



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:43 AM UTC

PDB ID : 8C0O / pdb_00008c0o
EMDB ID : EMD-16371
Title : African cichlid nakednavirus capsid at pH 5.5
Authors : Pfister, S.; Rabl, J.; Boehringer, D.; Meier, B.H.
Deposited on : 2022-12-19
Resolution : 3.90 Å(reported)

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:

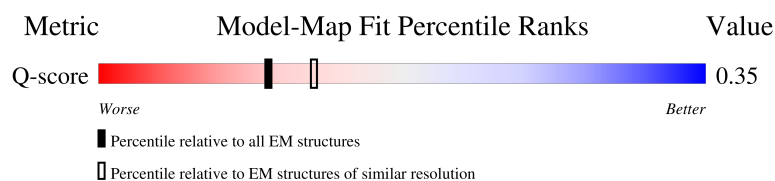
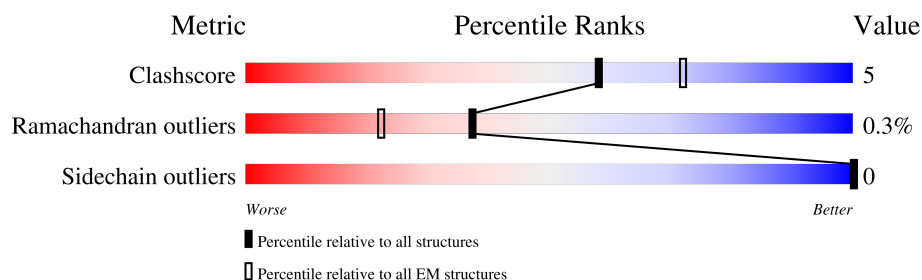
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.90 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	8855 (3.40 - 4.40)

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	1A	175	
1	1B	175	
1	1C	175	
1	2A	175	

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Mol	Chain	Length	Quality of chain
1	2B	175	
1	2C	175	
1	3A	175	
1	3B	175	
1	3C	175	
1	4A	175	
1	4B	175	
1	4C	175	
1	5A	175	
1	5B	175	
1	5C	175	
1	6A	175	
1	6B	175	
1	6C	175	
1	7A	175	
1	7B	175	
1	7C	175	
1	8A	175	
1	8B	175	
1	8C	175	
1	AA	175	
1	AB	175	
1	AC	175	
1	BA	175	
1	BB	175	

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Mol	Chain	Length	Quality of chain
1	BC	175	
1	CA	175	
1	CB	175	
1	CC	175	
1	DA	175	
1	DB	175	
1	DC	175	
1	EA	175	
1	EB	175	
1	EC	175	
1	FA	175	
1	FB	175	
1	FC	175	
1	GA	175	
1	GB	175	
1	GC	175	
1	HA	175	
1	HB	175	
1	HC	175	
1	IA	175	
1	IB	175	
1	IC	175	
1	JA	175	
1	JB	175	
1	JC	175	

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Mol	Chain	Length	Quality of chain
1	KA	175	
1	KB	175	
1	KC	175	
1	LA	175	
1	LB	175	
1	LC	175	
1	MA	175	
1	MB	175	
1	MC	175	
1	NA	175	
1	NB	175	
1	NC	175	
1	OA	175	
1	OB	175	
1	OC	175	
1	PA	175	
1	PB	175	
1	PC	175	
1	QA	175	
1	QB	175	
1	QC	175	
1	RA	175	
1	RB	175	
1	RC	175	
1	SA	175	

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Mol	Chain	Length	Quality of chain
1	SB	175	
1	SC	175	
1	TA	175	
1	TB	175	
1	TC	175	
1	UA	175	
1	UB	175	
1	UC	175	
1	VA	175	
1	VB	175	
1	VC	175	
1	WA	175	
1	WB	175	
1	WC	175	
1	XA	175	
1	XB	175	
1	XC	175	
1	YA	175	
1	YB	175	
1	YC	175	
1	ZA	175	
1	ZB	175	
1	ZC	175	
1	aA	175	
1	aB	175	

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Mol	Chain	Length	Quality of chain
1	aC	175	
1	bA	175	
1	bB	175	
1	bC	175	
1	cA	175	
1	cB	175	
1	cC	175	
1	dA	175	
1	dB	175	
1	dC	175	
1	eA	175	
1	eB	175	
1	eC	175	
1	fA	175	
1	fB	175	
1	fC	175	
1	gA	175	
1	gB	175	
1	gC	175	
1	hA	175	
1	hB	175	
1	hC	175	
1	iA	175	
1	iB	175	
1	iC	175	

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Mol	Chain	Length	Quality of chain
1	jA	175	
1	jB	175	
1	jC	175	
1	kA	175	
1	kB	175	
1	kC	175	
1	lA	175	
1	lB	175	
1	lC	175	
1	mA	175	
1	mB	175	
1	mC	175	
1	nA	175	
1	nB	175	
1	nC	175	
1	oA	175	
1	oB	175	
1	oC	175	
1	pA	175	
1	pB	175	
1	pC	175	
1	qA	175	
1	qB	175	
1	qC	175	
1	rA	175	

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Mol	Chain	Length	Quality of chain
1	rB	175	
1	rC	175	
1	sA	175	
1	sB	175	
1	sC	175	
1	tA	175	
1	tB	175	
1	tC	175	
1	uA	175	
1	uB	175	
1	uC	175	
1	vA	175	
1	vB	175	
1	vC	175	
1	wA	175	
1	wB	175	
1	wC	175	
1	xA	175	
1	xB	175	
1	xC	175	
1	yA	175	
1	yB	175	
1	yC	175	
1	zA	175	
1	zB	175	

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Mol	Chain	Length	Quality of chain
1	zC	175	23% 59% 9% 32%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 178320 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 C protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	AC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	BA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	BB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	BC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	CA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	CB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	CC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	DA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	DB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	DC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	EA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	EB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	EC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	FA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	FB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	FC	119	Total 974	C 635	N 166	O 165	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	GA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	GB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	GC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	HA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	HB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	HC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	IA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	IB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	IC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	JA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	1B	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	JB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	JC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	KA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	KB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	KC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	LA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	LB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	LC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	MA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	MB	122	Total 999	C 651	N 169	O 171	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	MC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	NA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	NB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	NC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	OA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	OB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	OC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	PA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	PB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	PC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	QA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	QB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	QC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	RA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	RB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	RC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	1C	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	SA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	SB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	SC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	TA	122	Total 999	C 651	N 169	O 171	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	TB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	TC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	UA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	UB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	UC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	VA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	VB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	VC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	WA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	WB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	WC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	XA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	XB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	XC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	YA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	YB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	YC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	ZA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	ZB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	ZC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	aA	122	Total 999	C 651	N 169	O 171	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	aB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	2A	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	aC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	bA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	bB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	bC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	cA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	cB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	cC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	dA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	dB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	dC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	eA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	eB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	eC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	fA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	fB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	fC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	gA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	gB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	gC	119	Total 974	C 635	N 166	O 165	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	hA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	hB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	hC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	iA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	iB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	iC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	jA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	2B	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	jB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	jC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	kA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	kB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	kC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	lA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	lB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	lC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	mA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	mB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	mC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	nA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	nB	122	Total 999	C 651	N 169	O 171	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	nC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	oA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	oB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	oC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	pA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	pB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	pC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	qA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	qB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	qC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	rA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	rB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	rC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	2C	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	sA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	sB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	sC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	tA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	tB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	tC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	uA	122	Total 999	C 651	N 169	O 171	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	uB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	uC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	vA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	vB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	vC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	wA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	wB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	wC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	xA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	xB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	xC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	yA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	yB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	yC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	zA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	zB	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	zC	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	3A	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	3B	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	3C	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	4A	122	Total 999	C 651	N 169	O 171	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	4B	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	4C	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	5A	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	5B	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	5C	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	6A	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	6B	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	6C	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	7A	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	7B	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	7C	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	8A	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	8B	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	8C	119	Total 974	C 635	N 166	O 165	S 8	0	0
1	AA	122	Total 999	C 651	N 169	O 171	S 8	0	0
1	AB	122	Total 999	C 651	N 169	O 171	S 8	0	0

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	1	GLY	-	insertion	UNP A0A3S9H6T3
AC	1	GLY	-	insertion	UNP A0A3S9H6T3
BA	1	GLY	-	insertion	UNP A0A3S9H6T3
BB	1	GLY	-	insertion	UNP A0A3S9H6T3
BC	1	GLY	-	insertion	UNP A0A3S9H6T3
CA	1	GLY	-	insertion	UNP A0A3S9H6T3
CB	1	GLY	-	insertion	UNP A0A3S9H6T3

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Chain	Residue	Modelled	Actual	Comment	Reference
CC	1	GLY	-	insertion	UNP A0A3S9H6T3
DA	1	GLY	-	insertion	UNP A0A3S9H6T3
DB	1	GLY	-	insertion	UNP A0A3S9H6T3
DC	1	GLY	-	insertion	UNP A0A3S9H6T3
EA	1	GLY	-	insertion	UNP A0A3S9H6T3
EB	1	GLY	-	insertion	UNP A0A3S9H6T3
EC	1	GLY	-	insertion	UNP A0A3S9H6T3
FA	1	GLY	-	insertion	UNP A0A3S9H6T3
FB	1	GLY	-	insertion	UNP A0A3S9H6T3
FC	1	GLY	-	insertion	UNP A0A3S9H6T3
GA	1	GLY	-	insertion	UNP A0A3S9H6T3
GB	1	GLY	-	insertion	UNP A0A3S9H6T3
GC	1	GLY	-	insertion	UNP A0A3S9H6T3
HA	1	GLY	-	insertion	UNP A0A3S9H6T3
HB	1	GLY	-	insertion	UNP A0A3S9H6T3
HC	1	GLY	-	insertion	UNP A0A3S9H6T3
IA	1	GLY	-	insertion	UNP A0A3S9H6T3
IB	1	GLY	-	insertion	UNP A0A3S9H6T3
IC	1	GLY	-	insertion	UNP A0A3S9H6T3
JA	1	GLY	-	insertion	UNP A0A3S9H6T3
1B	1	GLY	-	insertion	UNP A0A3S9H6T3
JB	1	GLY	-	insertion	UNP A0A3S9H6T3
JC	1	GLY	-	insertion	UNP A0A3S9H6T3
KA	1	GLY	-	insertion	UNP A0A3S9H6T3
KB	1	GLY	-	insertion	UNP A0A3S9H6T3
KC	1	GLY	-	insertion	UNP A0A3S9H6T3
LA	1	GLY	-	insertion	UNP A0A3S9H6T3
LB	1	GLY	-	insertion	UNP A0A3S9H6T3
LC	1	GLY	-	insertion	UNP A0A3S9H6T3
MA	1	GLY	-	insertion	UNP A0A3S9H6T3
MB	1	GLY	-	insertion	UNP A0A3S9H6T3
MC	1	GLY	-	insertion	UNP A0A3S9H6T3
NA	1	GLY	-	insertion	UNP A0A3S9H6T3
NB	1	GLY	-	insertion	UNP A0A3S9H6T3
NC	1	GLY	-	insertion	UNP A0A3S9H6T3
OA	1	GLY	-	insertion	UNP A0A3S9H6T3
OB	1	GLY	-	insertion	UNP A0A3S9H6T3
OC	1	GLY	-	insertion	UNP A0A3S9H6T3
PA	1	GLY	-	insertion	UNP A0A3S9H6T3
PB	1	GLY	-	insertion	UNP A0A3S9H6T3
PC	1	GLY	-	insertion	UNP A0A3S9H6T3
QA	1	GLY	-	insertion	UNP A0A3S9H6T3

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Chain	Residue	Modelled	Actual	Comment	Reference
QB	1	GLY	-	insertion	UNP A0A3S9H6T3
QC	1	GLY	-	insertion	UNP A0A3S9H6T3
RA	1	GLY	-	insertion	UNP A0A3S9H6T3
RB	1	GLY	-	insertion	UNP A0A3S9H6T3
RC	1	GLY	-	insertion	UNP A0A3S9H6T3
1C	1	GLY	-	insertion	UNP A0A3S9H6T3
SA	1	GLY	-	insertion	UNP A0A3S9H6T3
SB	1	GLY	-	insertion	UNP A0A3S9H6T3
SC	1	GLY	-	insertion	UNP A0A3S9H6T3
TA	1	GLY	-	insertion	UNP A0A3S9H6T3
TB	1	GLY	-	insertion	UNP A0A3S9H6T3
TC	1	GLY	-	insertion	UNP A0A3S9H6T3
UA	1	GLY	-	insertion	UNP A0A3S9H6T3
UB	1	GLY	-	insertion	UNP A0A3S9H6T3
UC	1	GLY	-	insertion	UNP A0A3S9H6T3
VA	1	GLY	-	insertion	UNP A0A3S9H6T3
VB	1	GLY	-	insertion	UNP A0A3S9H6T3
VC	1	GLY	-	insertion	UNP A0A3S9H6T3
WA	1	GLY	-	insertion	UNP A0A3S9H6T3
WB	1	GLY	-	insertion	UNP A0A3S9H6T3
WC	1	GLY	-	insertion	UNP A0A3S9H6T3
XA	1	GLY	-	insertion	UNP A0A3S9H6T3
XB	1	GLY	-	insertion	UNP A0A3S9H6T3
XC	1	GLY	-	insertion	UNP A0A3S9H6T3
YA	1	GLY	-	insertion	UNP A0A3S9H6T3
YB	1	GLY	-	insertion	UNP A0A3S9H6T3
YC	1	GLY	-	insertion	UNP A0A3S9H6T3
ZA	1	GLY	-	insertion	UNP A0A3S9H6T3
ZB	1	GLY	-	insertion	UNP A0A3S9H6T3
ZC	1	GLY	-	insertion	UNP A0A3S9H6T3
aA	1	GLY	-	insertion	UNP A0A3S9H6T3
aB	1	GLY	-	insertion	UNP A0A3S9H6T3
2A	1	GLY	-	insertion	UNP A0A3S9H6T3
aC	1	GLY	-	insertion	UNP A0A3S9H6T3
bA	1	GLY	-	insertion	UNP A0A3S9H6T3
bB	1	GLY	-	insertion	UNP A0A3S9H6T3
bC	1	GLY	-	insertion	UNP A0A3S9H6T3
cA	1	GLY	-	insertion	UNP A0A3S9H6T3
cB	1	GLY	-	insertion	UNP A0A3S9H6T3
cC	1	GLY	-	insertion	UNP A0A3S9H6T3
dA	1	GLY	-	insertion	UNP A0A3S9H6T3
dB	1	GLY	-	insertion	UNP A0A3S9H6T3

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Chain	Residue	Modelled	Actual	Comment	Reference
dC	1	GLY	-	insertion	UNP A0A3S9H6T3
eA	1	GLY	-	insertion	UNP A0A3S9H6T3
eB	1	GLY	-	insertion	UNP A0A3S9H6T3
eC	1	GLY	-	insertion	UNP A0A3S9H6T3
fA	1	GLY	-	insertion	UNP A0A3S9H6T3
fB	1	GLY	-	insertion	UNP A0A3S9H6T3
fC	1	GLY	-	insertion	UNP A0A3S9H6T3
gA	1	GLY	-	insertion	UNP A0A3S9H6T3
gB	1	GLY	-	insertion	UNP A0A3S9H6T3
gC	1	GLY	-	insertion	UNP A0A3S9H6T3
hA	1	GLY	-	insertion	UNP A0A3S9H6T3
hB	1	GLY	-	insertion	UNP A0A3S9H6T3
hC	1	GLY	-	insertion	UNP A0A3S9H6T3
iA	1	GLY	-	insertion	UNP A0A3S9H6T3
iB	1	GLY	-	insertion	UNP A0A3S9H6T3
iC	1	GLY	-	insertion	UNP A0A3S9H6T3
jA	1	GLY	-	insertion	UNP A0A3S9H6T3
2B	1	GLY	-	insertion	UNP A0A3S9H6T3
jB	1	GLY	-	insertion	UNP A0A3S9H6T3
jC	1	GLY	-	insertion	UNP A0A3S9H6T3
kA	1	GLY	-	insertion	UNP A0A3S9H6T3
kB	1	GLY	-	insertion	UNP A0A3S9H6T3
kC	1	GLY	-	insertion	UNP A0A3S9H6T3
lA	1	GLY	-	insertion	UNP A0A3S9H6T3
lB	1	GLY	-	insertion	UNP A0A3S9H6T3
lC	1	GLY	-	insertion	UNP A0A3S9H6T3
mA	1	GLY	-	insertion	UNP A0A3S9H6T3
mB	1	GLY	-	insertion	UNP A0A3S9H6T3
mC	1	GLY	-	insertion	UNP A0A3S9H6T3
nA	1	GLY	-	insertion	UNP A0A3S9H6T3
nB	1	GLY	-	insertion	UNP A0A3S9H6T3
nC	1	GLY	-	insertion	UNP A0A3S9H6T3
oA	1	GLY	-	insertion	UNP A0A3S9H6T3
oB	1	GLY	-	insertion	UNP A0A3S9H6T3
oC	1	GLY	-	insertion	UNP A0A3S9H6T3
pA	1	GLY	-	insertion	UNP A0A3S9H6T3
pB	1	GLY	-	insertion	UNP A0A3S9H6T3
pC	1	GLY	-	insertion	UNP A0A3S9H6T3
qA	1	GLY	-	insertion	UNP A0A3S9H6T3
qB	1	GLY	-	insertion	UNP A0A3S9H6T3
qC	1	GLY	-	insertion	UNP A0A3S9H6T3
rA	1	GLY	-	insertion	UNP A0A3S9H6T3

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Chain	Residue	Modelled	Actual	Comment	Reference
rB	1	GLY	-	insertion	UNP A0A3S9H6T3
rC	1	GLY	-	insertion	UNP A0A3S9H6T3
2C	1	GLY	-	insertion	UNP A0A3S9H6T3
sA	1	GLY	-	insertion	UNP A0A3S9H6T3
sB	1	GLY	-	insertion	UNP A0A3S9H6T3
sC	1	GLY	-	insertion	UNP A0A3S9H6T3
tA	1	GLY	-	insertion	UNP A0A3S9H6T3
tB	1	GLY	-	insertion	UNP A0A3S9H6T3
tC	1	GLY	-	insertion	UNP A0A3S9H6T3
uA	1	GLY	-	insertion	UNP A0A3S9H6T3
uB	1	GLY	-	insertion	UNP A0A3S9H6T3
uC	1	GLY	-	insertion	UNP A0A3S9H6T3
vA	1	GLY	-	insertion	UNP A0A3S9H6T3
vB	1	GLY	-	insertion	UNP A0A3S9H6T3
vC	1	GLY	-	insertion	UNP A0A3S9H6T3
wA	1	GLY	-	insertion	UNP A0A3S9H6T3
wB	1	GLY	-	insertion	UNP A0A3S9H6T3
wC	1	GLY	-	insertion	UNP A0A3S9H6T3
xA	1	GLY	-	insertion	UNP A0A3S9H6T3
xB	1	GLY	-	insertion	UNP A0A3S9H6T3
xC	1	GLY	-	insertion	UNP A0A3S9H6T3
yA	1	GLY	-	insertion	UNP A0A3S9H6T3
yB	1	GLY	-	insertion	UNP A0A3S9H6T3
yC	1	GLY	-	insertion	UNP A0A3S9H6T3
zA	1	GLY	-	insertion	UNP A0A3S9H6T3
zB	1	GLY	-	insertion	UNP A0A3S9H6T3
zC	1	GLY	-	insertion	UNP A0A3S9H6T3
3A	1	GLY	-	insertion	UNP A0A3S9H6T3
3B	1	GLY	-	insertion	UNP A0A3S9H6T3
3C	1	GLY	-	insertion	UNP A0A3S9H6T3
4A	1	GLY	-	insertion	UNP A0A3S9H6T3
4B	1	GLY	-	insertion	UNP A0A3S9H6T3
4C	1	GLY	-	insertion	UNP A0A3S9H6T3
5A	1	GLY	-	insertion	UNP A0A3S9H6T3
5B	1	GLY	-	insertion	UNP A0A3S9H6T3
5C	1	GLY	-	insertion	UNP A0A3S9H6T3
6A	1	GLY	-	insertion	UNP A0A3S9H6T3
6B	1	GLY	-	insertion	UNP A0A3S9H6T3
6C	1	GLY	-	insertion	UNP A0A3S9H6T3
7A	1	GLY	-	insertion	UNP A0A3S9H6T3
7B	1	GLY	-	insertion	UNP A0A3S9H6T3
7C	1	GLY	-	insertion	UNP A0A3S9H6T3

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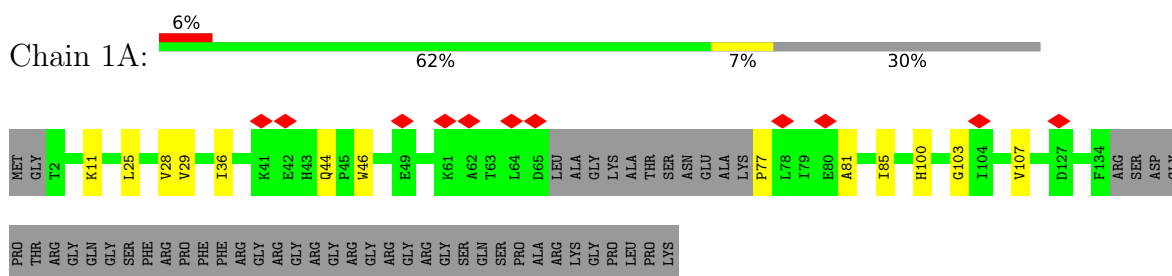
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Chain	Residue	Modelled	Actual	Comment	Reference
8A	1	GLY	-	insertion	UNP A0A3S9H6T3
8B	1	GLY	-	insertion	UNP A0A3S9H6T3
8C	1	GLY	-	insertion	UNP A0A3S9H6T3
AA	1	GLY	-	insertion	UNP A0A3S9H6T3
AB	1	GLY	-	insertion	UNP A0A3S9H6T3

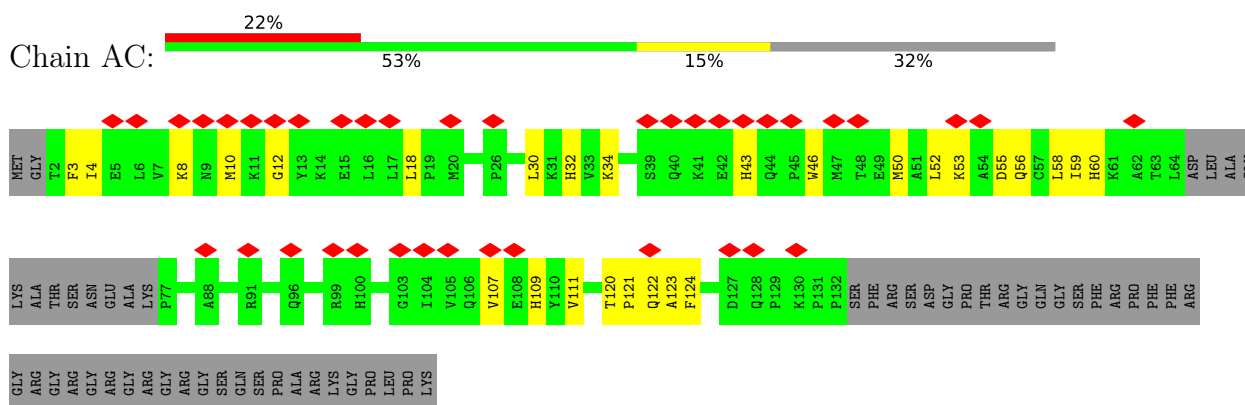
3 Residue-property plots [i](#)

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.

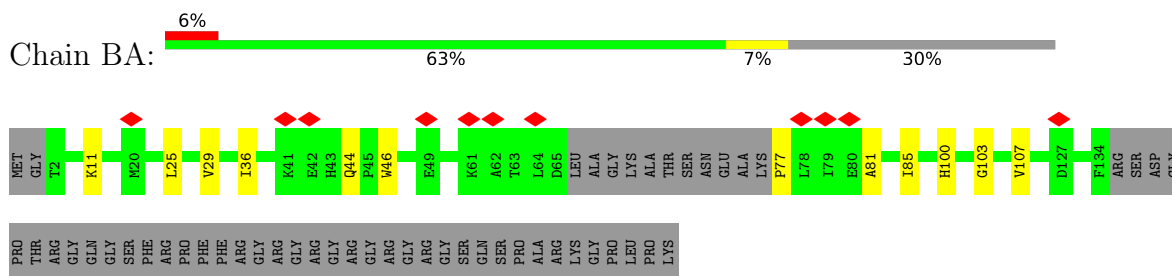
- Molecule 1: C protein



- Molecule 1: C protein

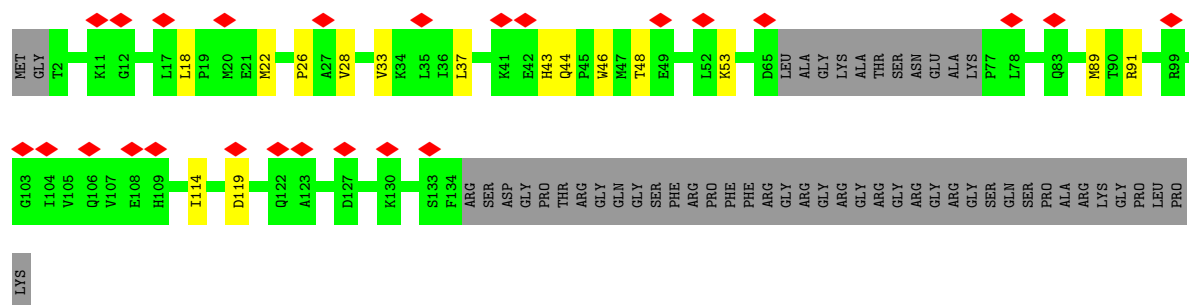


- Molecule 1: C protein

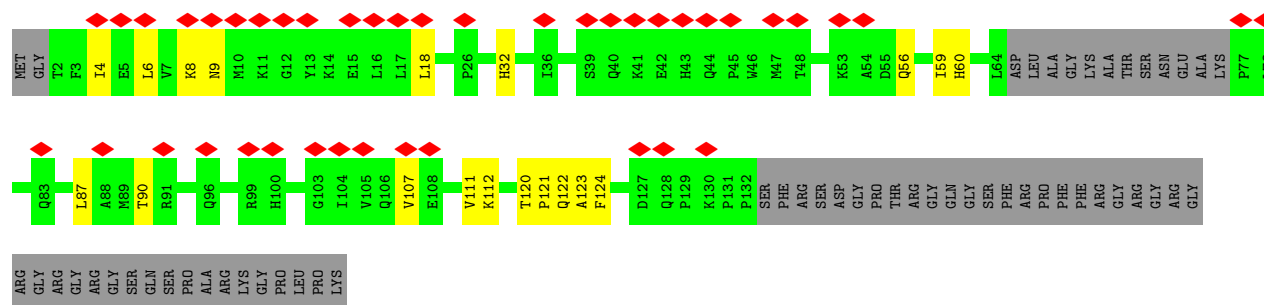


- Molecule 1: C protein

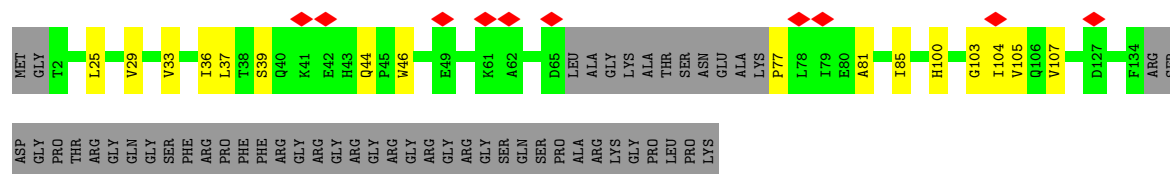




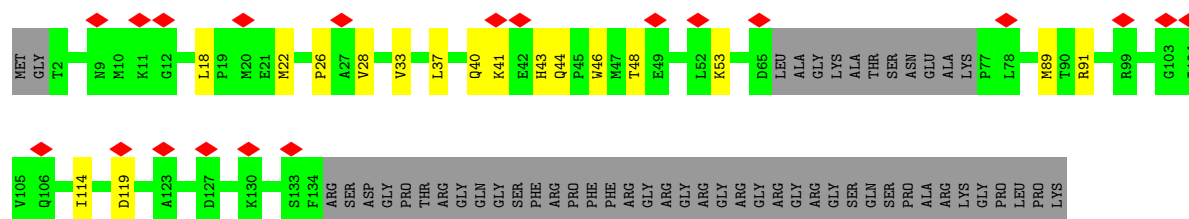
- Molecule 1: C protein



- Molecule 1: C protein

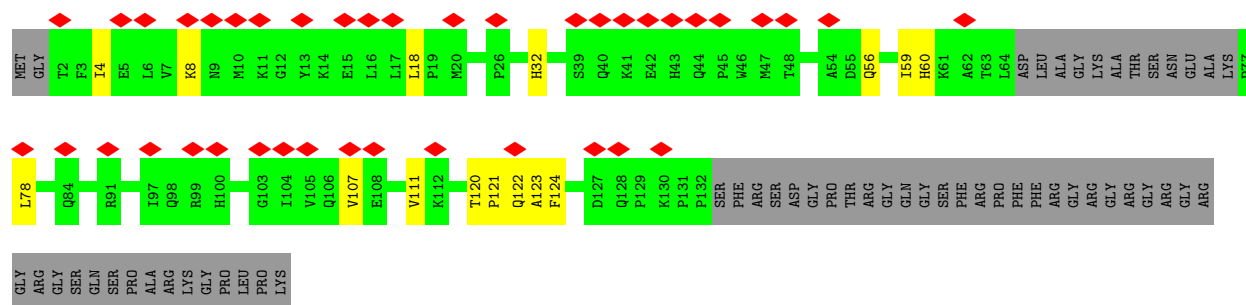


- Molecule 1: C protein

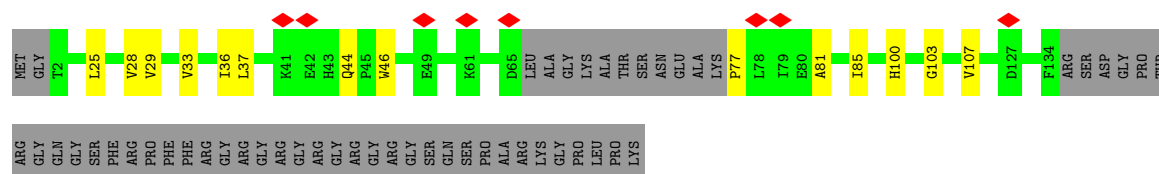


- Molecule 1: C protein

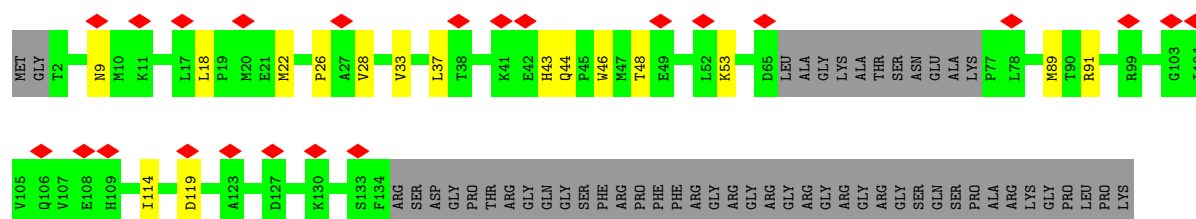




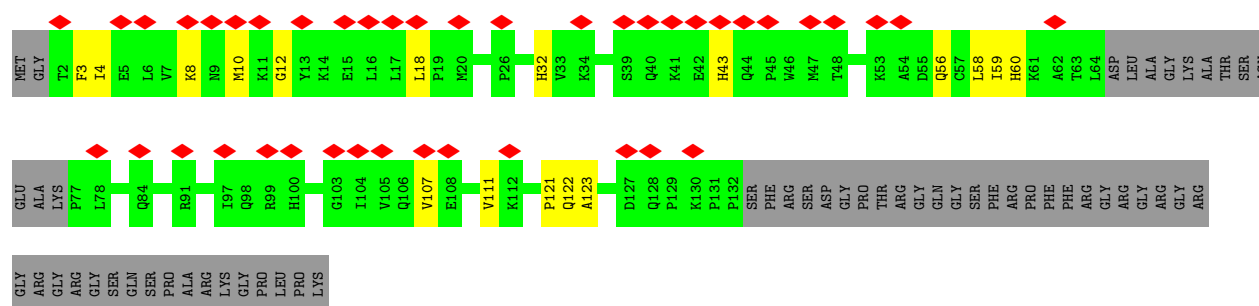
- Molecule 1: C protein



- Molecule 1: C protein



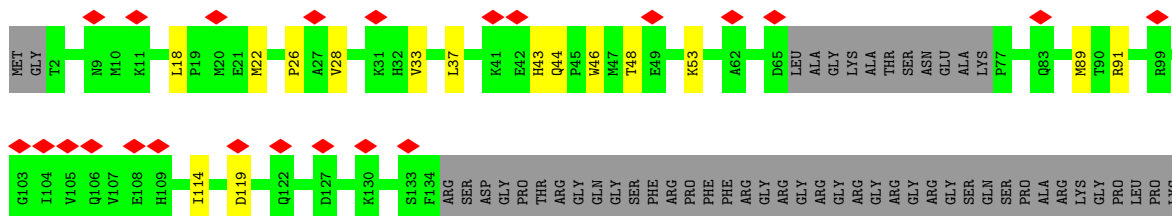
- Molecule 1: C protein



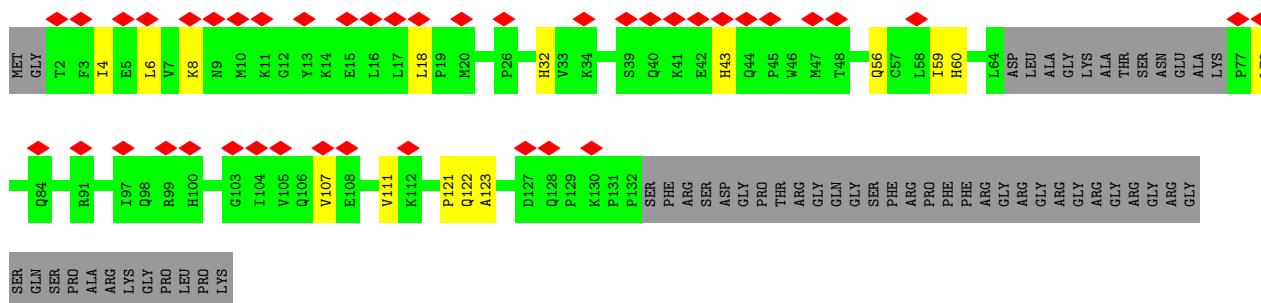
- Molecule 1: C protein



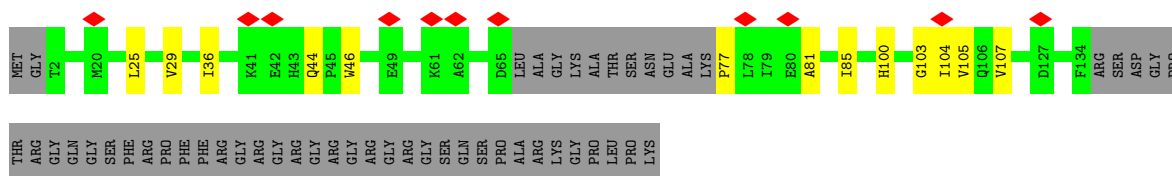
- Molecule 1: C protein



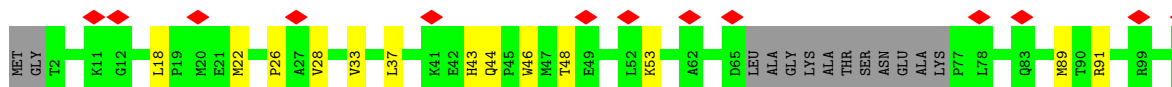
- Molecule 1: C protein

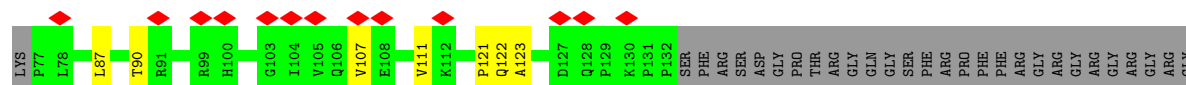


- Molecule 1: C protein



- Molecule 1: C protein

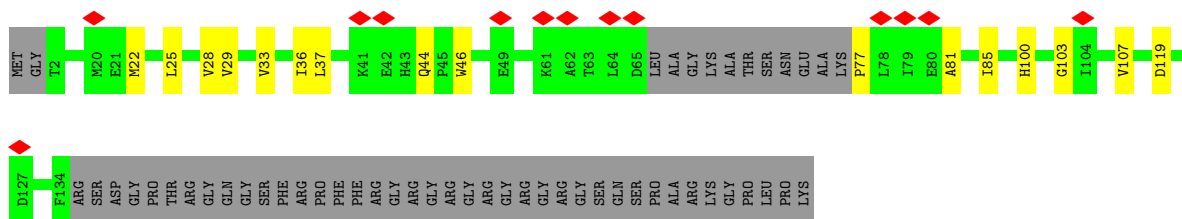




ARG
GLY
SER
GLN
PRO
PRO
ALA
ARG
LYS
GLY
PRO
LEU
PRO
LYS

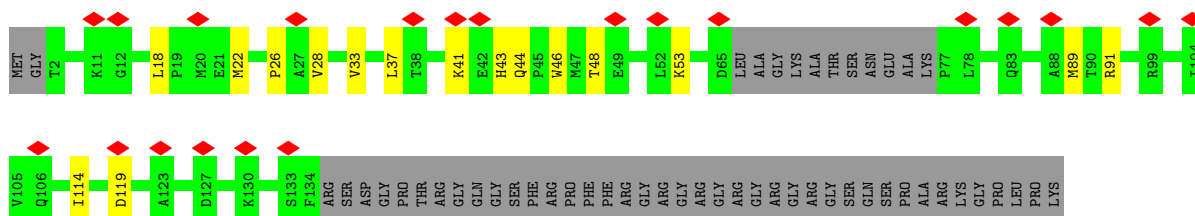
• Molecule 1: C protein

Chain HA: 7% 61% 9% 30%



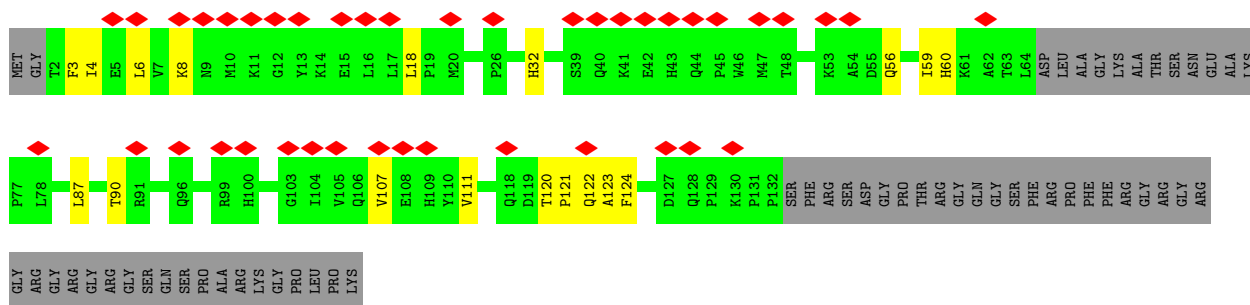
• Molecule 1: C protein

Chain HB: 12% 61% 9% 30%



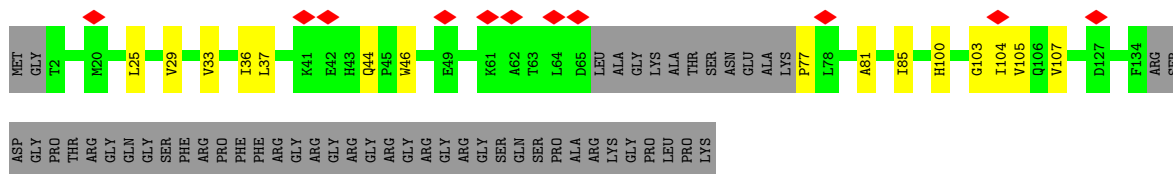
• Molecule 1: C protein

Chain HC: 23% 58% 10% 32%



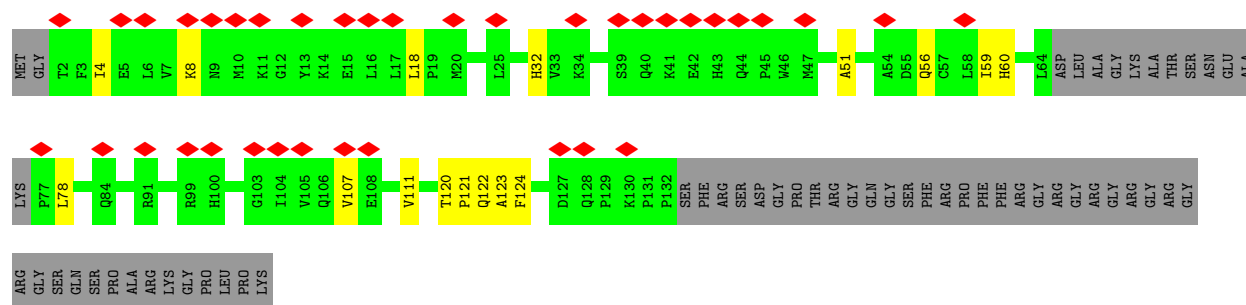
• Molecule 1: C protein

Chain IA: 6% 61% 9% 30%

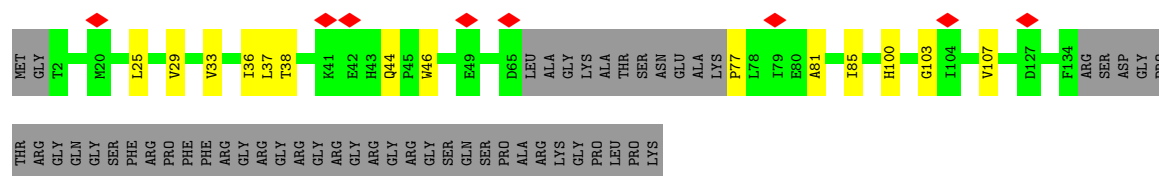


• Molecule 1: C protein

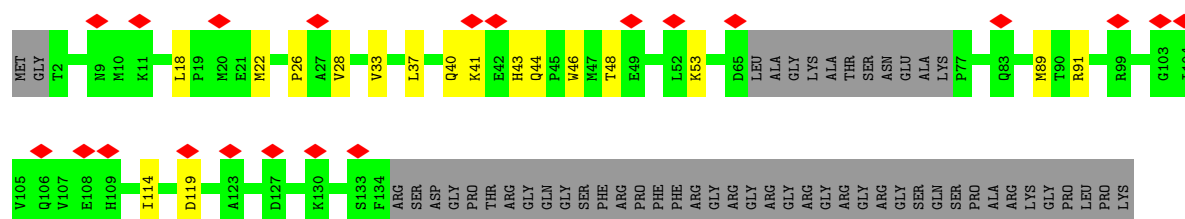




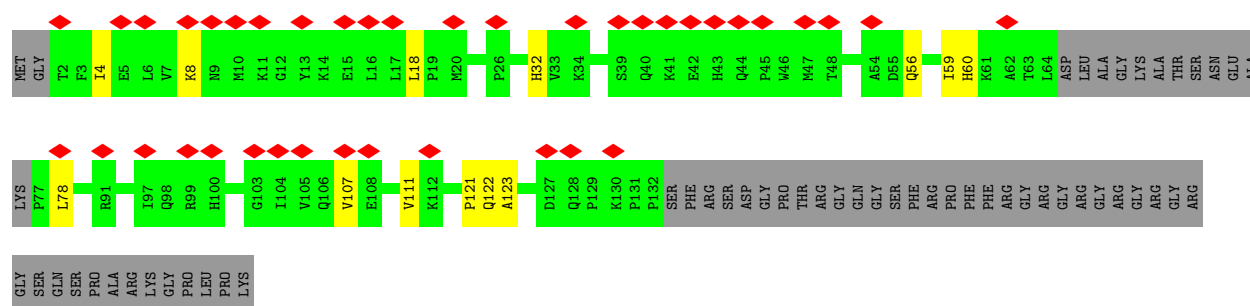
- Molecule 1: C protein



- Molecule 1: C protein

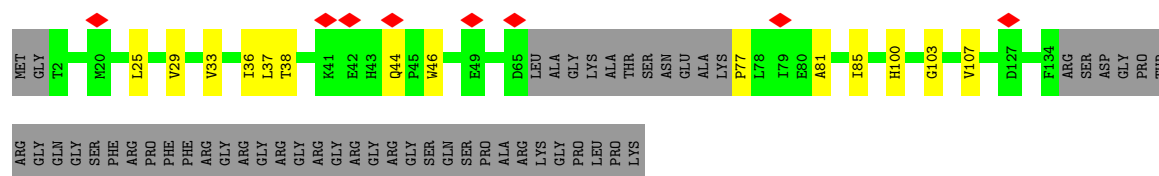


- Molecule 1: C protein

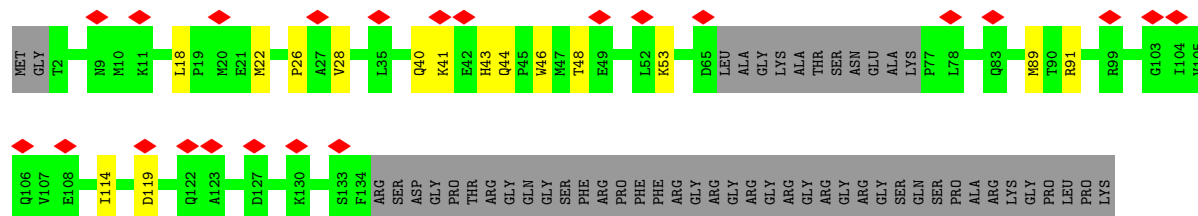


- Molecule 1: C protein

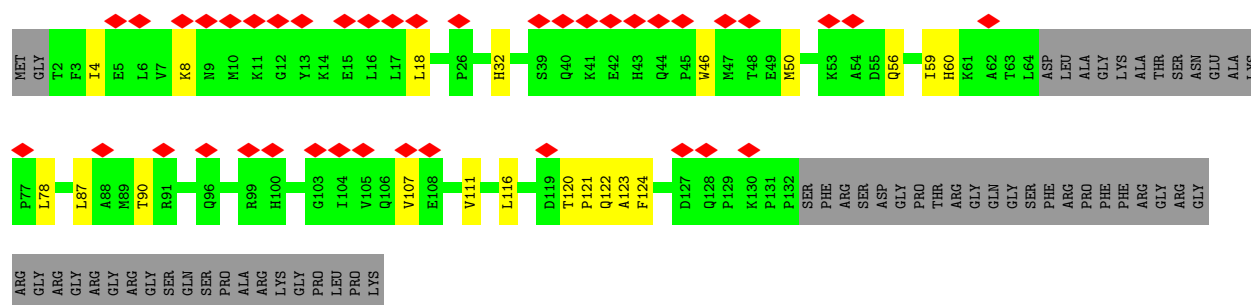




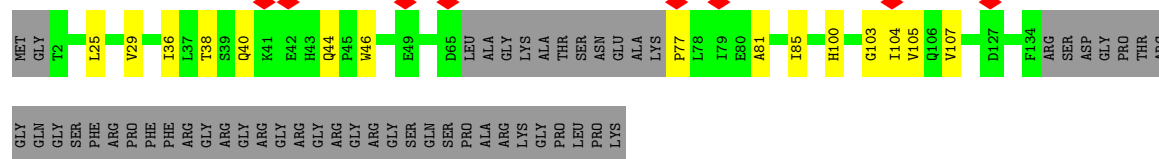
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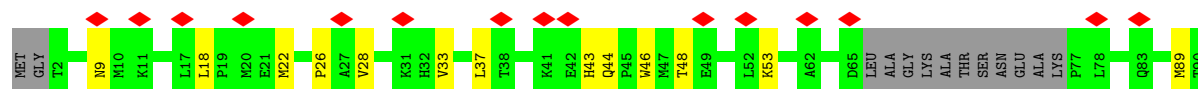
• Molecule 1: C protein

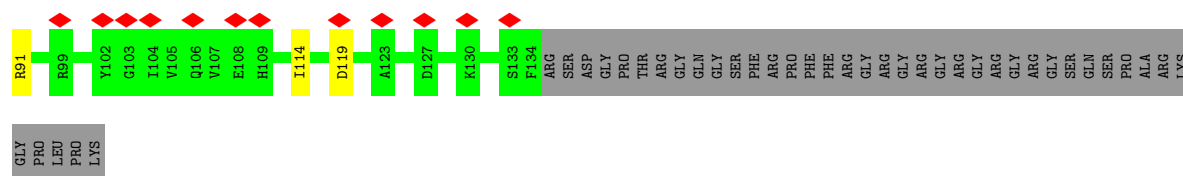


• Molecule 1: C protein

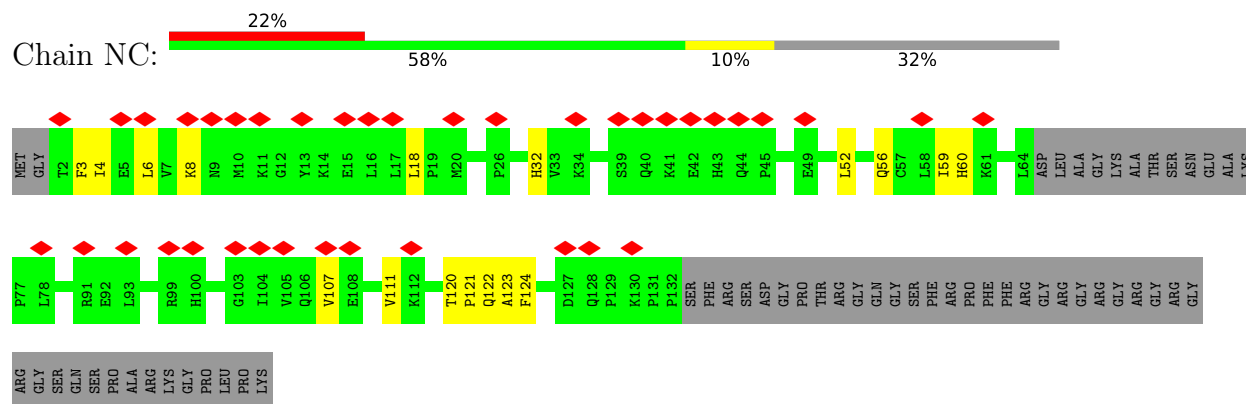


• Molecule 1: C protein

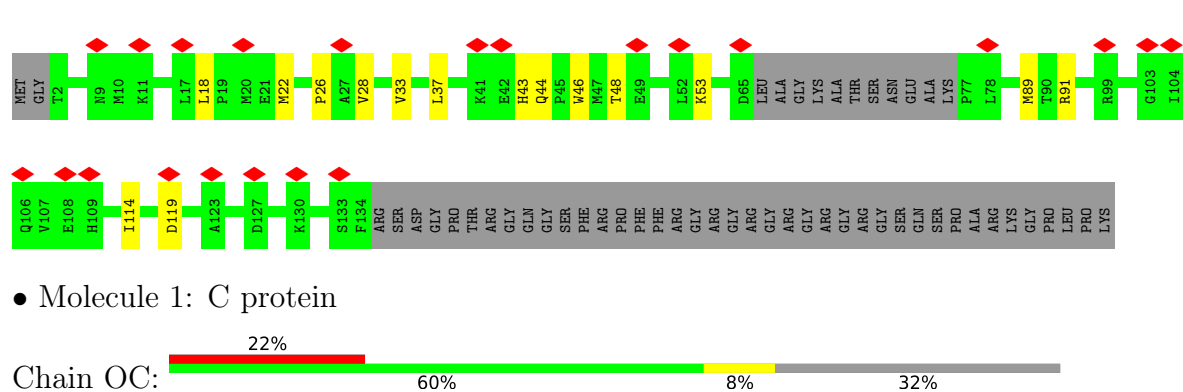
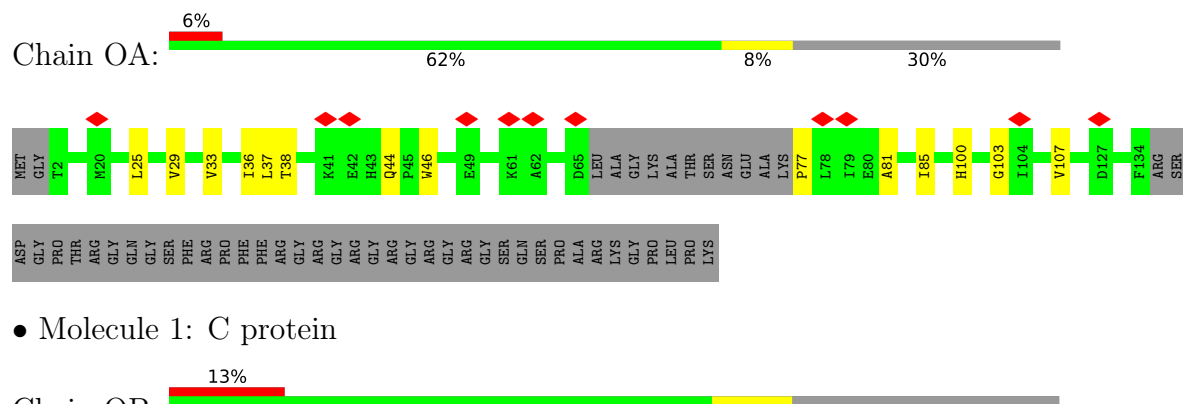




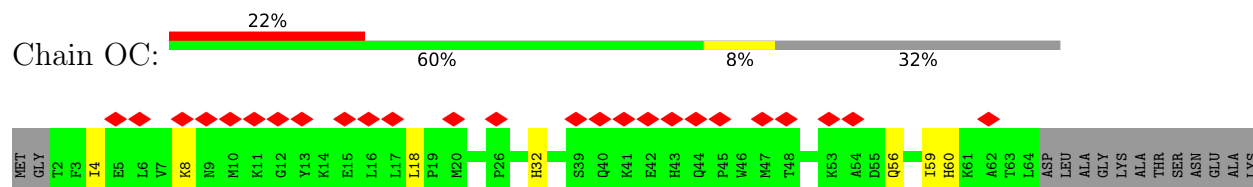
- Molecule 1: C protein

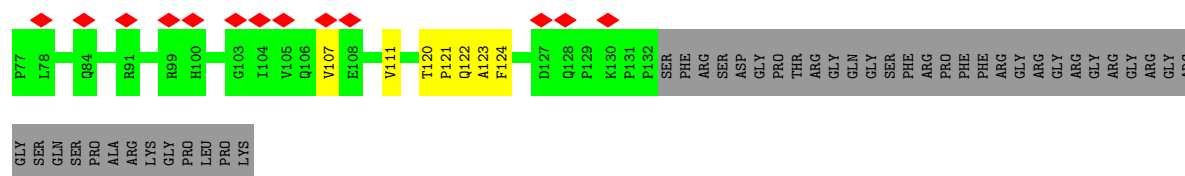


- Molecule 1: C protein

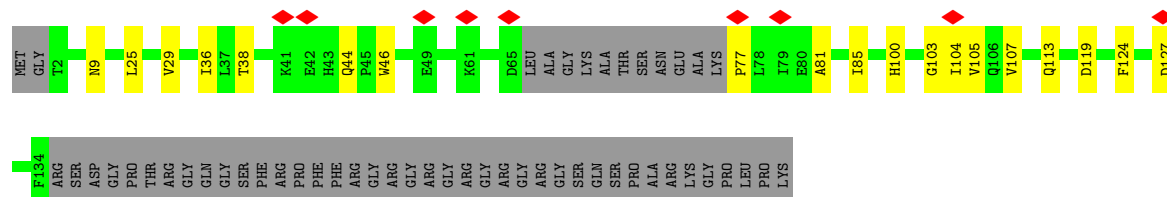


- Molecule 1: C protein

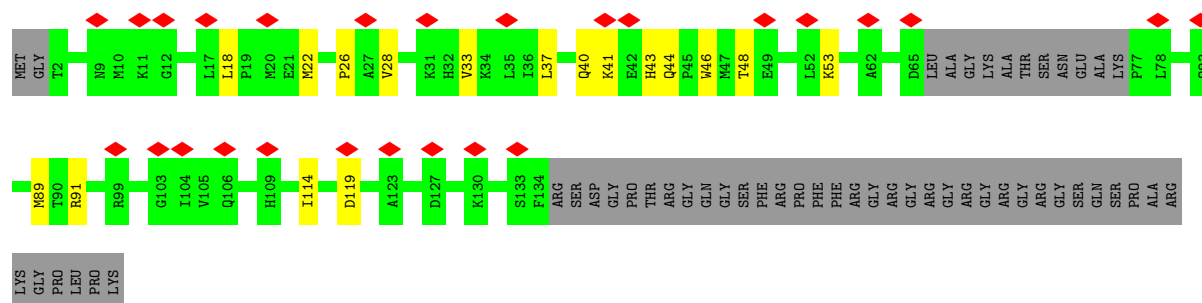




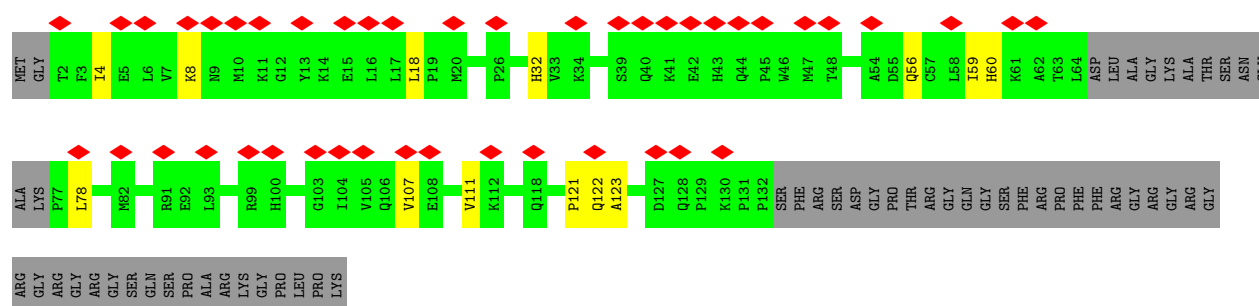
• Molecule 1: C protein



• Molecule 1: C protein

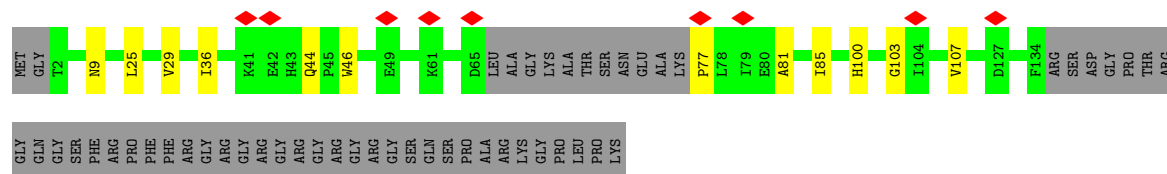


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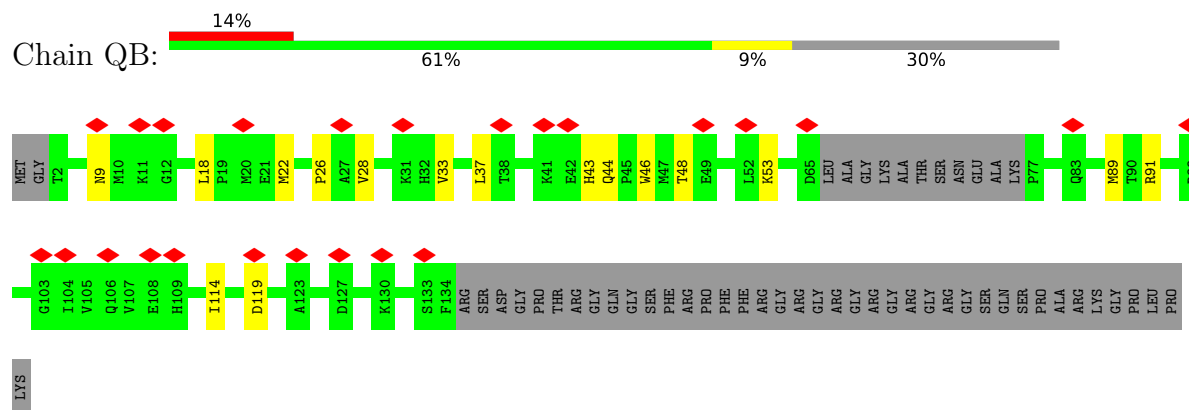


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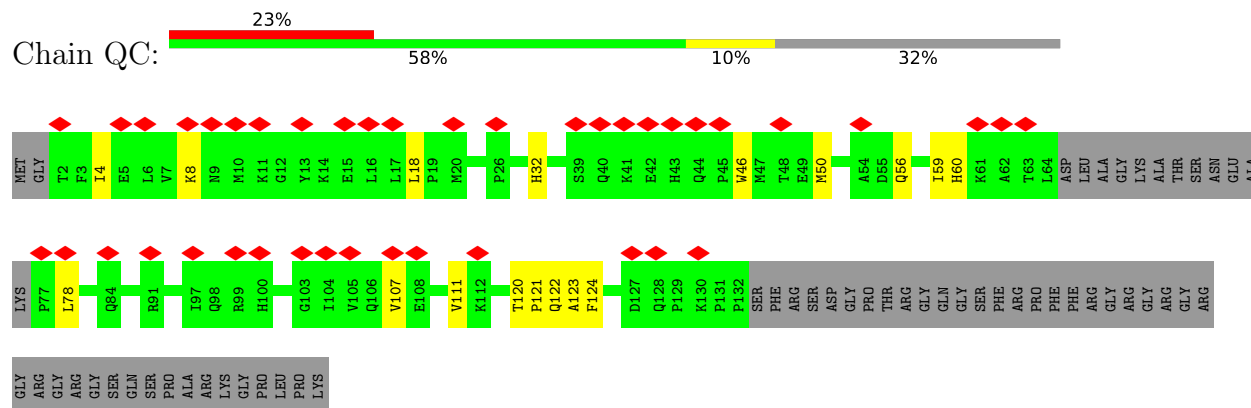




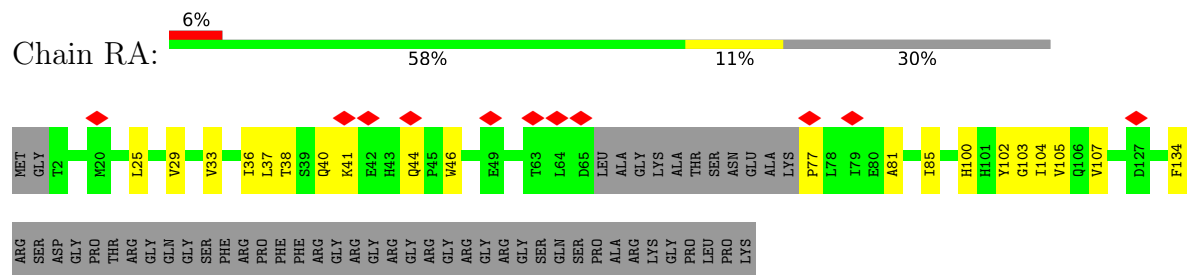
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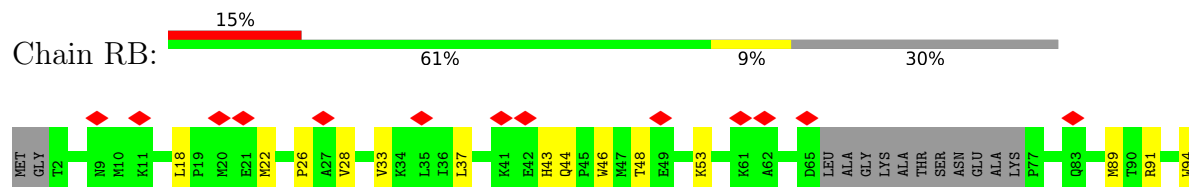
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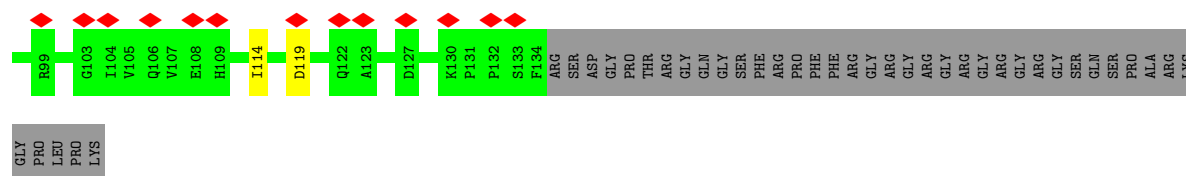


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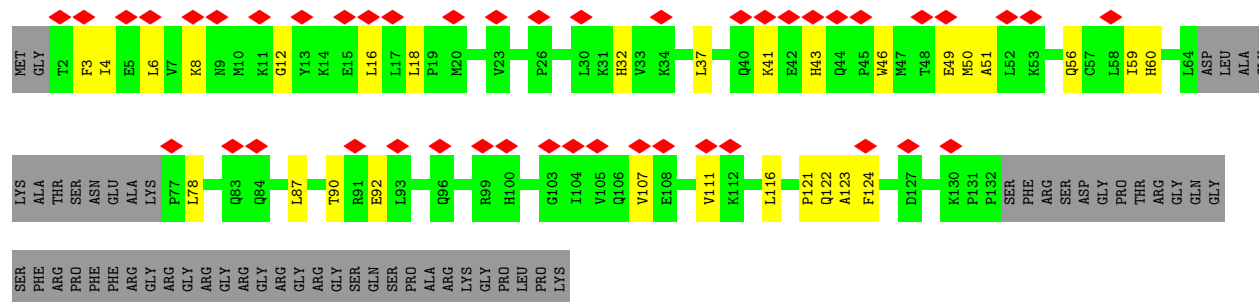


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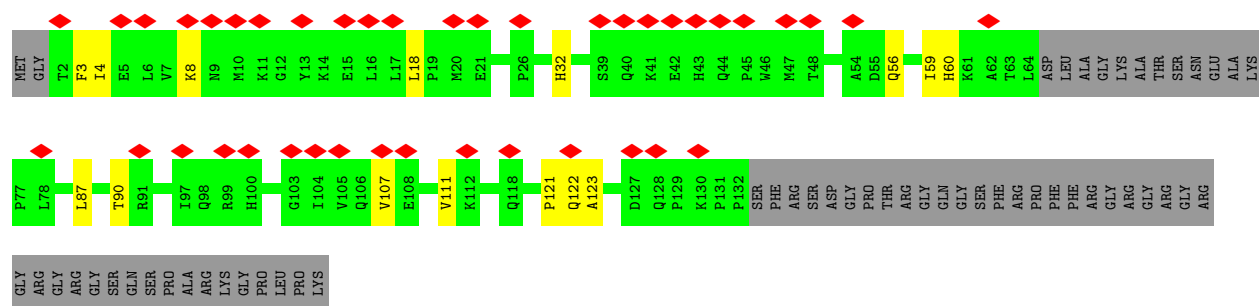




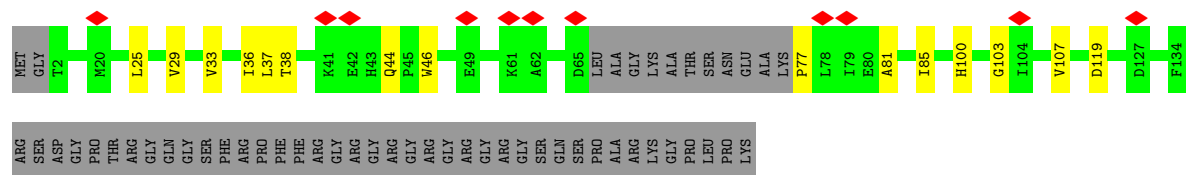
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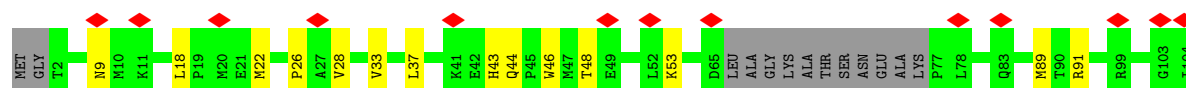
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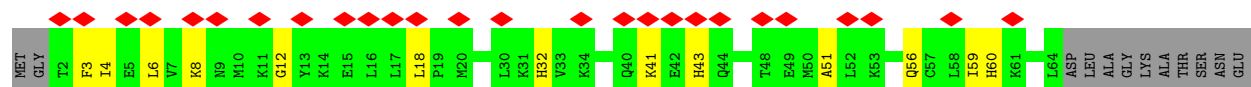


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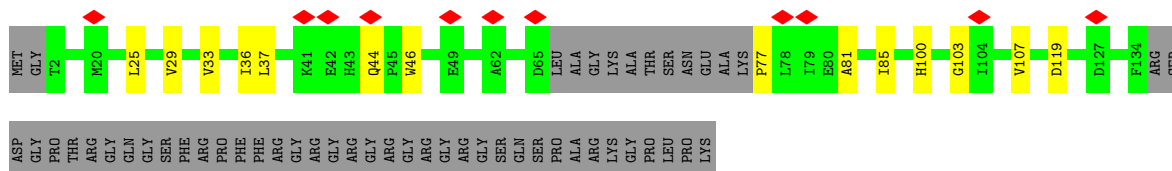


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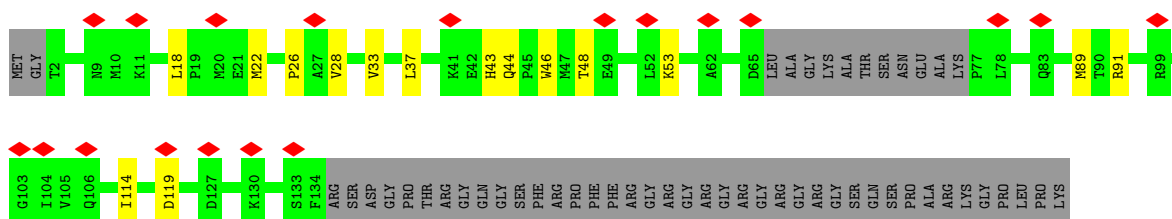




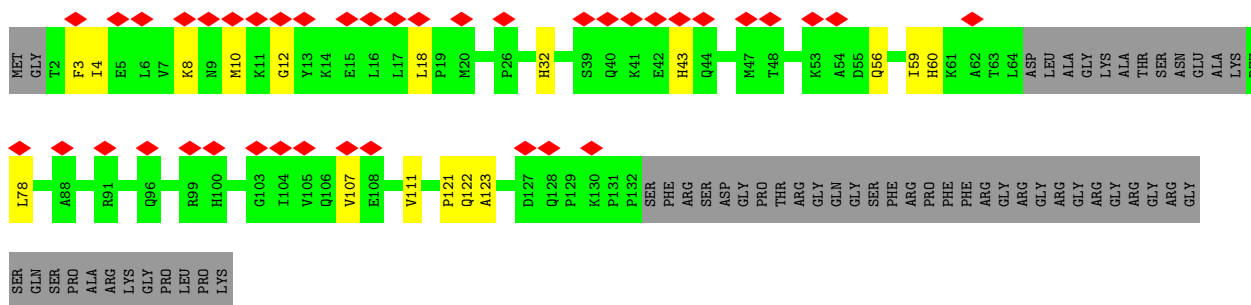
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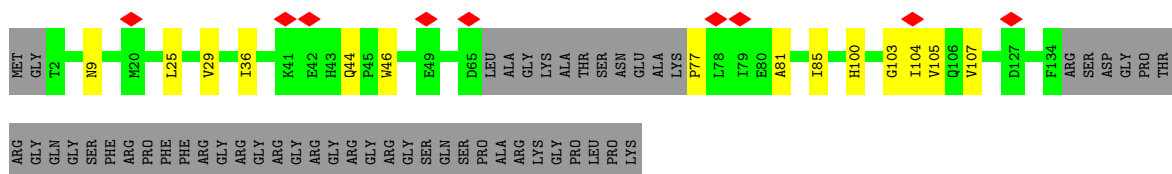
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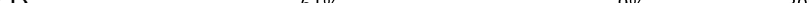


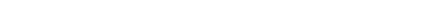
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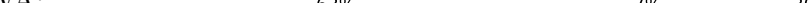


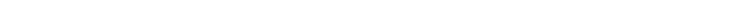
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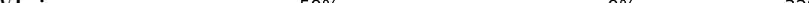


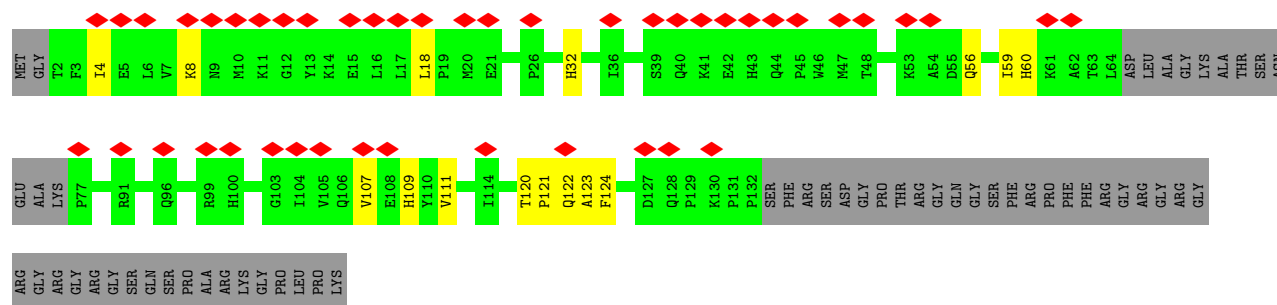
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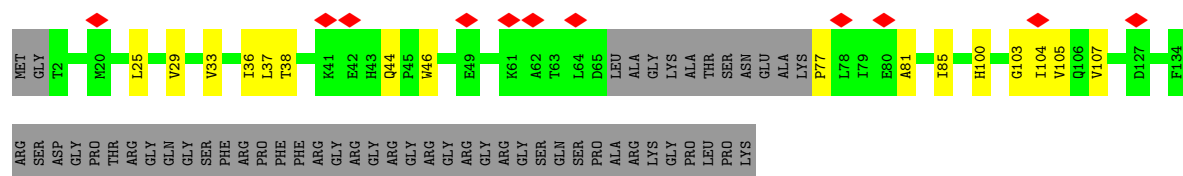
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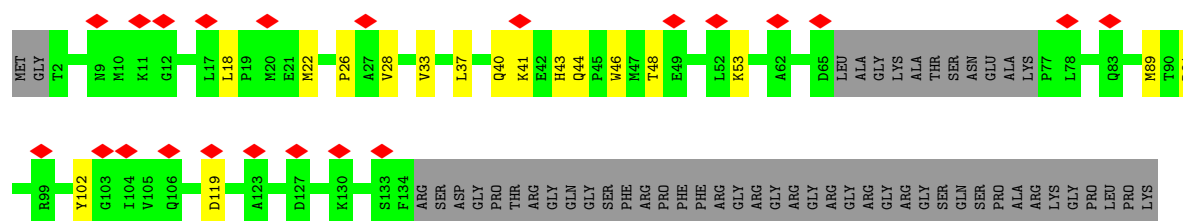
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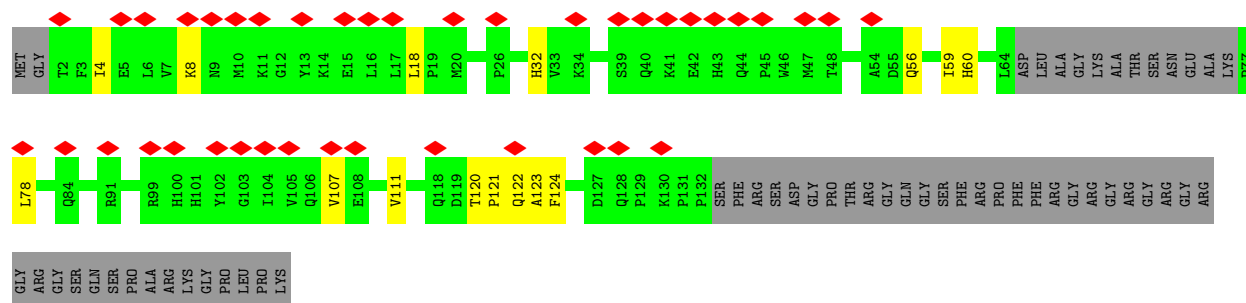
• Molecule 1: C protein



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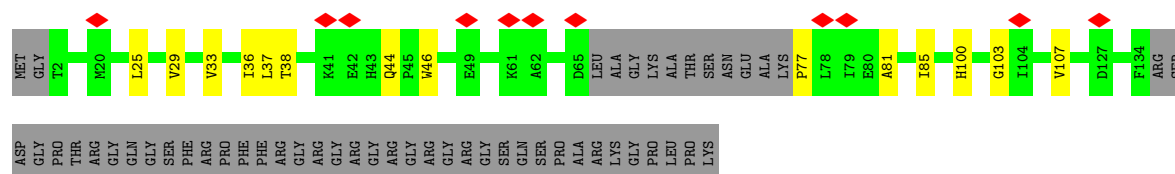


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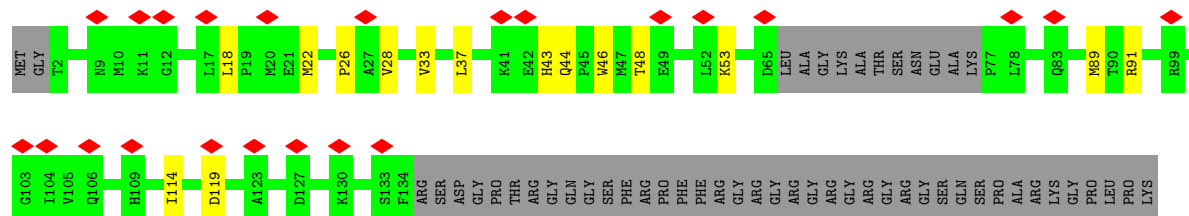


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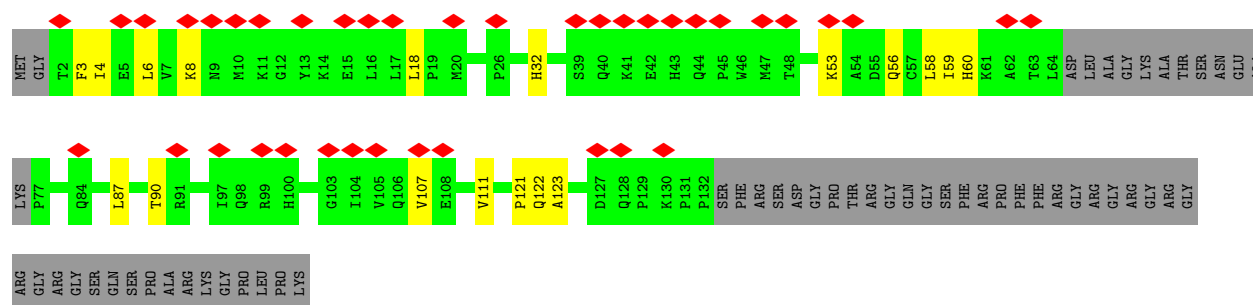




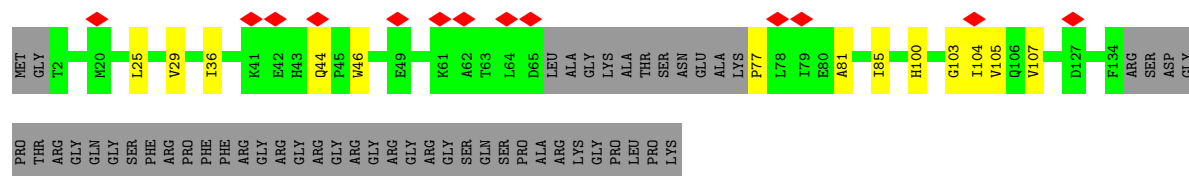
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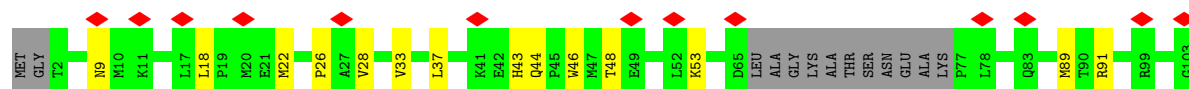
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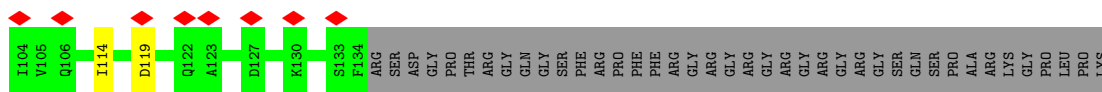


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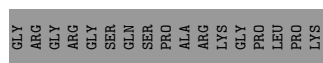
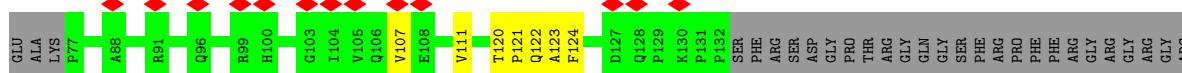
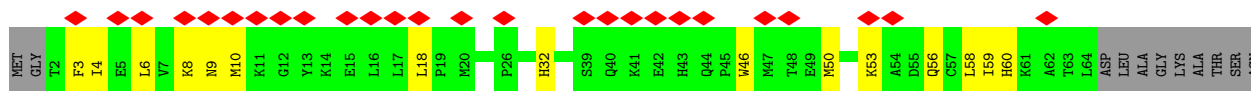


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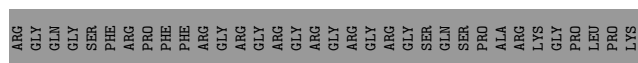
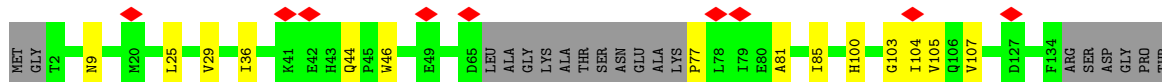




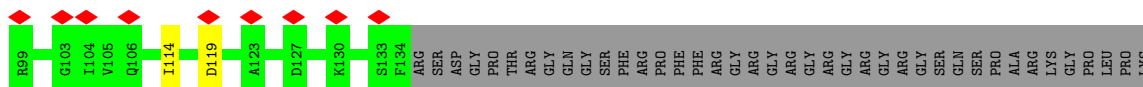
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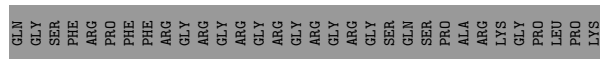
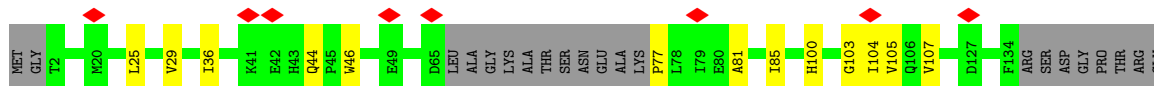
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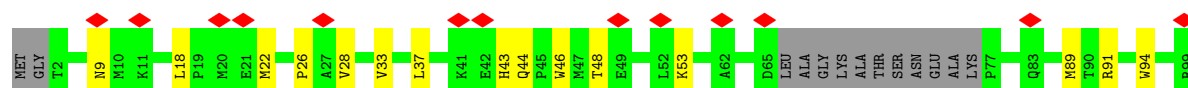
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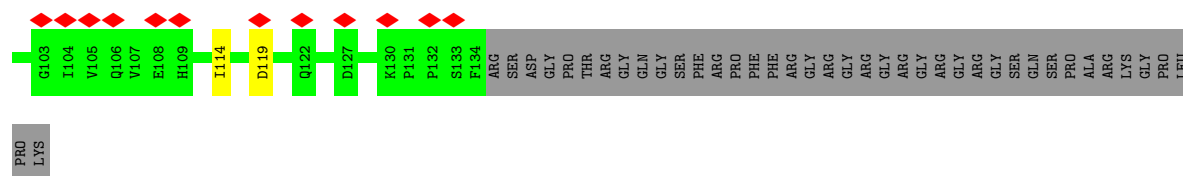


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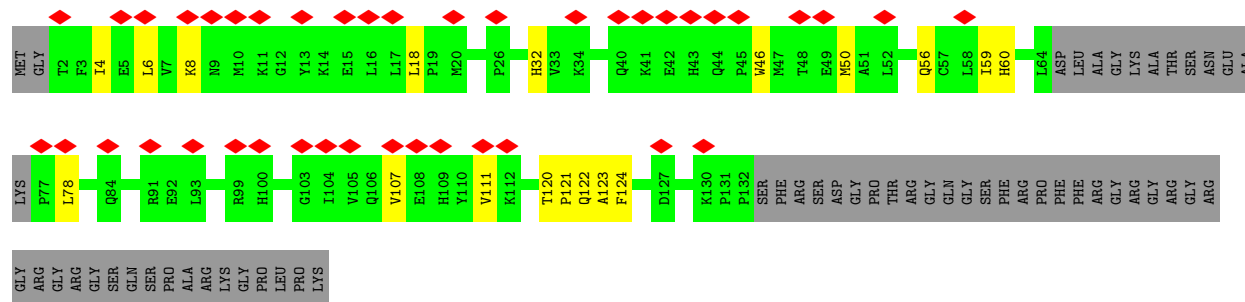


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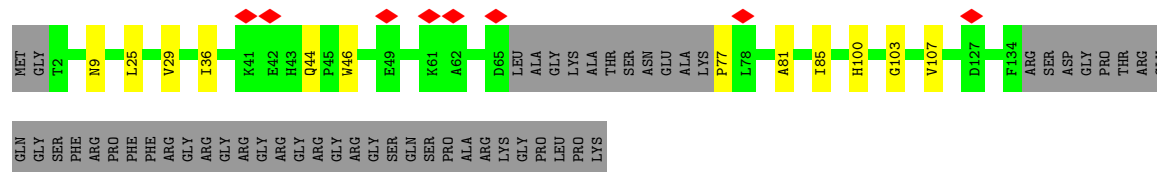




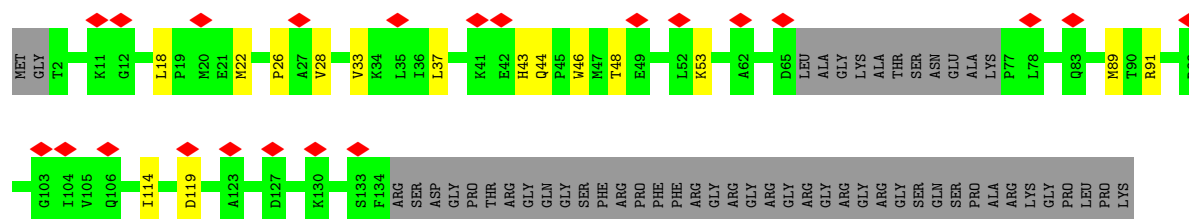
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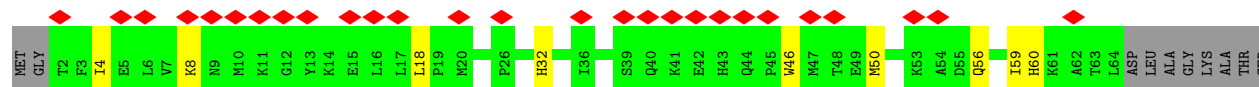
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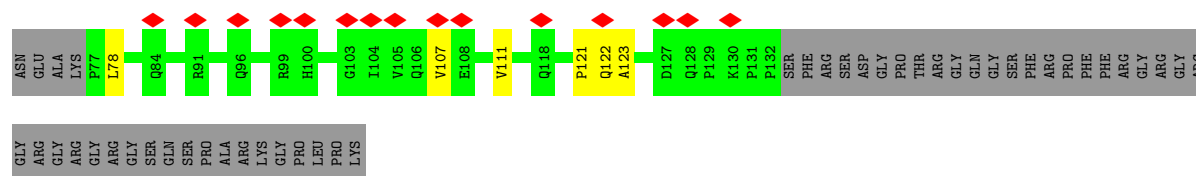


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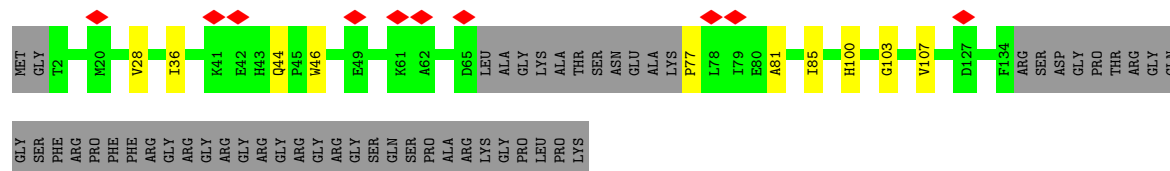


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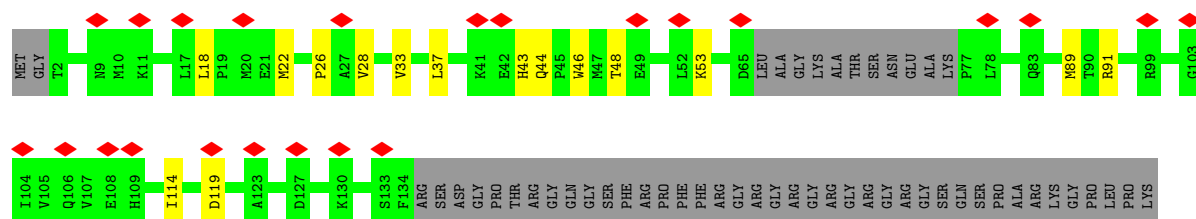




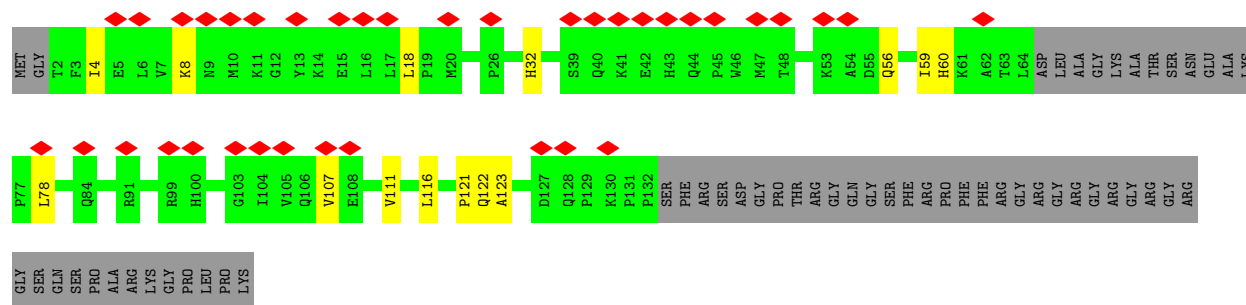
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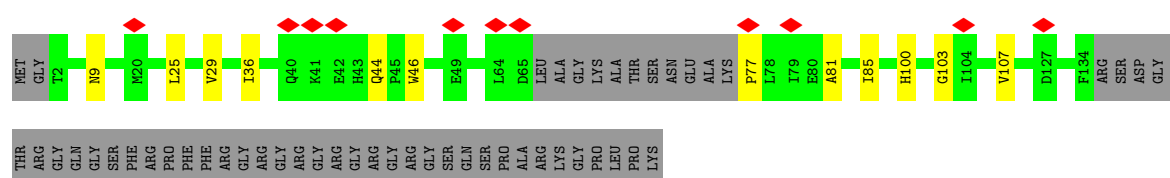
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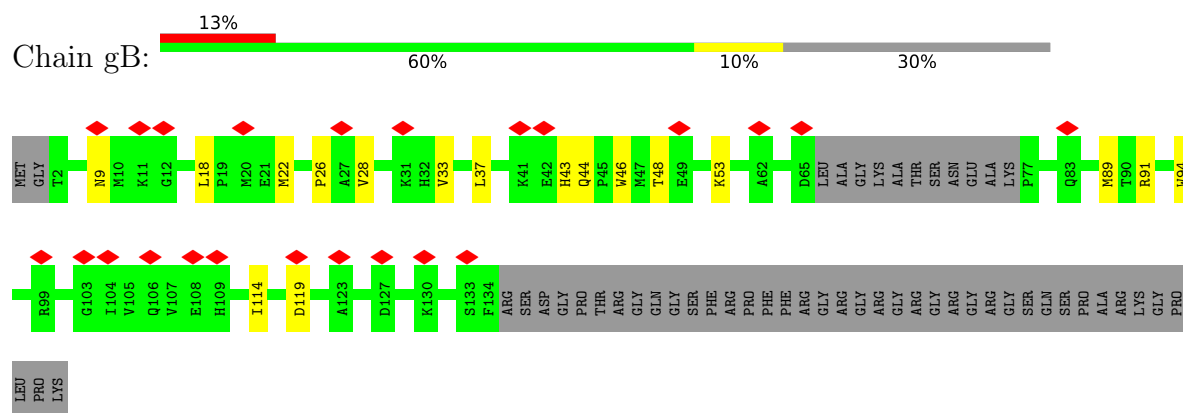
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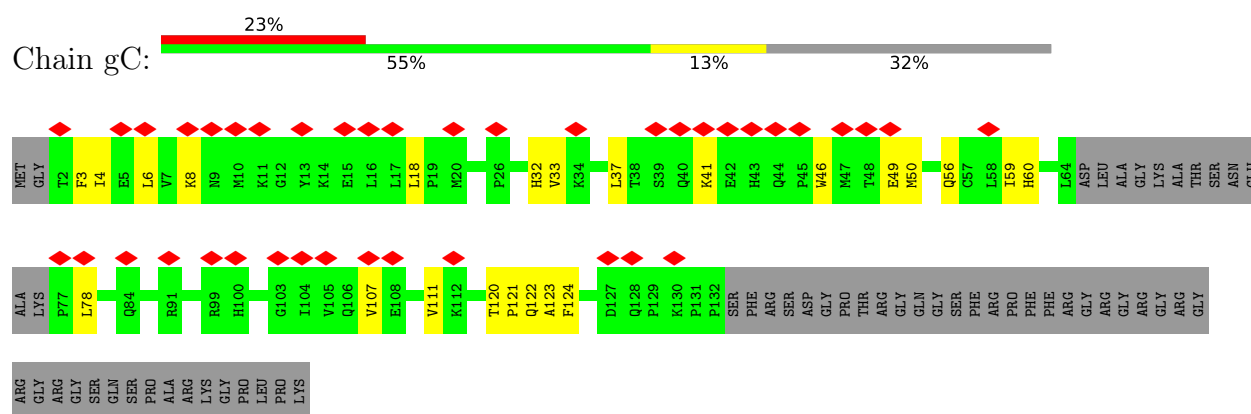
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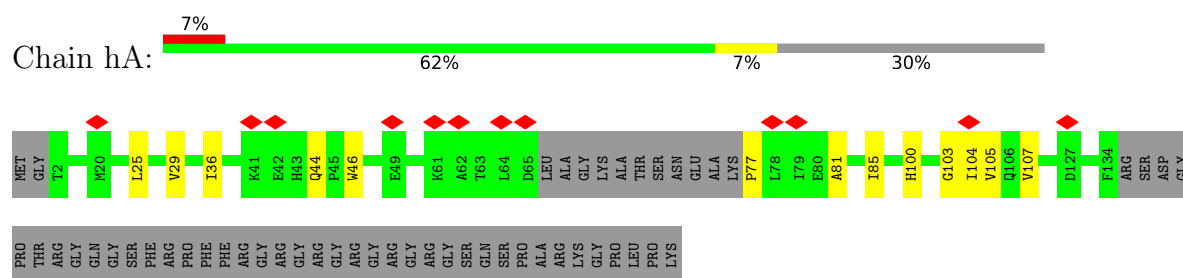
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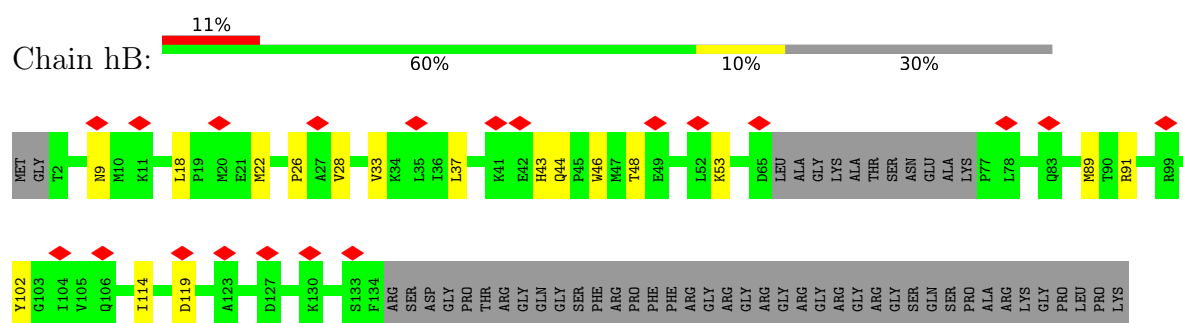
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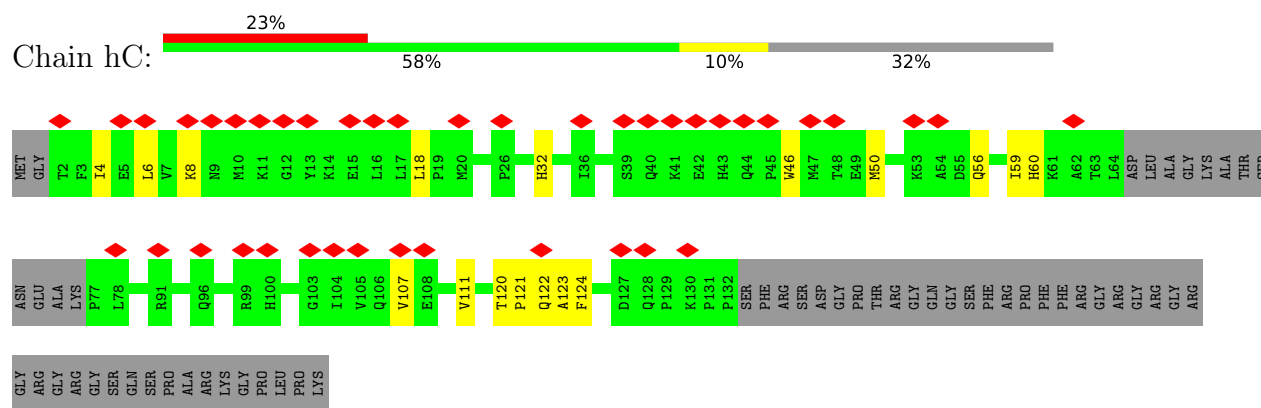
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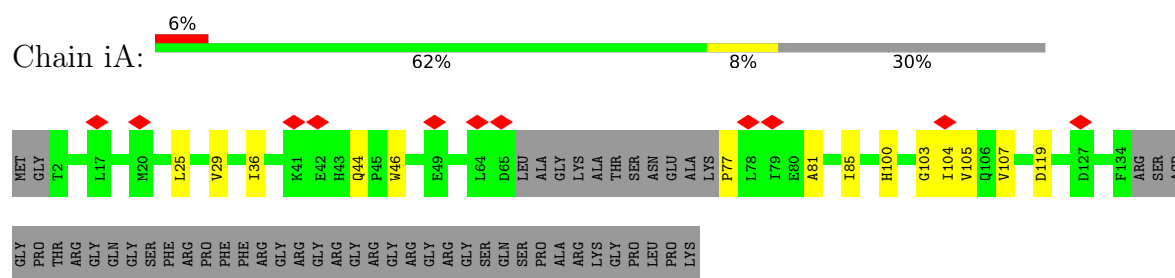
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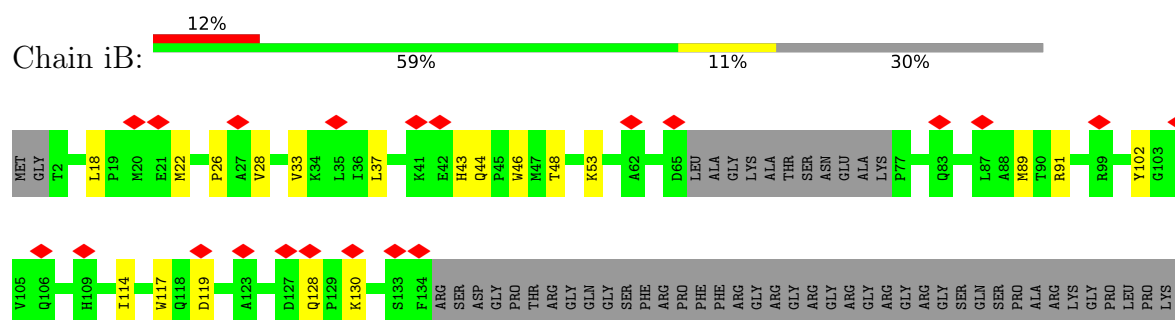
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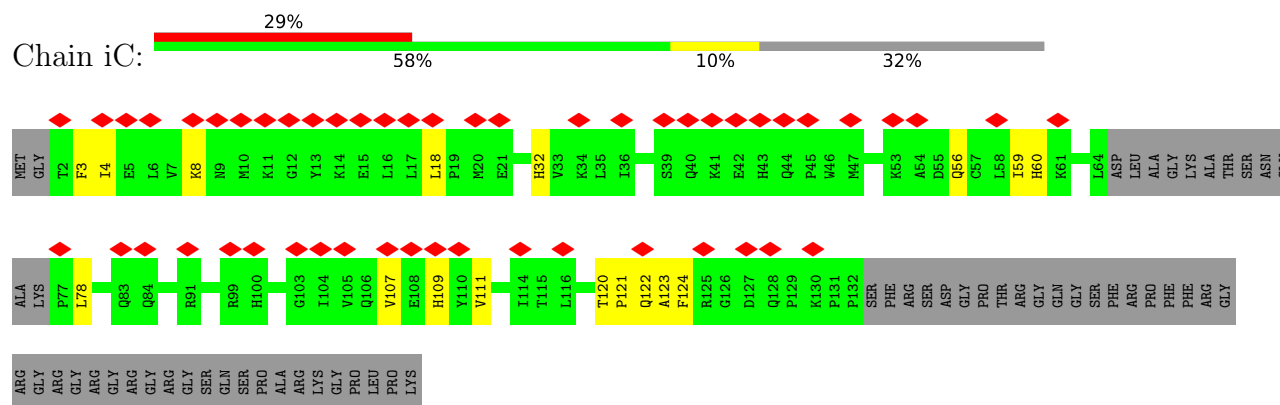
- Molecule 1: C protein



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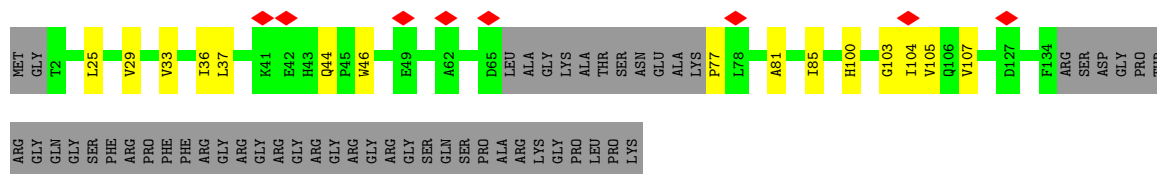
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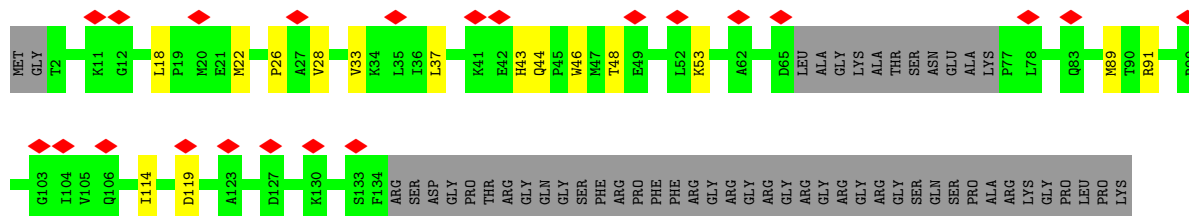
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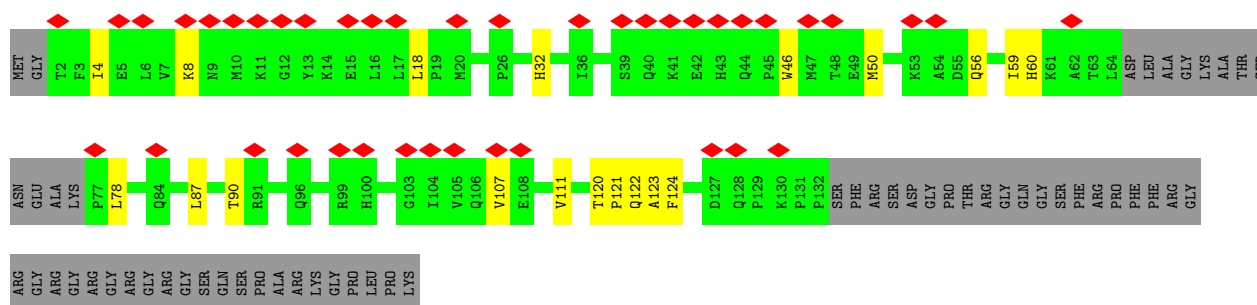




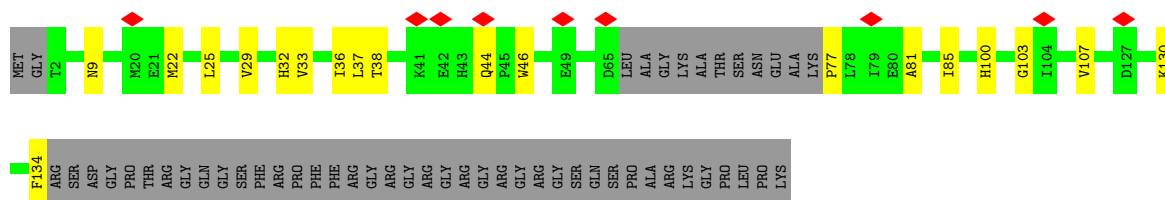
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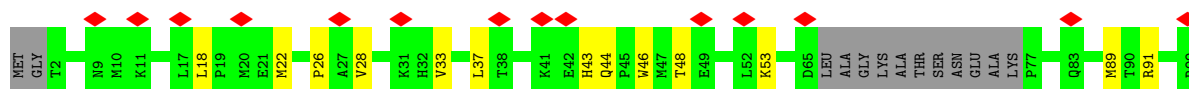
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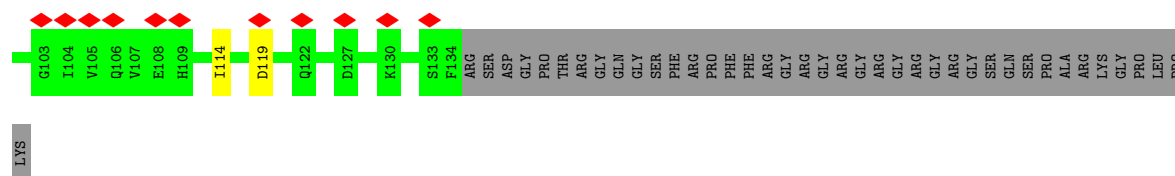


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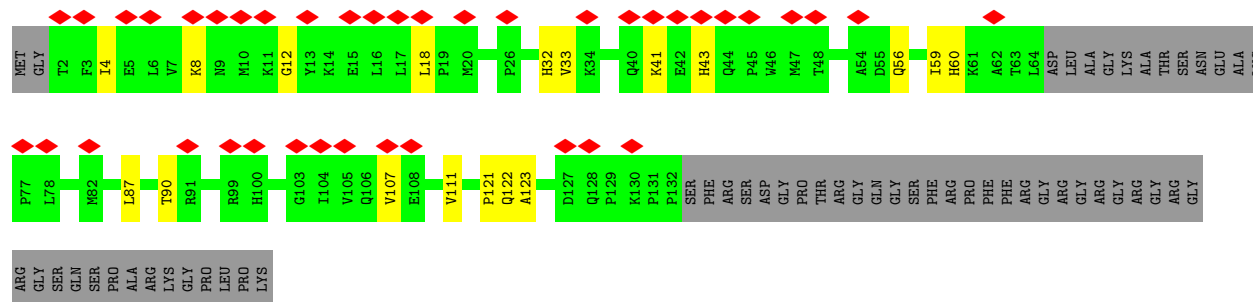


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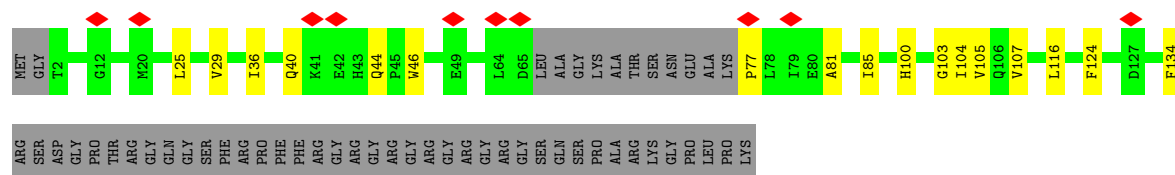




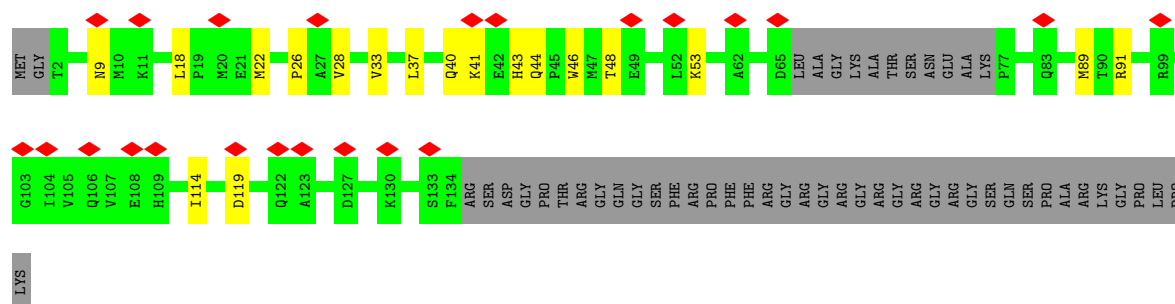
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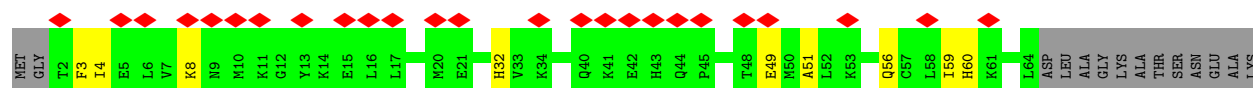
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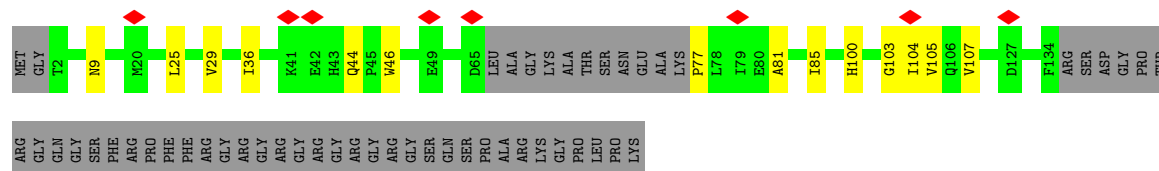
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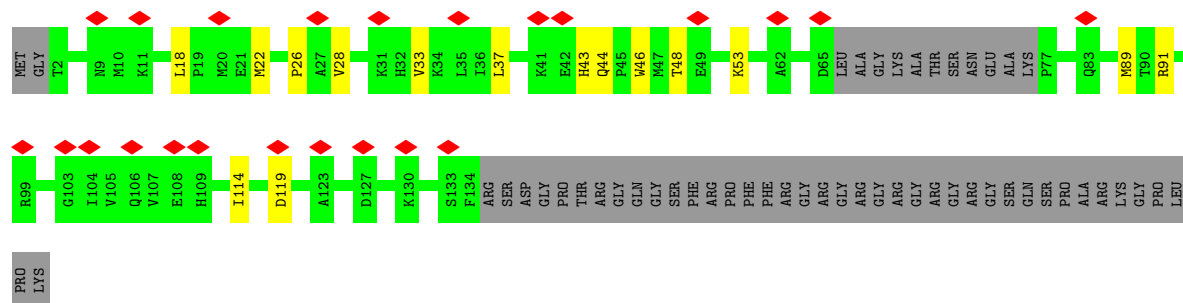
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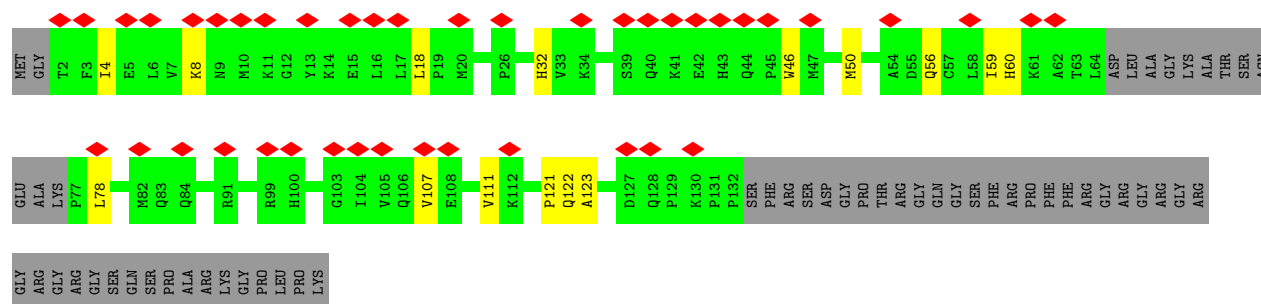
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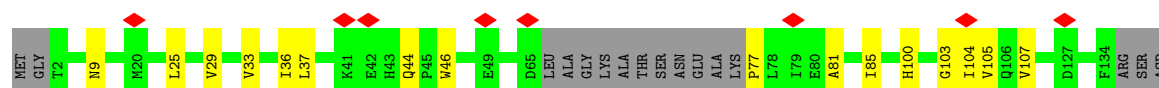
- Molecule 1: C protein



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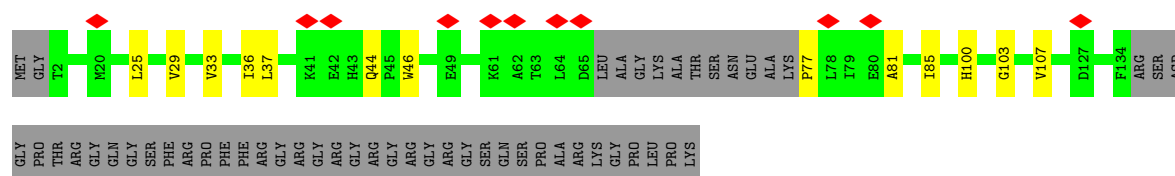
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Chain qA:

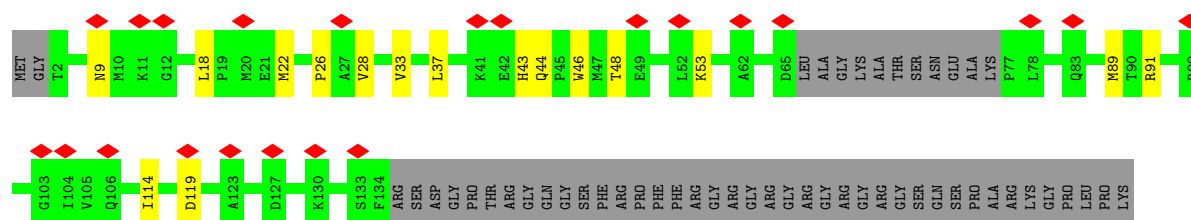
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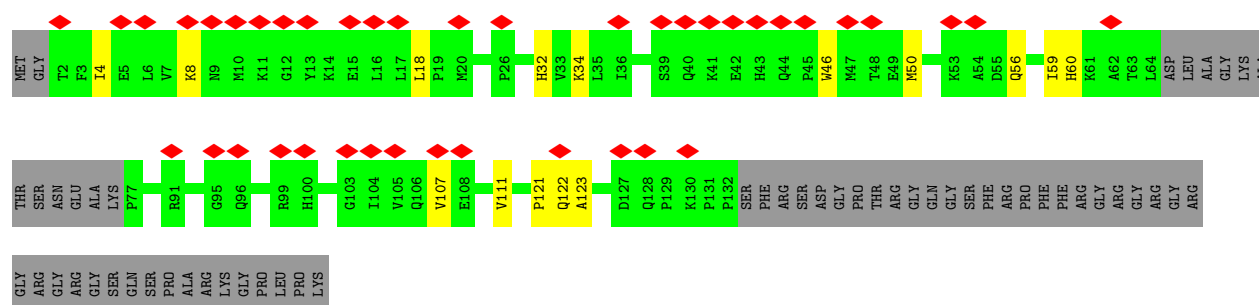
- Molecule 1: C protein



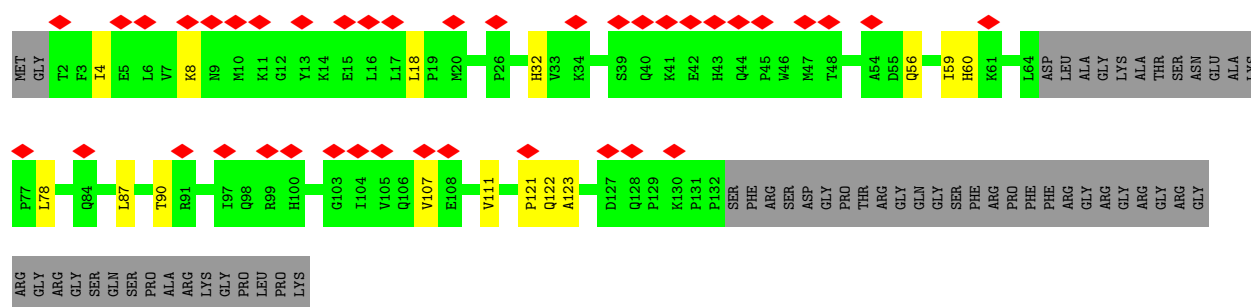
• Molecule 1: C protein



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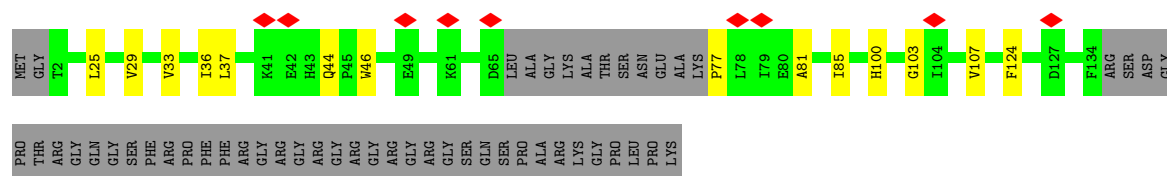


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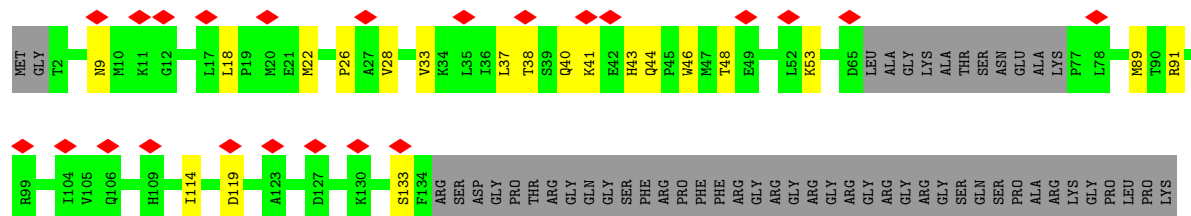


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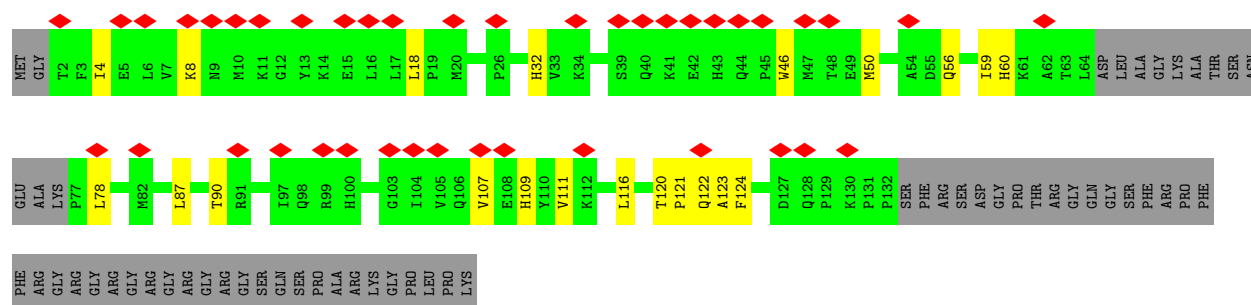




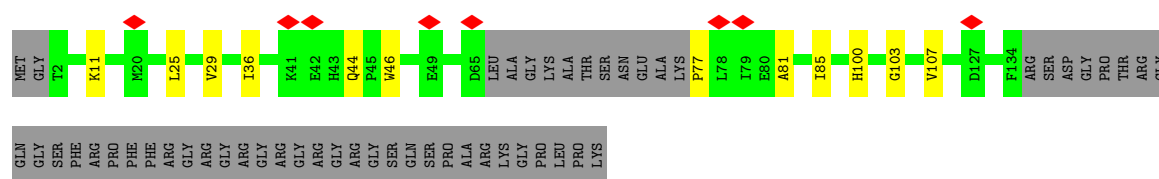
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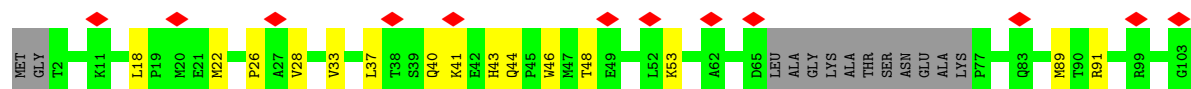
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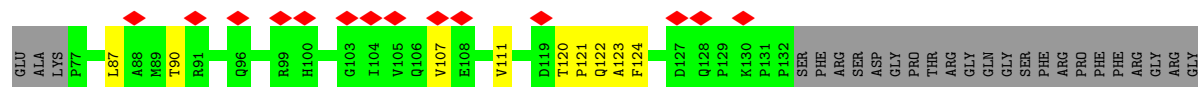


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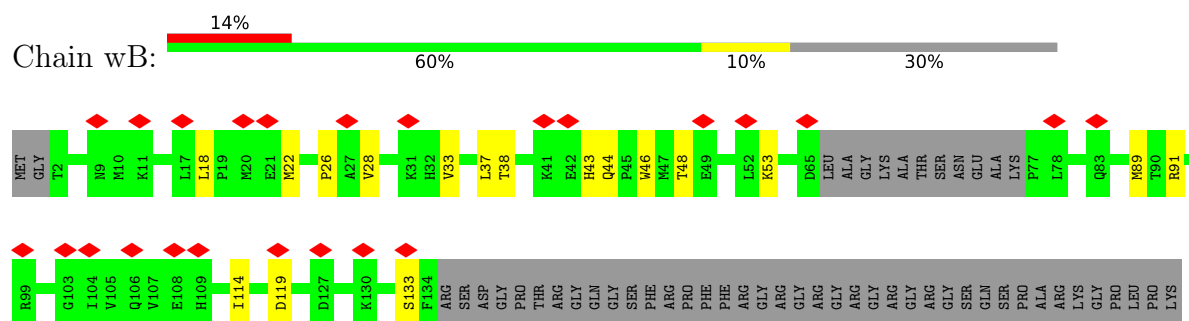


- Molecule 1: C protein

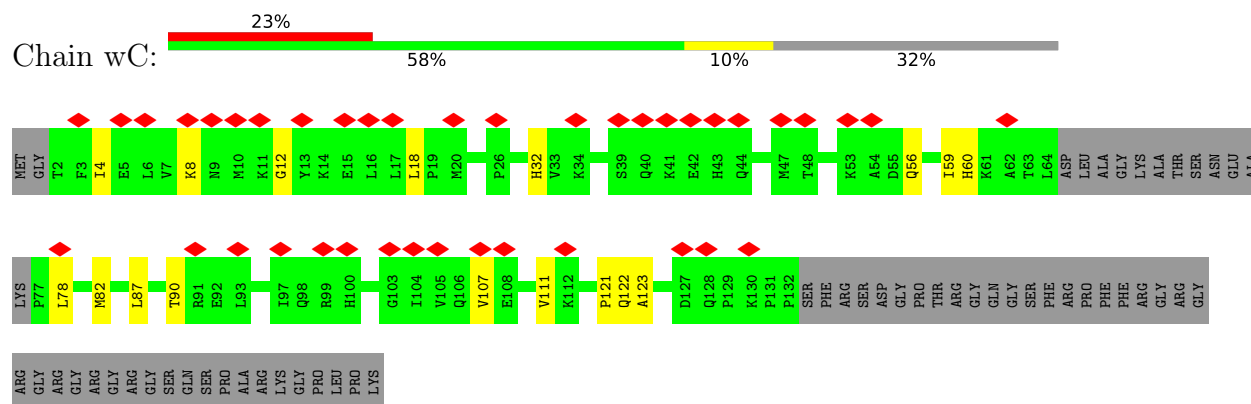




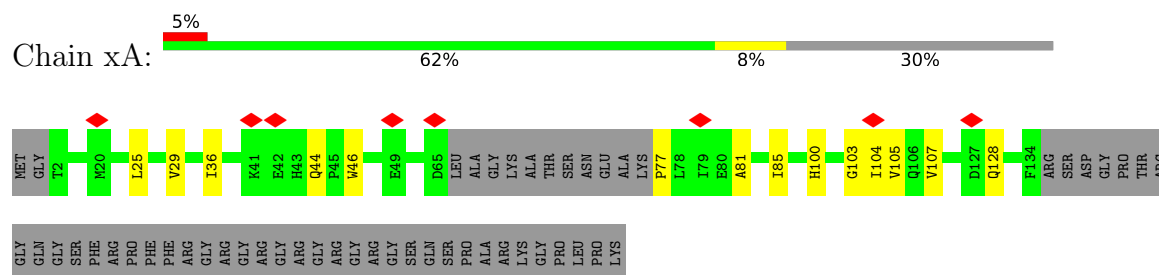
• Molecule 1: C protein



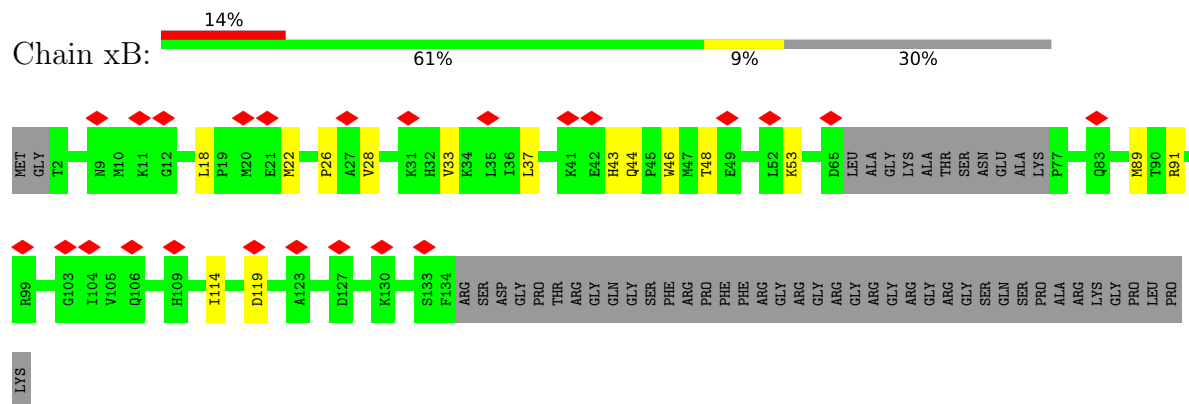
• Molecule 1: C protein



• Molecule 1: C protein

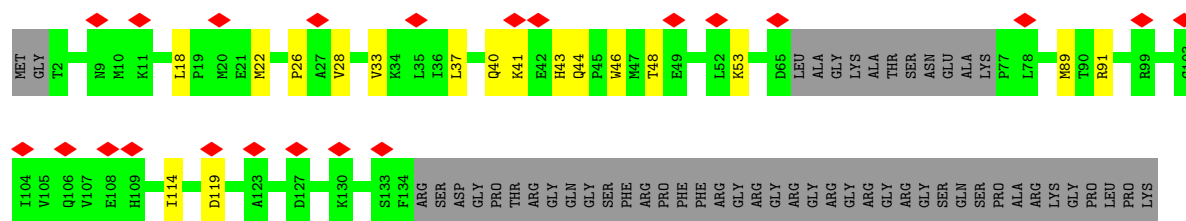


• Molecule 1: C protein

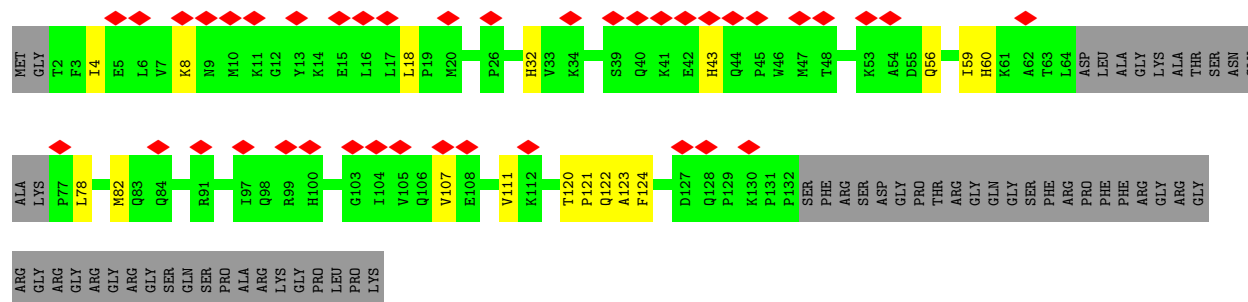


• Molecule 1: C protein

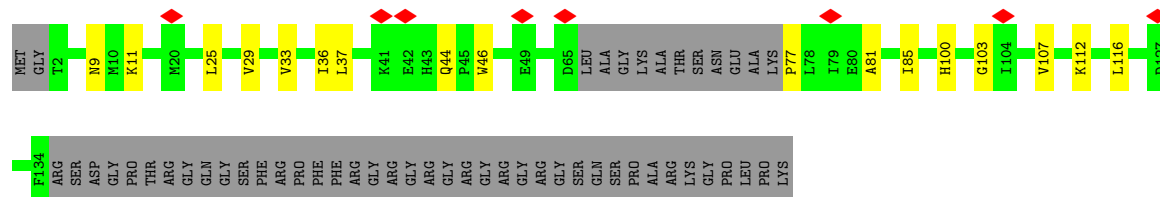




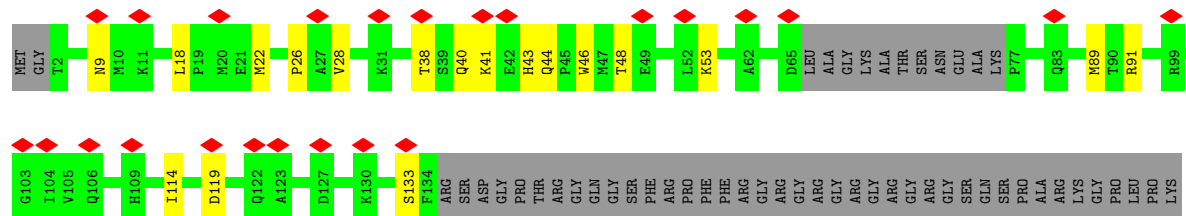
- Molecule 1: C protein



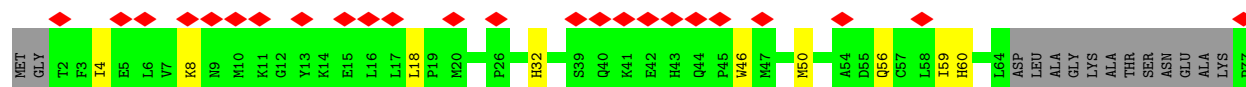
- Molecule 1: C protein

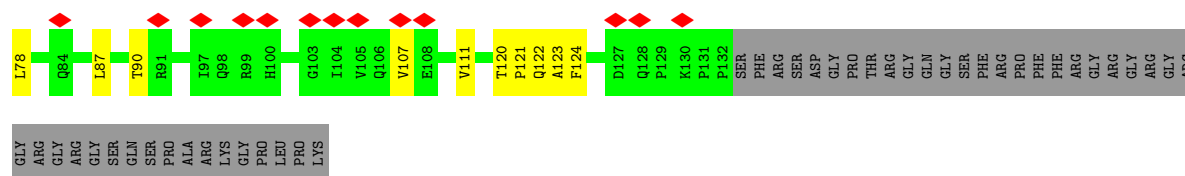


- Molecule 1: C protein

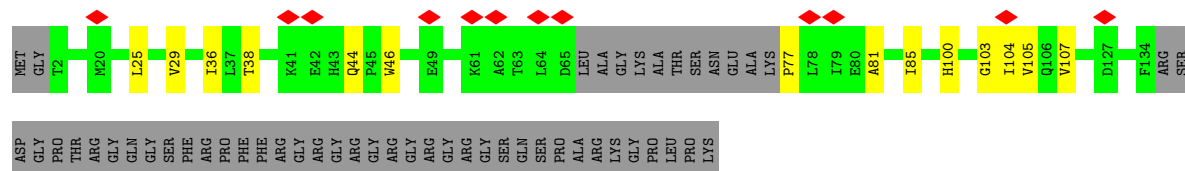


- Molecule 1: C protein

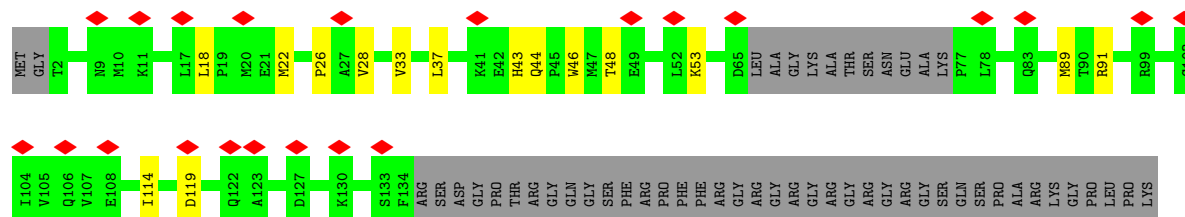




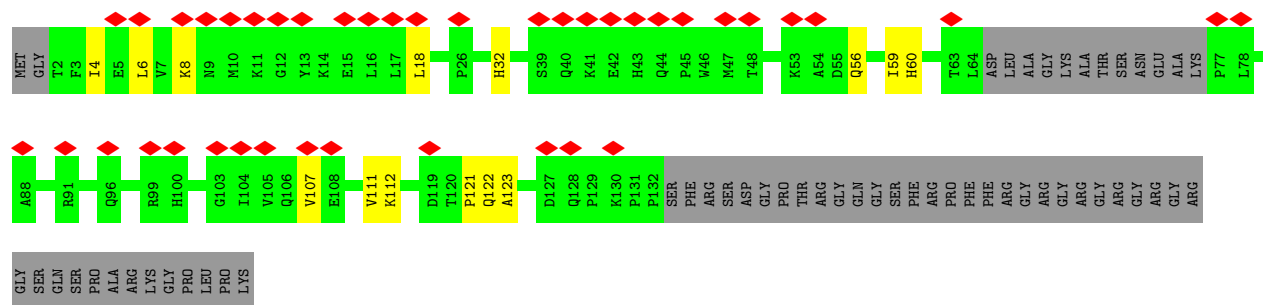
• Molecule 1: C protein



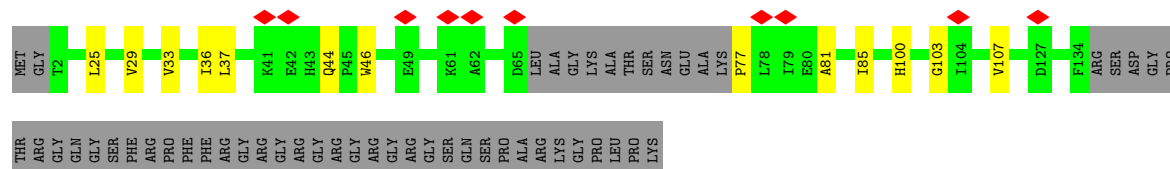
• Molecule 1: C protein



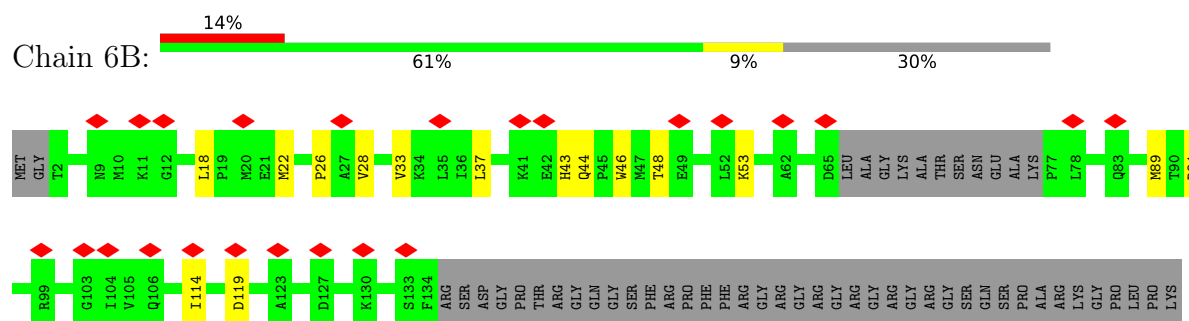
• Molecule 1: C protein



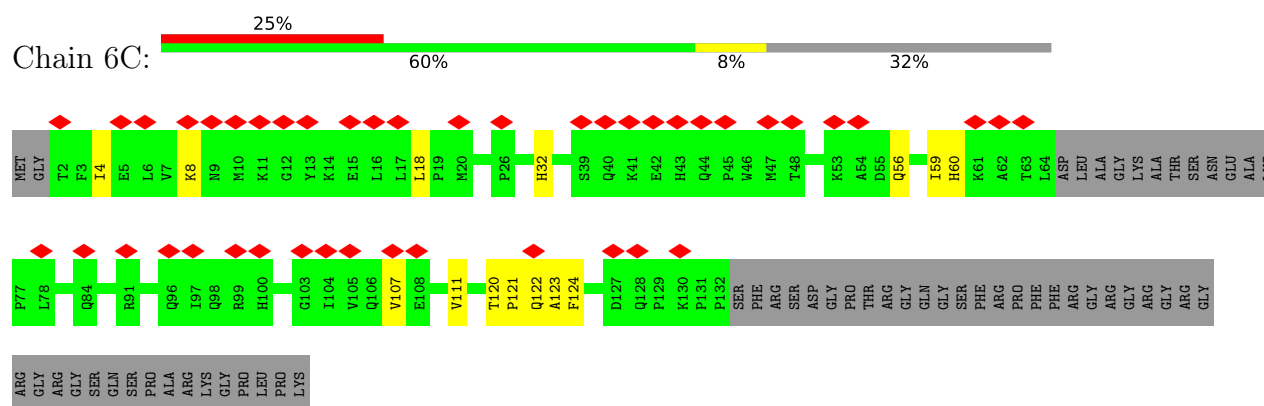
• Molecule 1: C protein



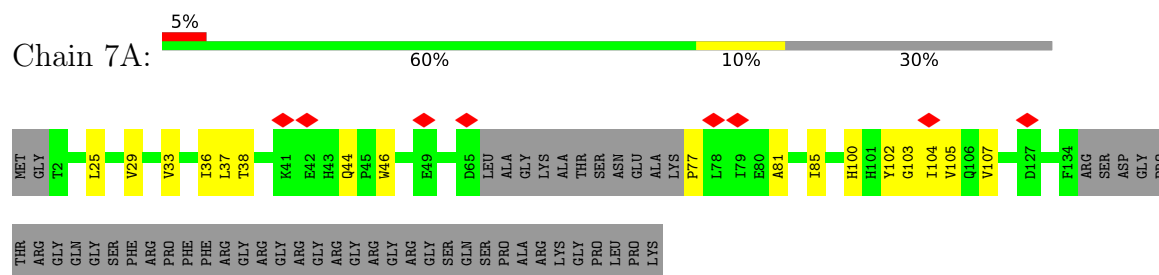
• Molecule 1: C protein



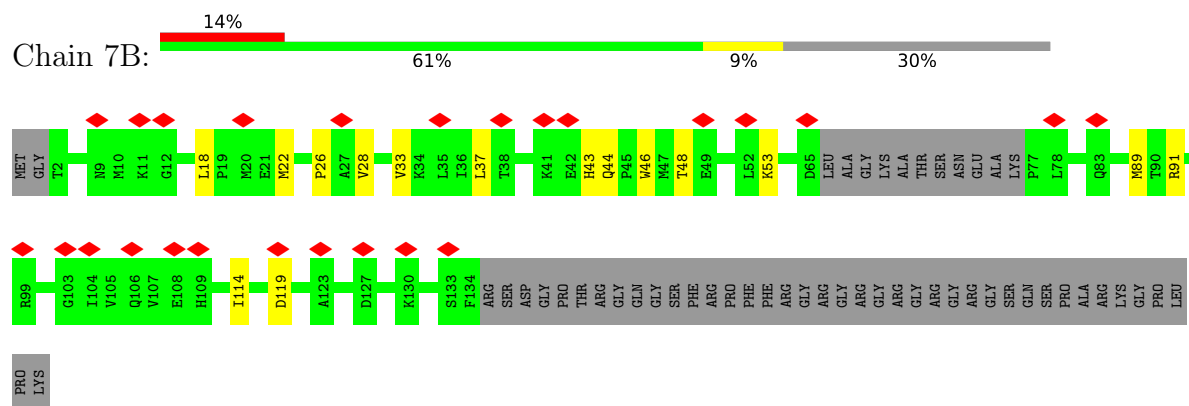
• Molecule 1: C protein



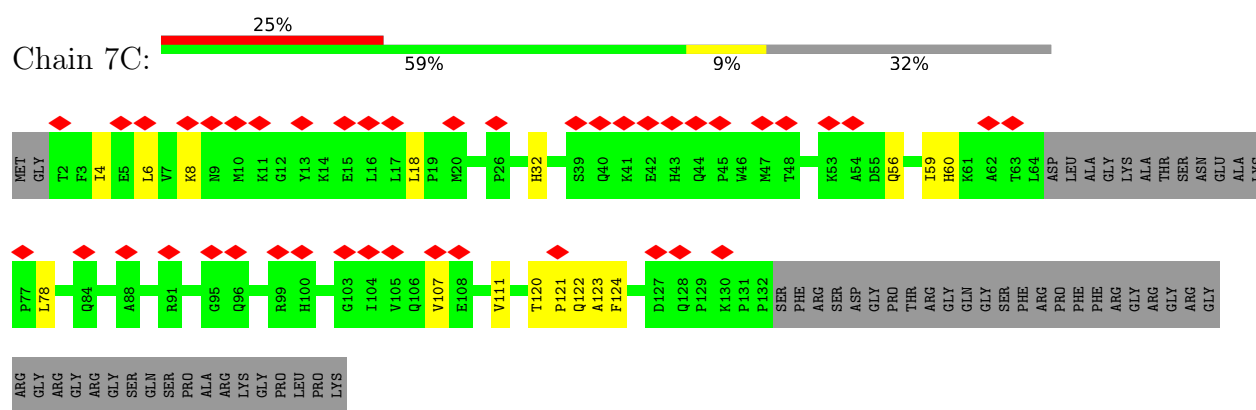
• Molecule 1: C protein



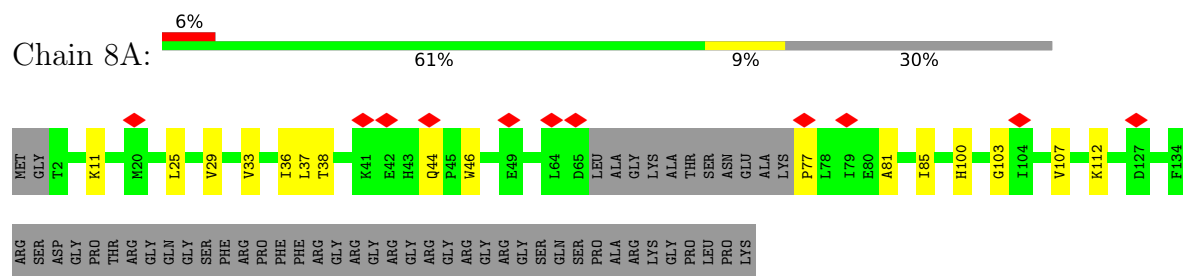
• Molecule 1: C protein



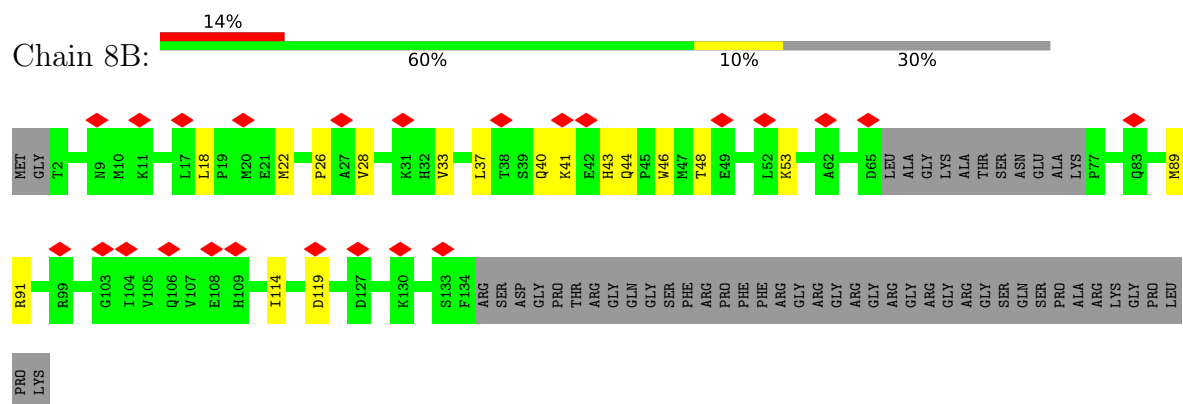
• Molecule 1: C protein



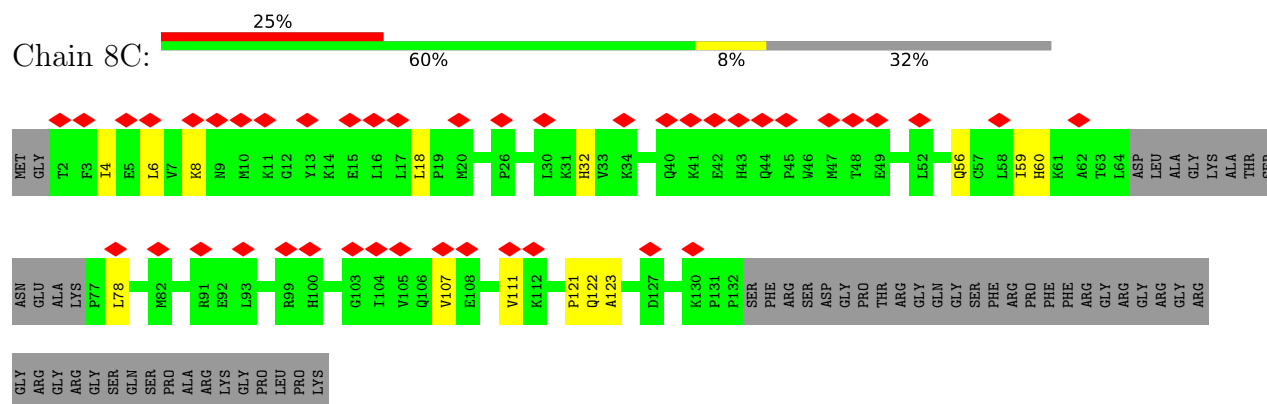
- Molecule 1: C protein



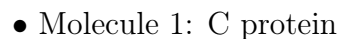
- Molecule 1: C protein



- Molecule 1: C protein



- Molecule 1: C protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	77129	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	166000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	362.87997, 362.87997, 362.87997	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8399999, 0.8399999, 0.8399999	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	1A	0.10	0/1024	0.20	0/1386
1	1B	0.09	0/1024	0.27	0/1386
1	1C	0.08	0/998	0.21	0/1351
1	2A	0.10	0/1024	0.20	0/1386
1	2B	0.09	0/1024	0.27	0/1386
1	2C	0.09	0/998	0.21	0/1351
1	3A	0.10	0/1024	0.20	0/1386
1	3B	0.09	0/1024	0.23	0/1386
1	3C	0.09	0/998	0.21	0/1351
1	4A	0.10	0/1024	0.20	0/1386
1	4B	0.09	0/1024	0.27	0/1386
1	4C	0.09	0/998	0.21	0/1351
1	5A	0.10	0/1024	0.20	0/1386
1	5B	0.09	0/1024	0.27	0/1386
1	5C	0.09	0/998	0.21	0/1351
1	6A	0.10	0/1024	0.20	0/1386
1	6B	0.09	0/1024	0.27	0/1386
1	6C	0.09	0/998	0.21	0/1351
1	7A	0.10	0/1024	0.20	0/1386
1	7B	0.09	0/1024	0.23	0/1386
1	7C	0.09	0/998	0.21	0/1351
1	8A	0.10	0/1024	0.20	0/1386
1	8B	0.09	0/1024	0.23	0/1386
1	8C	0.09	0/998	0.21	0/1351
1	AA	0.10	0/1024	0.20	0/1386
1	AB	0.09	0/1024	0.23	0/1386
1	AC	0.09	0/998	0.21	0/1351
1	BA	0.10	0/1024	0.20	0/1386
1	BB	0.09	0/1024	0.23	0/1386
1	BC	0.09	0/998	0.21	0/1351
1	CA	0.10	0/1024	0.20	0/1386
1	CB	0.09	0/1024	0.23	0/1386
1	CC	0.09	0/998	0.21	0/1351
1	DA	0.10	0/1024	0.20	0/1386

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	DB	0.09	0/1024	0.23	0/1386
1	DC	0.09	0/998	0.21	0/1351
1	EA	0.10	0/1024	0.20	0/1386
1	EB	0.09	0/1024	0.27	0/1386
1	EC	0.09	0/998	0.21	0/1351
1	FA	0.10	0/1024	0.20	0/1386
1	FB	0.09	0/1024	0.27	0/1386
1	FC	0.09	0/998	0.21	0/1351
1	GA	0.10	0/1024	0.20	0/1386
1	GB	0.09	0/1024	0.27	0/1386
1	GC	0.09	0/998	0.21	0/1351
1	HA	0.10	0/1024	0.20	0/1386
1	HB	0.10	0/1024	0.27	0/1386
1	HC	0.09	0/998	0.21	0/1351
1	IA	0.10	0/1024	0.20	0/1386
1	IB	0.09	0/1024	0.23	0/1386
1	IC	0.09	0/998	0.21	0/1351
1	JA	0.10	0/1024	0.20	0/1386
1	JB	0.09	0/1024	0.23	0/1386
1	JC	0.09	0/998	0.21	0/1351
1	KA	0.10	0/1024	0.20	0/1386
1	KB	0.10	0/1024	0.27	0/1386
1	KC	0.09	0/998	0.21	0/1351
1	LA	0.10	0/1024	0.20	0/1386
1	LB	0.09	0/1024	0.27	0/1386
1	LC	0.09	0/998	0.21	0/1351
1	MA	0.10	0/1024	0.20	0/1386
1	MB	0.09	0/1024	0.27	0/1386
1	MC	0.09	0/998	0.21	0/1351
1	NA	0.10	0/1024	0.20	0/1386
1	NB	0.09	0/1024	0.27	0/1386
1	NC	0.09	0/998	0.21	0/1351
1	OA	0.10	0/1024	0.20	0/1386
1	OB	0.09	0/1024	0.23	0/1386
1	OC	0.09	0/998	0.21	0/1351
1	PA	0.10	0/1024	0.20	0/1386
1	PB	0.09	0/1024	0.27	0/1386
1	PC	0.09	0/998	0.21	0/1351
1	QA	0.10	0/1024	0.20	0/1386
1	QB	0.09	0/1024	0.23	0/1386
1	QC	0.09	0/998	0.21	0/1351
1	RA	0.10	0/1024	0.20	0/1386
1	RB	0.09	0/1024	0.27	0/1386

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	RC	0.09	0/998	0.21	0/1351
1	SA	0.10	0/1024	0.20	0/1386
1	SB	0.09	0/1024	0.27	0/1386
1	SC	0.09	0/998	0.21	0/1351
1	TA	0.10	0/1024	0.20	0/1386
1	TB	0.09	0/1024	0.23	0/1386
1	TC	0.09	0/998	0.21	0/1351
1	UA	0.10	0/1024	0.20	0/1386
1	UB	0.10	0/1024	0.27	0/1386
1	UC	0.09	0/998	0.21	0/1351
1	VA	0.10	0/1024	0.20	0/1386
1	VB	0.09	0/1024	0.27	0/1386
1	VC	0.09	0/998	0.21	0/1351
1	WA	0.10	0/1024	0.20	0/1386
1	WB	0.09	0/1024	0.23	0/1386
1	WC	0.09	0/998	0.21	0/1351
1	XA	0.10	0/1024	0.20	0/1386
1	XB	0.09	0/1024	0.23	0/1386
1	XC	0.09	0/998	0.21	0/1351
1	YA	0.10	0/1024	0.20	0/1386
1	YB	0.09	0/1024	0.27	0/1386
1	YC	0.09	0/998	0.21	0/1351
1	ZA	0.10	0/1024	0.20	0/1386
1	ZB	0.09	0/1024	0.23	0/1386
1	ZC	0.09	0/998	0.21	0/1351
1	aA	0.10	0/1024	0.20	0/1386
1	aB	0.09	0/1024	0.27	0/1386
1	aC	0.09	0/998	0.21	0/1351
1	bA	0.10	0/1024	0.20	0/1386
1	bB	0.09	0/1024	0.23	0/1386
1	bC	0.09	0/998	0.21	0/1351
1	cA	0.10	0/1024	0.20	0/1386
1	cB	0.09	0/1024	0.27	0/1386
1	cC	0.09	0/998	0.21	0/1351
1	dA	0.10	0/1024	0.20	0/1386
1	dB	0.09	0/1024	0.27	0/1386
1	dC	0.09	0/998	0.21	0/1351
1	eA	0.10	0/1024	0.20	0/1386
1	eB	0.10	0/1024	0.27	0/1386
1	eC	0.09	0/998	0.21	0/1351
1	fA	0.10	0/1024	0.20	0/1386
1	fB	0.09	0/1024	0.27	0/1386
1	fC	0.09	0/998	0.21	0/1351

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	gA	0.10	0/1024	0.20	0/1386
1	gB	0.10	0/1024	0.27	0/1386
1	gC	0.09	0/998	0.21	0/1351
1	hA	0.10	0/1024	0.20	0/1386
1	hB	0.09	0/1024	0.27	0/1386
1	hC	0.09	0/998	0.21	0/1351
1	iA	0.10	0/1024	0.20	0/1386
1	iB	0.09	0/1024	0.23	0/1386
1	iC	0.09	0/998	0.21	0/1351
1	jA	0.10	0/1024	0.20	0/1386
1	jB	0.09	0/1024	0.23	0/1386
1	jC	0.09	0/998	0.21	0/1351
1	kA	0.10	0/1024	0.20	0/1386
1	kB	0.09	0/1024	0.27	0/1386
1	kC	0.09	0/998	0.21	0/1351
1	lA	0.10	0/1024	0.20	0/1386
1	lB	0.09	0/1024	0.23	0/1386
1	lC	0.09	0/998	0.21	0/1351
1	mA	0.10	0/1024	0.20	0/1386
1	mB	0.09	0/1024	0.23	0/1386
1	mC	0.09	0/998	0.21	0/1351
1	nA	0.10	0/1024	0.20	0/1386
1	nB	0.10	0/1024	0.27	0/1386
1	nC	0.09	0/998	0.21	0/1351
1	oA	0.10	0/1024	0.20	0/1386
1	oB	0.10	0/1024	0.27	0/1386
1	oC	0.08	0/998	0.21	0/1351
1	pA	0.10	0/1024	0.20	0/1386
1	pB	0.09	0/1024	0.23	0/1386
1	pC	0.09	0/998	0.21	0/1351
1	qA	0.10	0/1024	0.20	0/1386
1	qB	0.09	0/1024	0.27	0/1386
1	qC	0.09	0/998	0.21	0/1351
1	rA	0.10	0/1024	0.20	0/1386
1	rB	0.10	0/1024	0.27	0/1386
1	rC	0.09	0/998	0.21	0/1351
1	sA	0.10	0/1024	0.20	0/1386
1	sB	0.09	0/1024	0.27	0/1386
1	sC	0.09	0/998	0.21	0/1351
1	tA	0.10	0/1024	0.20	0/1386
1	tB	0.09	0/1024	0.27	0/1386
1	tC	0.09	0/998	0.21	0/1351
1	uA	0.10	0/1024	0.20	0/1386

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	uB	0.09	0/1024	0.23	0/1386
1	uC	0.09	0/998	0.21	0/1351
1	vA	0.10	0/1024	0.20	0/1386
1	vB	0.09	0/1024	0.27	0/1386
1	vC	0.09	0/998	0.21	0/1351
1	wA	0.10	0/1024	0.20	0/1386
1	wB	0.09	0/1024	0.27	0/1386
1	wC	0.09	0/998	0.21	0/1351
1	xA	0.10	0/1024	0.20	0/1386
1	xB	0.09	0/1024	0.27	0/1386
1	xC	0.09	0/998	0.21	0/1351
1	yA	0.10	0/1024	0.20	0/1386
1	yB	0.09	0/1024	0.23	0/1386
1	yC	0.09	0/998	0.21	0/1351
1	zA	0.10	0/1024	0.20	0/1386
1	zB	0.09	0/1024	0.27	0/1386
1	zC	0.09	0/998	0.21	0/1351
All	All	0.09	0/182760	0.22	0/247380

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	1A	999	0	1033	9	0
1	1B	999	0	1033	13	0
1	1C	974	0	1015	10	0
1	2A	999	0	1033	8	0
1	2B	999	0	1033	8	0
1	2C	974	0	1015	10	0
1	3A	999	0	1033	8	0
1	3B	999	0	1033	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3C	974	0	1015	12	0
1	4A	999	0	1033	14	0
1	4B	999	0	1033	13	0
1	4C	974	0	1015	12	0
1	5A	999	0	1033	9	0
1	5B	999	0	1033	8	0
1	5C	974	0	1015	11	0
1	6A	999	0	1033	8	0
1	6B	999	0	1033	8	0
1	6C	974	0	1015	9	0
1	7A	999	0	1033	12	0
1	7B	999	0	1033	8	0
1	7C	974	0	1015	11	0
1	8A	999	0	1033	12	0
1	8B	999	0	1033	9	0
1	8C	974	0	1015	13	0
1	AA	999	0	1033	9	0
1	AB	999	0	1033	11	0
1	AC	974	0	1015	34	0
1	BA	999	0	1033	8	0
1	BB	999	0	1033	8	0
1	BC	974	0	1015	17	0
1	CA	999	0	1033	10	0
1	CB	999	0	1033	10	0
1	CC	974	0	1015	10	0
1	DA	999	0	1033	9	0
1	DB	999	0	1033	9	0
1	DC	974	0	1015	16	0
1	EA	999	0	1033	9	0
1	EB	999	0	1033	8	0
1	EC	974	0	1015	12	0
1	FA	999	0	1033	8	0
1	FB	999	0	1033	8	0
1	FC	974	0	1015	14	0
1	GA	999	0	1033	7	0
1	GB	999	0	1033	7	0
1	GC	974	0	1015	10	0
1	HA	999	0	1033	11	0
1	HB	999	0	1033	9	0
1	HC	974	0	1015	12	0
1	IA	999	0	1033	9	0
1	IB	999	0	1033	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	IC	974	0	1015	10	0
1	JA	999	0	1033	9	0
1	JB	999	0	1033	9	0
1	JC	974	0	1015	16	0
1	KA	999	0	1033	14	0
1	KB	999	0	1033	10	0
1	KC	974	0	1015	11	0
1	LA	999	0	1033	9	0
1	LB	999	0	1033	9	0
1	LC	974	0	1015	9	0
1	MA	999	0	1033	9	0
1	MB	999	0	1033	9	0
1	MC	974	0	1015	13	0
1	NA	999	0	1033	11	0
1	NB	999	0	1033	9	0
1	NC	974	0	1015	13	0
1	OA	999	0	1033	9	0
1	OB	999	0	1033	8	0
1	OC	974	0	1015	9	0
1	PA	999	0	1033	19	0
1	PB	999	0	1033	9	0
1	PC	974	0	1015	9	0
1	QA	999	0	1033	8	0
1	QB	999	0	1033	9	0
1	QC	974	0	1015	11	0
1	RA	999	0	1033	15	0
1	RB	999	0	1033	10	0
1	RC	974	0	1015	35	0
1	SA	999	0	1033	10	0
1	SB	999	0	1033	9	0
1	SC	974	0	1015	11	0
1	TA	999	0	1033	11	0
1	TB	999	0	1033	11	0
1	TC	974	0	1015	26	0
1	UA	999	0	1033	9	0
1	UB	999	0	1033	8	0
1	UC	974	0	1015	16	0
1	VA	999	0	1033	9	0
1	VB	999	0	1033	9	0
1	VC	974	0	1015	11	0
1	WA	999	0	1033	8	0
1	WB	999	0	1033	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	WC	974	0	1015	11	0
1	XA	999	0	1033	10	0
1	XB	999	0	1033	11	0
1	XC	974	0	1015	10	0
1	YA	999	0	1033	9	0
1	YB	999	0	1033	8	0
1	YC	974	0	1015	16	0
1	ZA	999	0	1033	8	0
1	ZB	999	0	1033	10	0
1	ZC	974	0	1015	18	0
1	aA	999	0	1033	9	0
1	aB	999	0	1033	8	0
1	aC	974	0	1015	11	0
1	bA	999	0	1033	8	0
1	bB	999	0	1033	9	0
1	bC	974	0	1015	10	0
1	cA	999	0	1033	10	0
1	cB	999	0	1033	8	0
1	cC	974	0	1015	11	0
1	dA	999	0	1033	11	0
1	dB	999	0	1033	11	0
1	dC	974	0	1015	13	0
1	eA	999	0	1033	8	0
1	eB	999	0	1033	8	0
1	eC	974	0	1015	11	0
1	fA	999	0	1033	7	0
1	fB	999	0	1033	8	0
1	fC	974	0	1015	11	0
1	gA	999	0	1033	8	0
1	gB	999	0	1033	11	0
1	gC	974	0	1015	18	0
1	hA	999	0	1033	8	0
1	hB	999	0	1033	11	0
1	hC	974	0	1015	11	0
1	iA	999	0	1033	9	0
1	iB	999	0	1033	15	0
1	iC	974	0	1015	16	0
1	jA	999	0	1033	7	0
1	jB	999	0	1033	8	0
1	jC	974	0	1015	11	0
1	kA	999	0	1033	9	0
1	kB	999	0	1033	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	kC	974	0	1015	12	0
1	lA	999	0	1033	19	0
1	lB	999	0	1033	8	0
1	lC	974	0	1015	16	0
1	mA	999	0	1033	15	0
1	mB	999	0	1033	10	0
1	mC	974	0	1015	16	0
1	nA	999	0	1033	9	0
1	nB	999	0	1033	8	0
1	nC	974	0	1015	10	0
1	oA	999	0	1033	10	0
1	oB	999	0	1033	11	0
1	oC	974	0	1015	10	0
1	pA	999	0	1033	10	0
1	pB	999	0	1033	9	0
1	pC	974	0	1015	12	0
1	qA	999	0	1033	8	0
1	qB	999	0	1033	8	0
1	qC	974	0	1015	12	0
1	rA	999	0	1033	8	0
1	rB	999	0	1033	11	0
1	rC	974	0	1015	10	0
1	sA	999	0	1033	9	0
1	sB	999	0	1033	15	0
1	sC	974	0	1015	15	0
1	tA	999	0	1033	8	0
1	tB	999	0	1033	9	0
1	tC	974	0	1015	12	0
1	uA	999	0	1033	10	0
1	uB	999	0	1033	8	0
1	uC	974	0	1015	15	0
1	vA	999	0	1033	10	0
1	vB	999	0	1033	9	0
1	vC	974	0	1015	13	0
1	wA	999	0	1033	8	0
1	wB	999	0	1033	10	0
1	wC	974	0	1015	12	0
1	xA	999	0	1033	9	0
1	xB	999	0	1033	9	0
1	xC	974	0	1015	10	0
1	yA	999	0	1033	12	0
1	yB	999	0	1033	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	yC	974	0	1015	14	0
1	zA	999	0	1033	9	0
1	zB	999	0	1033	8	0
1	zC	974	0	1015	11	0
All	All	178320	0	184860	1691	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 (1691) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YC:58:LEU:HD11	1:mC:3:PHE:CE2	2.03	0.94
1:AC:58:LEU:HD11	1:RC:3:PHE:CD2	2.09	0.88
1:tB:53:LYS:NZ	1:tB:89:MET:SD	2.59	0.76
1:3B:53:LYS:NZ	1:3B:89:MET:SD	2.59	0.76
1:OB:53:LYS:NZ	1:OB:89:MET:SD	2.59	0.76
1:QB:53:LYS:NZ	1:QB:89:MET:SD	2.59	0.76
1:jB:53:LYS:NZ	1:jB:89:MET:SD	2.59	0.76
1:nB:53:LYS:NZ	1:nB:89:MET:SD	2.59	0.76
1:wB:53:LYS:NZ	1:wB:89:MET:SD	2.59	0.76
1:5B:53:LYS:NZ	1:5B:89:MET:SD	2.59	0.76
1:NB:53:LYS:NZ	1:NB:89:MET:SD	2.59	0.76
1:RB:53:LYS:NZ	1:RB:89:MET:SD	2.59	0.76
1:4B:53:LYS:NZ	1:4B:89:MET:SD	2.59	0.76
1:6B:53:LYS:NZ	1:6B:89:MET:SD	2.59	0.76
1:1B:53:LYS:NZ	1:1B:89:MET:SD	2.59	0.76
1:MB:53:LYS:NZ	1:MB:89:MET:SD	2.59	0.76
1:PB:53:LYS:NZ	1:PB:89:MET:SD	2.59	0.76
1:rB:53:LYS:NZ	1:rB:89:MET:SD	2.59	0.76
1:7B:53:LYS:NZ	1:7B:89:MET:SD	2.59	0.76
1:VB:53:LYS:NZ	1:VB:89:MET:SD	2.59	0.76
1:GB:53:LYS:NZ	1:GB:89:MET:SD	2.59	0.76
1:KB:53:LYS:NZ	1:KB:89:MET:SD	2.59	0.76
1:2B:53:LYS:NZ	1:2B:89:MET:SD	2.59	0.76
1:lB:53:LYS:NZ	1:lB:89:MET:SD	2.59	0.76
1:CB:53:LYS:NZ	1:CB:89:MET:SD	2.59	0.75
1:TB:53:LYS:NZ	1:TB:89:MET:SD	2.59	0.75
1:UB:53:LYS:NZ	1:UB:89:MET:SD	2.59	0.75
1:XB:53:LYS:NZ	1:XB:89:MET:SD	2.59	0.75
1:ZB:53:LYS:NZ	1:ZB:89:MET:SD	2.59	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:dB:53:LYS:NZ	1:dB:89:MET:SD	2.59	0.75
1:gB:53:LYS:NZ	1:gB:89:MET:SD	2.59	0.75
1:hB:53:LYS:NZ	1:hB:89:MET:SD	2.59	0.75
1:kB:53:LYS:NZ	1:kB:89:MET:SD	2.59	0.75
1:mB:53:LYS:NZ	1:mB:89:MET:SD	2.59	0.75
1:xB:53:LYS:NZ	1:xB:89:MET:SD	2.59	0.75
1:AB:53:LYS:NZ	1:AB:89:MET:SD	2.59	0.75
1:cB:53:LYS:NZ	1:cB:89:MET:SD	2.59	0.75
1:vB:53:LYS:NZ	1:vB:89:MET:SD	2.59	0.75
1:LB:53:LYS:NZ	1:LB:89:MET:SD	2.59	0.75
1:pB:53:LYS:NZ	1:pB:89:MET:SD	2.59	0.75
1:qB:53:LYS:NZ	1:qB:89:MET:SD	2.59	0.75
1:HB:53:LYS:NZ	1:HB:89:MET:SD	2.59	0.75
1:SB:53:LYS:NZ	1:SB:89:MET:SD	2.59	0.75
1:oB:53:LYS:NZ	1:oB:89:MET:SD	2.59	0.75
1:zB:53:LYS:NZ	1:zB:89:MET:SD	2.59	0.75
1:8B:53:LYS:NZ	1:8B:89:MET:SD	2.59	0.75
1:IB:53:LYS:NZ	1:IB:89:MET:SD	2.59	0.75
1:bB:53:LYS:NZ	1:bB:89:MET:SD	2.59	0.75
1:WB:53:LYS:NZ	1:WB:89:MET:SD	2.59	0.75
1:YB:53:LYS:NZ	1:YB:89:MET:SD	2.59	0.75
1:uB:53:LYS:NZ	1:uB:89:MET:SD	2.59	0.75
1:BB:53:LYS:NZ	1:BB:89:MET:SD	2.59	0.75
1:FB:53:LYS:NZ	1:FB:89:MET:SD	2.59	0.75
1:eB:53:LYS:NZ	1:eB:89:MET:SD	2.59	0.75
1:yB:53:LYS:NZ	1:yB:89:MET:SD	2.59	0.75
1:EB:53:LYS:NZ	1:EB:89:MET:SD	2.59	0.75
1:JB:53:LYS:NZ	1:JB:89:MET:SD	2.59	0.75
1:aB:53:LYS:NZ	1:aB:89:MET:SD	2.59	0.74
1:fB:53:LYS:NZ	1:fB:89:MET:SD	2.59	0.74
1:iB:53:LYS:NZ	1:iB:89:MET:SD	2.59	0.74
1:sB:53:LYS:NZ	1:sB:89:MET:SD	2.59	0.74
1:DB:53:LYS:NZ	1:DB:89:MET:SD	2.59	0.74
1:YC:58:LEU:HD11	1:mC:3:PHE:CD2	2.22	0.74
1:ZC:121:PRO:O	1:ZC:123:ALA:N	2.22	0.73
1:eC:121:PRO:O	1:eC:123:ALA:N	2.22	0.73
1:hC:121:PRO:O	1:hC:123:ALA:N	2.22	0.73
1:QC:121:PRO:O	1:QC:123:ALA:N	2.22	0.73
1:1C:121:PRO:O	1:1C:123:ALA:N	2.22	0.73
1:bC:121:PRO:O	1:bC:123:ALA:N	2.22	0.73
1:jC:121:PRO:O	1:jC:123:ALA:N	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:tC:121:PRO:O	1:tC:123:ALA:N	2.22	0.73
1:wC:121:PRO:O	1:wC:123:ALA:N	2.22	0.73
1:3C:121:PRO:O	1:3C:123:ALA:N	2.22	0.73
1:8C:121:PRO:O	1:8C:123:ALA:N	2.22	0.73
1:LC:121:PRO:O	1:LC:123:ALA:N	2.22	0.73
1:UC:121:PRO:O	1:UC:123:ALA:N	2.22	0.73
1:fC:121:PRO:O	1:fC:123:ALA:N	2.22	0.73
1:5C:121:PRO:O	1:5C:123:ALA:N	2.22	0.73
1:NC:121:PRO:O	1:NC:123:ALA:N	2.22	0.73
1:RC:121:PRO:O	1:RC:123:ALA:N	2.22	0.73
1:nC:121:PRO:O	1:nC:123:ALA:N	2.22	0.73
1:pC:121:PRO:O	1:pC:123:ALA:N	2.22	0.73
1:AC:121:PRO:O	1:AC:123:ALA:N	2.22	0.73
1:IC:121:PRO:O	1:IC:123:ALA:N	2.22	0.73
1:PC:121:PRO:O	1:PC:123:ALA:N	2.22	0.73
1:WC:121:PRO:O	1:WC:123:ALA:N	2.22	0.73
1:XC:121:PRO:O	1:XC:123:ALA:N	2.22	0.73
1:oC:121:PRO:O	1:oC:123:ALA:N	2.22	0.73
1:xC:121:PRO:O	1:xC:123:ALA:N	2.22	0.73
1:MC:121:PRO:O	1:MC:123:ALA:N	2.22	0.73
1:VC:121:PRO:O	1:VC:123:ALA:N	2.22	0.73
1:BC:121:PRO:O	1:BC:123:ALA:N	2.22	0.73
1:EC:121:PRO:O	1:EC:123:ALA:N	2.22	0.73
1:JC:121:PRO:O	1:JC:123:ALA:N	2.22	0.73
1:cC:121:PRO:O	1:cC:123:ALA:N	2.22	0.73
1:gC:121:PRO:O	1:gC:123:ALA:N	2.22	0.73
1:2C:121:PRO:O	1:2C:123:ALA:N	2.22	0.73
1:zC:121:PRO:O	1:zC:123:ALA:N	2.22	0.73
1:4C:121:PRO:O	1:4C:123:ALA:N	2.22	0.73
1:CC:121:PRO:O	1:CC:123:ALA:N	2.22	0.73
1:KC:121:PRO:O	1:KC:123:ALA:N	2.22	0.73
1:dC:121:PRO:O	1:dC:123:ALA:N	2.22	0.73
1:vC:121:PRO:O	1:vC:123:ALA:N	2.22	0.73
1:DC:121:PRO:O	1:DC:123:ALA:N	2.22	0.72
1:OC:121:PRO:O	1:OC:123:ALA:N	2.22	0.72
1:YC:121:PRO:O	1:YC:123:ALA:N	2.22	0.72
1:kC:121:PRO:O	1:kC:123:ALA:N	2.22	0.72
1:6C:121:PRO:O	1:6C:123:ALA:N	2.22	0.72
1:7C:121:PRO:O	1:7C:123:ALA:N	2.22	0.72
1:yC:121:PRO:O	1:yC:123:ALA:N	2.22	0.72
1:FC:121:PRO:O	1:FC:123:ALA:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SC:121:PRO:O	1:SC:123:ALA:N	2.22	0.72
1:uC:121:PRO:O	1:uC:123:ALA:N	2.22	0.72
1:aC:121:PRO:O	1:aC:123:ALA:N	2.22	0.72
1:qC:121:PRO:O	1:qC:123:ALA:N	2.22	0.72
1:sC:121:PRO:O	1:sC:123:ALA:N	2.22	0.72
1:TC:121:PRO:O	1:TC:123:ALA:N	2.22	0.72
1:iC:121:PRO:O	1:iC:123:ALA:N	2.22	0.72
1:mC:121:PRO:O	1:mC:123:ALA:N	2.22	0.72
1:GC:121:PRO:O	1:GC:123:ALA:N	2.22	0.72
1:HC:121:PRO:O	1:HC:123:ALA:N	2.22	0.72
1:lC:121:PRO:O	1:lC:123:ALA:N	2.22	0.72
1:rC:121:PRO:O	1:rC:123:ALA:N	2.22	0.71
1:vC:3:PHE:CE2	1:yC:58:LEU:HD11	2.27	0.69
1:rB:9:ASN:ND2	1:8C:6:LEU:HD22	2.07	0.69
1:DC:12:GLY:O	1:TC:43:HIS:CE1	2.47	0.67
1:BC:9:ASN:O	1:1B:41:LYS:HG3	1.94	0.66
1:KA:102:TYR:OH	1:mA:116:LEU:CD2	2.43	0.65
1:KA:102:TYR:OH	1:mA:116:LEU:HD23	1.97	0.65
1:TC:116:LEU:HD23	1:iB:102:TYR:OH	1.97	0.65
1:DC:43:HIS:CD2	1:TC:12:GLY:HA3	2.32	0.64
1:RC:124:PHE:CD2	1:XB:22:MET:HE2	2.33	0.63
1:AC:55:ASP:OD2	1:RC:4:ILE:HD11	1.98	0.63
1:AC:58:LEU:HD11	1:RC:3:PHE:CE2	2.33	0.62
1:AC:3:PHE:CD1	1:RC:37:LEU:HD12	2.34	0.62
1:RA:40:GLN:O	1:4A:11:LYS:HG2	2.00	0.62
1:YC:53:LYS:NZ	1:mC:49:GLU:OE1	2.32	0.62
1:RC:6:LEU:HD22	1:AB:9:ASN:ND2	2.16	0.61
1:kB:44:GLN:OE1	1:kB:46:TRP:NE1	2.34	0.61
1:yB:44:GLN:OE1	1:yB:46:TRP:NE1	2.34	0.61
1:FB:44:GLN:OE1	1:FB:46:TRP:NE1	2.34	0.61
1:YB:44:GLN:OE1	1:YB:46:TRP:NE1	2.34	0.61
1:2B:44:GLN:OE1	1:2B:46:TRP:NE1	2.34	0.61
1:qB:44:GLN:OE1	1:qB:46:TRP:NE1	2.34	0.61
1:uB:44:GLN:OE1	1:uB:46:TRP:NE1	2.34	0.61
1:xB:44:GLN:OE1	1:xB:46:TRP:NE1	2.34	0.61
1:DB:44:GLN:OE1	1:DB:46:TRP:NE1	2.34	0.61
1:WB:44:GLN:OE1	1:WB:46:TRP:NE1	2.34	0.61
1:pB:44:GLN:OE1	1:pB:46:TRP:NE1	2.34	0.61
1:SB:44:GLN:OE1	1:SB:46:TRP:NE1	2.34	0.60
1:lB:44:GLN:OE1	1:lB:46:TRP:NE1	2.34	0.60
1:BB:44:GLN:OE1	1:BB:46:TRP:NE1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PA:124:PHE:HB3	1:1A:22:MET:HE3	1.83	0.60
1:JB:44:GLN:OE1	1:JB:46:TRP:NE1	2.34	0.60
1:HB:41:LYS:HG3	1:aC:9:ASN:O	2.01	0.60
1:ZB:119:ASP:OD2	1:ZC:32:HIS:NE2	2.35	0.60
1:jB:119:ASP:OD2	1:jC:32:HIS:NE2	2.35	0.60
1:KB:44:GLN:OE1	1:KB:46:TRP:NE1	2.34	0.60
1:QB:119:ASP:OD2	1:QC:32:HIS:NE2	2.35	0.60
1:TB:119:ASP:OD2	1:TC:32:HIS:NE2	2.35	0.60
1:cB:44:GLN:OE1	1:cB:46:TRP:NE1	2.34	0.60
1:hB:119:ASP:OD2	1:hC:32:HIS:NE2	2.35	0.60
1:mB:119:ASP:OD2	1:mC:32:HIS:NE2	2.35	0.60
1:GB:119:ASP:OD2	1:GC:32:HIS:NE2	2.35	0.60
1:dB:119:ASP:OD2	1:dC:32:HIS:NE2	2.35	0.60
1:gB:119:ASP:OD2	1:gC:32:HIS:NE2	2.35	0.60
1:2B:119:ASP:OD2	1:2C:32:HIS:NE2	2.35	0.60
1:xB:119:ASP:OD2	1:xC:32:HIS:NE2	2.35	0.60
1:7B:44:GLN:OE1	1:7B:46:TRP:NE1	2.34	0.60
1:LB:119:ASP:OD2	1:LC:32:HIS:NE2	2.35	0.60
1:MB:119:ASP:OD2	1:MC:32:HIS:NE2	2.35	0.60
1:BC:6:LEU:HD22	1:QB:9:ASN:HB3	1.84	0.60
1:FB:119:ASP:OD2	1:FC:32:HIS:NE2	2.35	0.60
1:IB:119:ASP:OD2	1:IC:32:HIS:NE2	2.35	0.60
1:fB:44:GLN:OE1	1:fB:46:TRP:NE1	2.34	0.60
1:fB:119:ASP:OD2	1:fC:32:HIS:NE2	2.35	0.60
1:iB:119:ASP:OD2	1:iC:32:HIS:NE2	2.35	0.60
1:pB:119:ASP:OD2	1:pC:32:HIS:NE2	2.35	0.60
1:uB:119:ASP:OD2	1:uC:32:HIS:NE2	2.35	0.60
1:4B:119:ASP:OD2	1:4C:32:HIS:NE2	2.35	0.60
1:5B:119:ASP:OD2	1:5C:32:HIS:NE2	2.35	0.60
1:8B:119:ASP:OD2	1:8C:32:HIS:NE2	2.35	0.60
1:BB:119:ASP:OD2	1:BC:32:HIS:NE2	2.35	0.60
1:PB:44:GLN:OE1	1:PB:46:TRP:NE1	2.34	0.60
1:aB:44:GLN:OE1	1:aB:46:TRP:NE1	2.34	0.60
1:bB:119:ASP:OD2	1:bC:32:HIS:NE2	2.35	0.60
1:oB:119:ASP:OD2	1:oC:32:HIS:NE2	2.35	0.60
1:rB:119:ASP:OD2	1:rC:32:HIS:NE2	2.35	0.60
1:yB:119:ASP:OD2	1:yC:32:HIS:NE2	2.35	0.60
1:7B:119:ASP:OD2	1:7C:32:HIS:NE2	2.35	0.60
1:AC:32:HIS:NE2	1:AB:119:ASP:OD2	2.35	0.60
1:1B:119:ASP:OD2	1:1C:32:HIS:NE2	2.35	0.60
1:KB:119:ASP:OD2	1:KC:32:HIS:NE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TC:124:PHE:CD2	1:iB:22:MET:HE2	2.36	0.60
1:cB:119:ASP:OD2	1:cC:32:HIS:NE2	2.35	0.60
1:dB:44:GLN:OE1	1:dB:46:TRP:NE1	2.34	0.60
1:eB:119:ASP:OD2	1:eC:32:HIS:NE2	2.35	0.60
1:iB:44:GLN:OE1	1:iB:46:TRP:NE1	2.34	0.60
1:eB:44:GLN:OE1	1:eB:46:TRP:NE1	2.34	0.59
1:gB:44:GLN:OE1	1:gB:46:TRP:NE1	2.34	0.59
1:LB:44:GLN:OE1	1:LB:46:TRP:NE1	2.34	0.59
1:WB:119:ASP:OD2	1:WC:32:HIS:NE2	2.35	0.59
1:qB:119:ASP:OD2	1:qC:32:HIS:NE2	2.35	0.59
1:zB:44:GLN:OE1	1:zB:46:TRP:NE1	2.34	0.59
1:EB:119:ASP:OD2	1:EC:32:HIS:NE2	2.35	0.59
1:bB:44:GLN:OE1	1:bB:46:TRP:NE1	2.34	0.59
1:kB:119:ASP:OD2	1:kC:32:HIS:NE2	2.35	0.59
1:nB:44:GLN:OE1	1:nB:46:TRP:NE1	2.34	0.59
1:nB:119:ASP:OD2	1:nC:32:HIS:NE2	2.35	0.59
1:wB:119:ASP:OD2	1:wC:32:HIS:NE2	2.35	0.59
1:NB:119:ASP:OD2	1:NC:32:HIS:NE2	2.35	0.59
1:VB:119:ASP:OD2	1:VC:32:HIS:NE2	2.35	0.59
1:lB:119:ASP:OD2	1:lC:32:HIS:NE2	2.35	0.59
1:QA:44:GLN:OE1	1:QA:46:TRP:NE1	2.36	0.59
1:SB:119:ASP:OD2	1:SC:32:HIS:NE2	2.35	0.59
1:tA:44:GLN:OE1	1:tA:46:TRP:NE1	2.36	0.59
1:EB:44:GLN:OE1	1:EB:46:TRP:NE1	2.34	0.59
1:PB:119:ASP:OD2	1:PC:32:HIS:NE2	2.35	0.59
1:RB:119:ASP:OD2	1:RC:32:HIS:NE2	2.35	0.59
1:UB:119:ASP:OD2	1:UC:32:HIS:NE2	2.35	0.59
1:jA:44:GLN:OE1	1:jA:46:TRP:NE1	2.36	0.59
1:IB:44:GLN:OE1	1:IB:46:TRP:NE1	2.34	0.59
1:OB:119:ASP:OD2	1:OC:32:HIS:NE2	2.35	0.59
1:XB:44:GLN:OE1	1:XB:46:TRP:NE1	2.34	0.59
1:oB:44:GLN:OE1	1:oB:46:TRP:NE1	2.34	0.59
1:HB:44:GLN:OE1	1:HB:46:TRP:NE1	2.34	0.59
1:OA:44:GLN:OE1	1:OA:46:TRP:NE1	2.36	0.59
1:sB:44:GLN:OE1	1:sB:46:TRP:NE1	2.34	0.59
1:6A:44:GLN:OE1	1:6A:46:TRP:NE1	2.36	0.59
1:CB:44:GLN:OE1	1:CB:46:TRP:NE1	2.34	0.59
1:TA:44:GLN:OE1	1:TA:46:TRP:NE1	2.36	0.59
1:vB:44:GLN:OE1	1:vB:46:TRP:NE1	2.34	0.59
1:EA:44:GLN:OE1	1:EA:46:TRP:NE1	2.36	0.59
1:TB:44:GLN:OE1	1:TB:46:TRP:NE1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:mA:44:GLN:OE1	1:mA:46:TRP:NE1	2.36	0.59
1:mB:44:GLN:OE1	1:mB:46:TRP:NE1	2.34	0.59
1:pA:124:PHE:O	1:xA:128:GLN:NE2	2.24	0.59
1:zB:119:ASP:OD2	1:zC:32:HIS:NE2	2.35	0.59
1:GA:44:GLN:OE1	1:GA:46:TRP:NE1	2.36	0.58
1:YB:119:ASP:OD2	1:YC:32:HIS:NE2	2.35	0.58
1:aA:44:GLN:OE1	1:aA:46:TRP:NE1	2.36	0.58
1:wB:44:GLN:OE1	1:wB:46:TRP:NE1	2.34	0.58
1:3B:119:ASP:OD2	1:3C:32:HIS:NE2	2.35	0.58
1:6B:119:ASP:OD2	1:6C:32:HIS:NE2	2.35	0.58
1:CB:119:ASP:OD2	1:CC:32:HIS:NE2	2.35	0.58
1:UC:12:GLY:O	1:lC:43:HIS:NE2	2.37	0.58
1:DB:119:ASP:OD2	1:DC:32:HIS:NE2	2.35	0.58
1:GB:44:GLN:OE1	1:GB:46:TRP:NE1	2.34	0.58
1:MA:103:GLY:O	1:MA:107:VAL:HG23	2.04	0.58
1:ZA:44:GLN:OE1	1:ZA:46:TRP:NE1	2.36	0.58
1:iA:44:GLN:OE1	1:iA:46:TRP:NE1	2.36	0.58
1:tB:119:ASP:OD2	1:tC:32:HIS:NE2	2.35	0.58
1:GA:103:GLY:O	1:GA:107:VAL:HG23	2.04	0.58
1:NB:44:GLN:OE1	1:NB:46:TRP:NE1	2.34	0.58
1:rB:44:GLN:OE1	1:rB:46:TRP:NE1	2.34	0.58
1:tB:44:GLN:OE1	1:tB:46:TRP:NE1	2.34	0.58
1:4A:103:GLY:O	1:4A:107:VAL:HG23	2.04	0.58
1:HA:103:GLY:O	1:HA:107:VAL:HG23	2.04	0.58
1:JB:119:ASP:OD2	1:JC:32:HIS:NE2	2.35	0.58
1:KA:103:GLY:O	1:KA:107:VAL:HG23	2.04	0.58
1:MA:44:GLN:OE1	1:MA:46:TRP:NE1	2.36	0.58
1:VA:103:GLY:O	1:VA:107:VAL:HG23	2.04	0.58
1:VB:44:GLN:OE1	1:VB:46:TRP:NE1	2.34	0.58
1:XB:119:ASP:OD2	1:XC:32:HIS:NE2	2.35	0.58
1:hA:44:GLN:OE1	1:hA:46:TRP:NE1	2.36	0.58
1:sA:103:GLY:O	1:sA:107:VAL:HG23	2.04	0.58
1:vB:119:ASP:OD2	1:vC:32:HIS:NE2	2.35	0.58
1:AA:103:GLY:O	1:AA:107:VAL:HG23	2.04	0.58
1:CA:44:GLN:OE1	1:CA:46:TRP:NE1	2.36	0.58
1:DC:12:GLY:O	1:TC:43:HIS:NE2	2.35	0.58
1:HA:44:GLN:OE1	1:HA:46:TRP:NE1	2.36	0.58
1:RA:103:GLY:O	1:RA:107:VAL:HG23	2.04	0.58
1:UC:12:GLY:O	1:lC:43:HIS:CE1	2.56	0.58
1:pA:103:GLY:O	1:pA:107:VAL:HG23	2.04	0.58
1:rA:103:GLY:O	1:rA:107:VAL:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:wA:103:GLY:O	1:wA:107:VAL:HG23	2.04	0.58
1:FA:103:GLY:O	1:FA:107:VAL:HG23	2.04	0.58
1:1B:44:GLN:OE1	1:1B:46:TRP:NE1	2.34	0.58
1:XA:44:GLN:OE1	1:XA:46:TRP:NE1	2.36	0.58
1:jA:103:GLY:O	1:jA:107:VAL:HG23	2.04	0.58
1:4A:44:GLN:OE1	1:4A:46:TRP:NE1	2.36	0.58
1:7A:103:GLY:O	1:7A:107:VAL:HG23	2.04	0.58
1:AB:44:GLN:OE1	1:AB:46:TRP:NE1	2.34	0.58
1:1A:103:GLY:O	1:1A:107:VAL:HG23	2.04	0.58
1:BA:103:GLY:O	1:BA:107:VAL:HG23	2.04	0.58
1:NA:44:GLN:OE1	1:NA:46:TRP:NE1	2.36	0.58
1:QA:103:GLY:O	1:QA:107:VAL:HG23	2.04	0.58
1:TA:103:GLY:O	1:TA:107:VAL:HG23	2.04	0.58
1:WA:103:GLY:O	1:WA:107:VAL:HG23	2.04	0.58
1:hB:44:GLN:OE1	1:hB:46:TRP:NE1	2.34	0.58
1:mA:103:GLY:O	1:mA:107:VAL:HG23	2.04	0.58
1:JA:103:GLY:O	1:JA:107:VAL:HG23	2.04	0.58
1:PA:103:GLY:O	1:PA:107:VAL:HG23	2.04	0.58
1:UA:103:GLY:O	1:UA:107:VAL:HG23	2.04	0.58
1:kA:103:GLY:O	1:kA:107:VAL:HG23	2.04	0.58
1:nA:103:GLY:O	1:nA:107:VAL:HG23	2.04	0.58
1:3B:44:GLN:OE1	1:3B:46:TRP:NE1	2.34	0.58
1:8B:44:GLN:OE1	1:8B:46:TRP:NE1	2.34	0.58
1:AC:109:HIS:HE1	1:4B:133:SER:HB3	1.69	0.58
1:LA:103:GLY:O	1:LA:107:VAL:HG23	2.04	0.58
1:UB:44:GLN:OE1	1:UB:46:TRP:NE1	2.34	0.58
1:2A:103:GLY:O	1:2A:107:VAL:HG23	2.04	0.58
1:qA:103:GLY:O	1:qA:107:VAL:HG23	2.04	0.58
1:8A:103:GLY:O	1:8A:107:VAL:HG23	2.04	0.58
1:OA:103:GLY:O	1:OA:107:VAL:HG23	2.04	0.57
1:ZB:44:GLN:OE1	1:ZB:46:TRP:NE1	2.34	0.57
1:ZC:58:LEU:HD11	1:gC:3:PHE:CD2	2.39	0.57
1:2A:44:GLN:OE1	1:2A:46:TRP:NE1	2.36	0.57
1:cA:103:GLY:O	1:cA:107:VAL:HG23	2.04	0.57
1:dA:103:GLY:O	1:dA:107:VAL:HG23	2.04	0.57
1:gA:103:GLY:O	1:gA:107:VAL:HG23	2.04	0.57
1:iA:103:GLY:O	1:iA:107:VAL:HG23	2.04	0.57
1:kA:44:GLN:OE1	1:kA:46:TRP:NE1	2.36	0.57
1:oA:103:GLY:O	1:oA:107:VAL:HG23	2.04	0.57
1:vA:103:GLY:O	1:vA:107:VAL:HG23	2.04	0.57
1:5B:44:GLN:OE1	1:5B:46:TRP:NE1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:44:GLN:OE1	1:AA:46:TRP:NE1	2.36	0.57
1:CA:103:GLY:O	1:CA:107:VAL:HG23	2.04	0.57
1:HB:119:ASP:OD2	1:HC:32:HIS:NE2	2.35	0.57
1:IA:103:GLY:O	1:IA:107:VAL:HG23	2.04	0.57
1:MB:44:GLN:OE1	1:MB:46:TRP:NE1	2.34	0.57
1:XA:103:GLY:O	1:XA:107:VAL:HG23	2.04	0.57
1:aA:103:GLY:O	1:aA:107:VAL:HG23	2.04	0.57
1:xA:44:GLN:OE1	1:xA:46:TRP:NE1	2.36	0.57
1:xA:103:GLY:O	1:xA:107:VAL:HG23	2.04	0.57
1:4B:44:GLN:OE1	1:4B:46:TRP:NE1	2.34	0.57
1:6A:103:GLY:O	1:6A:107:VAL:HG23	2.04	0.57
1:IA:44:GLN:OE1	1:IA:46:TRP:NE1	2.36	0.57
1:dC:6:LEU:HD22	1:hB:9:ASN:ND2	2.18	0.57
1:wA:44:GLN:OE1	1:wA:46:TRP:NE1	2.36	0.57
1:1A:44:GLN:OE1	1:1A:46:TRP:NE1	2.36	0.57
1:EA:103:GLY:O	1:EA:107:VAL:HG23	2.04	0.57
1:YA:103:GLY:O	1:YA:107:VAL:HG23	2.04	0.57
1:ZA:103:GLY:O	1:ZA:107:VAL:HG23	2.04	0.57
1:fA:103:GLY:O	1:fA:107:VAL:HG23	2.04	0.57
1:sA:44:GLN:OE1	1:sA:46:TRP:NE1	2.36	0.57
1:tA:103:GLY:O	1:tA:107:VAL:HG23	2.04	0.57
1:zA:103:GLY:O	1:zA:107:VAL:HG23	2.04	0.57
1:DA:103:GLY:O	1:DA:107:VAL:HG23	2.04	0.57
1:NA:103:GLY:O	1:NA:107:VAL:HG23	2.04	0.57
1:hA:103:GLY:O	1:hA:107:VAL:HG23	2.04	0.57
1:nA:44:GLN:OE1	1:nA:46:TRP:NE1	2.36	0.57
1:oA:44:GLN:OE1	1:oA:46:TRP:NE1	2.36	0.57
1:vC:3:PHE:CD2	1:yC:58:LEU:HD11	2.40	0.57
1:3A:103:GLY:O	1:3A:107:VAL:HG23	2.04	0.57
1:VA:44:GLN:OE1	1:VA:46:TRP:NE1	2.36	0.57
1:bA:103:GLY:O	1:bA:107:VAL:HG23	2.04	0.57
1:sB:119:ASP:OD2	1:sC:32:HIS:NE2	2.35	0.57
1:RB:44:GLN:OE1	1:RB:46:TRP:NE1	2.34	0.57
1:eA:103:GLY:O	1:eA:107:VAL:HG23	2.04	0.57
1:jB:44:GLN:OE1	1:jB:46:TRP:NE1	2.34	0.57
1:uA:103:GLY:O	1:uA:107:VAL:HG23	2.04	0.57
1:JC:6:LEU:HD22	1:NB:9:ASN:HB3	1.86	0.57
1:SA:44:GLN:OE1	1:SA:46:TRP:NE1	2.36	0.57
1:yA:103:GLY:O	1:yA:107:VAL:HG23	2.04	0.57
1:BA:44:GLN:OE1	1:BA:46:TRP:NE1	2.36	0.57
1:LA:44:GLN:OE1	1:LA:46:TRP:NE1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QB:44:GLN:OE1	1:QB:46:TRP:NE1	2.34	0.57
1:aB:119:ASP:OD2	1:aC:32:HIS:NE2	2.35	0.57
1:PA:44:GLN:OE1	1:PA:46:TRP:NE1	2.36	0.57
1:dA:44:GLN:OE1	1:dA:46:TRP:NE1	2.36	0.57
1:gA:44:GLN:OE1	1:gA:46:TRP:NE1	2.36	0.57
1:UC:3:PHE:CZ	1:lC:33:VAL:HB	2.39	0.56
1:zA:44:GLN:OE1	1:zA:46:TRP:NE1	2.36	0.56
1:FA:44:GLN:OE1	1:FA:46:TRP:NE1	2.36	0.56
1:SA:119:ASP:HB3	1:yA:28:VAL:HG11	1.86	0.56
1:fA:44:GLN:OE1	1:fA:46:TRP:NE1	2.36	0.56
1:5A:103:GLY:O	1:5A:107:VAL:HG23	2.04	0.56
1:SA:103:GLY:O	1:SA:107:VAL:HG23	2.04	0.56
1:cA:44:GLN:OE1	1:cA:46:TRP:NE1	2.36	0.56
1:lA:103:GLY:O	1:lA:107:VAL:HG23	2.04	0.56
1:RA:44:GLN:OE1	1:RA:46:TRP:NE1	2.36	0.56
1:vA:44:GLN:OE1	1:vA:46:TRP:NE1	2.36	0.56
1:WA:44:GLN:OE1	1:WA:46:TRP:NE1	2.36	0.56
1:8A:44:GLN:OE1	1:8A:46:TRP:NE1	2.36	0.56
1:lA:44:GLN:OE1	1:lA:46:TRP:NE1	2.36	0.56
1:qA:44:GLN:OE1	1:qA:46:TRP:NE1	2.36	0.56
1:6B:44:GLN:OE1	1:6B:46:TRP:NE1	2.34	0.56
1:OB:44:GLN:OE1	1:OB:46:TRP:NE1	2.34	0.55
1:1A:28:VAL:HG11	1:UA:119:ASP:HB3	1.87	0.55
1:AC:53:LYS:NZ	1:RC:49:GLU:OE1	2.40	0.55
1:sB:18:LEU:O	1:sB:91:ARG:NE	2.40	0.55
1:vB:18:LEU:O	1:vB:91:ARG:NE	2.40	0.55
1:wB:18:LEU:O	1:wB:91:ARG:NE	2.40	0.55
1:yB:18:LEU:O	1:yB:91:ARG:NE	2.40	0.55
1:GB:18:LEU:O	1:GB:91:ARG:NE	2.40	0.55
1:HB:18:LEU:O	1:HB:91:ARG:NE	2.40	0.55
1:KA:44:GLN:OE1	1:KA:46:TRP:NE1	2.36	0.55
1:OB:18:LEU:O	1:OB:91:ARG:NE	2.40	0.55
1:aB:18:LEU:O	1:aB:91:ARG:NE	2.40	0.55
1:lB:18:LEU:O	1:lB:91:ARG:NE	2.39	0.55
1:uB:18:LEU:O	1:uB:91:ARG:NE	2.40	0.55
1:zB:18:LEU:O	1:zB:91:ARG:NE	2.40	0.55
1:6B:18:LEU:O	1:6B:91:ARG:NE	2.40	0.55
1:AC:3:PHE:CB	1:RC:51:ALA:HB1	2.37	0.55
1:JA:44:GLN:OE1	1:JA:46:TRP:NE1	2.36	0.55
1:1B:18:LEU:O	1:1B:91:ARG:NE	2.40	0.55
1:iB:18:LEU:O	1:iB:91:ARG:NE	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:rB:18:LEU:O	1:rB:91:ARG:NE	2.40	0.55
1:RB:18:LEU:O	1:RB:91:ARG:NE	2.40	0.55
1:XB:18:LEU:O	1:XB:91:ARG:NE	2.40	0.55
1:kB:18:LEU:O	1:kB:91:ARG:NE	2.40	0.55
1:FB:18:LEU:O	1:FB:91:ARG:NE	2.40	0.55
1:cB:18:LEU:O	1:cB:91:ARG:NE	2.40	0.55
1:CB:18:LEU:O	1:CB:91:ARG:NE	2.40	0.55
1:QB:18:LEU:O	1:QB:91:ARG:NE	2.40	0.55
1:TA:9:ASN:HA	1:7A:38:THR:HG21	1.89	0.55
1:rA:44:GLN:OE1	1:rA:46:TRP:NE1	2.36	0.55
1:vB:9:ASN:HB3	1:yC:6:LEU:HD22	1.88	0.55
1:EA:9:ASN:HA	1:wA:38:THR:HG21	1.88	0.55
1:SB:18:LEU:O	1:SB:91:ARG:NE	2.40	0.55
1:bA:44:GLN:OE1	1:bA:46:TRP:NE1	2.36	0.55
1:jB:18:LEU:O	1:jB:91:ARG:NE	2.40	0.55
1:EB:18:LEU:O	1:EB:91:ARG:NE	2.40	0.55
1:KA:128:GLN:NE2	1:mA:124:PHE:O	2.36	0.55
1:PB:18:LEU:O	1:PB:91:ARG:NE	2.40	0.55
1:ZB:18:LEU:O	1:ZB:91:ARG:NE	2.40	0.55
1:fB:18:LEU:O	1:fB:91:ARG:NE	2.40	0.55
1:qB:18:LEU:O	1:qB:91:ARG:NE	2.40	0.55
1:DB:18:LEU:O	1:DB:91:ARG:NE	2.40	0.55
1:hB:18:LEU:O	1:hB:91:ARG:NE	2.40	0.55
1:nB:18:LEU:O	1:nB:91:ARG:NE	2.40	0.55
1:5B:18:LEU:O	1:5B:91:ARG:NE	2.40	0.55
1:8B:18:LEU:O	1:8B:91:ARG:NE	2.40	0.55
1:BB:18:LEU:O	1:BB:91:ARG:NE	2.40	0.54
1:NB:18:LEU:O	1:NB:91:ARG:NE	2.40	0.54
1:UB:18:LEU:O	1:UB:91:ARG:NE	2.40	0.54
1:VB:18:LEU:O	1:VB:91:ARG:NE	2.39	0.54
1:YB:18:LEU:O	1:YB:91:ARG:NE	2.40	0.54
1:dB:18:LEU:O	1:dB:91:ARG:NE	2.40	0.54
1:eA:44:GLN:OE1	1:eA:46:TRP:NE1	2.36	0.54
1:4B:18:LEU:O	1:4B:91:ARG:NE	2.40	0.54
1:LB:18:LEU:O	1:LB:91:ARG:NE	2.40	0.54
1:MB:18:LEU:O	1:MB:91:ARG:NE	2.40	0.54
1:WB:18:LEU:O	1:WB:91:ARG:NE	2.40	0.54
1:bB:18:LEU:O	1:bB:91:ARG:NE	2.39	0.54
1:eB:18:LEU:O	1:eB:91:ARG:NE	2.40	0.54
1:gB:18:LEU:O	1:gB:91:ARG:NE	2.40	0.54
1:2B:18:LEU:O	1:2B:91:ARG:NE	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:mB:18:LEU:O	1:mB:91:ARG:NE	2.40	0.54
1:xB:18:LEU:O	1:xB:91:ARG:NE	2.40	0.54
1:DC:58:LEU:HD11	1:TC:3:PHE:CD2	2.43	0.54
1:7B:18:LEU:O	1:7B:91:ARG:NE	2.40	0.54
1:TB:18:LEU:O	1:TB:91:ARG:NE	2.40	0.54
1:oB:18:LEU:O	1:oB:91:ARG:NE	2.39	0.54
1:7A:44:GLN:OE1	1:7A:46:TRP:NE1	2.36	0.54
1:JB:18:LEU:O	1:JB:91:ARG:NE	2.40	0.54
1:YC:58:LEU:CD1	1:mC:3:PHE:CD2	2.91	0.54
1:IB:18:LEU:O	1:IB:91:ARG:NE	2.40	0.54
1:KB:18:LEU:O	1:KB:91:ARG:NE	2.40	0.54
1:tB:18:LEU:O	1:tB:91:ARG:NE	2.40	0.54
1:AB:18:LEU:O	1:AB:91:ARG:NE	2.40	0.54
1:pA:44:GLN:OE1	1:pA:46:TRP:NE1	2.36	0.54
1:pB:18:LEU:O	1:pB:91:ARG:NE	2.40	0.54
1:yA:44:GLN:OE1	1:yA:46:TRP:NE1	2.36	0.54
1:YA:44:GLN:OE1	1:YA:46:TRP:NE1	2.36	0.54
1:pB:9:ASN:HB3	1:5C:6:LEU:HD22	1.90	0.54
1:3B:18:LEU:O	1:3B:91:ARG:NE	2.40	0.54
1:AC:56:GLN:NE2	1:RC:92:GLU:OE2	2.42	0.54
1:uA:44:GLN:OE1	1:uA:46:TRP:NE1	2.36	0.54
1:AC:58:LEU:CD1	1:RC:3:PHE:CD2	2.85	0.53
1:DA:44:GLN:OE1	1:DA:46:TRP:NE1	2.36	0.53
1:UA:44:GLN:OE1	1:UA:46:TRP:NE1	2.36	0.53
1:YC:6:LEU:HD22	1:mB:9:ASN:HB3	1.90	0.53
1:ZC:58:LEU:HD11	1:gC:3:PHE:CE2	2.42	0.53
1:cA:128:GLN:NE2	1:sA:124:PHE:O	2.28	0.53
1:3A:44:GLN:OE1	1:3A:46:TRP:NE1	2.36	0.53
1:IC:107:VAL:O	1:IC:111:VAL:HG23	2.09	0.53
1:oC:107:VAL:O	1:oC:111:VAL:HG23	2.09	0.53
1:rC:107:VAL:O	1:rC:111:VAL:HG23	2.09	0.53
1:vC:107:VAL:O	1:vC:111:VAL:HG23	2.09	0.53
1:4C:107:VAL:O	1:4C:111:VAL:HG23	2.09	0.53
1:5C:107:VAL:O	1:5C:111:VAL:HG23	2.09	0.53
1:GC:107:VAL:O	1:GC:111:VAL:HG23	2.09	0.53
1:IC:107:VAL:O	1:IC:111:VAL:HG23	2.09	0.53
1:MC:107:VAL:O	1:MC:111:VAL:HG23	2.09	0.53
1:RC:107:VAL:O	1:RC:111:VAL:HG23	2.09	0.53
1:VC:107:VAL:O	1:VC:111:VAL:HG23	2.09	0.53
1:YC:107:VAL:O	1:YC:111:VAL:HG23	2.09	0.53
1:cC:107:VAL:O	1:cC:111:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:xC:107:VAL:O	1:xC:111:VAL:HG23	2.09	0.53
1:7C:107:VAL:O	1:7C:111:VAL:HG23	2.09	0.53
1:AC:58:LEU:HD21	1:RC:3:PHE:HE2	1.73	0.53
1:DC:107:VAL:O	1:DC:111:VAL:HG23	2.09	0.53
1:KC:107:VAL:O	1:KC:111:VAL:HG23	2.09	0.53
1:NC:107:VAL:O	1:NC:111:VAL:HG23	2.09	0.53
1:PA:119:ASP:OD2	1:IA:32:HIS:CE1	2.61	0.53
1:SC:107:VAL:O	1:SC:111:VAL:HG23	2.09	0.53
1:2C:107:VAL:O	1:2C:111:VAL:HG23	2.09	0.53
1:vC:49:GLU:OE1	1:yC:53:LYS:NZ	2.42	0.53
1:zC:107:VAL:O	1:zC:111:VAL:HG23	2.09	0.53
1:5A:44:GLN:OE1	1:5A:46:TRP:NE1	2.36	0.53
1:AC:107:VAL:O	1:AC:111:VAL:HG23	2.09	0.53
1:BC:112:LYS:HB3	1:1B:134:PHE:CZ	2.43	0.53
1:CC:107:VAL:O	1:CC:111:VAL:HG23	2.09	0.53
1:JC:107:VAL:O	1:JC:111:VAL:HG23	2.09	0.53
1:AC:109:HIS:CE1	1:4B:133:SER:HB3	2.43	0.53
1:WA:9:ASN:HA	1:pA:38:THR:HG21	1.91	0.53
1:XC:107:VAL:O	1:XC:111:VAL:HG23	2.09	0.53
1:qC:107:VAL:O	1:qC:111:VAL:HG23	2.09	0.53
1:yC:107:VAL:O	1:yC:111:VAL:HG23	2.09	0.53
1:FC:107:VAL:O	1:FC:111:VAL:HG23	2.09	0.53
1:YA:38:THR:HG21	1:aA:9:ASN:HA	1.91	0.53
1:aC:107:VAL:O	1:aC:111:VAL:HG23	2.09	0.53
1:eC:107:VAL:O	1:eC:111:VAL:HG23	2.09	0.53
1:fC:107:VAL:O	1:fC:111:VAL:HG23	2.09	0.53
1:hC:107:VAL:O	1:hC:111:VAL:HG23	2.09	0.53
1:iC:107:VAL:O	1:iC:111:VAL:HG23	2.09	0.53
1:pC:107:VAL:O	1:pC:111:VAL:HG23	2.09	0.53
1:uC:107:VAL:O	1:uC:111:VAL:HG23	2.09	0.53
1:8C:107:VAL:O	1:8C:111:VAL:HG23	2.09	0.53
1:ZC:107:VAL:O	1:ZC:111:VAL:HG23	2.09	0.53
1:bC:107:VAL:O	1:bC:111:VAL:HG23	2.09	0.53
1:dC:107:VAL:O	1:dC:111:VAL:HG23	2.09	0.53
1:iC:109:HIS:CE1	1:sB:133:SER:HB3	2.43	0.53
1:sC:107:VAL:O	1:sC:111:VAL:HG23	2.09	0.53
1:QC:107:VAL:O	1:QC:111:VAL:HG23	2.09	0.52
1:WC:107:VAL:O	1:WC:111:VAL:HG23	2.09	0.52
1:gC:107:VAL:O	1:gC:111:VAL:HG23	2.09	0.52
1:nC:107:VAL:O	1:nC:111:VAL:HG23	2.09	0.52
1:BC:107:VAL:O	1:BC:111:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PC:107:VAL:O	1:PC:111:VAL:HG23	2.09	0.52
1:kC:107:VAL:O	1:kC:111:VAL:HG23	2.09	0.52
1:6C:107:VAL:O	1:6C:111:VAL:HG23	2.09	0.52
1:HC:107:VAL:O	1:HC:111:VAL:HG23	2.09	0.52
1:LC:107:VAL:O	1:LC:111:VAL:HG23	2.09	0.52
1:wC:107:VAL:O	1:wC:111:VAL:HG23	2.09	0.52
1:EC:107:VAL:O	1:EC:111:VAL:HG23	2.09	0.52
1:UC:107:VAL:O	1:UC:111:VAL:HG23	2.09	0.52
1:iC:109:HIS:HE1	1:sB:133:SER:HB3	1.74	0.52
1:jC:107:VAL:O	1:jC:111:VAL:HG23	2.09	0.52
1:OC:107:VAL:O	1:OC:111:VAL:HG23	2.09	0.52
1:1C:107:VAL:O	1:1C:111:VAL:HG23	2.09	0.52
1:mC:107:VAL:O	1:mC:111:VAL:HG23	2.09	0.52
1:TC:107:VAL:O	1:TC:111:VAL:HG23	2.09	0.52
1:uC:6:LEU:HD22	1:zB:9:ASN:HB3	1.92	0.52
1:PA:113:GLN:HG2	1:lA:134:PHE:HE1	1.75	0.52
1:sB:9:ASN:HB3	1:7C:6:LEU:HD22	1.91	0.52
1:tC:107:VAL:O	1:tC:111:VAL:HG23	2.09	0.52
1:3C:107:VAL:O	1:3C:111:VAL:HG23	2.09	0.51
1:AC:3:PHE:HB3	1:RC:51:ALA:HB1	1.92	0.51
1:RA:102:TYR:OH	1:4A:116:LEU:CD2	2.59	0.51
1:UC:10:MET:HE1	1:lC:41:LYS:O	2.10	0.51
1:TC:124:PHE:CG	1:iB:22:MET:HE2	2.46	0.51
1:cC:51:ALA:HB1	1:iC:3:PHE:HB3	1.92	0.51
1:zA:9:ASN:HA	1:8A:38:THR:HG21	1.93	0.51
1:HA:28:VAL:HG11	1:yA:119:ASP:HB3	1.93	0.50
1:AC:43:HIS:CD2	1:RC:12:GLY:HA3	2.46	0.50
1:PA:9:ASN:HA	1:lA:38:THR:HG21	1.93	0.50
1:UC:43:HIS:NE2	1:lC:12:GLY:O	2.45	0.50
1:AC:30:LEU:HB3	1:RC:3:PHE:HZ	1.77	0.50
1:MC:56:GLN:O	1:MC:60:HIS:ND1	2.45	0.50
1:VB:43:HIS:HE2	1:VB:48:THR:HG1	1.60	0.50
1:3C:56:GLN:O	1:3C:60:HIS:ND1	2.45	0.50
1:8C:56:GLN:O	1:8C:60:HIS:ND1	2.45	0.50
1:GC:56:GLN:O	1:GC:60:HIS:ND1	2.45	0.50
1:WC:56:GLN:O	1:WC:60:HIS:ND1	2.45	0.50
1:aC:56:GLN:O	1:aC:60:HIS:ND1	2.45	0.50
1:rC:56:GLN:O	1:rC:60:HIS:ND1	2.45	0.50
1:xC:56:GLN:O	1:xC:60:HIS:ND1	2.45	0.50
1:4C:56:GLN:O	1:4C:60:HIS:ND1	2.45	0.50
1:DA:28:VAL:HG11	1:iA:119:ASP:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KC:56:GLN:O	1:KC:60:HIS:ND1	2.45	0.50
1:LC:56:GLN:O	1:LC:60:HIS:ND1	2.45	0.50
1:WB:26:PRO:O	1:WB:28:VAL:N	2.45	0.50
1:ZC:56:GLN:O	1:ZC:60:HIS:ND1	2.45	0.50
1:dC:124:PHE:CD2	1:xB:22:MET:HE2	2.46	0.50
1:iC:56:GLN:O	1:iC:60:HIS:ND1	2.45	0.50
1:2C:56:GLN:O	1:2C:60:HIS:ND1	2.45	0.50
1:tC:56:GLN:O	1:tC:60:HIS:ND1	2.45	0.50
1:7C:56:GLN:O	1:7C:60:HIS:ND1	2.45	0.50
1:BB:26:PRO:O	1:BB:28:VAL:N	2.45	0.50
1:BC:56:GLN:O	1:BC:60:HIS:ND1	2.45	0.50
1:1C:56:GLN:O	1:1C:60:HIS:ND1	2.45	0.50
1:TC:56:GLN:O	1:TC:60:HIS:ND1	2.45	0.50
1:bC:56:GLN:O	1:bC:60:HIS:ND1	2.45	0.50
1:eC:56:GLN:O	1:eC:60:HIS:ND1	2.45	0.50
1:hC:56:GLN:O	1:hC:60:HIS:ND1	2.45	0.50
1:mC:56:GLN:O	1:mC:60:HIS:ND1	2.45	0.50
1:wC:56:GLN:O	1:wC:60:HIS:ND1	2.45	0.50
1:6C:56:GLN:O	1:6C:60:HIS:ND1	2.45	0.50
1:EB:26:PRO:O	1:EB:28:VAL:N	2.45	0.49
1:RB:26:PRO:O	1:RB:28:VAL:N	2.45	0.49
1:TA:9:ASN:HA	1:7A:38:THR:CG2	2.42	0.49
1:UB:26:PRO:O	1:UB:28:VAL:N	2.45	0.49
1:XC:56:GLN:O	1:XC:60:HIS:ND1	2.45	0.49
1:kC:56:GLN:O	1:kC:60:HIS:ND1	2.45	0.49
1:nC:56:GLN:O	1:nC:60:HIS:ND1	2.45	0.49
1:vC:56:GLN:O	1:vC:60:HIS:ND1	2.45	0.49
1:zC:56:GLN:O	1:zC:60:HIS:ND1	2.45	0.49
1:CC:56:GLN:O	1:CC:60:HIS:ND1	2.45	0.49
1:NB:26:PRO:O	1:NB:28:VAL:N	2.45	0.49
1:NC:56:GLN:O	1:NC:60:HIS:ND1	2.45	0.49
1:OC:56:GLN:O	1:OC:60:HIS:ND1	2.45	0.49
1:RC:56:GLN:O	1:RC:60:HIS:ND1	2.45	0.49
1:UC:56:GLN:O	1:UC:60:HIS:ND1	2.45	0.49
1:iC:8:LYS:HB3	1:sB:38:THR:HG22	1.94	0.49
1:iC:8:LYS:O	1:sB:38:THR:O	2.30	0.49
1:lC:56:GLN:O	1:lC:60:HIS:ND1	2.45	0.49
1:oC:56:GLN:O	1:oC:60:HIS:ND1	2.45	0.49
1:5C:56:GLN:O	1:5C:60:HIS:ND1	2.45	0.49
1:8B:26:PRO:O	1:8B:28:VAL:N	2.45	0.49
1:FC:56:GLN:O	1:FC:60:HIS:ND1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HC:56:GLN:O	1:HC:60:HIS:ND1	2.45	0.49
1:IC:56:GLN:O	1:IC:60:HIS:ND1	2.45	0.49
1:SC:56:GLN:O	1:SC:60:HIS:ND1	2.45	0.49
1:fC:56:GLN:O	1:fC:60:HIS:ND1	2.45	0.49
1:rB:26:PRO:O	1:rB:28:VAL:N	2.45	0.49
1:sB:26:PRO:O	1:sB:28:VAL:N	2.45	0.49
1:uB:26:PRO:O	1:uB:28:VAL:N	2.45	0.49
1:GB:26:PRO:O	1:GB:28:VAL:N	2.45	0.49
1:PC:56:GLN:O	1:PC:60:HIS:ND1	2.45	0.49
1:cC:56:GLN:O	1:cC:60:HIS:ND1	2.45	0.49
1:2B:26:PRO:O	1:2B:28:VAL:N	2.45	0.49
1:pC:56:GLN:O	1:pC:60:HIS:ND1	2.45	0.49
1:qC:56:GLN:O	1:qC:60:HIS:ND1	2.45	0.49
1:sC:56:GLN:O	1:sC:60:HIS:ND1	2.45	0.49
1:xB:26:PRO:O	1:xB:28:VAL:N	2.45	0.49
1:LB:26:PRO:O	1:LB:28:VAL:N	2.45	0.49
1:RA:102:TYR:OH	1:4A:116:LEU:HD23	2.12	0.49
1:iB:26:PRO:O	1:iB:28:VAL:N	2.45	0.49
1:lB:26:PRO:O	1:lB:28:VAL:N	2.45	0.49
1:nB:26:PRO:O	1:nB:28:VAL:N	2.45	0.49
1:wC:82:MET:HE1	1:3C:82:MET:HE1	1.95	0.49
1:5B:26:PRO:O	1:5B:28:VAL:N	2.45	0.49
1:TC:129:PRO:HA	1:iB:130:LYS:HZ2	1.78	0.49
1:YC:56:GLN:O	1:YC:60:HIS:ND1	2.45	0.49
1:aB:26:PRO:O	1:aB:28:VAL:N	2.45	0.49
1:yB:26:PRO:O	1:yB:28:VAL:N	2.45	0.49
1:EC:56:GLN:O	1:EC:60:HIS:ND1	2.45	0.49
1:NA:40:GLN:O	1:dA:11:LYS:HG2	2.13	0.49
1:TB:94:TRP:HH2	1:sC:116:LEU:HD13	1.78	0.49
1:VC:56:GLN:O	1:VC:60:HIS:ND1	2.45	0.49
1:cB:26:PRO:O	1:cB:28:VAL:N	2.45	0.49
1:fB:26:PRO:O	1:fB:28:VAL:N	2.45	0.49
1:uC:56:GLN:O	1:uC:60:HIS:ND1	2.45	0.49
1:AC:56:GLN:O	1:AC:60:HIS:ND1	2.45	0.49
1:DC:56:GLN:O	1:DC:60:HIS:ND1	2.45	0.49
1:SA:77:PRO:O	1:SA:81:ALA:N	2.46	0.49
1:WC:8:LYS:HD3	1:wB:38:THR:CG2	2.43	0.49
1:XB:26:PRO:O	1:XB:28:VAL:N	2.45	0.49
1:oB:26:PRO:O	1:oB:28:VAL:N	2.45	0.49
1:tB:26:PRO:O	1:tB:28:VAL:N	2.45	0.49
1:BC:112:LYS:HB2	1:1B:134:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:9:ASN:ND2	1:TC:6:LEU:HD22	2.27	0.49
1:JC:56:GLN:O	1:JC:60:HIS:ND1	2.45	0.49
1:MC:116:LEU:HD23	1:hB:102:TYR:OH	2.12	0.49
1:PB:26:PRO:O	1:PB:28:VAL:N	2.45	0.49
1:kB:26:PRO:O	1:kB:28:VAL:N	2.45	0.49
1:yC:56:GLN:O	1:yC:60:HIS:ND1	2.45	0.49
1:CB:26:PRO:O	1:CB:28:VAL:N	2.45	0.48
1:HB:26:PRO:O	1:HB:28:VAL:N	2.45	0.48
1:UA:77:PRO:O	1:UA:81:ALA:N	2.46	0.48
1:gC:56:GLN:O	1:gC:60:HIS:ND1	2.45	0.48
1:wB:26:PRO:O	1:wB:28:VAL:N	2.45	0.48
1:xA:77:PRO:O	1:xA:81:ALA:N	2.46	0.48
1:JB:9:ASN:ND2	1:NC:6:LEU:HD22	2.28	0.48
1:SB:26:PRO:O	1:SB:28:VAL:N	2.45	0.48
1:2A:77:PRO:O	1:2A:81:ALA:N	2.46	0.48
1:dC:56:GLN:O	1:dC:60:HIS:ND1	2.45	0.48
1:lA:77:PRO:O	1:lA:81:ALA:N	2.46	0.48
1:3B:26:PRO:O	1:3B:28:VAL:N	2.45	0.48
1:4A:77:PRO:O	1:4A:81:ALA:N	2.46	0.48
1:FA:77:PRO:O	1:FA:81:ALA:N	2.46	0.48
1:IB:26:PRO:O	1:IB:28:VAL:N	2.45	0.48
1:MA:77:PRO:O	1:MA:81:ALA:N	2.46	0.48
1:NA:77:PRO:O	1:NA:81:ALA:N	2.46	0.48
1:TB:26:PRO:O	1:TB:28:VAL:N	2.45	0.48
1:pB:26:PRO:O	1:pB:28:VAL:N	2.45	0.48
1:1B:26:PRO:O	1:1B:28:VAL:N	2.45	0.48
1:MB:26:PRO:O	1:MB:28:VAL:N	2.45	0.48
1:QA:77:PRO:O	1:QA:81:ALA:N	2.46	0.48
1:mB:26:PRO:O	1:mB:28:VAL:N	2.45	0.48
1:EA:77:PRO:O	1:EA:81:ALA:N	2.46	0.48
1:GA:77:PRO:O	1:GA:81:ALA:N	2.46	0.48
1:OB:26:PRO:O	1:OB:28:VAL:N	2.45	0.48
1:RA:41:LYS:HA	1:4A:11:LYS:HD3	1.96	0.48
1:dB:26:PRO:O	1:dB:28:VAL:N	2.45	0.48
1:rA:77:PRO:O	1:rA:81:ALA:N	2.46	0.48
1:6B:26:PRO:O	1:6B:28:VAL:N	2.45	0.48
1:AA:77:PRO:O	1:AA:81:ALA:N	2.46	0.48
1:gB:26:PRO:O	1:gB:28:VAL:N	2.45	0.48
1:jB:26:PRO:O	1:jB:28:VAL:N	2.45	0.48
1:qA:77:PRO:O	1:qA:81:ALA:N	2.46	0.48
1:uA:77:PRO:O	1:uA:81:ALA:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4B:26:PRO:O	1:4B:28:VAL:N	2.45	0.48
1:PA:113:GLN:CG	1:1A:134:PHE:CE1	2.96	0.48
1:ZA:77:PRO:O	1:ZA:81:ALA:N	2.46	0.48
1:bA:77:PRO:O	1:bA:81:ALA:N	2.46	0.48
1:hB:26:PRO:O	1:hB:28:VAL:N	2.45	0.48
1:hB:43:HIS:HE2	1:hB:48:THR:HG1	1.60	0.48
1:jA:77:PRO:O	1:jA:81:ALA:N	2.46	0.48
1:jC:56:GLN:O	1:jC:60:HIS:ND1	2.45	0.48
1:yA:77:PRO:O	1:yA:81:ALA:N	2.46	0.48
1:5A:77:PRO:O	1:5A:81:ALA:N	2.46	0.48
1:HA:77:PRO:O	1:HA:81:ALA:N	2.46	0.48
1:KA:9:ASN:HA	1:bA:38:THR:HG21	1.95	0.48
1:QB:26:PRO:O	1:QB:28:VAL:N	2.45	0.48
1:QC:56:GLN:O	1:QC:60:HIS:ND1	2.45	0.48
1:RC:116:LEU:HD23	1:XB:102:TYR:OH	2.13	0.48
1:TC:124:PHE:CE2	1:iB:117:TRP:HZ3	2.31	0.48
1:VA:77:PRO:O	1:VA:81:ALA:N	2.46	0.48
1:ZB:26:PRO:O	1:ZB:28:VAL:N	2.45	0.48
1:fA:77:PRO:O	1:fA:81:ALA:N	2.46	0.48
1:hA:77:PRO:O	1:hA:81:ALA:N	2.46	0.48
1:JB:26:PRO:O	1:JB:28:VAL:N	2.45	0.48
1:YA:77:PRO:O	1:YA:81:ALA:N	2.46	0.48
1:sA:77:PRO:O	1:sA:81:ALA:N	2.46	0.48
1:DA:77:PRO:O	1:DA:81:ALA:N	2.46	0.48
1:1A:77:PRO:O	1:1A:81:ALA:N	2.46	0.47
1:DC:3:PHE:HB3	1:TC:51:ALA:HB1	1.96	0.47
1:PA:77:PRO:O	1:PA:81:ALA:N	2.46	0.47
1:pA:77:PRO:O	1:pA:81:ALA:N	2.46	0.47
1:pB:43:HIS:HE2	1:pB:48:THR:HG1	1.62	0.47
1:nA:77:PRO:O	1:nA:81:ALA:N	2.46	0.47
1:PA:113:GLN:HG3	1:1A:134:PHE:CE1	2.49	0.47
1:RA:77:PRO:O	1:RA:81:ALA:N	2.46	0.47
1:UC:4:ILE:O	1:UC:8:LYS:N	2.47	0.47
1:cA:77:PRO:O	1:cA:81:ALA:N	2.46	0.47
1:wA:77:PRO:O	1:wA:81:ALA:N	2.46	0.47
1:OC:4:ILE:O	1:OC:8:LYS:N	2.47	0.47
1:oA:77:PRO:O	1:oA:81:ALA:N	2.46	0.47
1:rC:34:LYS:HE3	1:8C:6:LEU:HD11	1.96	0.47
1:6C:4:ILE:O	1:6C:8:LYS:N	2.47	0.47
1:7A:77:PRO:O	1:7A:81:ALA:N	2.46	0.47
1:8A:77:PRO:O	1:8A:81:ALA:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IA:77:PRO:O	1:IA:81:ALA:N	2.46	0.47
1:ZB:43:HIS:HE2	1:ZB:48:THR:HG1	1.61	0.47
1:ZC:4:ILE:O	1:ZC:8:LYS:N	2.47	0.47
1:uC:4:ILE:O	1:uC:8:LYS:N	2.48	0.47
1:BC:4:ILE:O	1:BC:8:LYS:N	2.47	0.47
1:CA:77:PRO:O	1:CA:81:ALA:N	2.46	0.47
1:EC:43:HIS:NE2	1:SC:12:GLY:O	2.47	0.47
1:HC:4:ILE:O	1:HC:8:LYS:N	2.47	0.47
1:NA:38:THR:CG2	1:dA:9:ASN:HA	2.44	0.47
1:hC:4:ILE:O	1:hC:8:LYS:N	2.47	0.47
1:LA:77:PRO:O	1:LA:81:ALA:N	2.46	0.47
1:SC:4:ILE:O	1:SC:8:LYS:N	2.47	0.47
1:TC:124:PHE:HA	1:iB:128:GLN:OE1	2.14	0.47
1:TC:124:PHE:HE2	1:iB:117:TRP:HZ3	1.62	0.47
1:WB:134:PHE:CE1	1:5C:112:LYS:HB2	2.49	0.47
1:aA:77:PRO:O	1:aA:81:ALA:N	2.46	0.47
1:kA:77:PRO:O	1:kA:81:ALA:N	2.46	0.47
1:rB:9:ASN:ND2	1:8C:6:LEU:CD2	2.76	0.47
1:yC:4:ILE:O	1:yC:8:LYS:N	2.47	0.47
1:VB:26:PRO:O	1:VB:28:VAL:N	2.45	0.47
1:WC:4:ILE:O	1:WC:8:LYS:N	2.47	0.47
1:dA:77:PRO:O	1:dA:81:ALA:N	2.46	0.47
1:eA:77:PRO:O	1:eA:81:ALA:N	2.46	0.47
1:iA:77:PRO:O	1:iA:81:ALA:N	2.46	0.47
1:qB:43:HIS:NE2	1:qB:48:THR:OG1	2.48	0.47
1:sC:4:ILE:O	1:sC:8:LYS:N	2.47	0.47
1:tA:77:PRO:O	1:tA:81:ALA:N	2.46	0.47
1:BA:77:PRO:O	1:BA:81:ALA:N	2.46	0.47
1:CB:43:HIS:HE2	1:CB:48:THR:HG1	1.62	0.47
1:KA:77:PRO:O	1:KA:81:ALA:N	2.46	0.47
1:XA:77:PRO:O	1:XA:81:ALA:N	2.46	0.47
1:gA:77:PRO:O	1:gA:81:ALA:N	2.46	0.47
1:tC:4:ILE:O	1:tC:8:LYS:N	2.47	0.47
1:3A:77:PRO:O	1:3A:81:ALA:N	2.46	0.47
1:3C:4:ILE:O	1:3C:8:LYS:N	2.48	0.47
1:AB:43:HIS:HE2	1:AB:48:THR:HG1	1.63	0.47
1:EC:4:ILE:O	1:EC:8:LYS:N	2.47	0.47
1:FB:43:HIS:NE2	1:FB:48:THR:OG1	2.48	0.47
1:HC:3:PHE:HB3	1:KC:51:ALA:HB1	1.97	0.47
1:TA:77:PRO:O	1:TA:81:ALA:N	2.46	0.47
1:qB:26:PRO:O	1:qB:28:VAL:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:zA:77:PRO:O	1:zA:81:ALA:N	2.46	0.47
1:AB:26:PRO:O	1:AB:28:VAL:N	2.45	0.47
1:AC:4:ILE:O	1:AC:8:LYS:N	2.47	0.46
1:BC:9:ASN:O	1:1B:41:LYS:CG	2.63	0.46
1:DB:26:PRO:O	1:DB:28:VAL:N	2.45	0.46
1:WA:77:PRO:O	1:WA:81:ALA:N	2.46	0.46
1:dB:43:HIS:NE2	1:dB:48:THR:OG1	2.48	0.46
1:mA:77:PRO:O	1:mA:81:ALA:N	2.46	0.46
1:vA:77:PRO:O	1:vA:81:ALA:N	2.46	0.46
1:vB:26:PRO:O	1:vB:28:VAL:N	2.45	0.46
1:8C:4:ILE:O	1:8C:8:LYS:N	2.47	0.46
1:AC:3:PHE:CD1	1:RC:37:LEU:CD1	2.97	0.46
1:AC:10:MET:HE1	1:RC:41:LYS:O	2.14	0.46
1:LC:4:ILE:O	1:LC:8:LYS:N	2.48	0.46
1:eB:26:PRO:O	1:eB:28:VAL:N	2.45	0.46
1:gB:43:HIS:NE2	1:gB:48:THR:OG1	2.48	0.46
1:oB:43:HIS:NE2	1:oB:48:THR:OG1	2.48	0.46
1:5C:4:ILE:O	1:5C:8:LYS:N	2.47	0.46
1:BB:43:HIS:NE2	1:BB:48:THR:OG1	2.48	0.46
1:IB:43:HIS:NE2	1:IB:48:THR:OG1	2.48	0.46
1:PB:43:HIS:NE2	1:PB:48:THR:OG1	2.48	0.46
1:RC:4:ILE:O	1:RC:8:LYS:N	2.47	0.46
1:nB:43:HIS:NE2	1:nB:48:THR:OG1	2.48	0.46
1:zC:4:ILE:O	1:zC:8:LYS:N	2.47	0.46
1:FB:26:PRO:O	1:FB:28:VAL:N	2.45	0.46
1:JA:77:PRO:O	1:JA:81:ALA:N	2.46	0.46
1:OA:77:PRO:O	1:OA:81:ALA:N	2.46	0.46
1:VC:4:ILE:O	1:VC:8:LYS:N	2.48	0.46
1:XB:43:HIS:HE2	1:XB:48:THR:HG1	1.63	0.46
1:YB:26:PRO:O	1:YB:28:VAL:N	2.45	0.46
1:bB:26:PRO:O	1:bB:28:VAL:N	2.45	0.46
1:IC:4:ILE:O	1:IC:8:LYS:N	2.47	0.46
1:QC:4:ILE:O	1:QC:8:LYS:N	2.47	0.46
1:SA:38:THR:HG21	1:nA:9:ASN:HA	1.98	0.46
1:ZB:43:HIS:NE2	1:ZB:48:THR:OG1	2.48	0.46
1:hB:43:HIS:NE2	1:hB:48:THR:OG1	2.48	0.46
1:lC:4:ILE:O	1:lC:8:LYS:N	2.47	0.46
1:mC:4:ILE:O	1:mC:8:LYS:N	2.48	0.46
1:wC:4:ILE:O	1:wC:8:LYS:N	2.47	0.46
1:TC:4:ILE:O	1:TC:8:LYS:N	2.47	0.46
1:WB:134:PHE:CZ	1:5C:112:LYS:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JC:58:LEU:HD11	1:NC:3:PHE:CD2	2.50	0.46
1:jC:4:ILE:O	1:jC:8:LYS:N	2.47	0.46
1:kC:4:ILE:O	1:kC:8:LYS:N	2.47	0.46
1:lB:43:HIS:NE2	1:lB:48:THR:OG1	2.48	0.46
1:oC:4:ILE:O	1:oC:8:LYS:N	2.47	0.46
1:CC:4:ILE:O	1:CC:8:LYS:N	2.47	0.46
1:EB:43:HIS:NE2	1:EB:48:THR:OG1	2.48	0.46
1:RB:94:TRP:HH2	1:fC:116:LEU:HD13	1.79	0.46
1:RB:94:TRP:CH2	1:fC:116:LEU:HD13	2.51	0.46
1:TA:116:LEU:CD2	1:7A:102:TYR:OH	2.64	0.46
1:XC:4:ILE:O	1:XC:8:LYS:N	2.47	0.46
1:gA:9:ASN:HA	1:5A:38:THR:HG21	1.97	0.46
1:zB:26:PRO:O	1:zB:28:VAL:N	2.45	0.46
1:JC:116:LEU:HD13	1:dB:94:TRP:HH2	1.81	0.46
1:ZC:6:LEU:HD22	1:gB:9:ASN:HB3	1.98	0.46
1:aB:43:HIS:NE2	1:aB:48:THR:OG1	2.48	0.46
1:vC:4:ILE:O	1:vC:8:LYS:N	2.47	0.46
1:HA:119:ASP:HB3	1:fA:28:VAL:HG11	1.97	0.46
1:iB:43:HIS:NE2	1:iB:48:THR:OG1	2.48	0.46
1:pB:43:HIS:NE2	1:pB:48:THR:OG1	2.48	0.46
1:AC:12:GLY:O	1:RC:43:HIS:CE1	2.69	0.45
1:CB:43:HIS:NE2	1:CB:48:THR:OG1	2.48	0.45
1:iC:4:ILE:O	1:iC:8:LYS:N	2.47	0.45
1:rC:4:ILE:O	1:rC:8:LYS:N	2.47	0.45
1:6A:77:PRO:O	1:6A:81:ALA:N	2.46	0.45
1:GC:4:ILE:O	1:GC:8:LYS:N	2.47	0.45
1:JC:4:ILE:O	1:JC:8:LYS:N	2.47	0.45
1:KB:26:PRO:O	1:KB:28:VAL:N	2.45	0.45
1:1C:59:ILE:HD12	1:1C:59:ILE:H	1.82	0.45
1:jC:59:ILE:H	1:jC:59:ILE:HD12	1.82	0.45
1:LC:59:ILE:HD12	1:LC:59:ILE:H	1.82	0.45
1:OC:59:ILE:H	1:OC:59:ILE:HD12	1.82	0.45
1:1C:4:ILE:O	1:1C:8:LYS:N	2.47	0.45
1:SB:43:HIS:NE2	1:SB:48:THR:OG1	2.48	0.45
1:TB:43:HIS:NE2	1:TB:48:THR:OG1	2.48	0.45
1:TC:59:ILE:H	1:TC:59:ILE:HD12	1.82	0.45
1:aC:4:ILE:O	1:aC:8:LYS:N	2.47	0.45
1:5C:59:ILE:HD12	1:5C:59:ILE:H	1.82	0.45
1:8C:59:ILE:HD12	1:8C:59:ILE:H	1.82	0.45
1:NC:4:ILE:O	1:NC:8:LYS:N	2.47	0.45
1:CC:59:ILE:H	1:CC:59:ILE:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EC:59:ILE:HD12	1:EC:59:ILE:H	1.82	0.45
1:QC:59:ILE:HD12	1:QC:59:ILE:H	1.82	0.45
1:XC:59:ILE:HD12	1:XC:59:ILE:H	1.82	0.45
1:mB:43:HIS:NE2	1:mB:48:THR:OG1	2.48	0.45
1:rC:59:ILE:HD12	1:rC:59:ILE:H	1.82	0.45
1:4B:43:HIS:NE2	1:4B:48:THR:OG1	2.48	0.45
1:7C:59:ILE:H	1:7C:59:ILE:HD12	1.82	0.45
1:GC:59:ILE:HD12	1:GC:59:ILE:H	1.82	0.45
1:MB:43:HIS:HE2	1:MB:48:THR:HG1	1.63	0.45
1:MC:4:ILE:O	1:MC:8:LYS:N	2.47	0.45
1:NC:59:ILE:HD12	1:NC:59:ILE:H	1.82	0.45
1:UC:59:ILE:HD12	1:UC:59:ILE:H	1.82	0.45
1:cC:59:ILE:HD12	1:cC:59:ILE:H	1.82	0.45
1:eC:4:ILE:O	1:eC:8:LYS:N	2.47	0.45
1:mC:59:ILE:HD12	1:mC:59:ILE:H	1.82	0.45
1:qC:4:ILE:O	1:qC:8:LYS:N	2.47	0.45
1:wC:59:ILE:HD12	1:wC:59:ILE:H	1.82	0.45
1:6C:59:ILE:HD12	1:6C:59:ILE:H	1.82	0.45
1:AC:59:ILE:HD12	1:AC:59:ILE:H	1.82	0.45
1:KC:59:ILE:HD12	1:KC:59:ILE:H	1.82	0.45
1:MB:43:HIS:NE2	1:MB:48:THR:OG1	2.48	0.45
1:NB:43:HIS:NE2	1:NB:48:THR:OG1	2.48	0.45
1:OB:43:HIS:NE2	1:OB:48:THR:OG1	2.48	0.45
1:bC:4:ILE:O	1:bC:8:LYS:N	2.47	0.45
1:fC:59:ILE:HD12	1:fC:59:ILE:H	1.82	0.45
1:wC:12:GLY:O	1:3C:43:HIS:NE2	2.50	0.45
1:7B:26:PRO:O	1:7B:28:VAL:N	2.45	0.45
1:AC:52:LEU:HD11	1:RC:16:LEU:HD12	1.98	0.45
1:EC:43:HIS:CE1	1:SC:12:GLY:O	2.70	0.45
1:FC:4:ILE:O	1:FC:8:LYS:N	2.48	0.45
1:VC:59:ILE:HD12	1:VC:59:ILE:H	1.82	0.45
1:dC:59:ILE:HD12	1:dC:59:ILE:H	1.82	0.45
1:gC:4:ILE:O	1:gC:8:LYS:N	2.47	0.45
1:gC:59:ILE:HD12	1:gC:59:ILE:H	1.82	0.45
1:pC:59:ILE:HD12	1:pC:59:ILE:H	1.82	0.45
1:2C:59:ILE:H	1:2C:59:ILE:HD12	1.82	0.45
1:4B:43:HIS:HE2	1:4B:48:THR:HG1	1.63	0.45
1:4C:4:ILE:O	1:4C:8:LYS:N	2.47	0.45
1:6B:43:HIS:NE2	1:6B:48:THR:OG1	2.48	0.45
1:DC:4:ILE:O	1:DC:8:LYS:N	2.47	0.45
1:JB:43:HIS:NE2	1:JB:48:THR:OG1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JC:116:LEU:HD13	1:dB:94:TRP:CH2	2.52	0.45
1:iC:59:ILE:HD12	1:iC:59:ILE:H	1.82	0.45
1:kC:59:ILE:HD12	1:kC:59:ILE:H	1.82	0.45
1:oC:59:ILE:HD12	1:oC:59:ILE:H	1.82	0.45
1:pC:4:ILE:O	1:pC:8:LYS:N	2.47	0.45
1:xB:43:HIS:NE2	1:xB:48:THR:OG1	2.48	0.45
1:xC:59:ILE:HD12	1:xC:59:ILE:H	1.82	0.45
1:IC:59:ILE:HD12	1:IC:59:ILE:H	1.82	0.45
1:aC:59:ILE:HD12	1:aC:59:ILE:H	1.82	0.45
1:dC:4:ILE:O	1:dC:8:LYS:N	2.47	0.45
1:2C:4:ILE:O	1:2C:8:LYS:N	2.47	0.45
1:vC:59:ILE:H	1:vC:59:ILE:HD12	1.82	0.45
1:DC:43:HIS:NE2	1:TC:12:GLY:O	2.51	0.44
1:JC:59:ILE:HD12	1:JC:59:ILE:H	1.82	0.44
1:YC:4:ILE:O	1:YC:8:LYS:N	2.47	0.44
1:fC:4:ILE:O	1:fC:8:LYS:N	2.47	0.44
1:2B:43:HIS:NE2	1:2B:48:THR:OG1	2.48	0.44
1:nC:4:ILE:O	1:nC:8:LYS:N	2.47	0.44
1:zC:59:ILE:HD12	1:zC:59:ILE:H	1.82	0.44
1:FC:59:ILE:HD12	1:FC:59:ILE:H	1.82	0.44
1:ZC:3:PHE:CD1	1:gC:37:LEU:HD12	2.52	0.44
1:cC:4:ILE:O	1:cC:8:LYS:N	2.47	0.44
1:qC:59:ILE:HD12	1:qC:59:ILE:H	1.82	0.44
1:RC:59:ILE:HD12	1:RC:59:ILE:H	1.82	0.44
1:UB:43:HIS:NE2	1:UB:48:THR:OG1	2.48	0.44
1:WB:43:HIS:NE2	1:WB:48:THR:OG1	2.48	0.44
1:jB:43:HIS:NE2	1:jB:48:THR:OG1	2.48	0.44
1:CA:39:SER:HA	1:tA:11:LYS:HA	1.98	0.44
1:PC:59:ILE:HD12	1:PC:59:ILE:H	1.82	0.44
1:QB:43:HIS:NE2	1:QB:48:THR:OG1	2.48	0.44
1:xC:4:ILE:O	1:xC:8:LYS:N	2.47	0.44
1:MC:59:ILE:HD12	1:MC:59:ILE:H	1.82	0.44
1:eA:9:ASN:HA	1:vA:38:THR:HG21	2.00	0.44
1:sB:43:HIS:NE2	1:sB:48:THR:OG1	2.48	0.44
1:4C:59:ILE:HD12	1:4C:59:ILE:H	1.82	0.44
1:DC:10:MET:HE1	1:TC:41:LYS:O	2.17	0.44
1:HA:85:ILE:HD12	1:HA:85:ILE:H	1.83	0.44
1:PC:4:ILE:O	1:PC:8:LYS:N	2.47	0.44
1:RA:38:THR:CG2	1:4A:9:ASN:HA	2.48	0.44
1:TB:94:TRP:CH2	1:sC:116:LEU:HD13	2.52	0.44
1:VA:85:ILE:N	1:VA:85:ILE:HD12	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:bA:85:ILE:HD12	1:bA:85:ILE:H	1.83	0.44
1:sA:85:ILE:HD12	1:sA:85:ILE:H	1.83	0.44
1:AA:85:ILE:HD12	1:AA:85:ILE:N	2.33	0.44
1:DA:85:ILE:HD12	1:DA:85:ILE:H	1.83	0.44
1:DA:85:ILE:HD12	1:DA:85:ILE:N	2.33	0.44
1:YA:85:ILE:N	1:YA:85:ILE:HD12	2.33	0.44
1:YA:85:ILE:HD12	1:YA:85:ILE:H	1.83	0.44
1:bC:59:ILE:HD12	1:bC:59:ILE:H	1.82	0.44
1:eA:85:ILE:H	1:eA:85:ILE:HD12	1.83	0.44
1:hC:59:ILE:HD12	1:hC:59:ILE:H	1.82	0.44
1:qA:85:ILE:H	1:qA:85:ILE:HD12	1.83	0.44
1:yA:85:ILE:HD12	1:yA:85:ILE:H	1.83	0.44
1:yC:59:ILE:HD12	1:yC:59:ILE:H	1.82	0.44
1:5A:85:ILE:HD12	1:5A:85:ILE:N	2.33	0.44
1:BA:85:ILE:HD12	1:BA:85:ILE:H	1.83	0.44
1:EC:6:LEU:HD22	1:SB:9:ASN:ND2	2.33	0.44
1:FA:85:ILE:HD12	1:FA:85:ILE:H	1.83	0.44
1:GA:85:ILE:N	1:GA:85:ILE:HD12	2.33	0.44
1:KA:102:TYR:OH	1:mA:116:LEU:HD22	2.17	0.44
1:LB:43:HIS:NE2	1:LB:48:THR:OG1	2.48	0.44
1:NA:85:ILE:N	1:NA:85:ILE:HD12	2.33	0.44
1:UA:85:ILE:HD12	1:UA:85:ILE:N	2.33	0.44
1:WA:85:ILE:HD12	1:WA:85:ILE:H	1.83	0.44
1:XA:85:ILE:N	1:XA:85:ILE:HD12	2.33	0.44
1:gA:85:ILE:N	1:gA:85:ILE:HD12	2.33	0.44
1:lC:59:ILE:HD12	1:lC:59:ILE:H	1.82	0.44
1:uA:85:ILE:HD12	1:uA:85:ILE:H	1.83	0.44
1:8B:43:HIS:NE2	1:8B:48:THR:OG1	2.48	0.44
1:BC:59:ILE:HD12	1:BC:59:ILE:H	1.82	0.44
1:CA:85:ILE:HD12	1:CA:85:ILE:N	2.33	0.44
1:IA:85:ILE:HD12	1:IA:85:ILE:N	2.33	0.44
1:KA:85:ILE:HD12	1:KA:85:ILE:H	1.83	0.44
1:RB:43:HIS:NE2	1:RB:48:THR:OG1	2.48	0.44
1:YC:59:ILE:H	1:YC:59:ILE:HD12	1.82	0.44
1:ZC:59:ILE:HD12	1:ZC:59:ILE:H	1.82	0.44
1:cA:85:ILE:HD12	1:cA:85:ILE:N	2.33	0.44
1:dA:85:ILE:N	1:dA:85:ILE:HD12	2.33	0.44
1:eC:59:ILE:H	1:eC:59:ILE:HD12	1.82	0.44
1:mC:59:ILE:HD12	1:mC:59:ILE:H	1.82	0.44
1:oA:85:ILE:HD12	1:oA:85:ILE:N	2.33	0.44
1:rA:85:ILE:HD12	1:rA:85:ILE:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:sC:59:ILE:HD12	1:sC:59:ILE:H	1.82	0.44
1:6A:85:ILE:N	1:6A:85:ILE:HD12	2.33	0.44
1:DC:59:ILE:HD12	1:DC:59:ILE:H	1.82	0.43
1:LA:85:ILE:N	1:LA:85:ILE:HD12	2.33	0.43
1:OA:85:ILE:N	1:OA:85:ILE:HD12	2.33	0.43
1:PA:38:THR:HG21	1:cA:9:ASN:HA	1.99	0.43
1:WC:59:ILE:HD12	1:WC:59:ILE:N	2.33	0.43
1:bA:85:ILE:HD12	1:bA:85:ILE:N	2.33	0.43
1:eA:85:ILE:HD12	1:eA:85:ILE:N	2.33	0.43
1:fA:85:ILE:HD12	1:fA:85:ILE:N	2.33	0.43
1:kC:59:ILE:HD12	1:kC:59:ILE:N	2.33	0.43
1:rA:85:ILE:HD12	1:rA:85:ILE:N	2.33	0.43
1:tA:85:ILE:HD12	1:tA:85:ILE:N	2.33	0.43
1:zA:85:ILE:HD12	1:zA:85:ILE:H	1.83	0.43
1:7C:4:ILE:O	1:7C:8:LYS:N	2.47	0.43
1:GA:85:ILE:HD12	1:GA:85:ILE:H	1.83	0.43
1:HC:59:ILE:H	1:HC:59:ILE:HD12	1.82	0.43
1:RA:85:ILE:HD12	1:RA:85:ILE:N	2.33	0.43
1:SA:85:ILE:N	1:SA:85:ILE:HD12	2.33	0.43
1:VA:85:ILE:HD12	1:VA:85:ILE:H	1.83	0.43
1:ZA:85:ILE:HD12	1:ZA:85:ILE:N	2.33	0.43
1:ZC:53:LYS:NZ	1:gC:49:GLU:OE1	2.50	0.43
1:cC:59:ILE:HD12	1:cC:59:ILE:N	2.33	0.43
1:gA:85:ILE:HD12	1:gA:85:ILE:H	1.83	0.43
1:hA:85:ILE:HD12	1:hA:85:ILE:N	2.33	0.43
1:jC:59:ILE:HD12	1:jC:59:ILE:N	2.33	0.43
1:oC:59:ILE:HD12	1:oC:59:ILE:N	2.33	0.43
1:qC:6:LEU:HD22	1:4B:9:ASN:HB3	1.99	0.43
1:tC:59:ILE:HD12	1:tC:59:ILE:H	1.82	0.43
1:uC:59:ILE:HD12	1:uC:59:ILE:H	1.82	0.43
1:vC:59:ILE:HD12	1:vC:59:ILE:N	2.33	0.43
1:3A:85:ILE:HD12	1:3A:85:ILE:N	2.33	0.43
1:5A:85:ILE:HD12	1:5A:85:ILE:H	1.83	0.43
1:5B:43:HIS:NE2	1:5B:48:THR:OG1	2.48	0.43
1:BC:59:ILE:HD12	1:BC:59:ILE:N	2.33	0.43
1:HB:43:HIS:NE2	1:HB:48:THR:OG1	2.48	0.43
1:IC:59:ILE:HD12	1:IC:59:ILE:N	2.33	0.43
1:JC:59:ILE:HD12	1:JC:59:ILE:N	2.33	0.43
1:KC:59:ILE:HD12	1:KC:59:ILE:N	2.33	0.43
1:PA:85:ILE:HD12	1:PA:85:ILE:N	2.33	0.43
1:2A:85:ILE:HD12	1:2A:85:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:dA:85:ILE:HD12	1:dA:85:ILE:H	1.83	0.43
1:fC:59:ILE:HD12	1:fC:59:ILE:N	2.33	0.43
1:uA:85:ILE:HD12	1:uA:85:ILE:N	2.33	0.43
1:xA:85:ILE:N	1:xA:85:ILE:HD12	2.33	0.43
1:yA:85:ILE:HD12	1:yA:85:ILE:N	2.33	0.43
1:3C:59:ILE:HD12	1:3C:59:ILE:H	1.82	0.43
1:4A:85:ILE:N	1:4A:85:ILE:HD12	2.33	0.43
1:7A:85:ILE:HD12	1:7A:85:ILE:H	1.83	0.43
1:8A:85:ILE:N	1:8A:85:ILE:HD12	2.33	0.43
1:BA:85:ILE:HD12	1:BA:85:ILE:N	2.33	0.43
1:FA:85:ILE:HD12	1:FA:85:ILE:N	2.33	0.43
1:KA:85:ILE:HD12	1:KA:85:ILE:N	2.33	0.43
1:NC:59:ILE:HD12	1:NC:59:ILE:N	2.33	0.43
1:OC:59:ILE:HD12	1:OC:59:ILE:N	2.33	0.43
1:PA:85:ILE:HD12	1:PA:85:ILE:H	1.83	0.43
1:fA:85:ILE:HD12	1:fA:85:ILE:H	1.83	0.43
1:iC:59:ILE:HD12	1:iC:59:ILE:N	2.33	0.43
1:pC:59:ILE:HD12	1:pC:59:ILE:N	2.34	0.43
1:uC:59:ILE:HD12	1:uC:59:ILE:N	2.33	0.43
1:yC:59:ILE:HD12	1:yC:59:ILE:N	2.33	0.43
1:4C:59:ILE:HD12	1:4C:59:ILE:N	2.33	0.43
1:7C:59:ILE:HD12	1:7C:59:ILE:N	2.33	0.43
1:KC:4:ILE:O	1:KC:8:LYS:N	2.47	0.43
1:LA:85:ILE:HD12	1:LA:85:ILE:H	1.83	0.43
1:MA:85:ILE:HD12	1:MA:85:ILE:N	2.33	0.43
1:MC:59:ILE:HD12	1:MC:59:ILE:N	2.33	0.43
1:QA:85:ILE:N	1:QA:85:ILE:HD12	2.33	0.43
1:QC:59:ILE:HD12	1:QC:59:ILE:N	2.33	0.43
1:1C:59:ILE:HD12	1:1C:59:ILE:N	2.33	0.43
1:SC:59:ILE:HD12	1:SC:59:ILE:H	1.82	0.43
1:TA:85:ILE:H	1:TA:85:ILE:HD12	1.83	0.43
1:TA:85:ILE:HD12	1:TA:85:ILE:N	2.33	0.43
1:UA:85:ILE:HD12	1:UA:85:ILE:H	1.83	0.43
1:WA:85:ILE:HD12	1:WA:85:ILE:N	2.33	0.43
1:WC:109:HIS:HE1	1:wB:133:SER:HB3	1.84	0.43
1:aC:59:ILE:HD12	1:aC:59:ILE:N	2.33	0.43
1:jA:85:ILE:H	1:jA:85:ILE:HD12	1.83	0.43
1:mA:85:ILE:HD12	1:mA:85:ILE:H	1.83	0.43
1:mA:85:ILE:HD12	1:mA:85:ILE:N	2.33	0.43
1:qA:85:ILE:HD12	1:qA:85:ILE:N	2.33	0.43
1:sA:85:ILE:HD12	1:sA:85:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:vA:85:ILE:H	1:vA:85:ILE:HD12	1.83	0.43
1:wA:85:ILE:HD12	1:wA:85:ILE:H	1.83	0.43
1:wA:85:ILE:HD12	1:wA:85:ILE:N	2.33	0.43
1:zC:59:ILE:HD12	1:zC:59:ILE:N	2.33	0.43
1:6C:59:ILE:HD12	1:6C:59:ILE:N	2.34	0.43
1:8A:85:ILE:HD12	1:8A:85:ILE:H	1.83	0.43
1:AA:85:ILE:HD12	1:AA:85:ILE:H	1.83	0.43
1:VA:9:ASN:HA	1:dA:38:THR:HG21	2.00	0.43
1:WC:59:ILE:HD12	1:WC:59:ILE:H	1.82	0.43
1:jA:85:ILE:HD12	1:jA:85:ILE:N	2.33	0.43
1:nA:85:ILE:HD12	1:nA:85:ILE:H	1.83	0.43
1:qC:59:ILE:HD12	1:qC:59:ILE:N	2.34	0.43
1:3C:59:ILE:HD12	1:3C:59:ILE:N	2.33	0.43
1:6A:85:ILE:HD12	1:6A:85:ILE:H	1.83	0.43
1:7A:85:ILE:HD12	1:7A:85:ILE:N	2.33	0.43
1:AC:3:PHE:HB2	1:RC:51:ALA:HB1	2.00	0.43
1:IA:85:ILE:HD12	1:IA:85:ILE:H	1.83	0.43
1:JC:58:LEU:HD11	1:NC:3:PHE:CE2	2.54	0.43
1:PA:113:GLN:HG2	1:lA:134:PHE:CE1	2.53	0.43
1:2A:85:ILE:HD12	1:2A:85:ILE:H	1.83	0.43
1:cA:85:ILE:HD12	1:cA:85:ILE:H	1.83	0.43
1:lA:85:ILE:N	1:lA:85:ILE:HD12	2.33	0.43
1:sC:59:ILE:HD12	1:sC:59:ILE:N	2.33	0.43
1:tB:43:HIS:NE2	1:tB:48:THR:OG1	2.48	0.43
1:tC:59:ILE:HD12	1:tC:59:ILE:N	2.33	0.43
1:xA:85:ILE:HD12	1:xA:85:ILE:H	1.83	0.43
1:1A:85:ILE:N	1:1A:85:ILE:HD12	2.33	0.43
1:1A:85:ILE:HD12	1:1A:85:ILE:H	1.83	0.43
1:AC:59:ILE:HD12	1:AC:59:ILE:N	2.33	0.43
1:FC:59:ILE:HD12	1:FC:59:ILE:N	2.33	0.43
1:HC:6:LEU:HD22	1:KB:9:ASN:HB3	2.00	0.43
1:HC:59:ILE:HD12	1:HC:59:ILE:N	2.33	0.43
1:NA:38:THR:HG21	1:dA:9:ASN:HA	2.01	0.43
1:NA:85:ILE:HD12	1:NA:85:ILE:H	1.83	0.43
1:OA:85:ILE:HD12	1:OA:85:ILE:H	1.83	0.43
1:PA:124:PHE:CG	1:lA:22:MET:HG2	2.54	0.43
1:PC:59:ILE:HD12	1:PC:59:ILE:N	2.33	0.43
1:TC:59:ILE:HD12	1:TC:59:ILE:N	2.33	0.43
1:iA:85:ILE:HD12	1:iA:85:ILE:H	1.83	0.43
1:DC:59:ILE:HD12	1:DC:59:ILE:N	2.33	0.43
1:EA:85:ILE:N	1:EA:85:ILE:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GC:59:ILE:HD12	1:GC:59:ILE:N	2.34	0.43
1:QA:85:ILE:HD12	1:QA:85:ILE:H	1.83	0.43
1:RC:59:ILE:HD12	1:RC:59:ILE:N	2.33	0.43
1:SA:85:ILE:HD12	1:SA:85:ILE:H	1.83	0.43
1:VC:59:ILE:HD12	1:VC:59:ILE:N	2.33	0.43
1:eC:59:ILE:HD12	1:eC:59:ILE:N	2.33	0.43
1:hC:59:ILE:HD12	1:hC:59:ILE:N	2.33	0.43
1:mA:134:PHE:CE2	1:8A:112:LYS:HE3	2.54	0.43
1:nA:85:ILE:HD12	1:nA:85:ILE:N	2.33	0.43
1:pA:85:ILE:N	1:pA:85:ILE:HD12	2.33	0.43
1:rC:59:ILE:HD12	1:rC:59:ILE:N	2.33	0.43
1:uB:43:HIS:NE2	1:uB:48:THR:OG1	2.48	0.43
1:AC:34:LYS:HE3	1:RC:6:LEU:HD11	2.01	0.43
1:EC:59:ILE:HD12	1:EC:59:ILE:N	2.33	0.43
1:LC:59:ILE:HD12	1:LC:59:ILE:N	2.33	0.43
1:YC:59:ILE:HD12	1:YC:59:ILE:N	2.33	0.43
1:ZC:59:ILE:HD12	1:ZC:59:ILE:N	2.33	0.43
1:aA:85:ILE:HD12	1:aA:85:ILE:H	1.83	0.43
1:bC:59:ILE:HD12	1:bC:59:ILE:N	2.33	0.43
1:mA:40:GLN:O	1:8A:11:LYS:HG2	2.19	0.43
1:mC:59:ILE:HD12	1:mC:59:ILE:N	2.34	0.43
1:nC:59:ILE:HD12	1:nC:59:ILE:N	2.33	0.43
1:pA:85:ILE:HD12	1:pA:85:ILE:H	1.83	0.43
1:wC:59:ILE:HD12	1:wC:59:ILE:N	2.33	0.43
1:5C:59:ILE:HD12	1:5C:59:ILE:N	2.33	0.43
1:PA:25:LEU:O	1:PA:29:VAL:HG23	2.19	0.42
1:YC:58:LEU:CD1	1:mC:3:PHE:CE2	2.89	0.42
1:aA:85:ILE:HD12	1:aA:85:ILE:N	2.33	0.42
1:dC:59:ILE:HD12	1:dC:59:ILE:N	2.33	0.42
1:gC:59:ILE:HD12	1:gC:59:ILE:N	2.33	0.42
1:kA:85:ILE:HD12	1:kA:85:ILE:N	2.33	0.42
1:kB:43:HIS:NE2	1:kB:48:THR:OG1	2.48	0.42
1:yB:43:HIS:NE2	1:yB:48:THR:OG1	2.48	0.42
1:1A:11:LYS:HE3	1:BC:9:ASN:HD22	1.84	0.42
1:HA:85:ILE:HD12	1:HA:85:ILE:N	2.33	0.42
1:JA:25:LEU:O	1:JA:29:VAL:HG23	2.20	0.42
1:JA:85:ILE:N	1:JA:85:ILE:HD12	2.33	0.42
1:NA:25:LEU:O	1:NA:29:VAL:HG23	2.20	0.42
1:XB:43:HIS:NE2	1:XB:48:THR:OG1	2.48	0.42
1:eB:43:HIS:NE2	1:eB:48:THR:OG1	2.48	0.42
1:iA:85:ILE:HD12	1:iA:85:ILE:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:oA:85:ILE:HD12	1:oA:85:ILE:H	1.83	0.42
1:vA:85:ILE:HD12	1:vA:85:ILE:N	2.33	0.42
1:wB:43:HIS:NE2	1:wB:48:THR:OG1	2.48	0.42
1:yA:25:LEU:O	1:yA:29:VAL:HG23	2.20	0.42
1:5A:25:LEU:O	1:5A:29:VAL:HG23	2.20	0.42
1:8A:25:LEU:O	1:8A:29:VAL:HG23	2.20	0.42
1:8C:59:ILE:HD12	1:8C:59:ILE:N	2.33	0.42
1:LA:25:LEU:O	1:LA:29:VAL:HG23	2.20	0.42
1:RA:25:LEU:O	1:RA:29:VAL:HG23	2.20	0.42
1:SC:59:ILE:HD12	1:SC:59:ILE:N	2.33	0.42
1:rC:46:TRP:O	1:rC:50:MET:N	2.49	0.42
1:tA:85:ILE:HD12	1:tA:85:ILE:H	1.83	0.42
1:uA:25:LEU:O	1:uA:29:VAL:HG23	2.20	0.42
1:zA:85:ILE:HD12	1:zA:85:ILE:N	2.33	0.42
1:3A:85:ILE:HD12	1:3A:85:ILE:H	1.83	0.42
1:3B:43:HIS:NE2	1:3B:48:THR:OG1	2.48	0.42
1:4A:85:ILE:HD12	1:4A:85:ILE:H	1.83	0.42
1:CA:85:ILE:HD12	1:CA:85:ILE:H	1.83	0.42
1:CC:59:ILE:HD12	1:CC:59:ILE:N	2.33	0.42
1:EA:85:ILE:HD12	1:EA:85:ILE:H	1.83	0.42
1:MA:85:ILE:HD12	1:MA:85:ILE:H	1.83	0.42
1:RA:85:ILE:HD12	1:RA:85:ILE:H	1.83	0.42
1:XC:59:ILE:HD12	1:XC:59:ILE:N	2.33	0.42
1:bB:43:HIS:NE2	1:bB:48:THR:OG1	2.48	0.42
1:lC:59:ILE:HD12	1:lC:59:ILE:N	2.33	0.42
1:nA:25:LEU:O	1:nA:29:VAL:HG23	2.20	0.42
1:2C:59:ILE:HD12	1:2C:59:ILE:N	2.33	0.42
1:4A:25:LEU:O	1:4A:29:VAL:HG23	2.20	0.42
1:AC:34:LYS:HE3	1:RC:6:LEU:CD1	2.49	0.42
1:BC:9:ASN:O	1:1B:41:LYS:HB2	2.19	0.42
1:GC:46:TRP:O	1:GC:50:MET:N	2.49	0.42
1:KB:43:HIS:NE2	1:KB:48:THR:OG1	2.48	0.42
1:lA:85:ILE:HD12	1:lA:85:ILE:H	1.83	0.42
1:pA:25:LEU:O	1:pA:29:VAL:HG23	2.20	0.42
1:vA:25:LEU:O	1:vA:29:VAL:HG23	2.20	0.42
1:wA:25:LEU:O	1:wA:29:VAL:HG23	2.20	0.42
1:wC:87:LEU:O	1:wC:90:THR:OG1	2.36	0.42
1:FC:87:LEU:O	1:FC:90:THR:OG1	2.36	0.42
1:FC:109:HIS:HE1	1:oB:133:SER:HB3	1.85	0.42
1:MA:25:LEU:O	1:MA:29:VAL:HG23	2.20	0.42
1:XA:38:THR:HG21	1:3A:9:ASN:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZA:85:ILE:HD12	1:ZA:85:ILE:H	1.83	0.42
1:2A:25:LEU:O	1:2A:29:VAL:HG23	2.20	0.42
1:cB:43:HIS:NE2	1:cB:48:THR:OG1	2.48	0.42
1:dA:25:LEU:O	1:dA:29:VAL:HG23	2.20	0.42
1:gB:33:VAL:HG12	1:gB:37:LEU:HD12	2.02	0.42
1:hA:85:ILE:HD12	1:hA:85:ILE:H	1.83	0.42
1:kA:25:LEU:O	1:kA:29:VAL:HG23	2.20	0.42
1:nB:33:VAL:HG12	1:nB:37:LEU:HD12	2.02	0.42
1:oB:33:VAL:HG12	1:oB:37:LEU:HD12	2.02	0.42
1:qC:87:LEU:O	1:qC:90:THR:OG1	2.36	0.42
1:xA:25:LEU:O	1:xA:29:VAL:HG23	2.20	0.42
1:6A:25:LEU:O	1:6A:29:VAL:HG23	2.20	0.42
1:AA:25:LEU:O	1:AA:29:VAL:HG23	2.20	0.42
1:AC:46:TRP:O	1:AC:50:MET:N	2.49	0.42
1:GB:43:HIS:NE2	1:GB:48:THR:OG1	2.48	0.42
1:JC:92:GLU:OE2	1:NC:52:LEU:HB3	2.20	0.42
1:LB:33:VAL:HG12	1:LB:37:LEU:HD12	2.02	0.42
1:MB:40:GLN:OE1	1:MB:41:LYS:N	2.45	0.42
1:OA:25:LEU:O	1:OA:29:VAL:HG23	2.20	0.42
1:1C:87:LEU:O	1:1C:90:THR:OG1	2.36	0.42
1:TB:33:VAL:HG12	1:TB:37:LEU:HD12	2.02	0.42
1:UC:59:ILE:HD12	1:UC:59:ILE:N	2.33	0.42
1:XA:85:ILE:HD12	1:XA:85:ILE:H	1.83	0.42
1:YB:33:VAL:HG12	1:YB:37:LEU:HD12	2.02	0.42
1:bA:25:LEU:O	1:bA:29:VAL:HG23	2.20	0.42
1:bB:41:LYS:HG3	1:uC:9:ASN:O	2.19	0.42
1:dA:36:ILE:HG23	1:dA:100:HIS:CE1	2.55	0.42
1:gA:25:LEU:O	1:gA:29:VAL:HG23	2.20	0.42
1:jC:18:LEU:HD22	1:jC:111:VAL:HG21	2.02	0.42
1:jC:46:TRP:O	1:jC:50:MET:N	2.49	0.42
1:lB:33:VAL:HG12	1:lB:37:LEU:HD12	2.02	0.42
1:mB:33:VAL:HG12	1:mB:37:LEU:HD12	2.02	0.42
1:oA:25:LEU:O	1:oA:29:VAL:HG23	2.20	0.42
1:xC:59:ILE:HD12	1:xC:59:ILE:N	2.34	0.42
1:1A:25:LEU:O	1:1A:29:VAL:HG23	2.19	0.42
1:DB:33:VAL:HG12	1:DB:37:LEU:HD12	2.02	0.42
1:EA:36:ILE:HG23	1:EA:100:HIS:CE1	2.55	0.42
1:IA:25:LEU:O	1:IA:29:VAL:HG23	2.20	0.42
1:IB:33:VAL:HG12	1:IB:37:LEU:HD12	2.02	0.42
1:1B:43:HIS:NE2	1:1B:48:THR:OG1	2.48	0.42
1:NC:18:LEU:HD22	1:NC:111:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PA:36:ILE:HG23	1:PA:100:HIS:CE1	2.55	0.42
1:PB:33:VAL:HG12	1:PB:37:LEU:HD12	2.02	0.42
1:QC:18:LEU:HD22	1:QC:111:VAL:HG21	2.02	0.42
1:1C:18:LEU:HD22	1:1C:111:VAL:HG21	2.02	0.42
1:SB:33:VAL:HG12	1:SB:37:LEU:HD12	2.02	0.42
1:UC:43:HIS:CD2	1:1C:12:GLY:HA3	2.55	0.42
1:VA:25:LEU:O	1:VA:29:VAL:HG23	2.20	0.42
1:VC:46:TRP:O	1:VC:50:MET:N	2.49	0.42
1:dB:33:VAL:HG12	1:dB:37:LEU:HD12	2.02	0.42
1:eA:25:LEU:O	1:eA:29:VAL:HG23	2.20	0.42
1:gA:36:ILE:HG23	1:gA:100:HIS:CE1	2.55	0.42
1:kA:85:ILE:HD12	1:kA:85:ILE:H	1.83	0.42
1:lA:25:LEU:O	1:lA:29:VAL:HG23	2.20	0.42
1:lA:36:ILE:HG23	1:lA:100:HIS:CE1	2.55	0.42
1:lC:87:LEU:O	1:lC:90:THR:OG1	2.36	0.42
1:nA:36:ILE:HG23	1:nA:100:HIS:CE1	2.55	0.42
1:8B:33:VAL:HG12	1:8B:37:LEU:HD12	2.02	0.42
1:FA:25:LEU:O	1:FA:29:VAL:HG23	2.20	0.42
1:GC:87:LEU:O	1:GC:90:THR:OG1	2.36	0.42
1:HA:36:ILE:HG23	1:HA:100:HIS:CE1	2.55	0.42
1:JA:85:ILE:HD12	1:JA:85:ILE:H	1.83	0.42
1:KB:21:GLU:O	1:eC:121:PRO:HG2	2.19	0.42
1:LA:38:THR:HG21	1:vA:9:ASN:HA	2.01	0.42
1:MC:46:TRP:O	1:MC:50:MET:N	2.49	0.42
1:OA:38:THR:HG21	1:QA:9:ASN:HA	2.02	0.42
1:QA:36:ILE:HG23	1:QA:100:HIS:CE1	2.55	0.42
1:QC:46:TRP:O	1:QC:50:MET:N	2.49	0.42
1:SA:36:ILE:HG23	1:SA:100:HIS:CE1	2.55	0.42
1:aA:25:LEU:O	1:aA:29:VAL:HG23	2.20	0.42
1:cC:87:LEU:O	1:cC:90:THR:OG1	2.36	0.42
1:dC:46:TRP:O	1:dC:50:MET:N	2.49	0.42
1:gB:94:TRP:HH2	1:pC:116:LEU:HD13	1.85	0.42
1:iA:25:LEU:O	1:iA:29:VAL:HG23	2.20	0.42
1:qA:25:LEU:O	1:qA:29:VAL:HG23	2.20	0.42
1:sA:25:LEU:O	1:sA:29:VAL:HG23	2.20	0.42
1:sA:36:ILE:HG23	1:sA:100:HIS:CE1	2.55	0.42
1:sB:33:VAL:HG12	1:sB:37:LEU:HD12	2.02	0.42
1:tA:25:LEU:O	1:tA:29:VAL:HG23	2.20	0.42
1:uA:36:ILE:HG23	1:uA:100:HIS:CE1	2.55	0.42
1:uB:33:VAL:HG12	1:uB:37:LEU:HD12	2.02	0.42
1:vC:18:LEU:HD22	1:vC:111:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:zA:25:LEU:O	1:zA:29:VAL:HG23	2.20	0.42
1:zB:33:VAL:HG12	1:zB:37:LEU:HD12	2.02	0.42
1:3A:25:LEU:O	1:3A:29:VAL:HG23	2.20	0.42
1:7A:25:LEU:O	1:7A:29:VAL:HG23	2.20	0.42
1:AC:58:LEU:CD1	1:RC:3:PHE:HD2	2.31	0.42
1:CA:25:LEU:O	1:CA:29:VAL:HG23	2.20	0.42
1:DB:43:HIS:NE2	1:DB:48:THR:OG1	2.48	0.42
1:FA:36:ILE:HG23	1:FA:100:HIS:CE1	2.55	0.42
1:KA:25:LEU:O	1:KA:29:VAL:HG23	2.20	0.42
1:LC:18:LEU:HD22	1:LC:111:VAL:HG21	2.02	0.42
1:PC:18:LEU:HD22	1:PC:111:VAL:HG21	2.02	0.42
1:QA:25:LEU:O	1:QA:29:VAL:HG23	2.20	0.42
1:ZA:25:LEU:O	1:ZA:29:VAL:HG23	2.20	0.42
1:ZA:36:ILE:HG23	1:ZA:100:HIS:CE1	2.55	0.42
1:ZC:10:MET:HE1	1:gC:41:LYS:O	2.20	0.42
1:2A:36:ILE:HG23	1:2A:100:HIS:CE1	2.55	0.42
1:hA:25:LEU:O	1:hA:29:VAL:HG23	2.20	0.42
1:jA:36:ILE:HG23	1:jA:100:HIS:CE1	2.55	0.42
1:pA:36:ILE:HG23	1:pA:100:HIS:CE1	2.55	0.42
1:qA:36:ILE:HG23	1:qA:100:HIS:CE1	2.55	0.42
1:tA:36:ILE:HG23	1:tA:100:HIS:CE1	2.55	0.42
1:tB:40:GLN:OE1	1:tB:41:LYS:N	2.45	0.42
1:8C:18:LEU:HD22	1:8C:111:VAL:HG21	2.02	0.42
1:AC:3:PHE:HB3	1:RC:51:ALA:CB	2.50	0.41
1:DA:36:ILE:HG23	1:DA:100:HIS:CE1	2.55	0.41
1:EC:18:LEU:HD22	1:EC:111:VAL:HG21	2.02	0.41
1:HB:33:VAL:HG12	1:HB:37:LEU:HD12	2.02	0.41
1:KC:18:LEU:HD22	1:KC:111:VAL:HG21	2.02	0.41
1:QB:33:VAL:HG12	1:QB:37:LEU:HD12	2.02	0.41
1:XA:25:LEU:O	1:XA:29:VAL:HG23	2.20	0.41
1:XB:33:VAL:HG12	1:XB:37:LEU:HD12	2.02	0.41
1:YA:25:LEU:O	1:YA:29:VAL:HG23	2.20	0.41
1:bB:33:VAL:HG12	1:bB:37:LEU:HD12	2.02	0.41
1:eB:33:VAL:HG12	1:eB:37:LEU:HD12	2.02	0.41
1:fB:33:VAL:HG12	1:fB:37:LEU:HD12	2.02	0.41
1:gB:94:TRP:CH2	1:pC:116:LEU:HD13	2.54	0.41
1:hA:36:ILE:HG23	1:hA:100:HIS:CE1	2.55	0.41
1:nC:18:LEU:HD22	1:nC:111:VAL:HG21	2.02	0.41
1:vB:33:VAL:HG12	1:vB:37:LEU:HD12	2.02	0.41
1:wB:33:VAL:HG12	1:wB:37:LEU:HD12	2.02	0.41
1:wC:18:LEU:HD22	1:wC:111:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:xA:36:ILE:HG23	1:xA:100:HIS:CE1	2.55	0.41
1:yB:33:VAL:HG12	1:yB:37:LEU:HD12	2.02	0.41
1:zC:18:LEU:HD22	1:zC:111:VAL:HG21	2.02	0.41
1:4C:46:TRP:O	1:4C:50:MET:N	2.49	0.41
1:6A:36:ILE:HG23	1:6A:100:HIS:CE1	2.55	0.41
1:7C:18:LEU:HD22	1:7C:111:VAL:HG21	2.02	0.41
1:CB:33:VAL:HG12	1:CB:37:LEU:HD12	2.02	0.41
1:DA:25:LEU:O	1:DA:29:VAL:HG23	2.20	0.41
1:DC:58:LEU:HD11	1:TC:3:PHE:CE2	2.54	0.41
1:GB:22:MET:HE1	1:GB:114:ILE:HG23	2.02	0.41
1:HC:87:LEU:O	1:HC:90:THR:OG1	2.36	0.41
1:NA:36:ILE:HG23	1:NA:100:HIS:CE1	2.55	0.41
1:RB:22:MET:HE1	1:RB:114:ILE:HG23	2.03	0.41
1:SC:18:LEU:HD22	1:SC:111:VAL:HG21	2.02	0.41
1:UA:36:ILE:HG23	1:UA:100:HIS:CE1	2.55	0.41
1:YA:36:ILE:HG23	1:YA:100:HIS:CE1	2.55	0.41
1:YB:43:HIS:NE2	1:YB:48:THR:OG1	2.48	0.41
1:ZB:9:ASN:ND2	1:gC:6:LEU:HD22	2.34	0.41
1:ZC:18:LEU:HD22	1:ZC:111:VAL:HG21	2.02	0.41
1:cB:33:VAL:HG12	1:cB:37:LEU:HD12	2.02	0.41
1:gC:46:TRP:O	1:gC:50:MET:N	2.49	0.41
1:jA:25:LEU:O	1:jA:29:VAL:HG23	2.20	0.41
1:pC:18:LEU:HD22	1:pC:111:VAL:HG21	2.02	0.41
1:rA:36:ILE:HG23	1:rA:100:HIS:CE1	2.55	0.41
1:yA:36:ILE:HG23	1:yA:100:HIS:CE1	2.55	0.41
1:3A:36:ILE:HG23	1:3A:100:HIS:CE1	2.55	0.41
1:4A:36:ILE:HG23	1:4A:100:HIS:CE1	2.55	0.41
1:5A:36:ILE:HG23	1:5A:100:HIS:CE1	2.55	0.41
1:7B:43:HIS:NE2	1:7B:48:THR:OG1	2.48	0.41
1:GA:36:ILE:HG23	1:GA:100:HIS:CE1	2.55	0.41
1:HA:33:VAL:HG12	1:HA:37:LEU:HD12	2.03	0.41
1:JA:36:ILE:HG23	1:JA:100:HIS:CE1	2.55	0.41
1:1B:33:VAL:HG12	1:1B:37:LEU:HD12	2.02	0.41
1:LA:36:ILE:HG23	1:LA:100:HIS:CE1	2.55	0.41
1:LB:22:MET:HE1	1:LB:114:ILE:HG23	2.02	0.41
1:LB:40:GLN:OE1	1:LB:41:LYS:N	2.45	0.41
1:RC:46:TRP:O	1:RC:50:MET:N	2.49	0.41
1:SB:22:MET:HE1	1:SB:114:ILE:HG23	2.02	0.41
1:XC:18:LEU:HD22	1:XC:111:VAL:HG21	2.02	0.41
1:cB:22:MET:HE1	1:cB:114:ILE:HG23	2.03	0.41
1:cC:18:LEU:HD22	1:cC:111:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:iB:33:VAL:HG12	1:iB:37:LEU:HD12	2.02	0.41
1:2B:33:VAL:HG12	1:2B:37:LEU:HD12	2.02	0.41
1:jB:33:VAL:HG12	1:jB:37:LEU:HD12	2.02	0.41
1:kB:22:MET:HE1	1:kB:114:ILE:HG23	2.02	0.41
1:2C:18:LEU:HD22	1:2C:111:VAL:HG21	2.02	0.41
1:wA:36:ILE:HG23	1:wA:100:HIS:CE1	2.55	0.41
1:xC:18:LEU:HD22	1:xC:111:VAL:HG21	2.02	0.41
1:4B:40:GLN:OE1	1:4B:41:LYS:N	2.45	0.41
1:5C:18:LEU:HD22	1:5C:111:VAL:HG21	2.02	0.41
1:CB:40:GLN:OE1	1:CB:41:LYS:N	2.45	0.41
1:CC:18:LEU:HD22	1:CC:111:VAL:HG21	2.02	0.41
1:FC:109:HIS:CE1	1:oB:133:SER:HB3	2.56	0.41
1:HA:25:LEU:O	1:HA:29:VAL:HG23	2.20	0.41
1:IB:40:GLN:OE1	1:IB:41:LYS:N	2.45	0.41
1:MA:36:ILE:HG23	1:MA:100:HIS:CE1	2.55	0.41
1:OA:36:ILE:HG23	1:OA:100:HIS:CE1	2.55	0.41
1:PB:40:GLN:OE1	1:PB:41:LYS:N	2.45	0.41
1:RA:36:ILE:HG23	1:RA:100:HIS:CE1	2.55	0.41
1:UB:33:VAL:HG12	1:UB:37:LEU:HD12	2.02	0.41
1:UC:18:LEU:HD22	1:UC:111:VAL:HG21	2.02	0.41
1:WA:36:ILE:HG23	1:WA:100:HIS:CE1	2.55	0.41
1:aB:33:VAL:HG12	1:aB:37:LEU:HD12	2.02	0.41
1:bB:22:MET:HE1	1:bB:114:ILE:HG23	2.02	0.41
1:fC:18:LEU:HD22	1:fC:111:VAL:HG21	2.02	0.41
1:hC:18:LEU:HD22	1:hC:111:VAL:HG21	2.02	0.41
1:kC:87:LEU:O	1:kC:90:THR:OG1	2.36	0.41
1:mA:25:LEU:O	1:mA:29:VAL:HG23	2.20	0.41
1:pB:22:MET:HE1	1:pB:114:ILE:HG23	2.02	0.41
1:sA:33:VAL:HG12	1:sA:37:LEU:HD12	2.03	0.41
1:uC:18:LEU:HD22	1:uC:111:VAL:HG21	2.02	0.41
1:xB:33:VAL:HG12	1:xB:37:LEU:HD12	2.02	0.41
1:8A:36:ILE:HG23	1:8A:100:HIS:CE1	2.55	0.41
1:8B:22:MET:HE1	1:8B:114:ILE:HG23	2.03	0.41
1:BB:22:MET:HE1	1:BB:114:ILE:HG23	2.03	0.41
1:HB:22:MET:HE1	1:HB:114:ILE:HG23	2.03	0.41
1:JB:22:MET:HE1	1:JB:114:ILE:HG23	2.02	0.41
1:JC:18:LEU:HD22	1:JC:111:VAL:HG21	2.02	0.41
1:MB:22:MET:HE1	1:MB:114:ILE:HG23	2.03	0.41
1:OA:33:VAL:HG12	1:OA:37:LEU:HD12	2.03	0.41
1:RA:33:VAL:HG12	1:RA:37:LEU:HD12	2.03	0.41
1:RA:134:PHE:CZ	1:4A:112:LYS:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:25:LEU:O	1:SA:29:VAL:HG23	2.20	0.41
1:TA:25:LEU:O	1:TA:29:VAL:HG23	2.20	0.41
1:VA:36:ILE:HG23	1:VA:100:HIS:CE1	2.55	0.41
1:VB:43:HIS:NE2	1:VB:48:THR:OG1	2.48	0.41
1:WA:25:LEU:O	1:WA:29:VAL:HG23	2.20	0.41
1:eB:22:MET:HE1	1:eB:114:ILE:HG23	2.03	0.41
1:lB:22:MET:HE1	1:lB:114:ILE:HG23	2.02	0.41
1:nB:22:MET:HE1	1:nB:114:ILE:HG23	2.02	0.41
1:rB:22:MET:HE1	1:rB:114:ILE:HG23	2.02	0.41
1:sC:18:LEU:HD22	1:sC:111:VAL:HG21	2.02	0.41
1:uC:87:LEU:O	1:uC:90:THR:OG1	2.36	0.41
1:wB:22:MET:HE1	1:wB:114:ILE:HG23	2.03	0.41
1:AA:36:ILE:HG23	1:AA:100:HIS:CE1	2.55	0.41
1:1A:36:ILE:HG23	1:1A:100:HIS:CE1	2.55	0.41
1:BA:11:LYS:HA	1:JA:39:SER:HA	2.03	0.41
1:BA:25:LEU:O	1:BA:29:VAL:HG23	2.20	0.41
1:BA:36:ILE:HG23	1:BA:100:HIS:CE1	2.55	0.41
1:1B:22:MET:HE1	1:1B:114:ILE:HG23	2.02	0.41
1:XB:40:GLN:OE1	1:XB:41:LYS:N	2.45	0.41
1:XC:78:LEU:HD12	1:XC:78:LEU:H	1.86	0.41
1:aA:36:ILE:HG23	1:aA:100:HIS:CE1	2.55	0.41
1:dB:9:ASN:HB3	1:hC:6:LEU:HD22	2.01	0.41
1:fB:22:MET:HE1	1:fB:114:ILE:HG23	2.02	0.41
1:fC:78:LEU:H	1:fC:78:LEU:HD12	1.86	0.41
1:hB:33:VAL:HG12	1:hB:37:LEU:HD12	2.02	0.41
1:iA:36:ILE:HG23	1:iA:100:HIS:CE1	2.55	0.41
1:jC:78:LEU:HD12	1:jC:78:LEU:H	1.86	0.41
1:kC:78:LEU:HD12	1:kC:78:LEU:H	1.86	0.41
1:lC:18:LEU:HD22	1:lC:111:VAL:HG21	2.02	0.41
1:sB:22:MET:HE1	1:sB:114:ILE:HG23	2.03	0.41
1:yA:33:VAL:HG12	1:yA:37:LEU:HD12	2.03	0.41
1:yC:18:LEU:HD22	1:yC:111:VAL:HG21	2.02	0.41
1:3B:40:GLN:OE1	1:3B:41:LYS:N	2.45	0.41
1:5B:22:MET:HE1	1:5B:114:ILE:HG23	2.03	0.41
1:6A:33:VAL:HG12	1:6A:37:LEU:HD12	2.03	0.41
1:CC:78:LEU:H	1:CC:78:LEU:HD12	1.86	0.41
1:EA:25:LEU:O	1:EA:29:VAL:HG23	2.20	0.41
1:EA:33:VAL:HG12	1:EA:37:LEU:HD12	2.03	0.41
1:NB:22:MET:HE1	1:NB:114:ILE:HG23	2.03	0.41
1:OC:18:LEU:HD22	1:OC:111:VAL:HG21	2.02	0.41
1:RC:78:LEU:HD12	1:RC:78:LEU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RC:87:LEU:O	1:RC:90:THR:OG1	2.36	0.41
1:VB:22:MET:HE1	1:VB:114:ILE:HG23	2.03	0.41
1:WC:18:LEU:HD22	1:WC:111:VAL:HG21	2.02	0.41
1:ZB:33:VAL:HG12	1:ZB:37:LEU:HD12	2.02	0.41
1:ZC:9:ASN:O	1:AB:41:LYS:HG3	2.21	0.41
1:aC:18:LEU:HD22	1:aC:111:VAL:HG21	2.02	0.41
1:bA:36:ILE:HG23	1:bA:100:HIS:CE1	2.55	0.41
1:cA:36:ILE:HG23	1:cA:100:HIS:CE1	2.55	0.41
1:cC:78:LEU:H	1:cC:78:LEU:HD12	1.86	0.41
1:eA:36:ILE:HG23	1:eA:100:HIS:CE1	2.55	0.41
1:fA:36:ILE:HG23	1:fA:100:HIS:CE1	2.55	0.41
1:fB:43:HIS:NE2	1:fB:48:THR:OG1	2.48	0.41
1:kA:33:VAL:HG12	1:kA:37:LEU:HD12	2.03	0.41
1:kC:46:TRP:O	1:kC:50:MET:N	2.49	0.41
1:oB:40:GLN:OE1	1:oB:41:LYS:N	2.45	0.41
1:qC:78:LEU:H	1:qC:78:LEU:HD12	1.86	0.41
1:rB:43:HIS:NE2	1:rB:48:THR:OG1	2.48	0.41
1:2C:78:LEU:H	1:2C:78:LEU:HD12	1.86	0.41
1:uA:33:VAL:HG12	1:uA:37:LEU:HD12	2.03	0.41
1:uB:22:MET:HE1	1:uB:114:ILE:HG23	2.03	0.41
1:yB:22:MET:HE1	1:yB:114:ILE:HG23	2.02	0.41
1:yC:87:LEU:O	1:yC:90:THR:OG1	2.36	0.41
1:zA:36:ILE:HG23	1:zA:100:HIS:CE1	2.55	0.41
1:zC:78:LEU:HD12	1:zC:78:LEU:H	1.86	0.41
1:4A:33:VAL:HG12	1:4A:37:LEU:HD12	2.03	0.41
1:4B:22:MET:HE1	1:4B:114:ILE:HG23	2.03	0.41
1:6C:18:LEU:HD22	1:6C:111:VAL:HG21	2.02	0.41
1:AB:22:MET:HE1	1:AB:114:ILE:HG23	2.03	0.41
1:BB:33:VAL:HG12	1:BB:37:LEU:HD12	2.02	0.41
1:BC:18:LEU:HD22	1:BC:111:VAL:HG21	2.02	0.41
1:EC:78:LEU:H	1:EC:78:LEU:HD12	1.86	0.41
1:LC:78:LEU:HD12	1:LC:78:LEU:H	1.86	0.41
1:MC:87:LEU:O	1:MC:90:THR:OG1	2.36	0.41
1:PB:22:MET:HE1	1:PB:114:ILE:HG23	2.03	0.41
1:QC:78:LEU:HD12	1:QC:78:LEU:H	1.86	0.41
1:UA:25:LEU:O	1:UA:29:VAL:HG23	2.20	0.41
1:UC:43:HIS:CG	1:IC:12:GLY:HA3	2.56	0.41
1:WB:22:MET:HE1	1:WB:114:ILE:HG23	2.02	0.41
1:WB:33:VAL:HG12	1:WB:37:LEU:HD12	2.02	0.41
1:dC:18:LEU:HD22	1:dC:111:VAL:HG21	2.02	0.41
1:gC:18:LEU:HD22	1:gC:111:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:mA:134:PHE:HE2	1:8A:112:LYS:HD2	1.86	0.41
1:rA:25:LEU:O	1:rA:29:VAL:HG23	2.20	0.41
1:sB:40:GLN:OE1	1:sB:41:LYS:N	2.45	0.41
1:vC:78:LEU:HD12	1:vC:78:LEU:H	1.86	0.41
1:xC:78:LEU:H	1:xC:78:LEU:HD12	1.86	0.41
1:7A:36:ILE:HG23	1:7A:100:HIS:CE1	2.55	0.41
1:7B:33:VAL:HG12	1:7B:37:LEU:HD12	2.02	0.41
1:CA:36:ILE:HG23	1:CA:100:HIS:CE1	2.55	0.41
1:DB:22:MET:HE1	1:DB:114:ILE:HG23	2.02	0.41
1:EB:22:MET:HE1	1:EB:114:ILE:HG23	2.03	0.41
1:FB:33:VAL:HG12	1:FB:37:LEU:HD12	2.02	0.41
1:FC:18:LEU:HD22	1:FC:111:VAL:HG21	2.02	0.41
1:FC:78:LEU:H	1:FC:78:LEU:HD12	1.86	0.41
1:GA:25:LEU:O	1:GA:29:VAL:HG23	2.20	0.41
1:HC:120:THR:HG21	1:HC:124:PHE:O	2.21	0.41
1:IC:18:LEU:HD22	1:IC:111:VAL:HG21	2.02	0.41
1:JA:33:VAL:HG12	1:JA:37:LEU:HD12	2.03	0.41
1:JC:78:LEU:H	1:JC:78:LEU:HD12	1.86	0.41
1:KB:22:MET:HE1	1:KB:114:ILE:HG23	2.02	0.41
1:KB:33:VAL:HG12	1:KB:37:LEU:HD12	2.02	0.41
1:KC:78:LEU:HD12	1:KC:78:LEU:H	1.86	0.41
1:MA:33:VAL:HG12	1:MA:37:LEU:HD12	2.03	0.41
1:OB:22:MET:HE1	1:OB:114:ILE:HG23	2.03	0.41
1:PA:124:PHE:CB	1:lA:22:MET:HE3	2.49	0.41
1:TA:36:ILE:HG23	1:TA:100:HIS:CE1	2.55	0.41
1:TB:134:PHE:HD1	1:sC:109:HIS:HE1	1.68	0.41
1:UA:33:VAL:HG12	1:UA:37:LEU:HD12	2.03	0.41
1:UC:78:LEU:H	1:UC:78:LEU:HD12	1.86	0.41
1:VC:120:THR:HG21	1:VC:124:PHE:O	2.21	0.41
1:XA:36:ILE:HG23	1:XA:100:HIS:CE1	2.55	0.41
1:YB:22:MET:HE1	1:YB:114:ILE:HG23	2.03	0.41
1:ZB:22:MET:HE1	1:ZB:114:ILE:HG23	2.03	0.41
1:bC:18:LEU:HD22	1:bC:111:VAL:HG21	2.02	0.41
1:dB:22:MET:HE1	1:dB:114:ILE:HG23	2.03	0.41
1:gB:22:MET:HE1	1:gB:114:ILE:HG23	2.03	0.41
1:hB:22:MET:HE1	1:hB:114:ILE:HG23	2.02	0.41
1:hC:120:THR:HG21	1:hC:124:PHE:O	2.21	0.41
1:iC:18:LEU:HD22	1:iC:111:VAL:HG21	2.02	0.41
1:iC:120:THR:HG21	1:iC:124:PHE:O	2.21	0.41
1:2B:22:MET:HE1	1:2B:114:ILE:HG23	2.03	0.41
1:jB:22:MET:HE1	1:jB:114:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:kA:36:ILE:HG23	1:kA:100:HIS:CE1	2.55	0.41
1:mA:36:ILE:HG23	1:mA:100:HIS:CE1	2.55	0.41
1:nC:78:LEU:H	1:nC:78:LEU:HD12	1.86	0.41
1:oC:78:LEU:HD12	1:oC:78:LEU:H	1.86	0.41
1:pA:33:VAL:HG12	1:pA:37:LEU:HD12	2.03	0.41
1:qB:33:VAL:HG12	1:qB:37:LEU:HD12	2.02	0.41
1:sC:87:LEU:O	1:sC:90:THR:OG1	2.36	0.41
1:vA:36:ILE:HG23	1:vA:100:HIS:CE1	2.55	0.41
1:vB:43:HIS:NE2	1:vB:48:THR:OG1	2.48	0.41
1:xB:22:MET:HE1	1:xB:114:ILE:HG23	2.03	0.41
1:6B:22:MET:HE1	1:6B:114:ILE:HG23	2.02	0.41
1:6C:120:THR:HG21	1:6C:124:PHE:O	2.21	0.41
1:8B:40:GLN:OE1	1:8B:41:LYS:N	2.45	0.41
1:AC:8:LYS:HD3	1:4B:38:THR:CG2	2.51	0.41
1:AC:120:THR:HG21	1:AC:124:PHE:O	2.21	0.41
1:BC:120:THR:HG21	1:BC:124:PHE:O	2.21	0.41
1:EB:33:VAL:HG12	1:EB:37:LEU:HD12	2.02	0.41
1:HC:18:LEU:HD22	1:HC:111:VAL:HG21	2.02	0.41
1:JC:120:THR:HG21	1:JC:124:PHE:O	2.21	0.41
1:KA:36:ILE:HG23	1:KA:100:HIS:CE1	2.55	0.41
1:MC:120:THR:HG21	1:MC:124:PHE:O	2.21	0.41
1:NB:33:VAL:HG12	1:NB:37:LEU:HD12	2.02	0.41
1:NC:120:THR:HG21	1:NC:124:PHE:O	2.21	0.41
1:PC:78:LEU:H	1:PC:78:LEU:HD12	1.86	0.41
1:QC:120:THR:HG21	1:QC:124:PHE:O	2.21	0.41
1:RC:18:LEU:HD22	1:RC:111:VAL:HG21	2.02	0.41
1:TC:120:THR:HG21	1:TC:124:PHE:O	2.21	0.41
1:ZC:120:THR:HG21	1:ZC:124:PHE:O	2.21	0.41
1:aC:120:THR:HG21	1:aC:124:PHE:O	2.21	0.41
1:dC:78:LEU:HD12	1:dC:78:LEU:H	1.86	0.41
1:eC:18:LEU:HD22	1:eC:111:VAL:HG21	2.02	0.41
1:jC:120:THR:HG21	1:jC:124:PHE:O	2.21	0.41
1:kC:18:LEU:HD22	1:kC:111:VAL:HG21	2.02	0.41
1:mC:120:THR:HG21	1:mC:124:PHE:O	2.21	0.41
1:pC:120:THR:HG21	1:pC:124:PHE:O	2.21	0.41
1:qC:18:LEU:HD22	1:qC:111:VAL:HG21	2.02	0.41
1:tC:18:LEU:HD22	1:tC:111:VAL:HG21	2.02	0.41
1:tC:78:LEU:HD12	1:tC:78:LEU:H	1.86	0.41
1:3B:33:VAL:HG12	1:3B:37:LEU:HD12	2.02	0.41
1:3C:78:LEU:HD12	1:3C:78:LEU:H	1.86	0.41
1:4C:87:LEU:O	1:4C:90:THR:OG1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4C:120:THR:HG21	1:4C:124:PHE:O	2.21	0.41
1:7B:22:MET:HE1	1:7B:114:ILE:HG23	2.02	0.41
1:BC:87:LEU:O	1:BC:90:THR:OG1	2.36	0.40
1:DC:18:LEU:HD22	1:DC:111:VAL:HG21	2.02	0.40
1:FC:8:LYS:HD3	1:OB:38:THR:CG2	2.51	0.40
1:IC:78:LEU:HD12	1:IC:78:LEU:H	1.86	0.40
1:KC:120:THR:HG21	1:KC:124:PHE:O	2.21	0.40
1:MA:38:THR:HG21	1:OA:9:ASN:HA	2.04	0.40
1:MC:78:LEU:HD12	1:MC:78:LEU:H	1.86	0.40
1:OC:120:THR:HG21	1:OC:124:PHE:O	2.21	0.40
1:QB:22:MET:HE1	1:QB:114:ILE:HG23	2.02	0.40
1:RA:104:ILE:HG23	1:RA:105:VAL:N	2.37	0.40
1:TA:104:ILE:HG23	1:TA:105:VAL:N	2.36	0.40
1:VB:33:VAL:HG12	1:VB:37:LEU:HD12	2.02	0.40
1:VC:78:LEU:H	1:VC:78:LEU:HD12	1.86	0.40
1:XA:33:VAL:HG12	1:XA:37:LEU:HD12	2.03	0.40
1:YA:33:VAL:HG12	1:YA:37:LEU:HD12	2.03	0.40
1:YC:18:LEU:HD22	1:YC:111:VAL:HG21	2.02	0.40
1:aB:22:MET:HE1	1:aB:114:ILE:HG23	2.03	0.40
1:bC:46:TRP:O	1:bC:50:MET:N	2.49	0.40
1:gC:78:LEU:HD12	1:gC:78:LEU:H	1.86	0.40
1:iC:8:LYS:HD3	1:sB:38:THR:HG21	2.03	0.40
1:kB:33:VAL:HG12	1:kB:37:LEU:HD12	2.02	0.40
1:mB:40:GLN:OE1	1:mB:41:LYS:N	2.45	0.40
1:nA:104:ILE:HG23	1:nA:105:VAL:N	2.37	0.40
1:rC:18:LEU:HD22	1:rC:111:VAL:HG21	2.02	0.40
1:2C:87:LEU:O	1:2C:90:THR:OG1	2.36	0.40
1:sC:120:THR:HG21	1:sC:124:PHE:O	2.21	0.40
1:tB:33:VAL:HG12	1:tB:37:LEU:HD12	2.02	0.40
1:uA:104:ILE:HG23	1:uA:105:VAL:N	2.37	0.40
1:zA:33:VAL:HG12	1:zA:37:LEU:HD12	2.03	0.40
1:3B:22:MET:HE1	1:3B:114:ILE:HG23	2.02	0.40
1:3C:18:LEU:HD22	1:3C:111:VAL:HG21	2.02	0.40
1:6B:33:VAL:HG12	1:6B:37:LEU:HD12	2.02	0.40
1:7A:33:VAL:HG12	1:7A:37:LEU:HD12	2.03	0.40
1:7C:120:THR:HG21	1:7C:124:PHE:O	2.21	0.40
1:8C:78:LEU:HD12	1:8C:78:LEU:H	1.86	0.40
1:AB:33:VAL:HG12	1:AB:37:LEU:HD12	2.02	0.40
1:AC:18:LEU:HD22	1:AC:111:VAL:HG21	2.02	0.40
1:CA:33:VAL:HG12	1:CA:37:LEU:HD12	2.03	0.40
1:DA:33:VAL:HG12	1:DA:37:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GC:18:LEU:HD22	1:GC:111:VAL:HG21	2.02	0.40
1:HA:22:MET:HG2	1:yA:124:PHE:CB	2.51	0.40
1:IA:36:ILE:HG23	1:IA:100:HIS:CE1	2.55	0.40
1:IC:120:THR:HG21	1:IC:124:PHE:O	2.21	0.40
1:KA:33:VAL:HG12	1:KA:37:LEU:HD12	2.03	0.40
1:NA:104:ILE:HG23	1:NA:105:VAL:N	2.37	0.40
1:PA:104:ILE:HG23	1:PA:105:VAL:N	2.37	0.40
1:1C:3:PHE:HB3	1:tC:51:ALA:HB1	2.03	0.40
1:TB:40:GLN:OE1	1:TB:41:LYS:N	2.45	0.40
1:TC:87:LEU:O	1:TC:90:THR:OG1	2.36	0.40
1:WC:120:THR:HG21	1:WC:124:PHE:O	2.21	0.40
1:YC:3:PHE:HB3	1:mC:51:ALA:HB1	2.04	0.40
1:ZA:104:ILE:HG23	1:ZA:105:VAL:N	2.37	0.40
1:ZC:46:TRP:O	1:ZC:50:MET:N	2.49	0.40
1:aA:104:ILE:HG23	1:aA:105:VAL:N	2.37	0.40
1:2A:104:ILE:HG23	1:2A:105:VAL:N	2.37	0.40
1:cA:25:LEU:O	1:cA:29:VAL:HG23	2.20	0.40
1:eC:46:TRP:O	1:eC:50:MET:N	2.49	0.40
1:hC:46:TRP:O	1:hC:50:MET:N	2.49	0.40
1:iA:104:ILE:HG23	1:iA:105:VAL:N	2.37	0.40
1:iB:22:MET:HE1	1:iB:114:ILE:HG23	2.03	0.40
1:kA:104:ILE:HG23	1:kA:105:VAL:N	2.37	0.40
1:mA:104:ILE:HG23	1:mA:105:VAL:N	2.37	0.40
1:mC:87:LEU:O	1:mC:90:THR:OG1	2.36	0.40
1:nC:46:TRP:O	1:nC:50:MET:N	2.49	0.40
1:oC:18:LEU:HD22	1:oC:111:VAL:HG21	2.02	0.40
1:pC:78:LEU:H	1:pC:78:LEU:HD12	1.86	0.40
1:rB:9:ASN:HD22	1:8C:6:LEU:HD22	1.86	0.40
1:sC:78:LEU:H	1:sC:78:LEU:HD12	1.86	0.40
1:uC:46:TRP:O	1:uC:50:MET:N	2.49	0.40
1:vB:22:MET:HE1	1:vB:114:ILE:HG23	2.03	0.40
1:5A:104:ILE:HG23	1:5A:105:VAL:N	2.37	0.40
1:7C:78:LEU:HD12	1:7C:78:LEU:H	1.86	0.40
1:CA:104:ILE:HG23	1:CA:105:VAL:N	2.37	0.40
1:CC:120:THR:HG21	1:CC:124:PHE:O	2.21	0.40
1:FA:104:ILE:HG23	1:FA:105:VAL:N	2.37	0.40
1:LA:33:VAL:HG12	1:LA:37:LEU:HD12	2.03	0.40
1:PA:127:ASP:HB2	1:lA:130:LYS:HE2	2.03	0.40
1:RB:33:VAL:HG12	1:RB:37:LEU:HD12	2.02	0.40
1:SC:78:LEU:H	1:SC:78:LEU:HD12	1.86	0.40
1:UB:22:MET:HE1	1:UB:114:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:VA:104:ILE:HG23	1:VA:105:VAL:N	2.37	0.40
1:VC:18:LEU:HD22	1:VC:111:VAL:HG21	2.02	0.40
1:XA:104:ILE:HG23	1:XA:105:VAL:N	2.37	0.40
1:ZC:3:PHE:CZ	1:gC:33:VAL:HB	2.57	0.40
1:dC:120:THR:HG21	1:dC:124:PHE:O	2.21	0.40
1:eC:78:LEU:HD12	1:eC:78:LEU:H	1.86	0.40
1:gC:120:THR:HG21	1:gC:124:PHE:O	2.21	0.40
1:hA:104:ILE:HG23	1:hA:105:VAL:N	2.37	0.40
1:iC:78:LEU:HD12	1:iC:78:LEU:H	1.86	0.40
1:lA:33:VAL:HG12	1:lA:37:LEU:HD12	2.03	0.40
1:oA:104:ILE:HG23	1:oA:105:VAL:N	2.37	0.40
1:qC:120:THR:HG21	1:qC:124:PHE:O	2.21	0.40
1:rA:33:VAL:HG12	1:rA:37:LEU:HD12	2.03	0.40
1:vA:33:VAL:HG12	1:vA:37:LEU:HD12	2.03	0.40
1:yA:104:ILE:HG23	1:yA:105:VAL:N	2.37	0.40
1:3C:120:THR:HG21	1:3C:124:PHE:O	2.21	0.40
1:4C:18:LEU:HD22	1:4C:111:VAL:HG21	2.02	0.40
1:5B:33:VAL:HG12	1:5B:37:LEU:HD12	2.02	0.40
1:8A:33:VAL:HG12	1:8A:37:LEU:HD12	2.03	0.40
1:AA:33:VAL:HG12	1:AA:37:LEU:HD12	2.03	0.40
1:AB:43:HIS:NE2	1:AB:48:THR:OG1	2.48	0.40
1:IA:104:ILE:HG23	1:IA:105:VAL:N	2.37	0.40
1:JB:33:VAL:HG12	1:JB:37:LEU:HD12	2.02	0.40
1:OB:33:VAL:HG12	1:OB:37:LEU:HD12	2.02	0.40
1:XC:120:THR:HG21	1:XC:124:PHE:O	2.21	0.40
1:YC:87:LEU:O	1:YC:90:THR:OG1	2.36	0.40
1:aC:78:LEU:HD12	1:aC:78:LEU:H	1.86	0.40
1:bC:78:LEU:HD12	1:bC:78:LEU:H	1.86	0.40
1:kC:120:THR:HG21	1:kC:124:PHE:O	2.21	0.40
1:oA:33:VAL:HG12	1:oA:37:LEU:HD12	2.03	0.40
1:oA:36:ILE:HG23	1:oA:100:HIS:CE1	2.55	0.40
1:oC:120:THR:HG21	1:oC:124:PHE:O	2.21	0.40
1:qB:22:MET:HE1	1:qB:114:ILE:HG23	2.03	0.40
1:rB:33:VAL:HG12	1:rB:37:LEU:HD12	2.02	0.40
1:sC:46:TRP:O	1:sC:50:MET:N	2.49	0.40
1:tC:120:THR:HG21	1:tC:124:PHE:O	2.21	0.40
1:uC:3:PHE:HB3	1:zC:51:ALA:HB1	2.03	0.40
1:uC:120:THR:HG21	1:uC:124:PHE:O	2.21	0.40
1:xA:104:ILE:HG23	1:xA:105:VAL:N	2.37	0.40
1:xC:87:LEU:O	1:xC:90:THR:OG1	2.36	0.40
1:zB:22:MET:HE1	1:zB:114:ILE:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4C:78:LEU:HD12	1:4C:78:LEU:H	1.86	0.40
1:AA:104:ILE:HG23	1:AA:105:VAL:N	2.37	0.40
1:CB:22:MET:HE1	1:CB:114:ILE:HG23	2.03	0.40
1:FB:22:MET:HE1	1:FB:114:ILE:HG23	2.03	0.40
1:FC:120:THR:HG21	1:FC:124:PHE:O	2.21	0.40
1:IA:33:VAL:HG12	1:IA:37:LEU:HD12	2.03	0.40
1:KA:104:ILE:HG23	1:KA:105:VAL:N	2.37	0.40
1:MC:18:LEU:HD22	1:MC:111:VAL:HG21	2.02	0.40
1:SA:33:VAL:HG12	1:SA:37:LEU:HD12	2.03	0.40
1:TC:18:LEU:HD22	1:TC:111:VAL:HG21	2.02	0.40
1:cA:104:ILE:HG23	1:cA:105:VAL:N	2.37	0.40
1:lA:9:ASN:HA	1:uA:38:THR:HG21	2.03	0.40
1:mB:22:MET:HE1	1:mB:114:ILE:HG23	2.02	0.40
1:mC:78:LEU:H	1:mC:78:LEU:HD12	1.86	0.40
1:qA:104:ILE:HG23	1:qA:105:VAL:N	2.37	0.40
1:tB:22:MET:HE1	1:tB:114:ILE:HG23	2.03	0.40
1:tC:46:TRP:O	1:tC:50:MET:N	2.49	0.40
1:uC:58:LEU:HD11	1:zC:3:PHE:CE2	2.57	0.40
1:vC:120:THR:HG21	1:vC:124:PHE:O	2.21	0.40
1:wC:78:LEU:H	1:wC:78:LEU:HD12	1.86	0.40
1:yC:120:THR:HG21	1:yC:124:PHE:O	2.21	0.40
1:7A:104:ILE:HG23	1:7A:105:VAL:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	1B	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	1C	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2A	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	2B	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	2C	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	3A	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	3B	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	3C	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	4A	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	4B	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	4C	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	5A	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	5B	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	5C	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	6A	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	6B	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	6C	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	7A	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	7B	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	7C	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	8A	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	8B	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	8C	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	AA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	AB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	AC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	BA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	BB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	BC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	CA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	CB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	CC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	DA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	DC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	EA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	EB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	EC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	FA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	FB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	FC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	GA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	GB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	GC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	HA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	HB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	HC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	IA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	IB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	IC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	JA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	JB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	JC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	KA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	KB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	KC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	LA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	LB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	LC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	MA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	MB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	MC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	NA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	NB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	NC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	OA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	OB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	OC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	PA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	PB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	PC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	QA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	QB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	QC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	RA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	RB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	RC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	SA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	SB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	SC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	TA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	TB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	TC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	UA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	UB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	UC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	VA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	VB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	VC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	WA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	WB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	WC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	XA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	XB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	XC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	YA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	YB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	YC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	ZA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	ZB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	ZC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	aA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	aB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	aC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	bA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	bB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	bC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	cA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	cB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	cC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	dA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	dB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	dC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	eA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	eB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	eC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	fA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	fB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	fC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	gA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	gB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	gC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	hA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	hB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	hC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	iA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	iB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	iC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	jA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	jB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	jC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	kA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	kB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	kC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	lA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	lB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	lC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	mA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	mB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	mC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	nA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	nB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	nC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	oA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	oB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	oC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	pA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	pB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	pC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	qA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	qB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	qC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	rA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	rB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	rC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	sA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	sB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	sC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	tA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	tB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	tC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	uA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	uB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	uC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	vA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	vB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	vC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	wA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	wB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	wC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	xA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	xB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	xC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	yA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	yB	118/175 (67%)	110 (93%)	8 (7%)	0	100	100
1	yC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
1	zA	118/175 (67%)	113 (96%)	5 (4%)	0	100	100
1	zB	118/175 (67%)	111 (94%)	7 (6%)	0	100	100
1	zC	115/175 (66%)	109 (95%)	5 (4%)	1 (1%)	14	47
All	All	21060/31500 (67%)	19943 (95%)	1057 (5%)	60 (0%)	37	69

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AC	122	GLN
1	BC	122	GLN
1	CC	122	GLN
1	DC	122	GLN
1	EC	122	GLN
1	FC	122	GLN
1	GC	122	GLN

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Mol	Chain	Res	Type
1	HC	122	GLN
1	IC	122	GLN
1	JC	122	GLN
1	KC	122	GLN
1	LC	122	GLN
1	MC	122	GLN
1	NC	122	GLN
1	OC	122	GLN
1	PC	122	GLN
1	QC	122	GLN
1	RC	122	GLN
1	1C	122	GLN
1	SC	122	GLN
1	TC	122	GLN
1	UC	122	GLN
1	VC	122	GLN
1	WC	122	GLN
1	XC	122	GLN
1	YC	122	GLN
1	ZC	122	GLN
1	aC	122	GLN
1	bC	122	GLN
1	cC	122	GLN
1	dC	122	GLN
1	eC	122	GLN
1	fC	122	GLN
1	gC	122	GLN
1	hC	122	GLN
1	iC	122	GLN
1	jC	122	GLN
1	kC	122	GLN
1	lC	122	GLN
1	mC	122	GLN
1	nC	122	GLN
1	oC	122	GLN
1	pC	122	GLN
1	qC	122	GLN
1	rC	122	GLN
1	2C	122	GLN
1	sC	122	GLN
1	tC	122	GLN
1	uC	122	GLN

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Mol	Chain	Res	Type
1	vC	122	GLN
1	wC	122	GLN
1	xC	122	GLN
1	yC	122	GLN
1	zC	122	GLN
1	3C	122	GLN
1	4C	122	GLN
1	5C	122	GLN
1	6C	122	GLN
1	7C	122	GLN
1	8C	122	GLN

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	1A	111/148 (75%)	111 (100%)	0	100	100
1	1B	111/148 (75%)	111 (100%)	0	100	100
1	1C	108/148 (73%)	108 (100%)	0	100	100
1	2A	111/148 (75%)	111 (100%)	0	100	100
1	2B	111/148 (75%)	111 (100%)	0	100	100
1	2C	108/148 (73%)	108 (100%)	0	100	100
1	3A	111/148 (75%)	111 (100%)	0	100	100
1	3B	111/148 (75%)	111 (100%)	0	100	100
1	3C	108/148 (73%)	108 (100%)	0	100	100
1	4A	111/148 (75%)	111 (100%)	0	100	100
1	4B	111/148 (75%)	111 (100%)	0	100	100
1	4C	108/148 (73%)	108 (100%)	0	100	100
1	5A	111/148 (75%)	111 (100%)	0	100	100
1	5B	111/148 (75%)	111 (100%)	0	100	100
1	5C	108/148 (73%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6A	111/148 (75%)	111 (100%)	0	100	100
1	6B	111/148 (75%)	111 (100%)	0	100	100
1	6C	108/148 (73%)	108 (100%)	0	100	100
1	7A	111/148 (75%)	111 (100%)	0	100	100
1	7B	111/148 (75%)	111 (100%)	0	100	100
1	7C	108/148 (73%)	108 (100%)	0	100	100
1	8A	111/148 (75%)	111 (100%)	0	100	100
1	8B	111/148 (75%)	111 (100%)	0	100	100
1	8C	108/148 (73%)	108 (100%)	0	100	100
1	AA	111/148 (75%)	111 (100%)	0	100	100
1	AB	111/148 (75%)	111 (100%)	0	100	100
1	AC	108/148 (73%)	108 (100%)	0	100	100
1	BA	111/148 (75%)	111 (100%)	0	100	100
1	BB	111/148 (75%)	111 (100%)	0	100	100
1	BC	108/148 (73%)	108 (100%)	0	100	100
1	CA	111/148 (75%)	111 (100%)	0	100	100
1	CB	111/148 (75%)	111 (100%)	0	100	100
1	CC	108/148 (73%)	108 (100%)	0	100	100
1	DA	111/148 (75%)	111 (100%)	0	100	100
1	DB	111/148 (75%)	111 (100%)	0	100	100
1	DC	108/148 (73%)	108 (100%)	0	100	100
1	EA	111/148 (75%)	111 (100%)	0	100	100
1	EB	111/148 (75%)	111 (100%)	0	100	100
1	EC	108/148 (73%)	108 (100%)	0	100	100
1	FA	111/148 (75%)	111 (100%)	0	100	100
1	FB	111/148 (75%)	111 (100%)	0	100	100
1	FC	108/148 (73%)	108 (100%)	0	100	100
1	GA	111/148 (75%)	111 (100%)	0	100	100
1	GB	111/148 (75%)	111 (100%)	0	100	100
1	GC	108/148 (73%)	108 (100%)	0	100	100
1	HA	111/148 (75%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	HB	111/148 (75%)	111 (100%)	0	100	100
1	HC	108/148 (73%)	108 (100%)	0	100	100
1	IA	111/148 (75%)	111 (100%)	0	100	100
1	IB	111/148 (75%)	111 (100%)	0	100	100
1	IC	108/148 (73%)	108 (100%)	0	100	100
1	JA	111/148 (75%)	111 (100%)	0	100	100
1	JB	111/148 (75%)	111 (100%)	0	100	100
1	JC	108/148 (73%)	108 (100%)	0	100	100
1	KA	111/148 (75%)	111 (100%)	0	100	100
1	KB	111/148 (75%)	111 (100%)	0	100	100
1	KC	108/148 (73%)	108 (100%)	0	100	100
1	LA	111/148 (75%)	111 (100%)	0	100	100
1	LB	111/148 (75%)	111 (100%)	0	100	100
1	LC	108/148 (73%)	108 (100%)	0	100	100
1	MA	111/148 (75%)	111 (100%)	0	100	100
1	MB	111/148 (75%)	111 (100%)	0	100	100
1	MC	108/148 (73%)	108 (100%)	0	100	100
1	NA	111/148 (75%)	111 (100%)	0	100	100
1	NB	111/148 (75%)	111 (100%)	0	100	100
1	NC	108/148 (73%)	108 (100%)	0	100	100
1	OA	111/148 (75%)	111 (100%)	0	100	100
1	OB	111/148 (75%)	111 (100%)	0	100	100
1	OC	108/148 (73%)	108 (100%)	0	100	100
1	PA	111/148 (75%)	111 (100%)	0	100	100
1	PB	111/148 (75%)	111 (100%)	0	100	100
1	PC	108/148 (73%)	108 (100%)	0	100	100
1	QA	111/148 (75%)	111 (100%)	0	100	100
1	QB	111/148 (75%)	111 (100%)	0	100	100
1	QC	108/148 (73%)	108 (100%)	0	100	100
1	RA	111/148 (75%)	111 (100%)	0	100	100
1	RB	111/148 (75%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	RC	108/148 (73%)	108 (100%)	0	100	100
1	SA	111/148 (75%)	111 (100%)	0	100	100
1	SB	111/148 (75%)	111 (100%)	0	100	100
1	SC	108/148 (73%)	108 (100%)	0	100	100
1	TA	111/148 (75%)	111 (100%)	0	100	100
1	TB	111/148 (75%)	111 (100%)	0	100	100
1	TC	108/148 (73%)	108 (100%)	0	100	100
1	UA	111/148 (75%)	111 (100%)	0	100	100
1	UB	111/148 (75%)	111 (100%)	0	100	100
1	UC	108/148 (73%)	108 (100%)	0	100	100
1	VA	111/148 (75%)	111 (100%)	0	100	100
1	VB	111/148 (75%)	111 (100%)	0	100	100
1	VC	108/148 (73%)	108 (100%)	0	100	100
1	WA	111/148 (75%)	111 (100%)	0	100	100
1	WB	111/148 (75%)	111 (100%)	0	100	100
1	WC	108/148 (73%)	108 (100%)	0	100	100
1	XA	111/148 (75%)	111 (100%)	0	100	100
1	XB	111/148 (75%)	111 (100%)	0	100	100
1	XC	108/148 (73%)	108 (100%)	0	100	100
1	YA	111/148 (75%)	111 (100%)	0	100	100
1	YB	111/148 (75%)	111 (100%)	0	100	100
1	YC	108/148 (73%)	108 (100%)	0	100	100
1	ZA	111/148 (75%)	111 (100%)	0	100	100
1	ZB	111/148 (75%)	111 (100%)	0	100	100
1	ZC	108/148 (73%)	108 (100%)	0	100	100
1	aA	111/148 (75%)	111 (100%)	0	100	100
1	aB	111/148 (75%)	111 (100%)	0	100	100
1	aC	108/148 (73%)	108 (100%)	0	100	100
1	bA	111/148 (75%)	111 (100%)	0	100	100
1	bB	111/148 (75%)	111 (100%)	0	100	100
1	bC	108/148 (73%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	cA	111/148 (75%)	111 (100%)	0	100	100
1	cB	111/148 (75%)	111 (100%)	0	100	100
1	cC	108/148 (73%)	108 (100%)	0	100	100
1	dA	111/148 (75%)	111 (100%)	0	100	100
1	dB	111/148 (75%)	111 (100%)	0	100	100
1	dC	108/148 (73%)	108 (100%)	0	100	100
1	eA	111/148 (75%)	111 (100%)	0	100	100
1	eB	111/148 (75%)	111 (100%)	0	100	100
1	eC	108/148 (73%)	108 (100%)	0	100	100
1	fA	111/148 (75%)	111 (100%)	0	100	100
1	fB	111/148 (75%)	111 (100%)	0	100	100
1	fC	108/148 (73%)	108 (100%)	0	100	100
1	gA	111/148 (75%)	111 (100%)	0	100	100
1	gB	111/148 (75%)	111 (100%)	0	100	100
1	gC	108/148 (73%)	108 (100%)	0	100	100
1	hA	111/148 (75%)	111 (100%)	0	100	100
1	hB	111/148 (75%)	111 (100%)	0	100	100
1	hC	108/148 (73%)	108 (100%)	0	100	100
1	iA	111/148 (75%)	111 (100%)	0	100	100
1	iB	111/148 (75%)	111 (100%)	0	100	100
1	iC	108/148 (73%)	108 (100%)	0	100	100
1	jA	111/148 (75%)	111 (100%)	0	100	100
1	jB	111/148 (75%)	111 (100%)	0	100	100
1	jC	108/148 (73%)	108 (100%)	0	100	100
1	kA	111/148 (75%)	111 (100%)	0	100	100
1	kB	111/148 (75%)	111 (100%)	0	100	100
1	kC	108/148 (73%)	108 (100%)	0	100	100
1	lA	111/148 (75%)	111 (100%)	0	100	100
1	lB	111/148 (75%)	111 (100%)	0	100	100
1	lC	108/148 (73%)	108 (100%)	0	100	100
1	mA	111/148 (75%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	mB	111/148 (75%)	111 (100%)	0	100	100
1	mC	108/148 (73%)	108 (100%)	0	100	100
1	nA	111/148 (75%)	111 (100%)	0	100	100
1	nB	111/148 (75%)	111 (100%)	0	100	100
1	nC	108/148 (73%)	108 (100%)	0	100	100
1	oA	111/148 (75%)	111 (100%)	0	100	100
1	oB	111/148 (75%)	111 (100%)	0	100	100
1	oC	108/148 (73%)	108 (100%)	0	100	100
1	pA	111/148 (75%)	111 (100%)	0	100	100
1	pB	111/148 (75%)	111 (100%)	0	100	100
1	pC	108/148 (73%)	108 (100%)	0	100	100
1	qA	111/148 (75%)	111 (100%)	0	100	100
1	qB	111/148 (75%)	111 (100%)	0	100	100
1	qC	108/148 (73%)	108 (100%)	0	100	100
1	rA	111/148 (75%)	111 (100%)	0	100	100
1	rB	111/148 (75%)	111 (100%)	0	100	100
1	rC	108/148 (73%)	108 (100%)	0	100	100
1	sA	111/148 (75%)	111 (100%)	0	100	100
1	sB	111/148 (75%)	111 (100%)	0	100	100
1	sC	108/148 (73%)	108 (100%)	0	100	100
1	tA	111/148 (75%)	111 (100%)	0	100	100
1	tB	111/148 (75%)	111 (100%)	0	100	100
1	tC	108/148 (73%)	108 (100%)	0	100	100
1	uA	111/148 (75%)	111 (100%)	0	100	100
1	uB	111/148 (75%)	111 (100%)	0	100	100
1	uC	108/148 (73%)	108 (100%)	0	100	100
1	vA	111/148 (75%)	111 (100%)	0	100	100
1	vB	111/148 (75%)	111 (100%)	0	100	100
1	vC	108/148 (73%)	108 (100%)	0	100	100
1	wA	111/148 (75%)	111 (100%)	0	100	100
1	wB	111/148 (75%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	wC	108/148 (73%)	108 (100%)	0	100	100
1	xA	111/148 (75%)	111 (100%)	0	100	100
1	xB	111/148 (75%)	111 (100%)	0	100	100
1	xC	108/148 (73%)	108 (100%)	0	100	100
1	yA	111/148 (75%)	111 (100%)	0	100	100
1	yB	111/148 (75%)	111 (100%)	0	100	100
1	yC	108/148 (73%)	108 (100%)	0	100	100
1	zA	111/148 (75%)	111 (100%)	0	100	100
1	zB	111/148 (75%)	111 (100%)	0	100	100
1	zC	108/148 (73%)	108 (100%)	0	100	100
All	All	19800/26640 (74%)	19800 (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 (499) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	56	GLN
1	1A	84	GLN
1	1A	98	GLN
1	1A	101	HIS
1	AC	43	HIS
1	AC	101	HIS
1	AC	106	GLN
1	AC	109	HIS
1	BA	56	GLN
1	BA	84	GLN
1	BA	98	GLN
1	BA	101	HIS
1	BB	56	GLN
1	BB	113	GLN
1	BC	9	ASN
1	BC	101	HIS
1	BC	106	GLN
1	CA	56	GLN
1	CA	84	GLN
1	CA	98	GLN
1	CA	101	HIS

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Mol	Chain	Res	Type
1	CB	56	GLN
1	CB	113	GLN
1	CC	101	HIS
1	CC	106	GLN
1	DA	56	GLN
1	DA	84	GLN
1	DA	98	GLN
1	DA	101	HIS
1	DB	56	GLN
1	DB	113	GLN
1	DC	101	HIS
1	DC	106	GLN
1	EA	84	GLN
1	EA	101	HIS
1	EB	56	GLN
1	EB	113	GLN
1	EC	101	HIS
1	EC	106	GLN
1	FA	56	GLN
1	FA	84	GLN
1	FA	101	HIS
1	FB	56	GLN
1	FB	113	GLN
1	FC	43	HIS
1	FC	101	HIS
1	FC	106	GLN
1	FC	109	HIS
1	GA	56	GLN
1	GA	84	GLN
1	GA	98	GLN
1	GA	101	HIS
1	GB	56	GLN
1	GB	113	GLN
1	GC	101	HIS
1	HA	56	GLN
1	HA	84	GLN
1	HA	98	GLN
1	HA	101	HIS
1	HB	56	GLN
1	HB	113	GLN
1	HC	101	HIS
1	HC	106	GLN

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Mol	Chain	Res	Type
1	IA	56	GLN
1	IA	84	GLN
1	IA	98	GLN
1	IA	101	HIS
1	IB	56	GLN
1	IB	113	GLN
1	IC	100	HIS
1	IC	101	HIS
1	IC	106	GLN
1	JA	56	GLN
1	JA	84	GLN
1	JA	98	GLN
1	JA	101	HIS
1	1B	56	GLN
1	1B	113	GLN
1	JB	56	GLN
1	JB	113	GLN
1	JC	101	HIS
1	JC	106	GLN
1	KA	56	GLN
1	KA	84	GLN
1	KA	98	GLN
1	KA	101	HIS
1	KB	56	GLN
1	KB	113	GLN
1	KC	101	HIS
1	KC	106	GLN
1	LA	56	GLN
1	LA	84	GLN
1	LA	98	GLN
1	LA	101	HIS
1	LA	128	GLN
1	LB	56	GLN
1	LB	113	GLN
1	LC	101	HIS
1	LC	106	GLN
1	MA	32	HIS
1	MA	56	GLN
1	MA	84	GLN
1	MA	98	GLN
1	MA	101	HIS
1	MB	56	GLN

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Mol	Chain	Res	Type
1	MB	113	GLN
1	MC	43	HIS
1	MC	100	HIS
1	MC	101	HIS
1	NA	32	HIS
1	NA	56	GLN
1	NA	84	GLN
1	NA	98	GLN
1	NA	101	HIS
1	NB	56	GLN
1	NB	113	GLN
1	NC	101	HIS
1	NC	106	GLN
1	OA	32	HIS
1	OA	84	GLN
1	OA	98	GLN
1	OA	101	HIS
1	OB	56	GLN
1	OB	113	GLN
1	OC	43	HIS
1	OC	101	HIS
1	OC	106	GLN
1	PA	56	GLN
1	PA	84	GLN
1	PA	101	HIS
1	PB	56	GLN
1	PB	113	GLN
1	PC	101	HIS
1	PC	106	GLN
1	QA	56	GLN
1	QA	84	GLN
1	QA	101	HIS
1	QB	56	GLN
1	QB	113	GLN
1	QC	101	HIS
1	QC	106	GLN
1	RA	56	GLN
1	RA	84	GLN
1	RA	98	GLN
1	RA	101	HIS
1	RB	56	GLN
1	RB	113	GLN

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Mol	Chain	Res	Type
1	RC	43	HIS
1	RC	101	HIS
1	RC	106	GLN
1	1C	100	HIS
1	1C	101	HIS
1	1C	106	GLN
1	SA	56	GLN
1	SA	101	HIS
1	SB	113	GLN
1	SC	100	HIS
1	SC	101	HIS
1	SC	106	GLN
1	TA	32	HIS
1	TA	56	GLN
1	TA	84	GLN
1	TA	98	GLN
1	TA	101	HIS
1	TB	56	GLN
1	TB	113	GLN
1	TC	43	HIS
1	TC	101	HIS
1	TC	106	GLN
1	UA	56	GLN
1	UA	84	GLN
1	UA	98	GLN
1	UA	101	HIS
1	UB	56	GLN
1	UB	113	GLN
1	UC	101	HIS
1	UC	106	GLN
1	VA	56	GLN
1	VA	84	GLN
1	VA	98	GLN
1	VA	101	HIS
1	VB	56	GLN
1	VB	113	GLN
1	VC	43	HIS
1	VC	101	HIS
1	WA	56	GLN
1	WA	84	GLN
1	WA	98	GLN
1	WA	101	HIS

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Mol	Chain	Res	Type
1	WB	56	GLN
1	WB	113	GLN
1	WC	101	HIS
1	WC	106	GLN
1	XA	32	HIS
1	XA	56	GLN
1	XA	84	GLN
1	XA	98	GLN
1	XA	101	HIS
1	XB	56	GLN
1	XB	113	GLN
1	XC	101	HIS
1	XC	106	GLN
1	YA	56	GLN
1	YA	84	GLN
1	YA	98	GLN
1	YA	101	HIS
1	YB	56	GLN
1	YB	113	GLN
1	YC	101	HIS
1	YC	106	GLN
1	ZA	56	GLN
1	ZA	84	GLN
1	ZA	98	GLN
1	ZA	101	HIS
1	ZA	128	GLN
1	ZB	56	GLN
1	ZB	113	GLN
1	ZC	9	ASN
1	ZC	43	HIS
1	ZC	101	HIS
1	ZC	106	GLN
1	aA	32	HIS
1	aA	56	GLN
1	aA	84	GLN
1	aA	98	GLN
1	aA	101	HIS
1	aB	56	GLN
1	aB	113	GLN
1	2A	56	GLN
1	2A	84	GLN
1	2A	98	GLN

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Mol	Chain	Res	Type
1	2A	101	HIS
1	aC	101	HIS
1	bA	56	GLN
1	bA	84	GLN
1	bA	98	GLN
1	bA	101	HIS
1	bB	56	GLN
1	bB	113	GLN
1	bC	100	HIS
1	bC	101	HIS
1	bC	106	GLN
1	bC	109	HIS
1	cA	56	GLN
1	cA	84	GLN
1	cA	101	HIS
1	cB	56	GLN
1	cB	113	GLN
1	cC	100	HIS
1	cC	101	HIS
1	cC	106	GLN
1	dA	32	HIS
1	dA	56	GLN
1	dA	84	GLN
1	dA	98	GLN
1	dA	101	HIS
1	dA	128	GLN
1	dB	56	GLN
1	dB	113	GLN
1	dC	100	HIS
1	dC	101	HIS
1	dC	106	GLN
1	eA	56	GLN
1	eA	84	GLN
1	eA	98	GLN
1	eA	101	HIS
1	eB	56	GLN
1	eB	113	GLN
1	eC	100	HIS
1	eC	101	HIS
1	eC	106	GLN
1	fA	56	GLN
1	fA	84	GLN

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Mol	Chain	Res	Type
1	fA	98	GLN
1	fA	101	HIS
1	fB	56	GLN
1	fB	113	GLN
1	fC	43	HIS
1	fC	101	HIS
1	fC	106	GLN
1	gA	56	GLN
1	gA	84	GLN
1	gA	98	GLN
1	gA	101	HIS
1	gB	56	GLN
1	gB	113	GLN
1	gC	100	HIS
1	gC	101	HIS
1	gC	106	GLN
1	hA	56	GLN
1	hA	84	GLN
1	hA	98	GLN
1	hA	101	HIS
1	hB	56	GLN
1	hB	113	GLN
1	hC	101	HIS
1	hC	106	GLN
1	iA	56	GLN
1	iA	84	GLN
1	iA	98	GLN
1	iA	101	HIS
1	iA	128	GLN
1	iB	56	GLN
1	iB	113	GLN
1	iC	101	HIS
1	iC	109	HIS
1	jA	56	GLN
1	jA	101	HIS
1	2B	56	GLN
1	2B	113	GLN
1	jB	56	GLN
1	jB	113	GLN
1	jC	101	HIS
1	jC	106	GLN
1	kA	56	GLN

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Mol	Chain	Res	Type
1	kA	84	GLN
1	kA	98	GLN
1	kA	101	HIS
1	kB	56	GLN
1	kB	113	GLN
1	kC	43	HIS
1	kC	101	HIS
1	kC	106	GLN
1	lA	32	HIS
1	lA	56	GLN
1	lA	84	GLN
1	lA	98	GLN
1	lB	113	GLN
1	lC	100	HIS
1	lC	101	HIS
1	mA	32	HIS
1	mA	56	GLN
1	mA	84	GLN
1	mA	98	GLN
1	mA	101	HIS
1	mB	56	GLN
1	mB	113	GLN
1	mC	101	HIS
1	mC	106	GLN
1	nA	32	HIS
1	nA	56	GLN
1	nA	84	GLN
1	nA	101	HIS
1	nB	56	GLN
1	nB	113	GLN
1	nC	101	HIS
1	nC	106	GLN
1	oA	56	GLN
1	oA	84	GLN
1	oA	98	GLN
1	oA	101	HIS
1	oA	128	GLN
1	oB	56	GLN
1	oB	113	GLN
1	oC	100	HIS
1	oC	101	HIS
1	oC	106	GLN

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Mol	Chain	Res	Type
1	pA	56	GLN
1	pA	84	GLN
1	pA	98	GLN
1	pA	101	HIS
1	pB	56	GLN
1	pB	113	GLN
1	qA	56	GLN
1	qA	84	GLN
1	qA	101	HIS
1	qB	56	GLN
1	qB	113	GLN
1	qC	43	HIS
1	qC	101	HIS
1	qC	106	GLN
1	rA	56	GLN
1	rA	84	GLN
1	rA	98	GLN
1	rA	101	HIS
1	rB	9	ASN
1	rB	56	GLN
1	rB	113	GLN
1	rC	101	HIS
1	rC	106	GLN
1	2C	101	HIS
1	2C	106	GLN
1	sA	84	GLN
1	sA	98	GLN
1	sA	101	HIS
1	sB	56	GLN
1	sB	113	GLN
1	sC	101	HIS
1	sC	109	HIS
1	tA	84	GLN
1	tA	98	GLN
1	tA	101	HIS
1	tB	56	GLN
1	tB	113	GLN
1	tC	101	HIS
1	tC	106	GLN
1	uA	84	GLN
1	uA	98	GLN
1	uA	101	HIS

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Mol	Chain	Res	Type
1	uB	56	GLN
1	uB	113	GLN
1	uC	101	HIS
1	uC	106	GLN
1	vA	56	GLN
1	vA	84	GLN
1	vA	101	HIS
1	vB	56	GLN
1	vB	113	GLN
1	vC	101	HIS
1	vC	106	GLN
1	wA	32	HIS
1	wA	56	GLN
1	wA	84	GLN
1	wA	98	GLN
1	wA	101	HIS
1	wB	56	GLN
1	wB	113	GLN
1	wC	100	HIS
1	wC	101	HIS
1	wC	106	GLN
1	xA	56	GLN
1	xA	84	GLN
1	xA	98	GLN
1	xA	101	HIS
1	xB	56	GLN
1	xB	113	GLN
1	xC	101	HIS
1	xC	106	GLN
1	yA	84	GLN
1	yA	98	GLN
1	yA	101	HIS
1	yB	56	GLN
1	yB	113	GLN
1	yC	101	HIS
1	yC	106	GLN
1	yC	109	HIS
1	zA	56	GLN
1	zA	84	GLN
1	zA	101	HIS
1	zB	56	GLN
1	zB	113	GLN

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Mol	Chain	Res	Type
1	zC	101	HIS
1	3A	56	GLN
1	3A	84	GLN
1	3A	98	GLN
1	3A	101	HIS
1	3B	9	ASN
1	3B	56	GLN
1	3B	113	GLN
1	3C	101	HIS
1	4A	56	GLN
1	4A	84	GLN
1	4A	101	HIS
1	4B	56	GLN
1	4B	113	GLN
1	4C	43	HIS
1	4C	100	HIS
1	4C	101	HIS
1	5A	32	HIS
1	5A	84	GLN
1	5A	98	GLN
1	5A	101	HIS
1	5B	56	GLN
1	5B	113	GLN
1	5C	101	HIS
1	5C	106	GLN
1	6A	84	GLN
1	6A	98	GLN
1	6A	101	HIS
1	6A	128	GLN
1	6B	56	GLN
1	6B	113	GLN
1	6C	43	HIS
1	6C	101	HIS
1	6C	106	GLN
1	7A	32	HIS
1	7A	56	GLN
1	7A	84	GLN
1	7A	98	GLN
1	7A	101	HIS
1	7B	56	GLN
1	7B	113	GLN
1	7C	43	HIS

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Mol	Chain	Res	Type
1	7C	101	HIS
1	7C	106	GLN
1	8A	56	GLN
1	8A	84	GLN
1	8A	98	GLN
1	8A	101	HIS
1	8B	56	GLN
1	8B	113	GLN
1	8C	101	HIS
1	8C	106	GLN
1	AA	56	GLN
1	AA	84	GLN
1	AA	98	GLN
1	AA	101	HIS
1	AB	56	GLN
1	AB	113	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

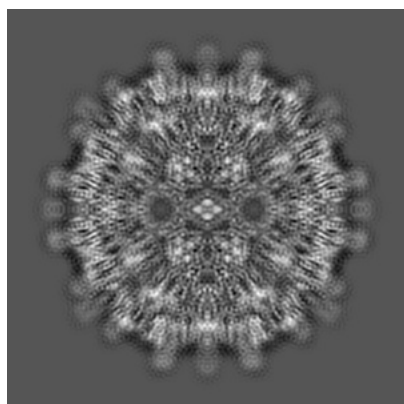
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16371. These allow visual inspection of the internal detail of the map and identification of artifacts.

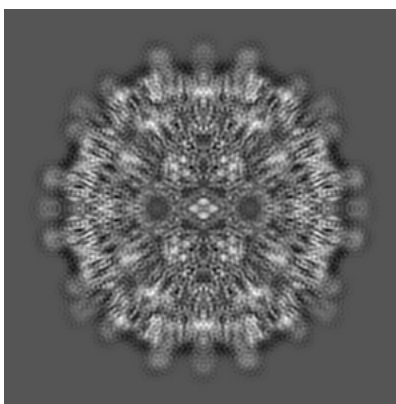
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

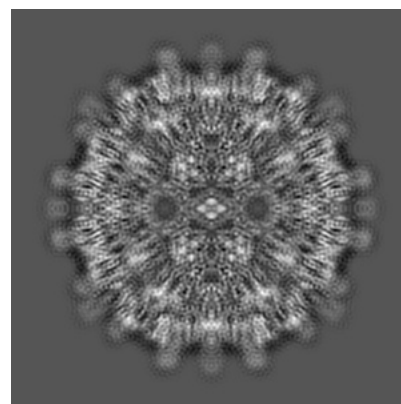
6.1.1 Primary map



X



Y



Z

6.1.2 Raw map



X



Y

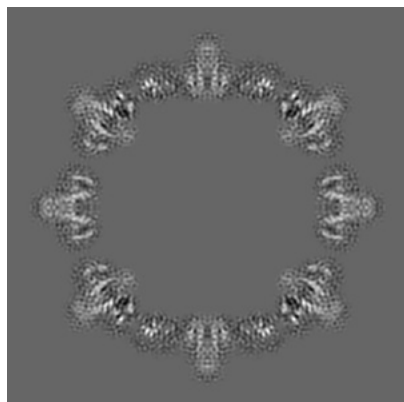


Z

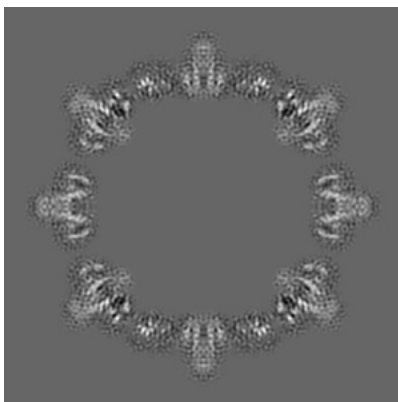
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

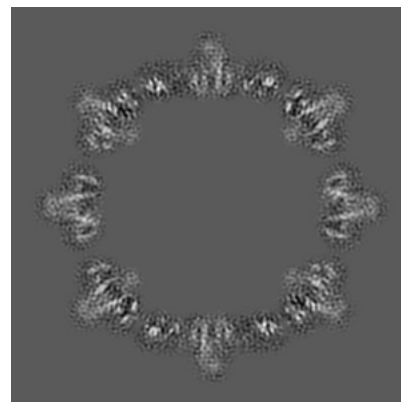
6.2.1 Primary map



X Index: 216

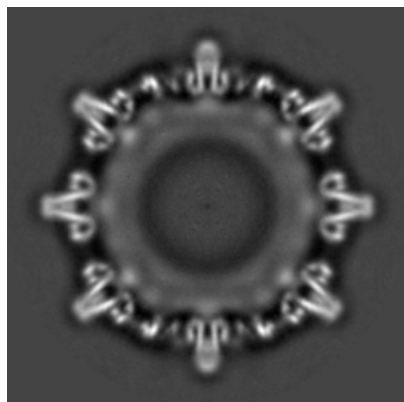


Y Index: 216

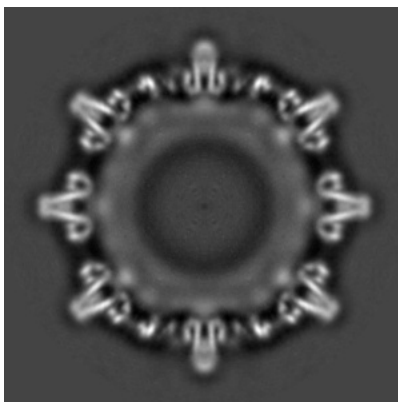


Z Index: 216

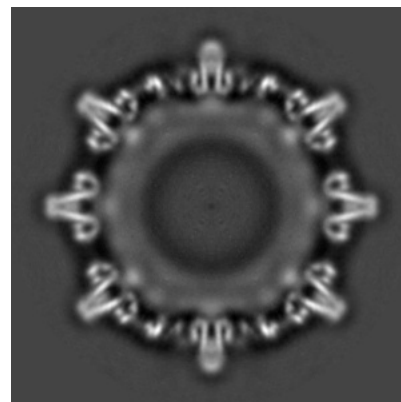
6.2.2 Raw map



X Index: 216



Y Index: 216

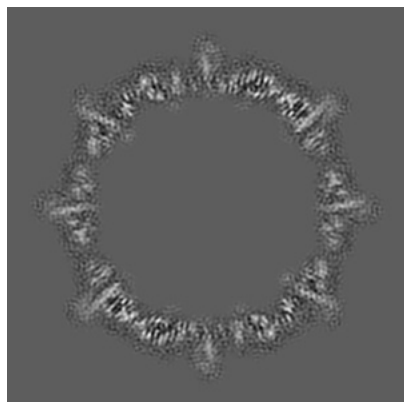


Z Index: 216

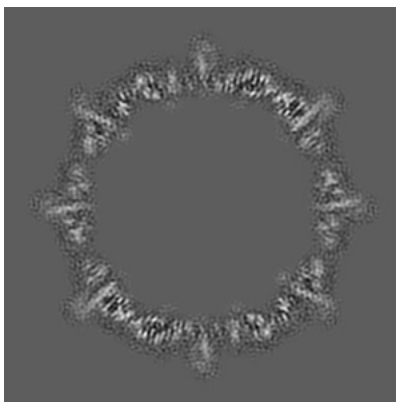
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

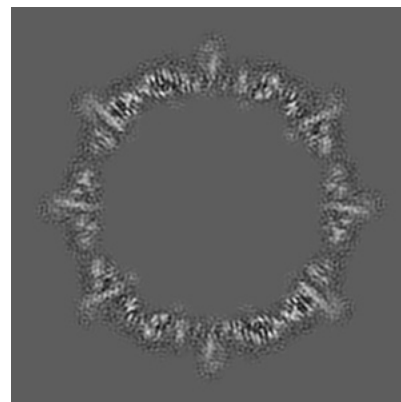
6.3.1 Primary map



X Index: 225

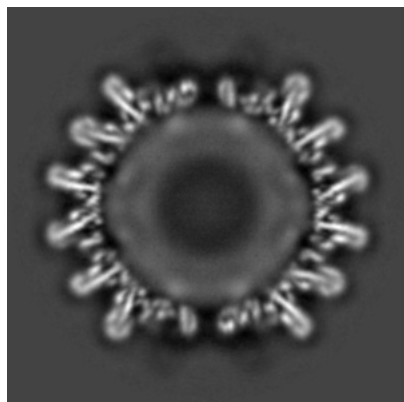


Y Index: 225

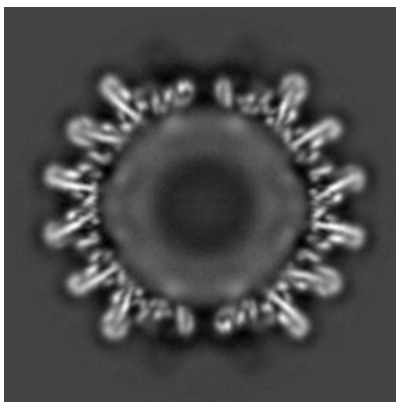


Z Index: 206

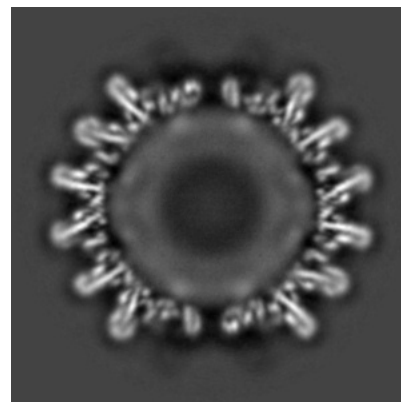
6.3.2 Raw map



X Index: 164



Y Index: 164

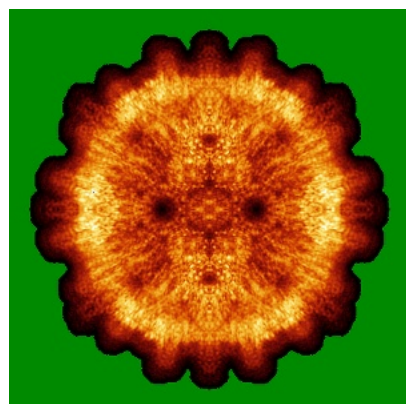


Z Index: 164

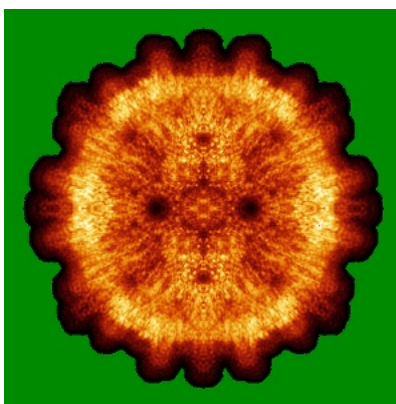
The images above show the largest variance slices of the map in three orthogonal directions.

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

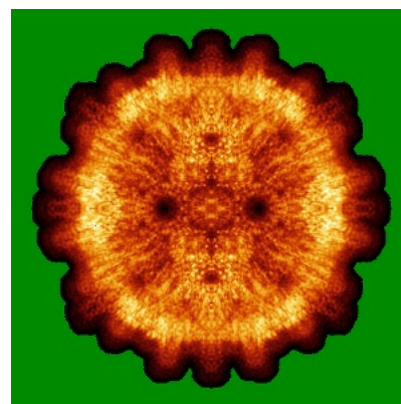
6.4.1 Primary map



X



Y



Z

6.4.2 Raw map



X



Y

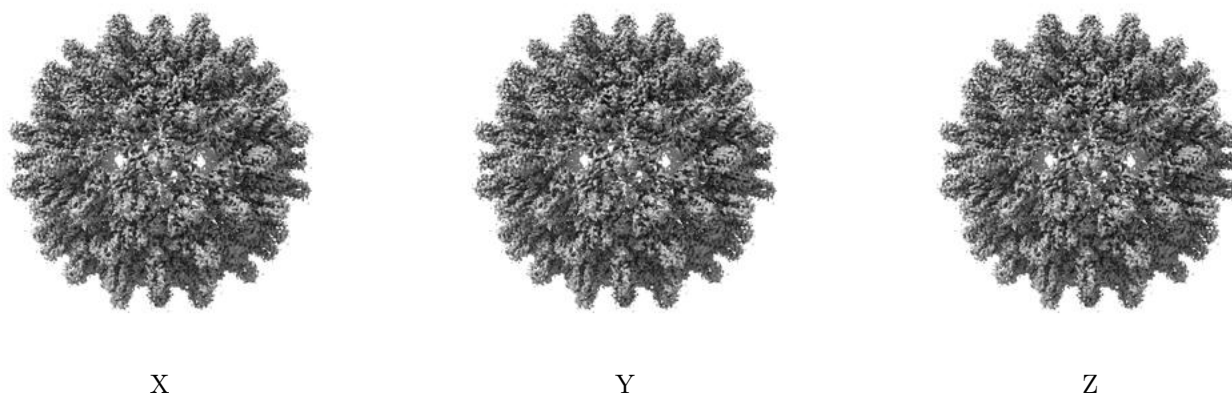


Z

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

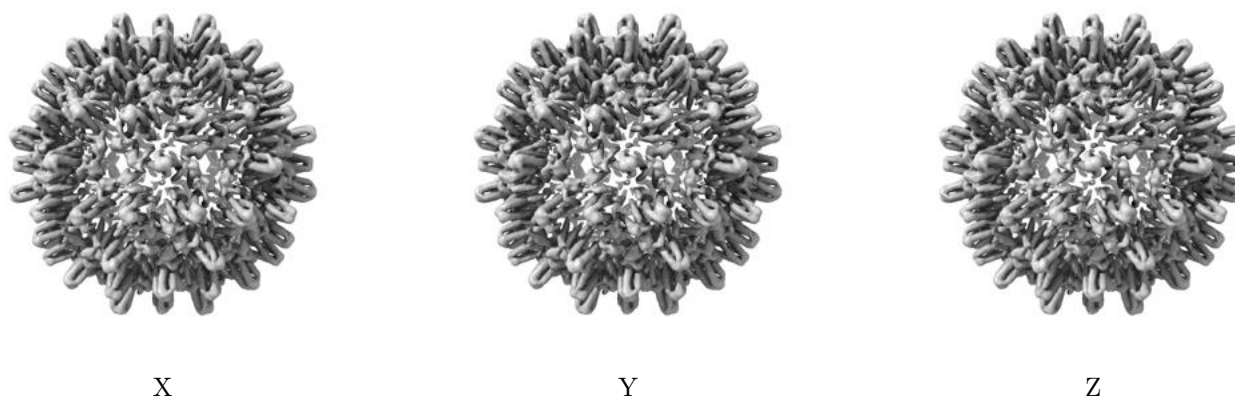
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

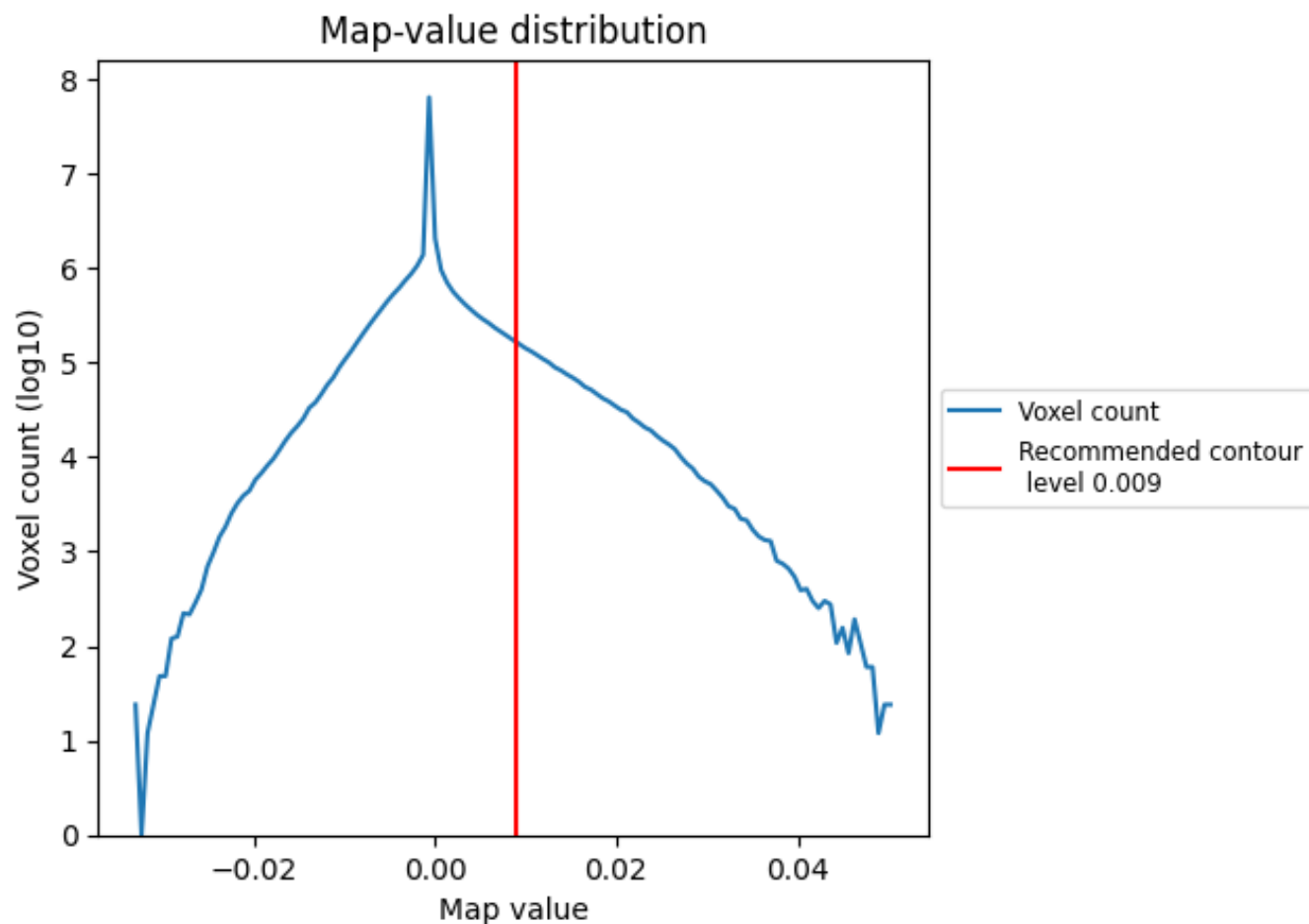
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

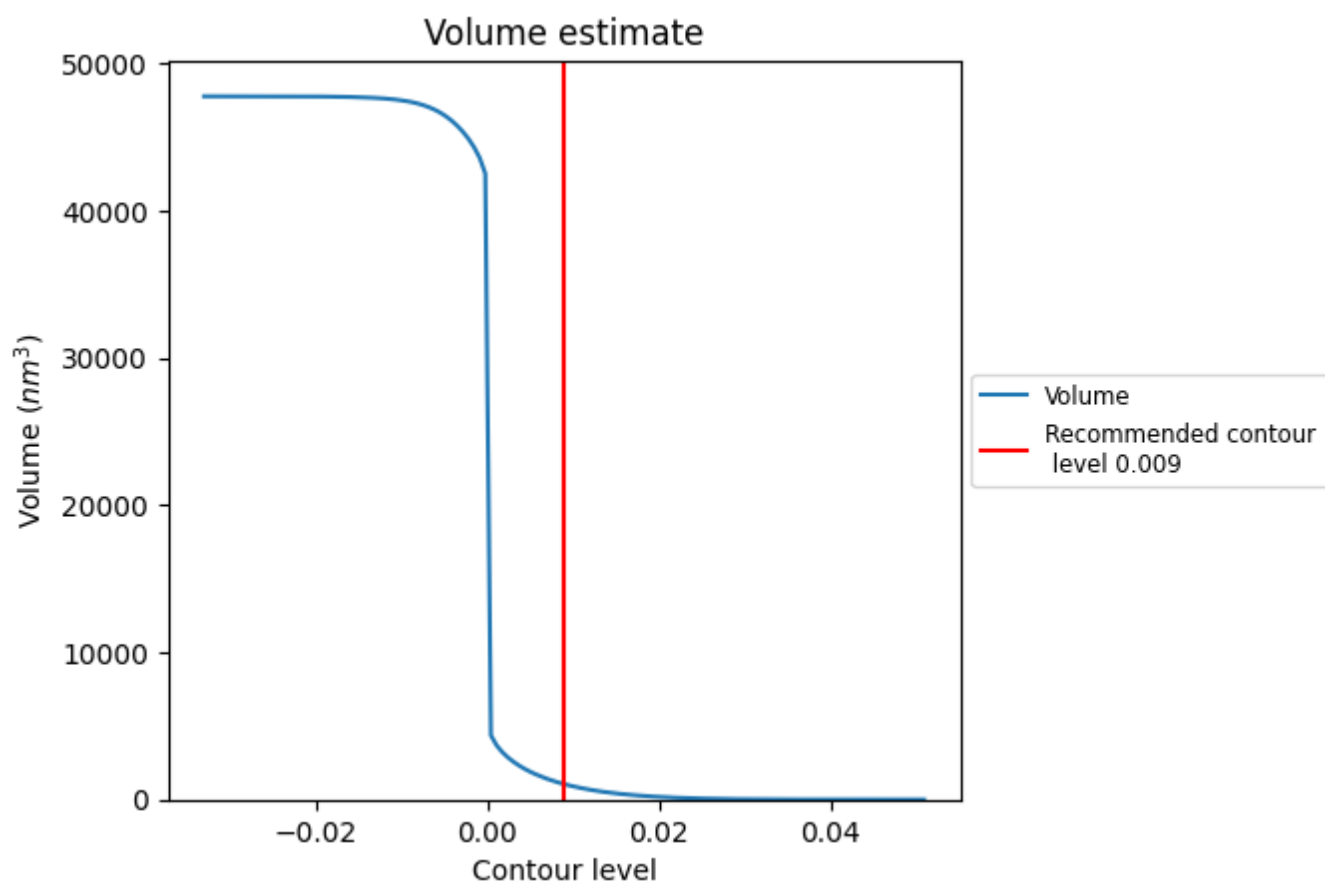
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

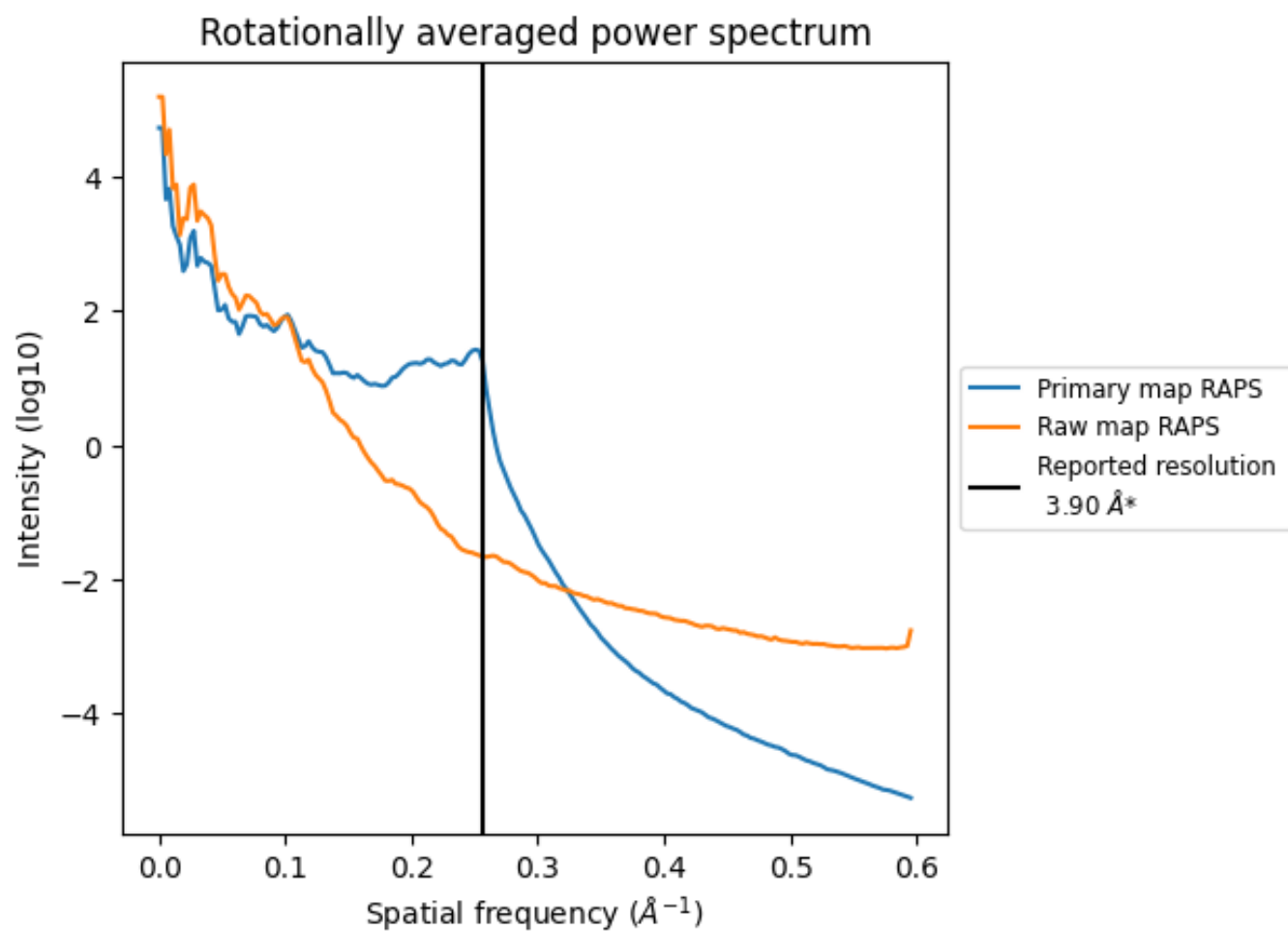
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1042 nm³; this corresponds to an approximate mass of 942 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 ⓘ

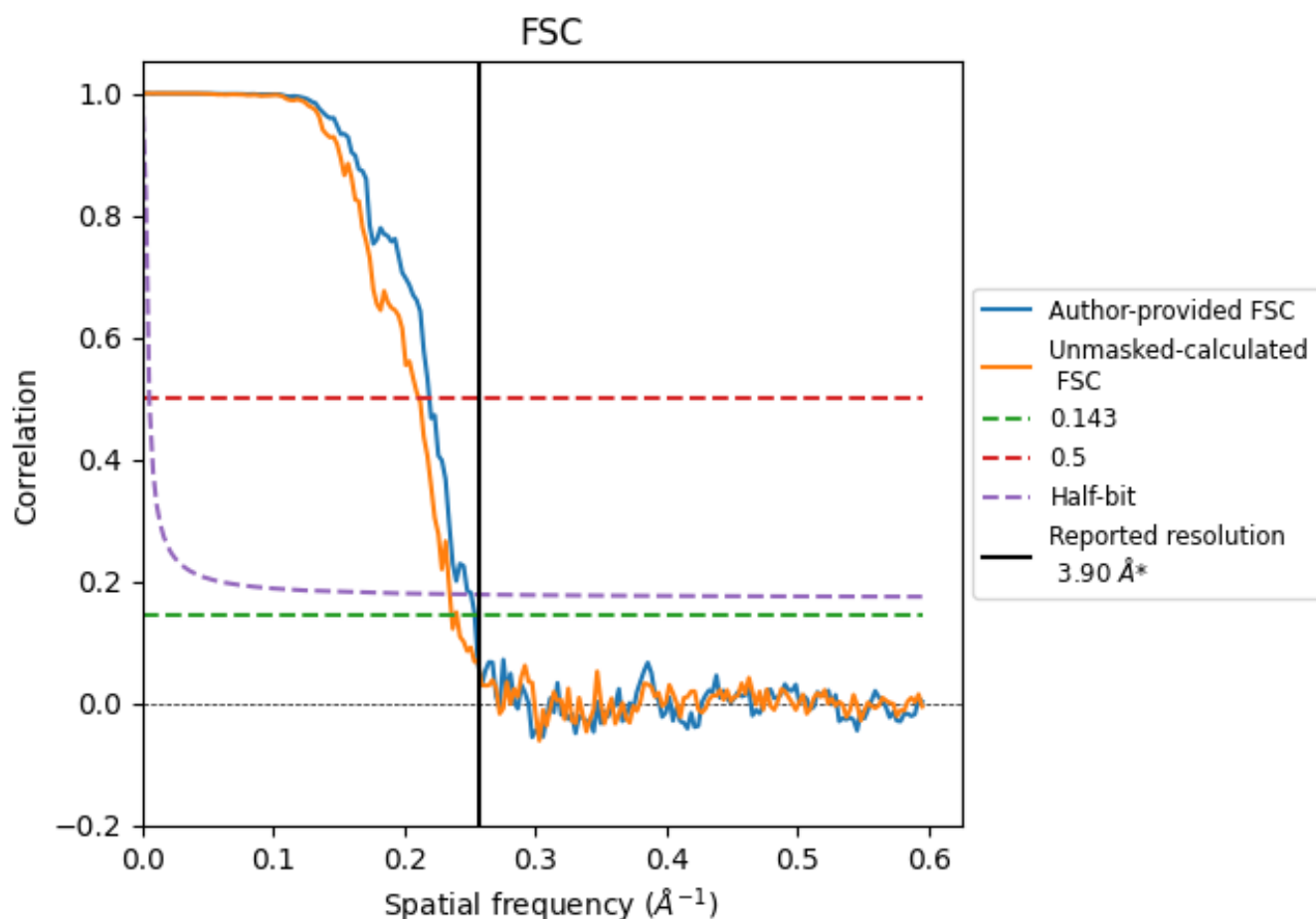


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.256 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

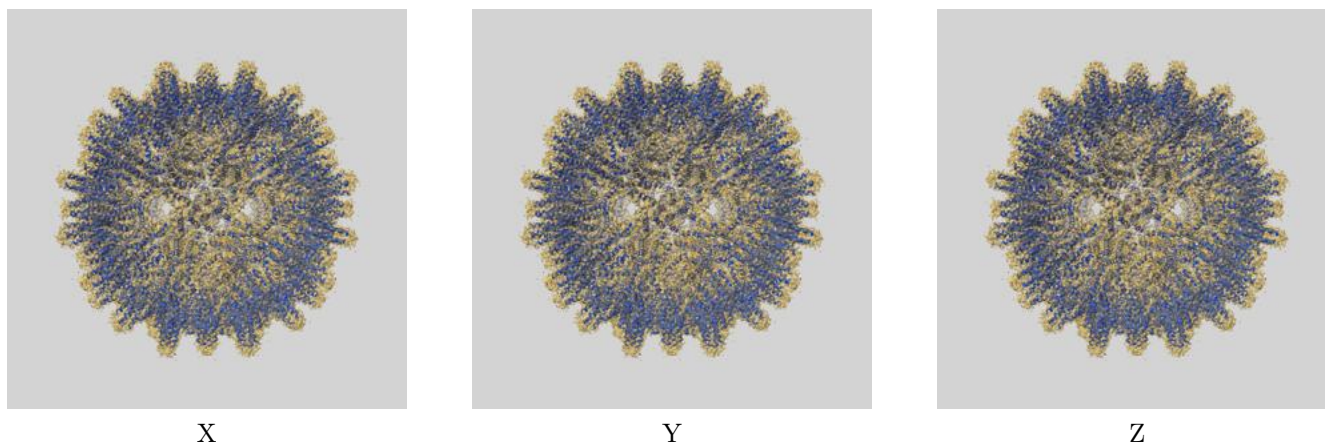
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.94	4.56	3.98
Unmasked-calculated*	4.24	4.73	4.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

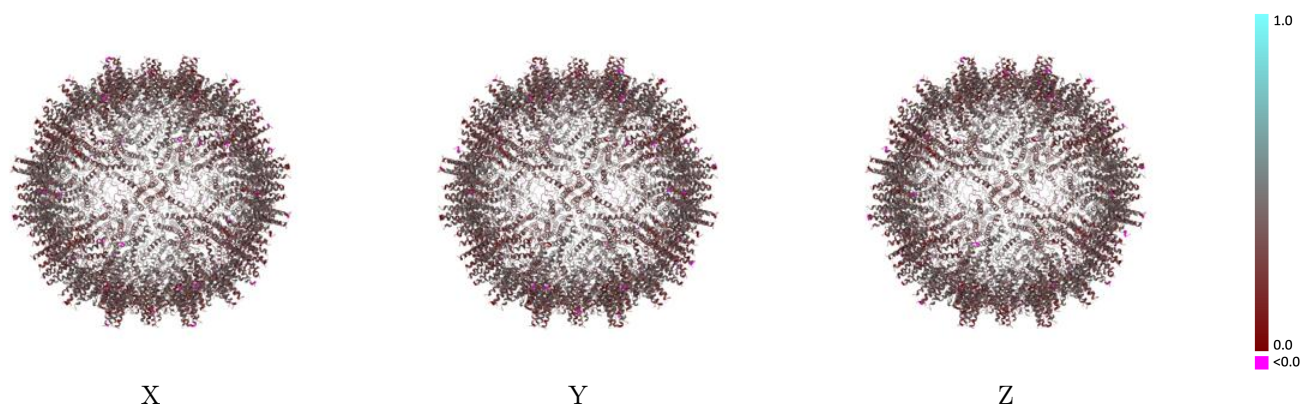
This section contains information regarding the fit between EMDB map EMD-16371 and PDB model 8C0O. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



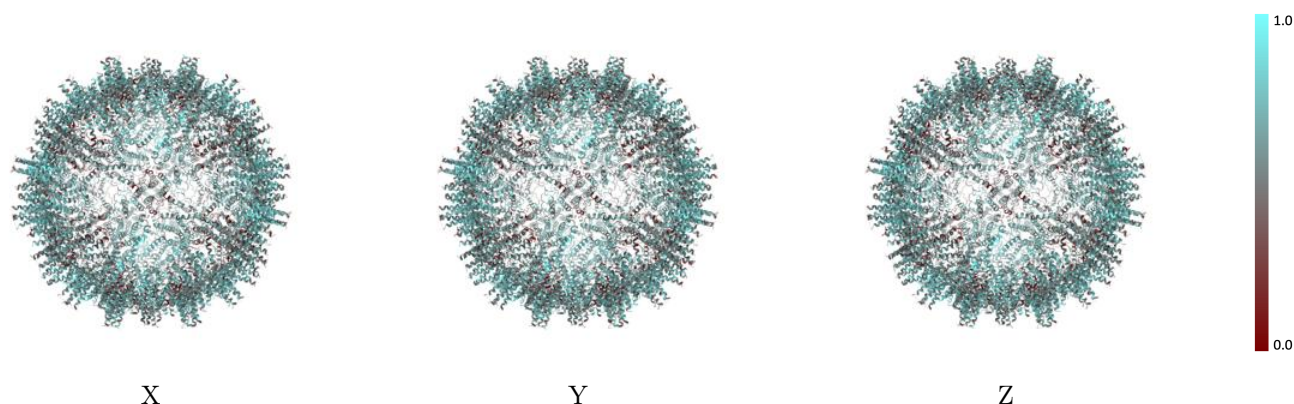
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



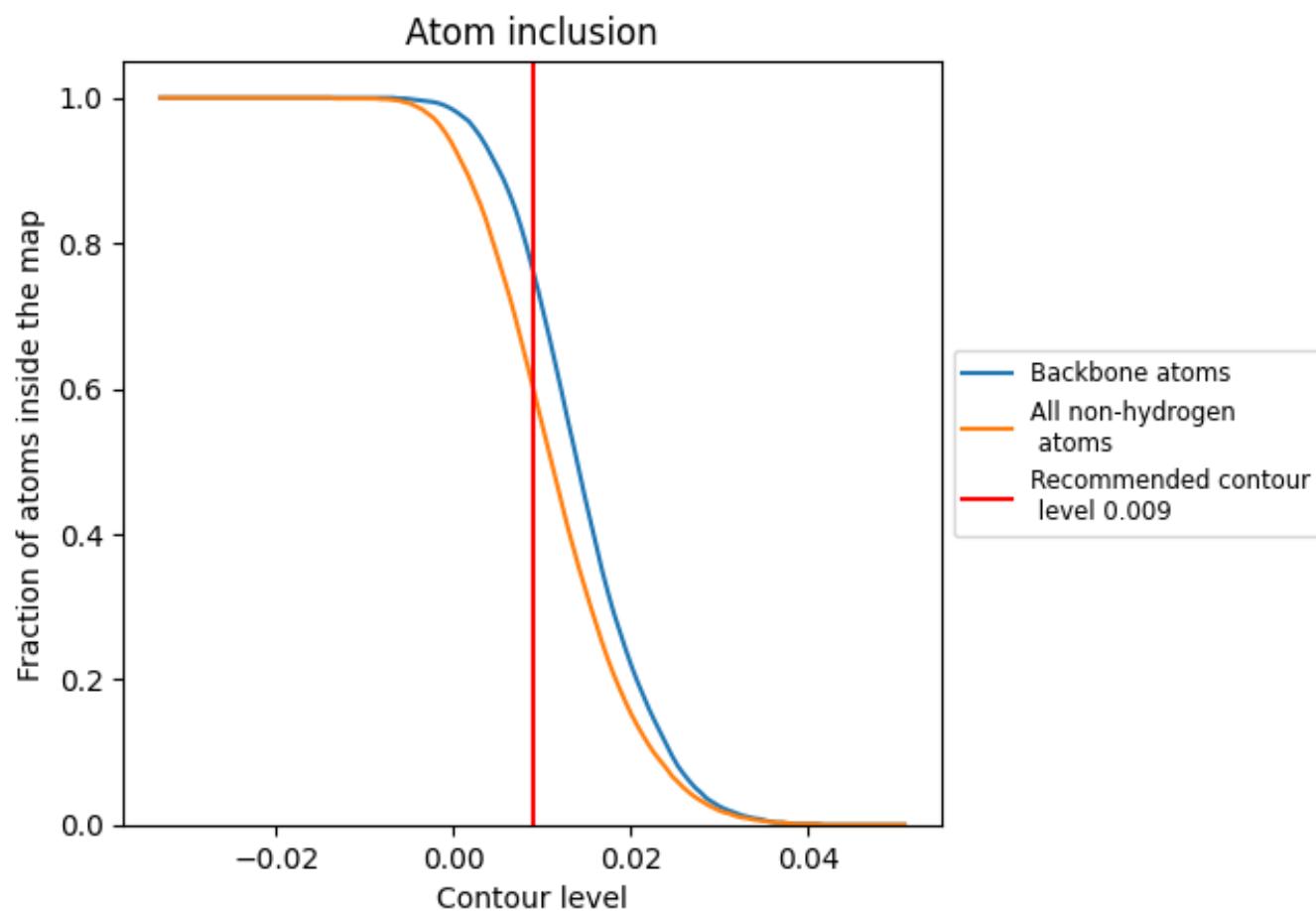
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 60% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6010	 0.3500
1A	 0.7070	 0.3930
1B	 0.6210	 0.3570
1C	 0.4850	 0.2980
2A	 0.7030	 0.3960
2B	 0.6130	 0.3580
2C	 0.4780	 0.3070
3A	 0.7060	 0.3990
3B	 0.6200	 0.3630
3C	 0.4820	 0.3140
4A	 0.7020	 0.3900
4B	 0.6140	 0.3550
4C	 0.4870	 0.2950
5A	 0.7040	 0.3930
5B	 0.6270	 0.3620
5C	 0.4770	 0.2970
6A	 0.7030	 0.3960
6B	 0.6200	 0.3560
6C	 0.4770	 0.2970
7A	 0.7050	 0.3940
7B	 0.6190	 0.3600
7C	 0.4780	 0.3050
8A	 0.6990	 0.3950
8B	 0.6060	 0.3510
8C	 0.4840	 0.3020
AA	 0.6940	 0.3870
AB	 0.6130	 0.3570
AC	 0.4720	 0.2910
BA	 0.6960	 0.3860
BB	 0.6150	 0.3540
BC	 0.4740	 0.2770
CA	 0.7080	 0.3990
CB	 0.6150	 0.3620
CC	 0.4860	 0.3100
DA	 0.7090	 0.3940



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Chain	Atom inclusion	Q-score
DB	 0.6180	 0.3590
DC	 0.4850	 0.3090
EA	 0.6960	 0.3900
EB	 0.6070	 0.3480
EC	 0.4860	 0.3060
FA	 0.7020	 0.3980
FB	 0.6270	 0.3590
FC	 0.4780	 0.2970
GA	 0.6960	 0.3890
GB	 0.6000	 0.3570
GC	 0.4950	 0.3130
HA	 0.6980	 0.3870
HB	 0.6110	 0.3500
HC	 0.4770	 0.3000
IA	 0.7090	 0.3930
IB	 0.6260	 0.3570
IC	 0.4730	 0.2970
JA	 0.7030	 0.3950
JB	 0.6150	 0.3620
JC	 0.4790	 0.3080
KA	 0.6990	 0.3950
KB	 0.6070	 0.3490
KC	 0.4840	 0.2970
LA	 0.7150	 0.3950
LB	 0.6180	 0.3580
LC	 0.4960	 0.3070
MA	 0.7110	 0.3890
MB	 0.6150	 0.3580
MC	 0.4770	 0.3010
NA	 0.7000	 0.3920
NB	 0.6030	 0.3540
NC	 0.4950	 0.3060
OA	 0.7080	 0.3960
OB	 0.6190	 0.3590
OC	 0.4860	 0.3060
PA	 0.6950	 0.3930
PB	 0.6030	 0.3580
PC	 0.4920	 0.3080
QA	 0.7030	 0.3910
QB	 0.6070	 0.3530
QC	 0.4850	 0.3080
RA	 0.6850	 0.3740

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Chain	Atom inclusion	Q-score
RB	 0.5920	 0.3250
RC	 0.4750	 0.2860
SA	 0.7080	 0.3970
SB	 0.6210	 0.3610
SC	 0.4850	 0.3120
TA	 0.6930	 0.3760
TB	 0.5900	 0.3300
TC	 0.4710	 0.2840
UA	 0.7020	 0.3920
UB	 0.6320	 0.3600
UC	 0.4850	 0.3050
VA	 0.7110	 0.4000
VB	 0.6190	 0.3650
VC	 0.4870	 0.3140
WA	 0.7040	 0.3910
WB	 0.6170	 0.3550
WC	 0.4700	 0.2820
XA	 0.7030	 0.3870
XB	 0.6300	 0.3580
XC	 0.4830	 0.2960
YA	 0.6980	 0.3930
YB	 0.6220	 0.3600
YC	 0.4850	 0.3100
ZA	 0.7070	 0.3880
ZB	 0.6210	 0.3580
ZC	 0.4820	 0.3070
aA	 0.7070	 0.3940
aB	 0.6190	 0.3590
aC	 0.4790	 0.3020
bA	 0.7080	 0.3990
bB	 0.6270	 0.3630
bC	 0.4780	 0.3020
cA	 0.6960	 0.3900
cB	 0.6020	 0.3550
cC	 0.4910	 0.2990
dA	 0.6880	 0.3870
dB	 0.5970	 0.3310
dC	 0.4830	 0.3000
eA	 0.7070	 0.3950
eB	 0.6230	 0.3610
eC	 0.4830	 0.3050
fA	 0.7120	 0.3990

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Chain	Atom inclusion	Q-score
fB	 0.6200	 0.3630
fC	 0.4840	 0.3110
gA	 0.7010	 0.3920
gB	 0.6030	 0.3460
gC	 0.4900	 0.2990
hA	 0.7040	 0.3960
hB	 0.6270	 0.3600
hC	 0.4850	 0.3030
iA	 0.6990	 0.3790
iB	 0.5890	 0.3270
iC	 0.4550	 0.2480
jA	 0.6980	 0.3880
jB	 0.6010	 0.3520
jC	 0.4900	 0.3040
kA	 0.7100	 0.3980
kB	 0.6270	 0.3590
kC	 0.4790	 0.3040
lA	 0.7060	 0.3930
lB	 0.6120	 0.3570
lC	 0.4900	 0.3100
mA	 0.6830	 0.3780
mB	 0.5990	 0.3400
mC	 0.4770	 0.2780
nA	 0.6980	 0.3930
nB	 0.6160	 0.3570
nC	 0.4890	 0.3050
oA	 0.7080	 0.3940
oB	 0.6160	 0.3550
oC	 0.4890	 0.3000
pA	 0.7030	 0.3920
pB	 0.6050	 0.3610
pC	 0.4900	 0.3090
qA	 0.7040	 0.3960
qB	 0.6200	 0.3570
qC	 0.4830	 0.3040
rA	 0.7050	 0.3870
rB	 0.6190	 0.3630
rC	 0.4810	 0.3040
sA	 0.7010	 0.3980
sB	 0.6110	 0.3630
sC	 0.4950	 0.3100
tA	 0.7060	 0.3890

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Chain	Atom inclusion	Q-score
tB	 0.6340	 0.3560
tC	 0.4800	 0.2920
uA	 0.7100	 0.3930
uB	 0.6190	 0.3580
uC	 0.4810	 0.2910
vA	 0.6980	 0.3900
vB	 0.6090	 0.3550
vC	 0.4780	 0.2920
wA	 0.7140	 0.3920
wB	 0.6280	 0.3600
wC	 0.4930	 0.3120
xA	 0.7080	 0.3980
xB	 0.6110	 0.3620
xC	 0.4820	 0.3100
yA	 0.7030	 0.3930
yB	 0.6200	 0.3610
yC	 0.4890	 0.3000
zA	 0.6980	 0.3920
zB	 0.6070	 0.3610
zC	 0.4820	 0.3020