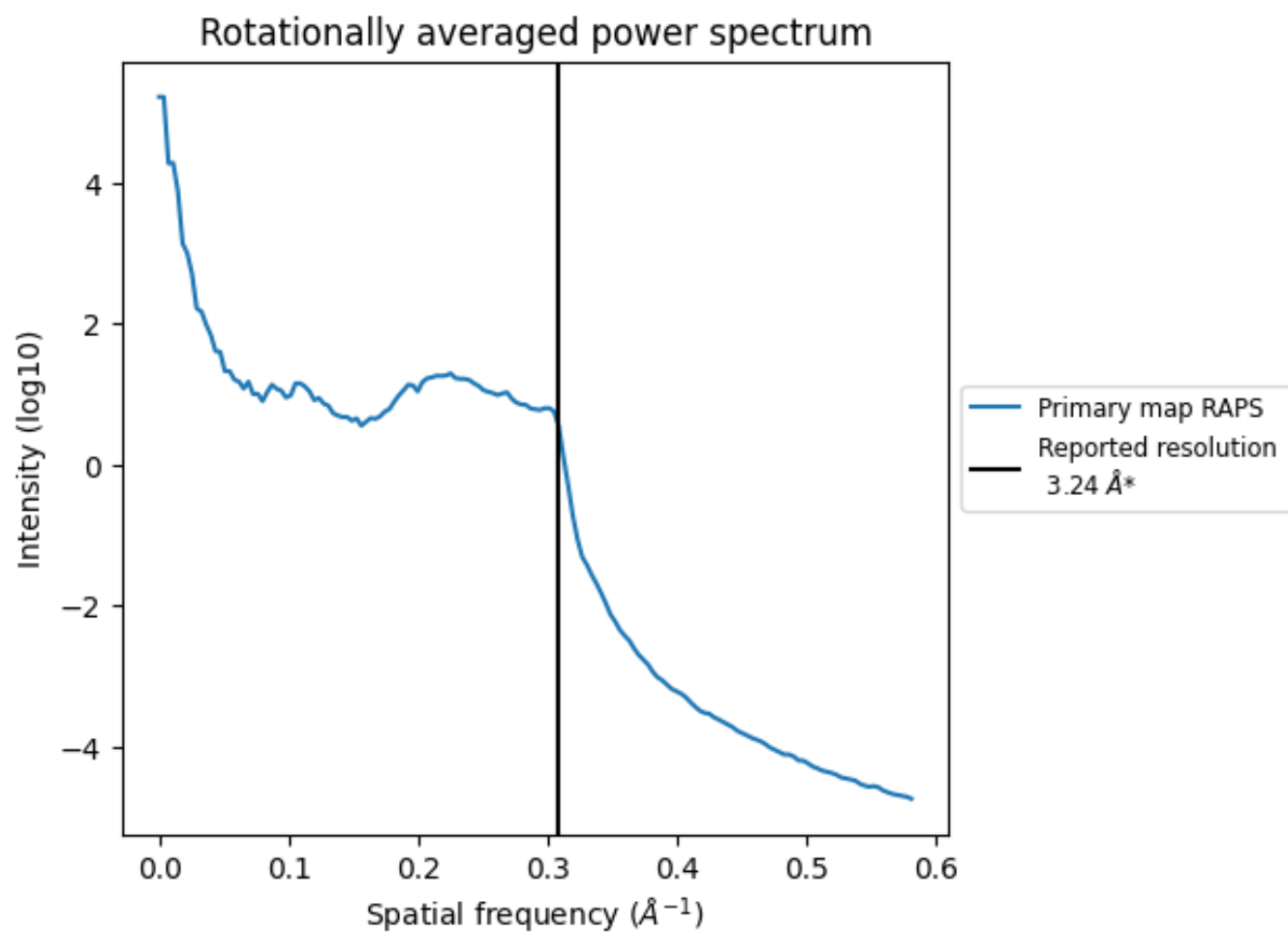
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 640 nm³; this corresponds to an approximate mass of 578 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 0.309 Å⁻¹

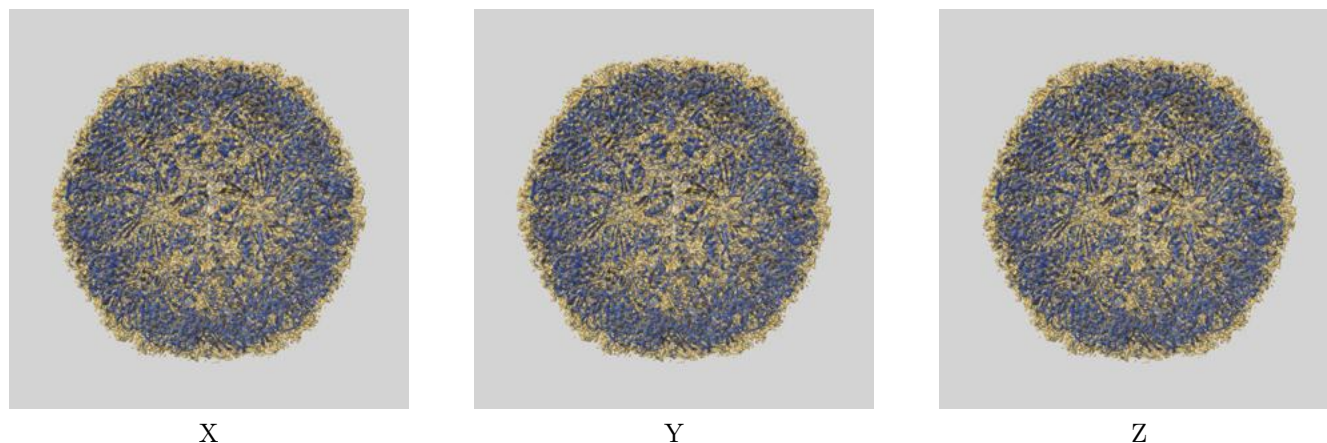
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

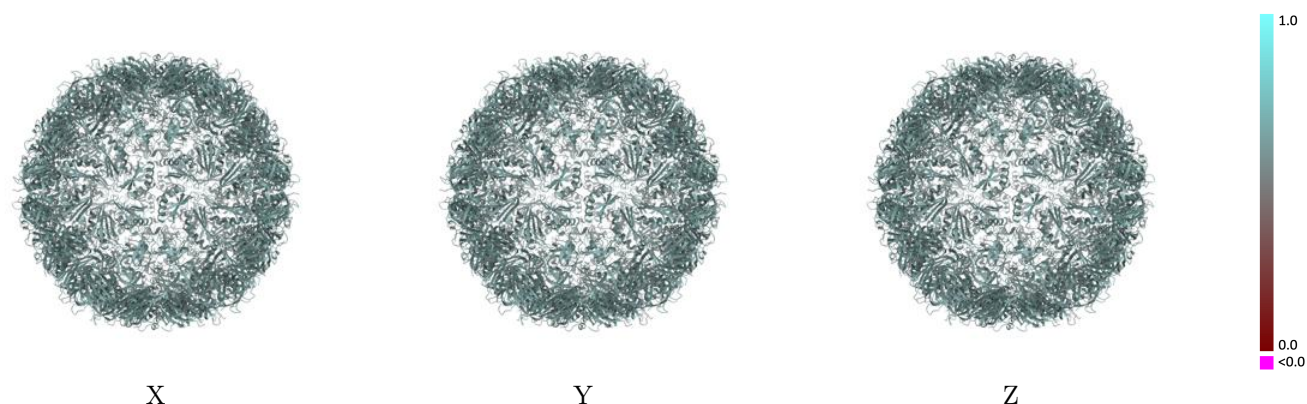
This section contains information regarding the fit between EMDB map EMD-30384 and PDB model 7CKB. Per-residue inclusion information can be found in section [3](#) on page [35](#).

9.1 Map-model overlay [i](#)



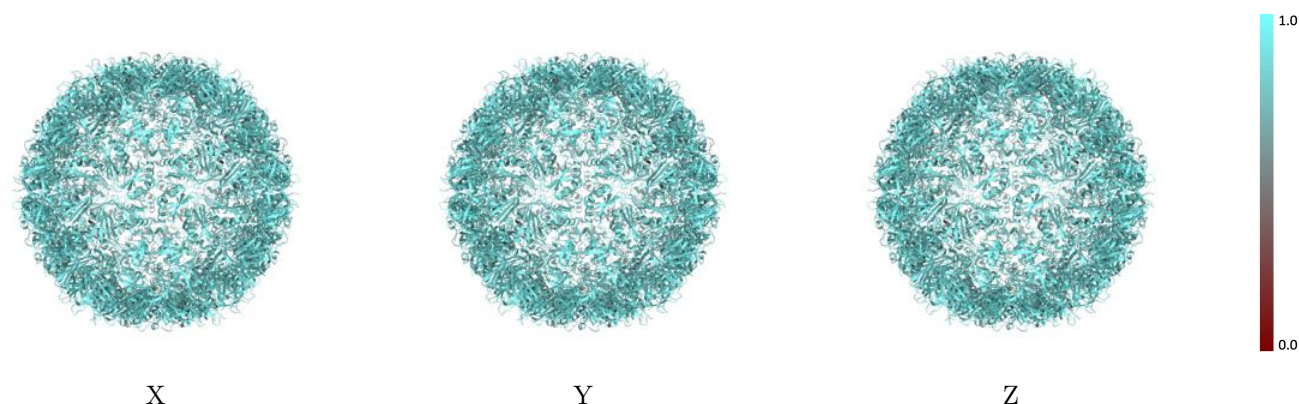
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



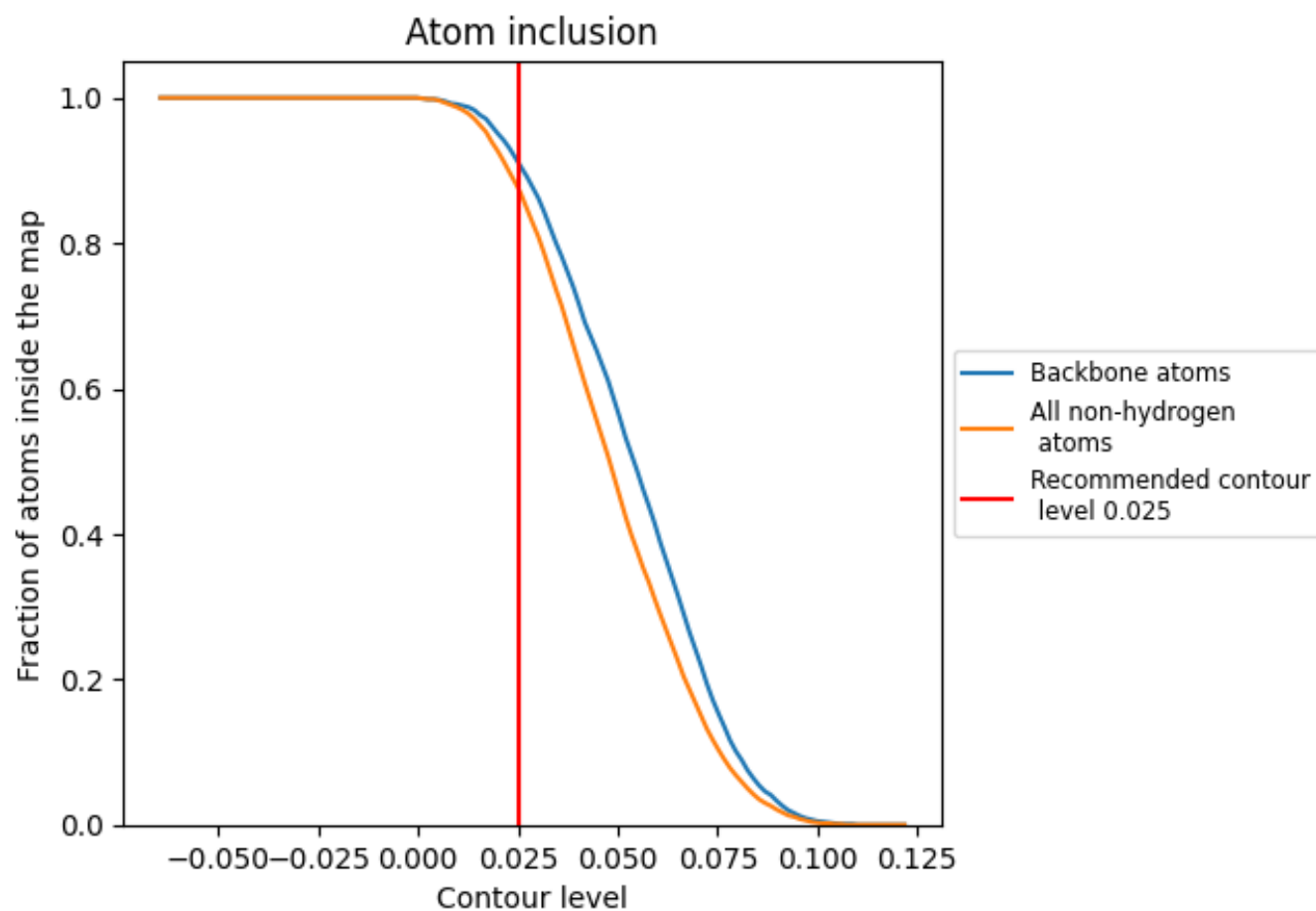
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.025).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8760	 0.5910
A0	 0.8890	 0.5960
A1	 0.8950	 0.5950
A2	 0.8890	 0.5960
A3	 0.8890	 0.5950
A4	 0.8940	 0.5940
A5	 0.8850	 0.5940
A6	 0.8900	 0.5970
A7	 0.8920	 0.5960
A8	 0.8940	 0.5940
A9	 0.8940	 0.5920
AA	 0.8900	 0.5940
AB	 0.8920	 0.5940
AC	 0.8920	 0.5910
AD	 0.8950	 0.5960
AE	 0.8950	 0.5930
AF	 0.8840	 0.5910
AG	 0.8940	 0.5980
AH	 0.8890	 0.5950
AI	 0.8950	 0.5960
AJ	 0.8920	 0.5960
AK	 0.8870	 0.5930
AL	 0.8900	 0.5940
AM	 0.8940	 0.5950
AN	 0.8870	 0.5950
AO	 0.8890	 0.5980
AP	 0.8850	 0.5920
AQ	 0.8970	 0.5950
AR	 0.8950	 0.5960
AS	 0.8920	 0.5930
AT	 0.8900	 0.5910
AV	 0.8890	 0.5970
AW	 0.8890	 0.5960
AX	 0.8920	 0.5940
AY	 0.8950	 0.5950























































































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Chain	Atom inclusion	Q-score
AZ	 0.8940	 0.5970
Aa	 0.8770	 0.5930
Ab	 0.8920	 0.5960
Ac	 0.8920	 0.5950
Ad	 0.8920	 0.5940
Ae	 0.8900	 0.5940
Af	 0.8900	 0.5940
Ag	 0.8940	 0.5950
Ah	 0.8890	 0.5950
Ai	 0.8950	 0.5950
Aj	 0.8890	 0.5950
Ak	 0.8870	 0.5970
Al	 0.8890	 0.5960
Am	 0.8950	 0.5970
An	 0.8900	 0.5930
Ao	 0.8920	 0.5960
Ap	 0.8850	 0.5980
Aq	 0.8870	 0.5930
Ar	 0.8940	 0.5930
As	 0.8920	 0.5940
At	 0.8900	 0.5970
Av	 0.8850	 0.5950
Aw	 0.8900	 0.5940
Ax	 0.8920	 0.5960
Ay	 0.8940	 0.5950
Az	 0.8950	 0.5950
B0	 0.8750	 0.5920
B1	 0.8750	 0.5880
B2	 0.8730	 0.5900
B3	 0.8780	 0.5930
B4	 0.8750	 0.5910
B5	 0.8750	 0.5900
B6	 0.8750	 0.5910
B7	 0.8720	 0.5890
B8	 0.8720	 0.5930
B9	 0.8770	 0.5910
BA	 0.8770	 0.5900
BB	 0.8770	 0.5880
BC	 0.8810	 0.5910
BD	 0.8750	 0.5890
BE	 0.8730	 0.5880
BF	 0.8730	 0.5890





















































































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Chain	Atom inclusion	Q-score
BG	 0.8800	 0.5910
BH	 0.8750	 0.5930
BI	 0.8730	 0.5930
BJ	 0.8750	 0.5880
BK	 0.8730	 0.5890
BL	 0.8750	 0.5900
BM	 0.8720	 0.5910
BN	 0.8720	 0.5920
BO	 0.8800	 0.5910
BP	 0.8730	 0.5900
BQ	 0.8720	 0.5900
BR	 0.8750	 0.5880
BS	 0.8770	 0.5900
BT	 0.8750	 0.5880
BV	 0.8750	 0.5910
BW	 0.8720	 0.5920
BX	 0.8730	 0.5930
BY	 0.8730	 0.5890
BZ	 0.8750	 0.5910
Ba	 0.8730	 0.5890
Bb	 0.8750	 0.5930
Bc	 0.8730	 0.5910
Bd	 0.8780	 0.5890
Be	 0.8750	 0.5890
Bf	 0.8750	 0.5870
Bg	 0.8770	 0.5900
Bh	 0.8770	 0.5920
Bi	 0.8720	 0.5920
Bj	 0.8750	 0.5920
Bk	 0.8770	 0.5920
Bl	 0.8800	 0.5900
Bm	 0.8770	 0.5890
Bn	 0.8730	 0.5910
Bo	 0.8730	 0.5910
Bp	 0.8750	 0.5920
Bq	 0.8800	 0.5900
Br	 0.8730	 0.5910
Bs	 0.8750	 0.5880
Bt	 0.8750	 0.5910
Bv	 0.8730	 0.5880
Bw	 0.8730	 0.5900
Bx	 0.8800	 0.5930









































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Chain	Atom inclusion	Q-score
By	 0.8750	 0.5910
Bz	 0.8770	 0.5890
C0	 0.8620	 0.5880
C1	 0.8640	 0.5870
C2	 0.8580	 0.5890
C3	 0.8590	 0.5870
C4	 0.8610	 0.5890
C5	 0.8660	 0.5870
C6	 0.8560	 0.5880
C7	 0.8640	 0.5920
C8	 0.8590	 0.5890
C9	 0.8590	 0.5900
CA	 0.8590	 0.5840
CB	 0.8590	 0.5890
CC	 0.8640	 0.5860
CD	 0.8660	 0.5890
CE	 0.8620	 0.5870
CF	 0.8670	 0.5880
CG	 0.8620	 0.5890
CH	 0.8610	 0.5860
CI	 0.8620	 0.5890
CJ	 0.8610	 0.5870
CK	 0.8660	 0.5870
CL	 0.8620	 0.5880
CM	 0.8620	 0.5900
CN	 0.8590	 0.5870
CO	 0.8620	 0.5890
CP	 0.8610	 0.5860
CQ	 0.8590	 0.5890
CR	 0.8640	 0.5850
CS	 0.8590	 0.5860
CT	 0.8590	 0.5870
CV	 0.8660	 0.5870
CW	 0.8620	 0.5860
CX	 0.8580	 0.5900
CY	 0.8670	 0.5860
CZ	 0.8620	 0.5910
Ca	 0.8660	 0.5900
Cb	 0.8610	 0.5860
Cc	 0.8620	 0.5850
Cd	 0.8610	 0.5880
Ce	 0.8640	 0.5900

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Chain	Atom inclusion	Q-score
Cf	 0.8640	 0.5900
Cg	 0.8620	 0.5910
Ch	 0.8620	 0.5890
Ci	 0.8610	 0.5870
Cj	 0.8610	 0.5860
Ck	 0.8640	 0.5880
Cl	 0.8590	 0.5910
Cm	 0.8640	 0.5900
Cn	 0.8590	 0.5900
Co	 0.8580	 0.5880
Cp	 0.8640	 0.5890
Cq	 0.8590	 0.5880
Cr	 0.8610	 0.5890
Cs	 0.8620	 0.5890
Ct	 0.8580	 0.5870
Cv	 0.8670	 0.5870
Cw	 0.8620	 0.5860
Cx	 0.8590	 0.5890
Cy	 0.8590	 0.5900
Cz	 0.8640	 0.5870