



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 03:18 AM UTC

PDB ID : 7CKC / pdb_00007ckc
EMDB ID : EMD-30385
Title : Simplified Alpha-Carboxysome, T=4
Authors : Tan, Y.Q.; Ali, S.; Xue, B.; Robinson, R.C.; Narita, A.; Yew, W.S.
Deposited on : 2020-07-16
Resolution : 2.90 Å (reported)
Based on initial models : 2EWH, 2RCF

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

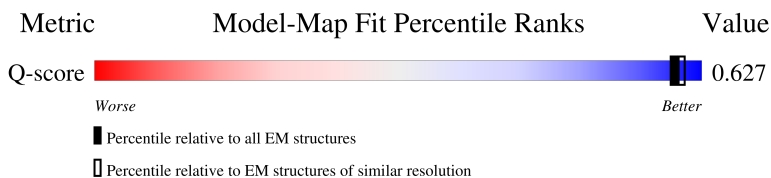
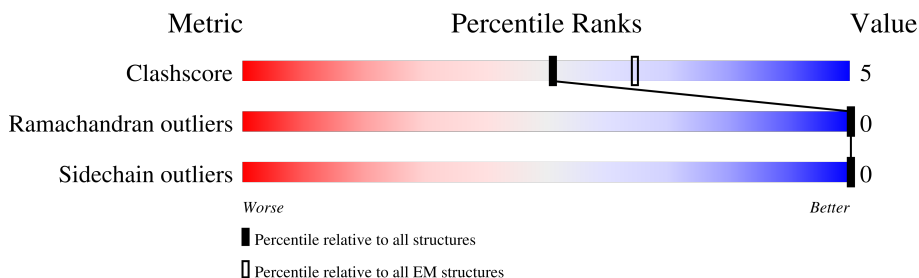
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



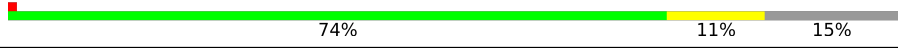
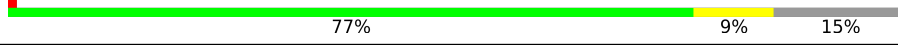
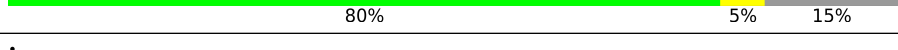
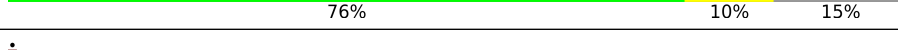
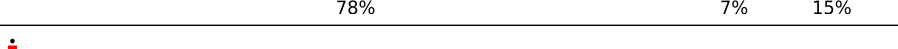
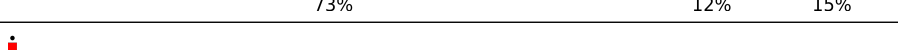
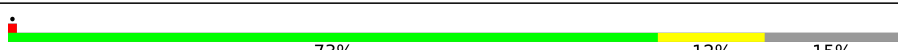
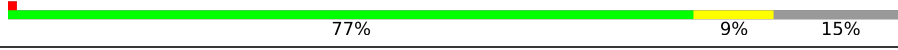
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	

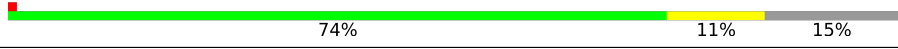
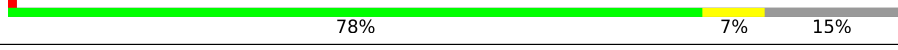
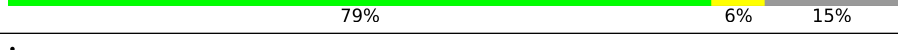
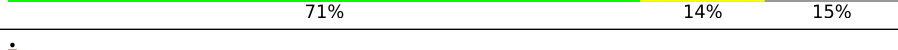
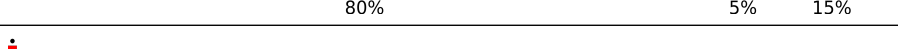
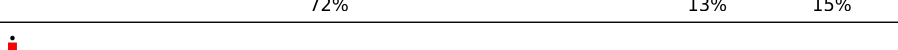
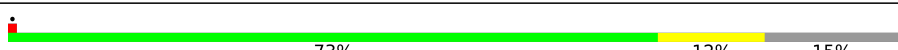
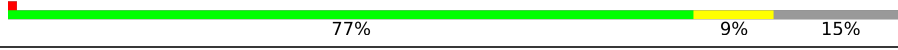
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Mol	Chain	Length	Quality of chain
1	A4	94	
1	A5	94	
1	A6	94	
1	A7	94	
1	A8	94	
1	A9	94	
1	AA	94	
1	AB	94	
1	AC	94	
1	AD	94	
1	AE	94	
1	AF	94	
1	AG	94	
1	AH	94	
1	AI	94	
1	AJ	94	
1	AK	94	
1	AL	94	
1	AM	94	
1	AN	94	
1	AO	94	
1	AP	94	
1	AQ	94	
1	AR	94	
1	AS	94	

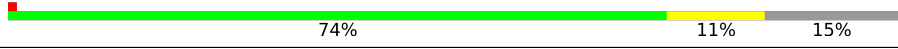
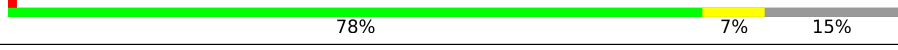
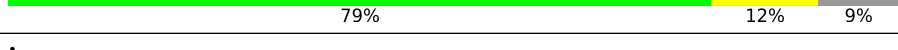
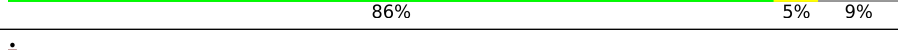
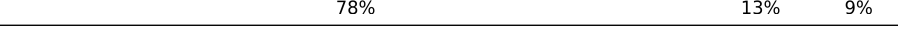
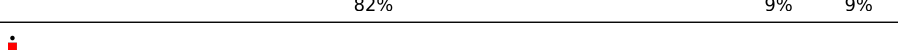
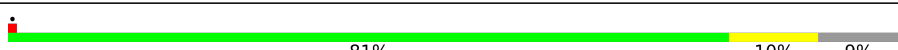
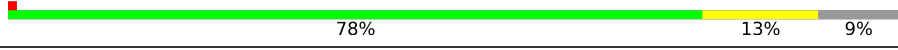
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Mol	Chain	Length	Quality of chain
1	AT	94	
1	AV	94	
1	AW	94	
1	AX	94	
1	AY	94	
1	AZ	94	
1	Aa	94	
1	Ab	94	
1	Ac	94	
1	Ad	94	
1	Ae	94	
1	Af	94	
1	Ag	94	
1	Ah	94	
1	Ai	94	
1	Aj	94	
1	Ak	94	
1	Al	94	
1	Am	94	
1	An	94	
1	Ao	94	
1	Ap	94	
1	Aq	94	
1	Ar	94	
1	As	94	

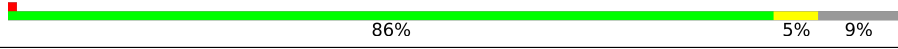
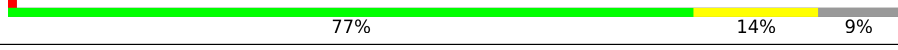
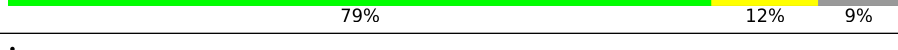
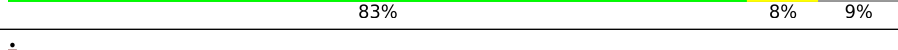
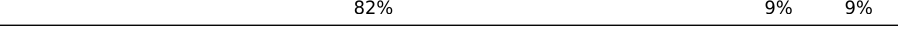
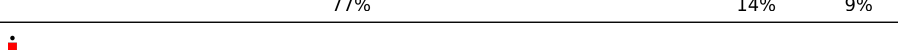
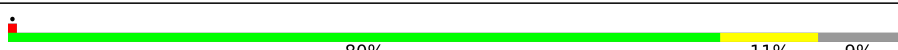
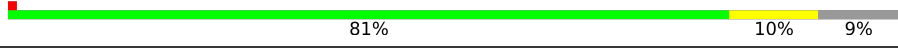
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Mol	Chain	Length	Quality of chain
1	At	94	
1	Av	94	
1	Aw	94	
1	Ax	94	
1	Ay	94	
1	Az	94	
2	B0	98	
2	B1	98	
2	B2	98	
2	B3	98	
2	B4	98	
2	B5	98	
2	B6	98	
2	B7	98	
2	B8	98	
2	B9	98	
2	BA	98	
2	BB	98	
2	BC	98	
2	BD	98	
2	BE	98	
2	BF	98	
2	BG	98	
2	BH	98	
2	BI	98	

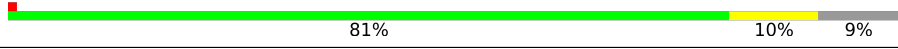
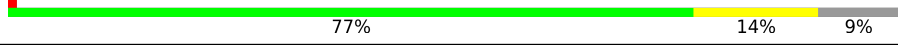
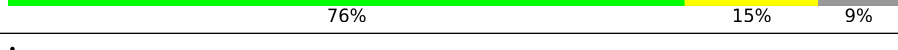
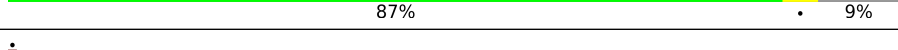
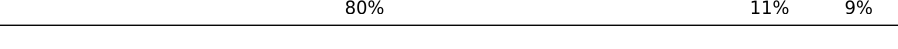
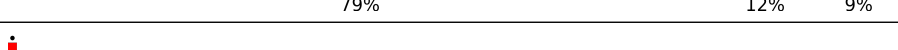
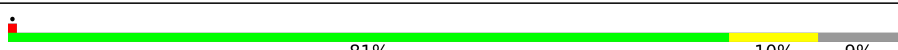
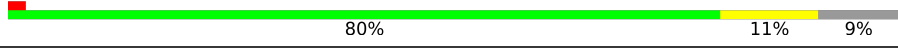
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Mol	Chain	Length	Quality of chain
2	BJ	98	
2	BK	98	
2	BL	98	
2	BM	98	
2	BN	98	
2	BO	98	
2	BP	98	
2	BQ	98	
2	BR	98	
2	BS	98	
2	BT	98	
2	BV	98	
2	BW	98	
2	BX	98	
2	BY	98	
2	BZ	98	
2	Ba	98	
2	Bb	98	
2	Bc	98	
2	Bd	98	
2	Be	98	
2	Bf	98	
2	Bg	98	
2	Bh	98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

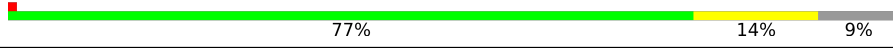
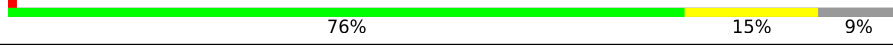
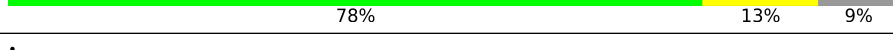
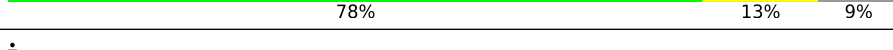
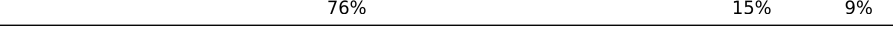
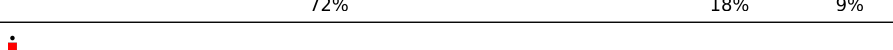
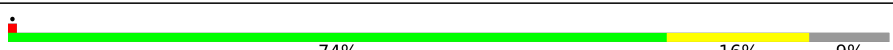
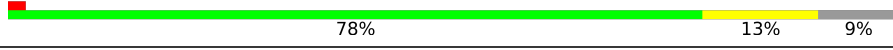
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Mol	Chain	Length	Quality of chain
2	Bj	98	
2	Bk	98	
2	Bl	98	
2	Bm	98	
2	Bn	98	
2	Bo	98	
2	Bp	98	
2	Bq	98	
2	Br	98	
2	Bs	98	
2	Bt	98	
2	Bv	98	
2	Bw	98	
2	Bx	98	
2	By	98	
2	Bz	98	
2	C0	98	
2	C1	98	
2	C2	98	
2	C3	98	
2	C4	98	
2	C5	98	
2	C6	98	
2	C7	98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

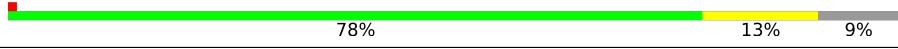
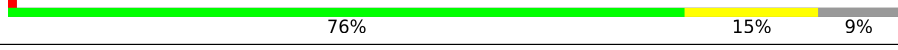
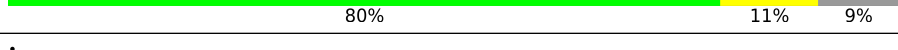
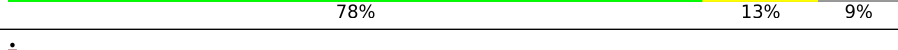
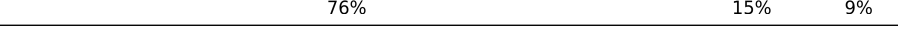
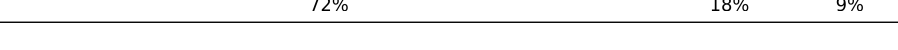
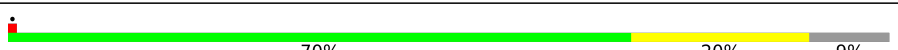
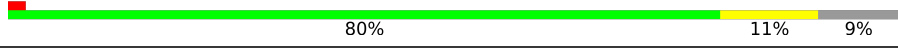
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Mol	Chain	Length	Quality of chain
2	C9	98	
2	CA	98	
2	CB	98	
2	CC	98	
2	CD	98	
2	CE	98	
2	CF	98	
2	CG	98	
2	CH	98	
2	CI	98	
2	CJ	98	
2	CK	98	
2	CL	98	
2	CM	98	
2	CN	98	
2	CO	98	
2	CP	98	
2	CQ	98	
2	CR	98	
2	CS	98	
2	CT	98	
2	CV	98	
2	CW	98	
2	CX	98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

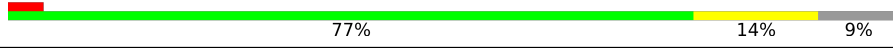
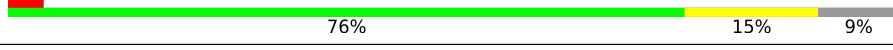
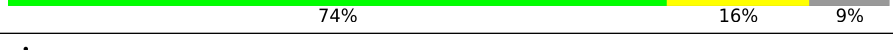
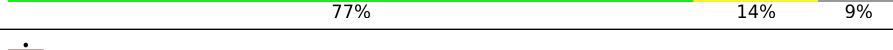
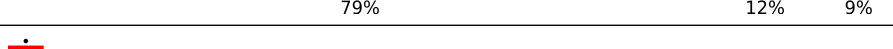
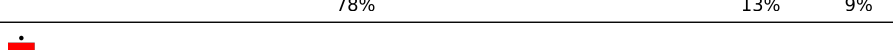
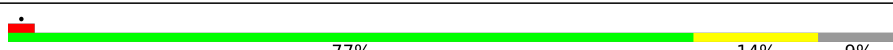
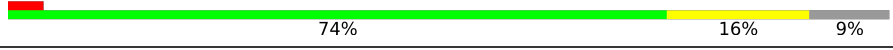
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Mol	Chain	Length	Quality of chain
2	CZ	98	
2	Ca	98	
2	Cb	98	
2	Cc	98	
2	Cd	98	
2	Ce	98	
2	Cf	98	
2	Cg	98	
2	Ch	98	
2	Ci	98	
2	Cj	98	
2	Ck	98	
2	Cl	98	
2	Cm	98	
2	Cn	98	
2	Co	98	
2	Cp	98	
2	Cq	98	
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2	Cx	98	
2	Cy	98	

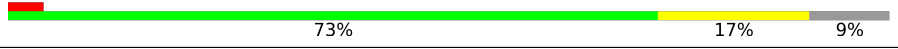
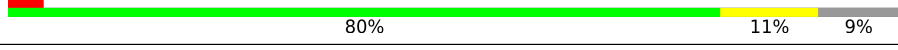
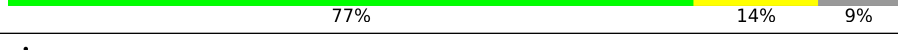
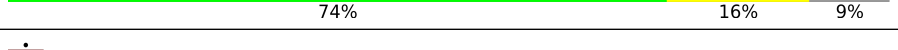
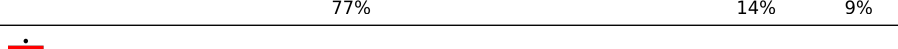
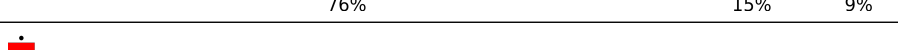
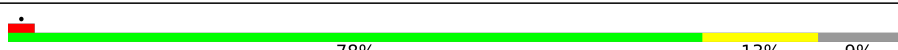
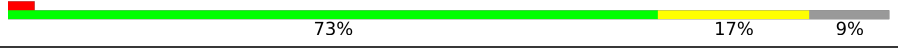
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Mol	Chain	Length	Quality of chain
2	Cz	98	
2	D0	98	
2	D1	98	
2	D2	98	
2	D3	98	
2	D4	98	
2	D5	98	
2	D6	98	
2	D7	98	
2	D8	98	
2	D9	98	
2	DA	98	
2	DB	98	
2	DC	98	
2	DD	98	
2	DE	98	
2	DF	98	
2	DG	98	
2	DH	98	
2	DI	98	
2	DJ	98	
2	DK	98	
2	DL	98	
2	DM	98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

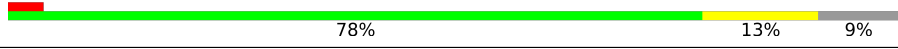
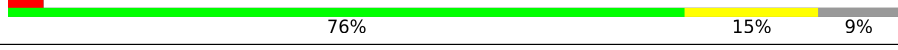
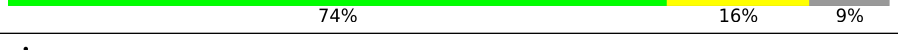
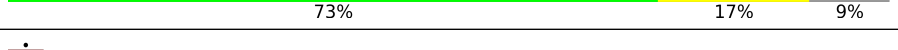
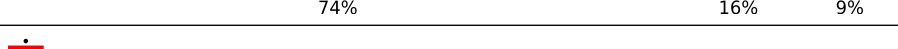
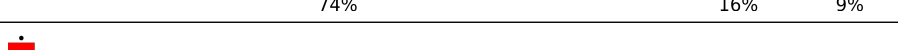
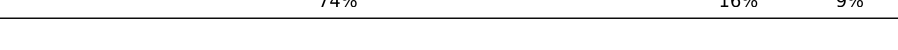
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Mol	Chain	Length	Quality of chain
2	DO	98	
2	DP	98	
2	DQ	98	
2	DR	98	
2	DS	98	
2	DT	98	
2	DV	98	
2	DW	98	
2	DX	98	
2	DY	98	
2	DZ	98	
2	Da	98	
2	Db	98	
2	Dc	98	
2	Dd	98	
2	De	98	
2	Df	98	
2	Dg	98	
2	Dh	98	
2	Di	98	
2	Dj	98	
2	Dk	98	
2	Dl	98	
2	Dm	98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

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Mol	Chain	Length	Quality of chain
2	Do	98	 77%14%9%
2	Dp	98	 77%14%9%
2	Dq	98	 78%13%9%
2	Dr	98	 76%15%9%
2	Ds	98	 74%16%9%
2	Dt	98	 78%13%9%
2	Dv	98	 74%16%9%
2	Dw	98	 73%17%9%
2	Dx	98	 74%16%9%
2	Dy	98	 74%16%9%
2	Dz	98	 74%16%9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 150300 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	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AB	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AC	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AD	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AE	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AF	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AG	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AH	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AI	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AJ	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AK	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AL	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AM	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AN	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AO	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AP	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AQ	80	Total 600	C 382	N 103	O 110	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AR	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AS	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AT	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AV	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AW	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AX	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AY	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	AZ	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Aa	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Ab	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Ac	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Ad	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Ae	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Af	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Ag	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Ah	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Ai	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Aj	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Ak	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Al	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Am	80	Total 600	C 382	N 103	O 110	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	An	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Ao	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Ap	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Aq	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Ar	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	As	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	At	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Av	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Aw	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Ax	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Ay	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	Az	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	A0	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	A1	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	A2	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	A3	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	A4	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	A5	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	A6	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	A7	80	Total 600	C 382	N 103	O 110	S 5	0	0
1	A8	80	Total 600	C 382	N 103	O 110	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	A9	80	Total	C	N	O	S	0	0
			600	382	103	110	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	89	Total	C	N	O	S	0	0
			635	395	119	118	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	CA	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DA	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BB	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CB	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DB	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BC	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CC	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DC	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BD	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CD	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DD	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BE	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CE	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DE	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BF	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CF	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DF	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BG	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CG	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DG	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BH	89	Total 635	C 395	N 119	O 118	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	CH	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DH	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BI	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CI	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DI	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BJ	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CJ	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DJ	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BK	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CK	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DK	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BL	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CL	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DL	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BM	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CM	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DM	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BN	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CN	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DN	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BO	89	Total 635	C 395	N 119	O 118	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	CO	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DO	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BP	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CP	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DP	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BQ	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CQ	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DQ	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BR	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CR	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DR	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BS	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CS	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DS	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BT	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CT	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DT	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BV	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CV	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DV	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BW	89	Total 635	C 395	N 119	O 118	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	CW	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DW	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BX	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CX	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DX	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BY	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CY	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DY	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	BZ	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	CZ	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	DZ	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Ba	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Ca	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Da	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bb	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Cb	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Db	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bc	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Cc	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dc	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bd	89	Total 635	C 395	N 119	O 118	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Cd	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dd	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Be	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Ce	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	De	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bf	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Cf	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Df	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bg	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Cg	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dg	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bh	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Ch	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dh	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bi	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Ci	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Di	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bj	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Cj	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dj	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bk	89	Total 635	C 395	N 119	O 118	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ck	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dk	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bl	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Cl	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dl	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bm	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Cm	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dm	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bn	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Cn	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dn	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bo	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Co	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Do	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bp	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Cp	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dp	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bq	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Cq	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dq	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Br	89	Total 635	C 395	N 119	O 118	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Cr	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dr	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bs	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Cs	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Ds	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bt	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Ct	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dt	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bv	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Cv	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dv	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bw	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Cw	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dw	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bx	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Cx	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dx	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	By	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Cy	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dy	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Bz	89	Total 635	C 395	N 119	O 118	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Cz	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	Dz	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	B0	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	C0	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	D0	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	B1	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	C1	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	D1	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	B2	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	C2	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	D2	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	B3	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	C3	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	D3	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	B4	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	C4	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	D4	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	B5	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	C5	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	D5	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	B6	89	Total 635	C 395	N 119	O 118	S 3	0	0

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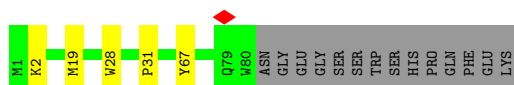
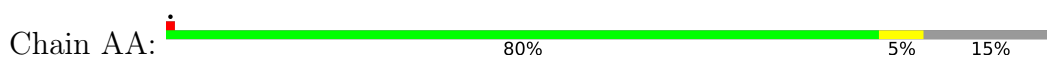
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	C6	89	Total 635	C 395	N 119	O 118	S 3	0	0
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2	B7	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	C7	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	D7	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	B8	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	C8	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	D8	89	Total 635	C 395	N 119	O 118	S 3	0	0
2	B9	89	Total 635	C 395	N 119	O 118	S 3	0	0
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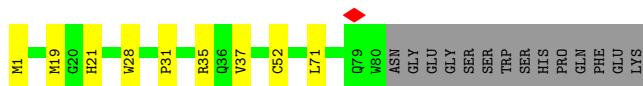
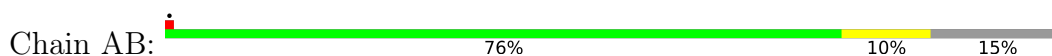
3 Residue-property plots [i](#)

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.

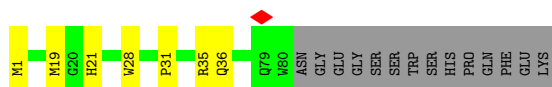
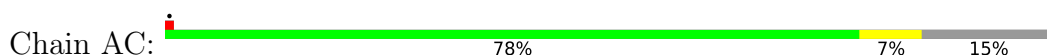
- Molecule 1: Unidentified carboxysome polypeptide



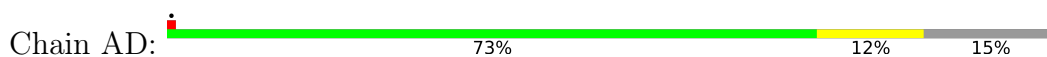
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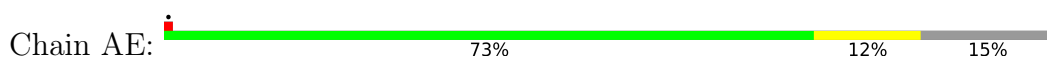
- Molecule 1: Unidentified carboxysome polypeptide



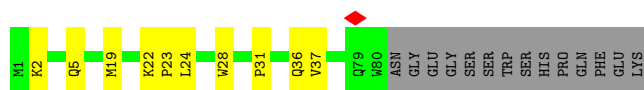
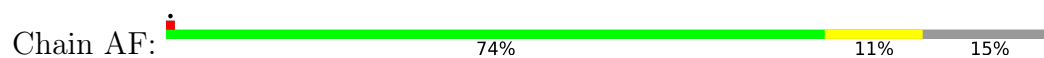
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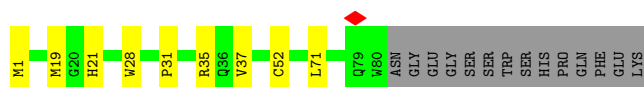
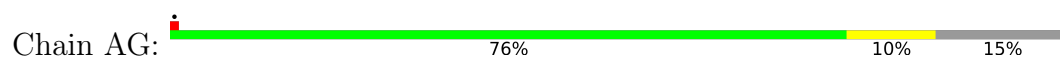
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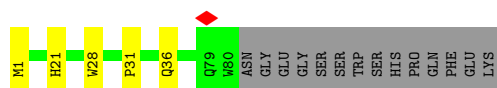
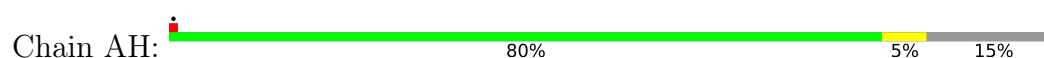
- Molecule 1: Unidentified carboxysome polypeptide



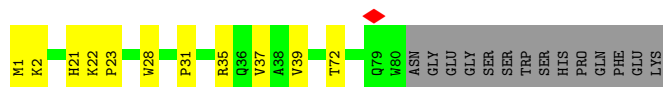
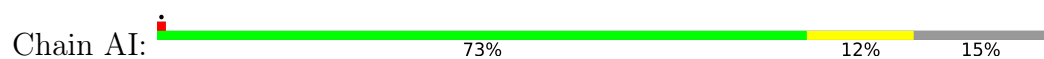
- Molecule 1: Unidentified carboxysome polypeptide



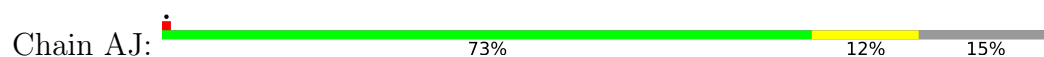
- Molecule 1: Unidentified carboxysome polypeptide



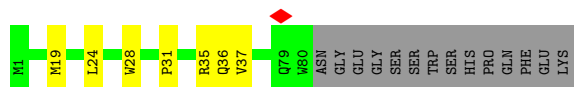
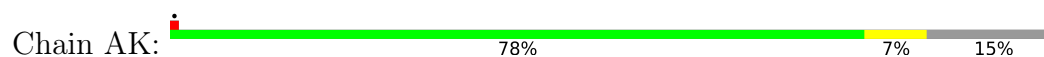
- Molecule 1: Unidentified carboxysome polypeptide



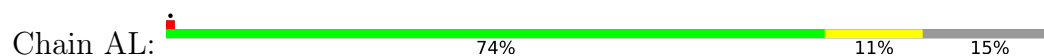
- Molecule 1: Unidentified carboxysome polypeptide

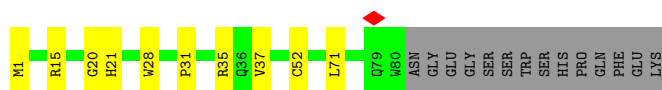


- Molecule 1: Unidentified carboxysome polypeptide

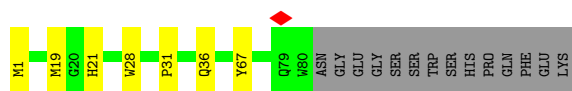
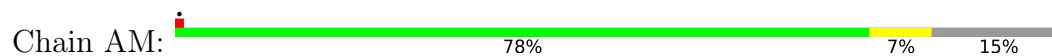


- Molecule 1: Unidentified carboxysome polypeptide

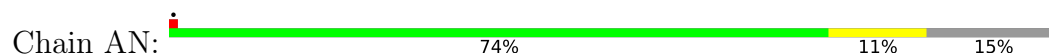




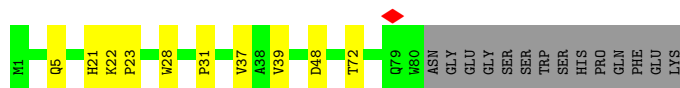
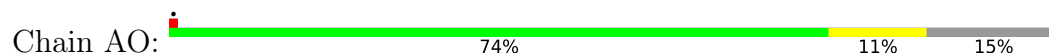
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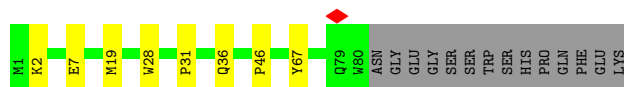
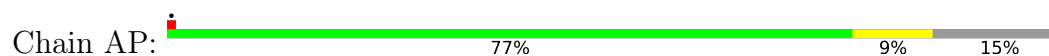
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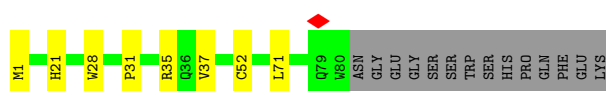
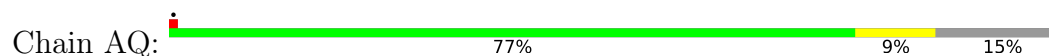
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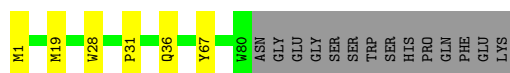
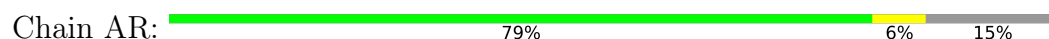
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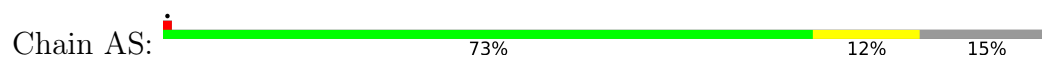
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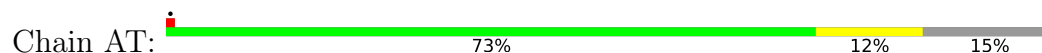
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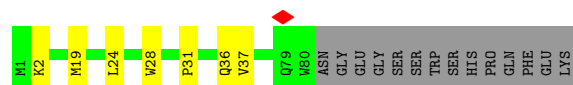
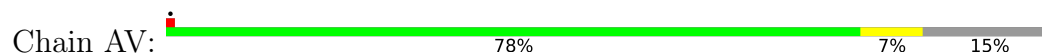
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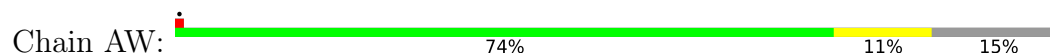
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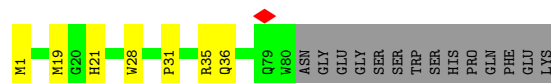
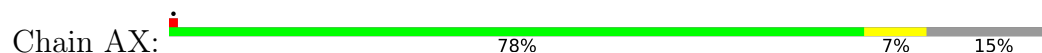
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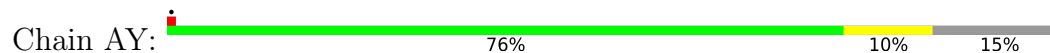
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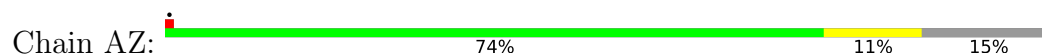
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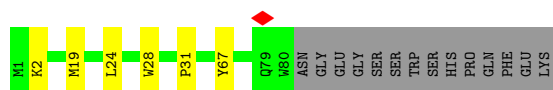
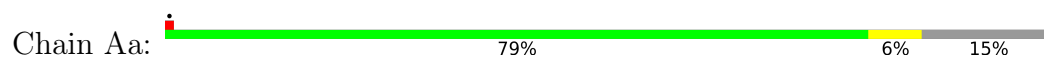
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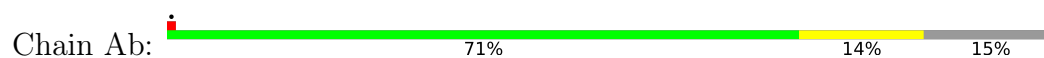
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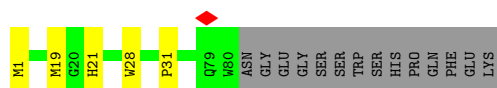
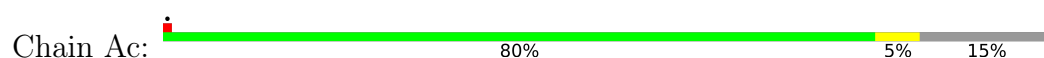
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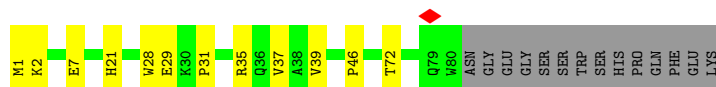
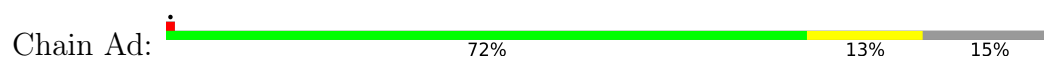
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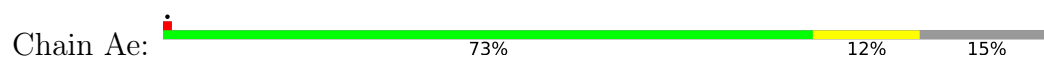
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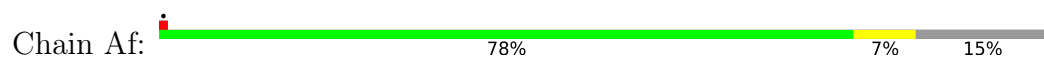
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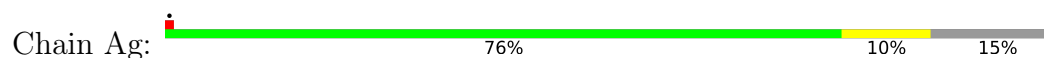
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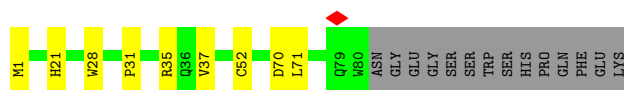


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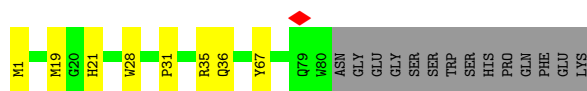
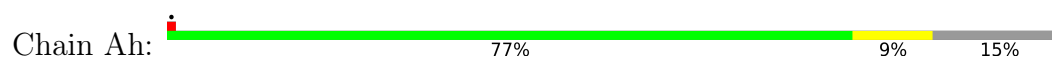


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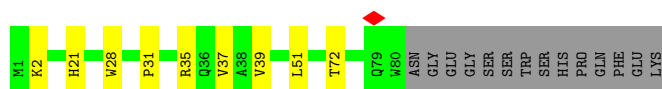
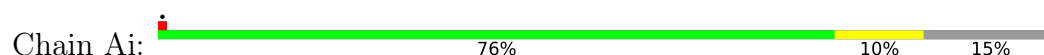




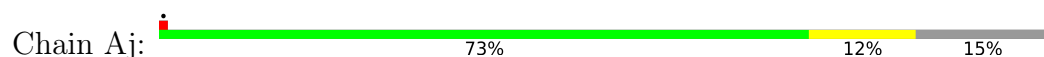
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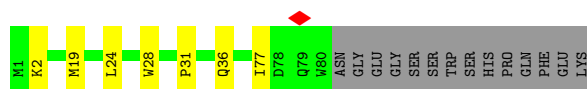
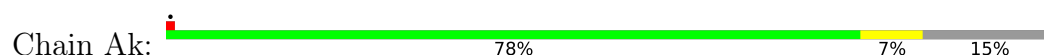
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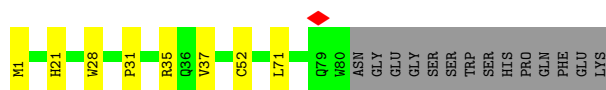
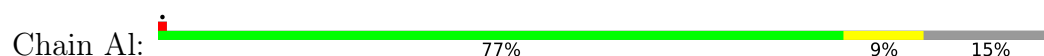
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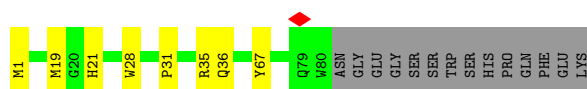
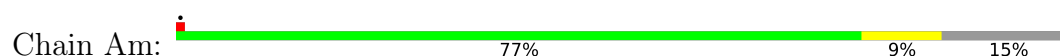
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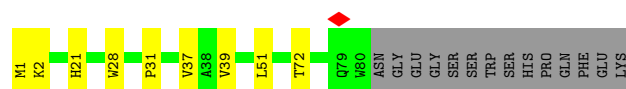
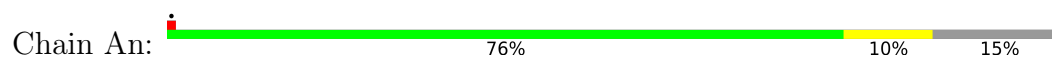
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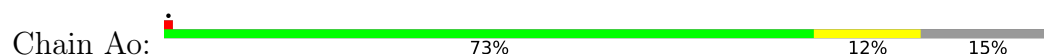
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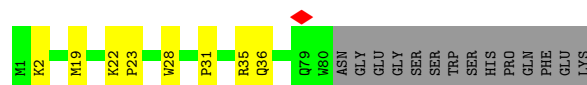
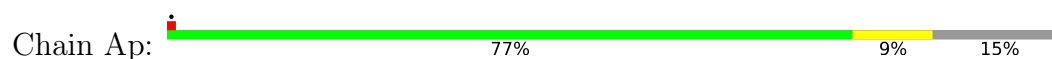
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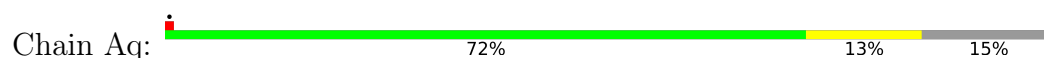
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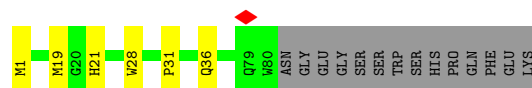
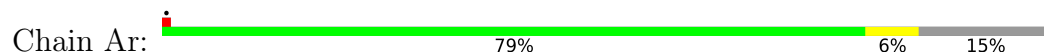
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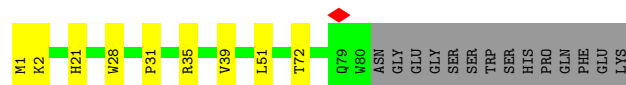
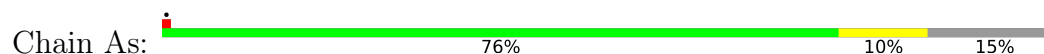
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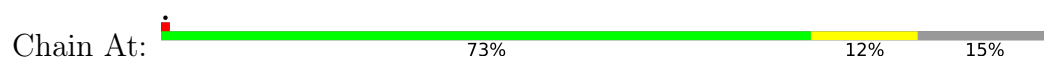
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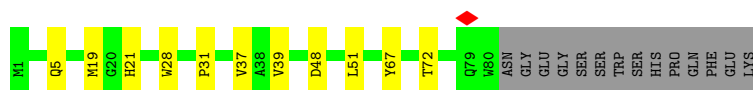


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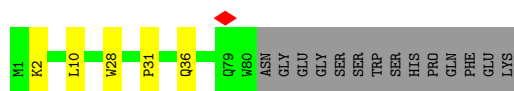
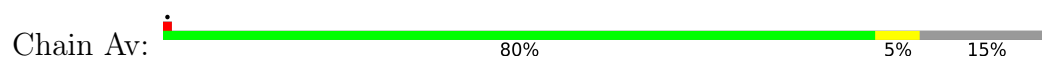


- Molecule 1: Unidentified carboxysome polypeptide

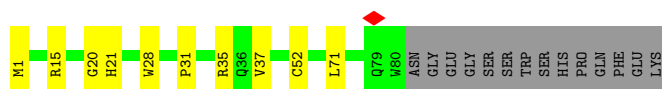
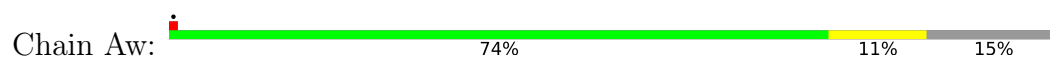




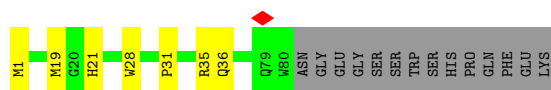
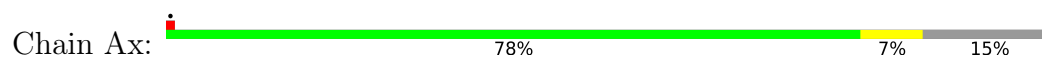
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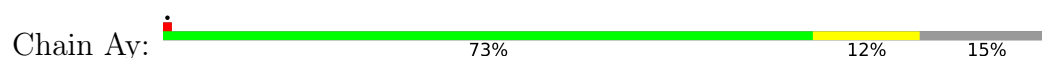
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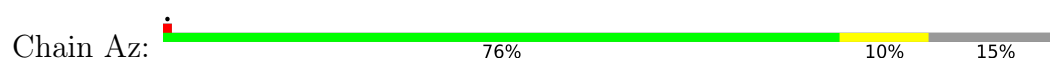
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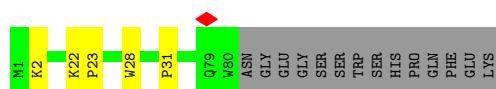
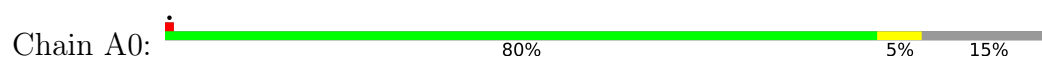
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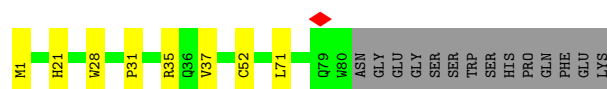
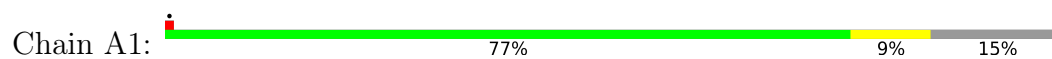
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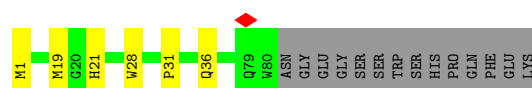
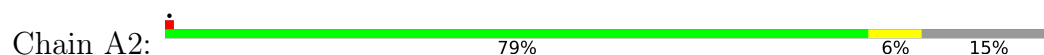
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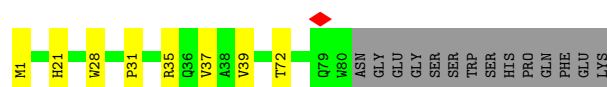
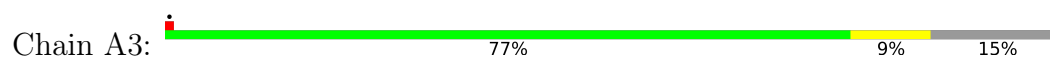
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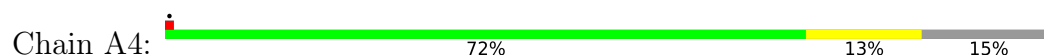
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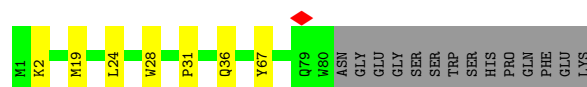
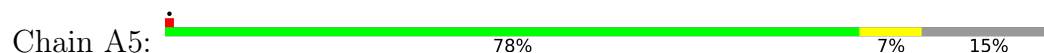
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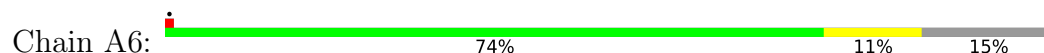
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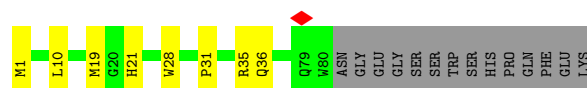
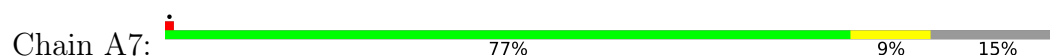
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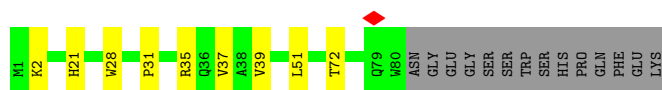
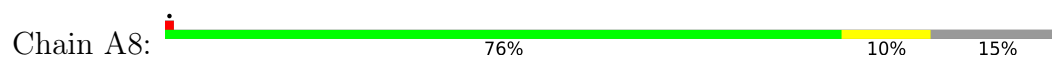
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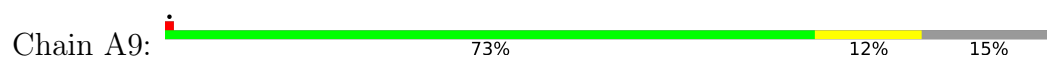
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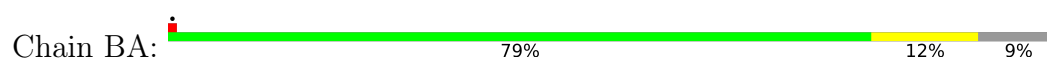
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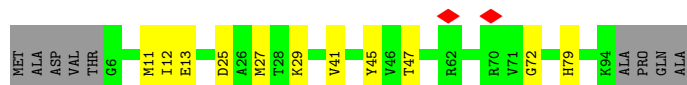
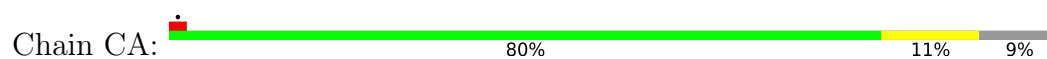
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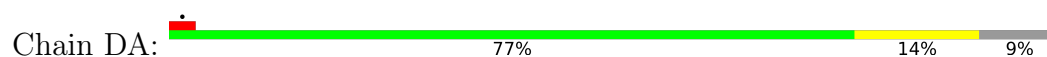
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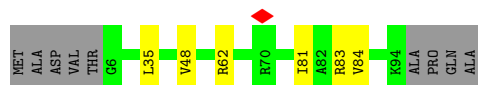
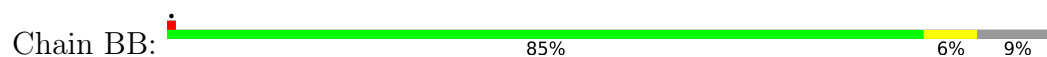
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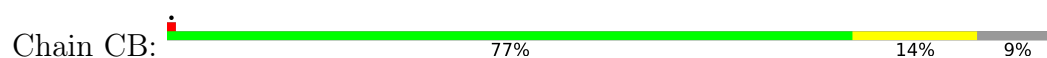
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A

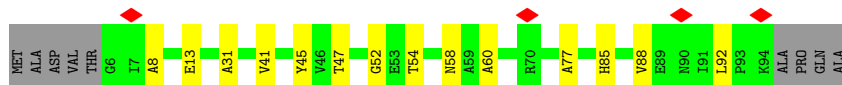
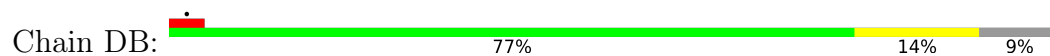


- Molecule 2: Major carboxysome shell protein 1A

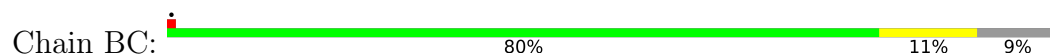




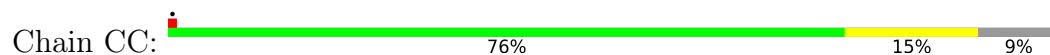
- Molecule 2: Major carboxysome shell protein 1A



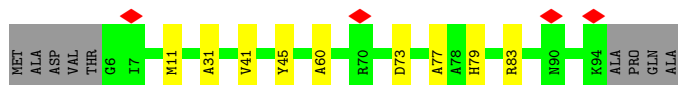
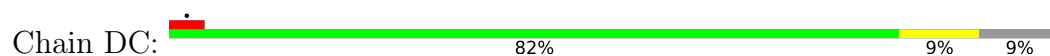
- Molecule 2: Major carboxysome shell protein 1A



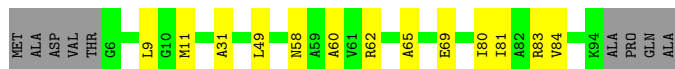
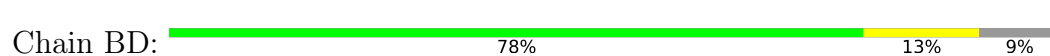
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A

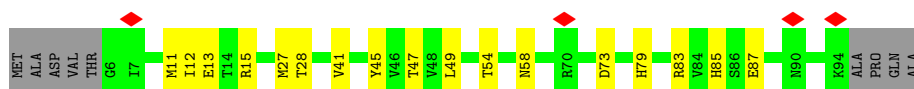


- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A

Chain DD:  73% 17% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain BE:  80% 11% 9%



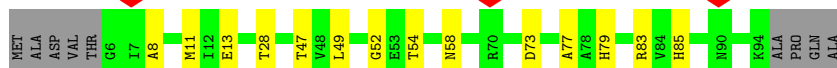
- Molecule 2: Major carboxysome shell protein 1A

Chain CE:  77% 14% 9%



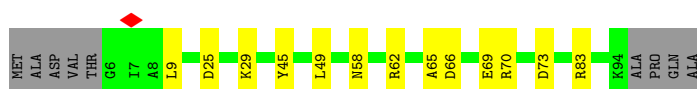
- Molecule 2: Major carboxysome shell protein 1A

Chain DE:  77% 14% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain BF:  78% 13% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain CF:  78% 13% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain DF:  77% 14% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain BG:  87% 9%



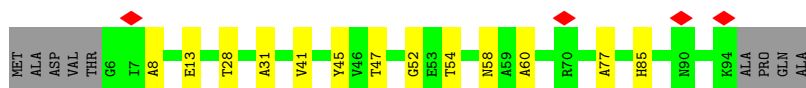
- Molecule 2: Major carboxysome shell protein 1A

Chain CG:  78% 13% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain DG:  78% 13% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain BH:  77% 14% 9%



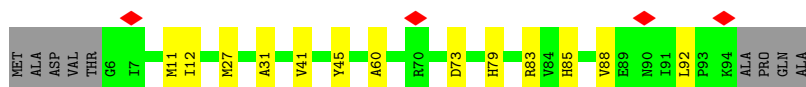
- Molecule 2: Major carboxysome shell protein 1A

Chain CH:  76% 15% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain DH:  78% 13% 9%



- Molecule 2: Major carboxysome shell protein 1A

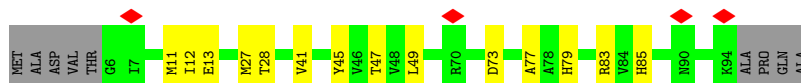
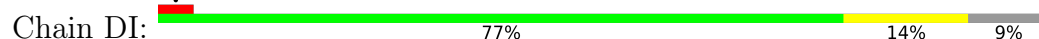
Chain BI:  77% 14% 9%



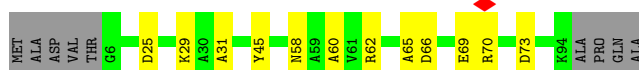
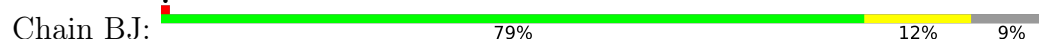
- Molecule 2: Major carboxysome shell protein 1A



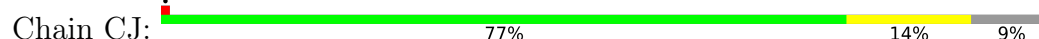
- Molecule 2: Major carboxysome shell protein 1A



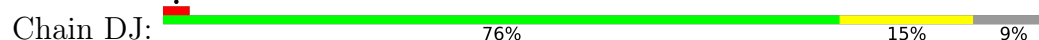
- Molecule 2: Major carboxysome shell protein 1A



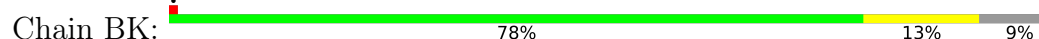
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A

Chain CK:  80% 11% 9%



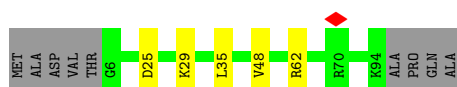
- Molecule 2: Major carboxysome shell protein 1A

Chain DK:  74% 16% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain BL:  86% 5% 9%



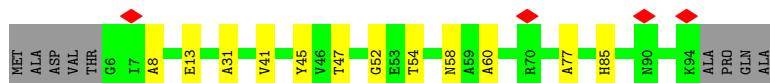
- Molecule 2: Major carboxysome shell protein 1A

Chain CL:  78% 13% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain DL:  79% 12% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain BM:  77% 14% 9%



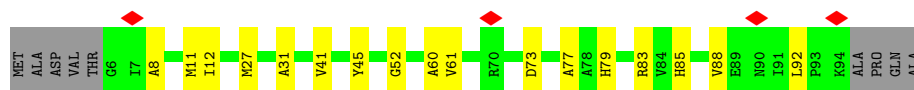
- Molecule 2: Major carboxysome shell protein 1A

Chain CM:  76% 15% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain DM:  73% 17% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain BN:  81% 10% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain CN:  72% 18% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain DN:  74% 16% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain BO:  80% 11% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain CO:  74% 16% 9%

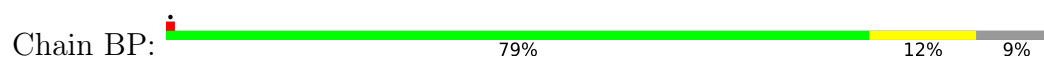


- Molecule 2: Major carboxysome shell protein 1A

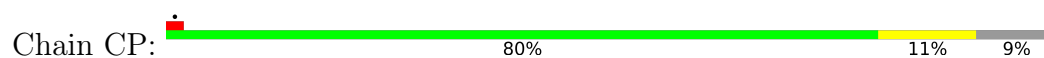
Chain DO:  78% 13% 9%



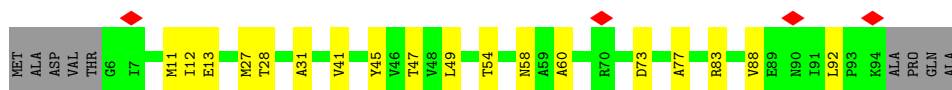
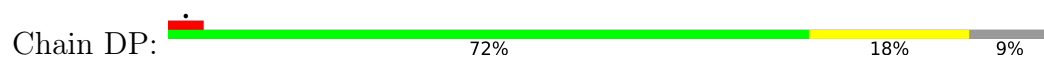
- Molecule 2: Major carboxysome shell protein 1A



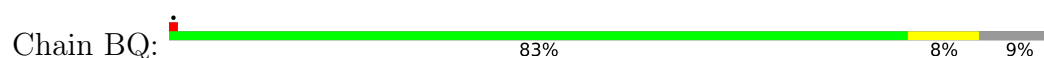
- Molecule 2: Major carboxysome shell protein 1A



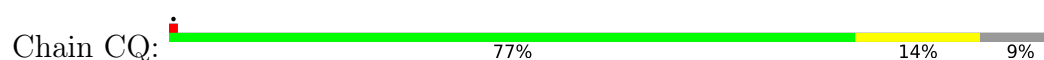
- Molecule 2: Major carboxysome shell protein 1A



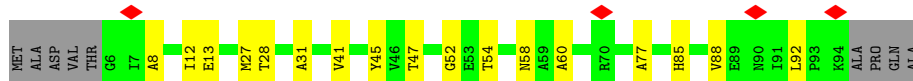
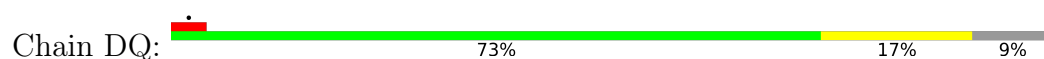
- Molecule 2: Major carboxysome shell protein 1A



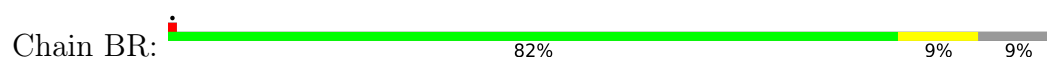
- Molecule 2: Major carboxysome shell protein 1A



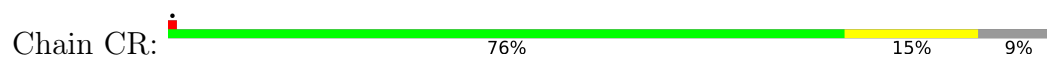
- Molecule 2: Major carboxysome shell protein 1A



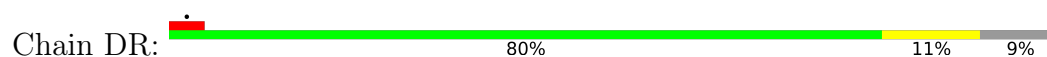
- Molecule 2: Major carboxysome shell protein 1A



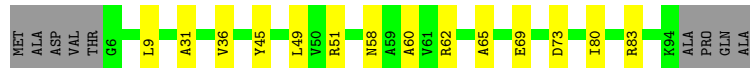
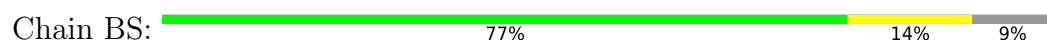
- Molecule 2: Major carboxysome shell protein 1A



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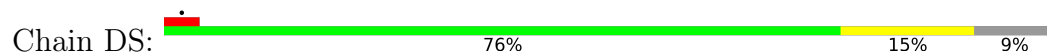
- Molecule 2: Major carboxysome shell protein 1A



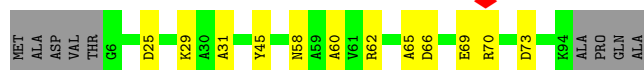
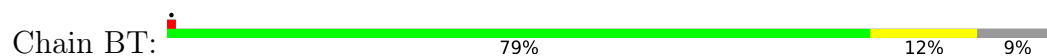
- Molecule 2: Major carboxysome shell protein 1A



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- Molecule 2: Major carboxysome shell protein 1A



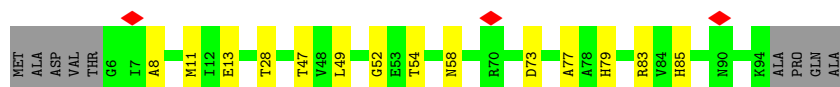
- Molecule 2: Major carboxysome shell protein 1A

Chain CT:  76% 15% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain DT:  77% 14% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain BV:  80% 11% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain CV:  78% 13% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain DV:  77% 14% 9%



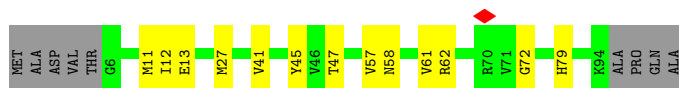
- Molecule 2: Major carboxysome shell protein 1A

Chain BW:  85% 6% 9%

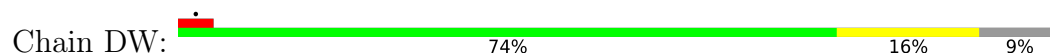


- Molecule 2: Major carboxysome shell protein 1A

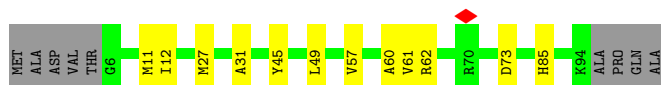
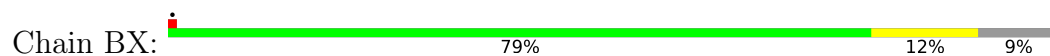
Chain CW:  78% 13% 9%



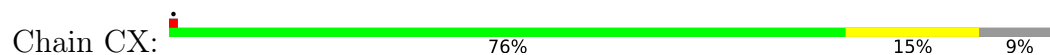
- Molecule 2: Major carboxysome shell protein 1A



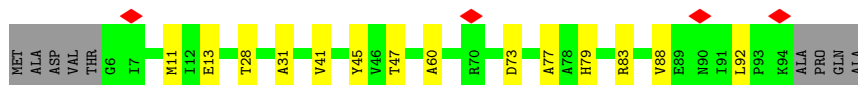
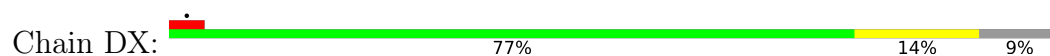
- Molecule 2: Major carboxysome shell protein 1A



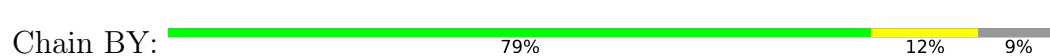
- Molecule 2: Major carboxysome shell protein 1A



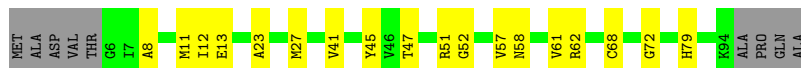
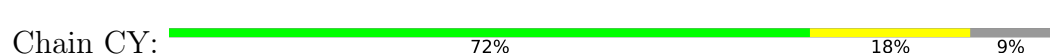
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A

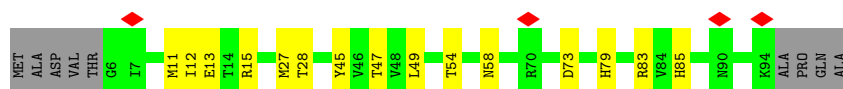


- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A

Chain DY:  76% 15% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain BZ:  80% 11% 9%



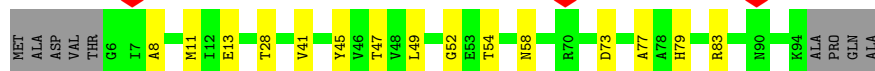
- Molecule 2: Major carboxysome shell protein 1A

Chain CZ:  77% 14% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain DZ:  76% 15% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Ba:  74% 16% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Ca:  78% 13% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Da:  76% 15% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Bb:  87% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Cb:  78% 13% 9%



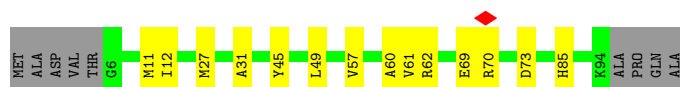
- Molecule 2: Major carboxysome shell protein 1A

Chain Db:  76% 15% 9%



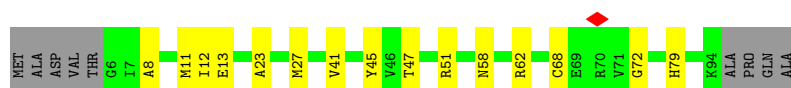
- Molecule 2: Major carboxysome shell protein 1A

Chain Bc:  77% 14% 9%



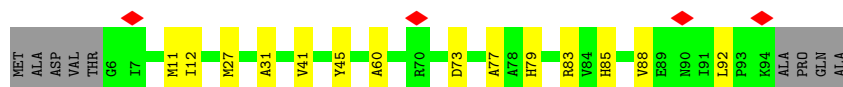
- Molecule 2: Major carboxysome shell protein 1A

Chain Cc:  76% 15% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Dc:  77% 14% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Bd:  80% 11% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Cd: 72% 18% 9%



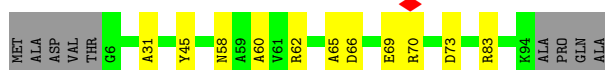
- Molecule 2: Major carboxysome shell protein 1A

Chain Dd: 77% 14% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Be: 80% 11% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Ce: 73% 17% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain De: 78% 13% 9%

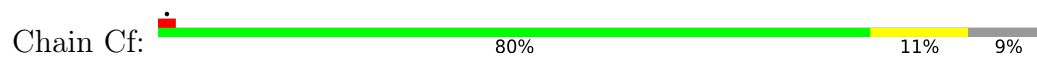


- Molecule 2: Major carboxysome shell protein 1A

Chain Bf: 81% 10% 9%



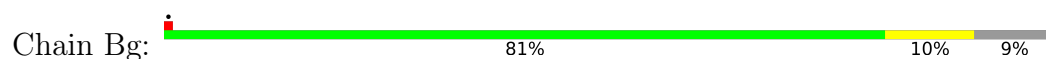
- Molecule 2: Major carboxysome shell protein 1A



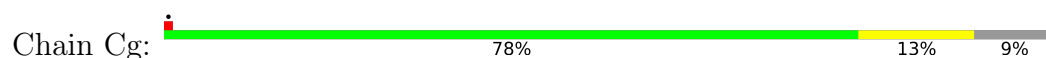
- Molecule 2: Major carboxysome shell protein 1A



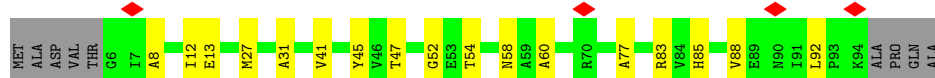
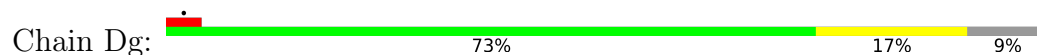
- Molecule 2: Major carboxysome shell protein 1A



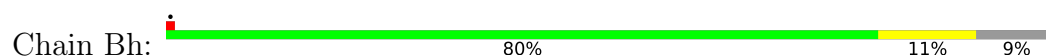
- Molecule 2: Major carboxysome shell protein 1A



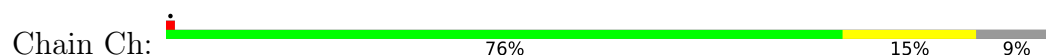
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A

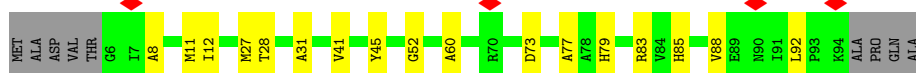
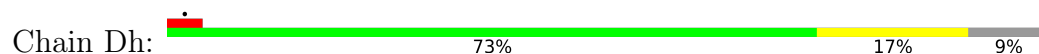


- Molecule 2: Major carboxysome shell protein 1A

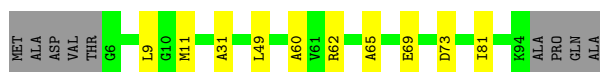
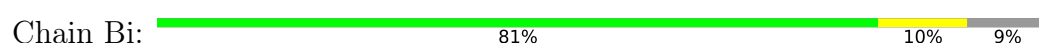




- Molecule 2: Major carboxysome shell protein 1A



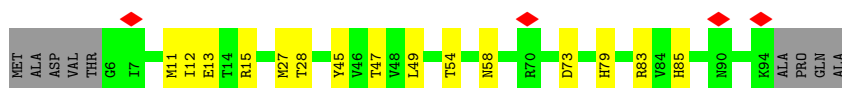
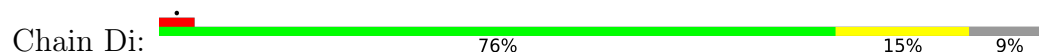
- Molecule 2: Major carboxysome shell protein 1A



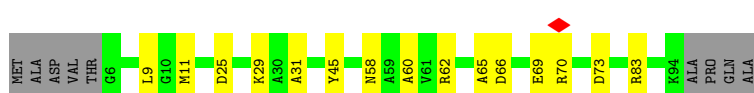
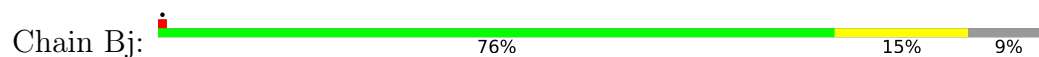
- Molecule 2: Major carboxysome shell protein 1A



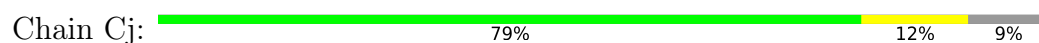
- Molecule 2: Major carboxysome shell protein 1A



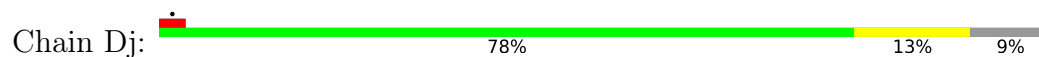
- Molecule 2: Major carboxysome shell protein 1A



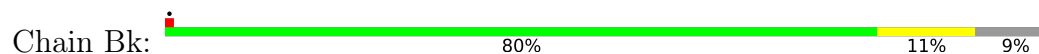
- Molecule 2: Major carboxysome shell protein 1A



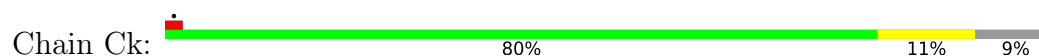
- Molecule 2: Major carboxysome shell protein 1A



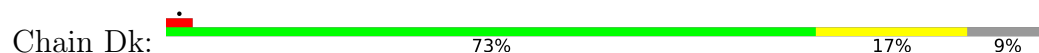
- Molecule 2: Major carboxysome shell protein 1A



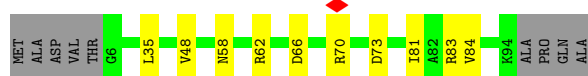
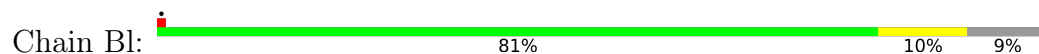
- Molecule 2: Major carboxysome shell protein 1A



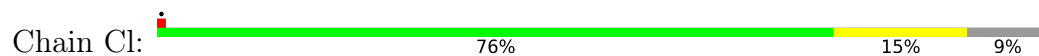
- Molecule 2: Major carboxysome shell protein 1A



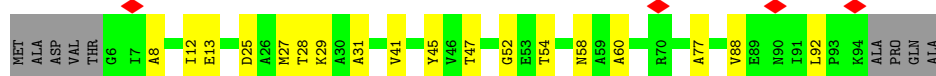
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A

Chain Bm:  77% 14% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Cm:  76% 15% 9%



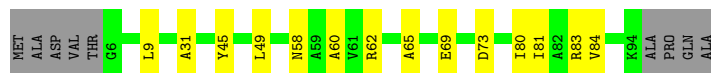
- Molecule 2: Major carboxysome shell protein 1A

Chain Dm:  80% 11% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Bn:  77% 14% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Cn:  72% 18% 9%



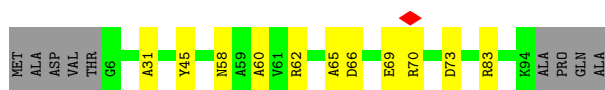
- Molecule 2: Major carboxysome shell protein 1A

Chain Dn:  76% 15% 9%



- Molecule 2: Major carboxysome shell protein 1A

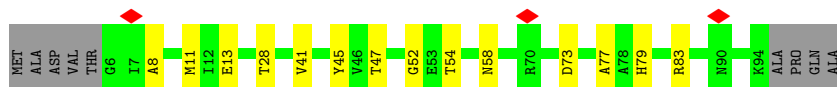
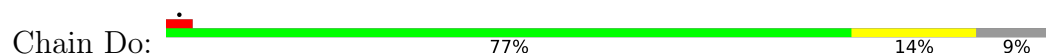
Chain Bo:  80% 11% 9%



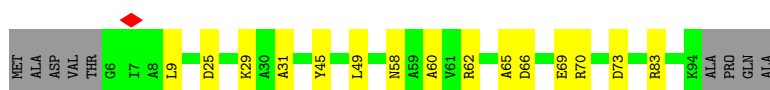
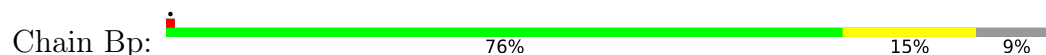
- Molecule 2: Major carboxysome shell protein 1A



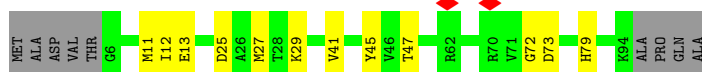
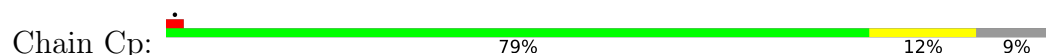
- Molecule 2: Major carboxysome shell protein 1A



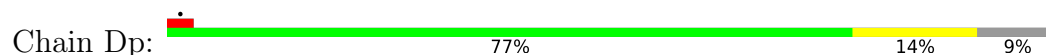
- Molecule 2: Major carboxysome shell protein 1A



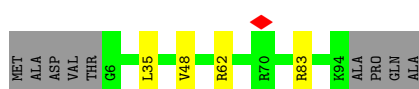
- Molecule 2: Major carboxysome shell protein 1A



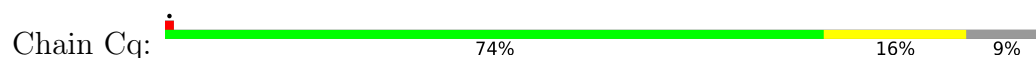
- Molecule 2: Major carboxysome shell protein 1A



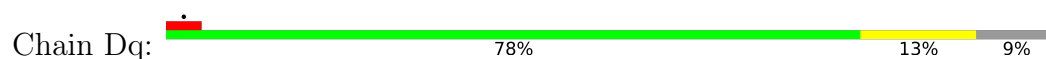
- Molecule 2: Major carboxysome shell protein 1A



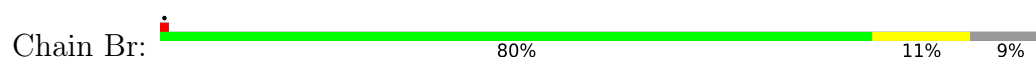
- Molecule 2: Major carboxysome shell protein 1A



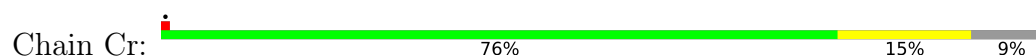
- Molecule 2: Major carboxysome shell protein 1A



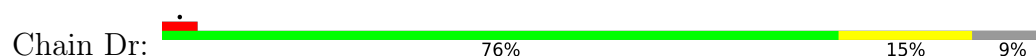
- Molecule 2: Major carboxysome shell protein 1A



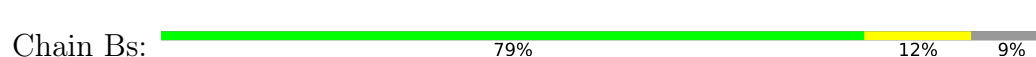
- Molecule 2: Major carboxysome shell protein 1A



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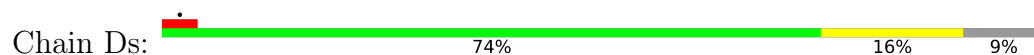


- Molecule 2: Major carboxysome shell protein 1A

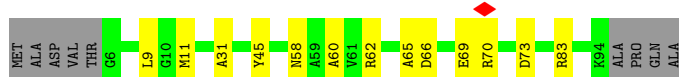
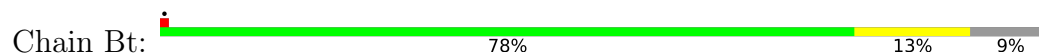




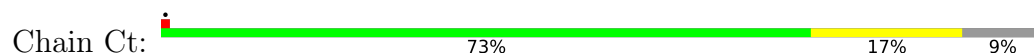
- Molecule 2: Major carboxysome shell protein 1A



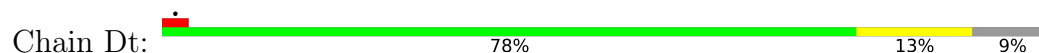
- Molecule 2: Major carboxysome shell protein 1A



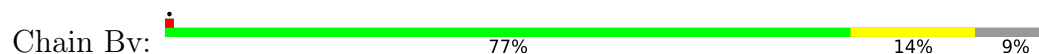
- Molecule 2: Major carboxysome shell protein 1A



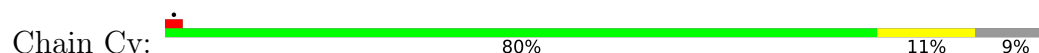
- Molecule 2: Major carboxysome shell protein 1A



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- Molecule 2: Major carboxysome shell protein 1A



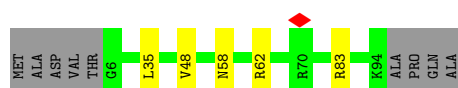
- Molecule 2: Major carboxysome shell protein 1A

Chain Dv:  74% 16% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Bw:  86% 5% 9%



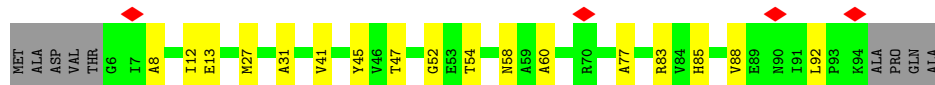
- Molecule 2: Major carboxysome shell protein 1A

Chain Cw:  78% 13% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Dw:  73% 17% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Bx:  79% 12% 9%



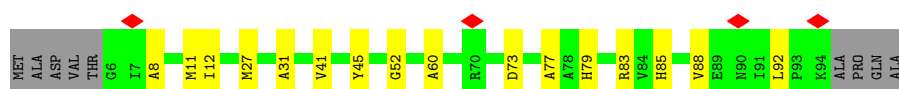
- Molecule 2: Major carboxysome shell protein 1A

Chain Cx:  76% 15% 9%



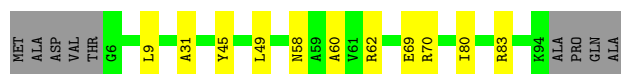
- Molecule 2: Major carboxysome shell protein 1A

Chain Dx:  74% 16% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain By:  80% 11% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Cy:  72% 18% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Dy:  74% 16% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Bz:  81% 10% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Cz:  74% 16% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain Dz:  74% 16% 9%

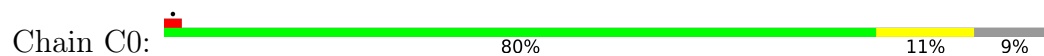


- Molecule 2: Major carboxysome shell protein 1A

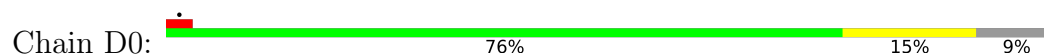
Chain B0:  79% 12% 9%



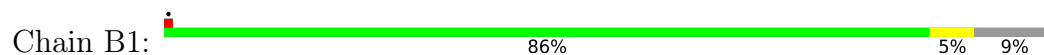
- Molecule 2: Major carboxysome shell protein 1A



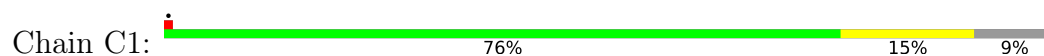
- Molecule 2: Major carboxysome shell protein 1A



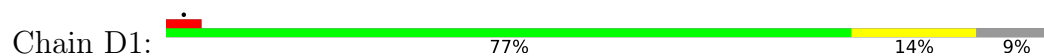
- Molecule 2: Major carboxysome shell protein 1A



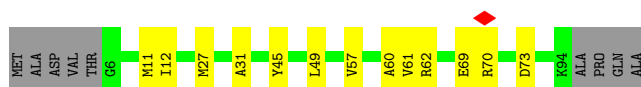
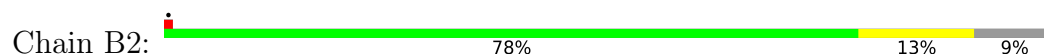
- Molecule 2: Major carboxysome shell protein 1A



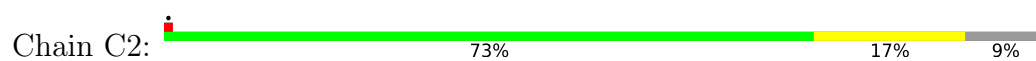
- Molecule 2: Major carboxysome shell protein 1A



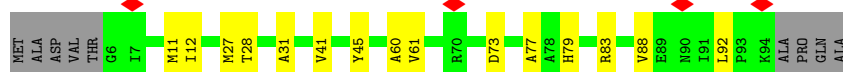
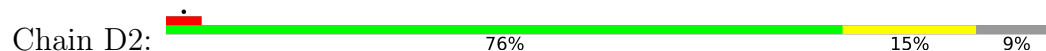
- Molecule 2: Major carboxysome shell protein 1A



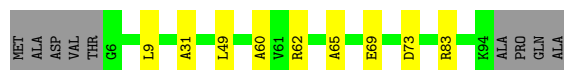
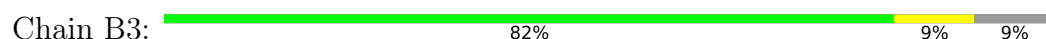
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A



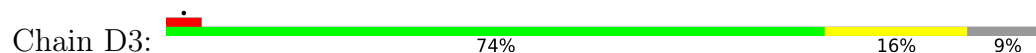
- Molecule 2: Major carboxysome shell protein 1A



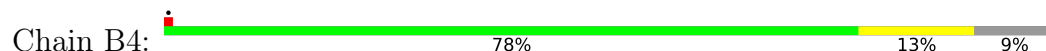
- Molecule 2: Major carboxysome shell protein 1A



- 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 D4:  78% 13% 9%



● Molecule 2: Major carboxysome shell protein 1A

Chain B5:  78% 13% 9%



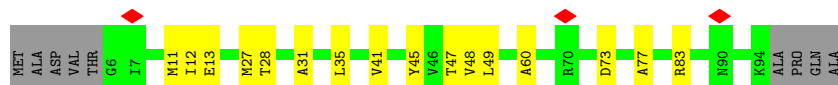
● Molecule 2: Major carboxysome shell protein 1A

Chain C5:  80% 11% 9%



● Molecule 2: Major carboxysome shell protein 1A

Chain D5:  74% 16% 9%



● Molecule 2: Major carboxysome shell protein 1A

Chain B6:  85% 6% 9%



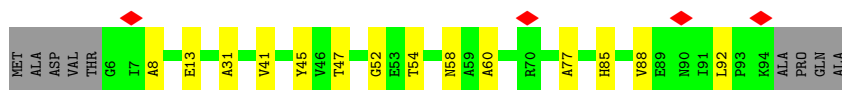
● Molecule 2: Major carboxysome shell protein 1A

Chain C6:  79% 12% 9%

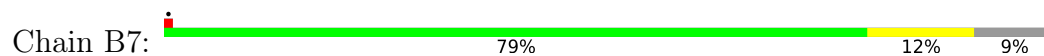


● Molecule 2: Major carboxysome shell protein 1A

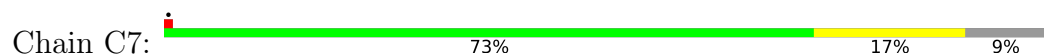
Chain D6:  77% 14% 9%



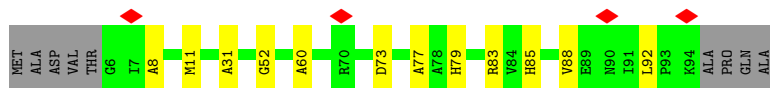
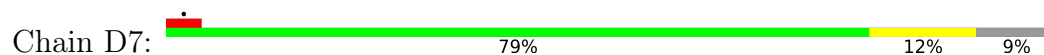
- Molecule 2: Major carboxysome shell protein 1A



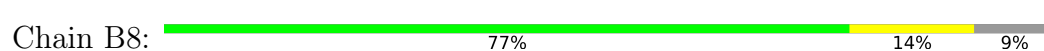
- Molecule 2: Major carboxysome shell protein 1A



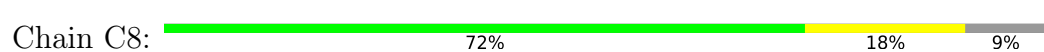
- Molecule 2: Major carboxysome shell protein 1A



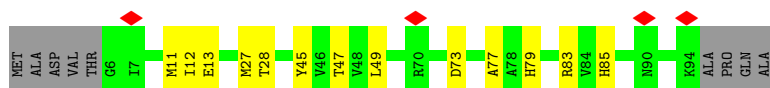
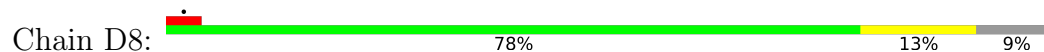
- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A

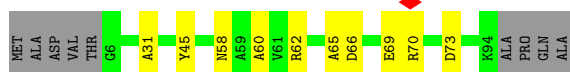


- Molecule 2: Major carboxysome shell protein 1A



- Molecule 2: Major carboxysome shell protein 1A

Chain B9:  81% 10% 9%



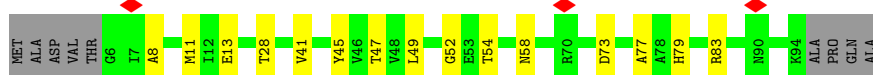
- Molecule 2: Major carboxysome shell protein 1A

Chain C9:  74% 16% 9%



- Molecule 2: Major carboxysome shell protein 1A

Chain D9:  76% 15% 9%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67192	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.123	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	258.0, 258.0, 258.0	wwPDB
Map dimensions	300, 300, 300	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	0.33	0/612	0.53	0/832
1	A1	0.32	0/612	0.54	0/832
1	A2	0.32	0/612	0.53	0/832
1	A3	0.32	0/612	0.54	0/832
1	A4	0.32	0/612	0.54	0/832
1	A5	0.33	0/612	0.53	0/832
1	A6	0.32	0/612	0.54	0/832
1	A7	0.32	0/612	0.53	0/832
1	A8	0.32	0/612	0.54	0/832
1	A9	0.32	0/612	0.54	0/832
1	AA	0.33	0/612	0.53	0/832
1	AB	0.32	0/612	0.53	0/832
1	AC	0.32	0/612	0.53	0/832
1	AD	0.32	0/612	0.54	0/832
1	AE	0.32	0/612	0.54	0/832
1	AF	0.32	0/612	0.53	0/832
1	AG	0.32	0/612	0.53	0/832
1	AH	0.32	0/612	0.51	0/832
1	AI	0.33	0/612	0.54	0/832
1	AJ	0.32	0/612	0.54	0/832
1	AK	0.32	0/612	0.53	0/832
1	AL	0.32	0/612	0.54	0/832
1	AM	0.32	0/612	0.52	0/832
1	AN	0.32	0/612	0.54	0/832
1	AO	0.32	0/612	0.54	0/832
1	AP	0.33	0/612	0.53	0/832
1	AQ	0.32	0/612	0.54	0/832
1	AR	0.32	0/612	0.52	0/832
1	AS	0.32	0/612	0.54	0/832
1	AT	0.32	0/612	0.54	0/832
1	AV	0.32	0/612	0.55	0/832
1	AW	0.33	0/612	0.54	0/832
1	AX	0.32	0/612	0.54	0/832
1	AY	0.32	0/612	0.54	0/832

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AZ	0.32	0/612	0.54	0/832
1	Aa	0.32	0/612	0.53	0/832
1	Ab	0.31	0/612	0.52	0/832
1	Ac	0.32	0/612	0.52	0/832
1	Ad	0.32	0/612	0.53	0/832
1	Ae	0.32	0/612	0.54	0/832
1	Af	0.33	0/612	0.54	0/832
1	Ag	0.32	0/612	0.53	0/832
1	Ah	0.32	0/612	0.53	0/832
1	Ai	0.32	0/612	0.54	0/832
1	Aj	0.32	0/612	0.54	0/832
1	Ak	0.33	0/612	0.53	0/832
1	Al	0.32	0/612	0.53	0/832
1	Am	0.32	0/612	0.52	0/832
1	An	0.32	0/612	0.55	0/832
1	Ao	0.32	0/612	0.54	0/832
1	Ap	0.32	0/612	0.54	0/832
1	Aq	0.32	0/612	0.52	0/832
1	Ar	0.32	0/612	0.53	0/832
1	As	0.32	0/612	0.54	0/832
1	At	0.32	0/612	0.54	0/832
1	Av	0.32	0/612	0.54	0/832
1	Aw	0.32	0/612	0.54	0/832
1	Ax	0.32	0/612	0.53	0/832
1	Ay	0.32	0/612	0.54	0/832
1	Az	0.32	0/612	0.53	0/832
2	B0	0.29	0/640	0.59	0/866
2	B1	0.29	0/640	0.55	0/866
2	B2	0.29	0/640	0.57	0/866
2	B3	0.30	0/640	0.58	0/866
2	B4	0.29	0/640	0.57	0/866
2	B5	0.29	0/640	0.59	0/866
2	B6	0.29	0/640	0.56	0/866
2	B7	0.28	0/640	0.57	0/866
2	B8	0.30	0/640	0.57	0/866
2	B9	0.28	0/640	0.57	0/866
2	BA	0.29	0/640	0.59	0/866
2	BB	0.29	0/640	0.55	0/866
2	BC	0.28	0/640	0.57	0/866
2	BD	0.30	0/640	0.58	0/866
2	BE	0.29	0/640	0.57	0/866
2	BF	0.29	0/640	0.59	0/866
2	BG	0.29	0/640	0.55	0/866

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	BH	0.29	0/640	0.57	0/866
2	BI	0.30	0/640	0.58	0/866
2	BJ	0.29	0/640	0.57	0/866
2	BK	0.29	0/640	0.58	0/866
2	BL	0.29	0/640	0.56	0/866
2	BM	0.29	0/640	0.57	0/866
2	BN	0.30	0/640	0.59	0/866
2	BO	0.29	0/640	0.58	0/866
2	BP	0.29	0/640	0.59	0/866
2	BQ	0.29	0/640	0.56	0/866
2	BR	0.28	0/640	0.56	0/866
2	BS	0.30	0/640	0.58	0/866
2	BT	0.29	0/640	0.57	0/866
2	BV	0.29	0/640	0.58	0/866
2	BW	0.29	0/640	0.55	0/866
2	BX	0.28	0/640	0.57	0/866
2	BY	0.30	0/640	0.59	0/866
2	BZ	0.28	0/640	0.56	0/866
2	Ba	0.29	0/640	0.58	0/866
2	Bb	0.29	0/640	0.55	0/866
2	Bc	0.28	0/640	0.56	0/866
2	Bd	0.30	0/640	0.58	0/866
2	Be	0.29	0/640	0.57	0/866
2	Bf	0.29	0/640	0.58	0/866
2	Bg	0.29	0/640	0.55	0/866
2	Bh	0.28	0/640	0.57	0/866
2	Bi	0.30	0/640	0.59	0/866
2	Bj	0.28	0/640	0.58	0/866
2	Bk	0.29	0/640	0.59	0/866
2	Bl	0.29	0/640	0.56	0/866
2	Bm	0.28	0/640	0.58	0/866
2	Bn	0.30	0/640	0.58	0/866
2	Bo	0.28	0/640	0.58	0/866
2	Bp	0.29	0/640	0.59	0/866
2	Bq	0.29	0/640	0.55	0/866
2	Br	0.28	0/640	0.57	0/866
2	Bs	0.30	0/640	0.58	0/866
2	Bt	0.29	0/640	0.57	0/866
2	Bv	0.29	0/640	0.59	0/866
2	Bw	0.29	0/640	0.55	0/866
2	Bx	0.28	0/640	0.57	0/866
2	By	0.30	0/640	0.58	0/866
2	Bz	0.28	0/640	0.57	0/866

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	C0	0.30	0/640	0.55	0/866
2	C1	0.29	0/640	0.54	0/866
2	C2	0.30	0/640	0.53	0/866
2	C3	0.29	0/640	0.55	0/866
2	C4	0.30	0/640	0.52	0/866
2	C5	0.30	0/640	0.55	0/866
2	C6	0.29	0/640	0.55	0/866
2	C7	0.30	0/640	0.53	0/866
2	C8	0.29	0/640	0.54	0/866
2	C9	0.29	0/640	0.51	0/866
2	CA	0.30	0/640	0.55	0/866
2	CB	0.29	0/640	0.54	0/866
2	CC	0.30	0/640	0.53	0/866
2	CD	0.29	0/640	0.54	0/866
2	CE	0.29	0/640	0.52	0/866
2	CF	0.30	0/640	0.55	0/866
2	CG	0.29	0/640	0.54	0/866
2	CH	0.30	0/640	0.53	0/866
2	CI	0.29	0/640	0.54	0/866
2	CJ	0.29	0/640	0.52	0/866
2	CK	0.29	0/640	0.55	0/866
2	CL	0.29	0/640	0.54	0/866
2	CM	0.29	0/640	0.54	0/866
2	CN	0.29	0/640	0.54	0/866
2	CO	0.30	0/640	0.52	0/866
2	CP	0.29	0/640	0.55	0/866
2	CQ	0.29	0/640	0.54	0/866
2	CR	0.30	0/640	0.53	0/866
2	CS	0.29	0/640	0.54	0/866
2	CT	0.30	0/640	0.53	0/866
2	CV	0.30	0/640	0.55	0/866
2	CW	0.30	0/640	0.54	0/866
2	CX	0.29	0/640	0.53	0/866
2	CY	0.29	0/640	0.54	0/866
2	CZ	0.30	0/640	0.52	0/866
2	Ca	0.29	0/640	0.55	0/866
2	Cb	0.29	0/640	0.56	0/866
2	Cc	0.30	0/640	0.53	0/866
2	Cd	0.30	0/640	0.54	0/866
2	Ce	0.30	0/640	0.52	0/866
2	Cf	0.30	0/640	0.55	0/866
2	Cg	0.29	0/640	0.54	0/866
2	Ch	0.30	0/640	0.53	0/866

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Ci	0.30	0/640	0.54	0/866
2	Cj	0.30	0/640	0.53	0/866
2	Ck	0.30	0/640	0.55	0/866
2	Cl	0.29	0/640	0.55	0/866
2	Cm	0.30	0/640	0.53	0/866
2	Cn	0.29	0/640	0.53	0/866
2	Co	0.30	0/640	0.52	0/866
2	Cp	0.30	0/640	0.55	0/866
2	Cq	0.29	0/640	0.55	0/866
2	Cr	0.29	0/640	0.53	0/866
2	Cs	0.30	0/640	0.54	0/866
2	Ct	0.30	0/640	0.52	0/866
2	Cv	0.30	0/640	0.55	0/866
2	Cw	0.29	0/640	0.54	0/866
2	Cx	0.30	0/640	0.53	0/866
2	Cy	0.30	0/640	0.54	0/866
2	Cz	0.30	0/640	0.53	0/866
2	D0	0.30	0/640	0.56	0/866
2	D1	0.29	0/640	0.54	0/866
2	D2	0.29	0/640	0.54	0/866
2	D3	0.29	0/640	0.54	0/866
2	D4	0.29	0/640	0.54	0/866
2	D5	0.29	0/640	0.55	0/866
2	D6	0.29	0/640	0.54	0/866
2	D7	0.28	0/640	0.53	0/866
2	D8	0.30	0/640	0.57	0/866
2	D9	0.28	0/640	0.54	0/866
2	DA	0.29	0/640	0.55	0/866
2	DB	0.29	0/640	0.54	0/866
2	DC	0.29	0/640	0.53	0/866
2	DD	0.30	0/640	0.56	0/866
2	DE	0.28	0/640	0.54	0/866
2	DF	0.29	0/640	0.55	0/866
2	DG	0.29	0/640	0.54	0/866
2	DH	0.29	0/640	0.54	0/866
2	DI	0.30	0/640	0.57	0/866
2	DJ	0.28	0/640	0.54	0/866
2	DK	0.29	0/640	0.55	0/866
2	DL	0.29	0/640	0.54	0/866
2	DM	0.29	0/640	0.54	0/866
2	DN	0.30	0/640	0.56	0/866
2	DO	0.29	0/640	0.55	0/866
2	DP	0.30	0/640	0.56	0/866

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	DQ	0.29	0/640	0.54	0/866
2	DR	0.28	0/640	0.53	0/866
2	DS	0.30	0/640	0.56	0/866
2	DT	0.29	0/640	0.54	0/866
2	DV	0.29	0/640	0.55	0/866
2	DW	0.29	0/640	0.55	0/866
2	DX	0.29	0/640	0.53	0/866
2	DY	0.30	0/640	0.56	0/866
2	DZ	0.28	0/640	0.55	0/866
2	Da	0.30	0/640	0.55	0/866
2	Db	0.29	0/640	0.54	0/866
2	Dc	0.30	0/640	0.54	0/866
2	Dd	0.30	0/640	0.56	0/866
2	De	0.28	0/640	0.54	0/866
2	Df	0.29	0/640	0.55	0/866
2	Dg	0.29	0/640	0.55	0/866
2	Dh	0.29	0/640	0.55	0/866
2	Di	0.30	0/640	0.55	0/866
2	Dj	0.28	0/640	0.54	0/866
2	Dk	0.29	0/640	0.55	0/866
2	Dl	0.29	0/640	0.55	0/866
2	Dm	0.28	0/640	0.53	0/866
2	Dn	0.30	0/640	0.56	0/866
2	Do	0.29	0/640	0.55	0/866
2	Dp	0.30	0/640	0.55	0/866
2	Dq	0.29	0/640	0.56	0/866
2	Dr	0.29	0/640	0.54	0/866
2	Ds	0.30	0/640	0.56	0/866
2	Dt	0.28	0/640	0.54	0/866
2	Dv	0.30	0/640	0.56	0/866
2	Dw	0.29	0/640	0.54	0/866
2	Dx	0.29	0/640	0.54	0/866
2	Dy	0.30	0/640	0.56	0/866
2	Dz	0.29	0/640	0.54	0/866
All	All	0.30	0/151920	0.55	0/205800

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 ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	600	0	619	3	0
1	A1	600	0	619	7	0
1	A2	600	0	619	6	0
1	A3	600	0	619	6	0
1	A4	600	0	619	8	0
1	A5	600	0	619	5	0
1	A6	600	0	619	8	0
1	A7	600	0	619	7	0
1	A8	600	0	619	8	0
1	A9	600	0	619	7	0
1	AA	600	0	619	3	0
1	AB	600	0	619	8	0
1	AC	600	0	619	6	0
1	AD	600	0	619	8	0
1	AE	600	0	619	7	0
1	AF	600	0	619	8	0
1	AG	600	0	619	7	0
1	AH	600	0	619	5	0
1	AI	600	0	619	8	0
1	AJ	600	0	619	7	0
1	AK	600	0	619	5	0
1	AL	600	0	619	8	0
1	AM	600	0	619	6	0
1	AN	600	0	619	8	0
1	AO	600	0	619	6	0
1	AP	600	0	619	5	0
1	AQ	600	0	619	7	0
1	AR	600	0	619	5	0
1	AS	600	0	619	8	0
1	AT	600	0	619	7	0
1	AV	600	0	619	5	0
1	AW	600	0	619	8	0
1	AX	600	0	619	6	0
1	AY	600	0	619	6	0
1	AZ	600	0	619	7	0
1	Aa	600	0	619	4	0
1	Ab	600	0	619	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ac	600	0	619	4	0
1	Ad	600	0	619	9	0
1	Ae	600	0	619	7	0
1	Af	600	0	619	5	0
1	Ag	600	0	619	7	0
1	Ah	600	0	619	7	0
1	Ai	600	0	619	7	0
1	Aj	600	0	619	7	0
1	Ak	600	0	619	5	0
1	Al	600	0	619	6	0
1	Am	600	0	619	8	0
1	An	600	0	619	7	0
1	Ao	600	0	619	7	0
1	Ap	600	0	619	6	0
1	Aq	600	0	619	10	0
1	Ar	600	0	619	5	0
1	As	600	0	619	7	0
1	At	600	0	619	7	0
1	Av	600	0	619	4	0
1	Aw	600	0	619	8	0
1	Ax	600	0	619	6	0
1	Ay	600	0	619	9	0
1	Az	600	0	619	6	0
2	B0	635	0	657	7	0
2	B1	635	0	657	4	0
2	B2	635	0	657	9	0
2	B3	635	0	657	7	0
2	B4	635	0	657	9	0
2	B5	635	0	657	8	0
2	B6	635	0	657	4	0
2	B7	635	0	657	8	0
2	B8	635	0	657	10	0
2	B9	635	0	657	7	0
2	BA	635	0	657	7	0
2	BB	635	0	657	4	0
2	BC	635	0	657	7	0
2	BD	635	0	657	9	0
2	BE	635	0	657	8	0
2	BF	635	0	657	9	0
2	BG	635	0	657	3	0
2	BH	635	0	657	10	0
2	BI	635	0	657	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BJ	635	0	657	8	0
2	BK	635	0	657	9	0
2	BL	635	0	657	3	0
2	BM	635	0	657	9	0
2	BN	635	0	657	9	0
2	BO	635	0	657	8	0
2	BP	635	0	657	7	0
2	BQ	635	0	657	5	0
2	BR	635	0	657	6	0
2	BS	635	0	657	9	0
2	BT	635	0	657	8	0
2	BV	635	0	657	6	0
2	BW	635	0	657	4	0
2	BX	635	0	657	8	0
2	BY	635	0	657	8	0
2	BZ	635	0	657	7	0
2	Ba	635	0	657	9	0
2	Bb	635	0	657	3	0
2	Bc	635	0	657	9	0
2	Bd	635	0	657	9	0
2	Be	635	0	657	8	0
2	Bf	635	0	657	6	0
2	Bg	635	0	657	8	0
2	Bh	635	0	657	8	0
2	Bi	635	0	657	7	0
2	Bj	635	0	657	10	0
2	Bk	635	0	657	6	0
2	Bl	635	0	657	7	0
2	Bm	635	0	657	10	0
2	Bn	635	0	657	9	0
2	Bo	635	0	657	8	0
2	Bp	635	0	657	9	0
2	Bq	635	0	657	3	0
2	Br	635	0	657	7	0
2	Bs	635	0	657	10	0
2	Bt	635	0	657	9	0
2	Bv	635	0	657	8	0
2	Bw	635	0	657	4	0
2	Bx	635	0	657	8	0
2	By	635	0	657	8	0
2	Bz	635	0	657	6	0
2	C0	635	0	657	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C1	635	0	657	10	0
2	C2	635	0	657	12	0
2	C3	635	0	657	12	0
2	C4	635	0	657	12	0
2	C5	635	0	657	7	0
2	C6	635	0	657	8	0
2	C7	635	0	657	12	0
2	C8	635	0	657	12	0
2	C9	635	0	657	10	0
2	CA	635	0	657	8	0
2	CB	635	0	657	8	0
2	CC	635	0	657	10	0
2	CD	635	0	657	13	0
2	CE	635	0	657	9	0
2	CF	635	0	657	8	0
2	CG	635	0	657	9	0
2	CH	635	0	657	11	0
2	CI	635	0	657	12	0
2	CJ	635	0	657	9	0
2	CK	635	0	657	7	0
2	CL	635	0	657	9	0
2	CM	635	0	657	11	0
2	CN	635	0	657	12	0
2	CO	635	0	657	10	0
2	CP	635	0	657	8	0
2	CQ	635	0	657	8	0
2	CR	635	0	657	10	0
2	CS	635	0	657	12	0
2	CT	635	0	657	10	0
2	CV	635	0	657	10	0
2	CW	635	0	657	8	0
2	CX	635	0	657	11	0
2	CY	635	0	657	11	0
2	CZ	635	0	657	9	0
2	Ca	635	0	657	10	0
2	Cb	635	0	657	9	0
2	Cc	635	0	657	11	0
2	Cd	635	0	657	11	0
2	Ce	635	0	657	11	0
2	Cf	635	0	657	8	0
2	Cg	635	0	657	10	0
2	Ch	635	0	657	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Ci	635	0	657	12	0
2	Cj	635	0	657	8	0
2	Ck	635	0	657	8	0
2	Cl	635	0	657	11	0
2	Cm	635	0	657	11	0
2	Cn	635	0	657	12	0
2	Co	635	0	657	13	0
2	Cp	635	0	657	8	0
2	Cq	635	0	657	12	0
2	Cr	635	0	657	11	0
2	Cs	635	0	657	12	0
2	Ct	635	0	657	11	0
2	Cv	635	0	657	7	0
2	Cw	635	0	657	9	0
2	Cx	635	0	657	11	0
2	Cy	635	0	657	12	0
2	Cz	635	0	657	10	0
2	D0	635	0	657	10	0
2	D1	635	0	657	8	0
2	D2	635	0	657	10	0
2	D3	635	0	657	11	0
2	D4	635	0	657	9	0
2	D5	635	0	657	11	0
2	D6	635	0	657	8	0
2	D7	635	0	657	8	0
2	D8	635	0	657	11	0
2	D9	635	0	657	10	0
2	DA	635	0	657	10	0
2	DB	635	0	657	8	0
2	DC	635	0	657	6	0
2	DD	635	0	657	11	0
2	DE	635	0	657	11	0
2	DF	635	0	657	9	0
2	DG	635	0	657	8	0
2	DH	635	0	657	8	0
2	DI	635	0	657	12	0
2	DJ	635	0	657	10	0
2	DK	635	0	657	10	0
2	DL	635	0	657	7	0
2	DM	635	0	657	11	0
2	DN	635	0	657	13	0
2	DO	635	0	657	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	DP	635	0	657	11	0
2	DQ	635	0	657	11	0
2	DR	635	0	657	7	0
2	DS	635	0	657	11	0
2	DT	635	0	657	11	0
2	DV	635	0	657	11	0
2	DW	635	0	657	9	0
2	DX	635	0	657	9	0
2	DY	635	0	657	11	0
2	DZ	635	0	657	10	0
2	Da	635	0	657	12	0
2	Db	635	0	657	9	0
2	Dc	635	0	657	9	0
2	Dd	635	0	657	11	0
2	De	635	0	657	9	0
2	Df	635	0	657	11	0
2	Dg	635	0	657	11	0
2	Dh	635	0	657	11	0
2	Di	635	0	657	11	0
2	Dj	635	0	657	9	0
2	Dk	635	0	657	10	0
2	Dl	635	0	657	11	0
2	Dm	635	0	657	7	0
2	Dn	635	0	657	12	0
2	Do	635	0	657	9	0
2	Dp	635	0	657	9	0
2	Dq	635	0	657	7	0
2	Dr	635	0	657	10	0
2	Ds	635	0	657	13	0
2	Dt	635	0	657	9	0
2	Dv	635	0	657	11	0
2	Dw	635	0	657	10	0
2	Dx	635	0	657	10	0
2	Dy	635	0	657	12	0
2	Dz	635	0	657	11	0
All	All	150300	0	155400	1679	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1679) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CW:12:ILE:HD12	2:CW:27:MET:HE3	1.50	0.93
2:CG:12:ILE:HD12	2:CG:27:MET:HE3	1.50	0.93
2:Cq:12:ILE:HD12	2:Cq:27:MET:HE3	1.50	0.90
2:C1:12:ILE:HD12	2:C1:27:MET:HE3	1.56	0.87
2:Cg:12:ILE:HD12	2:Cg:27:MET:HE3	1.56	0.86
2:Cb:12:ILE:HD12	2:Cb:27:MET:HE3	1.56	0.86
2:CL:12:ILE:HD12	2:CL:27:MET:HE3	1.56	0.85
2:Cw:12:ILE:HD12	2:Cw:27:MET:HE3	1.56	0.85
2:Cd:12:ILE:HD12	2:Cd:27:MET:HE3	1.56	0.84
2:C6:12:ILE:HD12	2:C6:27:MET:HE3	1.57	0.84
2:CQ:12:ILE:HD12	2:CQ:27:MET:HE3	1.58	0.84
2:CB:12:ILE:HD12	2:CB:27:MET:HE3	1.58	0.84
2:Do:54:THR:O	2:Do:58:ASN:ND2	2.10	0.84
2:D4:54:THR:O	2:D4:58:ASN:ND2	2.10	0.84
2:DO:54:THR:O	2:DO:58:ASN:ND2	2.10	0.84
2:Dj:54:THR:O	2:Dj:58:ASN:ND2	2.10	0.84
2:Cl:12:ILE:HD12	2:Cl:27:MET:HE3	1.59	0.84
2:Dz:54:THR:O	2:Dz:58:ASN:ND2	2.10	0.83
2:Dt:54:THR:O	2:Dt:58:ASN:ND2	2.10	0.83
2:D9:54:THR:O	2:D9:58:ASN:ND2	2.11	0.83
2:DJ:54:THR:O	2:DJ:58:ASN:ND2	2.10	0.83
2:DT:54:THR:O	2:DT:58:ASN:ND2	2.11	0.82
2:DE:54:THR:O	2:DE:58:ASN:ND2	2.10	0.82
2:DZ:54:THR:O	2:DZ:58:ASN:ND2	2.10	0.82
2:De:54:THR:O	2:De:58:ASN:ND2	2.10	0.82
2:CS:12:ILE:HD12	2:CS:27:MET:HE3	1.64	0.80
2:Cn:12:ILE:HD12	2:Cn:27:MET:HE3	1.64	0.80
2:Ci:12:ILE:HD12	2:Ci:27:MET:HE3	1.64	0.79
2:CD:12:ILE:HD12	2:CD:27:MET:HE3	1.64	0.79
2:CN:12:ILE:HD12	2:CN:27:MET:HE3	1.64	0.79
2:C3:12:ILE:HD12	2:C3:27:MET:HE3	1.64	0.79
2:Cs:12:ILE:HD12	2:Cs:27:MET:HE3	1.64	0.79
2:CI:12:ILE:HD12	2:CI:27:MET:HE3	1.64	0.79
2:Cy:12:ILE:HD12	2:Cy:27:MET:HE3	1.64	0.79
2:C8:12:ILE:HD12	2:C8:27:MET:HE3	1.63	0.78
2:Ck:12:ILE:HD12	2:Ck:27:MET:HE3	1.66	0.77
2:CY:12:ILE:HD12	2:CY:27:MET:HE3	1.63	0.77
2:Cp:12:ILE:HD12	2:Cp:27:MET:HE3	1.66	0.77
2:Cf:12:ILE:HD12	2:Cf:27:MET:HE3	1.66	0.77
2:C0:12:ILE:HD12	2:C0:27:MET:HE3	1.66	0.77
2:CV:12:ILE:HD12	2:CV:27:MET:HE3	1.66	0.76
2:Ca:12:ILE:HD12	2:Ca:27:MET:HE3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CP:12:ILE:HD12	2:CP:27:MET:HE3	1.66	0.76
2:CA:12:ILE:HD12	2:CA:27:MET:HE3	1.66	0.76
2:CK:12:ILE:HD12	2:CK:27:MET:HE3	1.66	0.76
2:CF:12:ILE:HD12	2:CF:27:MET:HE3	1.66	0.76
2:Cv:12:ILE:HD12	2:Cv:27:MET:HE3	1.66	0.75
2:C5:12:ILE:HD12	2:C5:27:MET:HE3	1.66	0.75
2:B2:69:GLU:OE1	2:B2:70:ARG:NH2	2.20	0.75
2:BH:69:GLU:OE1	2:BH:70:ARG:NH2	2.20	0.75
2:Bc:69:GLU:OE1	2:Bc:70:ARG:NH2	2.20	0.75
2:Di:54:THR:O	2:Di:58:ASN:ND2	2.20	0.74
2:C7:12:ILE:HD12	2:C7:27:MET:HE3	1.69	0.74
2:Cx:12:ILE:HD12	2:Cx:27:MET:HE3	1.69	0.74
2:C2:12:ILE:HD12	2:C2:27:MET:HE3	1.69	0.74
2:CH:12:ILE:HD12	2:CH:27:MET:HE3	1.69	0.74
2:Db:54:THR:O	2:Db:58:ASN:ND2	2.20	0.74
2:Cm:12:ILE:HD12	2:Cm:27:MET:HE3	1.69	0.74
2:CM:12:ILE:HD12	2:CM:27:MET:HE3	1.69	0.74
2:Ch:12:ILE:HD12	2:Ch:27:MET:HE3	1.69	0.74
2:Cr:12:ILE:HD12	2:Cr:27:MET:HE3	1.69	0.74
2:DW:54:THR:O	2:DW:58:ASN:ND2	2.20	0.73
2:DS:11:MET:HG2	2:DS:49:LEU:HD23	1.69	0.73
2:D1:54:THR:O	2:D1:58:ASN:ND2	2.20	0.73
2:DN:11:MET:HG2	2:DN:49:LEU:HD23	1.69	0.73
2:Dl:54:THR:O	2:Dl:58:ASN:ND2	2.20	0.73
2:CC:12:ILE:HD12	2:CC:27:MET:HE3	1.69	0.73
2:Dg:54:THR:O	2:Dg:58:ASN:ND2	2.20	0.73
2:CR:12:ILE:HD12	2:CR:27:MET:HE3	1.69	0.73
2:Dn:11:MET:HG2	2:Dn:49:LEU:HD23	1.69	0.73
2:Bm:69:GLU:OE1	2:Bm:70:ARG:NH2	2.20	0.73
2:DB:54:THR:O	2:DB:58:ASN:ND2	2.20	0.73
2:DQ:54:THR:O	2:DQ:58:ASN:ND2	2.20	0.72
2:Ds:11:MET:HG2	2:Ds:49:LEU:HD23	1.69	0.72
2:Dy:11:MET:HG2	2:Dy:49:LEU:HD23	1.69	0.72
2:DM:12:ILE:HD12	2:DM:27:MET:HE3	1.72	0.72
2:Cc:12:ILE:HD12	2:Cc:27:MET:HE3	1.69	0.72
2:Dd:11:MET:HG2	2:Dd:49:LEU:HD23	1.69	0.72
2:Dq:54:THR:O	2:Dq:58:ASN:ND2	2.21	0.72
2:CX:12:ILE:HD12	2:CX:27:MET:HE3	1.69	0.72
2:D3:54:THR:O	2:D3:58:ASN:ND2	2.20	0.72
2:DG:54:THR:O	2:DG:58:ASN:ND2	2.20	0.71
2:DY:54:THR:O	2:DY:58:ASN:ND2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DL:54:THR:O	2:DL:58:ASN:ND2	2.20	0.71
2:De:28:THR:O	2:Dr:83:ARG:NH2	2.24	0.71
2:D3:11:MET:HG2	2:D3:49:LEU:HD23	1.73	0.71
2:Dj:28:THR:O	2:Dx:83:ARG:NH2	2.24	0.71
2:DY:11:MET:HG2	2:DY:49:LEU:HD23	1.70	0.71
2:DE:28:THR:O	2:Dh:83:ARG:NH2	2.24	0.71
1:AN:77:ILE:HD12	1:Av:10:LEU:HD21	1.71	0.70
2:DO:28:THR:O	2:Dc:83:ARG:NH2	2.24	0.70
2:DC:83:ARG:NH2	2:Dz:28:THR:O	2.25	0.70
2:DJ:28:THR:O	2:DX:83:ARG:NH2	2.24	0.70
2:DR:83:ARG:NH2	2:D9:28:THR:O	2.25	0.70
2:Cl:13:GLU:OE2	2:Cl:47:THR:OG1	2.09	0.70
2:CQ:13:GLU:OE2	2:CQ:47:THR:OG1	2.09	0.70
2:DT:28:THR:O	2:Dm:83:ARG:NH2	2.24	0.70
2:Cg:13:GLU:OE2	2:Cg:47:THR:OG1	2.09	0.70
2:Cw:13:GLU:OE2	2:Cw:47:THR:OG1	2.09	0.70
2:C6:13:GLU:OE2	2:C6:47:THR:OG1	2.09	0.70
2:CW:13:GLU:OE2	2:CW:47:THR:OG1	2.09	0.70
2:Cb:13:GLU:OE2	2:Cb:47:THR:OG1	2.09	0.70
2:CB:13:GLU:OE2	2:CB:47:THR:OG1	2.10	0.70
2:DZ:28:THR:O	2:D2:83:ARG:NH2	2.25	0.70
2:D2:12:ILE:HD12	2:D2:27:MET:HE3	1.72	0.70
2:CG:13:GLU:OE2	2:CG:47:THR:OG1	2.09	0.70
2:DH:83:ARG:NH2	2:D4:28:THR:O	2.24	0.70
2:C1:13:GLU:OE2	2:C1:47:THR:OG1	2.09	0.70
2:Dw:54:THR:O	2:Dw:58:ASN:ND2	2.20	0.70
2:CL:13:GLU:OE2	2:CL:47:THR:OG1	2.09	0.69
2:Cq:13:GLU:OE2	2:Cq:47:THR:OG1	2.10	0.69
2:D6:54:THR:O	2:D6:58:ASN:ND2	2.20	0.69
2:Cm:58:ASN:HD21	2:Cm:62:ARG:HH21	1.41	0.69
2:DD:54:THR:O	2:DD:58:ASN:ND2	2.20	0.69
2:DI:11:MET:HE3	2:DI:79:HIS:HB3	1.75	0.68
2:D5:12:ILE:HD12	2:D5:27:MET:HE3	1.75	0.68
2:Df:12:ILE:HD12	2:Df:27:MET:HE3	1.75	0.68
2:Di:11:MET:HG2	2:Di:49:LEU:HD23	1.72	0.68
2:Dk:12:ILE:HD12	2:Dk:27:MET:HE3	1.76	0.68
2:DF:12:ILE:HD12	2:DF:27:MET:HE3	1.76	0.68
2:Cd:13:GLU:OE2	2:Cd:47:THR:OG1	2.12	0.68
2:Cx:13:GLU:OE2	2:Cx:47:THR:OG1	2.12	0.68
2:C7:13:GLU:OE2	2:C7:47:THR:OG1	2.12	0.68
2:CX:13:GLU:OE2	2:CX:47:THR:OG1	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dv:12:ILE:HD12	2:Dv:27:MET:HE3	1.76	0.68
2:D0:12:ILE:HD12	2:D0:27:MET:HE3	1.76	0.68
2:DK:12:ILE:HD12	2:DK:27:MET:HE3	1.76	0.68
2:CY:13:GLU:OE2	2:CY:47:THR:OG1	2.12	0.68
2:Cc:13:GLU:OE2	2:Cc:47:THR:OG1	2.12	0.68
2:Cd:11:MET:HE3	2:Cd:79:HIS:HB3	1.75	0.67
2:Di:11:MET:HE3	2:Di:79:HIS:HB3	1.76	0.67
2:Dp:12:ILE:HD12	2:Dp:27:MET:HE3	1.76	0.67
2:CS:13:GLU:OE2	2:CS:47:THR:OG1	2.12	0.67
2:By:69:GLU:OE1	2:By:70:ARG:NH2	2.28	0.67
2:C2:13:GLU:OE2	2:C2:47:THR:OG1	2.12	0.67
2:CD:13:GLU:OE2	2:CD:47:THR:OG1	2.12	0.67
2:CR:13:GLU:OE2	2:CR:47:THR:OG1	2.12	0.67
2:Cr:13:GLU:OE2	2:Cr:47:THR:OG1	2.12	0.67
2:DA:12:ILE:HD12	2:DA:27:MET:HE3	1.76	0.67
2:CC:13:GLU:OE2	2:CC:47:THR:OG1	2.12	0.67
2:DP:12:ILE:HD12	2:DP:27:MET:HE3	1.76	0.67
2:Do:28:THR:O	2:D7:83:ARG:NH2	2.28	0.67
2:Cs:13:GLU:OE2	2:Cs:47:THR:OG1	2.12	0.67
2:C3:13:GLU:OE2	2:C3:47:THR:OG1	2.12	0.67
2:D3:11:MET:HE3	2:D3:79:HIS:HB3	1.76	0.67
2:DD:11:MET:HE3	2:DD:79:HIS:HB3	1.77	0.67
2:CH:13:GLU:OE2	2:CH:47:THR:OG1	2.12	0.67
2:CM:13:GLU:OE2	2:CM:47:THR:OG1	2.12	0.67
2:Cy:13:GLU:OE2	2:Cy:47:THR:OG1	2.12	0.67
2:C8:13:GLU:OE2	2:C8:47:THR:OG1	2.12	0.67
2:Ch:13:GLU:OE2	2:Ch:47:THR:OG1	2.12	0.67
2:Cm:13:GLU:OE2	2:Cm:47:THR:OG1	2.12	0.67
2:BH:73:ASP:OD1	2:CH:45:TYR:OH	2.14	0.66
2:BM:73:ASP:OD2	2:CM:45:TYR:OH	2.14	0.66
1:AR:36:GLN:HG2	1:A5:2:LYS:HE3	1.78	0.66
2:DV:28:THR:O	2:De:83:ARG:NH2	2.29	0.66
2:DY:83:ARG:NH2	2:D3:28:THR:O	2.28	0.66
2:B2:73:ASP:OD2	2:C2:45:TYR:OH	2.14	0.66
2:DM:83:ARG:NH2	2:Dt:28:THR:O	2.28	0.66
2:DV:12:ILE:HD12	2:Dv:27:MET:HE3	1.76	0.66
2:BY:11:MET:HE1	2:BY:81:ILE:HD12	1.78	0.66
2:Bp:73:ASP:OD1	2:Cp:45:TYR:OH	2.13	0.66
2:C5:13:GLU:OE2	2:C5:47:THR:OG1	2.14	0.66
2:Da:12:ILE:HD12	2:Da:27:MET:HE3	1.76	0.66
2:Ci:13:GLU:OE2	2:Ci:47:THR:OG1	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Cp:13:GLU:OE2	2:Cp:47:THR:OG1	2.14	0.66
2:Cv:13:GLU:OE2	2:Cv:47:THR:OG1	2.14	0.66
2:DS:83:ARG:NH2	2:Dn:28:THR:O	2.29	0.66
2:C0:13:GLU:OE2	2:C0:47:THR:OG1	2.14	0.66
2:CI:13:GLU:OE2	2:CI:47:THR:OG1	2.12	0.66
2:Df:28:THR:O	2:Do:83:ARG:NH2	2.29	0.66
2:Cn:13:GLU:OE2	2:Cn:47:THR:OG1	2.12	0.66
2:Br:73:ASP:OD1	2:Cr:45:TYR:OH	2.14	0.66
2:D4:83:ARG:NH2	2:D5:28:THR:O	2.29	0.66
2:BD:11:MET:HE1	2:BD:81:ILE:HD12	1.78	0.65
2:CN:13:GLU:OE2	2:CN:47:THR:OG1	2.12	0.65
2:Dd:83:ARG:NH2	2:Ds:28:THR:O	2.29	0.65
2:B5:73:ASP:OD1	2:C5:45:TYR:OH	2.14	0.65
2:DI:83:ARG:NH2	2:DY:28:THR:O	2.29	0.65
2:DO:11:MET:HE3	2:DO:79:HIS:HB3	1.79	0.65
2:Bv:73:ASP:OD1	2:Cv:45:TYR:OH	2.14	0.65
2:D8:11:MET:HE3	2:D8:79:HIS:HB3	1.78	0.65
2:DD:28:THR:O	2:Dy:83:ARG:NH2	2.29	0.65
2:BX:73:ASP:OD1	2:CX:45:TYR:OH	2.14	0.65
2:DA:28:THR:O	2:DJ:83:ARG:NH2	2.29	0.65
2:DO:83:ARG:NH2	2:DP:28:THR:O	2.29	0.65
2:CF:11:MET:HE3	2:CF:79:HIS:HB3	1.77	0.65
2:Bc:73:ASP:OD1	2:Cc:45:TYR:OH	2.14	0.65
2:CP:13:GLU:OE2	2:CP:47:THR:OG1	2.14	0.65
2:DS:28:THR:O	2:D8:83:ARG:NH2	2.29	0.65
2:DD:83:ARG:NH2	2:Di:28:THR:O	2.30	0.65
2:DN:28:THR:O	2:Ds:83:ARG:NH2	2.29	0.65
2:Ca:13:GLU:OE2	2:Ca:47:THR:OG1	2.14	0.65
2:Bh:73:ASP:OD1	2:Ch:45:TYR:OH	2.14	0.65
2:Dp:28:THR:O	2:Dz:83:ARG:NH2	2.29	0.65
2:CA:13:GLU:OE2	2:CA:47:THR:OG1	2.14	0.65
2:DN:83:ARG:NH2	2:Dd:28:THR:O	2.29	0.65
2:CV:13:GLU:OE2	2:CV:47:THR:OG1	2.14	0.65
2:CF:13:GLU:OE2	2:CF:47:THR:OG1	2.14	0.65
2:CK:13:GLU:OE2	2:CK:47:THR:OG1	2.14	0.65
2:Bk:73:ASP:OD1	2:Ck:45:TYR:OH	2.14	0.65
2:Do:11:MET:HE3	2:Do:79:HIS:HB3	1.79	0.65
2:Dn:83:ARG:NH2	2:D8:28:THR:O	2.29	0.64
2:D4:11:MET:HE3	2:D4:79:HIS:HB3	1.79	0.64
2:Bm:73:ASP:OD2	2:Cm:45:TYR:OH	2.14	0.64
2:Ck:13:GLU:OE2	2:Ck:47:THR:OG1	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BR:73:ASP:OD1	2:CR:45:TYR:OH	2.14	0.64
2:Cf:13:GLU:OE2	2:Cf:47:THR:OG1	2.14	0.64
2:CV:11:MET:HE3	2:CV:79:HIS:HB3	1.80	0.64
2:B0:73:ASP:OD1	2:C0:45:TYR:OH	2.14	0.64
2:Ca:11:MET:HE3	2:Ca:79:HIS:HB3	1.80	0.64
2:BC:73:ASP:OD1	2:CC:45:TYR:OH	2.14	0.64
2:CK:11:MET:HE3	2:CK:79:HIS:HB3	1.80	0.64
2:C0:11:MET:HE3	2:C0:79:HIS:HB3	1.80	0.64
2:Cf:11:MET:HE3	2:Cf:79:HIS:HB3	1.80	0.63
2:Ck:11:MET:HE3	2:Ck:79:HIS:HB3	1.80	0.63
2:Cp:11:MET:HE3	2:Cp:79:HIS:HB3	1.80	0.63
2:Bf:73:ASP:OD1	2:Cf:45:TYR:OH	2.14	0.63
2:Dh:12:ILE:HD12	2:Dh:27:MET:HE3	1.81	0.63
2:DL:13:GLU:OE2	2:DL:47:THR:OG1	2.17	0.63
2:CW:11:MET:HE3	2:CW:79:HIS:HB3	1.81	0.63
1:A1:21:HIS:CD2	2:B1:62:ARG:HB3	2.34	0.63
2:CB:11:MET:HE3	2:CB:79:HIS:HB3	1.81	0.63
2:DG:13:GLU:OE2	2:DG:47:THR:OG1	2.17	0.63
2:CQ:11:MET:HE3	2:CQ:79:HIS:HB3	1.81	0.63
2:DW:13:GLU:OE2	2:DW:47:THR:OG1	2.17	0.63
2:DB:13:GLU:OE2	2:DB:47:THR:OG1	2.17	0.63
2:Dr:12:ILE:HD12	2:Dr:27:MET:HE3	1.81	0.63
2:C5:11:MET:HE3	2:C5:79:HIS:HB3	1.80	0.63
2:DI:28:THR:O	2:D3:83:ARG:NH2	2.31	0.63
2:Di:83:ARG:NH2	2:Dy:28:THR:O	2.31	0.63
1:Al:21:HIS:CD2	2:Bl:62:ARG:HB3	2.34	0.63
2:Cv:11:MET:HE3	2:Cv:79:HIS:HB3	1.80	0.63
1:Ag:21:HIS:CD2	2:Bg:62:ARG:HB3	2.34	0.63
1:Aw:21:HIS:CD2	2:Bw:62:ARG:HB3	2.34	0.63
1:A6:21:HIS:CD2	2:B6:62:ARG:HB3	2.34	0.63
1:AH:21:HIS:CD2	2:BH:62:ARG:HB3	2.33	0.62
1:AQ:21:HIS:CD2	2:BQ:62:ARG:HB3	2.34	0.62
1:AL:21:HIS:CD2	2:BL:62:ARG:HB3	2.34	0.62
2:BV:73:ASP:OD1	2:CV:45:TYR:OH	2.15	0.62
2:Dc:12:ILE:HD12	2:Dc:27:MET:HE3	1.81	0.62
1:AW:21:HIS:CD2	2:BW:62:ARG:HB3	2.34	0.62
2:BY:69:GLU:OE1	2:BY:70:ARG:NH2	2.31	0.62
2:Ba:73:ASP:OD1	2:Ca:45:TYR:OH	2.15	0.62
1:AB:21:HIS:CD2	2:BB:62:ARG:HB3	2.34	0.62
2:Dq:13:GLU:OE2	2:Dq:47:THR:OG1	2.17	0.62
2:Dw:13:GLU:OE2	2:Dw:47:THR:OG1	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bx:73:ASP:OD1	2:Cx:45:TYR:OH	2.14	0.62
2:Dx:12:ILE:HD12	2:Dx:27:MET:HE3	1.81	0.62
1:AG:21:HIS:CD2	2:BG:62:ARG:HB3	2.34	0.62
2:BS:45:TYR:OH	2:DS:73:ASP:OD1	2.16	0.62
2:D6:13:GLU:OE2	2:D6:47:THR:OG1	2.17	0.62
2:B7:73:ASP:OD2	2:C7:45:TYR:OH	2.14	0.62
2:BF:73:ASP:OD1	2:CF:45:TYR:OH	2.14	0.61
2:DH:12:ILE:HD12	2:DH:27:MET:HE3	1.81	0.61
2:CA:11:MET:HE3	2:CA:79:HIS:HB3	1.80	0.61
2:D1:13:GLU:OE2	2:D1:47:THR:OG1	2.17	0.61
2:CI:11:MET:HE3	2:CI:79:HIS:HB3	1.83	0.61
2:BM:69:GLU:OE1	2:BM:70:ARG:NH2	2.31	0.61
2:DQ:13:GLU:OE2	2:DQ:47:THR:OG1	2.17	0.61
2:Cn:11:MET:HE3	2:Cn:79:HIS:HB3	1.82	0.61
2:Cy:11:MET:HE3	2:Cy:79:HIS:HB3	1.82	0.61
2:CN:11:MET:HE3	2:CN:79:HIS:HB3	1.83	0.61
2:CP:11:MET:HE3	2:CP:79:HIS:HB3	1.80	0.61
2:Cx:11:MET:HE3	2:Cx:79:HIS:HB3	1.83	0.61
2:C7:11:MET:HE3	2:C7:79:HIS:HB3	1.83	0.61
2:BK:73:ASP:OD1	2:CK:45:TYR:OH	2.15	0.61
2:Ch:11:MET:HE3	2:Ch:79:HIS:HB3	1.83	0.61
2:Cm:11:MET:HE3	2:Cm:79:HIS:HB3	1.83	0.61
2:C8:11:MET:HE3	2:C8:79:HIS:HB3	1.83	0.61
2:CX:11:MET:HE3	2:CX:79:HIS:HB3	1.83	0.61
2:Ci:11:MET:HE3	2:Ci:79:HIS:HB3	1.83	0.61
2:BA:73:ASP:OD1	2:CA:45:TYR:OH	2.14	0.61
2:CR:11:MET:HE3	2:CR:79:HIS:HB3	1.83	0.61
2:Cc:11:MET:HE3	2:Cc:79:HIS:HB3	1.83	0.61
2:Bj:73:ASP:OD2	2:Cj:45:TYR:OH	2.18	0.61
2:CC:11:MET:HE3	2:CC:79:HIS:HB3	1.83	0.60
2:DX:13:GLU:OE2	2:DX:47:THR:OG1	2.17	0.60
2:B8:69:GLU:OE1	2:B8:70:ARG:NH2	2.30	0.60
2:BP:73:ASP:OD1	2:CP:45:TYR:OH	2.14	0.60
2:CY:11:MET:HE3	2:CY:79:HIS:HB3	1.83	0.60
2:Ct:11:MET:HE3	2:Ct:79:HIS:HB3	1.83	0.60
1:AM:21:HIS:CD2	2:BM:62:ARG:HB3	2.37	0.60
2:Cr:11:MET:HE3	2:Cr:79:HIS:HB3	1.83	0.60
2:C4:11:MET:HE3	2:C4:79:HIS:HB3	1.83	0.60
2:BH:45:TYR:OH	2:DH:73:ASP:OD1	2.16	0.60
2:Db:13:GLU:OE2	2:Db:47:THR:OG1	2.18	0.60
2:C2:11:MET:HE3	2:C2:79:HIS:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ad:28:TRP:CE2	1:Ad:31:PRO:HA	2.37	0.60
1:Ag:52:CYS:HB3	1:Ag:71:LEU:HD11	1.84	0.60
2:Cj:11:MET:HE3	2:Cj:79:HIS:HB3	1.83	0.60
2:C3:11:MET:HE3	2:C3:79:HIS:HB3	1.83	0.60
2:Cs:11:MET:HE3	2:Cs:79:HIS:HB3	1.83	0.60
2:Dt:11:MET:HE3	2:Dt:79:HIS:HB3	1.84	0.60
2:BM:45:TYR:OH	2:DM:73:ASP:OD1	2.16	0.60
2:Dl:28:THR:O	2:Dw:83:ARG:NH2	2.35	0.60
2:C9:11:MET:HE3	2:C9:79:HIS:HB3	1.83	0.60
2:DJ:11:MET:HE3	2:DJ:79:HIS:HB3	1.84	0.60
2:DK:11:MET:HG2	2:DK:49:LEU:HD22	1.83	0.60
2:CM:11:MET:HE3	2:CM:79:HIS:HB3	1.83	0.60
2:Cz:11:MET:HE3	2:Cz:79:HIS:HB3	1.83	0.60
2:B4:73:ASP:OD2	2:C4:45:TYR:OH	2.18	0.60
1:AB:52:CYS:HB3	1:AB:71:LEU:HD11	1.84	0.59
2:CD:11:MET:HE3	2:CD:79:HIS:HB3	1.82	0.59
2:CE:11:MET:HE3	2:CE:79:HIS:HB3	1.83	0.59
2:DE:11:MET:HE3	2:DE:79:HIS:HB3	1.84	0.59
2:CH:11:MET:HE3	2:CH:79:HIS:HB3	1.83	0.59
2:CJ:11:MET:HE3	2:CJ:79:HIS:HB3	1.83	0.59
2:CS:11:MET:HE3	2:CS:79:HIS:HB3	1.83	0.59
2:De:11:MET:HE3	2:De:79:HIS:HB3	1.84	0.59
2:Dg:13:GLU:OE2	2:Dg:47:THR:OG1	2.19	0.59
2:Dl:13:GLU:OE2	2:Dl:47:THR:OG1	2.19	0.59
2:Co:11:MET:HE3	2:Co:79:HIS:HB3	1.83	0.59
2:Dz:11:MET:HE3	2:Dz:79:HIS:HB3	1.84	0.59
2:CO:11:MET:HE3	2:CO:79:HIS:HB3	1.83	0.59
2:CT:11:MET:HE3	2:CT:79:HIS:HB3	1.83	0.59
2:DZ:11:MET:HE3	2:DZ:79:HIS:HB3	1.84	0.59
2:D9:11:MET:HE3	2:D9:79:HIS:HB3	1.84	0.59
2:DD:11:MET:HG2	2:DD:49:LEU:HD23	1.84	0.59
2:DT:11:MET:HE3	2:DT:79:HIS:HB3	1.84	0.59
2:Ce:11:MET:HE3	2:Ce:79:HIS:HB3	1.83	0.59
1:AQ:52:CYS:HB3	1:AQ:71:LEU:HD11	1.85	0.59
2:CZ:11:MET:HE3	2:CZ:79:HIS:HB3	1.83	0.59
2:Br:45:TYR:OH	2:Dr:73:ASP:OD1	2.16	0.59
2:BE:73:ASP:OD1	2:CE:45:TYR:OH	2.18	0.59
2:BT:73:ASP:OD1	2:CT:45:TYR:OH	2.18	0.59
1:Ab:52:CYS:HB3	1:Ab:71:LEU:HD11	1.84	0.59
1:Aw:52:CYS:HB3	1:Aw:71:LEU:HD11	1.85	0.59
1:A6:52:CYS:HB3	1:A6:71:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP:36:GLN:HG2	1:Ad:2:LYS:HE3	1.85	0.59
2:DS:11:MET:HE3	2:DS:79:HIS:HB3	1.85	0.59
1:Al:52:CYS:HB3	1:Al:71:LEU:HD11	1.85	0.59
1:Aq:52:CYS:HB3	1:Aq:71:LEU:HD11	1.84	0.59
2:Bx:45:TYR:OH	2:Dx:73:ASP:OD1	2.16	0.59
2:Dj:11:MET:HE3	2:Dj:79:HIS:HB3	1.84	0.59
1:As:28:TRP:CE2	1:As:31:PRO:HA	2.38	0.59
2:Ds:11:MET:HE3	2:Ds:79:HIS:HB3	1.85	0.59
2:DY:11:MET:HE3	2:DY:79:HIS:HB3	1.84	0.59
2:Dd:11:MET:HE3	2:Dd:79:HIS:HB3	1.84	0.59
1:AW:52:CYS:HB3	1:AW:71:LEU:HD11	1.85	0.58
1:A3:28:TRP:CE2	1:A3:31:PRO:HA	2.38	0.58
1:AN:28:TRP:CE2	1:AN:31:PRO:HA	2.38	0.58
1:AD:28:TRP:CE2	1:AD:31:PRO:HA	2.38	0.58
2:BI:45:TYR:OH	2:DI:73:ASP:OD1	2.18	0.58
2:DN:11:MET:HE3	2:DN:79:HIS:HB3	1.85	0.58
2:Be:73:ASP:OD1	2:Ce:45:TYR:OH	2.18	0.58
1:A1:52:CYS:HB3	1:A1:71:LEU:HD11	1.85	0.58
2:DP:11:MET:HG2	2:DP:49:LEU:HD22	1.85	0.58
1:AS:28:TRP:CE2	1:AS:31:PRO:HA	2.38	0.58
1:AY:28:TRP:CE2	1:AY:31:PRO:HA	2.39	0.58
1:Ay:28:TRP:CE2	1:Ay:31:PRO:HA	2.38	0.58
2:Bz:73:ASP:OD1	2:Cz:45:TYR:OH	2.18	0.58
2:B9:73:ASP:OD1	2:C9:45:TYR:OH	2.18	0.58
2:BC:45:TYR:OH	2:DC:73:ASP:OD1	2.17	0.58
2:DG:28:THR:O	2:Dg:83:ARG:NH2	2.37	0.58
2:BY:9:LEU:HG	2:BY:11:MET:HE2	1.86	0.58
1:Al:28:TRP:CE2	1:Al:31:PRO:HA	2.39	0.58
2:Dv:11:MET:HG2	2:Dv:49:LEU:HD22	1.86	0.58
2:BJ:73:ASP:OD1	2:CJ:45:TYR:OH	2.18	0.58
1:Ab:28:TRP:CE2	1:Ab:31:PRO:HA	2.39	0.58
2:By:45:TYR:OH	2:Dy:73:ASP:OD1	2.18	0.58
2:BN:9:LEU:HG	2:BN:11:MET:HE2	1.86	0.58
2:D4:13:GLU:OE2	2:D4:47:THR:OG1	2.22	0.58
1:A8:28:TRP:CE2	1:A8:31:PRO:HA	2.39	0.58
1:AG:52:CYS:HB3	1:AG:71:LEU:HD11	1.85	0.58
1:AH:21:HIS:HD2	2:BH:62:ARG:HB3	1.68	0.58
1:AL:52:CYS:HB3	1:AL:71:LEU:HD11	1.85	0.58
2:BR:45:TYR:OH	2:DR:73:ASP:OD1	2.16	0.58
2:Da:11:MET:HG2	2:Da:49:LEU:HD22	1.85	0.58
1:Ai:28:TRP:CE2	1:Ai:31:PRO:HA	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bm:45:TYR:OH	2:Dm:73:ASP:OD1	2.16	0.58
2:Dn:11:MET:HE3	2:Dn:79:HIS:HB3	1.84	0.58
2:Dy:11:MET:HE3	2:Dy:79:HIS:HB3	1.85	0.58
2:D5:11:MET:HG2	2:D5:49:LEU:HD22	1.86	0.58
2:DV:11:MET:HG2	2:DV:49:LEU:HD22	1.85	0.57
2:Bo:73:ASP:OD1	2:Co:45:TYR:OH	2.18	0.57
2:Dp:11:MET:HG2	2:Dp:49:LEU:HD22	1.85	0.57
2:BZ:73:ASP:OD2	2:CZ:45:TYR:OH	2.18	0.57
2:Bh:45:TYR:OH	2:Dh:73:ASP:OD2	2.16	0.57
2:DA:11:MET:HG2	2:DA:49:LEU:HD22	1.86	0.57
2:Bt:73:ASP:OD1	2:Ct:45:TYR:OH	2.18	0.57
1:AB:28:TRP:CE2	1:AB:31:PRO:HA	2.40	0.57
2:DF:11:MET:HG2	2:DF:49:LEU:HD22	1.86	0.57
1:A2:21:HIS:CD2	2:B2:62:ARG:HB3	2.40	0.57
2:BN:45:TYR:OH	2:DN:73:ASP:OD2	2.18	0.57
2:D0:11:MET:HG2	2:D0:49:LEU:HD22	1.86	0.57
1:AD:2:LYS:HE3	1:Ap:36:GLN:HG2	1.86	0.57
2:Bd:9:LEU:HG	2:Bd:11:MET:HE2	1.87	0.57
1:Ak:36:GLN:HG2	1:Ay:2:LYS:HE3	1.87	0.57
1:AV:36:GLN:HG2	1:As:2:LYS:HE3	1.86	0.57
2:Bs:9:LEU:HG	2:Bs:11:MET:HE2	1.87	0.57
2:B8:45:TYR:OH	2:D8:73:ASP:OD1	2.19	0.57
1:AN:2:LYS:HE3	1:Av:36:GLN:HG2	1.85	0.57
1:Aq:28:TRP:CE2	1:Aq:31:PRO:HA	2.39	0.57
2:BI:9:LEU:HG	2:BI:11:MET:HE2	1.87	0.57
2:DI:12:ILE:HD12	2:DI:27:MET:HE3	1.87	0.57
1:Am:21:HIS:CD2	2:Bm:62:ARG:HB3	2.40	0.57
2:Bn:45:TYR:OH	2:Dn:73:ASP:OD2	2.18	0.57
1:Ap:28:TRP:CE2	1:Ap:31:PRO:HA	2.40	0.57
2:DO:13:GLU:OE2	2:DO:47:THR:OG1	2.22	0.56
1:AI:28:TRP:CE2	1:AI:31:PRO:HA	2.40	0.56
2:Do:13:GLU:OE2	2:Do:47:THR:OG1	2.23	0.56
2:Bq:35:LEU:HD11	2:Bq:48:VAL:HG13	1.88	0.56
2:B7:45:TYR:OH	2:D7:73:ASP:OD1	2.17	0.56
2:DY:12:ILE:HD12	2:DY:27:MET:HE3	1.88	0.56
2:Bl:35:LEU:HD11	2:Bl:48:VAL:HG13	1.88	0.56
2:B1:35:LEU:HD11	2:B1:48:VAL:HG13	1.88	0.56
1:AG:28:TRP:CE2	1:AG:31:PRO:HA	2.40	0.56
1:Ag:28:TRP:CE2	1:Ag:31:PRO:HA	2.41	0.56
2:Bg:35:LEU:HD11	2:Bg:48:VAL:HG13	1.88	0.56
2:Bi:9:LEU:HD11	2:Bi:49:LEU:HD23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dd:12:ILE:HD12	2:Dd:27:MET:HE3	1.88	0.56
2:Bc:45:TYR:OH	2:Dc:73:ASP:OD1	2.16	0.56
2:Bi:9:LEU:HG	2:Bi:11:MET:HE2	1.87	0.56
1:Aw:28:TRP:CE2	1:Aw:31:PRO:HA	2.41	0.56
1:A6:28:TRP:CE2	1:A6:31:PRO:HA	2.41	0.56
2:BX:45:TYR:OH	2:DX:73:ASP:OD2	2.16	0.56
1:Ar:28:TRP:CE2	1:Ar:31:PRO:HA	2.41	0.56
1:AH:28:TRP:CE2	1:AH:31:PRO:HA	2.41	0.56
2:BW:35:LEU:HD11	2:BW:48:VAL:HG13	1.88	0.56
2:Df:11:MET:HG2	2:Df:49:LEU:HD22	1.86	0.56
1:AI:2:LYS:HE3	1:A5:36:GLN:HG2	1.87	0.55
2:BD:9:LEU:HG	2:BD:11:MET:HE2	1.86	0.55
1:An:28:TRP:CE2	1:An:31:PRO:HA	2.41	0.55
2:Ds:12:ILE:HD12	2:Ds:27:MET:HE3	1.88	0.55
1:Av:28:TRP:CE2	1:Av:31:PRO:HA	2.41	0.55
2:BL:35:LEU:HD11	2:BL:48:VAL:HG13	1.88	0.55
2:BN:9:LEU:HD11	2:BN:49:LEU:HD23	1.88	0.55
1:AX:28:TRP:CE2	1:AX:31:PRO:HA	2.41	0.55
2:Bb:35:LEU:HD11	2:Bb:48:VAL:HG13	1.88	0.55
2:Dk:11:MET:HG2	2:Dk:49:LEU:HD22	1.86	0.55
2:Bn:9:LEU:HD11	2:Bn:49:LEU:HD23	1.89	0.55
2:D8:12:ILE:HD12	2:D8:27:MET:HE3	1.87	0.55
2:BG:35:LEU:HD11	2:BG:48:VAL:HG13	1.88	0.55
1:AL:28:TRP:CE2	1:AL:31:PRO:HA	2.41	0.55
1:Ac:28:TRP:CE2	1:Ac:31:PRO:HA	2.41	0.55
1:A1:28:TRP:CE2	1:A1:31:PRO:HA	2.41	0.55
1:A7:28:TRP:CE2	1:A7:31:PRO:HA	2.41	0.55
2:DD:12:ILE:HD12	2:DD:27:MET:HE3	1.88	0.55
2:DN:12:ILE:HD12	2:DN:27:MET:HE3	1.88	0.55
1:AW:28:TRP:CE2	1:AW:31:PRO:HA	2.41	0.55
2:DZ:83:ARG:NH2	2:Da:28:THR:O	2.40	0.55
1:Af:28:TRP:CE2	1:Af:31:PRO:HA	2.41	0.55
1:Ah:28:TRP:CE2	1:Ah:31:PRO:HA	2.41	0.55
1:Aq:21:HIS:CD2	2:Bq:62:ARG:HB3	2.42	0.55
2:D3:12:ILE:HD12	2:D3:27:MET:HE3	1.88	0.55
2:BD:9:LEU:HD11	2:BD:49:LEU:HD23	1.89	0.55
1:AQ:28:TRP:CE2	1:AQ:31:PRO:HA	2.41	0.55
2:Bd:9:LEU:HD11	2:Bd:49:LEU:HD23	1.88	0.55
2:Bs:9:LEU:HD11	2:Bs:49:LEU:HD23	1.88	0.55
1:Ax:28:TRP:CE2	1:Ax:31:PRO:HA	2.41	0.55
1:AP:28:TRP:CE2	1:AP:31:PRO:HA	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Cc:58:ASN:HD21	2:Cc:62:ARG:HH21	1.55	0.55
1:AA:28:TRP:CE2	1:AA:31:PRO:HA	2.42	0.55
2:DS:12:ILE:HD12	2:DS:27:MET:HE3	1.88	0.55
1:Aa:28:TRP:CE2	1:Aa:31:PRO:HA	2.42	0.55
2:Bw:35:LEU:HD11	2:Bw:48:VAL:HG13	1.88	0.55
1:AC:28:TRP:CE2	1:AC:31:PRO:HA	2.41	0.55
1:AK:28:TRP:CE2	1:AK:31:PRO:HA	2.41	0.55
1:AM:28:TRP:CE2	1:AM:31:PRO:HA	2.42	0.55
2:CX:58:ASN:HD21	2:CX:62:ARG:HH21	1.55	0.55
2:Dy:12:ILE:HD12	2:Dy:27:MET:HE3	1.88	0.55
2:B6:35:LEU:HD11	2:B6:48:VAL:HG13	1.88	0.55
2:BO:73:ASP:OD1	2:CO:45:TYR:OH	2.21	0.54
2:Di:12:ILE:HD12	2:Di:27:MET:HE3	1.88	0.54
2:Dn:12:ILE:HD12	2:Dn:27:MET:HE3	1.88	0.54
1:A0:28:TRP:CE2	1:A0:31:PRO:HA	2.42	0.54
1:AN:51:LEU:HG	1:AN:77:ILE:HD11	1.88	0.54
2:BS:9:LEU:HD11	2:BS:49:LEU:HD23	1.89	0.54
1:Am:28:TRP:CE2	1:Am:31:PRO:HA	2.42	0.54
2:Bs:73:ASP:OD1	2:Cs:45:TYR:OH	2.20	0.54
2:Dt:83:ARG:NH2	2:Dv:28:THR:O	2.40	0.54
2:Ch:58:ASN:HD21	2:Ch:62:ARG:HH21	1.55	0.54
2:Dj:83:ARG:NH2	2:Dk:28:THR:O	2.40	0.54
2:C2:58:ASN:HD21	2:C2:62:ARG:HH21	1.55	0.54
2:B3:9:LEU:HD11	2:B3:49:LEU:HD23	1.89	0.54
2:BO:45:TYR:OH	2:DO:73:ASP:OD1	2.23	0.54
1:AV:2:LYS:HE2	1:A2:36:GLN:HG2	1.89	0.54
1:AV:28:TRP:CE2	1:AV:31:PRO:HA	2.43	0.54
2:Cr:58:ASN:HD21	2:Cr:62:ARG:HH21	1.55	0.54
2:BI:9:LEU:HD11	2:BI:49:LEU:HD23	1.89	0.54
2:BQ:35:LEU:HD11	2:BQ:48:VAL:HG13	1.88	0.54
2:Bo:83:ARG:NH2	2:D7:85:HIS:HE1	2.06	0.54
2:D0:28:THR:O	2:D9:83:ARG:NH2	2.40	0.54
2:DE:83:ARG:NH2	2:DF:28:THR:O	2.40	0.54
2:DK:28:THR:O	2:DT:83:ARG:NH2	2.40	0.54
1:AX:21:HIS:CD2	2:BX:62:ARG:HB3	2.43	0.54
2:BY:9:LEU:HD11	2:BY:49:LEU:HD23	1.89	0.54
1:Ac:21:HIS:CD2	2:Bc:62:ARG:HB3	2.43	0.54
1:Ar:21:HIS:CD2	2:Br:62:ARG:HB3	2.43	0.54
2:Cx:58:ASN:HD21	2:Cx:62:ARG:HH21	1.55	0.54
2:By:9:LEU:HD11	2:By:49:LEU:HD23	1.89	0.54
2:BB:35:LEU:HD11	2:BB:48:VAL:HG13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:21:HIS:CD2	2:B7:62:ARG:HB3	2.43	0.54
2:B8:9:LEU:HD11	2:B8:49:LEU:HD23	1.89	0.54
1:AM:36:GLN:HG2	1:Ap:2:LYS:HE2	1.90	0.54
1:Ah:21:HIS:CD2	2:Bh:62:ARG:HB3	2.43	0.54
2:C7:58:ASN:HD21	2:C7:62:ARG:HH21	1.55	0.54
2:CC:58:ASN:HD21	2:CC:62:ARG:HH21	1.55	0.54
2:CR:58:ASN:HD21	2:CR:62:ARG:HH21	1.55	0.54
1:Ax:21:HIS:CD2	2:Bx:62:ARG:HB3	2.43	0.54
1:AC:21:HIS:CD2	2:BC:62:ARG:HB3	2.43	0.53
2:CH:58:ASN:HD21	2:CH:62:ARG:HH21	1.55	0.53
2:Bt:9:LEU:HG	2:Bt:11:MET:HE2	1.90	0.53
1:AR:28:TRP:CE2	1:AR:31:PRO:HA	2.44	0.53
1:A2:28:TRP:CE2	1:A2:31:PRO:HA	2.43	0.53
1:AF:2:LYS:HE2	1:AX:36:GLN:HG2	1.91	0.53
1:Ak:28:TRP:CE2	1:Ak:31:PRO:HA	2.42	0.53
1:AC:36:GLN:HG2	1:Av:2:LYS:HE2	1.91	0.53
1:AI:21:HIS:ND1	2:BI:62:ARG:HB3	2.24	0.53
2:CM:58:ASN:HD21	2:CM:62:ARG:HH21	1.55	0.53
1:AN:21:HIS:ND1	2:BN:62:ARG:HB3	2.24	0.53
2:B4:9:LEU:HG	2:B4:11:MET:HE2	1.91	0.53
1:Am:21:HIS:HD2	2:Bm:62:ARG:HB3	1.74	0.53
1:An:21:HIS:ND1	2:Bn:62:ARG:HB3	2.24	0.53
2:CG:41:VAL:HB	2:CG:45:TYR:HB2	1.91	0.53
2:DM:85:HIS:HE1	2:Bt:83:ARG:NH2	2.07	0.53
1:A5:28:TRP:CE2	1:A5:31:PRO:HA	2.43	0.53
2:Be:83:ARG:NH2	2:Dr:85:HIS:HE1	2.07	0.53
1:AS:21:HIS:ND1	2:BS:62:ARG:HB3	2.24	0.53
2:Bn:73:ASP:OD1	2:Cn:45:TYR:OH	2.21	0.53
2:BO:83:ARG:NH2	2:Dc:85:HIS:HE1	2.07	0.53
2:CZ:13:GLU:OE2	2:CZ:47:THR:OG1	2.27	0.53
2:Bj:83:ARG:NH2	2:Dx:85:HIS:HE1	2.07	0.53
1:AD:21:HIS:ND1	2:BD:62:ARG:HB3	2.24	0.52
2:Ce:13:GLU:OE2	2:Ce:47:THR:OG1	2.28	0.52
2:Bi:73:ASP:OD1	2:Ci:45:TYR:OH	2.21	0.52
2:BI:58:ASN:HD22	2:BI:80:ILE:HD13	1.74	0.52
2:DN:45:TYR:OH	2:Ct:73:ASP:OD1	2.25	0.52
1:As:21:HIS:ND1	2:Bs:62:ARG:HB3	2.24	0.52
2:CE:13:GLU:OE2	2:CE:47:THR:OG1	2.27	0.52
2:DI:45:TYR:OH	2:C4:73:ASP:OD1	2.25	0.52
2:BV:66:ASP:O	2:BV:70:ARG:NH2	2.42	0.52
2:Bf:66:ASP:O	2:Bf:70:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C4:13:GLU:OE2	2:C4:47:THR:OG1	2.27	0.52
2:B5:9:LEU:HD11	2:B5:49:LEU:HD23	1.92	0.52
1:AB:1:MET:SD	1:AB:1:MET:N	2.79	0.52
2:BI:73:ASP:OD1	2:CI:45:TYR:OH	2.21	0.52
1:AQ:1:MET:SD	1:AQ:1:MET:N	2.79	0.52
2:CT:13:GLU:OE2	2:CT:47:THR:OG1	2.27	0.52
2:Ct:13:GLU:OE2	2:Ct:47:THR:OG1	2.28	0.52
2:Bv:9:LEU:HD11	2:Bv:49:LEU:HD23	1.92	0.52
2:C0:25:ASP:OD1	2:C0:29:LYS:HE3	2.10	0.52
2:BS:58:ASN:HD22	2:BS:80:ILE:HD13	1.74	0.52
2:Bk:25:ASP:O	2:Bk:29:LYS:HG3	2.10	0.52
2:BD:58:ASN:HD22	2:BD:80:ILE:HD13	1.74	0.52
2:DH:85:HIS:HE1	2:B4:83:ARG:NH2	2.07	0.52
2:Bo:45:TYR:OH	2:Do:73:ASP:OD2	2.22	0.52
2:B0:9:LEU:HD11	2:B0:49:LEU:HD23	1.92	0.52
2:B8:58:ASN:HD22	2:B8:80:ILE:HD13	1.74	0.52
2:Ba:66:ASP:O	2:Ba:70:ARG:NH2	2.42	0.52
2:Bn:58:ASN:HD22	2:Bn:80:ILE:HD13	1.74	0.52
2:BE:83:ARG:NH2	2:Dh:85:HIS:HE1	2.07	0.52
2:BN:73:ASP:OD1	2:CN:45:TYR:OH	2.21	0.52
2:BP:25:ASP:O	2:BP:29:LYS:HG3	2.10	0.52
2:Cj:13:GLU:OE2	2:Cj:47:THR:OG1	2.27	0.52
2:Bk:66:ASP:O	2:Bk:70:ARG:NH2	2.43	0.52
2:Bv:25:ASP:O	2:Bv:29:LYS:HG3	2.10	0.52
2:BA:9:LEU:HD11	2:BA:49:LEU:HD23	1.92	0.52
2:BY:58:ASN:HD22	2:BY:80:ILE:HD13	1.74	0.52
2:Bp:9:LEU:HD11	2:Bp:49:LEU:HD23	1.92	0.52
2:Bs:58:ASN:HD22	2:Bs:80:ILE:HD13	1.74	0.52
2:By:58:ASN:HD22	2:By:80:ILE:HD13	1.74	0.52
2:B0:66:ASP:O	2:B0:70:ARG:NH2	2.43	0.52
2:B5:25:ASP:O	2:B5:29:LYS:HG3	2.10	0.52
1:AW:1:MET:SD	1:AW:1:MET:N	2.79	0.51
2:Bd:58:ASN:HD22	2:Bd:80:ILE:HD13	1.74	0.51
2:C9:41:VAL:HB	2:C9:45:TYR:HB2	1.93	0.51
2:BA:25:ASP:O	2:BA:29:LYS:HG3	2.10	0.51
2:BP:9:LEU:HD11	2:BP:49:LEU:HD23	1.92	0.51
2:Cl:41:VAL:HB	2:Cl:45:TYR:HB2	1.92	0.51
2:Cm:58:ASN:ND2	2:Cm:62:ARG:HH21	2.08	0.51
2:Bp:66:ASP:O	2:Bp:70:ARG:NH2	2.43	0.51
2:Bv:66:ASP:O	2:Bv:70:ARG:NH2	2.43	0.51
2:CL:41:VAL:HB	2:CL:45:TYR:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ci:41:VAL:HB	2:Ci:45:TYR:HB2	1.93	0.51
2:Co:13:GLU:OE2	2:Co:47:THR:OG1	2.28	0.51
2:B5:66:ASP:O	2:B5:70:ARG:NH2	2.43	0.51
2:C6:41:VAL:HB	2:C6:45:TYR:HB2	1.92	0.51
1:AF:28:TRP:CE2	1:AF:31:PRO:HA	2.44	0.51
2:BF:66:ASP:O	2:BF:70:ARG:NH2	2.43	0.51
2:Bf:9:LEU:HD11	2:Bf:49:LEU:HD23	1.92	0.51
2:Cg:41:VAL:HB	2:Cg:45:TYR:HB2	1.92	0.51
2:Bk:9:LEU:HD11	2:Bk:49:LEU:HD23	1.92	0.51
2:Cn:41:VAL:HB	2:Cn:45:TYR:HB2	1.93	0.51
2:Cw:41:VAL:HB	2:Cw:45:TYR:HB2	1.92	0.51
2:Cz:13:GLU:OE2	2:Cz:47:THR:OG1	2.27	0.51
2:Cz:41:VAL:HB	2:Cz:45:TYR:HB2	1.93	0.51
2:C9:13:GLU:OE2	2:C9:47:THR:OG1	2.27	0.51
1:AE:19:MET:O	1:AE:67:TYR:OH	2.25	0.51
2:Cq:51:ARG:HG2	2:Cq:51:ARG:HH11	1.76	0.51
2:C5:25:ASP:OD1	2:C5:29:LYS:HE3	2.10	0.51
1:AJ:28:TRP:CE2	1:AJ:31:PRO:HA	2.46	0.51
2:BK:66:ASP:O	2:BK:70:ARG:NH2	2.43	0.51
2:DM:27:MET:HE2	2:DM:61:VAL:HA	1.92	0.51
2:CS:41:VAL:HB	2:CS:45:TYR:HB2	1.93	0.51
2:Bd:45:TYR:OH	2:Dd:73:ASP:OD2	2.18	0.51
1:A2:21:HIS:HD2	2:B2:62:ARG:HB3	1.74	0.51
2:B2:45:TYR:OH	2:D2:73:ASP:OD1	2.16	0.51
2:BA:45:TYR:OH	2:DA:73:ASP:OD1	2.22	0.51
2:CJ:13:GLU:OE2	2:CJ:47:THR:OG1	2.27	0.51
1:AO:28:TRP:CE2	1:AO:31:PRO:HA	2.46	0.51
2:CO:13:GLU:OE2	2:CO:47:THR:OG1	2.27	0.51
1:Aq:15:ARG:NH2	1:Aq:20:GLY:O	2.44	0.51
2:CD:41:VAL:HB	2:CD:45:TYR:HB2	1.93	0.51
2:BV:9:LEU:HD11	2:BV:49:LEU:HD23	1.92	0.51
2:Bf:25:ASP:O	2:Bf:29:LYS:HG3	2.11	0.51
1:At:28:TRP:CE2	1:At:31:PRO:HA	2.46	0.51
2:B0:25:ASP:O	2:B0:29:LYS:HG3	2.11	0.51
2:BP:66:ASP:O	2:BP:70:ARG:NH2	2.43	0.51
2:CY:41:VAL:HB	2:CY:45:TYR:HB2	1.93	0.51
2:Ba:9:LEU:HD11	2:Ba:49:LEU:HD23	1.92	0.51
2:Ds:13:GLU:OE2	2:Ds:47:THR:OG1	2.29	0.51
1:A4:28:TRP:CE2	1:A4:31:PRO:HA	2.46	0.51
1:A9:28:TRP:CE2	1:A9:31:PRO:HA	2.46	0.51
2:D9:8:ALA:HB3	2:D9:52:GLY:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CI:41:VAL:HB	2:CI:45:TYR:HB2	1.93	0.51
2:DS:13:GLU:OE2	2:DS:47:THR:OG1	2.29	0.51
2:DV:77:ALA:HB2	2:Ca:72:GLY:HA2	1.93	0.51
2:Cd:41:VAL:HB	2:Cd:45:TYR:HB2	1.93	0.51
2:Dd:13:GLU:OE2	2:Dd:47:THR:OG1	2.29	0.51
2:Cj:41:VAL:HB	2:Cj:45:TYR:HB2	1.93	0.51
2:Bp:25:ASP:O	2:Bp:29:LYS:HG3	2.11	0.51
1:A9:19:MET:O	1:A9:67:TYR:OH	2.25	0.51
2:BA:66:ASP:O	2:BA:70:ARG:NH2	2.43	0.50
2:CB:41:VAL:HB	2:CB:45:TYR:HB2	1.92	0.50
2:DD:13:GLU:OE2	2:DD:47:THR:OG1	2.29	0.50
1:AH:1:MET:HE2	1:Ag:37:VAL:HG12	1.93	0.50
2:BK:25:ASP:O	2:BK:29:LYS:HG3	2.11	0.50
2:CN:41:VAL:HB	2:CN:45:TYR:HB2	1.93	0.50
2:CQ:41:VAL:HB	2:CQ:45:TYR:HB2	1.92	0.50
1:AT:28:TRP:CE2	1:AT:31:PRO:HA	2.46	0.50
2:BW:73:ASP:OD1	2:CW:45:TYR:OH	2.27	0.50
2:DY:13:GLU:OE2	2:DY:47:THR:OG1	2.29	0.50
1:AZ:19:MET:O	1:AZ:67:TYR:OH	2.25	0.50
1:Ae:19:MET:O	1:Ae:67:TYR:OH	2.25	0.50
2:Cq:41:VAL:HB	2:Cq:45:TYR:HB2	1.92	0.50
2:Dy:13:GLU:OE2	2:Dy:47:THR:OG1	2.29	0.50
1:AA:19:MET:O	1:AA:67:TYR:OH	2.29	0.50
2:Dn:13:GLU:OE2	2:Dn:47:THR:OG1	2.29	0.50
2:Co:41:VAL:HB	2:Co:45:TYR:HB2	1.93	0.50
2:Do:8:ALA:HB3	2:Do:52:GLY:O	2.11	0.50
2:Dt:8:ALA:HB3	2:Dt:52:GLY:O	2.11	0.50
2:C1:41:VAL:HB	2:C1:45:TYR:HB2	1.92	0.50
2:D3:13:GLU:OE2	2:D3:47:THR:OG1	2.30	0.50
2:C6:70:ARG:NH1	2:C6:71:VAL:HG23	2.26	0.50
2:BF:25:ASP:O	2:BF:29:LYS:HG3	2.11	0.50
2:BM:12:ILE:HD12	2:BM:27:MET:HE3	1.94	0.50
1:AZ:28:TRP:CE2	1:AZ:31:PRO:HA	2.46	0.50
1:Aj:28:TRP:CE2	1:Aj:31:PRO:HA	2.46	0.50
2:Cs:41:VAL:HB	2:Cs:45:TYR:HB2	1.93	0.50
1:Az:28:TRP:CE2	1:Az:31:PRO:HA	2.46	0.50
1:A1:1:MET:SD	1:A1:1:MET:N	2.79	0.50
2:C3:41:VAL:HB	2:C3:45:TYR:HB2	1.93	0.50
2:C8:41:VAL:HB	2:C8:45:TYR:HB2	1.93	0.50
2:BF:9:LEU:HD11	2:BF:49:LEU:HD23	1.92	0.50
1:AI:28:TRP:HZ3	1:AI:35:ARG:HE	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CV:72:GLY:HA2	2:Da:77:ALA:HB2	1.94	0.50
2:Cb:41:VAL:HB	2:Cb:45:TYR:HB2	1.92	0.50
1:Ae:28:TRP:CE2	1:Ae:31:PRO:HA	2.46	0.50
1:Ao:28:TRP:CE2	1:Ao:31:PRO:HA	2.46	0.50
2:Cq:70:ARG:NH1	2:Cq:71:VAL:HG23	2.27	0.50
2:Ct:41:VAL:HB	2:Ct:45:TYR:HB2	1.93	0.50
2:Cy:41:VAL:HB	2:Cy:45:TYR:HB2	1.93	0.50
2:C4:41:VAL:HB	2:C4:45:TYR:HB2	1.93	0.50
2:D4:8:ALA:HB3	2:D4:52:GLY:O	2.12	0.50
1:AE:28:TRP:CE2	1:AE:31:PRO:HA	2.46	0.50
2:CQ:70:ARG:NH1	2:CQ:70:ARG:HB2	2.27	0.50
2:CW:41:VAL:HB	2:CW:45:TYR:HB2	1.92	0.50
2:Cw:70:ARG:NH1	2:Cw:71:VAL:HG23	2.27	0.50
2:BH:12:ILE:HD12	2:BH:27:MET:HE3	1.94	0.50
2:Bj:45:TYR:OH	2:Dj:73:ASP:OD2	2.28	0.50
2:CA:72:GLY:HA2	2:DF:77:ALA:HB2	1.94	0.50
2:BK:9:LEU:HD11	2:BK:49:LEU:HD23	1.92	0.50
2:BV:25:ASP:O	2:BV:29:LYS:HG3	2.11	0.50
2:Ba:25:ASP:O	2:Ba:29:LYS:HG3	2.11	0.50
2:Cb:70:ARG:NH1	2:Cb:71:VAL:HG23	2.27	0.50
1:Az:19:MET:O	1:Az:67:TYR:OH	2.26	0.50
2:C1:70:ARG:NH1	2:C1:71:VAL:HG23	2.27	0.50
2:D8:13:GLU:OE2	2:D8:47:THR:OG1	2.30	0.50
2:CB:70:ARG:NH1	2:CB:70:ARG:HB2	2.27	0.50
2:CE:41:VAL:HB	2:CE:45:TYR:HB2	1.93	0.50
2:DA:77:ALA:HB2	2:CF:72:GLY:HA2	1.94	0.50
2:CT:41:VAL:HB	2:CT:45:TYR:HB2	1.93	0.50
2:Cf:72:GLY:HA2	2:Dk:77:ALA:HB2	1.94	0.50
2:Di:13:GLU:OE2	2:Di:47:THR:OG1	2.30	0.50
2:Bm:11:MET:HG2	2:Bm:49:LEU:HG	1.94	0.50
2:D2:27:MET:HE2	2:D2:61:VAL:HA	1.93	0.50
1:A8:39:VAL:HG23	1:A8:72:THR:HG23	1.94	0.50
2:DD:85:HIS:HD2	2:DD:87:GLU:H	1.60	0.49
2:CH:58:ASN:ND2	2:CH:62:ARG:HH21	2.10	0.49
2:Ce:41:VAL:HB	2:Ce:45:TYR:HB2	1.93	0.49
2:Cl:70:ARG:NH1	2:Cl:71:VAL:HG23	2.27	0.49
2:CM:58:ASN:ND2	2:CM:62:ARG:HH21	2.10	0.49
2:CZ:41:VAL:HB	2:CZ:45:TYR:HB2	1.93	0.49
2:DZ:77:ALA:HB2	2:C3:72:GLY:HA2	1.95	0.49
1:Ay:39:VAL:HG23	1:Ay:72:THR:HG23	1.94	0.49
2:Dz:8:ALA:HB3	2:Dz:52:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DE:85:HIS:HE1	2:BF:83:ARG:HH21	1.60	0.49
2:CR:58:ASN:ND2	2:CR:62:ARG:HH21	2.10	0.49
2:Cg:70:ARG:NH1	2:Cg:71:VAL:HG23	2.27	0.49
2:D1:8:ALA:HB3	2:D1:52:GLY:O	2.13	0.49
2:CI:72:GLY:HA2	2:D4:77:ALA:HB2	1.94	0.49
2:DK:77:ALA:HB2	2:CP:72:GLY:HA2	1.94	0.49
2:BM:85:HIS:HE1	2:Dv:83:ARG:HH22	1.59	0.49
2:DO:8:ALA:HB3	2:DO:52:GLY:O	2.13	0.49
2:CC:58:ASN:ND2	2:CC:62:ARG:HH21	2.10	0.49
1:AD:39:VAL:HG23	1:AD:72:THR:HG23	1.95	0.49
2:DJ:8:ALA:HB3	2:DJ:52:GLY:O	2.13	0.49
2:BK:83:ARG:HH21	2:DT:85:HIS:HE1	1.61	0.49
2:BN:11:MET:HE1	2:BN:81:ILE:HD12	1.95	0.49
1:AT:19:MET:O	1:AT:67:TYR:OH	2.25	0.49
1:AZ:37:VAL:HG12	1:Ab:1:MET:HE2	1.94	0.49
1:Ab:1:MET:SD	1:Ab:1:MET:N	2.81	0.49
2:Bi:11:MET:HE1	2:Bi:81:ILE:HD12	1.94	0.49
2:DJ:77:ALA:HB2	2:CY:72:GLY:HA2	1.95	0.49
1:AN:39:VAL:HG23	1:AN:72:THR:HG23	1.94	0.49
2:DN:13:GLU:OE2	2:DN:47:THR:OG1	2.29	0.49
2:Db:8:ALA:HB3	2:Db:52:GLY:O	2.12	0.49
2:Df:77:ALA:HB2	2:Ck:72:GLY:HA2	1.94	0.49
2:Dj:8:ALA:HB3	2:Dj:52:GLY:O	2.13	0.49
2:Bt:45:TYR:OH	2:Dt:73:ASP:OD2	2.28	0.49
2:B2:11:MET:HG2	2:B2:49:LEU:HG	1.94	0.49
2:CD:72:GLY:HA2	2:Dz:77:ALA:HB2	1.94	0.49
1:AI:39:VAL:HG23	1:AI:72:THR:HG23	1.94	0.49
2:CK:72:GLY:HA2	2:DP:77:ALA:HB2	1.94	0.49
2:CL:70:ARG:NH1	2:CL:71:VAL:HG23	2.27	0.49
2:BX:12:ILE:HD12	2:BX:27:MET:HE3	1.94	0.49
2:Cc:58:ASN:ND2	2:Cc:62:ARG:HH21	2.10	0.49
2:De:77:ALA:HB2	2:Cs:72:GLY:HA2	1.95	0.49
2:DB:8:ALA:HB3	2:DB:52:GLY:O	2.13	0.49
2:CJ:73:ASP:OD1	2:DY:45:TYR:OH	2.25	0.49
2:BN:83:ARG:NH2	2:Ds:85:HIS:HE1	2.10	0.49
2:CS:72:GLY:HA2	2:D9:77:ALA:HB2	1.94	0.49
2:Ch:58:ASN:ND2	2:Ch:62:ARG:HH21	2.10	0.49
1:AI:39:VAL:HG23	1:AI:72:THR:HG23	1.94	0.49
1:An:39:VAL:HG23	1:An:72:THR:HG23	1.94	0.49
2:CG:70:ARG:NH1	2:CG:71:VAL:HG23	2.27	0.49
2:DO:77:ALA:HB2	2:Cd:72:GLY:HA2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DQ:8:ALA:HB3	2:DQ:52:GLY:O	2.13	0.49
2:DT:8:ALA:HB3	2:DT:52:GLY:O	2.12	0.49
2:BI:11:MET:HE1	2:BI:81:ILE:HD12	1.95	0.49
1:AJ:21:HIS:CD2	2:BJ:62:ARG:HB3	2.48	0.49
2:CO:41:VAL:HB	2:CO:45:TYR:HB2	1.93	0.49
2:BS:73:ASP:OD1	2:CS:45:TYR:OH	2.20	0.49
2:B4:45:TYR:OH	2:D4:73:ASP:OD2	2.29	0.49
2:B7:12:ILE:HD12	2:B7:27:MET:HE3	1.94	0.49
2:B8:73:ASP:OD1	2:C8:45:TYR:OH	2.21	0.49
1:AE:39:VAL:HG23	1:AE:72:THR:HG23	1.95	0.48
2:DE:8:ALA:HB3	2:DE:52:GLY:O	2.12	0.48
2:DI:13:GLU:OE2	2:DI:47:THR:OG1	2.30	0.48
2:CJ:41:VAL:HB	2:CJ:45:TYR:HB2	1.93	0.48
2:CX:58:ASN:ND2	2:CX:62:ARG:HH21	2.10	0.48
2:Br:12:ILE:HD12	2:Br:27:MET:HE3	1.94	0.48
2:BC:12:ILE:HD12	2:BC:27:MET:HE3	1.94	0.48
2:DL:8:ALA:HB3	2:DL:52:GLY:O	2.13	0.48
1:AO:21:HIS:CD2	2:BO:62:ARG:HB3	2.48	0.48
2:CO:73:ASP:OD1	2:Dd:45:TYR:OH	2.25	0.48
1:Ao:19:MET:O	1:Ao:67:TYR:OH	2.25	0.48
2:Cp:72:GLY:HA2	2:Dv:77:ALA:HB2	1.94	0.48
2:Bx:12:ILE:HD12	2:Bx:27:MET:HE3	1.94	0.48
2:D0:77:ALA:HB2	2:C5:72:GLY:HA2	1.94	0.48
2:D6:8:ALA:HB3	2:D6:52:GLY:O	2.13	0.48
2:DE:77:ALA:HB2	2:Ci:72:GLY:HA2	1.95	0.48
2:DG:8:ALA:HB3	2:DG:52:GLY:O	2.13	0.48
2:DW:8:ALA:HB3	2:DW:52:GLY:O	2.13	0.48
2:Bc:12:ILE:HD12	2:Bc:27:MET:HE3	1.94	0.48
2:Cj:73:ASP:OD1	2:Dy:45:TYR:OH	2.24	0.48
1:A9:21:HIS:CD2	2:B9:62:ARG:HB3	2.48	0.48
2:BE:45:TYR:OH	2:DE:73:ASP:OD2	2.28	0.48
2:De:8:ALA:HB3	2:De:52:GLY:O	2.12	0.48
1:At:21:HIS:CD2	2:Bt:62:ARG:HB3	2.48	0.48
2:C0:72:GLY:HA2	2:D5:77:ALA:HB2	1.94	0.48
2:C2:58:ASN:ND2	2:C2:62:ARG:HH21	2.10	0.48
1:A4:21:HIS:CD2	2:B4:62:ARG:HB3	2.48	0.48
1:AS:39:VAL:HG23	1:AS:72:THR:HG23	1.96	0.48
2:BT:45:TYR:OH	2:DT:73:ASP:OD2	2.28	0.48
2:DT:77:ALA:HB2	2:Cn:72:GLY:HA2	1.95	0.48
1:AY:39:VAL:HG23	1:AY:72:THR:HG23	1.94	0.48
2:DZ:8:ALA:HB3	2:DZ:52:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aj:21:HIS:CD2	2:Bj:62:ARG:HB3	2.48	0.48
2:Co:73:ASP:OD1	2:D8:45:TYR:OH	2.25	0.48
1:Az:39:VAL:HG23	1:Az:72:THR:HG23	1.96	0.48
2:B2:12:ILE:HD12	2:B2:27:MET:HE3	1.94	0.48
2:CN:72:GLY:HA2	2:Dt:77:ALA:HB2	1.95	0.48
2:CT:73:ASP:OD1	2:Dn:45:TYR:OH	2.25	0.48
1:Aj:19:MET:O	1:Aj:67:TYR:OH	2.25	0.48
1:Ao:21:HIS:CD2	2:Bo:62:ARG:HB3	2.48	0.48
2:Dp:77:ALA:HB2	2:Cv:72:GLY:HA2	1.94	0.48
2:Cr:58:ASN:ND2	2:Cr:62:ARG:HH21	2.10	0.48
1:A3:39:VAL:HG23	1:A3:72:THR:HG23	1.94	0.48
2:Bp:45:TYR:OH	2:Dp:73:ASP:OD1	2.22	0.48
1:As:39:VAL:HG23	1:As:72:THR:HG23	1.94	0.48
2:Bs:45:TYR:OH	2:Ds:73:ASP:OD1	2.18	0.48
2:CD:70:ARG:NH1	2:CD:70:ARG:HB2	2.28	0.48
2:Bh:12:ILE:HD12	2:Bh:27:MET:HE3	1.94	0.48
2:Bm:12:ILE:HD12	2:Bm:27:MET:HE3	1.94	0.48
2:Dq:8:ALA:HB3	2:Dq:52:GLY:O	2.14	0.48
2:Cz:70:ARG:NH1	2:Cz:70:ARG:HB2	2.29	0.48
2:C9:70:ARG:NH1	2:C9:70:ARG:HB2	2.29	0.48
1:AT:39:VAL:HG23	1:AT:72:THR:HG23	1.96	0.48
2:Ce:73:ASP:OD1	2:Ds:45:TYR:OH	2.25	0.48
2:Bs:11:MET:HE1	2:Bs:81:ILE:HD12	1.96	0.48
1:At:39:VAL:HG23	1:At:72:THR:HG23	1.96	0.48
2:Dw:8:ALA:HB3	2:Dw:52:GLY:O	2.13	0.48
1:AE:21:HIS:CD2	2:BE:62:ARG:HB3	2.48	0.48
1:AT:21:HIS:CD2	2:BT:62:ARG:HB3	2.48	0.48
1:Ad:39:VAL:HG23	1:Ad:72:THR:HG23	1.95	0.48
2:Bf:45:TYR:OH	2:Df:73:ASP:OD2	2.22	0.48
2:Co:70:ARG:NH1	2:Co:70:ARG:HB2	2.29	0.48
2:Cp:73:ASP:OD1	2:Dv:45:TYR:OH	2.26	0.48
1:A9:39:VAL:HG23	1:A9:72:THR:HG23	1.96	0.48
2:Ct:70:ARG:NH1	2:Ct:70:ARG:HB2	2.29	0.47
2:Cx:58:ASN:ND2	2:Cx:62:ARG:HH21	2.10	0.47
1:Aj:39:VAL:HG23	1:Aj:72:THR:HG23	1.96	0.47
2:DE:85:HIS:HE1	2:BF:83:ARG:NH2	2.12	0.47
2:BK:83:ARG:NH2	2:DT:85:HIS:HE1	2.12	0.47
2:Dj:77:ALA:HB2	2:Cy:72:GLY:HA2	1.95	0.47
1:Al:28:TRP:HZ3	1:Al:35:ARG:HE	1.61	0.47
1:At:37:VAL:HG12	1:Aw:1:MET:HE2	1.96	0.47
2:C4:70:ARG:NH1	2:C4:70:ARG:HB2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BD:65:ALA:O	2:BD:69:GLU:HG3	2.14	0.47
2:CE:73:ASP:OD1	2:Di:45:TYR:OH	2.25	0.47
2:BI:65:ALA:O	2:BI:69:GLU:HG3	2.14	0.47
2:BS:65:ALA:O	2:BS:69:GLU:HG3	2.14	0.47
1:Ao:39:VAL:HG23	1:Ao:72:THR:HG23	1.96	0.47
1:Aq:1:MET:HE2	1:Az:37:VAL:HG12	1.96	0.47
1:Ay:16:ILE:HG13	1:Ay:19:MET:HG3	1.97	0.47
1:A4:37:VAL:HG12	1:A6:1:MET:HE2	1.97	0.47
1:A4:39:VAL:HG23	1:A4:72:THR:HG23	1.96	0.47
2:C7:58:ASN:ND2	2:C7:62:ARG:HH21	2.10	0.47
2:BR:85:HIS:HE1	2:D0:83:ARG:HH22	1.62	0.47
1:Ap:28:TRP:HZ3	1:Ap:35:ARG:HE	1.61	0.47
2:Cq:58:ASN:HD21	2:Cq:62:ARG:NH2	2.13	0.47
2:BD:83:ARG:NH2	2:Dy:85:HIS:HE1	2.11	0.47
2:DI:11:MET:HG2	2:DI:49:LEU:HD23	1.97	0.47
2:BL:25:ASP:O	2:BL:29:LYS:HG3	2.14	0.47
2:DS:85:HIS:HE1	2:Bn:83:ARG:NH2	2.11	0.47
1:AW:1:MET:HE2	1:Ae:37:VAL:HG12	1.97	0.47
2:CW:58:ASN:HD21	2:CW:62:ARG:NH2	2.13	0.47
2:CZ:70:ARG:NH1	2:CZ:70:ARG:HB2	2.29	0.47
1:Ae:21:HIS:CD2	2:Be:62:ARG:HB3	2.48	0.47
2:Ce:70:ARG:NH1	2:Ce:70:ARG:HB2	2.29	0.47
2:Cl:70:ARG:HD3	2:Cl:70:ARG:H	1.80	0.47
2:Do:77:ALA:HB2	2:C8:72:GLY:HA2	1.96	0.47
2:Cq:70:ARG:HD3	2:Cq:70:ARG:H	1.80	0.47
1:AG:28:TRP:HZ3	1:AG:35:ARG:HE	1.63	0.47
1:AO:37:VAL:HG12	1:AQ:1:MET:HE2	1.96	0.47
1:AO:39:VAL:HG23	1:AO:72:THR:HG23	1.95	0.47
2:CT:70:ARG:NH1	2:CT:70:ARG:HB2	2.29	0.47
1:AZ:21:HIS:CD2	2:BZ:62:ARG:HB3	2.48	0.47
2:Cg:70:ARG:H	2:Cg:70:ARG:HD3	1.80	0.47
2:CE:70:ARG:NH1	2:CE:70:ARG:HB2	2.29	0.47
2:BQ:25:ASP:O	2:BQ:29:LYS:HG3	2.14	0.47
2:C1:70:ARG:HD3	2:C1:70:ARG:H	1.80	0.47
1:AB:1:MET:HE2	1:AJ:37:VAL:HG12	1.97	0.47
2:BT:25:ASP:OD1	2:BT:29:LYS:HE3	2.15	0.47
2:Cq:51:ARG:HG2	2:Cq:51:ARG:NH1	2.29	0.47
2:BJ:45:TYR:OH	2:DJ:73:ASP:OD2	2.28	0.46
2:BP:45:TYR:OH	2:DP:73:ASP:OD1	2.22	0.46
2:B0:45:TYR:OH	2:D0:73:ASP:OD1	2.23	0.46
1:A1:1:MET:HE2	1:A9:37:VAL:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A8:21:HIS:ND1	2:B8:62:ARG:HB3	2.30	0.46
1:AJ:39:VAL:HG23	1:AJ:72:THR:HG23	1.96	0.46
2:CJ:70:ARG:NH1	2:CJ:70:ARG:HB2	2.29	0.46
1:AM:19:MET:O	1:AM:67:TYR:OH	2.30	0.46
2:CO:70:ARG:NH1	2:CO:70:ARG:HB2	2.29	0.46
2:DR:11:MET:HE3	2:DR:79:HIS:HB3	1.98	0.46
2:Bd:11:MET:HE1	2:Bd:81:ILE:HD12	1.95	0.46
2:Dg:8:ALA:HB3	2:Dg:52:GLY:O	2.15	0.46
2:B9:45:TYR:OH	2:D9:73:ASP:OD2	2.28	0.46
1:Aa:19:MET:O	1:Aa:67:TYR:OH	2.28	0.46
2:Dl:8:ALA:HB3	2:Dl:52:GLY:O	2.15	0.46
2:B3:65:ALA:O	2:B3:69:GLU:HG3	2.15	0.46
1:A5:19:MET:O	1:A5:67:TYR:OH	2.28	0.46
2:B5:45:TYR:OH	2:D5:73:ASP:OD1	2.22	0.46
2:D7:11:MET:HE3	2:D7:79:HIS:HB3	1.97	0.46
2:DC:11:MET:HE3	2:DC:79:HIS:HB3	1.98	0.46
2:CG:70:ARG:HD3	2:CG:70:ARG:H	1.80	0.46
2:BJ:25:ASP:OD1	2:BJ:29:LYS:HE3	2.15	0.46
2:CL:70:ARG:H	2:CL:70:ARG:HD3	1.80	0.46
1:Ab:28:TRP:HZ3	1:Ab:35:ARG:HE	1.64	0.46
2:Bd:65:ALA:O	2:Bd:69:GLU:HG3	2.15	0.46
1:Ae:39:VAL:HG23	1:Ae:72:THR:HG23	1.96	0.46
2:Bi:65:ALA:O	2:Bi:69:GLU:HG3	2.14	0.46
2:C3:8:ALA:HB3	2:C3:52:GLY:O	2.16	0.46
2:CZ:73:ASP:OD1	2:D3:45:TYR:OH	2.25	0.46
2:Cf:25:ASP:OD2	2:Cf:29:LYS:HE3	2.16	0.46
2:Ck:25:ASP:OD2	2:Ck:29:LYS:HE3	2.16	0.46
2:Dm:11:MET:HE3	2:Dm:79:HIS:HB3	1.98	0.46
2:Cn:58:ASN:HD21	2:Cn:62:ARG:NH2	2.14	0.46
2:Cp:41:VAL:HB	2:Cp:45:TYR:HB2	1.98	0.46
2:Cs:8:ALA:HB3	2:Cs:52:GLY:O	2.16	0.46
1:Ay:21:HIS:ND1	2:By:62:ARG:HB3	2.30	0.46
2:Bz:45:TYR:OH	2:Dz:73:ASP:OD2	2.28	0.46
2:C8:8:ALA:HB3	2:C8:52:GLY:O	2.16	0.46
2:CP:25:ASP:OD2	2:CP:29:LYS:HE3	2.16	0.46
1:AY:21:HIS:ND1	2:BY:62:ARG:HB3	2.31	0.46
1:Ai:21:HIS:ND1	2:Bi:62:ARG:HB3	2.31	0.46
1:A6:1:MET:SD	1:A6:1:MET:N	2.79	0.46
2:DI:85:HIS:HE1	2:BY:83:ARG:NH2	2.14	0.46
1:AK:28:TRP:HZ3	1:AK:35:ARG:HE	1.64	0.46
1:AL:1:MET:SD	1:AL:1:MET:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CS:12:ILE:CD1	2:CS:27:MET:HE3	2.42	0.46
1:Ag:1:MET:HE2	1:Ao:37:VAL:HG12	1.96	0.46
1:Aj:37:VAL:HG12	1:Al:1:MET:HE2	1.96	0.46
2:Cp:25:ASP:OD2	2:Cp:29:LYS:HE3	2.16	0.46
2:Bs:65:ALA:O	2:Bs:69:GLU:HG3	2.15	0.46
2:Cy:58:ASN:HD21	2:Cy:62:ARG:NH2	2.14	0.46
2:CA:25:ASP:OD2	2:CA:29:LYS:HE3	2.16	0.46
2:CI:8:ALA:HB3	2:CI:52:GLY:O	2.16	0.46
2:CN:8:ALA:HB3	2:CN:52:GLY:O	2.16	0.46
2:CP:41:VAL:HB	2:CP:45:TYR:HB2	1.98	0.46
1:AZ:39:VAL:HG23	1:AZ:72:THR:HG23	1.96	0.46
2:BZ:45:TYR:OH	2:DZ:73:ASP:OD2	2.28	0.46
2:Bn:65:ALA:O	2:Bn:69:GLU:HG3	2.15	0.46
2:CA:41:VAL:HB	2:CA:45:TYR:HB2	1.98	0.46
2:CD:12:ILE:CD1	2:CD:27:MET:HE3	2.41	0.46
2:BS:83:ARG:NH2	2:D8:85:HIS:HE1	2.14	0.46
2:CY:8:ALA:HB3	2:CY:52:GLY:O	2.16	0.46
2:BZ:36:VAL:HG11	2:BZ:51:ARG:HG3	1.98	0.46
1:Ad:21:HIS:ND1	2:Bd:62:ARG:HB3	2.31	0.46
2:Cd:58:ASN:HD21	2:Cd:62:ARG:NH2	2.14	0.46
2:Ck:41:VAL:HB	2:Ck:45:TYR:HB2	1.98	0.46
2:Dm:31:ALA:HB3	2:Dm:60:ALA:HB2	1.98	0.46
2:C0:41:VAL:HB	2:C0:45:TYR:HB2	1.98	0.46
2:CB:58:ASN:HD21	2:CB:62:ARG:NH2	2.13	0.46
2:CK:25:ASP:OD2	2:CK:29:LYS:HE3	2.16	0.46
2:BN:83:ARG:HH22	2:Ds:85:HIS:HE1	1.64	0.46
2:CQ:72:GLY:HA2	2:Dc:77:ALA:HB2	1.98	0.46
2:DR:31:ALA:HB3	2:DR:60:ALA:HB2	1.98	0.46
2:Cb:70:ARG:H	2:Cb:70:ARG:HD3	1.80	0.46
2:Be:45:TYR:OH	2:De:73:ASP:OD2	2.28	0.46
2:DG:77:ALA:HB2	2:Ch:72:GLY:HA2	1.98	0.45
2:CQ:58:ASN:HD21	2:CQ:62:ARG:NH2	2.13	0.45
2:CS:8:ALA:HB3	2:CS:52:GLY:O	2.16	0.45
2:Cf:41:VAL:HB	2:Cf:45:TYR:HB2	1.98	0.45
1:As:28:TRP:HZ3	1:As:35:ARG:HE	1.64	0.45
2:Cv:25:ASP:OD2	2:Cv:29:LYS:HE3	2.16	0.45
1:Aw:1:MET:SD	1:Aw:1:MET:N	2.79	0.45
2:DC:31:ALA:HB3	2:DC:60:ALA:HB2	1.99	0.45
1:AD:28:TRP:HZ3	1:AD:35:ARG:HE	1.64	0.45
2:CG:58:ASN:HD21	2:CG:62:ARG:NH2	2.13	0.45
2:Cb:23:ALA:HB2	2:Cb:68:CYS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Cg:23:ALA:HB2	2:Cg:68:CYS:HB3	1.97	0.45
1:Ah:19:MET:O	1:Ah:67:TYR:OH	2.30	0.45
1:Am:1:MET:HE2	1:Aw:37:VAL:HG12	1.99	0.45
2:C3:12:ILE:CD1	2:C3:27:MET:HE3	2.42	0.45
2:C6:70:ARG:HD3	2:C6:70:ARG:H	1.80	0.45
1:AL:1:MET:HE2	1:AT:37:VAL:HG12	1.96	0.45
1:AR:19:MET:O	1:AR:67:TYR:OH	2.31	0.45
2:CV:41:VAL:HB	2:CV:45:TYR:HB2	1.98	0.45
1:A3:21:HIS:ND1	2:B3:62:ARG:HB3	2.31	0.45
1:AB:37:VAL:HG12	1:Ar:1:MET:HE2	1.99	0.45
2:CE:58:ASN:ND2	2:CE:62:ARG:HH21	2.15	0.45
2:CT:58:ASN:ND2	2:CT:62:ARG:HH21	2.15	0.45
2:DW:31:ALA:HB3	2:DW:60:ALA:HB2	1.99	0.45
2:Ca:41:VAL:HB	2:Ca:45:TYR:HB2	1.98	0.45
2:Cs:12:ILE:CD1	2:Cs:27:MET:HE3	2.42	0.45
2:Cw:70:ARG:HD3	2:Cw:70:ARG:H	1.80	0.45
2:DL:77:ALA:HB2	2:Cm:72:GLY:HA2	1.99	0.45
1:AQ:37:VAL:HG12	1:A2:1:MET:HE2	1.99	0.45
1:AS:28:TRP:HZ3	1:AS:35:ARG:HE	1.64	0.45
2:DT:11:MET:HG2	2:DT:49:LEU:HD22	1.99	0.45
2:DX:31:ALA:HB3	2:DX:60:ALA:HB2	1.98	0.45
2:Da:92:LEU:HD23	2:Da:92:LEU:HA	1.83	0.45
1:Ah:1:MET:HE2	1:A6:37:VAL:HG12	1.99	0.45
2:Dh:11:MET:HE3	2:Dh:79:HIS:HB3	1.99	0.45
2:DE:11:MET:HG2	2:DE:49:LEU:HD22	1.99	0.45
2:BF:45:TYR:OH	2:DF:73:ASP:OD1	2.22	0.45
2:CZ:58:ASN:ND2	2:CZ:62:ARG:HH21	2.15	0.45
2:Bh:11:MET:HE3	2:Bh:11:MET:HB2	1.91	0.45
2:Bv:45:TYR:OH	2:Dv:73:ASP:OD1	2.22	0.45
2:Cx:12:ILE:CD1	2:Cx:27:MET:HE3	2.45	0.45
2:C1:23:ALA:HB2	2:C1:68:CYS:HB3	1.99	0.45
2:CB:72:GLY:HA2	2:DX:77:ALA:HB2	1.98	0.45
1:AE:37:VAL:HG12	1:AG:1:MET:HE2	1.97	0.45
1:Ac:19:MET:HE2	1:Ac:19:MET:HB3	1.90	0.45
2:Dg:77:ALA:HB2	2:C7:72:GLY:HA2	1.99	0.45
2:Cl:58:ASN:HD21	2:Cl:62:ARG:NH2	2.14	0.45
2:DI:77:ALA:HB2	2:Cx:72:GLY:HA2	1.99	0.45
1:Aq:1:MET:SD	1:Aq:1:MET:N	2.79	0.45
2:Ct:58:ASN:ND2	2:Ct:62:ARG:HH21	2.15	0.45
2:Dt:11:MET:HG2	2:Dt:49:LEU:HD22	1.99	0.45
2:Cv:41:VAL:HB	2:Cv:45:TYR:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C4:58:ASN:ND2	2:C4:62:ARG:HH21	2.15	0.45
2:CF:58:ASN:HD21	2:CF:62:ARG:NH2	2.15	0.45
2:CI:23:ALA:HB2	2:CI:68:CYS:HB3	1.99	0.45
2:DJ:11:MET:HG2	2:DJ:49:LEU:HD22	1.99	0.45
2:CO:58:ASN:ND2	2:CO:62:ARG:HH21	2.15	0.45
2:DQ:77:ALA:HB2	2:Cc:72:GLY:HA2	1.99	0.45
2:Ca:25:ASP:OD2	2:Ca:29:LYS:HE3	2.16	0.45
2:Ci:8:ALA:HB3	2:Ci:52:GLY:O	2.16	0.45
2:Bj:31:ALA:HB3	2:Bj:60:ALA:HB2	1.98	0.45
1:An:1:MET:SD	1:An:1:MET:N	2.85	0.45
2:Co:23:ALA:HB2	2:Co:68:CYS:HB3	1.99	0.45
2:C1:31:ALA:HB3	2:C1:60:ALA:HB2	1.99	0.45
1:AI:1:MET:SD	1:AI:1:MET:N	2.83	0.45
2:CJ:58:ASN:ND2	2:CJ:62:ARG:HH21	2.15	0.45
2:CK:41:VAL:HB	2:CK:45:TYR:HB2	1.98	0.45
2:CM:72:GLY:HA2	2:Dw:77:ALA:HB2	1.99	0.45
1:AY:28:TRP:HZ3	1:AY:35:ARG:HE	1.65	0.45
1:Aa:2:LYS:HE2	1:Ar:36:GLN:HG2	1.99	0.45
2:Dd:34:ARG:HH21	2:Dd:51:ARG:HB2	1.82	0.45
2:Ce:58:ASN:ND2	2:Ce:62:ARG:HH21	2.15	0.45
2:Dj:11:MET:HG2	2:Dj:49:LEU:HD22	1.99	0.45
2:C5:41:VAL:HB	2:C5:45:TYR:HB2	1.98	0.45
2:C7:12:ILE:CD1	2:C7:27:MET:HE3	2.45	0.45
1:AR:1:MET:HE2	1:Ab:37:VAL:HG12	1.98	0.45
2:CV:25:ASP:OD2	2:CV:29:LYS:HE3	2.16	0.45
2:BZ:31:ALA:HB3	2:BZ:60:ALA:HB2	1.99	0.45
2:C4:23:ALA:HB2	2:C4:68:CYS:HB3	1.99	0.45
2:D8:11:MET:HG2	2:D8:49:LEU:HD23	1.99	0.45
2:DB:77:ALA:HB2	2:CX:72:GLY:HA2	1.99	0.44
2:CC:72:GLY:HA2	2:Dq:77:ALA:HB2	1.98	0.44
2:CH:72:GLY:HA2	2:D6:77:ALA:HB2	1.99	0.44
2:CL:31:ALA:HB3	2:CL:60:ALA:HB2	1.99	0.44
2:Co:58:ASN:ND2	2:Co:62:ARG:HH21	2.15	0.44
2:Dx:11:MET:HE3	2:Dx:79:HIS:HB3	1.99	0.44
2:C2:8:ALA:O	2:C2:51:ARG:HA	2.17	0.44
2:DD:45:TYR:OH	2:Cz:73:ASP:OD1	2.25	0.44
1:AV:19:MET:HE1	1:AV:24:LEU:HD21	1.99	0.44
2:Ce:23:ALA:HB2	2:Ce:68:CYS:HB3	1.99	0.44
1:Af:19:MET:HE1	1:Af:24:LEU:HD21	2.00	0.44
2:Dh:31:ALA:HB3	2:Dh:60:ALA:HB2	2.00	0.44
2:Cr:8:ALA:O	2:Cr:51:ARG:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Cz:23:ALA:HB2	2:Cz:68:CYS:HB3	1.99	0.44
2:D7:31:ALA:HB3	2:D7:60:ALA:HB2	1.98	0.44
1:AF:19:MET:HE1	1:AF:24:LEU:HD21	1.99	0.44
2:CR:72:GLY:HA2	2:D1:77:ALA:HB2	1.98	0.44
1:AX:19:MET:HE2	1:AX:19:MET:HB3	1.90	0.44
2:Db:31:ALA:HB3	2:Db:60:ALA:HB2	2.00	0.44
2:Dn:34:ARG:HH21	2:Dn:51:ARG:HB2	1.82	0.44
2:C7:87:GLU:O	2:C7:90:ASN:ND2	2.50	0.44
2:CC:8:ALA:O	2:CC:51:ARG:HA	2.18	0.44
2:CF:41:VAL:HB	2:CF:45:TYR:HB2	1.99	0.44
1:AG:37:VAL:HG12	1:A7:1:MET:HE2	1.99	0.44
1:AP:19:MET:O	1:AP:67:TYR:OH	2.29	0.44
2:CR:8:ALA:O	2:CR:51:ARG:HA	2.18	0.44
2:DS:34:ARG:HH21	2:DS:51:ARG:HB2	1.82	0.44
2:Ch:8:ALA:O	2:Ch:51:ARG:HA	2.18	0.44
2:Di:85:HIS:HE1	2:By:83:ARG:NH2	2.16	0.44
1:As:1:MET:SD	1:As:1:MET:N	2.83	0.44
2:Ct:23:ALA:HB2	2:Ct:68:CYS:HB3	1.99	0.44
2:Cz:58:ASN:ND2	2:Cz:62:ARG:HH21	2.15	0.44
2:C9:23:ALA:HB2	2:C9:68:CYS:HB3	1.99	0.44
2:BK:45:TYR:OH	2:DK:73:ASP:OD1	2.23	0.44
1:AL:37:VAL:HG12	1:Ax:1:MET:HE2	1.99	0.44
1:AM:19:MET:HE2	1:AM:19:MET:HB3	1.90	0.44
1:Ac:1:MET:HE2	1:A1:37:VAL:HG12	1.99	0.44
2:Cl:23:ALA:HB2	2:Cl:68:CYS:HB3	1.99	0.44
1:Ay:19:MET:HE2	1:Ay:19:MET:HB3	1.93	0.44
1:A3:28:TRP:HZ3	1:A3:35:ARG:HE	1.66	0.44
2:C9:58:ASN:ND2	2:C9:62:ARG:HH21	2.15	0.44
1:AG:19:MET:HE2	1:AG:19:MET:HB3	1.89	0.44
2:CH:8:ALA:O	2:CH:51:ARG:HA	2.17	0.44
2:DN:85:HIS:HE1	2:Bd:83:ARG:NH2	2.16	0.44
2:Dc:31:ALA:HB3	2:Dc:60:ALA:HB2	1.99	0.44
2:Cm:8:ALA:O	2:Cm:51:ARG:HA	2.18	0.44
2:Cn:8:ALA:O	2:Cn:51:ARG:HA	2.18	0.44
2:Dn:85:HIS:HE1	2:B8:83:ARG:NH2	2.16	0.44
1:Aq:28:TRP:HZ3	1:Aq:35:ARG:HE	1.65	0.44
2:Dr:11:MET:HE3	2:Dr:79:HIS:HB3	2.00	0.44
2:CD:23:ALA:HB2	2:CD:68:CYS:HB3	1.99	0.44
2:CI:12:ILE:CD1	2:CI:27:MET:HE3	2.42	0.44
2:BM:57:VAL:O	2:BM:61:VAL:HG23	2.18	0.44
2:DS:45:TYR:OH	2:C9:73:ASP:OD1	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dd:85:HIS:HE1	2:Bs:83:ARG:NH2	2.16	0.44
2:Bj:9:LEU:HG	2:Bj:11:MET:HE2	1.99	0.44
2:Cs:8:ALA:O	2:Cs:51:ARG:HA	2.18	0.44
2:Dz:11:MET:HG2	2:Dz:49:LEU:HD22	1.99	0.44
2:C6:31:ALA:HB3	2:C6:60:ALA:HB2	1.99	0.44
2:C9:8:ALA:O	2:C9:51:ARG:HA	2.18	0.44
2:D9:11:MET:HG2	2:D9:49:LEU:HD22	1.99	0.44
2:CE:23:ALA:HB2	2:CE:68:CYS:HB3	1.99	0.44
2:CG:31:ALA:HB3	2:CG:60:ALA:HB2	2.00	0.44
2:BH:57:VAL:O	2:BH:61:VAL:HG23	2.18	0.44
2:CL:23:ALA:HB2	2:CL:68:CYS:HB3	1.99	0.44
2:CS:8:ALA:O	2:CS:51:ARG:HA	2.18	0.44
2:CS:23:ALA:HB2	2:CS:68:CYS:HB3	1.99	0.44
1:AX:1:MET:HE2	1:Aq:37:VAL:HG12	1.99	0.44
2:C3:8:ALA:O	2:C3:51:ARG:HA	2.18	0.44
1:A4:19:MET:O	1:A4:67:TYR:OH	2.25	0.44
2:C8:8:ALA:O	2:C8:51:ARG:HA	2.18	0.44
2:DB:31:ALA:HB3	2:DB:60:ALA:HB2	2.00	0.44
2:CM:8:ALA:O	2:CM:51:ARG:HA	2.18	0.44
2:DQ:31:ALA:HB3	2:DQ:60:ALA:HB2	2.00	0.44
2:BR:31:ALA:HB3	2:BR:60:ALA:HB2	2.00	0.44
2:DX:11:MET:HE3	2:DX:79:HIS:HB3	1.98	0.44
2:DY:85:HIS:HE1	2:B3:83:ARG:NH2	2.16	0.44
1:AZ:36:GLN:HG2	1:Ab:2:LYS:HE3	2.00	0.44
2:DZ:11:MET:HG2	2:DZ:49:LEU:HD22	1.99	0.44
2:Ba:45:TYR:OH	2:Da:73:ASP:OD1	2.22	0.44
1:Ai:28:TRP:HZ3	1:Ai:35:ARG:HE	1.66	0.44
2:Ci:8:ALA:O	2:Ci:51:ARG:HA	2.18	0.44
1:Am:28:TRP:HZ3	1:Am:35:ARG:HE	1.65	0.44
2:Cw:23:ALA:HB2	2:Cw:68:CYS:HB3	1.99	0.44
2:Cy:8:ALA:O	2:Cy:51:ARG:HA	2.18	0.44
1:Az:1:MET:SD	1:Az:1:MET:N	2.82	0.44
2:CD:8:ALA:HB3	2:CD:52:GLY:O	2.18	0.43
2:BJ:66:ASP:O	2:BJ:70:ARG:NH2	2.51	0.43
2:DK:31:ALA:HB3	2:DK:60:ALA:HB2	2.00	0.43
1:AR:19:MET:HE2	1:AR:19:MET:HB3	1.91	0.43
2:CT:23:ALA:HB2	2:CT:68:CYS:HB3	2.00	0.43
2:CW:72:GLY:HA2	2:Dr:77:ALA:HB2	2.00	0.43
2:CY:8:ALA:O	2:CY:51:ARG:HA	2.18	0.43
2:Cd:8:ALA:HB3	2:Cd:52:GLY:O	2.18	0.43
2:Cd:8:ALA:O	2:Cd:51:ARG:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:De:11:MET:HG2	2:De:49:LEU:HD22	1.99	0.43
1:Ap:19:MET:HE2	1:Ap:19:MET:HB3	1.91	0.43
2:Cw:31:ALA:HB3	2:Cw:60:ALA:HB2	1.99	0.43
1:Ay:28:TRP:HZ3	1:Ay:35:ARG:HE	1.66	0.43
2:Dy:34:ARG:HH21	2:Dy:51:ARG:HB2	1.82	0.43
2:D0:92:LEU:HD23	2:D0:92:LEU:HA	1.82	0.43
1:AC:19:MET:HE2	1:AC:19:MET:HB3	1.90	0.43
2:DF:41:VAL:HB	2:DF:45:TYR:HB2	2.00	0.43
2:CN:12:ILE:CD1	2:CN:27:MET:HE3	2.42	0.43
2:Be:66:ASP:O	2:Be:70:ARG:NH2	2.51	0.43
2:Cy:8:ALA:HB3	2:Cy:52:GLY:O	2.18	0.43
2:Cz:8:ALA:O	2:Cz:51:ARG:HA	2.19	0.43
2:D2:11:MET:HE3	2:D2:79:HIS:HB3	2.00	0.43
2:D2:31:ALA:HB3	2:D2:60:ALA:HB2	1.99	0.43
2:C6:23:ALA:HB2	2:C6:68:CYS:HB3	1.99	0.43
1:AC:1:MET:HE2	1:AW:37:VAL:HG12	1.99	0.43
1:AM:1:MET:HE2	1:Al:37:VAL:HG12	1.99	0.43
2:CX:8:ALA:O	2:CX:51:ARG:HA	2.18	0.43
2:Db:41:VAL:HB	2:Db:45:TYR:HB2	2.01	0.43
2:Be:31:ALA:HB3	2:Be:60:ALA:HB2	2.00	0.43
2:Dl:31:ALA:HB3	2:Dl:60:ALA:HB2	2.00	0.43
1:At:19:MET:O	1:At:67:TYR:OH	2.25	0.43
2:C7:8:ALA:O	2:C7:51:ARG:HA	2.18	0.43
1:A8:28:TRP:HZ3	1:A8:35:ARG:HE	1.66	0.43
2:CJ:23:ALA:HB2	2:CJ:68:CYS:HB3	1.99	0.43
2:DM:31:ALA:HB3	2:DM:60:ALA:HB2	1.99	0.43
2:CO:23:ALA:HB2	2:CO:68:CYS:HB3	1.99	0.43
2:DP:31:ALA:HB3	2:DP:60:ALA:HB2	2.00	0.43
1:AQ:28:TRP:HZ3	1:AQ:35:ARG:HE	1.67	0.43
2:DW:77:ALA:HB2	2:Cr:72:GLY:HA2	1.99	0.43
1:Ad:1:MET:SD	1:Ad:1:MET:N	2.83	0.43
1:Af:2:LYS:HE2	1:Ax:36:GLN:HG2	1.99	0.43
2:Dg:31:ALA:HB3	2:Dg:60:ALA:HB2	2.00	0.43
2:Cl:31:ALA:HB3	2:Cl:60:ALA:HB2	1.99	0.43
2:Dp:92:LEU:HD23	2:Dp:92:LEU:HA	1.82	0.43
2:Dq:31:ALA:HB3	2:Dq:60:ALA:HB2	1.99	0.43
2:Dq:41:VAL:HB	2:Dq:45:TYR:HB2	2.00	0.43
2:Dr:31:ALA:HB3	2:Dr:60:ALA:HB2	2.00	0.43
2:Bx:57:VAL:O	2:Bx:61:VAL:HG23	2.19	0.43
1:A7:19:MET:HE2	1:A7:19:MET:HB3	1.90	0.43
2:B9:66:ASP:O	2:B9:70:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AF:5:GLN:HE21	1:AF:28:TRP:HE1	1.67	0.43
1:AP:2:LYS:HE2	1:Am:36:GLN:HG2	1.99	0.43
2:DW:41:VAL:HB	2:DW:45:TYR:HB2	2.01	0.43
2:Ba:35:LEU:HD11	2:Ba:48:VAL:HG13	2.01	0.43
2:Db:77:ALA:HB2	2:C2:72:GLY:HA2	1.99	0.43
2:Bc:57:VAL:O	2:Bc:61:VAL:HG23	2.18	0.43
2:Dd:85:HIS:HE1	2:Bs:83:ARG:HH22	1.67	0.43
1:Aq:70:ASP:OD2	1:Aq:70:ASP:N	2.52	0.43
1:Aw:28:TRP:HZ3	1:Aw:35:ARG:HE	1.67	0.43
2:Dw:41:VAL:HB	2:Dw:45:TYR:HB2	2.00	0.43
2:Cx:8:ALA:O	2:Cx:51:ARG:HA	2.18	0.43
1:A6:28:TRP:HZ3	1:A6:35:ARG:HE	1.67	0.43
2:B7:57:VAL:O	2:B7:61:VAL:HG23	2.19	0.43
1:AA:2:LYS:HE2	1:Ah:36:GLN:HG2	1.99	0.43
1:AF:19:MET:HE2	1:AF:19:MET:HB3	1.91	0.43
2:DF:31:ALA:HB3	2:DF:60:ALA:HB2	2.01	0.43
2:DH:31:ALA:HB3	2:DH:60:ALA:HB2	1.99	0.43
2:DP:88:VAL:HG12	2:DP:92:LEU:HG	2.01	0.43
2:DQ:41:VAL:HB	2:DQ:45:TYR:HB2	2.01	0.43
2:BZ:66:ASP:O	2:BZ:70:ARG:NH2	2.51	0.43
2:Ds:34:ARG:HH21	2:Ds:51:ARG:HB2	1.82	0.43
2:Dx:31:ALA:HB3	2:Dx:60:ALA:HB2	1.99	0.43
2:D9:13:GLU:OE2	2:D9:47:THR:OG1	2.37	0.43
2:DB:41:VAL:HB	2:DB:45:TYR:HB2	2.01	0.43
2:BC:31:ALA:HB3	2:BC:60:ALA:HB2	2.01	0.43
2:BJ:31:ALA:HB3	2:BJ:60:ALA:HB2	2.00	0.43
2:DN:34:ARG:HH21	2:DN:51:ARG:HB2	1.82	0.43
2:DZ:13:GLU:OE2	2:DZ:47:THR:OG1	2.37	0.43
2:Cg:31:ALA:HB3	2:Cg:60:ALA:HB2	1.99	0.43
1:Am:19:MET:O	1:Am:67:TYR:OH	2.30	0.43
2:Dn:85:HIS:HE1	2:B8:83:ARG:HH22	1.67	0.43
2:Dz:13:GLU:OE2	2:Dz:47:THR:OG1	2.37	0.43
2:DA:31:ALA:HB3	2:DA:60:ALA:HB2	2.01	0.43
2:DG:31:ALA:HB3	2:DG:60:ALA:HB2	2.00	0.43
2:CI:8:ALA:O	2:CI:51:ARG:HA	2.18	0.43
1:AL:28:TRP:HZ3	1:AL:35:ARG:HE	1.67	0.43
2:CM:12:ILE:CD1	2:CM:27:MET:HE3	2.45	0.43
2:CN:8:ALA:O	2:CN:51:ARG:HA	2.18	0.43
2:DV:31:ALA:HB3	2:DV:60:ALA:HB2	2.01	0.43
2:Da:31:ALA:HB3	2:Da:60:ALA:HB2	2.01	0.43
2:Cc:8:ALA:O	2:Cc:51:ARG:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dk:31:ALA:HB3	2:Dk:60:ALA:HB2	2.01	0.43
2:Bv:65:ALA:O	2:Bv:69:GLU:HG3	2.19	0.43
1:Ay:1:MET:SD	1:Ay:1:MET:N	2.83	0.43
2:D1:31:ALA:HB3	2:D1:60:ALA:HB2	2.00	0.43
2:CH:12:ILE:CD1	2:CH:27:MET:HE3	2.44	0.43
2:BI:83:ARG:NH2	2:D3:85:HIS:HE1	2.17	0.43
2:CL:70:ARG:HH11	2:CL:71:VAL:HG23	1.84	0.43
2:CN:23:ALA:HB2	2:CN:68:CYS:HB3	2.01	0.43
1:AS:19:MET:HE1	1:AS:24:LEU:HD21	2.01	0.43
1:AY:19:MET:O	1:AY:67:TYR:OH	2.33	0.43
1:Ad:28:TRP:HZ3	1:Ad:35:ARG:HE	1.67	0.43
2:Cd:23:ALA:O	2:Cd:27:MET:HG3	2.19	0.43
2:Df:31:ALA:HB3	2:Df:60:ALA:HB2	2.01	0.43
2:Bm:31:ALA:HB3	2:Bm:60:ALA:HB2	2.00	0.43
2:Bz:66:ASP:O	2:Bz:70:ARG:NH2	2.51	0.43
2:D1:41:VAL:HB	2:D1:45:TYR:HB2	2.01	0.43
2:C2:12:ILE:CD1	2:C2:27:MET:HE3	2.44	0.43
2:B5:65:ALA:O	2:B5:69:GLU:HG3	2.19	0.43
2:CG:70:ARG:HH11	2:CG:71:VAL:HG23	1.84	0.43
2:DH:11:MET:HE3	2:DH:79:HIS:HB3	2.00	0.43
2:DL:31:ALA:HB3	2:DL:60:ALA:HB2	2.00	0.43
2:DR:88:VAL:HG12	2:DR:92:LEU:HG	2.01	0.43
2:CX:41:VAL:HB	2:CX:45:TYR:HB2	2.01	0.43
2:CZ:8:ALA:O	2:CZ:51:ARG:HA	2.19	0.43
2:Cb:31:ALA:HB3	2:Cb:60:ALA:HB2	1.99	0.43
2:Cc:41:VAL:HB	2:Cc:45:TYR:HB2	2.01	0.43
2:De:13:GLU:OE2	2:De:47:THR:OG1	2.37	0.43
2:Dg:12:ILE:HD12	2:Dg:27:MET:HE3	2.01	0.43
2:Bh:31:ALA:HB3	2:Bh:60:ALA:HB2	2.01	0.43
2:Dk:41:VAL:HB	2:Dk:45:TYR:HB2	2.01	0.43
2:Cn:12:ILE:CD1	2:Cn:27:MET:HE3	2.41	0.43
2:Bo:66:ASP:O	2:Bo:70:ARG:NH2	2.51	0.43
2:Dw:31:ALA:HB3	2:Dw:60:ALA:HB2	1.99	0.43
1:Ax:19:MET:HE2	1:Ax:19:MET:HB3	1.90	0.43
1:A1:28:TRP:HZ3	1:A1:35:ARG:HE	1.67	0.43
2:C1:70:ARG:HH11	2:C1:71:VAL:HG23	1.84	0.43
2:B4:31:ALA:HB3	2:B4:60:ALA:HB2	1.99	0.43
1:A5:19:MET:HE1	1:A5:24:LEU:HD21	2.01	0.43
2:DD:15:ARG:HB2	2:DD:73:ASP:HB2	2.01	0.42
2:DE:13:GLU:OE2	2:DE:47:THR:OG1	2.37	0.42
2:BF:65:ALA:O	2:BF:69:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BH:85:HIS:HE1	2:D5:83:ARG:HH22	1.67	0.42
2:CI:58:ASN:HD21	2:CI:62:ARG:NH2	2.17	0.42
2:BK:65:ALA:O	2:BK:69:GLU:HG3	2.18	0.42
2:BM:11:MET:HG2	2:BM:49:LEU:HG	2.01	0.42
2:CN:58:ASN:HD21	2:CN:62:ARG:NH2	2.17	0.42
2:DX:88:VAL:HG12	2:DX:92:LEU:HG	2.01	0.42
1:Ab:70:ASP:OD2	1:Ab:70:ASP:N	2.52	0.42
2:Ce:8:ALA:O	2:Ce:51:ARG:HA	2.19	0.42
2:Df:13:GLU:OE2	2:Df:47:THR:OG1	2.37	0.42
2:Df:41:VAL:HB	2:Df:45:TYR:HB2	2.01	0.42
2:Dk:13:GLU:OE2	2:Dk:47:THR:OG1	2.37	0.42
2:Cn:23:ALA:HB2	2:Cn:68:CYS:HB3	2.01	0.42
2:Dw:12:ILE:HD12	2:Dw:27:MET:HE3	2.01	0.42
2:C4:8:ALA:O	2:C4:51:ARG:HA	2.19	0.42
2:CF:25:ASP:OD1	2:CF:29:LYS:HE3	2.19	0.42
2:CJ:8:ALA:O	2:CJ:51:ARG:HA	2.18	0.42
2:DK:83:ARG:HH22	2:Bm:85:HIS:HE1	1.67	0.42
2:BO:31:ALA:HB3	2:BO:60:ALA:HB2	2.00	0.42
2:DP:83:ARG:HH22	2:Bc:85:HIS:HE1	1.68	0.42
2:BT:31:ALA:HB3	2:BT:60:ALA:HB2	2.00	0.42
2:DW:88:VAL:HG12	2:DW:92:LEU:HG	2.01	0.42
2:Cl:70:ARG:HH11	2:Cl:71:VAL:HG23	1.84	0.42
2:Bo:31:ALA:HB3	2:Bo:60:ALA:HB2	2.00	0.42
2:Co:8:ALA:O	2:Co:51:ARG:HA	2.19	0.42
2:Dp:31:ALA:HB3	2:Dp:60:ALA:HB2	2.01	0.42
2:Cq:70:ARG:HH11	2:Cq:71:VAL:HG23	1.84	0.42
2:BE:31:ALA:HB3	2:BE:60:ALA:HB2	2.00	0.42
2:DG:41:VAL:HB	2:DG:45:TYR:HB2	2.01	0.42
2:DK:41:VAL:HB	2:DK:45:TYR:HB2	2.01	0.42
2:DL:41:VAL:HB	2:DL:45:TYR:HB2	2.01	0.42
2:DM:11:MET:HE3	2:DM:79:HIS:HB3	2.00	0.42
2:DQ:12:ILE:HD12	2:DQ:27:MET:HE3	2.01	0.42
2:BX:57:VAL:O	2:BX:61:VAL:HG23	2.19	0.42
2:CY:23:ALA:HB2	2:CY:68:CYS:HB3	2.01	0.42
2:Da:83:ARG:NH2	2:D2:28:THR:O	2.53	0.42
2:Dc:88:VAL:HG12	2:Dc:92:LEU:HG	2.01	0.42
2:Bf:65:ALA:O	2:Bf:69:GLU:HG3	2.18	0.42
2:Bm:57:VAL:O	2:Bm:61:VAL:HG23	2.19	0.42
2:Ct:8:ALA:O	2:Ct:51:ARG:HA	2.19	0.42
2:Bv:58:ASN:O	2:Bv:62:ARG:HG3	2.20	0.42
2:Dv:31:ALA:HB3	2:Dv:60:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D0:31:ALA:HB3	2:D0:60:ALA:HB2	2.01	0.42
1:AB:19:MET:HE2	1:AB:19:MET:HB3	1.89	0.42
2:CD:8:ALA:O	2:CD:51:ARG:HA	2.20	0.42
2:BO:66:ASP:O	2:BO:70:ARG:NH2	2.52	0.42
2:CO:8:ALA:O	2:CO:51:ARG:HA	2.19	0.42
2:DV:41:VAL:HB	2:DV:45:TYR:HB2	2.02	0.42
2:Da:41:VAL:HB	2:Da:45:TYR:HB2	2.02	0.42
2:Cb:70:ARG:HH11	2:Cb:71:VAL:HG23	1.84	0.42
1:Af:36:GLN:HG2	1:A8:2:LYS:HE3	2.01	0.42
2:Cg:70:ARG:HH11	2:Cg:71:VAL:HG23	1.84	0.42
2:Bh:57:VAL:O	2:Bh:61:VAL:HG23	2.19	0.42
2:Ci:58:ASN:HD21	2:Ci:62:ARG:NH2	2.17	0.42
2:Bj:66:ASP:O	2:Bj:70:ARG:NH2	2.51	0.42
2:Dm:88:VAL:HG12	2:Dm:92:LEU:HG	2.01	0.42
2:Cn:57:VAL:O	2:Cn:61:VAL:HG23	2.20	0.42
2:Cr:12:ILE:CD1	2:Cr:27:MET:HE3	2.44	0.42
2:Bt:31:ALA:HB3	2:Bt:60:ALA:HB2	2.00	0.42
2:Dt:13:GLU:OE2	2:Dt:47:THR:OG1	2.37	0.42
2:Dv:41:VAL:HB	2:Dv:45:TYR:HB2	2.01	0.42
2:BA:58:ASN:O	2:BA:62:ARG:HG3	2.20	0.42
2:CC:41:VAL:HB	2:CC:45:TYR:HB2	2.01	0.42
1:AD:19:MET:O	1:AD:67:TYR:OH	2.33	0.42
2:DH:88:VAL:HG12	2:DH:92:LEU:HG	2.01	0.42
1:AK:19:MET:HE1	1:AK:24:LEU:HD21	2.00	0.42
2:DM:8:ALA:HB3	2:DM:52:GLY:O	2.20	0.42
2:DV:92:LEU:HD23	2:DV:92:LEU:HA	1.82	0.42
1:Ag:28:TRP:HZ3	1:Ag:35:ARG:HE	1.67	0.42
2:Dl:12:ILE:HD12	2:Dl:27:MET:HE3	2.02	0.42
2:Br:57:VAL:O	2:Br:61:VAL:HG23	2.19	0.42
2:Dr:88:VAL:HG12	2:Dr:92:LEU:HG	2.01	0.42
2:D2:88:VAL:HG12	2:D2:92:LEU:HG	2.02	0.42
2:D5:41:VAL:HB	2:D5:45:TYR:HB2	2.01	0.42
2:C6:70:ARG:HH11	2:C6:71:VAL:HG23	1.84	0.42
2:D6:41:VAL:HB	2:D6:45:TYR:HB2	2.01	0.42
2:C7:23:ALA:HB2	2:C7:68:CYS:HB3	2.01	0.42
2:C8:58:ASN:HD21	2:C8:62:ARG:NH2	2.17	0.42
2:CH:23:ALA:HB2	2:CH:68:CYS:HB3	2.02	0.42
2:CH:41:VAL:HB	2:CH:45:TYR:HB2	2.01	0.42
2:CM:23:ALA:HB2	2:CM:68:CYS:HB3	2.02	0.42
2:CR:23:ALA:HB2	2:CR:68:CYS:HB3	2.02	0.42
2:Dc:11:MET:HE3	2:Dc:79:HIS:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ad:7:GLU:O	1:Ad:46:PRO:HB3	2.20	0.42
2:Dj:13:GLU:OE2	2:Dj:47:THR:OG1	2.37	0.42
2:Cn:8:ALA:HB3	2:Cn:52:GLY:O	2.19	0.42
2:B2:31:ALA:HB3	2:B2:60:ALA:HB2	2.00	0.42
2:B2:57:VAL:O	2:B2:61:VAL:HG23	2.19	0.42
2:B5:58:ASN:O	2:B5:62:ARG:HG3	2.20	0.42
2:D5:31:ALA:HB3	2:D5:60:ALA:HB2	2.01	0.42
2:B7:31:ALA:HB3	2:B7:60:ALA:HB2	2.00	0.42
2:CC:23:ALA:HB2	2:CC:68:CYS:HB3	2.02	0.42
1:AH:36:GLN:HG2	1:A0:2:LYS:HE2	2.02	0.42
2:DM:77:ALA:HB2	2:Cw:72:GLY:HA2	2.02	0.42
1:AN:28:TRP:HZ3	1:AN:35:ARG:HE	1.66	0.42
2:BP:58:ASN:O	2:BP:62:ARG:HG3	2.20	0.42
2:DQ:28:THR:O	2:Db:83:ARG:NH2	2.53	0.42
2:CR:41:VAL:HB	2:CR:45:TYR:HB2	2.02	0.42
2:BZ:65:ALA:O	2:BZ:69:GLU:HG3	2.20	0.42
1:Aa:19:MET:HE1	1:Aa:24:LEU:HD21	2.02	0.42
1:Ag:70:ASP:N	1:Ag:70:ASP:OD2	2.52	0.42
2:Bg:25:ASP:OD1	2:Bg:29:LYS:HE3	2.20	0.42
2:Dg:41:VAL:HB	2:Dg:45:TYR:HB2	2.02	0.42
2:Ci:12:ILE:CD1	2:Ci:27:MET:HE3	2.42	0.42
2:Ci:23:ALA:HB2	2:Ci:68:CYS:HB3	2.01	0.42
2:Ci:57:VAL:O	2:Ci:61:VAL:HG23	2.20	0.42
2:Ck:12:ILE:CD1	2:Ck:27:MET:HE3	2.45	0.42
2:Cr:23:ALA:HB2	2:Cr:68:CYS:HB3	2.02	0.42
2:Bt:66:ASP:O	2:Bt:70:ARG:NH2	2.51	0.42
2:Bx:31:ALA:HB3	2:Bx:60:ALA:HB2	2.00	0.42
2:Cx:23:ALA:HB2	2:Cx:68:CYS:HB3	2.02	0.42
2:B0:65:ALA:O	2:B0:69:GLU:HG3	2.19	0.42
2:C2:23:ALA:HB2	2:C2:68:CYS:HB3	2.02	0.42
2:C3:23:ALA:HB2	2:C3:68:CYS:HB3	2.01	0.42
2:D7:8:ALA:HB3	2:D7:52:GLY:O	2.19	0.42
2:D7:88:VAL:HG12	2:D7:92:LEU:HG	2.00	0.42
2:B9:31:ALA:HB3	2:B9:60:ALA:HB2	2.00	0.42
2:BA:65:ALA:O	2:BA:69:GLU:HG3	2.19	0.42
2:CE:8:ALA:O	2:CE:51:ARG:HA	2.18	0.42
2:CM:41:VAL:HB	2:CM:45:TYR:HB2	2.02	0.42
2:DM:88:VAL:HG12	2:DM:92:LEU:HG	2.01	0.42
2:BR:57:VAL:O	2:BR:61:VAL:HG23	2.18	0.42
2:DT:13:GLU:OE2	2:DT:47:THR:OG1	2.38	0.42
2:Ba:58:ASN:O	2:Ba:62:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ab:22:LYS:HA	1:Ab:23:PRO:HD3	1.93	0.42
2:Dc:41:VAL:HB	2:Dc:45:TYR:HB2	2.02	0.42
2:Di:85:HIS:HE1	2:By:83:ARG:HH22	1.68	0.42
1:Ak:19:MET:HE1	1:Ak:24:LEU:HD21	2.01	0.42
2:Dl:88:VAL:HG12	2:Dl:92:LEU:HG	2.02	0.42
2:Cs:23:ALA:HB2	2:Cs:68:CYS:HB3	2.01	0.42
2:CA:12:ILE:CD1	2:CA:27:MET:HE3	2.45	0.42
2:BE:66:ASP:O	2:BE:70:ARG:NH2	2.51	0.42
2:BO:65:ALA:O	2:BO:69:GLU:HG3	2.20	0.42
2:BP:65:ALA:O	2:BP:69:GLU:HG3	2.19	0.42
2:DP:41:VAL:HB	2:DP:45:TYR:HB2	2.01	0.42
2:DQ:92:LEU:HD23	2:DQ:92:LEU:HA	1.89	0.42
2:BS:36:VAL:HG11	2:BS:51:ARG:HG3	2.02	0.42
2:BV:58:ASN:O	2:BV:62:ARG:HG3	2.20	0.42
1:AW:28:TRP:HZ3	1:AW:35:ARG:HE	1.67	0.42
2:DX:41:VAL:HB	2:DX:45:TYR:HB2	2.02	0.42
2:Cf:12:ILE:CD1	2:Cf:27:MET:HE3	2.45	0.42
2:Bg:73:ASP:OD2	2:Cg:45:TYR:OH	2.26	0.42
2:Cj:58:ASN:ND2	2:Cj:62:ARG:HH21	2.17	0.42
2:Bk:65:ALA:O	2:Bk:69:GLU:HG3	2.19	0.42
2:Bl:73:ASP:OD1	2:Cl:45:TYR:OH	2.26	0.42
2:Dl:41:VAL:HB	2:Dl:45:TYR:HB2	2.02	0.42
2:Bp:65:ALA:O	2:Bp:69:GLU:HG3	2.19	0.42
1:AN:37:VAL:HG21	1:Ae:51:LEU:HD21	2.02	0.42
2:CP:12:ILE:CD1	2:CP:27:MET:HE3	2.45	0.42
1:AS:19:MET:O	1:AS:67:TYR:OH	2.33	0.42
2:DV:13:GLU:OE2	2:DV:47:THR:OG1	2.38	0.42
2:DV:83:ARG:NH2	2:Dr:28:THR:O	2.53	0.42
2:BY:36:VAL:HG11	2:BY:51:ARG:HG3	2.02	0.42
2:Cd:57:VAL:O	2:Cd:61:VAL:HG23	2.20	0.42
2:Be:65:ALA:O	2:Be:69:GLU:HG3	2.20	0.42
2:Df:83:ARG:HH22	2:B7:85:HIS:HE1	1.67	0.42
2:Dk:83:ARG:HH22	2:Bx:85:HIS:HE1	1.67	0.42
2:Cs:57:VAL:O	2:Cs:61:VAL:HG23	2.20	0.42
2:Dw:88:VAL:HG12	2:Dw:92:LEU:HG	2.02	0.42
1:A3:1:MET:SD	1:A3:1:MET:N	2.85	0.42
2:C3:57:VAL:O	2:C3:61:VAL:HG23	2.20	0.42
2:B4:65:ALA:O	2:B4:69:GLU:HG3	2.20	0.42
2:B4:66:ASP:O	2:B4:70:ARG:NH2	2.52	0.42
2:D6:31:ALA:HB3	2:D6:60:ALA:HB2	2.00	0.42
2:DC:77:ALA:HB2	2:Cq:72:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Da:13:GLU:OE2	2:Da:47:THR:OG1	2.38	0.41
2:Bc:31:ALA:HB3	2:Bc:60:ALA:HB2	2.00	0.41
2:Dg:88:VAL:HG12	2:Dg:92:LEU:HG	2.02	0.41
2:Ch:41:VAL:HB	2:Ch:45:TYR:HB2	2.01	0.41
1:Ak:2:LYS:HE2	1:A7:36:GLN:HG2	2.01	0.41
2:Cm:41:VAL:HB	2:Cm:45:TYR:HB2	2.01	0.41
2:Br:31:ALA:HB3	2:Br:60:ALA:HB2	2.01	0.41
2:Cw:70:ARG:HH11	2:Cw:71:VAL:HG23	1.84	0.41
2:Dx:88:VAL:HG12	2:Dx:92:LEU:HG	2.01	0.41
2:Cy:23:ALA:HB2	2:Cy:68:CYS:HB3	2.01	0.41
1:AC:28:TRP:HZ3	1:AC:35:ARG:HE	1.68	0.41
2:BC:11:MET:HG2	2:BC:49:LEU:HG	2.02	0.41
2:BC:57:VAL:O	2:BC:61:VAL:HG23	2.19	0.41
2:BJ:65:ALA:O	2:BJ:69:GLU:HG3	2.20	0.41
2:BS:31:ALA:HB3	2:BS:60:ALA:HB2	2.02	0.41
2:DY:85:HIS:HE1	2:B3:83:ARG:HH22	1.68	0.41
2:Dh:88:VAL:HG12	2:Dh:92:LEU:HG	2.02	0.41
2:Cm:23:ALA:HB2	2:Cm:68:CYS:HB3	2.01	0.41
2:Bt:65:ALA:O	2:Bt:69:GLU:HG3	2.20	0.41
2:Dv:13:GLU:OE2	2:Dv:47:THR:OG1	2.38	0.41
2:D0:13:GLU:OE2	2:D0:47:THR:OG1	2.38	0.41
2:D3:15:ARG:HB2	2:D3:73:ASP:HB2	2.01	0.41
2:D5:13:GLU:OE2	2:D5:47:THR:OG1	2.38	0.41
2:CD:57:VAL:O	2:CD:61:VAL:HG23	2.20	0.41
2:BF:58:ASN:O	2:BF:62:ARG:HG3	2.20	0.41
1:Al:37:VAL:HG21	1:AZ:51:LEU:HD21	2.02	0.41
2:BJ:58:ASN:O	2:BJ:62:ARG:HG3	2.20	0.41
2:DJ:13:GLU:OE2	2:DJ:47:THR:OG1	2.37	0.41
2:BO:58:ASN:O	2:BO:62:ARG:HG3	2.20	0.41
2:CV:12:ILE:CD1	2:CV:27:MET:HE3	2.45	0.41
2:CX:12:ILE:HD12	2:CX:27:MET:CE	2.47	0.41
1:AY:37:VAL:HG21	1:A4:51:LEU:HD21	2.02	0.41
2:CY:57:VAL:O	2:CY:61:VAL:HG23	2.20	0.41
2:Ca:12:ILE:CD1	2:Ca:27:MET:HE3	2.45	0.41
2:Ch:12:ILE:CD1	2:Ch:27:MET:HE3	2.44	0.41
2:Dr:41:VAL:HB	2:Dr:45:TYR:HB2	2.02	0.41
2:C3:58:ASN:HD21	2:C3:62:ARG:NH2	2.17	0.41
2:DA:41:VAL:HB	2:DA:45:TYR:HB2	2.02	0.41
1:AD:19:MET:HE1	1:AD:24:LEU:HD21	2.02	0.41
2:CD:58:ASN:HD21	2:CD:62:ARG:NH2	2.18	0.41
2:DF:13:GLU:OE2	2:DF:47:THR:OG1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DF:83:ARG:NH2	2:Dh:28:THR:O	2.53	0.41
2:BH:11:MET:HG2	2:BH:49:LEU:HG	2.03	0.41
2:DH:41:VAL:HB	2:DH:45:TYR:HB2	2.02	0.41
2:DK:13:GLU:OE2	2:DK:47:THR:OG1	2.38	0.41
2:BQ:83:ARG:NH2	2:Db:85:HIS:HE1	2.19	0.41
2:CS:57:VAL:O	2:CS:61:VAL:HG23	2.20	0.41
2:CS:58:ASN:HD21	2:CS:62:ARG:NH2	2.17	0.41
2:BT:65:ALA:O	2:BT:69:GLU:HG3	2.20	0.41
2:BT:66:ASP:O	2:BT:70:ARG:NH2	2.51	0.41
2:CY:58:ASN:HD21	2:CY:62:ARG:NH2	2.17	0.41
2:DY:15:ARG:HB2	2:DY:73:ASP:HB2	2.01	0.41
2:Cd:23:ALA:HB2	2:Cd:68:CYS:HB3	2.02	0.41
2:Ch:23:ALA:HB2	2:Ch:68:CYS:HB3	2.02	0.41
2:Di:25:ASP:OD1	2:Di:29:LYS:HE3	2.20	0.41
1:Am:19:MET:HE2	1:Am:19:MET:HB3	1.91	0.41
2:Dp:13:GLU:OE2	2:Dp:47:THR:OG1	2.38	0.41
2:Cs:58:ASN:HD21	2:Cs:62:ARG:NH2	2.17	0.41
2:Bt:58:ASN:O	2:Bt:62:ARG:HG3	2.20	0.41
2:Bz:31:ALA:HB3	2:Bz:60:ALA:HB2	2.01	0.41
2:Cz:81:ILE:HG21	2:Cz:84:VAL:HG12	2.03	0.41
1:A0:22:LYS:HA	1:A0:23:PRO:HD3	1.95	0.41
1:A7:28:TRP:HZ3	1:A7:35:ARG:HE	1.69	0.41
2:C8:23:ALA:HB2	2:C8:68:CYS:HB3	2.01	0.41
2:BB:83:ARG:NH2	2:DW:85:HIS:HE1	2.19	0.41
1:AE:5:GLN:HG3	1:AE:48:ASP:O	2.21	0.41
1:AF:36:GLN:HG2	1:Ai:2:LYS:HE3	2.03	0.41
2:BK:58:ASN:O	2:BK:62:ARG:HG3	2.20	0.41
2:DM:41:VAL:HB	2:DM:45:TYR:HB2	2.02	0.41
2:CN:57:VAL:O	2:CN:61:VAL:HG23	2.20	0.41
2:DN:85:HIS:HE1	2:Bd:83:ARG:HH22	1.67	0.41
2:DO:11:MET:HG2	2:DO:49:LEU:HD23	2.03	0.41
2:BR:11:MET:HG2	2:BR:49:LEU:HG	2.03	0.41
2:CT:8:ALA:O	2:CT:51:ARG:HA	2.19	0.41
2:Cc:12:ILE:HD12	2:Cc:27:MET:CE	2.47	0.41
1:Ad:37:VAL:HG21	1:At:51:LEU:HD21	2.02	0.41
2:Bg:81:ILE:HG21	2:Bg:84:VAL:HG12	2.03	0.41
1:Ah:28:TRP:HZ3	1:Ah:35:ARG:HE	1.68	0.41
2:Bj:25:ASP:OD1	2:Bj:29:LYS:HE3	2.20	0.41
2:Dm:41:VAL:HB	2:Dm:45:TYR:HB2	2.02	0.41
2:Bv:31:ALA:HB3	2:Bv:60:ALA:HB2	2.02	0.41
2:Dv:35:LEU:HD11	2:Dv:48:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D0:41:VAL:HB	2:D0:45:TYR:HB2	2.01	0.41
2:D3:41:VAL:HB	2:D3:45:TYR:HB2	2.02	0.41
1:A4:1:MET:SD	1:A4:1:MET:N	2.79	0.41
2:BD:31:ALA:HB3	2:BD:60:ALA:HB2	2.03	0.41
2:BE:65:ALA:O	2:BE:69:GLU:HG3	2.20	0.41
2:BH:31:ALA:HB3	2:BH:60:ALA:HB2	2.01	0.41
2:CI:57:VAL:O	2:CI:61:VAL:HG23	2.20	0.41
2:DI:11:MET:HB3	2:C4:18:VAL:HG22	2.02	0.41
2:DI:77:ALA:HB2	2:C4:72:GLY:HA2	2.03	0.41
1:AT:5:GLN:HG3	1:AT:48:ASP:O	2.20	0.41
2:BX:11:MET:HG2	2:BX:49:LEU:HG	2.02	0.41
2:Bh:11:MET:HG2	2:Bh:49:LEU:HG	2.02	0.41
2:Dh:41:VAL:HB	2:Dh:45:TYR:HB2	2.03	0.41
2:Bk:58:ASN:O	2:Bk:62:ARG:HG3	2.20	0.41
2:Bl:81:ILE:HG21	2:Bl:84:VAL:HG12	2.03	0.41
2:Cm:12:ILE:CD1	2:Cm:27:MET:HE3	2.44	0.41
2:Bp:83:ARG:NH2	2:Dz:85:HIS:HE1	2.19	0.41
2:Cy:57:VAL:O	2:Cy:61:VAL:HG23	2.20	0.41
2:D2:41:VAL:HB	2:D2:45:TYR:HB2	2.02	0.41
2:B9:58:ASN:O	2:B9:62:ARG:HG3	2.20	0.41
2:DD:41:VAL:HB	2:DD:45:TYR:HB2	2.03	0.41
2:CG:72:GLY:HA2	2:Dh:77:ALA:HB2	2.02	0.41
2:DN:77:ALA:HB2	2:Ct:72:GLY:HA2	2.03	0.41
2:BV:65:ALA:O	2:BV:69:GLU:HG3	2.19	0.41
2:BX:31:ALA:HB3	2:BX:60:ALA:HB2	2.01	0.41
2:Bj:58:ASN:O	2:Bj:62:ARG:HG3	2.21	0.41
2:Dl:92:LEU:HD23	2:Dl:92:LEU:HA	1.89	0.41
1:An:37:VAL:HG21	1:A9:51:LEU:HD21	2.02	0.41
2:Bz:65:ALA:O	2:Bz:69:GLU:HG3	2.20	0.41
2:B9:65:ALA:O	2:B9:69:GLU:HG3	2.20	0.41
1:AE:51:LEU:HD21	1:Ay:37:VAL:HG21	2.02	0.41
1:AK:36:GLN:HG2	1:An:2:LYS:HE3	2.02	0.41
2:BM:31:ALA:HB3	2:BM:60:ALA:HB2	2.01	0.41
2:DR:77:ALA:HB2	2:C1:72:GLY:HA2	2.02	0.41
1:AT:51:LEU:HD21	1:A8:37:VAL:HG21	2.02	0.41
2:DV:45:TYR:OH	2:Ca:73:ASP:OD2	2.27	0.41
2:Ba:65:ALA:O	2:Ba:69:GLU:HG3	2.19	0.41
1:Ab:21:HIS:ND1	2:Bb:62:ARG:HB3	2.36	0.41
2:Bb:83:ARG:NH2	2:D1:85:HIS:HE1	2.19	0.41
2:Cc:23:ALA:HB2	2:Cc:68:CYS:HB3	2.01	0.41
1:Ah:19:MET:HE2	1:Ah:19:MET:HB3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bi:31:ALA:HB3	2:Bi:60:ALA:HB2	2.02	0.41
1:Aj:5:GLN:HG3	1:Aj:48:ASP:O	2.20	0.41
2:Cj:12:ILE:HD12	2:Cj:27:MET:HE3	2.03	0.41
1:Ao:5:GLN:HG3	1:Ao:48:ASP:O	2.20	0.41
2:Co:12:ILE:HD12	2:Co:27:MET:HE3	2.03	0.41
2:Dp:41:VAL:HB	2:Dp:45:TYR:HB2	2.02	0.41
2:Cq:23:ALA:HB2	2:Cq:68:CYS:HB3	2.03	0.41
1:At:5:GLN:HG3	1:At:48:ASP:O	2.20	0.41
1:Ax:28:TRP:HZ3	1:Ax:35:ARG:HE	1.69	0.41
2:Bz:58:ASN:O	2:Bz:62:ARG:HG3	2.21	0.41
2:D5:35:LEU:HD11	2:D5:48:VAL:CG1	2.51	0.41
2:C9:12:ILE:HD12	2:C9:27:MET:HE3	2.03	0.41
1:AD:37:VAL:HG21	1:Aj:51:LEU:HD21	2.02	0.41
2:BE:58:ASN:O	2:BE:62:ARG:HG3	2.20	0.41
1:AF:22:LYS:HA	1:AF:23:PRO:HD3	1.95	0.41
1:AF:37:VAL:HG21	1:AI:51:LEU:HD21	2.03	0.41
1:AI:22:LYS:HA	1:AI:23:PRO:HD3	1.96	0.41
2:BI:36:VAL:HG11	2:BI:51:ARG:HG3	2.02	0.41
2:DI:41:VAL:HB	2:DI:45:TYR:HB2	2.03	0.41
1:AK:37:VAL:HG21	1:An:51:LEU:HD21	2.03	0.41
2:DK:88:VAL:HG12	2:DK:92:LEU:HG	2.03	0.41
1:AO:22:LYS:HA	1:AO:23:PRO:HD3	1.94	0.41
2:CQ:57:VAL:O	2:CQ:61:VAL:HG23	2.20	0.41
2:BT:58:ASN:O	2:BT:62:ARG:HG3	2.20	0.41
2:CV:73:ASP:OD2	2:Da:45:TYR:OH	2.27	0.41
1:AW:22:LYS:HA	1:AW:23:PRO:HD3	1.93	0.41
2:CX:23:ALA:HB2	2:CX:68:CYS:HB3	2.02	0.41
2:CY:12:ILE:CD1	2:CY:27:MET:HE3	2.42	0.41
1:Ab:19:MET:HE2	1:Ab:19:MET:HB3	1.89	0.41
2:Cb:72:GLY:HA2	2:D2:77:ALA:HB2	2.02	0.41
2:Db:88:VAL:HG12	2:Db:92:LEU:HG	2.03	0.41
2:Be:58:ASN:O	2:Be:62:ARG:HG3	2.20	0.41
2:Ce:72:GLY:HA2	2:Ds:77:ALA:HB2	2.03	0.41
2:Df:35:LEU:HD11	2:Df:48:VAL:CG1	2.51	0.41
2:Df:88:VAL:HG12	2:Df:92:LEU:HG	2.03	0.41
2:Bg:25:ASP:O	2:Bg:29:LYS:HG3	2.20	0.41
2:Dg:92:LEU:HD23	2:Dg:92:LEU:HA	1.90	0.41
2:Di:15:ARG:HB2	2:Di:73:ASP:HB2	2.01	0.41
2:Bj:65:ALA:O	2:Bj:69:GLU:HG3	2.20	0.41
2:Dk:35:LEU:HD11	2:Dk:48:VAL:CG1	2.51	0.41
2:Bo:58:ASN:O	2:Bo:62:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Co:81:ILE:HG21	2:Co:84:VAL:HG12	2.03	0.41
1:Ap:22:LYS:HA	1:Ap:23:PRO:HD3	1.95	0.41
2:Bp:31:ALA:HB3	2:Bp:60:ALA:HB2	2.03	0.41
1:Ar:19:MET:HE2	1:Ar:19:MET:HB3	1.90	0.41
2:Br:11:MET:HG2	2:Br:49:LEU:HG	2.02	0.41
1:Aw:15:ARG:NH2	1:Aw:20:GLY:O	2.54	0.41
2:Cy:23:ALA:O	2:Cy:27:MET:HG3	2.21	0.41
2:Dy:35:LEU:HD12	2:Dy:35:LEU:HA	1.91	0.41
1:A6:15:ARG:NH2	1:A6:20:GLY:O	2.54	0.41
2:C7:41:VAL:HB	2:C7:45:TYR:HB2	2.01	0.41
2:C8:57:VAL:O	2:C8:61:VAL:HG23	2.20	0.41
2:CB:31:ALA:HB3	2:CB:60:ALA:HB2	2.02	0.41
2:DB:85:HIS:HE1	2:Bq:83:ARG:NH2	2.19	0.41
1:AP:7:GLU:O	1:AP:46:PRO:HB3	2.21	0.41
2:DR:41:VAL:HB	2:DR:45:TYR:HB2	2.03	0.41
1:AS:37:VAL:HG21	1:Ao:51:LEU:HD21	2.02	0.41
2:CV:18:VAL:HG22	2:Da:11:MET:HB3	2.03	0.41
1:AX:28:TRP:HZ3	1:AX:35:ARG:HE	1.68	0.41
1:Ai:37:VAL:HG21	1:Az:51:LEU:HD21	2.02	0.41
2:Cl:72:GLY:HA2	2:Dx:77:ALA:HB2	2.04	0.41
2:Bn:31:ALA:HB3	2:Bn:60:ALA:HB2	2.02	0.41
2:Cq:57:VAL:O	2:Cq:61:VAL:HG23	2.21	0.41
2:Ct:81:ILE:HG21	2:Ct:84:VAL:HG12	2.03	0.41
2:Cx:41:VAL:HB	2:Cx:45:TYR:HB2	2.02	0.41
1:A4:5:GLN:HG3	1:A4:48:ASP:O	2.21	0.41
2:B4:58:ASN:O	2:B4:62:ARG:HG3	2.21	0.41
2:C4:81:ILE:HG21	2:C4:84:VAL:HG12	2.03	0.41
2:D4:11:MET:HG2	2:D4:49:LEU:HD23	2.03	0.41
2:D6:88:VAL:HG12	2:D6:92:LEU:HG	2.03	0.41
1:AB:28:TRP:HZ3	1:AB:35:ARG:HE	1.69	0.40
2:DC:41:VAL:HB	2:DC:45:TYR:HB2	2.03	0.40
2:BD:81:ILE:HG21	2:BD:84:VAL:HG12	2.03	0.40
2:DG:85:HIS:HE1	2:B6:83:ARG:NH2	2.19	0.40
1:AJ:51:LEU:HD21	1:A3:37:VAL:HG21	2.02	0.40
2:DN:41:VAL:HB	2:DN:45:TYR:HB2	2.03	0.40
2:DP:13:GLU:OE2	2:DP:47:THR:OG1	2.38	0.40
2:DQ:85:HIS:HE1	2:B1:83:ARG:NH2	2.19	0.40
2:DV:11:MET:HB3	2:Ca:18:VAL:HG22	2.03	0.40
2:Dh:8:ALA:HB3	2:Dh:52:GLY:O	2.21	0.40
2:Cj:72:GLY:HA2	2:Dy:77:ALA:HB2	2.03	0.40
2:Dk:88:VAL:HG12	2:Dk:92:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bn:81:ILE:HG21	2:Bn:84:VAL:HG12	2.03	0.40
2:Bp:58:ASN:O	2:Bp:62:ARG:HG3	2.20	0.40
2:Dx:8:ALA:HB3	2:Dx:52:GLY:O	2.21	0.40
2:By:31:ALA:HB3	2:By:60:ALA:HB2	2.03	0.40
2:C2:87:GLU:O	2:C2:90:ASN:ND2	2.54	0.40
1:A8:2:LYS:HA	1:A8:2:LYS:HD3	1.89	0.40
2:DA:83:ARG:NH2	2:DX:28:THR:O	2.54	0.40
2:DB:88:VAL:HG12	2:DB:92:LEU:HG	2.03	0.40
1:AJ:22:LYS:HA	1:AJ:23:PRO:HD3	1.94	0.40
2:DJ:41:VAL:HB	2:DJ:45:TYR:HB2	2.04	0.40
2:CL:72:GLY:HA2	2:Dm:77:ALA:HB2	2.02	0.40
1:AO:5:GLN:HG3	1:AO:48:ASP:O	2.20	0.40
2:DO:11:MET:HG2	2:DO:49:LEU:CD2	2.52	0.40
2:BQ:66:ASP:O	2:BQ:70:ARG:NH2	2.54	0.40
1:AV:37:VAL:HG21	1:As:51:LEU:HD21	2.04	0.40
2:CZ:81:ILE:HG21	2:CZ:84:VAL:HG12	2.03	0.40
1:Ab:2:LYS:HD3	1:Ab:2:LYS:HA	1.91	0.40
2:Cg:72:GLY:HA2	2:D7:77:ALA:HB2	2.04	0.40
1:Ak:77:ILE:HG12	1:A7:10:LEU:HD21	2.04	0.40
2:Bl:66:ASP:O	2:Bl:70:ARG:NH2	2.54	0.40
2:Ds:41:VAL:HB	2:Ds:45:TYR:HB2	2.03	0.40
2:Bw:58:ASN:O	2:Bw:62:ARG:HG3	2.22	0.40
2:C2:41:VAL:HB	2:C2:45:TYR:HB2	2.01	0.40
2:B3:73:ASP:OD1	2:C3:45:TYR:OH	2.21	0.40
2:B8:31:ALA:HB3	2:B8:60:ALA:HB2	2.03	0.40
2:B8:36:VAL:HG11	2:B8:51:ARG:HG3	2.02	0.40
2:DA:13:GLU:OE2	2:DA:47:THR:OG1	2.38	0.40
2:BB:81:ILE:HG21	2:BB:84:VAL:HG12	2.03	0.40
2:BG:83:ARG:NH2	2:Dg:85:HIS:HE1	2.19	0.40
2:CO:81:ILE:HG21	2:CO:84:VAL:HG12	2.03	0.40
2:DQ:88:VAL:HG12	2:DQ:92:LEU:HG	2.03	0.40
2:DS:41:VAL:HB	2:DS:45:TYR:HB2	2.03	0.40
2:CT:72:GLY:HA2	2:Dn:77:ALA:HB2	2.03	0.40
2:BW:81:ILE:HG21	2:BW:84:VAL:HG12	2.03	0.40
2:Ba:31:ALA:HB3	2:Ba:60:ALA:HB2	2.03	0.40
2:Ce:81:ILE:HG21	2:Ce:84:VAL:HG12	2.03	0.40
2:Bg:83:ARG:NH2	2:D6:85:HIS:HE1	2.19	0.40
2:Co:72:GLY:HA2	2:D8:77:ALA:HB2	2.03	0.40
2:Cr:41:VAL:HB	2:Cr:45:TYR:HB2	2.02	0.40
2:Dz:41:VAL:HB	2:Dz:45:TYR:HB2	2.04	0.40
2:B0:58:ASN:O	2:B0:62:ARG:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D5:35:LEU:HD12	2:D5:35:LEU:HA	1.90	0.40
2:B7:11:MET:HG2	2:B7:49:LEU:HG	2.02	0.40
2:D9:41:VAL:HB	2:D9:45:TYR:HB2	2.04	0.40
2:DA:83:ARG:HH22	2:BX:85:HIS:HE1	1.70	0.40
1:AL:15:ARG:NH2	1:AL:20:GLY:O	2.54	0.40
2:DP:54:THR:O	2:DP:58:ASN:OD1	2.40	0.40
1:AS:2:LYS:HD3	1:AS:2:LYS:HA	1.89	0.40
2:DW:12:ILE:HD12	2:DW:27:MET:HE3	2.02	0.40
1:Ad:2:LYS:HD2	1:Ad:29:GLU:OE2	2.20	0.40
1:Ae:5:GLN:HG3	1:Ae:48:ASP:O	2.21	0.40
2:Bl:83:ARG:NH2	2:Dw:85:HIS:HE1	2.19	0.40
2:Bo:65:ALA:O	2:Bo:69:GLU:HG3	2.20	0.40
2:Co:18:VAL:HG22	2:D8:11:MET:HB3	2.02	0.40
2:Dq:88:VAL:HG12	2:Dq:92:LEU:HG	2.03	0.40
2:Dx:41:VAL:HB	2:Dx:45:TYR:HB2	2.02	0.40
2:Cy:12:ILE:CD1	2:Cy:27:MET:HE3	2.41	0.40
2:B1:58:ASN:O	2:B1:62:ARG:HG3	2.22	0.40
1:A2:19:MET:HE2	1:A2:19:MET:HB3	1.90	0.40
2:CD:23:ALA:O	2:CD:27:MET:HG3	2.21	0.40
1:AJ:5:GLN:HG3	1:AJ:48:ASP:O	2.21	0.40
2:DL:85:HIS:HE1	2:Bw:83:ARG:NH2	2.19	0.40
2:BN:31:ALA:HB3	2:BN:60:ALA:HB2	2.02	0.40
2:CW:57:VAL:O	2:CW:61:VAL:HG23	2.21	0.40
2:DZ:41:VAL:HB	2:DZ:45:TYR:HB2	2.04	0.40
2:Bc:11:MET:HG2	2:Bc:49:LEU:HG	2.03	0.40
1:Af:37:VAL:HG21	1:A8:51:LEU:HD21	2.03	0.40
2:Bg:58:ASN:O	2:Bg:62:ARG:HG3	2.22	0.40
2:Bl:58:ASN:O	2:Bl:62:ARG:HG3	2.22	0.40
2:Do:41:VAL:HB	2:Do:45:TYR:HB2	2.04	0.40
1:Aq:19:MET:HE2	1:Aq:19:MET:HB3	1.88	0.40
2:Bx:11:MET:HG2	2:Bx:49:LEU:HG	2.02	0.40
2:C1:58:ASN:HD21	2:C1:62:ARG:NH2	2.20	0.40
2:D1:88:VAL:HG12	2:D1:92:LEU:HG	2.03	0.40
2:B3:31:ALA:HB3	2:B3:60:ALA:HB2	2.02	0.40
2:B5:83:ARG:HH11	2:B5:83:ARG:HD2	1.78	0.40
2:B6:66:ASP:O	2:B6:70:ARG:NH2	2.54	0.40
2:C8:12:ILE:CD1	2:C8:27:MET:HE3	2.42	0.40
1:A9:5:GLN:HG3	1:A9:48:ASP:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	A1	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	A2	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	A3	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	A4	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	A5	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	A6	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	A7	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	A8	78/94 (83%)	74 (95%)	4 (5%)	0	100	100
1	A9	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	AA	78/94 (83%)	74 (95%)	4 (5%)	0	100	100
1	AB	78/94 (83%)	74 (95%)	4 (5%)	0	100	100
1	AC	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	AD	78/94 (83%)	74 (95%)	4 (5%)	0	100	100
1	AE	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	AF	78/94 (83%)	75 (96%)	3 (4%)	0	100	100
1	AG	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	AH	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	AI	78/94 (83%)	74 (95%)	4 (5%)	0	100	100
1	AJ	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	AK	78/94 (83%)	75 (96%)	3 (4%)	0	100	100
1	AL	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	AM	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	AN	78/94 (83%)	74 (95%)	4 (5%)	0	100	100
1	AO	78/94 (83%)	73 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AP	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	AQ	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	AR	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	AS	78/94 (83%)	74 (95%)	4 (5%)	0	100	100
1	AT	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	AV	78/94 (83%)	75 (96%)	3 (4%)	0	100	100
1	AW	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	AX	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	AY	78/94 (83%)	74 (95%)	4 (5%)	0	100	100
1	AZ	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Aa	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Ab	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Ac	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Ad	78/94 (83%)	74 (95%)	4 (5%)	0	100	100
1	Ae	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Af	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Ag	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Ah	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Ai	78/94 (83%)	74 (95%)	4 (5%)	0	100	100
1	Aj	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Ak	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Al	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Am	78/94 (83%)	74 (95%)	4 (5%)	0	100	100
1	An	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Ao	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Ap	78/94 (83%)	74 (95%)	4 (5%)	0	100	100
1	Aq	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Ar	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	As	78/94 (83%)	74 (95%)	4 (5%)	0	100	100
1	At	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Av	78/94 (83%)	74 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aw	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Ax	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
1	Ay	78/94 (83%)	74 (95%)	4 (5%)	0	100	100
1	Az	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
2	B0	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	B1	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	B2	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	B3	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	B4	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	B5	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	B6	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	B7	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	B8	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	B9	87/98 (89%)	87 (100%)	0	0	100	100
2	BA	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BB	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BC	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BD	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BE	87/98 (89%)	87 (100%)	0	0	100	100
2	BF	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BG	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BH	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BI	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BJ	87/98 (89%)	87 (100%)	0	0	100	100
2	BK	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BL	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BM	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BN	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BO	87/98 (89%)	87 (100%)	0	0	100	100
2	BP	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BQ	87/98 (89%)	86 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BR	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BS	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BT	87/98 (89%)	87 (100%)	0	0	100	100
2	BV	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BW	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BX	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BY	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	BZ	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Ba	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bb	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bc	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bd	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Be	87/98 (89%)	87 (100%)	0	0	100	100
2	Bf	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bg	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bh	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bi	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bj	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bk	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bl	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bm	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bn	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bo	87/98 (89%)	87 (100%)	0	0	100	100
2	Bp	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bq	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Br	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bs	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bt	87/98 (89%)	87 (100%)	0	0	100	100
2	Bv	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bw	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bx	87/98 (89%)	86 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	By	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Bz	87/98 (89%)	87 (100%)	0	0	100	100
2	C0	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	C1	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	C2	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	C3	87/98 (89%)	87 (100%)	0	0	100	100
2	C4	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	C5	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	C6	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	C7	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	C8	87/98 (89%)	87 (100%)	0	0	100	100
2	C9	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CA	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CB	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CC	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CD	87/98 (89%)	87 (100%)	0	0	100	100
2	CE	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CF	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CG	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CH	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CI	87/98 (89%)	87 (100%)	0	0	100	100
2	CJ	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CK	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CL	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CM	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CN	87/98 (89%)	87 (100%)	0	0	100	100
2	CO	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CP	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CQ	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CR	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CS	87/98 (89%)	87 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CT	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CV	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CW	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CX	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	CY	87/98 (89%)	87 (100%)	0	0	100	100
2	CZ	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Ca	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cb	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cc	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cd	87/98 (89%)	87 (100%)	0	0	100	100
2	Ce	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cf	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cg	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Ch	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Ci	87/98 (89%)	87 (100%)	0	0	100	100
2	Cj	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Ck	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cl	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cm	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cn	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Co	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cp	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cq	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cr	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cs	87/98 (89%)	87 (100%)	0	0	100	100
2	Ct	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cv	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cw	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cx	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cy	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Cz	87/98 (89%)	86 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D0	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	D1	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	D2	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	D3	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	D4	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	D5	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	D6	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	D7	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	D8	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	D9	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DA	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DB	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DC	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DD	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DE	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DF	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DG	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DH	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DI	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DJ	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DK	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DL	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DM	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DN	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DO	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DP	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DQ	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DR	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DS	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DT	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DV	87/98 (89%)	86 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	DW	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DX	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DY	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	DZ	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Da	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Db	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dc	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dd	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	De	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Df	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dg	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dh	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Di	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dj	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dk	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dl	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dm	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dn	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Do	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dp	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dq	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dr	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Ds	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dt	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dv	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dw	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dx	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dy	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
2	Dz	87/98 (89%)	86 (99%)	1 (1%)	0	100	100
All	All	20340/23280 (87%)	19900 (98%)	440 (2%)	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	65/77 (84%)	65 (100%)	0	100	100
1	A1	65/77 (84%)	65 (100%)	0	100	100
1	A2	65/77 (84%)	65 (100%)	0	100	100
1	A3	65/77 (84%)	65 (100%)	0	100	100
1	A4	65/77 (84%)	65 (100%)	0	100	100
1	A5	65/77 (84%)	65 (100%)	0	100	100
1	A6	65/77 (84%)	65 (100%)	0	100	100
1	A7	65/77 (84%)	65 (100%)	0	100	100
1	A8	65/77 (84%)	65 (100%)	0	100	100
1	A9	65/77 (84%)	65 (100%)	0	100	100
1	AA	65/77 (84%)	65 (100%)	0	100	100
1	AB	65/77 (84%)	65 (100%)	0	100	100
1	AC	65/77 (84%)	65 (100%)	0	100	100
1	AD	65/77 (84%)	65 (100%)	0	100	100
1	AE	65/77 (84%)	65 (100%)	0	100	100
1	AF	65/77 (84%)	65 (100%)	0	100	100
1	AG	65/77 (84%)	65 (100%)	0	100	100
1	AH	65/77 (84%)	65 (100%)	0	100	100
1	AI	65/77 (84%)	65 (100%)	0	100	100
1	AJ	65/77 (84%)	65 (100%)	0	100	100
1	AK	65/77 (84%)	65 (100%)	0	100	100
1	AL	65/77 (84%)	65 (100%)	0	100	100
1	AM	65/77 (84%)	65 (100%)	0	100	100
1	AN	65/77 (84%)	65 (100%)	0	100	100
1	AO	65/77 (84%)	65 (100%)	0	100	100
1	AP	65/77 (84%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AQ	65/77 (84%)	65 (100%)	0	100	100
1	AR	65/77 (84%)	65 (100%)	0	100	100
1	AS	65/77 (84%)	65 (100%)	0	100	100
1	AT	65/77 (84%)	65 (100%)	0	100	100
1	AV	65/77 (84%)	65 (100%)	0	100	100
1	AW	65/77 (84%)	65 (100%)	0	100	100
1	AX	65/77 (84%)	65 (100%)	0	100	100
1	AY	65/77 (84%)	65 (100%)	0	100	100
1	AZ	65/77 (84%)	65 (100%)	0	100	100
1	Aa	65/77 (84%)	65 (100%)	0	100	100
1	Ab	65/77 (84%)	65 (100%)	0	100	100
1	Ac	65/77 (84%)	65 (100%)	0	100	100
1	Ad	65/77 (84%)	65 (100%)	0	100	100
1	Ae	65/77 (84%)	65 (100%)	0	100	100
1	Af	65/77 (84%)	65 (100%)	0	100	100
1	Ag	65/77 (84%)	65 (100%)	0	100	100
1	Ah	65/77 (84%)	65 (100%)	0	100	100
1	Ai	65/77 (84%)	65 (100%)	0	100	100
1	Aj	65/77 (84%)	65 (100%)	0	100	100
1	Ak	65/77 (84%)	65 (100%)	0	100	100
1	Al	65/77 (84%)	65 (100%)	0	100	100
1	Am	65/77 (84%)	65 (100%)	0	100	100
1	An	65/77 (84%)	65 (100%)	0	100	100
1	Ao	65/77 (84%)	65 (100%)	0	100	100
1	Ap	65/77 (84%)	65 (100%)	0	100	100
1	Aq	65/77 (84%)	65 (100%)	0	100	100
1	Ar	65/77 (84%)	65 (100%)	0	100	100
1	As	65/77 (84%)	65 (100%)	0	100	100
1	At	65/77 (84%)	65 (100%)	0	100	100
1	Av	65/77 (84%)	65 (100%)	0	100	100
1	Aw	65/77 (84%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ax	65/77 (84%)	65 (100%)	0	100	100
1	Ay	65/77 (84%)	65 (100%)	0	100	100
1	Az	65/77 (84%)	65 (100%)	0	100	100
2	B0	61/67 (91%)	61 (100%)	0	100	100
2	B1	61/67 (91%)	61 (100%)	0	100	100
2	B2	61/67 (91%)	61 (100%)	0	100	100
2	B3	61/67 (91%)	61 (100%)	0	100	100
2	B4	61/67 (91%)	61 (100%)	0	100	100
2	B5	61/67 (91%)	61 (100%)	0	100	100
2	B6	61/67 (91%)	61 (100%)	0	100	100
2	B7	61/67 (91%)	61 (100%)	0	100	100
2	B8	61/67 (91%)	61 (100%)	0	100	100
2	B9	61/67 (91%)	61 (100%)	0	100	100
2	BA	61/67 (91%)	61 (100%)	0	100	100
2	BB	61/67 (91%)	61 (100%)	0	100	100
2	BC	61/67 (91%)	61 (100%)	0	100	100
2	BD	61/67 (91%)	61 (100%)	0	100	100
2	BE	61/67 (91%)	61 (100%)	0	100	100
2	BF	61/67 (91%)	61 (100%)	0	100	100
2	BG	61/67 (91%)	61 (100%)	0	100	100
2	BH	61/67 (91%)	61 (100%)	0	100	100
2	BI	61/67 (91%)	61 (100%)	0	100	100
2	BJ	61/67 (91%)	61 (100%)	0	100	100
2	BK	61/67 (91%)	61 (100%)	0	100	100
2	BL	61/67 (91%)	61 (100%)	0	100	100
2	BM	61/67 (91%)	61 (100%)	0	100	100
2	BN	61/67 (91%)	61 (100%)	0	100	100
2	BO	61/67 (91%)	61 (100%)	0	100	100
2	BP	61/67 (91%)	61 (100%)	0	100	100
2	BQ	61/67 (91%)	61 (100%)	0	100	100
2	BR	61/67 (91%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BS	61/67 (91%)	61 (100%)	0	100	100
2	BT	61/67 (91%)	61 (100%)	0	100	100
2	BV	61/67 (91%)	61 (100%)	0	100	100
2	BW	61/67 (91%)	61 (100%)	0	100	100
2	BX	61/67 (91%)	61 (100%)	0	100	100
2	BY	61/67 (91%)	61 (100%)	0	100	100
2	BZ	61/67 (91%)	61 (100%)	0	100	100
2	Ba	61/67 (91%)	61 (100%)	0	100	100
2	Bb	61/67 (91%)	61 (100%)	0	100	100
2	Bc	61/67 (91%)	61 (100%)	0	100	100
2	Bd	61/67 (91%)	61 (100%)	0	100	100
2	Be	61/67 (91%)	61 (100%)	0	100	100
2	Bf	61/67 (91%)	61 (100%)	0	100	100
2	Bg	61/67 (91%)	61 (100%)	0	100	100
2	Bh	61/67 (91%)	61 (100%)	0	100	100
2	Bi	61/67 (91%)	61 (100%)	0	100	100
2	Bj	61/67 (91%)	61 (100%)	0	100	100
2	Bk	61/67 (91%)	61 (100%)	0	100	100
2	Bl	61/67 (91%)	61 (100%)	0	100	100
2	Bm	61/67 (91%)	61 (100%)	0	100	100
2	Bn	61/67 (91%)	61 (100%)	0	100	100
2	Bo	61/67 (91%)	61 (100%)	0	100	100
2	Bp	61/67 (91%)	61 (100%)	0	100	100
2	Bq	61/67 (91%)	61 (100%)	0	100	100
2	Br	61/67 (91%)	61 (100%)	0	100	100
2	Bs	61/67 (91%)	61 (100%)	0	100	100
2	Bt	61/67 (91%)	61 (100%)	0	100	100
2	Bv	61/67 (91%)	61 (100%)	0	100	100
2	Bw	61/67 (91%)	61 (100%)	0	100	100
2	Bx	61/67 (91%)	61 (100%)	0	100	100
2	By	61/67 (91%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Bz	61/67 (91%)	61 (100%)	0	100	100
2	C0	61/67 (91%)	61 (100%)	0	100	100
2	C1	61/67 (91%)	61 (100%)	0	100	100
2	C2	61/67 (91%)	61 (100%)	0	100	100
2	C3	61/67 (91%)	61 (100%)	0	100	100
2	C4	61/67 (91%)	61 (100%)	0	100	100
2	C5	61/67 (91%)	61 (100%)	0	100	100
2	C6	61/67 (91%)	61 (100%)	0	100	100
2	C7	61/67 (91%)	61 (100%)	0	100	100
2	C8	61/67 (91%)	61 (100%)	0	100	100
2	C9	61/67 (91%)	61 (100%)	0	100	100
2	CA	61/67 (91%)	61 (100%)	0	100	100
2	CB	61/67 (91%)	61 (100%)	0	100	100
2	CC	61/67 (91%)	61 (100%)	0	100	100
2	CD	61/67 (91%)	61 (100%)	0	100	100
2	CE	61/67 (91%)	61 (100%)	0	100	100
2	CF	61/67 (91%)	61 (100%)	0	100	100
2	CG	61/67 (91%)	61 (100%)	0	100	100
2	CH	61/67 (91%)	61 (100%)	0	100	100
2	CI	61/67 (91%)	61 (100%)	0	100	100
2	CJ	61/67 (91%)	61 (100%)	0	100	100
2	CK	61/67 (91%)	61 (100%)	0	100	100
2	CL	61/67 (91%)	61 (100%)	0	100	100
2	CM	61/67 (91%)	61 (100%)	0	100	100
2	CN	61/67 (91%)	61 (100%)	0	100	100
2	CO	61/67 (91%)	61 (100%)	0	100	100
2	CP	61/67 (91%)	61 (100%)	0	100	100
2	CQ	61/67 (91%)	61 (100%)	0	100	100
2	CR	61/67 (91%)	61 (100%)	0	100	100
2	CS	61/67 (91%)	61 (100%)	0	100	100
2	CT	61/67 (91%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	CV	61/67 (91%)	61 (100%)	0	100	100
2	CW	61/67 (91%)	61 (100%)	0	100	100
2	CX	61/67 (91%)	61 (100%)	0	100	100
2	CY	61/67 (91%)	61 (100%)	0	100	100
2	CZ	61/67 (91%)	61 (100%)	0	100	100
2	Ca	61/67 (91%)	61 (100%)	0	100	100
2	Cb	61/67 (91%)	61 (100%)	0	100	100
2	Cc	61/67 (91%)	61 (100%)	0	100	100
2	Cd	61/67 (91%)	61 (100%)	0	100	100
2	Ce	61/67 (91%)	61 (100%)	0	100	100
2	Cf	61/67 (91%)	61 (100%)	0	100	100
2	Cg	61/67 (91%)	61 (100%)	0	100	100
2	Ch	61/67 (91%)	61 (100%)	0	100	100
2	Ci	61/67 (91%)	61 (100%)	0	100	100
2	Cj	61/67 (91%)	61 (100%)	0	100	100
2	Ck	61/67 (91%)	61 (100%)	0	100	100
2	Cl	61/67 (91%)	61 (100%)	0	100	100
2	Cm	61/67 (91%)	61 (100%)	0	100	100
2	Cn	61/67 (91%)	61 (100%)	0	100	100
2	Co	61/67 (91%)	61 (100%)	0	100	100
2	Cp	61/67 (91%)	61 (100%)	0	100	100
2	Cq	61/67 (91%)	61 (100%)	0	100	100
2	Cr	61/67 (91%)	61 (100%)	0	100	100
2	Cs	61/67 (91%)	61 (100%)	0	100	100
2	Ct	61/67 (91%)	61 (100%)	0	100	100
2	Cv	61/67 (91%)	61 (100%)	0	100	100
2	Cw	61/67 (91%)	61 (100%)	0	100	100
2	Cx	61/67 (91%)	61 (100%)	0	100	100
2	Cy	61/67 (91%)	61 (100%)	0	100	100
2	Cz	61/67 (91%)	61 (100%)	0	100	100
2	D0	61/67 (91%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D1	61/67 (91%)	61 (100%)	0	100	100
2	D2	61/67 (91%)	61 (100%)	0	100	100
2	D3	61/67 (91%)	61 (100%)	0	100	100
2	D4	61/67 (91%)	61 (100%)	0	100	100
2	D5	61/67 (91%)	61 (100%)	0	100	100
2	D6	61/67 (91%)	61 (100%)	0	100	100
2	D7	61/67 (91%)	61 (100%)	0	100	100
2	D8	61/67 (91%)	61 (100%)	0	100	100
2	D9	61/67 (91%)	61 (100%)	0	100	100
2	DA	61/67 (91%)	61 (100%)	0	100	100
2	DB	61/67 (91%)	61 (100%)	0	100	100
2	DC	61/67 (91%)	61 (100%)	0	100	100
2	DD	61/67 (91%)	61 (100%)	0	100	100
2	DE	61/67 (91%)	61 (100%)	0	100	100
2	DF	61/67 (91%)	61 (100%)	0	100	100
2	DG	61/67 (91%)	61 (100%)	0	100	100
2	DH	61/67 (91%)	61 (100%)	0	100	100
2	DI	61/67 (91%)	61 (100%)	0	100	100
2	DJ	61/67 (91%)	61 (100%)	0	100	100
2	DK	61/67 (91%)	61 (100%)	0	100	100
2	DL	61/67 (91%)	61 (100%)	0	100	100
2	DM	61/67 (91%)	61 (100%)	0	100	100
2	DN	61/67 (91%)	61 (100%)	0	100	100
2	DO	61/67 (91%)	61 (100%)	0	100	100
2	DP	61/67 (91%)	61 (100%)	0	100	100
2	DQ	61/67 (91%)	61 (100%)	0	100	100
2	DR	61/67 (91%)	61 (100%)	0	100	100
2	DS	61/67 (91%)	61 (100%)	0	100	100
2	DT	61/67 (91%)	61 (100%)	0	100	100
2	DV	61/67 (91%)	61 (100%)	0	100	100
2	DW	61/67 (91%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	DX	61/67 (91%)	61 (100%)	0	100	100
2	DY	61/67 (91%)	61 (100%)	0	100	100
2	DZ	61/67 (91%)	61 (100%)	0	100	100
2	Da	61/67 (91%)	61 (100%)	0	100	100
2	Db	61/67 (91%)	61 (100%)	0	100	100
2	Dc	61/67 (91%)	61 (100%)	0	100	100
2	Dd	61/67 (91%)	61 (100%)	0	100	100
2	De	61/67 (91%)	61 (100%)	0	100	100
2	Df	61/67 (91%)	61 (100%)	0	100	100
2	Dg	61/67 (91%)	61 (100%)	0	100	100
2	Dh	61/67 (91%)	61 (100%)	0	100	100
2	Di	61/67 (91%)	61 (100%)	0	100	100
2	Dj	61/67 (91%)	61 (100%)	0	100	100
2	Dk	61/67 (91%)	61 (100%)	0	100	100
2	Dl	61/67 (91%)	61 (100%)	0	100	100
2	Dm	61/67 (91%)	61 (100%)	0	100	100
2	Dn	61/67 (91%)	61 (100%)	0	100	100
2	Do	61/67 (91%)	61 (100%)	0	100	100
2	Dp	61/67 (91%)	61 (100%)	0	100	100
2	Dq	61/67 (91%)	61 (100%)	0	100	100
2	Dr	61/67 (91%)	61 (100%)	0	100	100
2	Ds	61/67 (91%)	61 (100%)	0	100	100
2	Dt	61/67 (91%)	61 (100%)	0	100	100
2	Dv	61/67 (91%)	61 (100%)	0	100	100
2	Dw	61/67 (91%)	61 (100%)	0	100	100
2	Dx	61/67 (91%)	61 (100%)	0	100	100
2	Dy	61/67 (91%)	61 (100%)	0	100	100
2	Dz	61/67 (91%)	61 (100%)	0	100	100
All	All	14880/16680 (89%)	14880 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (336)

such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	5	GLN
2	BA	79	HIS
2	BA	90	ASN
2	DA	58	ASN
1	AB	5	GLN
1	AB	21	HIS
2	BB	85	HIS
2	CB	58	ASN
2	CB	85	HIS
2	DB	85	HIS
1	AC	5	GLN
2	BC	58	ASN
2	BC	85	HIS
2	BC	90	ASN
2	CC	58	ASN
2	CC	85	HIS
2	DC	58	ASN
1	AD	5	GLN
2	BD	58	ASN
2	CD	58	ASN
2	DD	85	HIS
1	AE	5	GLN
1	AE	21	HIS
1	AE	36	GLN
2	BE	90	ASN
2	CE	85	HIS
2	DE	85	HIS
1	AF	5	GLN
2	BF	79	HIS
2	BF	90	ASN
2	CF	58	ASN
2	CF	90	ASN
2	DF	58	ASN
1	AG	5	GLN
1	AG	21	HIS
2	CG	58	ASN
2	DG	85	HIS
1	AH	5	GLN
1	AH	21	HIS
1	AH	36	GLN
2	BH	58	ASN
2	BH	85	HIS

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Mol	Chain	Res	Type
2	BH	90	ASN
2	CH	58	ASN
2	CH	85	HIS
2	DH	58	ASN
2	DH	85	HIS
1	AI	5	GLN
2	BI	58	ASN
2	BI	90	ASN
2	CI	58	ASN
2	DI	58	ASN
2	DI	85	HIS
1	AJ	5	GLN
1	AJ	21	HIS
2	BJ	90	ASN
2	CJ	85	HIS
2	DJ	85	HIS
2	BK	79	HIS
2	BK	90	ASN
2	DK	58	ASN
2	DK	85	HIS
1	AL	5	GLN
1	AL	21	HIS
2	CL	58	ASN
2	CL	85	HIS
2	DL	85	HIS
1	AM	5	GLN
2	BM	58	ASN
2	BM	85	HIS
2	BM	90	ASN
2	CM	58	ASN
2	CM	85	HIS
2	DM	58	ASN
2	DM	85	HIS
1	AN	5	GLN
2	CN	58	ASN
2	DN	58	ASN
2	DN	85	HIS
1	AO	5	GLN
1	AO	21	HIS
1	AO	36	GLN
2	BO	90	ASN
2	CO	85	HIS

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Mol	Chain	Res	Type
2	DO	85	HIS
1	AP	5	GLN
2	BP	79	HIS
2	BP	90	ASN
1	AQ	5	GLN
1	AQ	21	HIS
2	BQ	90	ASN
2	CQ	58	ASN
2	DQ	85	HIS
1	AR	5	GLN
1	AR	36	GLN
2	BR	58	ASN
2	BR	85	HIS
2	BR	90	ASN
2	CR	58	ASN
2	CR	85	HIS
2	DR	58	ASN
1	AS	5	GLN
2	BS	58	ASN
2	BS	90	ASN
2	CS	58	ASN
2	DS	58	ASN
2	DS	85	HIS
1	AT	5	GLN
1	AT	21	HIS
2	BT	90	ASN
2	CT	85	HIS
2	DT	85	HIS
2	BV	79	HIS
2	BV	90	ASN
2	DV	58	ASN
1	AW	5	GLN
1	AW	21	HIS
2	CW	58	ASN
2	CW	85	HIS
2	DW	85	HIS
1	AX	5	GLN
2	BX	58	ASN
2	BX	85	HIS
2	BX	90	ASN
2	CX	58	ASN
2	CX	85	HIS

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Mol	Chain	Res	Type
2	DX	58	ASN
1	AY	5	GLN
2	BY	58	ASN
2	BY	90	ASN
2	CY	58	ASN
2	DY	85	HIS
1	AZ	5	GLN
1	AZ	21	HIS
2	BZ	90	ASN
2	CZ	85	HIS
2	DZ	79	HIS
2	DZ	85	HIS
1	Aa	5	GLN
2	Ba	79	HIS
2	Ba	90	ASN
2	Da	58	ASN
1	Ab	5	GLN
2	Bb	85	HIS
2	Cb	58	ASN
2	Cb	85	HIS
2	Db	85	HIS
1	Ac	5	GLN
2	Bc	58	ASN
2	Bc	79	HIS
2	Bc	85	HIS
2	Bc	90	ASN
2	Cc	58	ASN
2	Cc	85	HIS
2	Dc	58	ASN
2	Dc	85	HIS
1	Ad	36	GLN
2	Bd	58	ASN
2	Bd	90	ASN
2	Cd	58	ASN
2	Dd	58	ASN
2	Dd	85	HIS
1	Ae	5	GLN
1	Ae	21	HIS
2	Be	90	ASN
2	Ce	85	HIS
2	De	79	HIS
2	De	85	HIS

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Mol	Chain	Res	Type
1	Af	5	GLN
2	Bf	79	HIS
2	Bf	90	ASN
2	Df	58	ASN
2	Df	85	HIS
1	Ag	5	GLN
1	Ag	21	HIS
2	Cg	58	ASN
2	Cg	85	HIS
2	Dg	85	HIS
1	Ah	5	GLN
2	Bh	58	ASN
2	Bh	85	HIS
2	Bh	90	ASN
2	Ch	58	ASN
2	Ch	85	HIS
2	Dh	58	ASN
2	Dh	85	HIS
1	Ai	5	GLN
2	Bi	90	ASN
2	Ci	58	ASN
2	Di	85	HIS
1	Aj	5	GLN
1	Aj	21	HIS
1	Aj	36	GLN
2	Bj	90	ASN
2	Cj	85	HIS
2	Dj	85	HIS
1	Ak	5	GLN
2	Bk	79	HIS
2	Bk	90	ASN
2	Dk	58	ASN
2	Dk	85	HIS
1	Al	5	GLN
1	Al	21	HIS
2	Bl	90	ASN
2	Cl	58	ASN
2	Cl	85	HIS
1	Am	5	GLN
1	Am	21	HIS
2	Bm	58	ASN
2	Bm	85	HIS

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Mol	Chain	Res	Type
2	Bm	90	ASN
2	Cm	58	ASN
2	Cm	85	HIS
2	Dm	58	ASN
1	An	5	GLN
1	An	36	GLN
2	Bn	58	ASN
2	Cn	58	ASN
2	Dn	58	ASN
2	Dn	85	HIS
1	Ao	5	GLN
1	Ao	21	HIS
2	Bo	90	ASN
2	Co	85	HIS
2	Do	85	HIS
2	Bp	79	HIS
2	Bp	90	ASN
2	Dp	58	ASN
1	Aq	5	GLN
1	Aq	21	HIS
2	Bq	85	HIS
2	Cq	58	ASN
1	Ar	5	GLN
2	Br	58	ASN
2	Br	85	HIS
2	Br	90	ASN
2	Cr	58	ASN
2	Cr	85	HIS
2	Dr	58	ASN
2	Dr	85	HIS
1	As	5	GLN
2	Bs	58	ASN
2	Cs	58	ASN
2	Ds	58	ASN
2	Ds	85	HIS
1	At	5	GLN
1	At	21	HIS
1	At	36	GLN
2	Bt	90	ASN
2	Ct	85	HIS
2	Dt	85	HIS
2	Bv	79	HIS

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Mol	Chain	Res	Type
2	Bv	90	ASN
2	Dv	58	ASN
1	Aw	5	GLN
1	Aw	21	HIS
2	Cw	58	ASN
2	Cw	85	HIS
2	Dw	85	HIS
1	Ax	5	GLN
2	Bx	58	ASN
2	Bx	85	HIS
2	Bx	90	ASN
2	Cx	58	ASN
2	Cx	85	HIS
2	Dx	58	ASN
2	Dx	85	HIS
1	Ay	5	GLN
2	By	58	ASN
2	By	90	ASN
2	Cy	58	ASN
2	Dy	58	ASN
2	Dy	85	HIS
1	Az	5	GLN
1	Az	21	HIS
2	Bz	90	ASN
2	Cz	85	HIS
2	Dz	85	HIS
1	A0	5	GLN
2	B0	79	HIS
2	B0	90	ASN
2	D0	58	ASN
2	D0	85	HIS
1	A1	5	GLN
1	A1	21	HIS
2	B1	85	HIS
2	C1	58	ASN
2	C1	85	HIS
2	D1	85	HIS
1	A2	5	GLN
1	A2	21	HIS
2	B2	58	ASN
2	B2	85	HIS
2	B2	90	ASN

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Mol	Chain	Res	Type
2	C2	58	ASN
2	C2	85	HIS
2	C2	90	ASN
2	D2	58	ASN
1	A3	5	GLN
2	B3	90	ASN
2	C3	58	ASN
2	D3	85	HIS
1	A4	5	GLN
1	A4	21	HIS
1	A4	36	GLN
2	B4	90	ASN
2	C4	85	HIS
1	A5	5	GLN
2	B5	79	HIS
2	B5	90	ASN
2	D5	58	ASN
2	D5	85	HIS
1	A6	5	GLN
1	A6	21	HIS
2	C6	58	ASN
2	C6	85	HIS
2	D6	85	HIS
1	A7	5	GLN
2	B7	58	ASN
2	B7	85	HIS
2	B7	90	ASN
2	C7	58	ASN
2	C7	85	HIS
2	D7	58	ASN
2	D7	85	HIS
1	A8	5	GLN
2	B8	58	ASN
2	B8	90	ASN
2	C8	58	ASN
2	D8	58	ASN
2	D8	85	HIS
1	A9	5	GLN
1	A9	21	HIS
2	B9	90	ASN
2	C9	85	HIS
2	D9	85	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

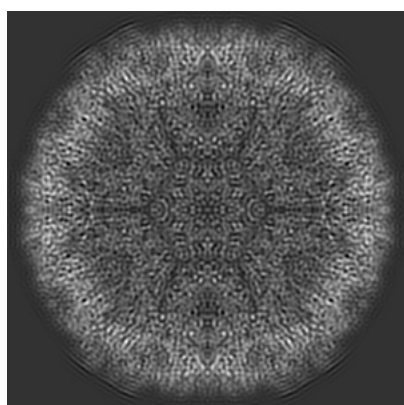
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30385. These allow visual inspection of the internal detail of the map and identification of artifacts.

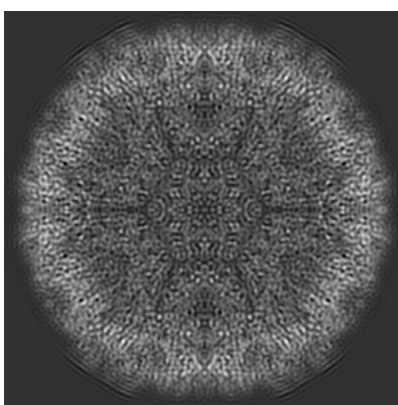
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

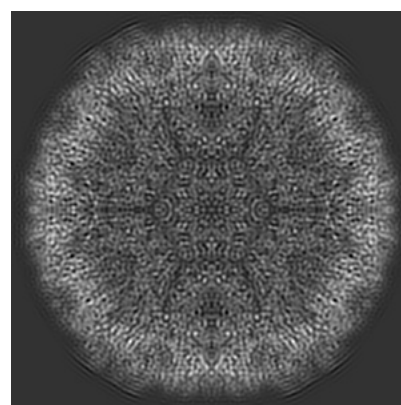
6.1.1 Primary map



X



Y

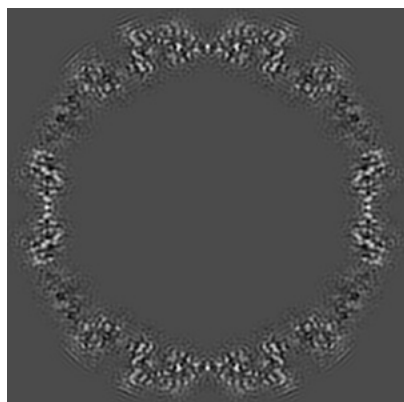


Z

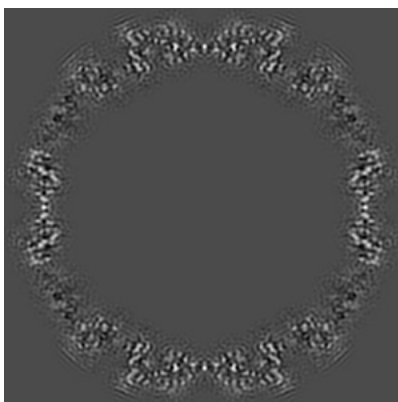
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

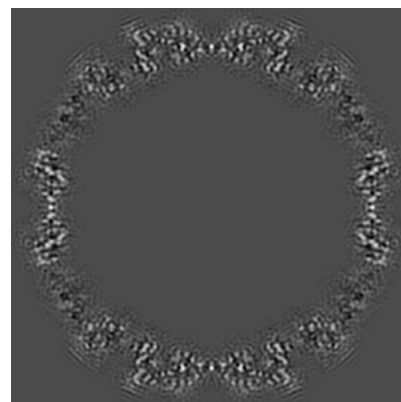
6.2.1 Primary map



X Index: 150



Y Index: 150

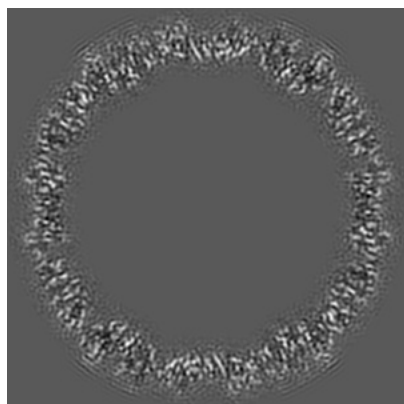


Z Index: 150

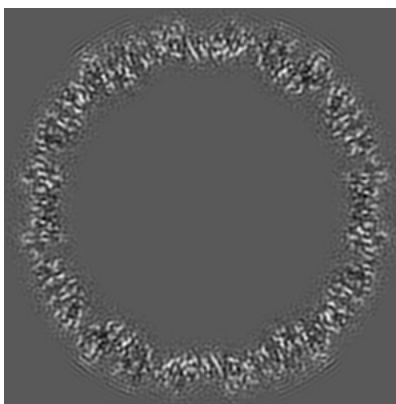
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

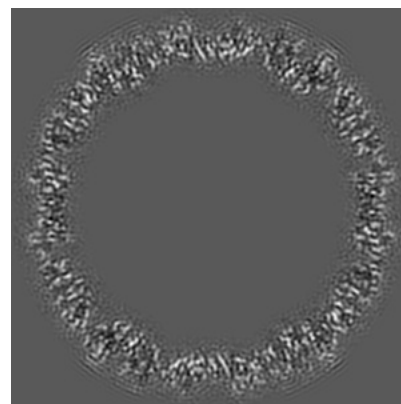
6.3.1 Primary map



X Index: 162



Y Index: 162

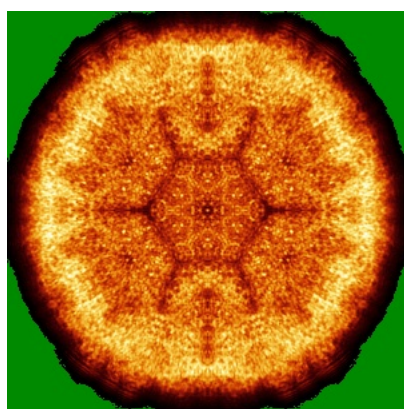


Z Index: 162

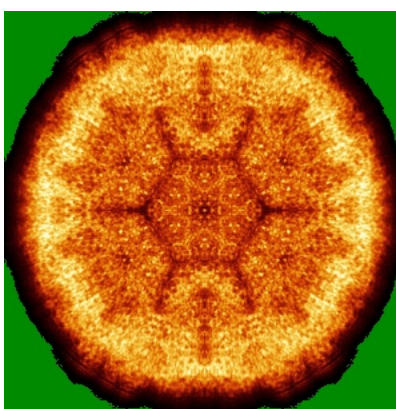
The images above show the largest variance slices of the map in three orthogonal directions.

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

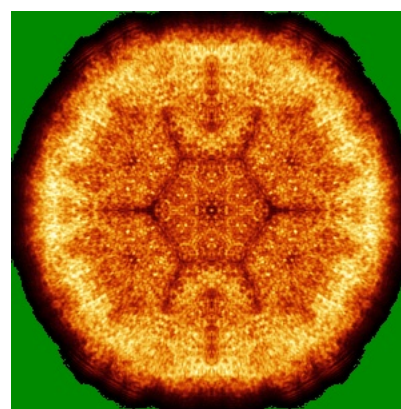
6.4.1 Primary map



X



Y

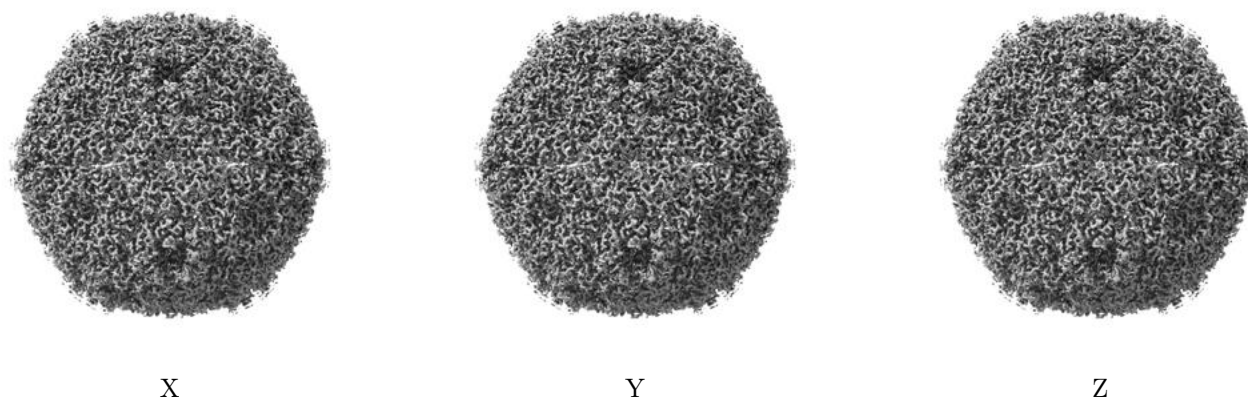


Z

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.

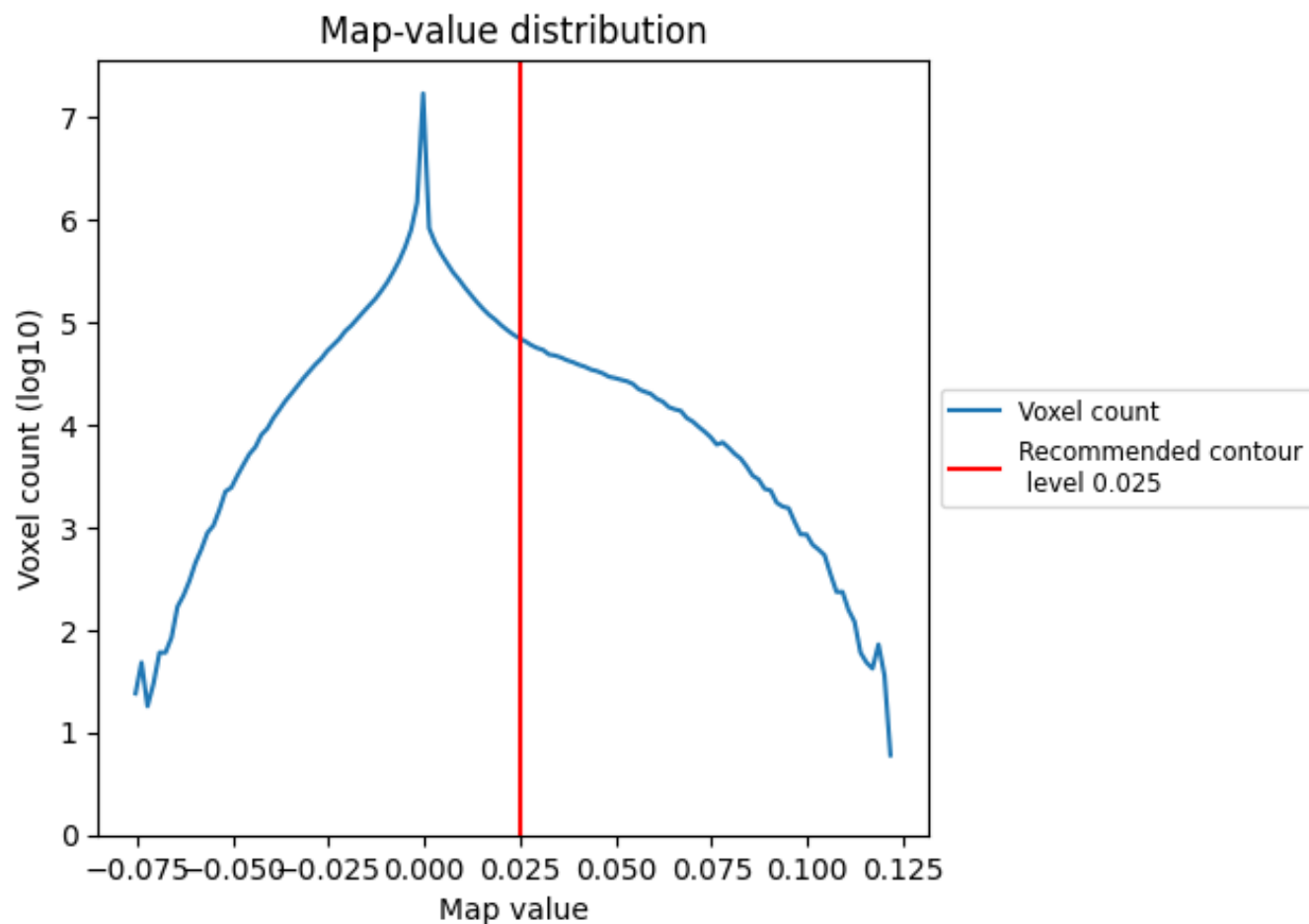
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

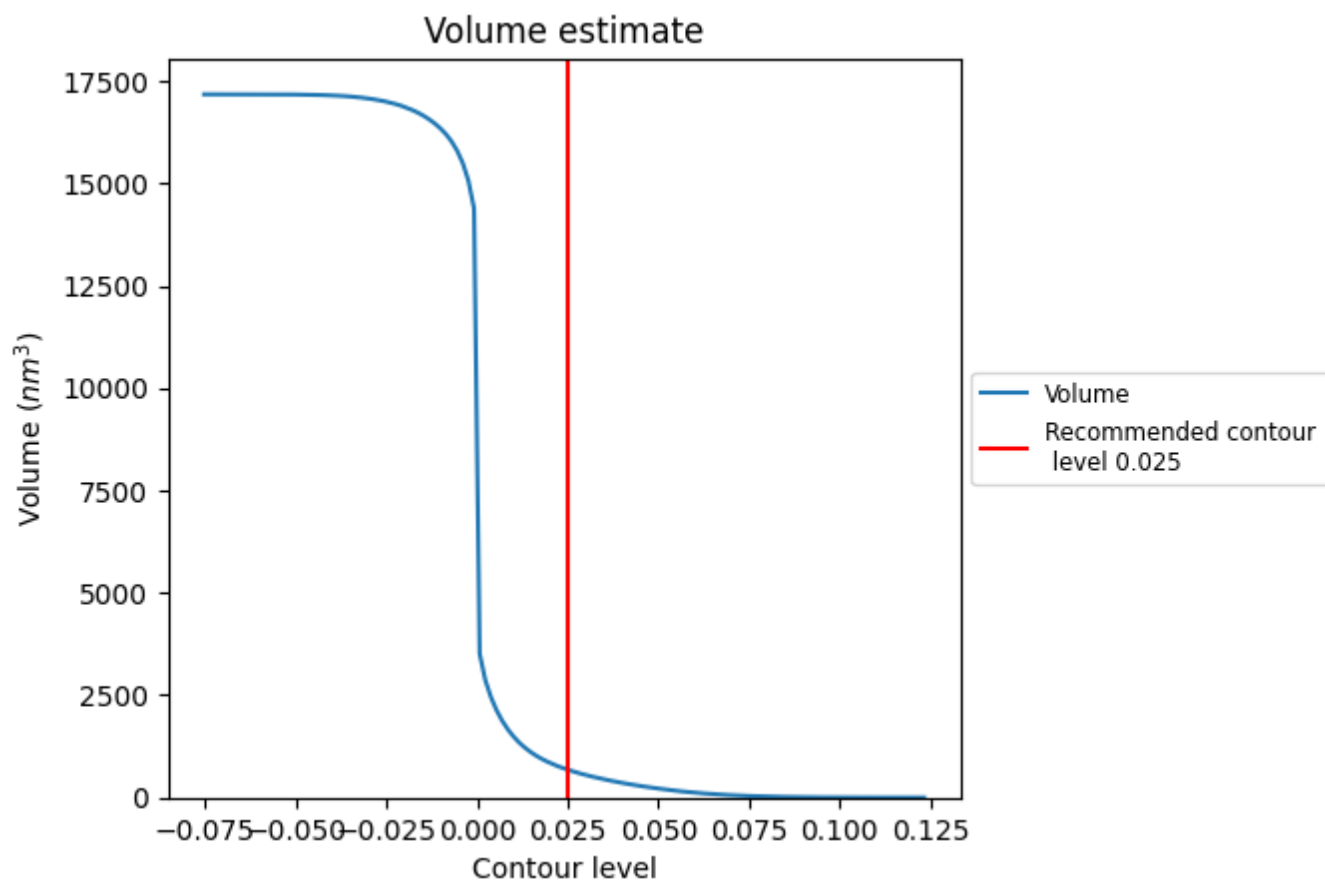
This section contains the results of statistical analysis of the map.

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.

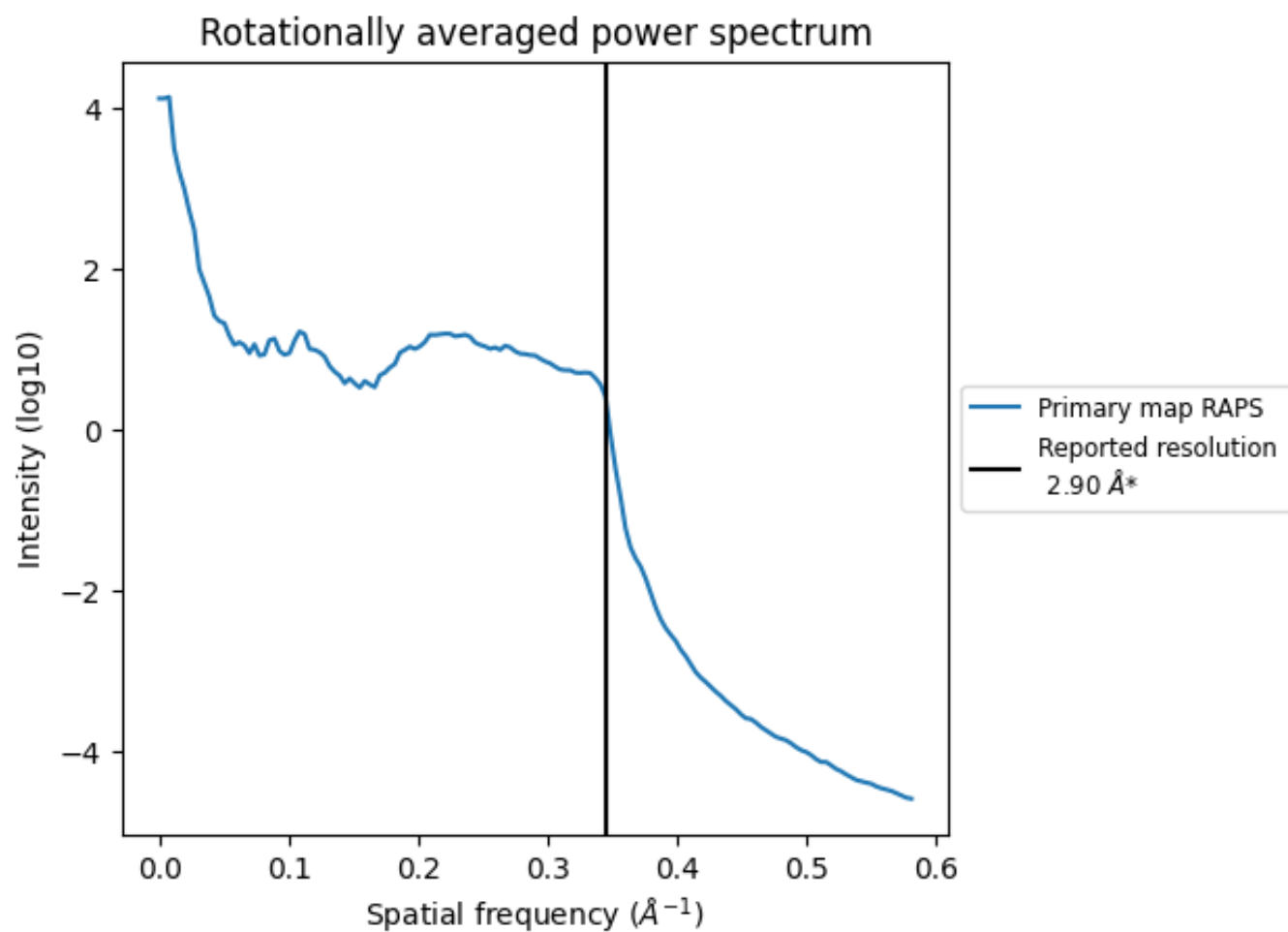
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 679 nm³; this corresponds to an approximate mass of 613 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 0.345 $\text{\AA}^{-1}$

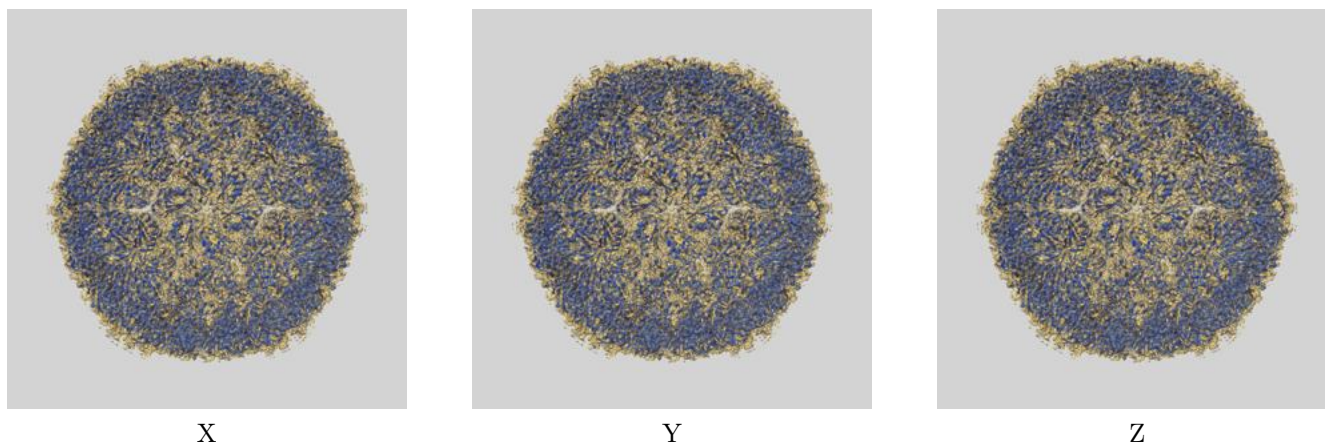
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

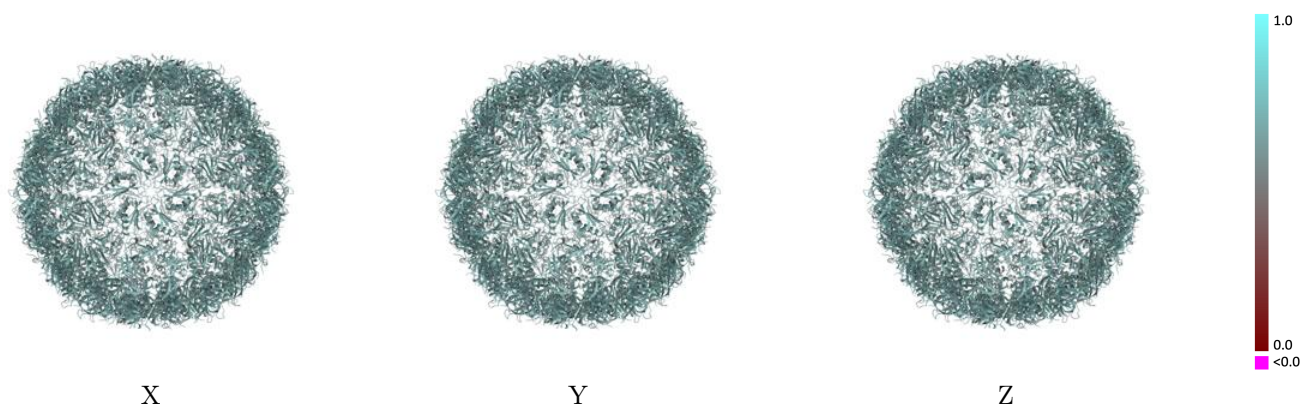
This section contains information regarding the fit between EMDB map EMD-30385 and PDB model 7CKC. Per-residue inclusion information can be found in section [3](#) on page [41](#).

9.1 Map-model overlay [i](#)



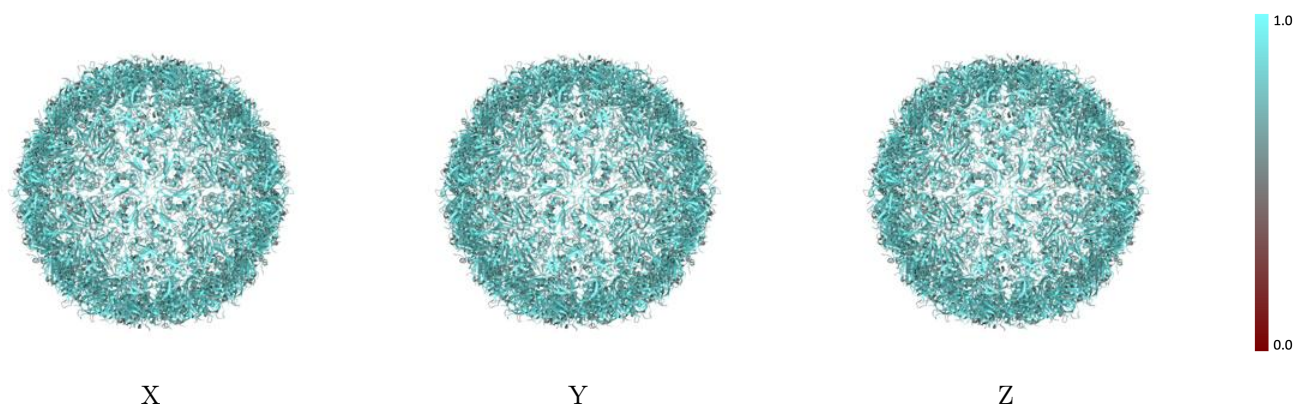
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



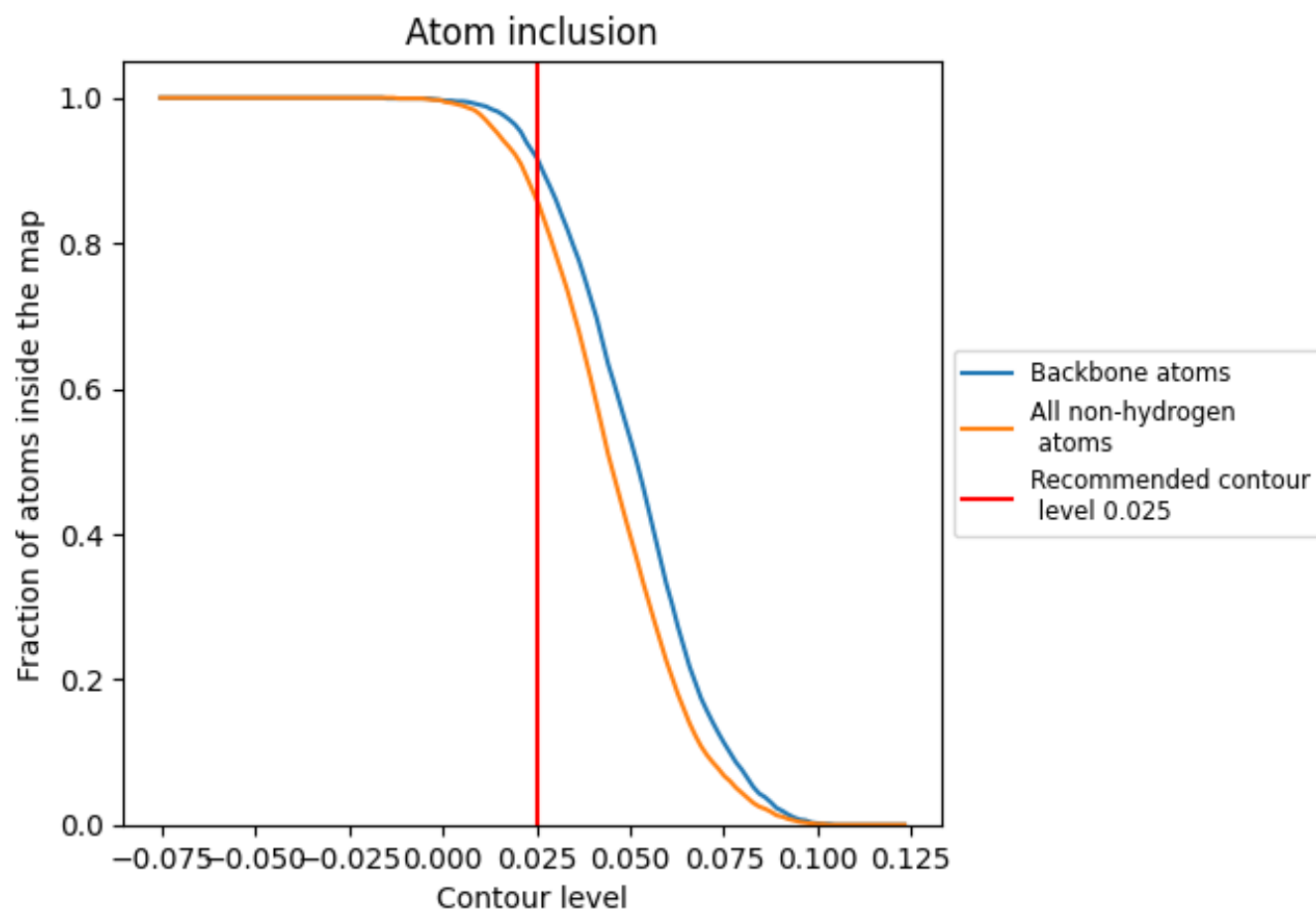
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 92% of all backbone atoms, 86% 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	 0.8600	 0.6270
A0	 0.8730	 0.6290
A1	 0.8680	 0.6290
A2	 0.8750	 0.6320
A3	 0.8660	 0.6340
A4	 0.8880	 0.6320
A5	 0.8700	 0.6310
A6	 0.8680	 0.6300
A7	 0.8730	 0.6330
A8	 0.8680	 0.6340
A9	 0.8880	 0.6310
AA	 0.8710	 0.6280
AB	 0.8680	 0.6320
AC	 0.8730	 0.6330
AD	 0.8680	 0.6340
AE	 0.8880	 0.6300
AF	 0.8680	 0.6280
AG	 0.8680	 0.6290
AH	 0.8780	 0.6320
AI	 0.8630	 0.6330
AJ	 0.8880	 0.6310
AK	 0.8750	 0.6310
AL	 0.8640	 0.6330
AM	 0.8750	 0.6330
AN	 0.8660	 0.6330
AO	 0.8880	 0.6290
AP	 0.8710	 0.6260
AQ	 0.8660	 0.6270
AR	 0.8760	 0.6340
AS	 0.8660	 0.6360
AT	 0.8880	 0.6340
AV	 0.8710	 0.6320
AW	 0.8680	 0.6320
AX	 0.8730	 0.6300
AY	 0.8700	 0.6320



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Chain	Atom inclusion	Q-score
AZ	 0.8860	 0.6320
Aa	 0.8710	 0.6300
Ab	 0.8660	 0.6320
Ac	 0.8750	 0.6280
Ad	 0.8680	 0.6310
Ae	 0.8880	 0.6310
Af	 0.8660	 0.6310
Ag	 0.8660	 0.6300
Ah	 0.8730	 0.6300
Ai	 0.8680	 0.6310
Aj	 0.8880	 0.6320
Ak	 0.8710	 0.6300
Al	 0.8680	 0.6330
Am	 0.8750	 0.6320
An	 0.8610	 0.6300
Ao	 0.8880	 0.6360
Ap	 0.8730	 0.6330
Aq	 0.8710	 0.6310
Ar	 0.8730	 0.6340
As	 0.8640	 0.6330
At	 0.8880	 0.6330
Av	 0.8750	 0.6320
Aw	 0.8700	 0.6290
Ax	 0.8730	 0.6330
Ay	 0.8680	 0.6340
Az	 0.8860	 0.6320
B0	 0.8730	 0.6280
B1	 0.8660	 0.6270
B2	 0.8630	 0.6280
B3	 0.8680	 0.6260
B4	 0.8630	 0.6290
B5	 0.8710	 0.6260
B6	 0.8680	 0.6260
B7	 0.8630	 0.6240
B8	 0.8680	 0.6280
B9	 0.8650	 0.6240
BA	 0.8710	 0.6250
BB	 0.8660	 0.6280
BC	 0.8630	 0.6270
BD	 0.8690	 0.6260
BE	 0.8650	 0.6240
BF	 0.8730	 0.6210

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Chain	Atom inclusion	Q-score
BG	 0.8680	 0.6290
BH	 0.8650	 0.6260
BI	 0.8660	 0.6260
BJ	 0.8650	 0.6260
BK	 0.8690	 0.6240
BL	 0.8660	 0.6290
BM	 0.8650	 0.6280
BN	 0.8680	 0.6300
BO	 0.8650	 0.6250
BP	 0.8710	 0.6240
BQ	 0.8660	 0.6270
BR	 0.8630	 0.6280
BS	 0.8680	 0.6260
BT	 0.8650	 0.6240
BV	 0.8680	 0.6250
BW	 0.8660	 0.6290
BX	 0.8650	 0.6240
BY	 0.8660	 0.6260
BZ	 0.8610	 0.6260
Ba	 0.8680	 0.6250
Bb	 0.8660	 0.6280
Bc	 0.8630	 0.6260
Bd	 0.8660	 0.6250
Be	 0.8650	 0.6280
Bf	 0.8730	 0.6250
Bg	 0.8660	 0.6290
Bh	 0.8650	 0.6260
Bi	 0.8660	 0.6260
Bj	 0.8610	 0.6250
Bk	 0.8710	 0.6260
Bl	 0.8660	 0.6300
Bm	 0.8630	 0.6250
Bn	 0.8710	 0.6260
Bo	 0.8630	 0.6240
Bp	 0.8710	 0.6260
Bq	 0.8660	 0.6280
Br	 0.8630	 0.6300
Bs	 0.8680	 0.6240
Bt	 0.8650	 0.6270
Bv	 0.8710	 0.6250
Bw	 0.8680	 0.6270
Bx	 0.8630	 0.6250

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Chain	Atom inclusion	Q-score
By	 0.8680	 0.6260
Bz	 0.8650	 0.6240
C0	 0.8480	 0.6230
C1	 0.8570	 0.6240
C2	 0.8610	 0.6230
C3	 0.8570	 0.6280
C4	 0.8650	 0.6230
C5	 0.8500	 0.6240
C6	 0.8570	 0.6260
C7	 0.8600	 0.6240
C8	 0.8550	 0.6250
C9	 0.8600	 0.6250
CA	 0.8500	 0.6210
CB	 0.8530	 0.6250
CC	 0.8610	 0.6240
CD	 0.8570	 0.6240
CE	 0.8630	 0.6240
CF	 0.8530	 0.6220
CG	 0.8530	 0.6260
CH	 0.8600	 0.6250
CI	 0.8550	 0.6260
CJ	 0.8630	 0.6240
CK	 0.8480	 0.6210
CL	 0.8570	 0.6260
CM	 0.8610	 0.6250
CN	 0.8550	 0.6250
CO	 0.8650	 0.6240
CP	 0.8480	 0.6210
CQ	 0.8530	 0.6260
CR	 0.8610	 0.6240
CS	 0.8570	 0.6260
CT	 0.8650	 0.6250
CV	 0.8480	 0.6220
CW	 0.8520	 0.6280
CX	 0.8610	 0.6220
CY	 0.8550	 0.6230
CZ	 0.8630	 0.6240
Ca	 0.8480	 0.6250
Cb	 0.8580	 0.6260
Cc	 0.8610	 0.6230
Cd	 0.8550	 0.6220
Ce	 0.8630	 0.6240

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Chain	Atom inclusion	Q-score
Cf	 0.8480	 0.6250
Cg	 0.8550	 0.6270
Ch	 0.8610	 0.6240
Ci	 0.8550	 0.6210
Cj	 0.8610	 0.6260
Ck	 0.8480	 0.6240
Cl	 0.8550	 0.6260
Cm	 0.8610	 0.6250
Cn	 0.8530	 0.6210
Co	 0.8650	 0.6260
Cp	 0.8480	 0.6230
Cq	 0.8610	 0.6210
Cr	 0.8610	 0.6250
Cs	 0.8550	 0.6270
Ct	 0.8650	 0.6230
Cv	 0.8480	 0.6230
Cw	 0.8570	 0.6240
Cx	 0.8610	 0.6250
Cy	 0.8530	 0.6220
Cz	 0.8650	 0.6250
D0	 0.8570	 0.6290
D1	 0.8500	 0.6290
D2	 0.8360	 0.6250
D3	 0.8440	 0.6280
D4	 0.8450	 0.6250
D5	 0.8550	 0.6270
D6	 0.8500	 0.6250
D7	 0.8360	 0.6260
D8	 0.8440	 0.6270
D9	 0.8470	 0.6250
DA	 0.8550	 0.6250
DB	 0.8500	 0.6260
DC	 0.8360	 0.6260
DD	 0.8450	 0.6250
DE	 0.8470	 0.6270
DF	 0.8550	 0.6250
DG	 0.8500	 0.6260
DH	 0.8370	 0.6290
DI	 0.8440	 0.6270
DJ	 0.8470	 0.6250
DK	 0.8530	 0.6270
DL	 0.8500	 0.6270

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Chain	Atom inclusion	Q-score
DM	 0.8370	 0.6270
DN	 0.8440	 0.6250
DO	 0.8450	 0.6240
DP	 0.8500	 0.6240
DQ	 0.8520	 0.6250
DR	 0.8360	 0.6260
DS	 0.8440	 0.6250
DT	 0.8470	 0.6270
DV	 0.8530	 0.6290
DW	 0.8520	 0.6290
DX	 0.8370	 0.6260
DY	 0.8440	 0.6250
DZ	 0.8470	 0.6270
Da	 0.8530	 0.6270
Db	 0.8500	 0.6250
Dc	 0.8370	 0.6230
Dd	 0.8440	 0.6240
De	 0.8470	 0.6270
Df	 0.8570	 0.6260
Dg	 0.8480	 0.6230
Dh	 0.8340	 0.6240
Di	 0.8440	 0.6270
Dj	 0.8470	 0.6270
Dk	 0.8570	 0.6260
Dl	 0.8480	 0.6260
Dm	 0.8360	 0.6260
Dn	 0.8440	 0.6260
Do	 0.8450	 0.6290
Dp	 0.8530	 0.6250
Dq	 0.8470	 0.6280
Dr	 0.8370	 0.6250
Ds	 0.8440	 0.6280
Dt	 0.8470	 0.6240
Dv	 0.8520	 0.6260
Dw	 0.8520	 0.6260
Dx	 0.8370	 0.6250
Dy	 0.8440	 0.6250
Dz	 0.8470	 0.6280