



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:56 PM UTC

PDB ID : 8AAC / pdb\_00008aac  
EMDB ID : EMD-15295  
Title : African cichlid nakednavirus capsid at pH 7.5  
Authors : Pfister, S.; Rabl, J.; Boehringer, D.; Meier, B.H.  
Deposited on : 2022-07-01  
Resolution : 3.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

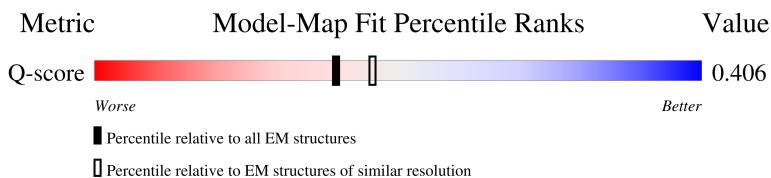
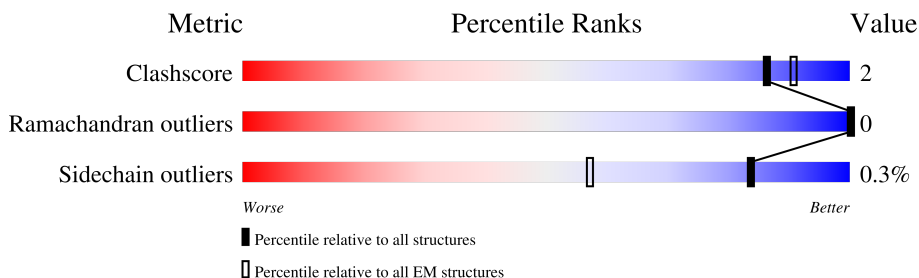
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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	11569 ( 3.20 - 4.20 )

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

Mol	Chain	Length	Quality of chain
1	1A	175	9% (red), 69% (green), 27% (grey), 5% (yellow)
1	1B	175	9% (red), 67% (green), 28% (grey), 5% (yellow)
1	1C	175	15% (red), 69% (green), 27% (grey), 5% (yellow)
1	2A	175	7% (red), 70% (green), 27% (grey), 5% (yellow)

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Mol	Chain	Length	Quality of chain		
1	2B	175	9%	68%	28%
1	2C	175	13%	68%	27%
1	3A	175	9%	69%	27%
1	3B	175	9%	68%	28%
1	3C	175	13%	67%	27%
1	4A	175	7%	69%	27%
1	4B	175	9%	67%	28%
1	4C	175	12%	68%	27%
1	5A	175	9%	69%	27%
1	5B	175	7%	67%	28%
1	5C	175	11%	67%	27%
1	6A	175	7%	69%	27%
1	6B	175	7%	68%	28%
1	6C	175	15%	68%	27%
1	7A	175	9%	69%	27%
1	7B	175	10%	67%	28%
1	7C	175	13%	69%	27%
1	8A	175	7%	69%	27%
1	8B	175	9%	68%	28%
1	8C	175	13%	68%	27%
1	AA	175	8%	69%	27%
1	AB	175	9%	67%	28%
1	AC	175	13%	68%	27%
1	BA	175	9%	69%	27%
1	BB	175	7%	68%	28%

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Mol	Chain	Length	Quality of chain			
1	BC	175	11%	68%	5%	27%
1	CA	175	7%	69%	•	27%
1	CB	175	9%	68%	•	28%
1	CC	175	16%	69%	•	27%
1	DA	175	9%	69%	•	27%
1	DB	175	9%	66%	6%	28%
1	DC	175	13%	69%	•	27%
1	EA	175	7%	69%	•	27%
1	EB	175	9%	68%	•	28%
1	EC	175	16%	67%	6%	27%
1	FA	175	7%	70%	•	27%
1	FB	175	9%	68%	•	28%
1	FC	175	13%	68%	5%	27%
1	GA	175	9%	69%	•	27%
1	GB	175	9%	67%	5%	28%
1	GC	175	13%	69%	•	27%
1	HA	175	8%	69%	•	27%
1	HB	175	7%	67%	5%	28%
1	HC	175	11%	68%	5%	27%
1	IA	175	8%	70%	•	27%
1	IB	175	9%	68%	•	28%
1	IC	175	15%	69%	•	27%
1	JA	175	9%	69%	•	27%
1	JB	175	10%	68%	•	28%
1	JC	175	14%	68%	5%	27%

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Mol	Chain	Length	Quality of chain		
1	KA	175	8%	70%	27%
1	KB	175	9%	67%	28%
1	KC	175	14%	68%	27%
1	LA	175	7%	69%	27%
1	LB	175	10%	68%	28%
1	LC	175	14%	69%	27%
1	MA	175	7%	69%	27%
1	MB	175	9%	67%	28%
1	MC	175	11%	68%	27%
1	NA	175	9%	69%	27%
1	NB	175	8%	67%	28%
1	NC	175	11%	67%	27%
1	OA	175	8%	69%	27%
1	OB	175	9%	68%	28%
1	OC	175	13%	68%	27%
1	PA	175	7%	69%	27%
1	PB	175	7%	68%	28%
1	PC	175	13%	69%	27%
1	QA	175	7%	69%	27%
1	QB	175	10%	68%	28%
1	QC	175	14%	69%	27%
1	RA	175	7%	70%	27%
1	RB	175	9%	68%	28%
1	RC	175	14%	68%	27%
1	SA	175	7%	69%	27%

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Mol	Chain	Length	Quality of chain		
1	SB	175	9%	68%	28%
1	SC	175	12%	67%	27%
1	TA	175	9%	69%	27%
1	TB	175	7%	68%	28%
1	TC	175	10%	69%	27%
1	UA	175	7%	69%	27%
1	UB	175	9%	68%	28%
1	UC	175	13%	68%	27%
1	VA	175	8%	69%	27%
1	VB	175	9%	67%	28%
1	VC	175	13%	69%	27%
1	WA	175	8%	70%	27%
1	WB	175	8%	68%	28%
1	WC	175	11%	69%	27%
1	XA	175	8%	69%	27%
1	XB	175	9%	68%	28%
1	XC	175	14%	68%	27%
1	YA	175	9%	69%	27%
1	YB	175	9%	67%	28%
1	YC	175	13%	69%	27%
1	ZA	175	8%	69%	27%
1	ZB	175	10%	68%	28%
1	ZC	175	12%	68%	27%
1	aA	175	8%	69%	27%
1	aB	175	7%	67%	28%

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Mol	Chain	Length	Quality of chain		
1	aC	175	11%	69%	27%
1	bA	175	8%	69%	27%
1	bB	175	9%	68%	28%
1	bC	175	14%	69%	27%
1	cA	175	7%	70%	27%
1	cB	175	10%	67%	28%
1	cC	175	14%	68%	27%
1	dA	175	7%	69%	27%
1	dB	175	9%	68%	28%
1	dC	175	13%	68%	27%
1	eA	175	8%	69%	27%
1	eB	175	9%	68%	28%
1	eC	175	13%	69%	27%
1	fA	175	9%	70%	27%
1	fB	175	9%	66%	28%
1	fC	175	15%	69%	27%
1	gA	175	7%	69%	27%
1	gB	175	9%	68%	28%
1	gC	175	13%	68%	27%
1	hA	175	8%	69%	27%
1	hB	175	9%	68%	28%
1	hC	175	11%	68%	27%
1	iA	175	9%	69%	27%
1	iB	175	8%	67%	28%
1	iC	175	14%	69%	27%

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Mol	Chain	Length	Quality of chain		
1	jA	175	8%	69%	27%
1	jB	175	9%	68%	28%
1	jC	175	14%	69%	27%
1	kA	175	7%	70%	27%
1	kB	175	9%	67%	28%
1	kC	175	14%	69%	27%
1	lA	175	7%	69%	27%
1	lB	175	10%	68%	28%
1	lC	175	13%	68%	27%
1	mA	175	9%	69%	27%
1	mB	175	7%	68%	28%
1	mC	175	10%	69%	27%
1	nA	175	8%	69%	27%
1	nB	175	9%	68%	28%
1	nC	175	14%	69%	27%
1	oA	175	7%	70%	27%
1	oB	175	8%	68%	28%
1	oC	175	15%	69%	27%
1	pA	175	9%	69%	27%
1	pB	175	9%	68%	28%
1	pC	175	14%	68%	27%
1	qA	175	7%	70%	27%
1	qB	175	9%	68%	28%
1	qC	175	13%	68%	27%
1	rA	175	9%	69%	27%

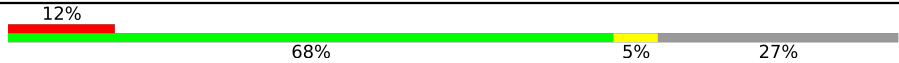
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Mol	Chain	Length	Quality of chain			
1	rB	175	10%	67%	5%	28%
1	rC	175	11%	68%	5%	27%
1	sA	175	9%	69%	•	27%
1	sB	175	7%	68%	•	28%
1	sC	175	13%	69%	•	27%
1	tA	175	7%	69%	•	27%
1	tB	175	10%	68%	•	28%
1	tC	175	14%	68%	5%	27%
1	uA	175	7%	69%	•	27%
1	uB	175	9%	67%	5%	28%
1	uC	175	13%	68%	5%	27%
1	vA	175	8%	69%	•	27%
1	vB	175	9%	67%	5%	28%
1	vC	175	14%	69%	•	27%
1	wA	175	8%	69%	•	27%
1	wB	175	8%	68%	•	28%
1	wC	175	11%	68%	5%	27%
1	xA	175	8%	70%	•	27%
1	xB	175	9%	68%	•	28%
1	xC	175	13%	69%	•	27%
1	yA	175	8%	69%	•	27%
1	yB	175	9%	67%	5%	28%
1	yC	175	13%	69%	•	27%
1	zA	175	8%	69%	•	27%
1	zB	175	9%	68%	•	28%

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Mol	Chain	Length	Quality of chain
1	zC	175	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '12%', a large green segment labeled '68%', a small yellow segment labeled '5%', and a grey segment on the right labeled '27%'.</p>

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 185940 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
			Total	C	N	O	S		
1	1A	127	1034	671	178	177	8	0	0
1	AC	127	1037	673	178	178	8	0	0
1	BA	127	1034	671	178	177	8	0	0
1	BB	126	1028	668	177	175	8	0	0
1	BC	127	1037	673	178	178	8	0	0
1	CA	127	1034	671	178	177	8	0	0
1	CB	126	1028	668	177	175	8	0	0
1	CC	127	1037	673	178	178	8	0	0
1	DA	127	1034	671	178	177	8	0	0
1	DB	126	1028	668	177	175	8	0	0
1	DC	127	1037	673	178	178	8	0	0
1	EA	127	1034	671	178	177	8	0	0
1	EB	126	1028	668	177	175	8	0	0
1	EC	127	1037	673	178	178	8	0	0
1	FA	127	1034	671	178	177	8	0	0
1	FB	126	1028	668	177	175	8	0	0
1	FC	127	1037	673	178	178	8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	GA	127	1034	671	178	177	8	0	0
1	GB	126	1028	668	177	175	8	0	0
1	GC	127	1037	673	178	178	8	0	0
1	HA	127	1034	671	178	177	8	0	0
1	HB	126	1028	668	177	175	8	0	0
1	HC	127	1037	673	178	178	8	0	0
1	IA	127	1034	671	178	177	8	0	0
1	IB	126	1028	668	177	175	8	0	0
1	IC	127	1037	673	178	178	8	0	0
1	JA	127	1034	671	178	177	8	0	0
1	1B	126	1028	668	177	175	8	0	0
1	JB	126	1028	668	177	175	8	0	0
1	JC	127	1037	673	178	178	8	0	0
1	KA	127	1034	671	178	177	8	0	0
1	KB	126	1028	668	177	175	8	0	0
1	KC	127	1037	673	178	178	8	0	0
1	LA	127	1034	671	178	177	8	0	0
1	LB	126	1028	668	177	175	8	0	0
1	LC	127	1037	673	178	178	8	0	0
1	MA	127	1034	671	178	177	8	0	0
1	MB	126	1028	668	177	175	8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	MC	127	1037	673	178	178	8	0	0
1	NA	127	1034	671	178	177	8	0	0
1	NB	126	1028	668	177	175	8	0	0
1	NC	127	1037	673	178	178	8	0	0
1	OA	127	1034	671	178	177	8	0	0
1	OB	126	1028	668	177	175	8	0	0
1	OC	127	1037	673	178	178	8	0	0
1	PA	127	1034	671	178	177	8	0	0
1	PB	126	1028	668	177	175	8	0	0
1	PC	127	1037	673	178	178	8	0	0
1	QA	127	1034	671	178	177	8	0	0
1	QB	126	1028	668	177	175	8	0	0
1	QC	127	1037	673	178	178	8	0	0
1	RA	127	1034	671	178	177	8	0	0
1	RB	126	1028	668	177	175	8	0	0
1	RC	127	1037	673	178	178	8	0	0
1	1C	127	1037	673	178	178	8	0	0
1	SA	127	1034	671	178	177	8	0	0
1	SB	126	1028	668	177	175	8	0	0
1	SC	127	1037	673	178	178	8	0	0
1	TA	127	1034	671	178	177	8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	TB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	TC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	UA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	UB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	UC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	VA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	VB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	VC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	WA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	WB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	WC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	XA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	XB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	XC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	YA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	YB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	YC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	ZA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	ZB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	ZC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	aA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	aB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	2A	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	aC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	bA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	bB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	bC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	cA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	cB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	cC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	dA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	dB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	dC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	eA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	eB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	eC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	fA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	fB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	fC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	gA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	gB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	gC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	hA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	hB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	hC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	iA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	iB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	iC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	jA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	2B	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	jB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	jC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	kA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	kB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	kC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	lA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	lB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	lC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	mA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	mB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	mC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	nA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	nB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	nC	127	Total 1037	C 673	N 178	O 178	S 8	0	0
1	oA	127	Total 1034	C 671	N 178	O 177	S 8	0	0
1	oB	126	Total 1028	C 668	N 177	O 175	S 8	0	0
1	oC	127	Total 1037	C 673	N 178	O 178	S 8	0	0
1	pA	127	Total 1034	C 671	N 178	O 177	S 8	0	0
1	pB	126	Total 1028	C 668	N 177	O 175	S 8	0	0
1	pC	127	Total 1037	C 673	N 178	O 178	S 8	0	0
1	qA	127	Total 1034	C 671	N 178	O 177	S 8	0	0
1	qB	126	Total 1028	C 668	N 177	O 175	S 8	0	0
1	qC	127	Total 1037	C 673	N 178	O 178	S 8	0	0
1	rA	127	Total 1034	C 671	N 178	O 177	S 8	0	0
1	rB	126	Total 1028	C 668	N 177	O 175	S 8	0	0
1	rC	127	Total 1037	C 673	N 178	O 178	S 8	0	0
1	2C	127	Total 1037	C 673	N 178	O 178	S 8	0	0
1	sA	127	Total 1034	C 671	N 178	O 177	S 8	0	0
1	sB	126	Total 1028	C 668	N 177	O 175	S 8	0	0
1	sC	127	Total 1037	C 673	N 178	O 178	S 8	0	0
1	tA	127	Total 1034	C 671	N 178	O 177	S 8	0	0
1	tB	126	Total 1028	C 668	N 177	O 175	S 8	0	0
1	tC	127	Total 1037	C 673	N 178	O 178	S 8	0	0
1	uA	127	Total 1034	C 671	N 178	O 177	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	uB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	uC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	vA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	vB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	vC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	wA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	wB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	wC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	xA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	xB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	xC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	yA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	yB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	yC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	zA	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	zB	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	zC	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	3A	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		
1	3B	126	Total	C	N	O	S	0	0
			1028	668	177	175	8		
1	3C	127	Total	C	N	O	S	0	0
			1037	673	178	178	8		
1	4A	127	Total	C	N	O	S	0	0
			1034	671	178	177	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	4B	126	1028	668	177	175	8	0	0
1	4C	127	1037	673	178	178	8	0	0
1	5A	127	1034	671	178	177	8	0	0
1	5B	126	1028	668	177	175	8	0	0
1	5C	127	1037	673	178	178	8	0	0
1	6A	127	1034	671	178	177	8	0	0
1	6B	126	1028	668	177	175	8	0	0
1	6C	127	1037	673	178	178	8	0	0
1	7A	127	1034	671	178	177	8	0	0
1	7B	126	1028	668	177	175	8	0	0
1	7C	127	1037	673	178	178	8	0	0
1	8A	127	1034	671	178	177	8	0	0
1	8B	126	1028	668	177	175	8	0	0
1	8C	127	1037	673	178	178	8	0	0
1	AA	127	1034	671	178	177	8	0	0
1	AB	126	1028	668	177	175	8	0	0

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
1A	0	GLY	-	expression tag	UNP A0A3S9H6T3
AC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
AC	0	GLY	-	expression tag	UNP A0A3S9H6T3
BA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
BA	0	GLY	-	expression tag	UNP A0A3S9H6T3
BB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3

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Chain	Residue	Modelled	Actual	Comment	Reference
BB	0	GLY	-	expression tag	UNP A0A3S9H6T3
BC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
BC	0	GLY	-	expression tag	UNP A0A3S9H6T3
CA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
CA	0	GLY	-	expression tag	UNP A0A3S9H6T3
CB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
CB	0	GLY	-	expression tag	UNP A0A3S9H6T3
CC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
CC	0	GLY	-	expression tag	UNP A0A3S9H6T3
DA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
DA	0	GLY	-	expression tag	UNP A0A3S9H6T3
DB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
DB	0	GLY	-	expression tag	UNP A0A3S9H6T3
DC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
DC	0	GLY	-	expression tag	UNP A0A3S9H6T3
EA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
EA	0	GLY	-	expression tag	UNP A0A3S9H6T3
EB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
EB	0	GLY	-	expression tag	UNP A0A3S9H6T3
EC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
EC	0	GLY	-	expression tag	UNP A0A3S9H6T3
FA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
FA	0	GLY	-	expression tag	UNP A0A3S9H6T3
FB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
FB	0	GLY	-	expression tag	UNP A0A3S9H6T3
FC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
FC	0	GLY	-	expression tag	UNP A0A3S9H6T3
GA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
GA	0	GLY	-	expression tag	UNP A0A3S9H6T3
GB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
GB	0	GLY	-	expression tag	UNP A0A3S9H6T3
GC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
GC	0	GLY	-	expression tag	UNP A0A3S9H6T3
HA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
HA	0	GLY	-	expression tag	UNP A0A3S9H6T3
HB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
HB	0	GLY	-	expression tag	UNP A0A3S9H6T3
HC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
HC	0	GLY	-	expression tag	UNP A0A3S9H6T3
IA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
IA	0	GLY	-	expression tag	UNP A0A3S9H6T3
IB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3

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Chain	Residue	Modelled	Actual	Comment	Reference
IB	0	GLY	-	expression tag	UNP A0A3S9H6T3
IC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
IC	0	GLY	-	expression tag	UNP A0A3S9H6T3
JA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
JA	0	GLY	-	expression tag	UNP A0A3S9H6T3
1B	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
1B	0	GLY	-	expression tag	UNP A0A3S9H6T3
JB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
JB	0	GLY	-	expression tag	UNP A0A3S9H6T3
JC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
JC	0	GLY	-	expression tag	UNP A0A3S9H6T3
KA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
KA	0	GLY	-	expression tag	UNP A0A3S9H6T3
KB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
KB	0	GLY	-	expression tag	UNP A0A3S9H6T3
KC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
KC	0	GLY	-	expression tag	UNP A0A3S9H6T3
LA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
LA	0	GLY	-	expression tag	UNP A0A3S9H6T3
LB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
LB	0	GLY	-	expression tag	UNP A0A3S9H6T3
LC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
LC	0	GLY	-	expression tag	UNP A0A3S9H6T3
MA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
MA	0	GLY	-	expression tag	UNP A0A3S9H6T3
MB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
MB	0	GLY	-	expression tag	UNP A0A3S9H6T3
MC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
MC	0	GLY	-	expression tag	UNP A0A3S9H6T3
NA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
NA	0	GLY	-	expression tag	UNP A0A3S9H6T3
NB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
NB	0	GLY	-	expression tag	UNP A0A3S9H6T3
NC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
NC	0	GLY	-	expression tag	UNP A0A3S9H6T3
OA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
OA	0	GLY	-	expression tag	UNP A0A3S9H6T3
OB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
OB	0	GLY	-	expression tag	UNP A0A3S9H6T3
OC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
OC	0	GLY	-	expression tag	UNP A0A3S9H6T3
PA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3

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Chain	Residue	Modelled	Actual	Comment	Reference
PA	0	GLY	-	expression tag	UNP A0A3S9H6T3
PB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
PB	0	GLY	-	expression tag	UNP A0A3S9H6T3
PC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
PC	0	GLY	-	expression tag	UNP A0A3S9H6T3
QA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
QA	0	GLY	-	expression tag	UNP A0A3S9H6T3
QB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
QB	0	GLY	-	expression tag	UNP A0A3S9H6T3
QC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
QC	0	GLY	-	expression tag	UNP A0A3S9H6T3
RA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
RA	0	GLY	-	expression tag	UNP A0A3S9H6T3
RB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
RB	0	GLY	-	expression tag	UNP A0A3S9H6T3
RC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
RC	0	GLY	-	expression tag	UNP A0A3S9H6T3
1C	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
1C	0	GLY	-	expression tag	UNP A0A3S9H6T3
SA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
SA	0	GLY	-	expression tag	UNP A0A3S9H6T3
SB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
SB	0	GLY	-	expression tag	UNP A0A3S9H6T3
SC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
SC	0	GLY	-	expression tag	UNP A0A3S9H6T3
TA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
TA	0	GLY	-	expression tag	UNP A0A3S9H6T3
TB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
TB	0	GLY	-	expression tag	UNP A0A3S9H6T3
TC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
TC	0	GLY	-	expression tag	UNP A0A3S9H6T3
UA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
UA	0	GLY	-	expression tag	UNP A0A3S9H6T3
UB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
UB	0	GLY	-	expression tag	UNP A0A3S9H6T3
UC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
UC	0	GLY	-	expression tag	UNP A0A3S9H6T3
VA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
VA	0	GLY	-	expression tag	UNP A0A3S9H6T3
VB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
VB	0	GLY	-	expression tag	UNP A0A3S9H6T3
VC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3

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Chain	Residue	Modelled	Actual	Comment	Reference
VC	0	GLY	-	expression tag	UNP A0A3S9H6T3
WA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
WA	0	GLY	-	expression tag	UNP A0A3S9H6T3
WB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
WB	0	GLY	-	expression tag	UNP A0A3S9H6T3
WC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
WC	0	GLY	-	expression tag	UNP A0A3S9H6T3
XA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
XA	0	GLY	-	expression tag	UNP A0A3S9H6T3
XB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
XB	0	GLY	-	expression tag	UNP A0A3S9H6T3
XC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
XC	0	GLY	-	expression tag	UNP A0A3S9H6T3
YA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
YA	0	GLY	-	expression tag	UNP A0A3S9H6T3
YB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
YB	0	GLY	-	expression tag	UNP A0A3S9H6T3
YC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
YC	0	GLY	-	expression tag	UNP A0A3S9H6T3
ZA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
ZA	0	GLY	-	expression tag	UNP A0A3S9H6T3
ZB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
ZB	0	GLY	-	expression tag	UNP A0A3S9H6T3
ZC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
ZC	0	GLY	-	expression tag	UNP A0A3S9H6T3
aA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
aA	0	GLY	-	expression tag	UNP A0A3S9H6T3
aB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
aB	0	GLY	-	expression tag	UNP A0A3S9H6T3
2A	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
2A	0	GLY	-	expression tag	UNP A0A3S9H6T3
aC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
aC	0	GLY	-	expression tag	UNP A0A3S9H6T3
bA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
bA	0	GLY	-	expression tag	UNP A0A3S9H6T3
bB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
bB	0	GLY	-	expression tag	UNP A0A3S9H6T3
bC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
bC	0	GLY	-	expression tag	UNP A0A3S9H6T3
cA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
cA	0	GLY	-	expression tag	UNP A0A3S9H6T3
cB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3

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Chain	Residue	Modelled	Actual	Comment	Reference
cB	0	GLY	-	expression tag	UNP A0A3S9H6T3
cC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
cC	0	GLY	-	expression tag	UNP A0A3S9H6T3
dA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
dA	0	GLY	-	expression tag	UNP A0A3S9H6T3
dB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
dB	0	GLY	-	expression tag	UNP A0A3S9H6T3
dC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
dC	0	GLY	-	expression tag	UNP A0A3S9H6T3
eA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
eA	0	GLY	-	expression tag	UNP A0A3S9H6T3
eB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
eB	0	GLY	-	expression tag	UNP A0A3S9H6T3
eC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
eC	0	GLY	-	expression tag	UNP A0A3S9H6T3
fA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
fA	0	GLY	-	expression tag	UNP A0A3S9H6T3
fB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
fB	0	GLY	-	expression tag	UNP A0A3S9H6T3
fC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
fC	0	GLY	-	expression tag	UNP A0A3S9H6T3
gA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
gA	0	GLY	-	expression tag	UNP A0A3S9H6T3
gB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
gB	0	GLY	-	expression tag	UNP A0A3S9H6T3
gC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
gC	0	GLY	-	expression tag	UNP A0A3S9H6T3
hA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
hA	0	GLY	-	expression tag	UNP A0A3S9H6T3
hB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
hB	0	GLY	-	expression tag	UNP A0A3S9H6T3
hC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
hC	0	GLY	-	expression tag	UNP A0A3S9H6T3
iA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
iA	0	GLY	-	expression tag	UNP A0A3S9H6T3
iB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
iB	0	GLY	-	expression tag	UNP A0A3S9H6T3
iC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
iC	0	GLY	-	expression tag	UNP A0A3S9H6T3
jA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
jA	0	GLY	-	expression tag	UNP A0A3S9H6T3
2B	-1	MET	-	initiating methionine	UNP A0A3S9H6T3

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Chain	Residue	Modelled	Actual	Comment	Reference
2B	0	GLY	-	expression tag	UNP A0A3S9H6T3
jB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
jB	0	GLY	-	expression tag	UNP A0A3S9H6T3
jC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
jC	0	GLY	-	expression tag	UNP A0A3S9H6T3
kA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
kA	0	GLY	-	expression tag	UNP A0A3S9H6T3
kB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
kB	0	GLY	-	expression tag	UNP A0A3S9H6T3
kC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
kC	0	GLY	-	expression tag	UNP A0A3S9H6T3
lA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
lA	0	GLY	-	expression tag	UNP A0A3S9H6T3
lB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
lB	0	GLY	-	expression tag	UNP A0A3S9H6T3
lC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
lC	0	GLY	-	expression tag	UNP A0A3S9H6T3
mA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
mA	0	GLY	-	expression tag	UNP A0A3S9H6T3
mB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
mB	0	GLY	-	expression tag	UNP A0A3S9H6T3
mC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
mC	0	GLY	-	expression tag	UNP A0A3S9H6T3
nA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
nA	0	GLY	-	expression tag	UNP A0A3S9H6T3
nB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
nB	0	GLY	-	expression tag	UNP A0A3S9H6T3
nC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
nC	0	GLY	-	expression tag	UNP A0A3S9H6T3
oA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
oA	0	GLY	-	expression tag	UNP A0A3S9H6T3
oB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
oB	0	GLY	-	expression tag	UNP A0A3S9H6T3
oC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
oC	0	GLY	-	expression tag	UNP A0A3S9H6T3
pA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
pA	0	GLY	-	expression tag	UNP A0A3S9H6T3
pB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
pB	0	GLY	-	expression tag	UNP A0A3S9H6T3
pC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
pC	0	GLY	-	expression tag	UNP A0A3S9H6T3
qA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3

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Chain	Residue	Modelled	Actual	Comment	Reference
qA	0	GLY	-	expression tag	UNP A0A3S9H6T3
qB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
qB	0	GLY	-	expression tag	UNP A0A3S9H6T3
qC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
qC	0	GLY	-	expression tag	UNP A0A3S9H6T3
rA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
rA	0	GLY	-	expression tag	UNP A0A3S9H6T3
rB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
rB	0	GLY	-	expression tag	UNP A0A3S9H6T3
rC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
rC	0	GLY	-	expression tag	UNP A0A3S9H6T3
2C	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
2C	0	GLY	-	expression tag	UNP A0A3S9H6T3
sA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
sA	0	GLY	-	expression tag	UNP A0A3S9H6T3
sB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
sB	0	GLY	-	expression tag	UNP A0A3S9H6T3
sC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
sC	0	GLY	-	expression tag	UNP A0A3S9H6T3
tA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
tA	0	GLY	-	expression tag	UNP A0A3S9H6T3
tB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
tB	0	GLY	-	expression tag	UNP A0A3S9H6T3
tC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
tC	0	GLY	-	expression tag	UNP A0A3S9H6T3
uA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
uA	0	GLY	-	expression tag	UNP A0A3S9H6T3
uB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
uB	0	GLY	-	expression tag	UNP A0A3S9H6T3
uC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
uC	0	GLY	-	expression tag	UNP A0A3S9H6T3
vA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
vA	0	GLY	-	expression tag	UNP A0A3S9H6T3
vB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
vB	0	GLY	-	expression tag	UNP A0A3S9H6T3
vC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
vC	0	GLY	-	expression tag	UNP A0A3S9H6T3
wA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
wA	0	GLY	-	expression tag	UNP A0A3S9H6T3
wB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
wB	0	GLY	-	expression tag	UNP A0A3S9H6T3
wC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3

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Chain	Residue	Modelled	Actual	Comment	Reference
wC	0	GLY	-	expression tag	UNP A0A3S9H6T3
xA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
xA	0	GLY	-	expression tag	UNP A0A3S9H6T3
xB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
xB	0	GLY	-	expression tag	UNP A0A3S9H6T3
xC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
xC	0	GLY	-	expression tag	UNP A0A3S9H6T3
yA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
yA	0	GLY	-	expression tag	UNP A0A3S9H6T3
yB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
yB	0	GLY	-	expression tag	UNP A0A3S9H6T3
yC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
yC	0	GLY	-	expression tag	UNP A0A3S9H6T3
zA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
zA	0	GLY	-	expression tag	UNP A0A3S9H6T3
zB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
zB	0	GLY	-	expression tag	UNP A0A3S9H6T3
zC	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
zC	0	GLY	-	expression tag	UNP A0A3S9H6T3
3A	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
3A	0	GLY	-	expression tag	UNP A0A3S9H6T3
3B	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
3B	0	GLY	-	expression tag	UNP A0A3S9H6T3
3C	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
3C	0	GLY	-	expression tag	UNP A0A3S9H6T3
4A	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
4A	0	GLY	-	expression tag	UNP A0A3S9H6T3
4B	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
4B	0	GLY	-	expression tag	UNP A0A3S9H6T3
4C	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
4C	0	GLY	-	expression tag	UNP A0A3S9H6T3
5A	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
5A	0	GLY	-	expression tag	UNP A0A3S9H6T3
5B	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
5B	0	GLY	-	expression tag	UNP A0A3S9H6T3
5C	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
5C	0	GLY	-	expression tag	UNP A0A3S9H6T3
6A	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
6A	0	GLY	-	expression tag	UNP A0A3S9H6T3
6B	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
6B	0	GLY	-	expression tag	UNP A0A3S9H6T3
6C	-1	MET	-	initiating methionine	UNP A0A3S9H6T3

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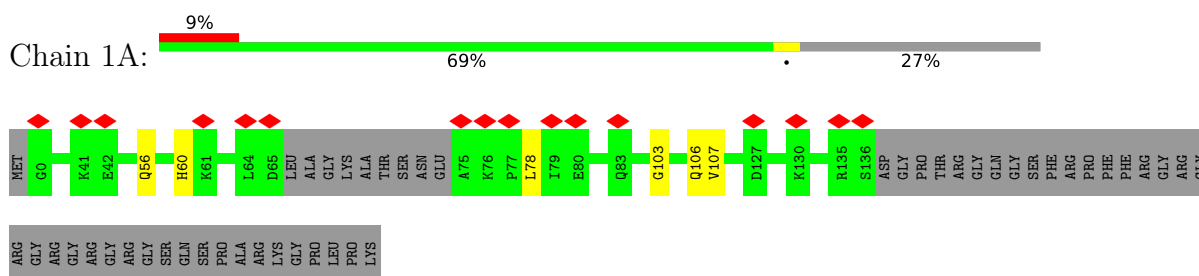
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Chain	Residue	Modelled	Actual	Comment	Reference
6C	0	GLY	-	expression tag	UNP A0A3S9H6T3
7A	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
7A	0	GLY	-	expression tag	UNP A0A3S9H6T3
7B	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
7B	0	GLY	-	expression tag	UNP A0A3S9H6T3
7C	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
7C	0	GLY	-	expression tag	UNP A0A3S9H6T3
8A	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
8A	0	GLY	-	expression tag	UNP A0A3S9H6T3
8B	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
8B	0	GLY	-	expression tag	UNP A0A3S9H6T3
8C	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
8C	0	GLY	-	expression tag	UNP A0A3S9H6T3
AA	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
AA	0	GLY	-	expression tag	UNP A0A3S9H6T3
AB	-1	MET	-	initiating methionine	UNP A0A3S9H6T3
AB	0	GLY	-	expression tag	UNP A0A3S9H6T3

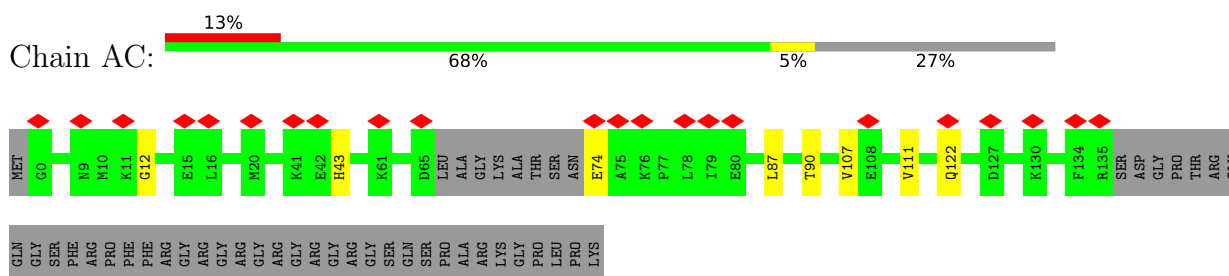
### 3 Residue-property plots [i](#)

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.

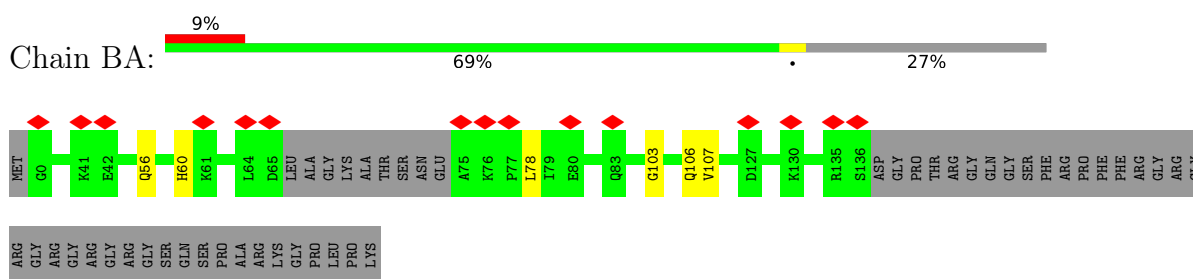
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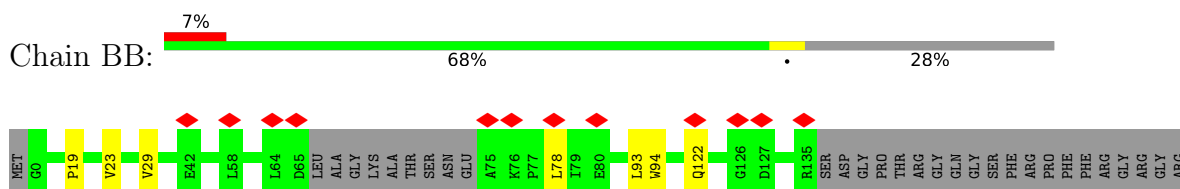
- Molecule 1: C protein



- Molecule 1: C protein

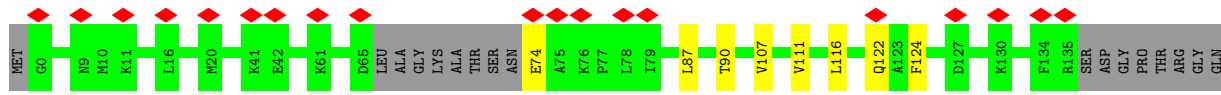


- Molecule 1: C protein



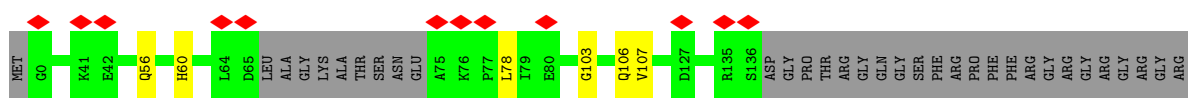
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PRO  
PRO  
LYS

• Molecule 1: C protein



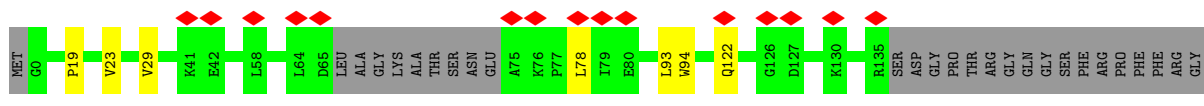
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ALA  
ARG  
LYS  
THR  
SER  
GLY  
PRO  
LEU  
LYS

• Molecule 1: C protein



GLY  
ARG  
GLY  
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PRO  
LYS

• Molecule 1: C protein



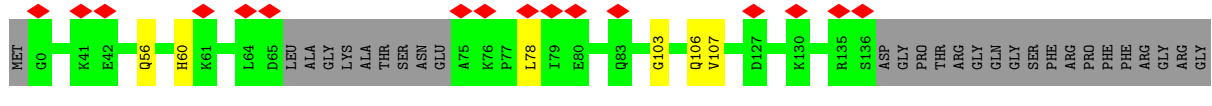
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PRO  
LEU  
LYS

• Molecule 1: C protein



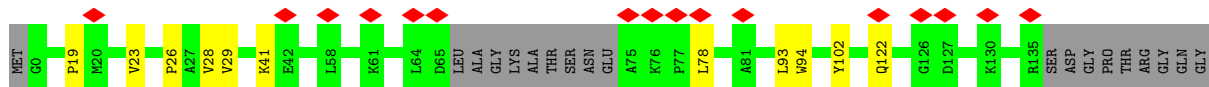
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• Molecule 1: C protein



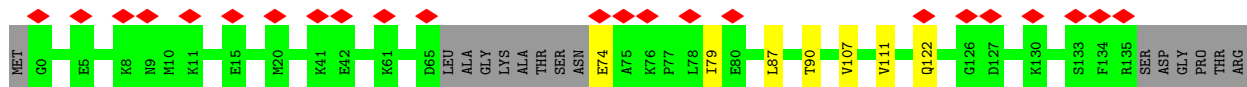
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LYS

• Molecule 1: C protein



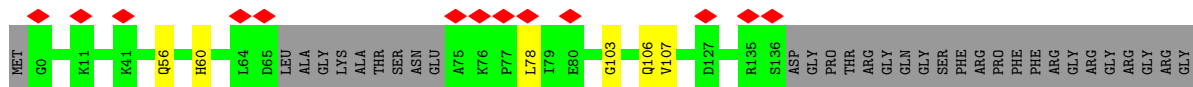
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GLN  
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LYS

• Molecule 1: C protein



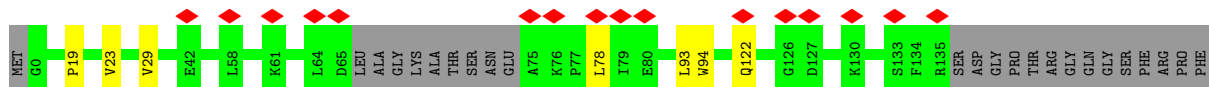
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LYS

• Molecule 1: C protein



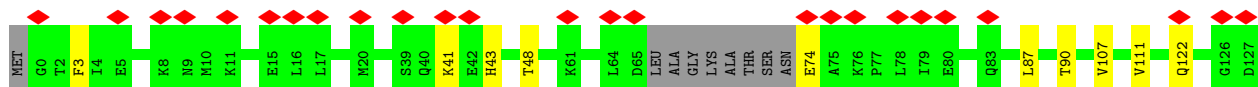
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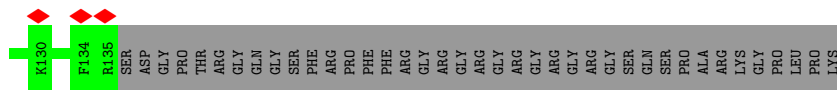
• Molecule 1: C protein



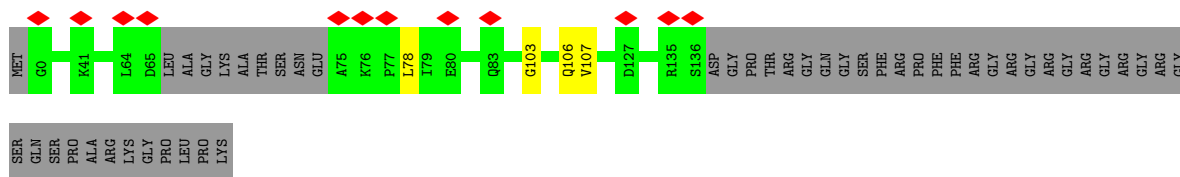
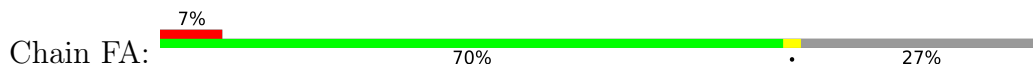
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• Molecule 1: C protein

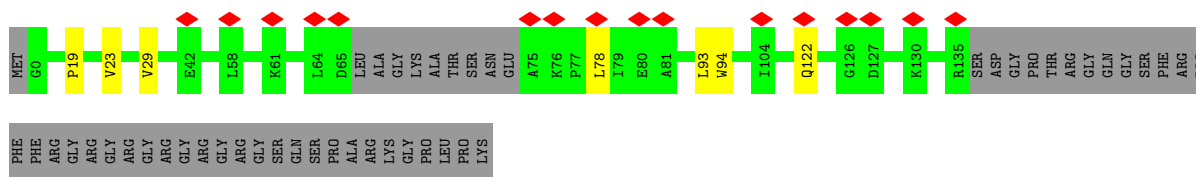




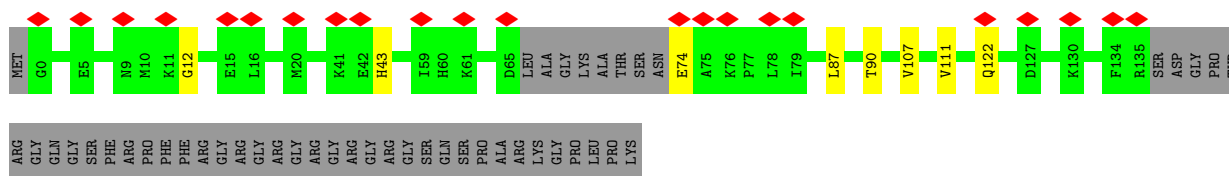
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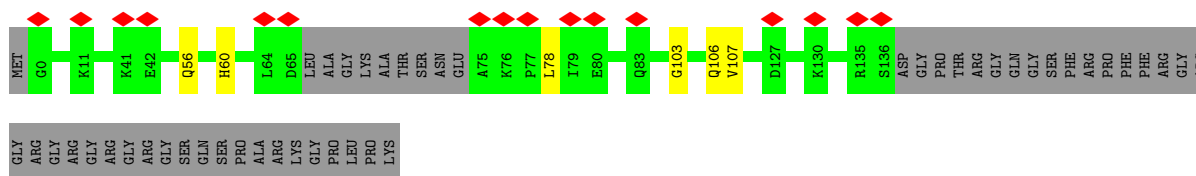
• Molecule 1: C protein



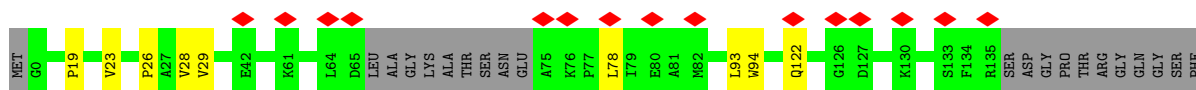
• Molecule 1: C protein



• Molecule 1: C protein



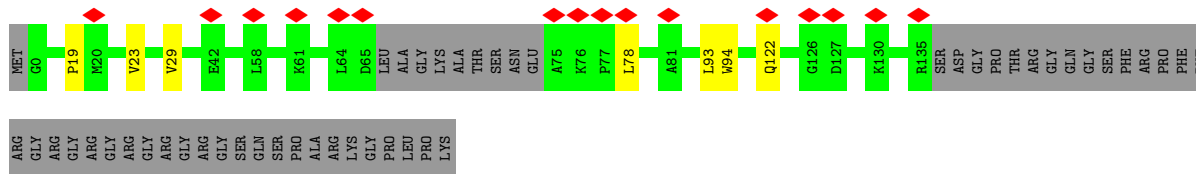
• Molecule 1: C protein





GLY  
SER  
GLN  
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PRO  
LYS

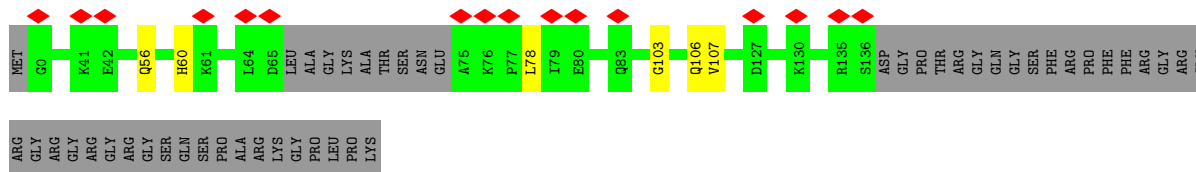
• Molecule 1: C protein



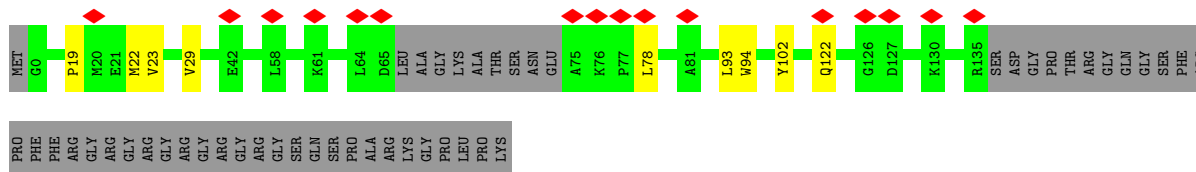
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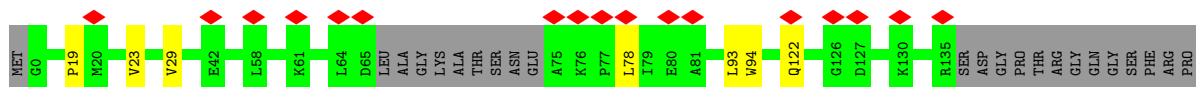
• Molecule 1: C protein



• Molecule 1: C protein



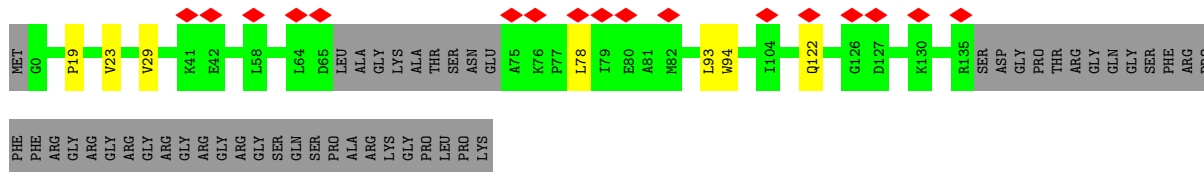
• Molecule 1: C protein



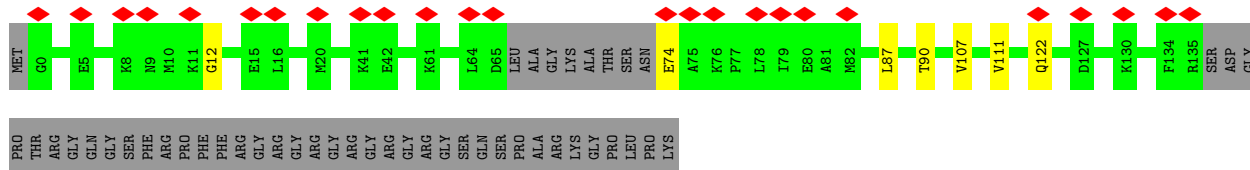


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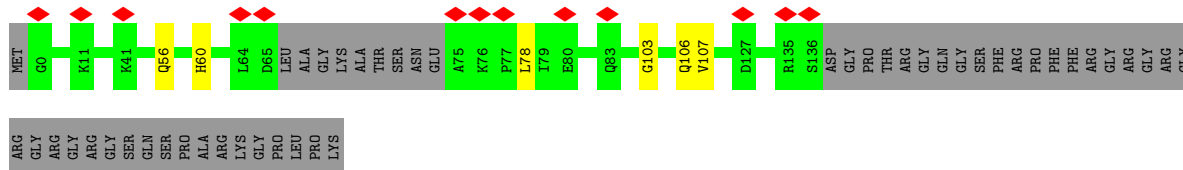
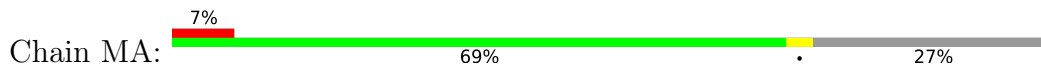
• Molecule 1: C protein



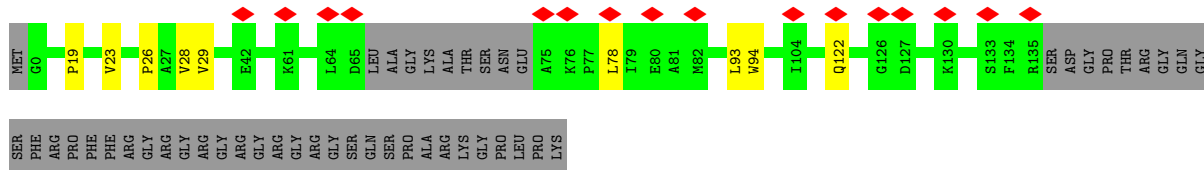
• Molecule 1: C protein



• Molecule 1: C protein



• Molecule 1: C protein

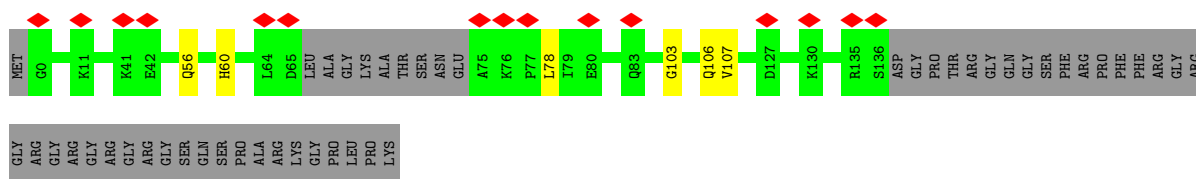
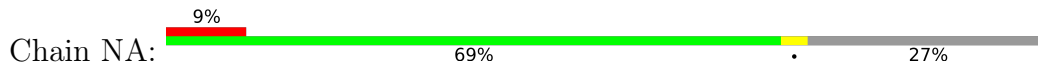


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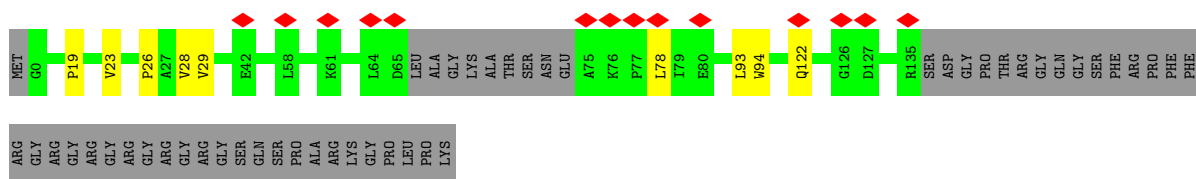


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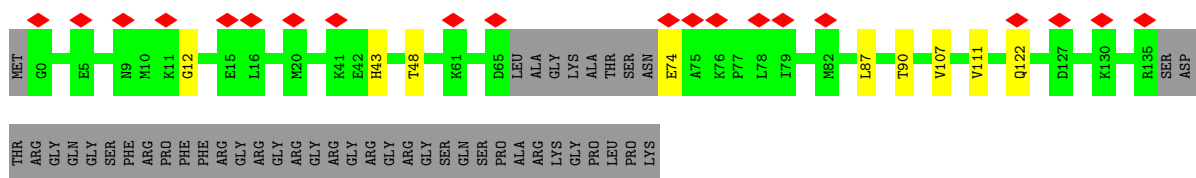
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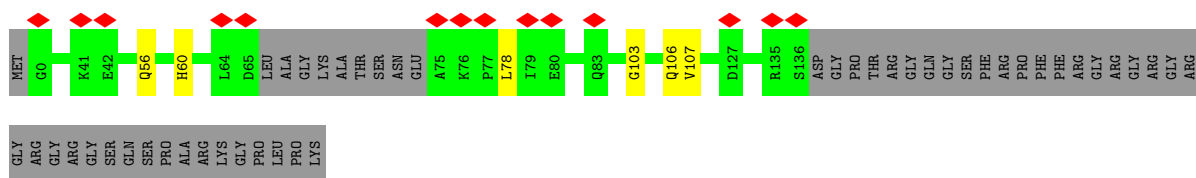
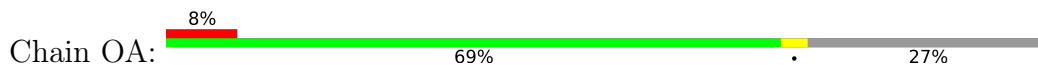
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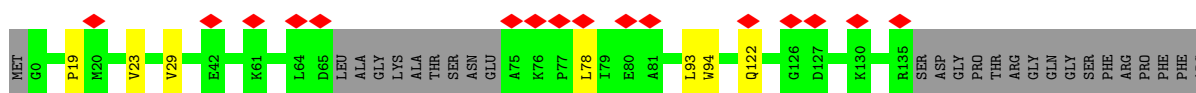
• Molecule 1: C protein



• Molecule 1: C protein



• Molecule 1: C protein



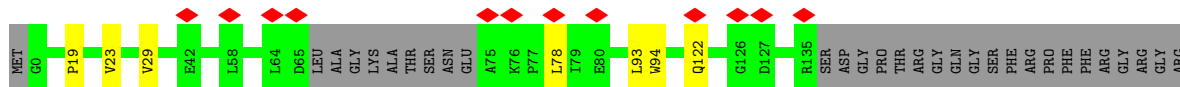






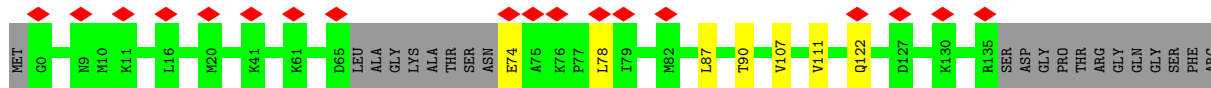
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• Molecule 1: C protein



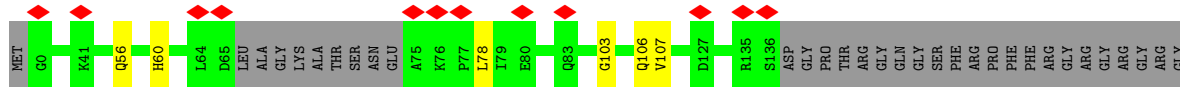
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• Molecule 1: C protein



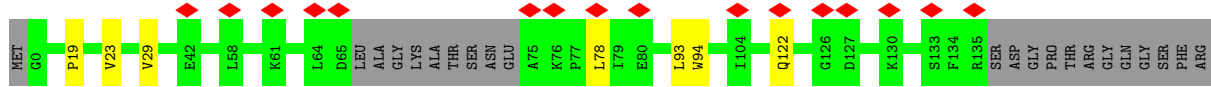
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• Molecule 1: C protein



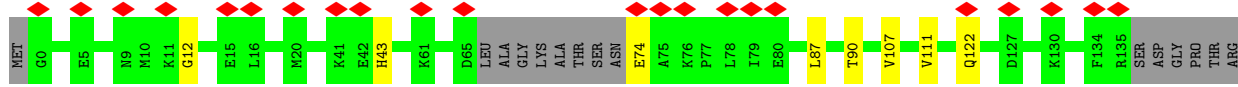
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• Molecule 1: C protein



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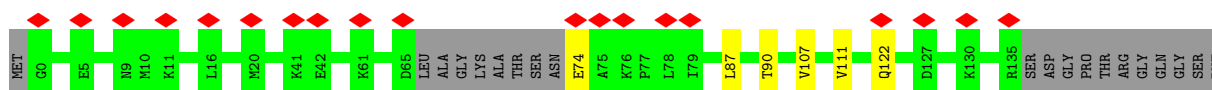
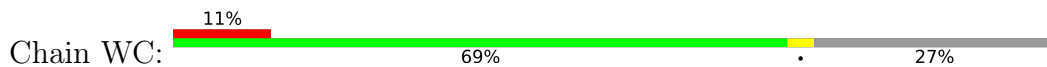
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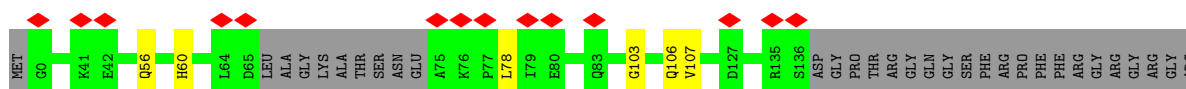
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• Molecule 1: C protein



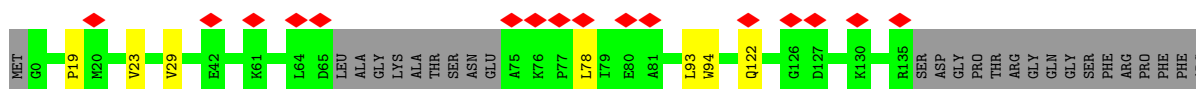
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• Molecule 1: C protein



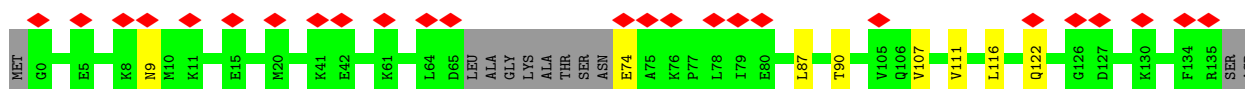
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• Molecule 1: C protein



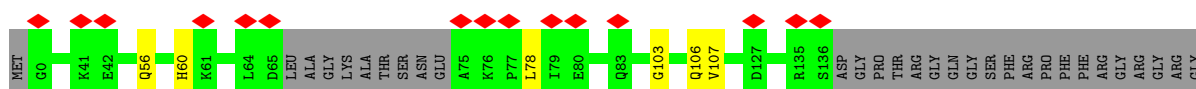
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• Molecule 1: C protein



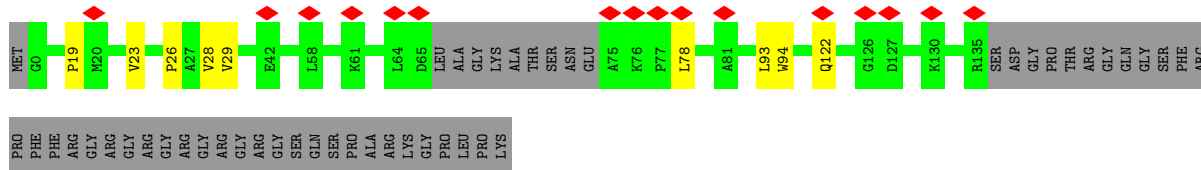
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• Molecule 1: C protein

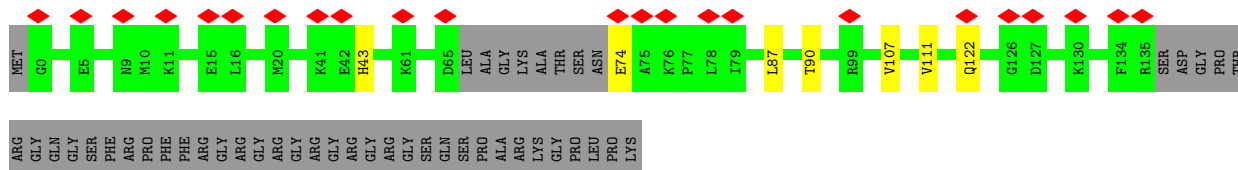


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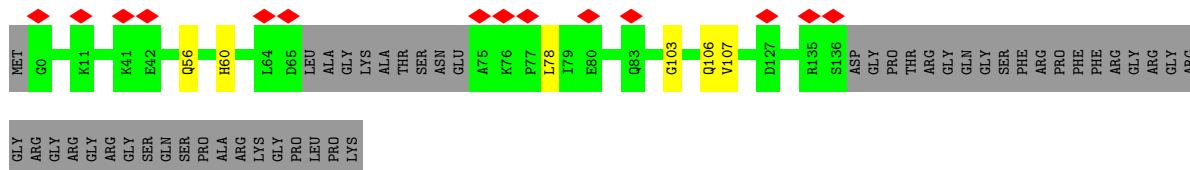
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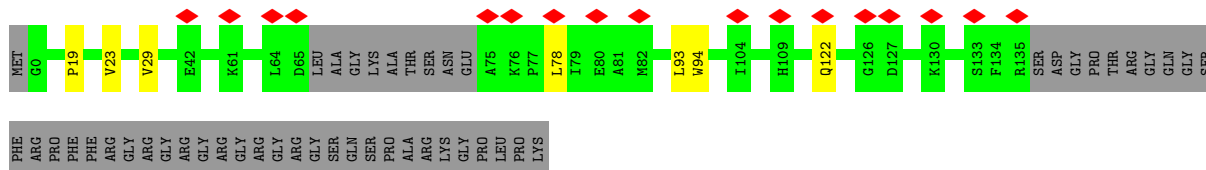
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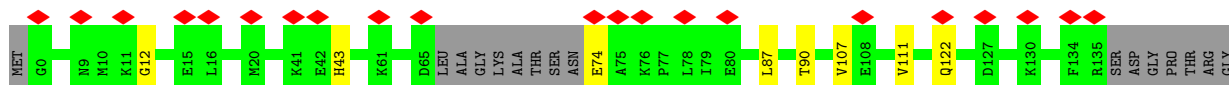
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• Molecule 1: C protein



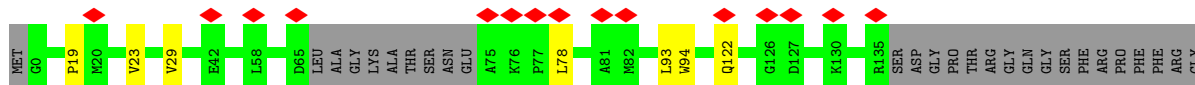
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• Molecule 1: C protein



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• Molecule 1: C protein



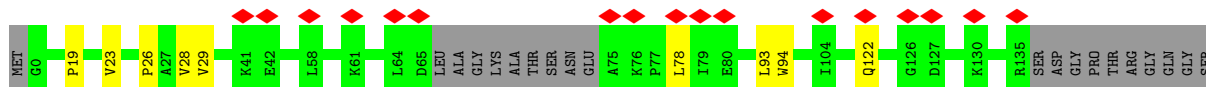
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• Molecule 1: C protein



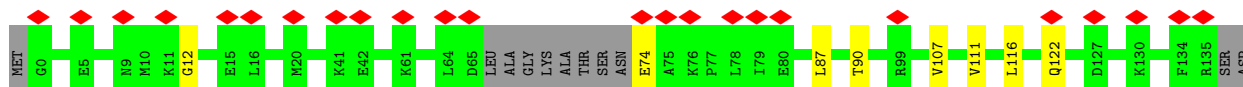
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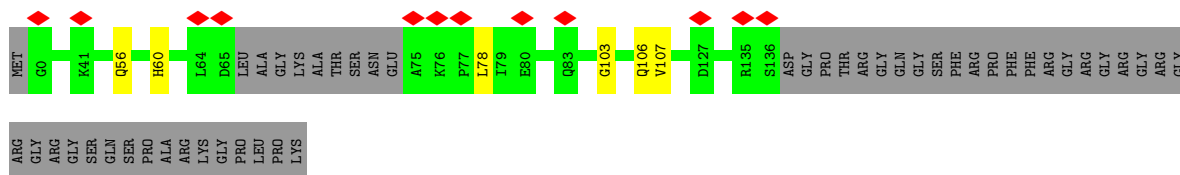
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• Molecule 1: C protein

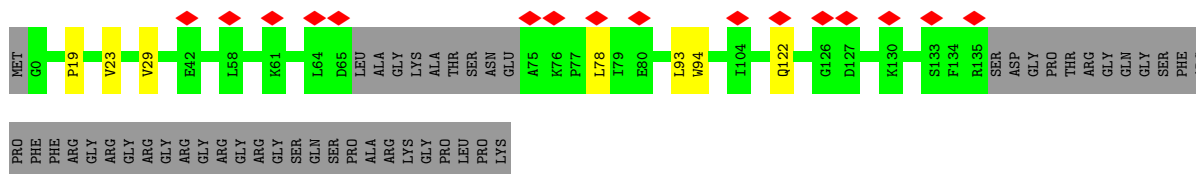


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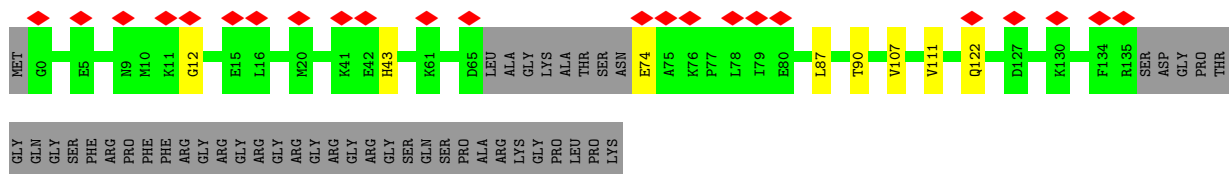
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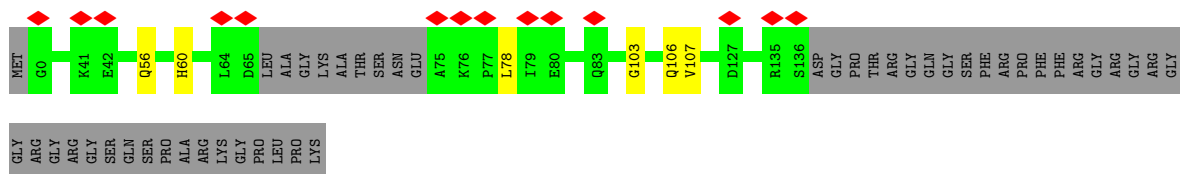
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• Molecule 1: C protein



• Molecule 1: C protein



• Molecule 1: C protein



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• Molecule 1: C protein



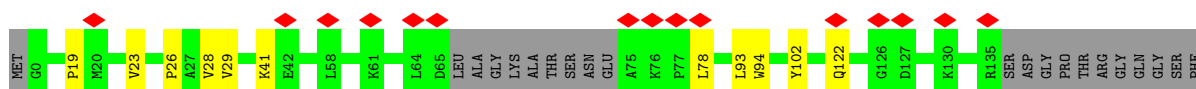
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• Molecule 1: C protein



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• Molecule 1: C protein



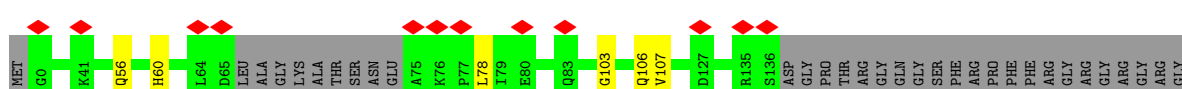
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• Molecule 1: C protein



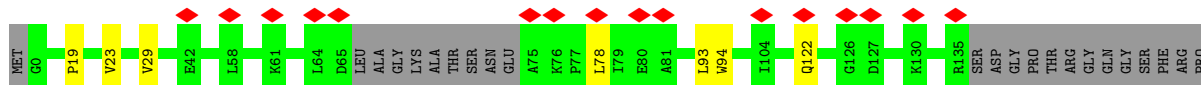
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• Molecule 1: C protein



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• Molecule 1: C protein



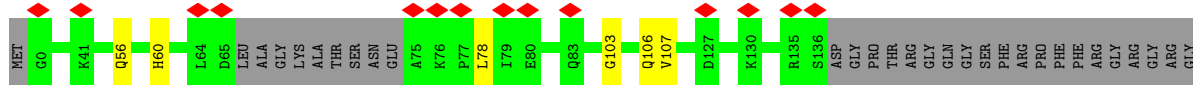
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• Molecule 1: C protein



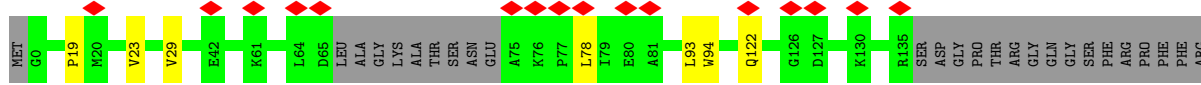
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• Molecule 1: C protein



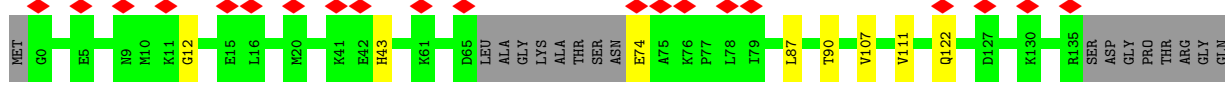
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• Molecule 1: C protein



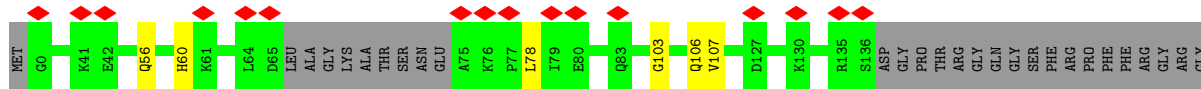
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• Molecule 1: C protein



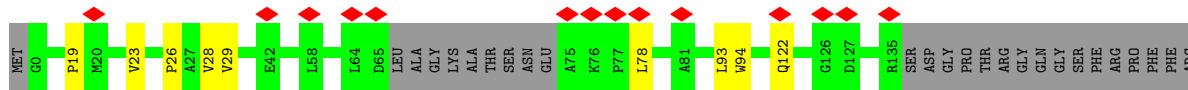
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• Molecule 1: C protein



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• Molecule 1: C protein



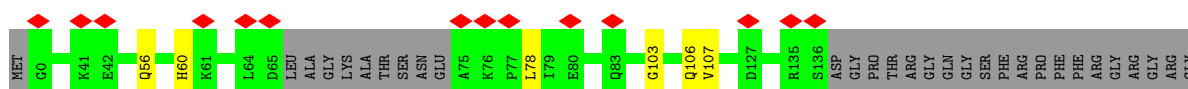
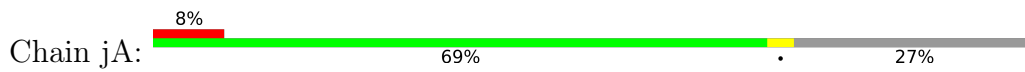
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• Molecule 1: C protein



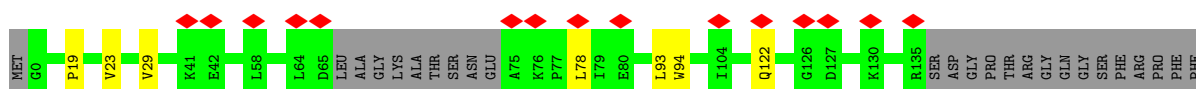
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• Molecule 1: C protein



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• Molecule 1: C protein

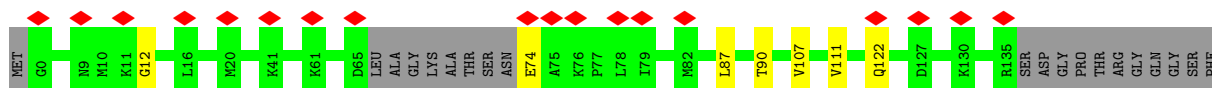






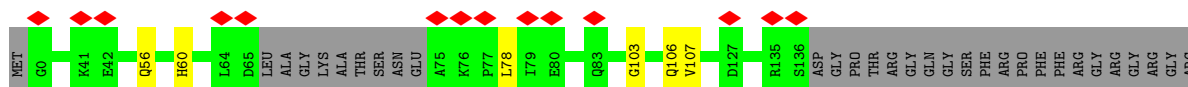
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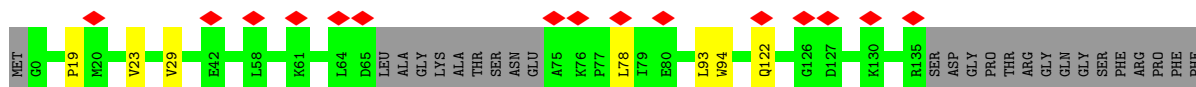
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• Molecule 1: C protein



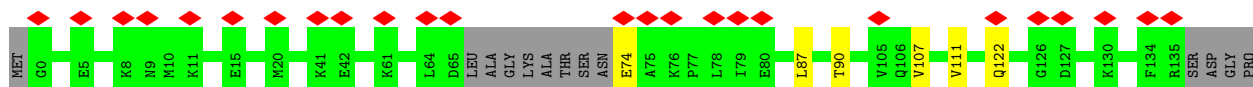
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GLY  
LYS  
PRO  
LEU  
PRO  
LYS

• Molecule 1: C protein



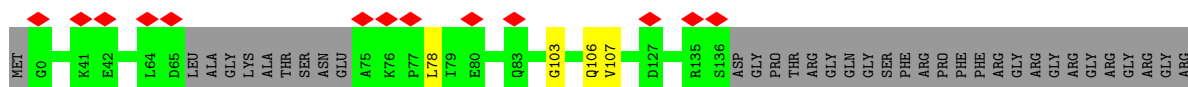
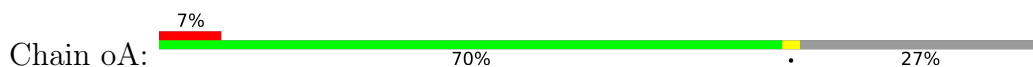
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PRO  
LEU  
PRO  
LYS

• Molecule 1: C protein



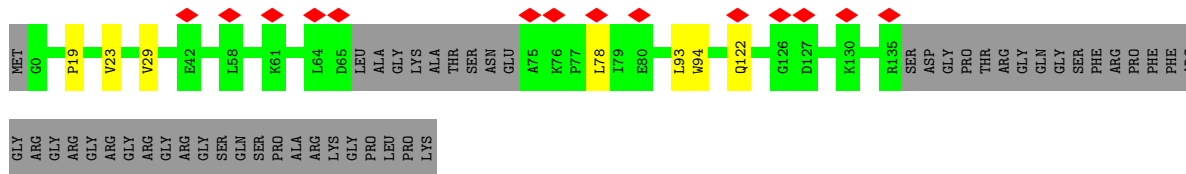
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LYS  
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LYS  
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ARG  
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GLY  
LEU  
PRO  
LYS

• Molecule 1: C protein

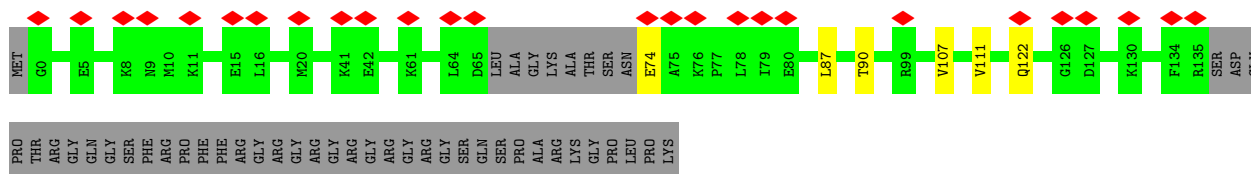


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ALA  
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PRO  
LYS

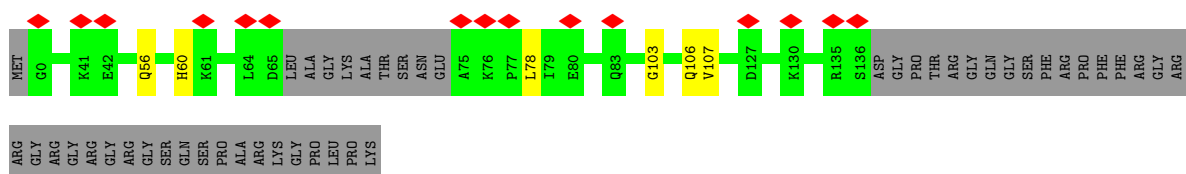
• Molecule 1: C protein



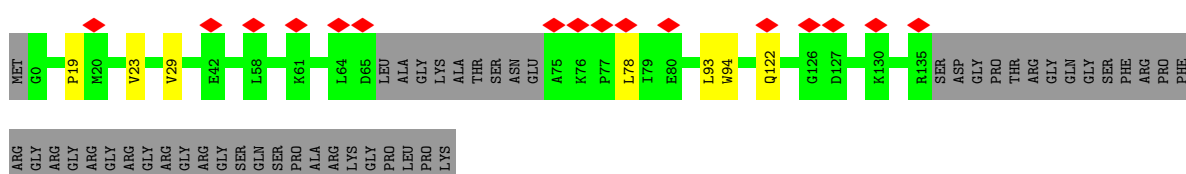
• Molecule 1: C protein



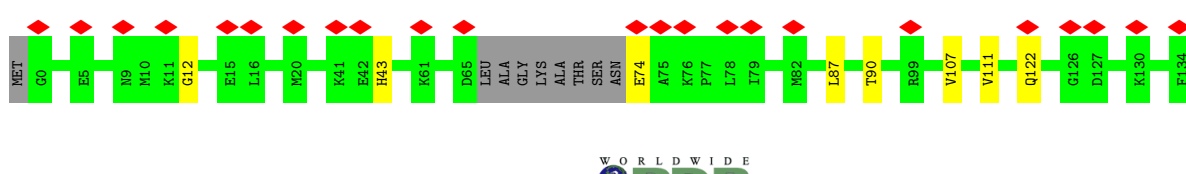
• Molecule 1: C protein



• Molecule 1: C protein



• Molecule 1: C protein

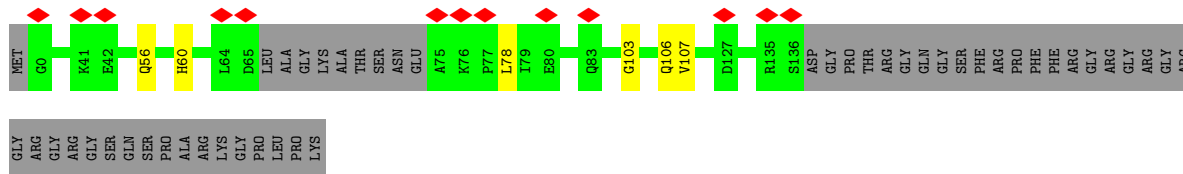




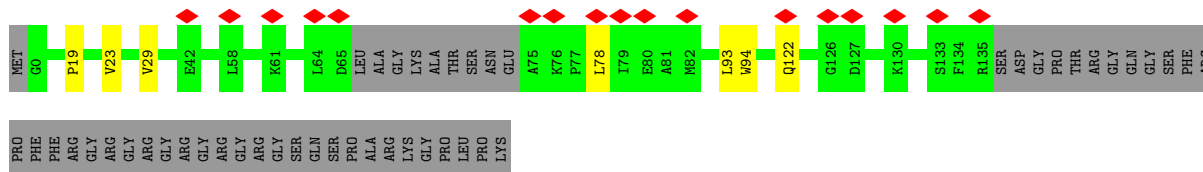


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SER  
ASN  
GLU  
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L78  
I79  
E80  
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G103  
Q106  
V107  
D127  
R135  
S136  
ASP  
GLY  
PRO  
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ARG  
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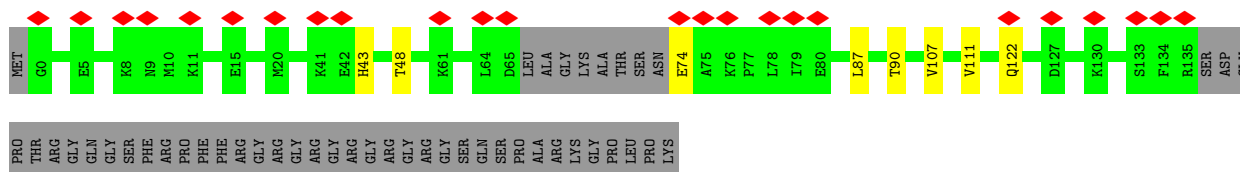
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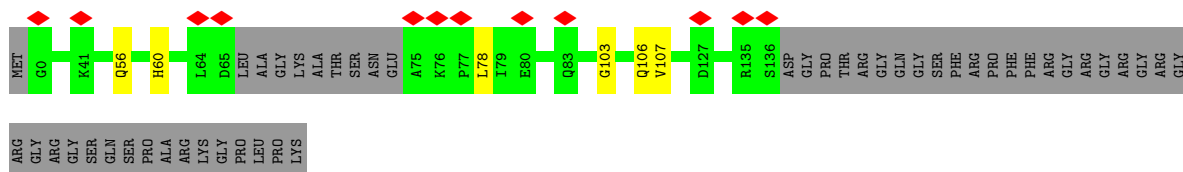
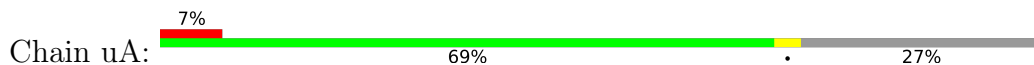
• Molecule 1: C protein



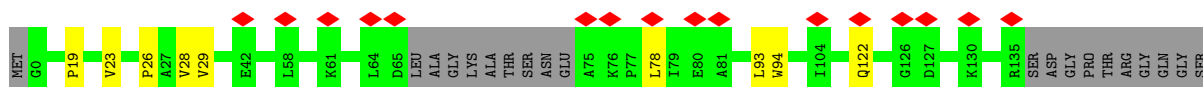
• Molecule 1: C protein



• Molecule 1: C protein



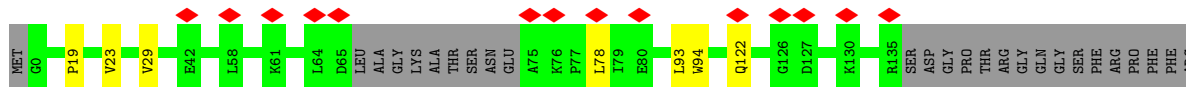
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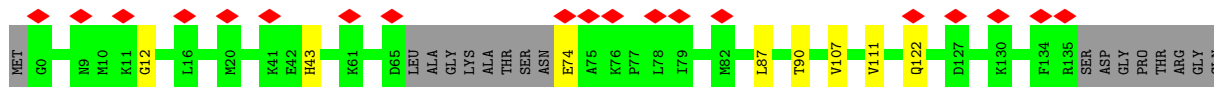
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LEU  
LEU  
PRO  
LYS

• Molecule 1: C protein



GLY  
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PRO  
LYS

• Molecule 1: C protein



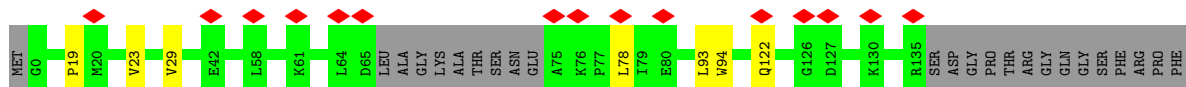
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ALA  
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LEU  
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LYS

• Molecule 1: C protein



GLY  
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LYS

• Molecule 1: C protein



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LEU  
PRO  
LYS

• Molecule 1: C protein

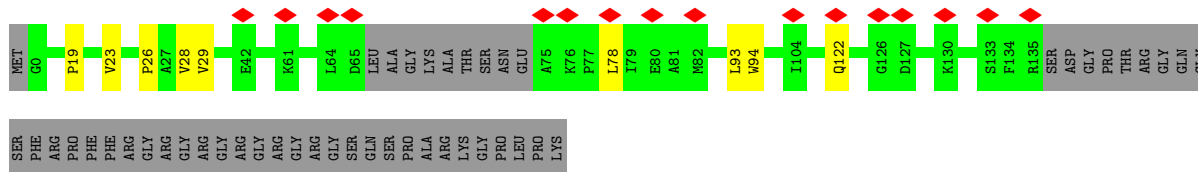




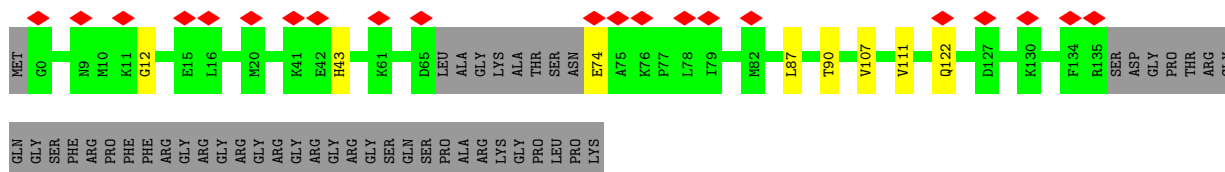


ARG  
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ARG  
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LYS  
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LYS

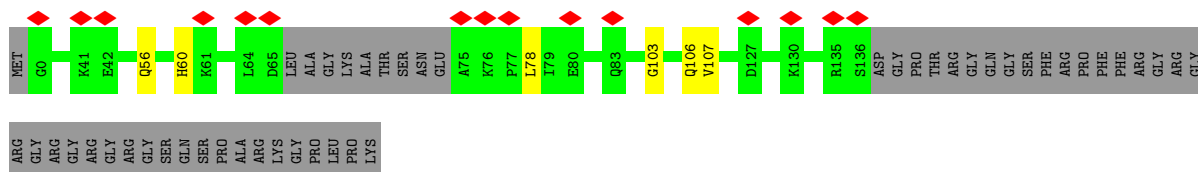
• Molecule 1: C protein



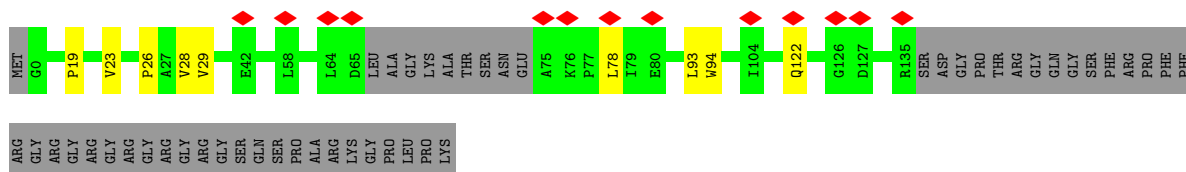
• Molecule 1: C protein



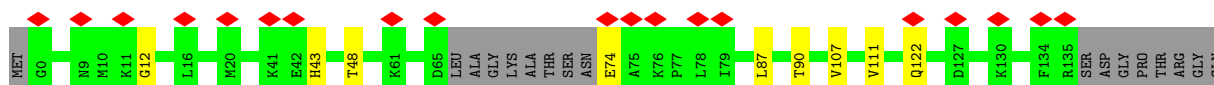
• Molecule 1: C protein



• Molecule 1: C protein



• Molecule 1: C protein







ARG  
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ALA  
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GLY  
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PRO  
LYS

• Molecule 1: C protein



SER  
PHE  
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ALA  
PRO  
GLY  
LYS  
ALA  
ARG  
LYS  
THR  
SER  
ASN  
GLU  
PRO  
PRO  
LYS

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	70868	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 ( $e^-/\text{\AA}^2$ )	76	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.043	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0103	Depositor
Map size (Å)	462.24002, 462.24002, 462.24002	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.09	0/1059	0.21	0/1432
1	1B	0.11	0/1053	0.24	0/1424
1	1C	0.08	0/1062	0.20	0/1436
1	2A	0.09	0/1059	0.22	0/1432
1	2B	0.11	0/1053	0.24	0/1424
1	2C	0.08	0/1062	0.20	0/1436
1	3A	0.09	0/1059	0.22	0/1432
1	3B	0.11	0/1053	0.24	0/1424
1	3C	0.08	0/1062	0.20	0/1436
1	4A	0.09	0/1059	0.21	0/1432
1	4B	0.11	0/1053	0.24	0/1424
1	4C	0.08	0/1062	0.20	0/1436
1	5A	0.09	0/1059	0.21	0/1432
1	5B	0.11	0/1053	0.24	0/1424
1	5C	0.08	0/1062	0.20	0/1436
1	6A	0.09	0/1059	0.21	0/1432
1	6B	0.11	0/1053	0.24	0/1424
1	6C	0.08	0/1062	0.20	0/1436
1	7A	0.09	0/1059	0.22	0/1432
1	7B	0.11	0/1053	0.24	0/1424
1	7C	0.08	0/1062	0.20	0/1436
1	8A	0.09	0/1059	0.21	0/1432
1	8B	0.11	0/1053	0.24	0/1424
1	8C	0.08	0/1062	0.20	0/1436
1	AA	0.09	0/1059	0.21	0/1432
1	AB	0.11	0/1053	0.24	0/1424
1	AC	0.08	0/1062	0.20	0/1436
1	BA	0.09	0/1059	0.21	0/1432
1	BB	0.11	0/1053	0.24	0/1424
1	BC	0.08	0/1062	0.20	0/1436
1	CA	0.09	0/1059	0.22	0/1432
1	CB	0.11	0/1053	0.24	0/1424
1	CC	0.08	0/1062	0.20	0/1436
1	DA	0.09	0/1059	0.21	0/1432

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	DB	0.11	0/1053	0.24	0/1424
1	DC	0.08	0/1062	0.20	0/1436
1	EA	0.09	0/1059	0.21	0/1432
1	EB	0.11	0/1053	0.24	0/1424
1	EC	0.08	0/1062	0.20	0/1436
1	FA	0.09	0/1059	0.21	0/1432
1	FB	0.11	0/1053	0.24	0/1424
1	FC	0.08	0/1062	0.20	0/1436
1	GA	0.09	0/1059	0.21	0/1432
1	GB	0.11	0/1053	0.24	0/1424
1	GC	0.08	0/1062	0.20	0/1436
1	HA	0.08	0/1059	0.21	0/1432
1	HB	0.11	0/1053	0.24	0/1424
1	HC	0.08	0/1062	0.20	0/1436
1	IA	0.09	0/1059	0.21	0/1432
1	IB	0.11	0/1053	0.24	0/1424
1	IC	0.08	0/1062	0.20	0/1436
1	JA	0.09	0/1059	0.21	0/1432
1	JB	0.11	0/1053	0.24	0/1424
1	JC	0.08	0/1062	0.20	0/1436
1	KA	0.09	0/1059	0.22	0/1432
1	KB	0.11	0/1053	0.24	0/1424
1	KC	0.08	0/1062	0.20	0/1436
1	LA	0.09	0/1059	0.21	0/1432
1	LB	0.11	0/1053	0.24	0/1424
1	LC	0.08	0/1062	0.20	0/1436
1	MA	0.09	0/1059	0.21	0/1432
1	MB	0.11	0/1053	0.24	0/1424
1	MC	0.08	0/1062	0.20	0/1436
1	NA	0.09	0/1059	0.22	0/1432
1	NB	0.11	0/1053	0.24	0/1424
1	NC	0.08	0/1062	0.20	0/1436
1	OA	0.09	0/1059	0.21	0/1432
1	OB	0.11	0/1053	0.24	0/1424
1	OC	0.08	0/1062	0.20	0/1436
1	PA	0.09	0/1059	0.22	0/1432
1	PB	0.11	0/1053	0.24	0/1424
1	PC	0.08	0/1062	0.20	0/1436
1	QA	0.08	0/1059	0.22	0/1432
1	QB	0.11	0/1053	0.24	0/1424
1	QC	0.08	0/1062	0.20	0/1436
1	RA	0.09	0/1059	0.21	0/1432
1	RB	0.11	0/1053	0.24	0/1424

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	RC	0.08	0/1062	0.20	0/1436
1	SA	0.09	0/1059	0.21	0/1432
1	SB	0.11	0/1053	0.24	0/1424
1	SC	0.08	0/1062	0.20	0/1436
1	TA	0.09	0/1059	0.22	0/1432
1	TB	0.11	0/1053	0.24	0/1424
1	TC	0.08	0/1062	0.20	0/1436
1	UA	0.09	0/1059	0.21	0/1432
1	UB	0.11	0/1053	0.24	0/1424
1	UC	0.08	0/1062	0.20	0/1436
1	VA	0.09	0/1059	0.22	0/1432
1	VB	0.11	0/1053	0.24	0/1424
1	VC	0.08	0/1062	0.20	0/1436
1	WA	0.09	0/1059	0.21	0/1432
1	WB	0.11	0/1053	0.24	0/1424
1	WC	0.08	0/1062	0.20	0/1436
1	XA	0.09	0/1059	0.22	0/1432
1	XB	0.11	0/1053	0.24	0/1424
1	XC	0.08	0/1062	0.20	0/1436
1	YA	0.09	0/1059	0.21	0/1432
1	YB	0.11	0/1053	0.24	0/1424
1	YC	0.08	0/1062	0.20	0/1436
1	ZA	0.09	0/1059	0.22	0/1432
1	ZB	0.11	0/1053	0.24	0/1424
1	ZC	0.08	0/1062	0.20	0/1436
1	aA	0.09	0/1059	0.21	0/1432
1	aB	0.11	0/1053	0.24	0/1424
1	aC	0.08	0/1062	0.20	0/1436
1	bA	0.09	0/1059	0.22	0/1432
1	bB	0.11	0/1053	0.24	0/1424
1	bC	0.08	0/1062	0.20	0/1436
1	cA	0.09	0/1059	0.21	0/1432
1	cB	0.11	0/1053	0.24	0/1424
1	cC	0.08	0/1062	0.20	0/1436
1	dA	0.09	0/1059	0.21	0/1432
1	dB	0.11	0/1053	0.24	0/1424
1	dC	0.08	0/1062	0.20	0/1436
1	eA	0.09	0/1059	0.22	0/1432
1	eB	0.11	0/1053	0.24	0/1424
1	eC	0.08	0/1062	0.20	0/1436
1	fA	0.09	0/1059	0.21	0/1432
1	fB	0.11	0/1053	0.24	0/1424
1	fC	0.08	0/1062	0.20	0/1436

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	gA	0.09	0/1059	0.21	0/1432
1	gB	0.11	0/1053	0.24	0/1424
1	gC	0.08	0/1062	0.20	0/1436
1	hA	0.09	0/1059	0.22	0/1432
1	hB	0.11	0/1053	0.24	0/1424
1	hC	0.08	0/1062	0.20	0/1436
1	iA	0.09	0/1059	0.21	0/1432
1	iB	0.11	0/1053	0.24	0/1424
1	iC	0.08	0/1062	0.20	0/1436
1	jA	0.09	0/1059	0.21	0/1432
1	jB	0.11	0/1053	0.24	0/1424
1	jC	0.08	0/1062	0.20	0/1436
1	kA	0.09	0/1059	0.22	0/1432
1	kB	0.11	0/1053	0.24	0/1424
1	kC	0.08	0/1062	0.20	0/1436
1	lA	0.09	0/1059	0.21	0/1432
1	lB	0.11	0/1053	0.24	0/1424
1	lC	0.08	0/1062	0.20	0/1436
1	mA	0.09	0/1059	0.22	0/1432
1	mB	0.11	0/1053	0.24	0/1424
1	mC	0.08	0/1062	0.20	0/1436
1	nA	0.09	0/1059	0.21	0/1432
1	nB	0.11	0/1053	0.24	0/1424
1	nC	0.08	0/1062	0.20	0/1436
1	oA	0.09	0/1059	0.21	0/1432
1	oB	0.11	0/1053	0.24	0/1424
1	oC	0.08	0/1062	0.20	0/1436
1	pA	0.09	0/1059	0.21	0/1432
1	pB	0.11	0/1053	0.24	0/1424
1	pC	0.08	0/1062	0.20	0/1436
1	qA	0.09	0/1059	0.21	0/1432
1	qB	0.11	0/1053	0.24	0/1424
1	qC	0.08	0/1062	0.20	0/1436
1	rA	0.09	0/1059	0.22	0/1432
1	rB	0.11	0/1053	0.24	0/1424
1	rC	0.08	0/1062	0.20	0/1436
1	sA	0.09	0/1059	0.21	0/1432
1	sB	0.11	0/1053	0.24	0/1424
1	sC	0.08	0/1062	0.20	0/1436
1	tA	0.09	0/1059	0.22	0/1432
1	tB	0.11	0/1053	0.24	0/1424
1	tC	0.08	0/1062	0.20	0/1436
1	uA	0.09	0/1059	0.21	0/1432

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	uB	0.11	0/1053	0.24	0/1424
1	uC	0.08	0/1062	0.20	0/1436
1	vA	0.09	0/1059	0.22	0/1432
1	vB	0.11	0/1053	0.24	0/1424
1	vC	0.08	0/1062	0.20	0/1436
1	wA	0.09	0/1059	0.21	0/1432
1	wB	0.11	0/1053	0.24	0/1424
1	wC	0.08	0/1062	0.20	0/1436
1	xA	0.09	0/1059	0.21	0/1432
1	xB	0.11	0/1053	0.24	0/1424
1	xC	0.08	0/1062	0.20	0/1436
1	yA	0.09	0/1059	0.22	0/1432
1	yB	0.11	0/1053	0.24	0/1424
1	yC	0.08	0/1062	0.20	0/1436
1	zA	0.09	0/1059	0.22	0/1432
1	zB	0.11	0/1053	0.24	0/1424
1	zC	0.08	0/1062	0.20	0/1436
All	All	0.09	0/190440	0.22	0/257520

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	1034	0	1074	5	0
1	1B	1028	0	1069	6	0
1	1C	1037	0	1075	4	0
1	2A	1034	0	1074	4	0
1	2B	1028	0	1069	4	0
1	2C	1037	0	1075	5	0
1	3A	1034	0	1074	5	0
1	3B	1028	0	1069	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3C	1037	0	1075	7	0
1	4A	1034	0	1074	5	0
1	4B	1028	0	1069	5	0
1	4C	1037	0	1075	6	0
1	5A	1034	0	1074	5	0
1	5B	1028	0	1069	5	0
1	5C	1037	0	1075	7	0
1	6A	1034	0	1074	5	0
1	6B	1028	0	1069	4	0
1	6C	1037	0	1075	6	0
1	7A	1034	0	1074	5	0
1	7B	1028	0	1069	5	0
1	7C	1037	0	1075	5	0
1	8A	1034	0	1074	5	0
1	8B	1028	0	1069	4	0
1	8C	1037	0	1075	6	0
1	AA	1034	0	1074	5	0
1	AB	1028	0	1069	5	0
1	AC	1037	0	1075	6	0
1	BA	1034	0	1074	5	0
1	BB	1028	0	1069	4	0
1	BC	1037	0	1075	6	0
1	CA	1034	0	1074	5	0
1	CB	1028	0	1069	4	0
1	CC	1037	0	1075	4	0
1	DA	1034	0	1074	5	0
1	DB	1028	0	1069	7	0
1	DC	1037	0	1075	6	0
1	EA	1034	0	1074	5	0
1	EB	1028	0	1069	4	0
1	EC	1037	0	1075	12	0
1	FA	1034	0	1074	4	0
1	FB	1028	0	1069	4	0
1	FC	1037	0	1075	6	0
1	GA	1034	0	1074	5	0
1	GB	1028	0	1069	5	0
1	GC	1037	0	1075	5	0
1	HA	1034	0	1074	5	0
1	HB	1028	0	1069	5	0
1	HC	1037	0	1075	6	0
1	IA	1034	0	1074	4	0
1	IB	1028	0	1069	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	IC	1037	0	1075	4	0
1	JA	1034	0	1074	5	0
1	JB	1028	0	1069	4	0
1	JC	1037	0	1075	7	0
1	KA	1034	0	1074	4	0
1	KB	1028	0	1069	5	0
1	KC	1037	0	1075	6	0
1	LA	1034	0	1074	5	0
1	LB	1028	0	1069	4	0
1	LC	1037	0	1075	5	0
1	MA	1034	0	1074	5	0
1	MB	1028	0	1069	5	0
1	MC	1037	0	1075	6	0
1	NA	1034	0	1074	5	0
1	NB	1028	0	1069	5	0
1	NC	1037	0	1075	8	0
1	OA	1034	0	1074	5	0
1	OB	1028	0	1069	4	0
1	OC	1037	0	1075	5	0
1	PA	1034	0	1074	5	0
1	PB	1028	0	1069	4	0
1	PC	1037	0	1075	4	0
1	QA	1034	0	1074	5	0
1	QB	1028	0	1069	4	0
1	QC	1037	0	1075	4	0
1	RA	1034	0	1074	4	0
1	RB	1028	0	1069	4	0
1	RC	1037	0	1075	6	0
1	SA	1034	0	1074	5	0
1	SB	1028	0	1069	4	0
1	SC	1037	0	1075	11	0
1	TA	1034	0	1074	5	0
1	TB	1028	0	1069	4	0
1	TC	1037	0	1075	6	0
1	UA	1034	0	1074	5	0
1	UB	1028	0	1069	4	0
1	UC	1037	0	1075	6	0
1	VA	1034	0	1074	5	0
1	VB	1028	0	1069	5	0
1	VC	1037	0	1075	4	0
1	WA	1034	0	1074	4	0
1	WB	1028	0	1069	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	WC	1037	0	1075	4	0
1	XA	1034	0	1074	5	0
1	XB	1028	0	1069	4	0
1	XC	1037	0	1075	6	0
1	YA	1034	0	1074	5	0
1	YB	1028	0	1069	5	0
1	YC	1037	0	1075	5	0
1	ZA	1034	0	1074	5	0
1	ZB	1028	0	1069	4	0
1	ZC	1037	0	1075	6	0
1	aA	1034	0	1074	5	0
1	aB	1028	0	1069	5	0
1	aC	1037	0	1075	4	0
1	bA	1034	0	1074	5	0
1	bB	1028	0	1069	4	0
1	bC	1037	0	1075	5	0
1	cA	1034	0	1074	4	0
1	cB	1028	0	1069	5	0
1	cC	1037	0	1075	6	0
1	dA	1034	0	1074	5	0
1	dB	1028	0	1069	4	0
1	dC	1037	0	1075	6	0
1	eA	1034	0	1074	5	0
1	eB	1028	0	1069	4	0
1	eC	1037	0	1075	5	0
1	fA	1034	0	1074	4	0
1	fB	1028	0	1069	7	0
1	fC	1037	0	1075	4	0
1	gA	1034	0	1074	5	0
1	gB	1028	0	1069	4	0
1	gC	1037	0	1075	6	0
1	hA	1034	0	1074	5	0
1	hB	1028	0	1069	4	0
1	hC	1037	0	1075	6	0
1	iA	1034	0	1074	5	0
1	iB	1028	0	1069	5	0
1	iC	1037	0	1075	5	0
1	jA	1034	0	1074	5	0
1	jB	1028	0	1069	4	0
1	jC	1037	0	1075	4	0
1	kA	1034	0	1074	4	0
1	kB	1028	0	1069	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	kC	1037	0	1075	4	0
1	lA	1034	0	1074	5	0
1	lB	1028	0	1069	4	0
1	lC	1037	0	1075	6	0
1	mA	1034	0	1074	5	0
1	mB	1028	0	1069	4	0
1	mC	1037	0	1075	5	0
1	nA	1034	0	1074	5	0
1	nB	1028	0	1069	4	0
1	nC	1037	0	1075	4	0
1	oA	1034	0	1074	4	0
1	oB	1028	0	1069	4	0
1	oC	1037	0	1075	4	0
1	pA	1034	0	1074	5	0
1	pB	1028	0	1069	4	0
1	pC	1037	0	1075	6	0
1	qA	1034	0	1074	4	0
1	qB	1028	0	1069	4	0
1	qC	1037	0	1075	6	0
1	rA	1034	0	1074	5	0
1	rB	1028	0	1069	5	0
1	rC	1037	0	1075	6	0
1	sA	1034	0	1074	5	0
1	sB	1028	0	1069	4	0
1	sC	1037	0	1075	5	0
1	tA	1034	0	1074	5	0
1	tB	1028	0	1069	4	0
1	tC	1037	0	1075	5	0
1	uA	1034	0	1074	5	0
1	uB	1028	0	1069	5	0
1	uC	1037	0	1075	6	0
1	vA	1034	0	1074	5	0
1	vB	1028	0	1069	5	0
1	vC	1037	0	1075	5	0
1	wA	1034	0	1074	5	0
1	wB	1028	0	1069	4	0
1	wC	1037	0	1075	6	0
1	xA	1034	0	1074	4	0
1	xB	1028	0	1069	4	0
1	xC	1037	0	1075	4	0
1	yA	1034	0	1074	5	0
1	yB	1028	0	1069	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	yC	1037	0	1075	5	0
1	zA	1034	0	1074	5	0
1	zB	1028	0	1069	4	0
1	zC	1037	0	1075	6	0
All	All	185940	0	193080	782	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 2.

All (782) 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:CC:74:GLU:OE1	1:CC:74:GLU:N	2.24	0.71
1:ZC:74:GLU:N	1:ZC:74:GLU:OE1	2.24	0.71
1:hC:74:GLU:N	1:hC:74:GLU:OE1	2.24	0.71
1:pC:74:GLU:N	1:pC:74:GLU:OE1	2.24	0.71
1:WC:74:GLU:N	1:WC:74:GLU:OE1	2.24	0.71
1:XC:74:GLU:N	1:XC:74:GLU:OE1	2.24	0.71
1:jC:74:GLU:OE1	1:jC:74:GLU:N	2.24	0.71
1:2C:74:GLU:OE1	1:2C:74:GLU:N	2.24	0.71
1:xC:74:GLU:OE1	1:xC:74:GLU:N	2.24	0.71
1:5C:74:GLU:N	1:5C:74:GLU:OE1	2.24	0.71
1:BC:74:GLU:N	1:BC:74:GLU:OE1	2.24	0.71
1:GC:74:GLU:N	1:GC:74:GLU:OE1	2.24	0.71
1:JC:74:GLU:OE1	1:JC:74:GLU:N	2.24	0.71
1:NC:74:GLU:N	1:NC:74:GLU:OE1	2.24	0.71
1:QC:74:GLU:OE1	1:QC:74:GLU:N	2.24	0.71
1:1C:74:GLU:N	1:1C:74:GLU:OE1	2.24	0.71
1:nC:74:GLU:N	1:nC:74:GLU:OE1	2.24	0.71
1:PC:74:GLU:N	1:PC:74:GLU:OE1	2.24	0.71
1:rC:74:GLU:N	1:rC:74:GLU:OE1	2.24	0.71
1:fC:74:GLU:N	1:fC:74:GLU:OE1	2.24	0.71
1:wC:74:GLU:N	1:wC:74:GLU:OE1	2.24	0.71
1:TC:74:GLU:OE1	1:TC:74:GLU:N	2.24	0.71
1:gC:74:GLU:OE1	1:gC:74:GLU:N	2.24	0.71
1:IC:74:GLU:N	1:IC:74:GLU:OE1	2.24	0.71
1:KC:74:GLU:N	1:KC:74:GLU:OE1	2.24	0.71
1:dC:74:GLU:N	1:dC:74:GLU:OE1	2.24	0.71
1:mC:74:GLU:N	1:mC:74:GLU:OE1	2.24	0.71
1:DC:74:GLU:N	1:DC:74:GLU:OE1	2.24	0.70
1:YC:74:GLU:OE1	1:YC:74:GLU:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:cC:74:GLU:N	1:cC:74:GLU:OE1	2.24	0.70
1:oC:74:GLU:N	1:oC:74:GLU:OE1	2.24	0.70
1:MC:74:GLU:N	1:MC:74:GLU:OE1	2.24	0.70
1:vC:74:GLU:OE1	1:vC:74:GLU:N	2.24	0.70
1:7C:74:GLU:OE1	1:7C:74:GLU:N	2.24	0.70
1:zC:74:GLU:N	1:zC:74:GLU:OE1	2.24	0.70
1:4C:74:GLU:OE1	1:4C:74:GLU:N	2.24	0.70
1:6C:74:GLU:N	1:6C:74:GLU:OE1	2.24	0.70
1:tC:74:GLU:N	1:tC:74:GLU:OE1	2.24	0.70
1:8C:74:GLU:N	1:8C:74:GLU:OE1	2.24	0.70
1:AC:74:GLU:N	1:AC:74:GLU:OE1	2.24	0.70
1:HC:74:GLU:OE1	1:HC:74:GLU:N	2.24	0.70
1:LC:74:GLU:N	1:LC:74:GLU:OE1	2.24	0.70
1:iC:74:GLU:N	1:iC:74:GLU:OE1	2.24	0.70
1:sC:74:GLU:OE1	1:sC:74:GLU:N	2.24	0.70
1:OC:74:GLU:OE1	1:OC:74:GLU:N	2.24	0.70
1:SC:74:GLU:N	1:SC:74:GLU:OE1	2.24	0.70
1:aC:74:GLU:N	1:aC:74:GLU:OE1	2.24	0.70
1:3C:74:GLU:N	1:3C:74:GLU:OE1	2.24	0.70
1:EC:74:GLU:OE1	1:EC:74:GLU:N	2.24	0.70
1:UC:74:GLU:N	1:UC:74:GLU:OE1	2.24	0.70
1:VC:74:GLU:OE1	1:VC:74:GLU:N	2.24	0.70
1:uC:74:GLU:N	1:uC:74:GLU:OE1	2.24	0.70
1:yC:74:GLU:N	1:yC:74:GLU:OE1	2.24	0.70
1:RC:74:GLU:N	1:RC:74:GLU:OE1	2.24	0.70
1:bC:74:GLU:OE1	1:bC:74:GLU:N	2.24	0.70
1:kC:74:GLU:N	1:kC:74:GLU:OE1	2.24	0.70
1:eC:74:GLU:OE1	1:eC:74:GLU:N	2.24	0.69
1:lC:74:GLU:OE1	1:lC:74:GLU:N	2.24	0.69
1:FC:74:GLU:N	1:FC:74:GLU:OE1	2.24	0.69
1:qC:74:GLU:OE1	1:qC:74:GLU:N	2.24	0.69
1:lB:19:PRO:O	1:lB:23:VAL:HG23	1.97	0.65
1:WB:19:PRO:O	1:WB:23:VAL:HG23	1.97	0.65
1:rB:19:PRO:O	1:rB:23:VAL:HG23	1.97	0.65
1:7B:19:PRO:O	1:7B:23:VAL:HG23	1.97	0.65
1:BB:19:PRO:O	1:BB:23:VAL:HG23	1.97	0.65
1:EB:19:PRO:O	1:EB:23:VAL:HG23	1.97	0.65
1:GB:19:PRO:O	1:GB:23:VAL:HG23	1.97	0.65
1:SB:19:PRO:O	1:SB:23:VAL:HG23	1.97	0.65
1:AB:19:PRO:O	1:AB:23:VAL:HG23	1.97	0.65
1:HB:19:PRO:O	1:HB:23:VAL:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KB:19:PRO:O	1:KB:23:VAL:HG23	1.97	0.65
1:VB:19:PRO:O	1:VB:23:VAL:HG23	1.97	0.65
1:ZB:19:PRO:O	1:ZB:23:VAL:HG23	1.97	0.65
1:cB:19:PRO:O	1:cB:23:VAL:HG23	1.97	0.65
1:vB:19:PRO:O	1:vB:23:VAL:HG23	1.97	0.65
1:UB:19:PRO:O	1:UB:23:VAL:HG23	1.97	0.65
1:fB:19:PRO:O	1:fB:23:VAL:HG23	1.97	0.65
1:gB:19:PRO:O	1:gB:23:VAL:HG23	1.97	0.65
1:hB:19:PRO:O	1:hB:23:VAL:HG23	1.97	0.65
1:mB:19:PRO:O	1:mB:23:VAL:HG23	1.97	0.65
1:sB:19:PRO:O	1:sB:23:VAL:HG23	1.97	0.65
1:zB:19:PRO:O	1:zB:23:VAL:HG23	1.97	0.65
1:TB:19:PRO:O	1:TB:23:VAL:HG23	1.97	0.65
1:oB:19:PRO:O	1:oB:23:VAL:HG23	1.97	0.65
1:IB:19:PRO:O	1:IB:23:VAL:HG23	1.97	0.65
1:QB:19:PRO:O	1:QB:23:VAL:HG23	1.97	0.65
1:dB:19:PRO:O	1:dB:23:VAL:HG23	1.97	0.65
1:jB:19:PRO:O	1:jB:23:VAL:HG23	1.97	0.65
1:RB:19:PRO:O	1:RB:23:VAL:HG23	1.97	0.65
1:yB:19:PRO:O	1:yB:23:VAL:HG23	1.97	0.65
1:bB:19:PRO:O	1:bB:23:VAL:HG23	1.97	0.64
1:kB:19:PRO:O	1:kB:23:VAL:HG23	1.97	0.64
1:uB:19:PRO:O	1:uB:23:VAL:HG23	1.97	0.64
1:FB:19:PRO:O	1:FB:23:VAL:HG23	1.97	0.64
1:eB:19:PRO:O	1:eB:23:VAL:HG23	1.97	0.64
1:xB:19:PRO:O	1:xB:23:VAL:HG23	1.97	0.64
1:2B:19:PRO:O	1:2B:23:VAL:HG23	1.97	0.64
1:qB:19:PRO:O	1:qB:23:VAL:HG23	1.97	0.64
1:CB:19:PRO:O	1:CB:23:VAL:HG23	1.97	0.64
1:1B:19:PRO:O	1:1B:23:VAL:HG23	1.97	0.64
1:MB:19:PRO:O	1:MB:23:VAL:HG23	1.97	0.64
1:wB:19:PRO:O	1:wB:23:VAL:HG23	1.97	0.64
1:4B:19:PRO:O	1:4B:23:VAL:HG23	1.97	0.64
1:8B:19:PRO:O	1:8B:23:VAL:HG23	1.97	0.64
1:LB:19:PRO:O	1:LB:23:VAL:HG23	1.97	0.64
1:XB:19:PRO:O	1:XB:23:VAL:HG23	1.97	0.64
1:nB:19:PRO:O	1:nB:23:VAL:HG23	1.97	0.64
1:6B:19:PRO:O	1:6B:23:VAL:HG23	1.97	0.64
1:JB:19:PRO:O	1:JB:23:VAL:HG23	1.97	0.64
1:PB:19:PRO:O	1:PB:23:VAL:HG23	1.97	0.64
1:OB:19:PRO:O	1:OB:23:VAL:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:pB:19:PRO:O	1:pB:23:VAL:HG23	1.97	0.64
1:YB:19:PRO:O	1:YB:23:VAL:HG23	1.97	0.63
1:iB:19:PRO:O	1:iB:23:VAL:HG23	1.97	0.63
1:DB:19:PRO:O	1:DB:23:VAL:HG23	1.97	0.63
1:aB:19:PRO:O	1:aB:23:VAL:HG23	1.97	0.63
1:EA:106:GLN:N	1:EA:106:GLN:OE1	2.32	0.63
1:NB:19:PRO:O	1:NB:23:VAL:HG23	1.97	0.63
1:5B:19:PRO:O	1:5B:23:VAL:HG23	1.97	0.63
1:QA:106:GLN:N	1:QA:106:GLN:OE1	2.32	0.63
1:ZA:106:GLN:N	1:ZA:106:GLN:OE1	2.32	0.63
1:eA:106:GLN:N	1:eA:106:GLN:OE1	2.32	0.63
1:hA:106:GLN:OE1	1:hA:106:GLN:N	2.32	0.63
1:jA:106:GLN:N	1:jA:106:GLN:OE1	2.32	0.63
1:tB:19:PRO:O	1:tB:23:VAL:HG23	1.97	0.63
1:3B:19:PRO:O	1:3B:23:VAL:HG23	1.97	0.63
1:NA:106:GLN:N	1:NA:106:GLN:OE1	2.32	0.63
1:UA:106:GLN:OE1	1:UA:106:GLN:N	2.32	0.63
1:6A:106:GLN:N	1:6A:106:GLN:OE1	2.32	0.63
1:OA:106:GLN:N	1:OA:106:GLN:OE1	2.32	0.63
1:bA:106:GLN:N	1:bA:106:GLN:OE1	2.32	0.63
1:kA:106:GLN:N	1:kA:106:GLN:OE1	2.32	0.63
1:5A:106:GLN:OE1	1:5A:106:GLN:N	2.32	0.63
1:RA:106:GLN:OE1	1:RA:106:GLN:N	2.32	0.63
1:nA:106:GLN:N	1:nA:106:GLN:OE1	2.32	0.63
1:PA:106:GLN:OE1	1:PA:106:GLN:N	2.32	0.63
1:fA:106:GLN:OE1	1:fA:106:GLN:N	2.32	0.63
1:GA:106:GLN:N	1:GA:106:GLN:OE1	2.32	0.63
1:VA:106:GLN:N	1:VA:106:GLN:OE1	2.32	0.63
1:zA:106:GLN:N	1:zA:106:GLN:OE1	2.32	0.63
1:AC:43:HIS:ND1	1:RC:12:GLY:O	2.32	0.62
1:cA:106:GLN:OE1	1:cA:106:GLN:N	2.32	0.62
1:qA:106:GLN:N	1:qA:106:GLN:OE1	2.32	0.62
1:rA:106:GLN:OE1	1:rA:106:GLN:N	2.32	0.62
1:vA:106:GLN:N	1:vA:106:GLN:OE1	2.32	0.62
1:FA:106:GLN:OE1	1:FA:106:GLN:N	2.32	0.62
1:KA:106:GLN:OE1	1:KA:106:GLN:N	2.32	0.62
1:uA:106:GLN:N	1:uA:106:GLN:OE1	2.32	0.62
1:AA:106:GLN:OE1	1:AA:106:GLN:N	2.32	0.62
1:MA:106:GLN:OE1	1:MA:106:GLN:N	2.32	0.62
1:7A:106:GLN:N	1:7A:106:GLN:OE1	2.32	0.62
1:SA:106:GLN:N	1:SA:106:GLN:OE1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IA:106:GLN:N	1:IA:106:GLN:OE1	2.32	0.62
1:sA:106:GLN:N	1:sA:106:GLN:OE1	2.32	0.62
1:tA:106:GLN:OE1	1:tA:106:GLN:N	2.32	0.62
1:HA:106:GLN:N	1:HA:106:GLN:OE1	2.32	0.62
1:YA:106:GLN:N	1:YA:106:GLN:OE1	2.32	0.62
1:mA:106:GLN:OE1	1:mA:106:GLN:N	2.32	0.62
1:yA:106:GLN:OE1	1:yA:106:GLN:N	2.32	0.62
1:3A:106:GLN:N	1:3A:106:GLN:OE1	2.32	0.62
1:IA:106:GLN:N	1:IA:106:GLN:OE1	2.32	0.62
1:TA:106:GLN:N	1:TA:106:GLN:OE1	2.32	0.62
1:gA:106:GLN:N	1:gA:106:GLN:OE1	2.32	0.62
1:4A:106:GLN:N	1:4A:106:GLN:OE1	2.32	0.62
1:LA:106:GLN:N	1:LA:106:GLN:OE1	2.32	0.62
1:dA:106:GLN:N	1:dA:106:GLN:OE1	2.32	0.62
1:aA:106:GLN:OE1	1:aA:106:GLN:N	2.32	0.62
1:iA:106:GLN:N	1:iA:106:GLN:OE1	2.32	0.62
1:wC:12:GLY:O	1:3C:43:HIS:ND1	2.33	0.62
1:8A:106:GLN:N	1:8A:106:GLN:OE1	2.32	0.62
1:CA:106:GLN:N	1:CA:106:GLN:OE1	2.32	0.61
1:DA:106:GLN:OE1	1:DA:106:GLN:N	2.32	0.61
1:WA:106:GLN:OE1	1:WA:106:GLN:N	2.32	0.61
1:XA:106:GLN:N	1:XA:106:GLN:OE1	2.32	0.61
1:BA:106:GLN:N	1:BA:106:GLN:OE1	2.32	0.61
1:pA:106:GLN:N	1:pA:106:GLN:OE1	2.32	0.61
1:1A:106:GLN:N	1:1A:106:GLN:OE1	2.32	0.61
1:oA:106:GLN:OE1	1:oA:106:GLN:N	2.32	0.61
1:JA:106:GLN:N	1:JA:106:GLN:OE1	2.32	0.61
1:fB:29:VAL:HG23	1:fB:94:TRP:HE3	1.66	0.61
1:7B:29:VAL:HG23	1:7B:94:TRP:HE3	1.66	0.61
1:BB:29:VAL:HG23	1:BB:94:TRP:HE3	1.66	0.61
1:CB:29:VAL:HG23	1:CB:94:TRP:HE3	1.66	0.61
1:IB:29:VAL:HG23	1:IB:94:TRP:HE3	1.66	0.61
1:OB:29:VAL:HG23	1:OB:94:TRP:HE3	1.66	0.61
1:TB:29:VAL:HG23	1:TB:94:TRP:HE3	1.66	0.61
1:XB:29:VAL:HG23	1:XB:94:TRP:HE3	1.66	0.61
1:cB:29:VAL:HG23	1:cB:94:TRP:HE3	1.66	0.61
1:mB:29:VAL:HG23	1:mB:94:TRP:HE3	1.66	0.61
1:oB:29:VAL:HG23	1:oB:94:TRP:HE3	1.66	0.61
1:uB:29:VAL:HG23	1:uB:94:TRP:HE3	1.66	0.61
1:vB:29:VAL:HG23	1:vB:94:TRP:HE3	1.66	0.61
1:yB:29:VAL:HG23	1:yB:94:TRP:HE3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:zB:29:VAL:HG23	1:zB:94:TRP:HE3	1.66	0.61
1:5B:29:VAL:HG23	1:5B:94:TRP:HE3	1.66	0.61
1:EB:29:VAL:HG23	1:EB:94:TRP:HE3	1.66	0.61
1:MB:29:VAL:HG23	1:MB:94:TRP:HE3	1.66	0.61
1:NB:29:VAL:HG23	1:NB:94:TRP:HE3	1.66	0.61
1:UB:29:VAL:HG23	1:UB:94:TRP:HE3	1.66	0.61
1:wA:106:GLN:OE1	1:wA:106:GLN:N	2.32	0.61
1:AC:12:GLY:O	1:RC:43:HIS:ND1	2.34	0.61
1:KB:29:VAL:HG23	1:KB:94:TRP:HE3	1.66	0.61
1:WB:29:VAL:HG23	1:WB:94:TRP:HE3	1.66	0.61
1:2A:106:GLN:N	1:2A:106:GLN:OE1	2.32	0.61
1:xA:106:GLN:N	1:xA:106:GLN:OE1	2.32	0.61
1:4B:29:VAL:HG23	1:4B:94:TRP:HE3	1.66	0.61
1:6B:29:VAL:HG23	1:6B:94:TRP:HE3	1.66	0.61
1:RB:29:VAL:HG23	1:RB:94:TRP:HE3	1.66	0.60
1:SB:29:VAL:HG23	1:SB:94:TRP:HE3	1.66	0.60
1:YB:29:VAL:HG23	1:YB:94:TRP:HE3	1.66	0.60
1:kB:29:VAL:HG23	1:kB:94:TRP:HE3	1.66	0.60
1:jB:29:VAL:HG23	1:jB:94:TRP:HE3	1.66	0.60
1:lB:29:VAL:HG23	1:lB:94:TRP:HE3	1.66	0.60
1:ZC:12:GLY:O	1:gC:43:HIS:ND1	2.34	0.60
1:ZC:43:HIS:ND1	1:gC:12:GLY:O	2.34	0.60
1:dB:29:VAL:HG23	1:dB:94:TRP:HE3	1.66	0.60
1:iB:29:VAL:HG23	1:iB:94:TRP:HE3	1.66	0.60
1:DB:29:VAL:HG23	1:DB:94:TRP:HE3	1.66	0.60
1:EC:3:PHE:CE2	1:SC:58:LEU:HD11	2.36	0.60
1:QB:29:VAL:HG23	1:QB:94:TRP:HE3	1.66	0.60
1:aB:29:VAL:HG23	1:aB:94:TRP:HE3	1.66	0.60
1:gB:29:VAL:HG23	1:gB:94:TRP:HE3	1.66	0.60
1:tB:29:VAL:HG23	1:tB:94:TRP:HE3	1.66	0.60
1:3B:29:VAL:HG23	1:3B:94:TRP:HE3	1.66	0.60
1:rB:29:VAL:HG23	1:rB:94:TRP:HE3	1.66	0.60
1:VB:29:VAL:HG23	1:VB:94:TRP:HE3	1.66	0.60
1:nB:29:VAL:HG23	1:nB:94:TRP:HE3	1.66	0.60
1:GB:29:VAL:HG23	1:GB:94:TRP:HE3	1.66	0.60
1:1B:29:VAL:HG23	1:1B:94:TRP:HE3	1.66	0.60
1:PB:29:VAL:HG23	1:PB:94:TRP:HE3	1.66	0.60
1:FC:43:HIS:ND1	1:MC:12:GLY:O	2.35	0.59
1:hB:29:VAL:HG23	1:hB:94:TRP:HE3	1.66	0.59
1:HB:29:VAL:HG23	1:HB:94:TRP:HE3	1.66	0.59
1:JB:29:VAL:HG23	1:JB:94:TRP:HE3	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LB:29:VAL:HG23	1:LB:94:TRP:HE3	1.66	0.59
1:ZB:29:VAL:HG23	1:ZB:94:TRP:HE3	1.66	0.59
1:pB:29:VAL:HG23	1:pB:94:TRP:HE3	1.66	0.59
1:qB:29:VAL:HG23	1:qB:94:TRP:HE3	1.66	0.59
1:AB:29:VAL:HG23	1:AB:94:TRP:HE3	1.66	0.59
1:FB:29:VAL:HG23	1:FB:94:TRP:HE3	1.66	0.59
1:sB:29:VAL:HG23	1:sB:94:TRP:HE3	1.66	0.59
1:wB:29:VAL:HG23	1:wB:94:TRP:HE3	1.66	0.59
1:8B:29:VAL:HG23	1:8B:94:TRP:HE3	1.66	0.59
1:bB:29:VAL:HG23	1:bB:94:TRP:HE3	1.66	0.59
1:2B:29:VAL:HG23	1:2B:94:TRP:HE3	1.66	0.59
1:wC:43:HIS:ND1	1:3C:12:GLY:O	2.35	0.59
1:eB:29:VAL:HG23	1:eB:94:TRP:HE3	1.66	0.59
1:xB:29:VAL:HG23	1:xB:94:TRP:HE3	1.66	0.59
1:rC:122:GLN:N	1:rC:122:GLN:OE1	2.36	0.58
1:xC:122:GLN:N	1:xC:122:GLN:OE1	2.36	0.58
1:WC:122:GLN:N	1:WC:122:GLN:OE1	2.36	0.58
1:2C:122:GLN:OE1	1:2C:122:GLN:N	2.36	0.58
1:BC:122:GLN:N	1:BC:122:GLN:OE1	2.36	0.58
1:GC:122:GLN:N	1:GC:122:GLN:OE1	2.36	0.58
1:sC:122:GLN:N	1:sC:122:GLN:OE1	2.36	0.58
1:HC:122:GLN:OE1	1:HC:122:GLN:N	2.36	0.58
1:UC:122:GLN:N	1:UC:122:GLN:OE1	2.36	0.58
1:FC:12:GLY:O	1:MC:43:HIS:ND1	2.37	0.58
1:UC:43:HIS:ND1	1:IC:12:GLY:O	2.37	0.58
1:EC:122:GLN:OE1	1:EC:122:GLN:N	2.36	0.58
1:yC:122:GLN:OE1	1:yC:122:GLN:N	2.36	0.58
1:IC:122:GLN:N	1:IC:122:GLN:OE1	2.36	0.57
1:QC:122:GLN:N	1:QC:122:GLN:OE1	2.36	0.57
1:uC:122:GLN:N	1:uC:122:GLN:OE1	2.36	0.57
1:3C:122:GLN:N	1:3C:122:GLN:OE1	2.36	0.57
1:FC:122:GLN:N	1:FC:122:GLN:OE1	2.36	0.57
1:fC:122:GLN:N	1:fC:122:GLN:OE1	2.36	0.57
1:PC:122:GLN:N	1:PC:122:GLN:OE1	2.36	0.57
1:jC:122:GLN:OE1	1:jC:122:GLN:N	2.36	0.57
1:qC:122:GLN:OE1	1:qC:122:GLN:N	2.36	0.57
1:zC:122:GLN:N	1:zC:122:GLN:OE1	2.36	0.57
1:MC:122:GLN:N	1:MC:122:GLN:OE1	2.36	0.57
1:cC:122:GLN:OE1	1:cC:122:GLN:N	2.36	0.57
1:uC:43:HIS:ND1	1:zC:12:GLY:O	2.37	0.57
1:NC:122:GLN:N	1:NC:122:GLN:OE1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:nC:122:GLN:N	1:nC:122:GLN:OE1	2.36	0.57
1:wC:122:GLN:N	1:wC:122:GLN:OE1	2.36	0.57
1:4C:122:GLN:OE1	1:4C:122:GLN:N	2.36	0.57
1:5C:122:GLN:N	1:5C:122:GLN:OE1	2.36	0.57
1:OC:122:GLN:OE1	1:OC:122:GLN:N	2.36	0.57
1:tC:122:GLN:OE1	1:tC:122:GLN:N	2.36	0.57
1:vC:122:GLN:OE1	1:vC:122:GLN:N	2.36	0.57
1:SC:122:GLN:N	1:SC:122:GLN:OE1	2.36	0.57
1:NB:122:GLN:OE1	1:NB:122:GLN:N	2.38	0.57
1:bC:122:GLN:N	1:bC:122:GLN:OE1	2.36	0.57
1:qB:122:GLN:OE1	1:qB:122:GLN:N	2.38	0.57
1:5B:122:GLN:OE1	1:5B:122:GLN:N	2.38	0.57
1:6C:122:GLN:N	1:6C:122:GLN:OE1	2.36	0.57
1:FB:122:GLN:OE1	1:FB:122:GLN:N	2.38	0.56
1:TC:122:GLN:OE1	1:TC:122:GLN:N	2.36	0.56
1:mC:122:GLN:N	1:mC:122:GLN:OE1	2.36	0.56
1:pC:122:GLN:N	1:pC:122:GLN:OE1	2.36	0.56
1:JC:122:GLN:OE1	1:JC:122:GLN:N	2.36	0.56
1:RC:122:GLN:N	1:RC:122:GLN:OE1	2.36	0.56
1:aC:122:GLN:N	1:aC:122:GLN:OE1	2.36	0.56
1:hC:122:GLN:N	1:hC:122:GLN:OE1	2.36	0.56
1:PB:122:GLN:OE1	1:PB:122:GLN:N	2.38	0.56
1:UB:122:GLN:OE1	1:UB:122:GLN:N	2.38	0.56
1:ZB:122:GLN:OE1	1:ZB:122:GLN:N	2.38	0.56
1:ZC:122:GLN:N	1:ZC:122:GLN:OE1	2.36	0.56
1:eC:122:GLN:OE1	1:eC:122:GLN:N	2.36	0.56
1:hB:122:GLN:OE1	1:hB:122:GLN:N	2.38	0.56
1:iC:122:GLN:N	1:iC:122:GLN:OE1	2.36	0.56
1:kC:122:GLN:N	1:kC:122:GLN:OE1	2.36	0.56
1:lC:122:GLN:N	1:lC:122:GLN:OE1	2.36	0.56
1:nB:122:GLN:OE1	1:nB:122:GLN:N	2.38	0.56
1:wB:122:GLN:OE1	1:wB:122:GLN:N	2.38	0.56
1:3B:122:GLN:OE1	1:3B:122:GLN:N	2.38	0.56
1:uC:12:GLY:O	1:zC:43:HIS:ND1	2.39	0.56
1:dC:122:GLN:N	1:dC:122:GLN:OE1	2.36	0.56
1:8C:122:GLN:N	1:8C:122:GLN:OE1	2.36	0.56
1:EB:122:GLN:OE1	1:EB:122:GLN:N	2.38	0.56
1:gC:122:GLN:N	1:gC:122:GLN:OE1	2.36	0.56
1:DB:102:TYR:OH	1:6C:116:LEU:CD2	2.54	0.56
1:DC:122:GLN:N	1:DC:122:GLN:OE1	2.36	0.56
1:GB:122:GLN:OE1	1:GB:122:GLN:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LC:122:GLN:N	1:LC:122:GLN:OE1	2.36	0.56
1:SB:122:GLN:OE1	1:SB:122:GLN:N	2.38	0.56
1:WB:122:GLN:OE1	1:WB:122:GLN:N	2.38	0.56
1:dB:122:GLN:OE1	1:dB:122:GLN:N	2.38	0.56
1:gB:122:GLN:OE1	1:gB:122:GLN:N	2.38	0.56
1:lB:122:GLN:OE1	1:lB:122:GLN:N	2.38	0.56
1:tB:122:GLN:OE1	1:tB:122:GLN:N	2.38	0.56
1:BB:122:GLN:OE1	1:BB:122:GLN:N	2.38	0.56
1:bB:122:GLN:OE1	1:bB:122:GLN:N	2.38	0.56
1:rB:122:GLN:OE1	1:rB:122:GLN:N	2.38	0.56
1:HB:122:GLN:OE1	1:HB:122:GLN:N	2.38	0.56
1:7C:122:GLN:OE1	1:7C:122:GLN:N	2.36	0.56
1:JB:122:GLN:N	1:JB:122:GLN:OE1	2.38	0.55
1:YC:122:GLN:OE1	1:YC:122:GLN:N	2.36	0.55
1:rC:43:HIS:ND1	1:8C:12:GLY:O	2.38	0.55
1:QB:122:GLN:N	1:QB:122:GLN:OE1	2.38	0.55
1:XC:122:GLN:N	1:XC:122:GLN:OE1	2.36	0.55
1:pB:122:GLN:N	1:pB:122:GLN:OE1	2.38	0.55
1:sB:122:GLN:OE1	1:sB:122:GLN:N	2.38	0.55
1:cB:122:GLN:OE1	1:cB:122:GLN:N	2.38	0.55
1:xB:122:GLN:N	1:xB:122:GLN:OE1	2.38	0.55
1:DB:122:GLN:N	1:DB:122:GLN:OE1	2.38	0.55
1:KC:122:GLN:N	1:KC:122:GLN:OE1	2.36	0.55
1:2B:122:GLN:OE1	1:2B:122:GLN:N	2.38	0.55
1:jB:122:GLN:N	1:jB:122:GLN:OE1	2.38	0.55
1:WA:103:GLY:O	1:WA:107:VAL:HG23	2.07	0.55
1:2A:103:GLY:O	1:2A:107:VAL:HG23	2.07	0.55
1:eB:122:GLN:N	1:eB:122:GLN:OE1	2.38	0.55
1:lA:103:GLY:O	1:lA:107:VAL:HG23	2.07	0.55
1:xA:103:GLY:O	1:xA:107:VAL:HG23	2.07	0.55
1:zA:103:GLY:O	1:zA:107:VAL:HG23	2.07	0.55
1:DA:103:GLY:O	1:DA:107:VAL:HG23	2.07	0.55
1:SA:103:GLY:O	1:SA:107:VAL:HG23	2.07	0.55
1:UC:12:GLY:O	1:lC:43:HIS:ND1	2.40	0.55
1:YA:103:GLY:O	1:YA:107:VAL:HG23	2.07	0.55
1:ZA:103:GLY:O	1:ZA:107:VAL:HG23	2.07	0.55
1:bA:103:GLY:O	1:bA:107:VAL:HG23	2.07	0.55
1:dC:12:GLY:O	1:hC:43:HIS:ND1	2.39	0.55
1:fB:122:GLN:N	1:fB:122:GLN:OE1	2.38	0.55
1:hA:103:GLY:O	1:hA:107:VAL:HG23	2.07	0.55
1:8B:122:GLN:OE1	1:8B:122:GLN:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:122:GLN:N	1:AC:122:GLN:OE1	2.36	0.55
1:BA:103:GLY:O	1:BA:107:VAL:HG23	2.07	0.55
1:CC:122:GLN:OE1	1:CC:122:GLN:N	2.36	0.55
1:MA:103:GLY:O	1:MA:107:VAL:HG23	2.07	0.55
1:OA:103:GLY:O	1:OA:107:VAL:HG23	2.07	0.55
1:UA:103:GLY:O	1:UA:107:VAL:HG23	2.07	0.55
1:VC:122:GLN:OE1	1:VC:122:GLN:N	2.36	0.55
1:XA:103:GLY:O	1:XA:107:VAL:HG23	2.07	0.55
1:uA:103:GLY:O	1:uA:107:VAL:HG23	2.07	0.55
1:vA:103:GLY:O	1:vA:107:VAL:HG23	2.07	0.55
1:3A:103:GLY:O	1:3A:107:VAL:HG23	2.07	0.55
1:4A:103:GLY:O	1:4A:107:VAL:HG23	2.07	0.55
1:6A:103:GLY:O	1:6A:107:VAL:HG23	2.07	0.55
1:CA:103:GLY:O	1:CA:107:VAL:HG23	2.07	0.55
1:EC:41:LYS:O	1:SC:10:MET:HE1	2.05	0.55
1:NA:103:GLY:O	1:NA:107:VAL:HG23	2.07	0.55
1:jA:103:GLY:O	1:jA:107:VAL:HG23	2.07	0.55
1:tA:103:GLY:O	1:tA:107:VAL:HG23	2.07	0.55
1:5A:103:GLY:O	1:5A:107:VAL:HG23	2.07	0.55
1:EA:103:GLY:O	1:EA:107:VAL:HG23	2.07	0.55
1:LB:122:GLN:OE1	1:LB:122:GLN:N	2.38	0.55
1:QA:103:GLY:O	1:QA:107:VAL:HG23	2.07	0.55
1:aA:103:GLY:O	1:aA:107:VAL:HG23	2.07	0.55
1:iA:103:GLY:O	1:iA:107:VAL:HG23	2.07	0.55
1:qC:43:HIS:ND1	1:4C:12:GLY:O	2.40	0.55
1:JA:103:GLY:O	1:JA:107:VAL:HG23	2.07	0.55
1:eA:103:GLY:O	1:eA:107:VAL:HG23	2.07	0.55
1:mA:103:GLY:O	1:mA:107:VAL:HG23	2.07	0.55
1:yA:103:GLY:O	1:yA:107:VAL:HG23	2.07	0.55
1:GA:103:GLY:O	1:GA:107:VAL:HG23	2.07	0.54
1:TA:103:GLY:O	1:TA:107:VAL:HG23	2.07	0.54
1:oB:122:GLN:OE1	1:oB:122:GLN:N	2.38	0.54
1:pA:103:GLY:O	1:pA:107:VAL:HG23	2.07	0.54
1:qA:103:GLY:O	1:qA:107:VAL:HG23	2.07	0.54
1:rA:103:GLY:O	1:rA:107:VAL:HG23	2.07	0.54
1:1A:103:GLY:O	1:1A:107:VAL:HG23	2.07	0.54
1:FA:103:GLY:O	1:FA:107:VAL:HG23	2.07	0.54
1:IA:103:GLY:O	1:IA:107:VAL:HG23	2.07	0.54
1:IC:122:GLN:N	1:IC:122:GLN:OE1	2.36	0.54
1:IB:122:GLN:OE1	1:IB:122:GLN:N	2.38	0.54
1:gA:103:GLY:O	1:gA:107:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:oA:103:GLY:O	1:oA:107:VAL:HG23	2.07	0.54
1:wA:103:GLY:O	1:wA:107:VAL:HG23	2.07	0.54
1:8A:103:GLY:O	1:8A:107:VAL:HG23	2.07	0.54
1:LA:103:GLY:O	1:LA:107:VAL:HG23	2.07	0.54
1:dA:103:GLY:O	1:dA:107:VAL:HG23	2.07	0.54
1:oC:122:GLN:OE1	1:oC:122:GLN:N	2.36	0.54
1:cA:103:GLY:O	1:cA:107:VAL:HG23	2.07	0.54
1:PA:103:GLY:O	1:PA:107:VAL:HG23	2.07	0.54
1:fA:103:GLY:O	1:fA:107:VAL:HG23	2.07	0.54
1:MB:122:GLN:OE1	1:MB:122:GLN:N	2.38	0.54
1:nA:103:GLY:O	1:nA:107:VAL:HG23	2.07	0.54
1:HA:103:GLY:O	1:HA:107:VAL:HG23	2.07	0.54
1:KA:103:GLY:O	1:KA:107:VAL:HG23	2.07	0.54
1:sA:103:GLY:O	1:sA:107:VAL:HG23	2.07	0.54
1:JC:107:VAL:O	1:JC:111:VAL:HG23	2.08	0.54
1:RA:103:GLY:O	1:RA:107:VAL:HG23	2.07	0.54
1:1C:107:VAL:O	1:1C:111:VAL:HG23	2.09	0.54
1:VA:103:GLY:O	1:VA:107:VAL:HG23	2.07	0.54
1:XB:122:GLN:N	1:XB:122:GLN:OE1	2.38	0.54
1:hC:107:VAL:O	1:hC:111:VAL:HG23	2.08	0.54
1:kA:103:GLY:O	1:kA:107:VAL:HG23	2.07	0.54
1:uC:107:VAL:O	1:uC:111:VAL:HG23	2.08	0.54
1:wC:107:VAL:O	1:wC:111:VAL:HG23	2.08	0.54
1:yC:107:VAL:O	1:yC:111:VAL:HG23	2.08	0.54
1:4B:122:GLN:N	1:4B:122:GLN:OE1	2.38	0.54
1:MC:107:VAL:O	1:MC:111:VAL:HG23	2.09	0.53
1:ZC:107:VAL:O	1:ZC:111:VAL:HG23	2.09	0.53
1:aC:107:VAL:O	1:aC:111:VAL:HG23	2.08	0.53
1:iC:107:VAL:O	1:iC:111:VAL:HG23	2.08	0.53
1:pC:107:VAL:O	1:pC:111:VAL:HG23	2.08	0.53
1:4C:107:VAL:O	1:4C:111:VAL:HG23	2.09	0.53
1:7A:103:GLY:O	1:7A:107:VAL:HG23	2.07	0.53
1:AA:103:GLY:O	1:AA:107:VAL:HG23	2.07	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	2.08	0.53
1:UC:107:VAL:O	1:UC:111:VAL:HG23	2.08	0.53
1:fC:107:VAL:O	1:fC:111:VAL:HG23	2.08	0.53
1:jC:107:VAL:O	1:jC:111:VAL:HG23	2.08	0.53
1:nC:107:VAL:O	1:nC:111:VAL:HG23	2.08	0.53
1:QC:107:VAL:O	1:QC:111:VAL:HG23	2.09	0.53
1:WC:107:VAL:O	1:WC:111:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:cC:107:VAL:O	1:cC:111:VAL:HG23	2.08	0.53
1:qC:107:VAL:O	1:qC:111:VAL:HG23	2.08	0.53
1:rA:78:LEU:HD22	1:rB:78:LEU:HD23	1.91	0.53
1:uB:122:GLN:OE1	1:uB:122:GLN:N	2.38	0.53
1:yA:78:LEU:HD22	1:yB:78:LEU:HD23	1.91	0.53
1:zB:122:GLN:OE1	1:zB:122:GLN:N	2.38	0.53
1:AC:107:VAL:O	1:AC:111:VAL:HG23	2.09	0.53
1:BC:107:VAL:O	1:BC:111:VAL:HG23	2.09	0.53
1:CB:122:GLN:OE1	1:CB:122:GLN:N	2.38	0.53
1:GA:78:LEU:HD22	1:GB:78:LEU:HD23	1.91	0.53
1:PC:107:VAL:O	1:PC:111:VAL:HG23	2.08	0.53
1:VC:107:VAL:O	1:VC:111:VAL:HG23	2.09	0.53
1:mC:107:VAL:O	1:mC:111:VAL:HG23	2.08	0.53
1:uA:78:LEU:HD22	1:uB:78:LEU:HD23	1.91	0.53
1:vB:122:GLN:OE1	1:vB:122:GLN:N	2.38	0.53
1:7A:78:LEU:HD22	1:7B:78:LEU:HD23	1.91	0.53
1:IC:107:VAL:O	1:IC:111:VAL:HG23	2.09	0.53
1:KA:78:LEU:HD22	1:KB:78:LEU:HD23	1.91	0.53
1:TC:107:VAL:O	1:TC:111:VAL:HG23	2.09	0.53
1:dC:107:VAL:O	1:dC:111:VAL:HG23	2.08	0.53
1:gC:107:VAL:O	1:gC:111:VAL:HG23	2.09	0.53
1:6A:78:LEU:HD22	1:6B:78:LEU:HD23	1.91	0.53
1:EA:78:LEU:HD22	1:EB:78:LEU:HD23	1.91	0.53
1:JC:43:HIS:ND1	1:NC:12:GLY:O	2.42	0.53
1:RB:122:GLN:OE1	1:RB:122:GLN:N	2.38	0.53
1:gA:78:LEU:HD22	1:gB:78:LEU:HD23	1.91	0.53
1:kB:122:GLN:OE1	1:kB:122:GLN:N	2.38	0.53
1:IA:78:LEU:HD22	1:IB:78:LEU:HD23	1.91	0.53
1:oC:107:VAL:O	1:oC:111:VAL:HG23	2.09	0.53
1:2C:107:VAL:O	1:2C:111:VAL:HG23	2.08	0.53
1:vC:107:VAL:O	1:vC:111:VAL:HG23	2.08	0.53
1:xC:107:VAL:O	1:xC:111:VAL:HG23	2.08	0.53
1:KB:122:GLN:OE1	1:KB:122:GLN:N	2.38	0.53
1:OA:78:LEU:HD22	1:OB:78:LEU:HD23	1.91	0.53
1:RA:78:LEU:HD22	1:RB:78:LEU:HD23	1.91	0.53
1:YC:107:VAL:O	1:YC:111:VAL:HG23	2.09	0.53
1:iB:122:GLN:OE1	1:iB:122:GLN:N	2.38	0.53
1:kA:78:LEU:HD22	1:kB:78:LEU:HD23	1.91	0.53
1:zC:107:VAL:O	1:zC:111:VAL:HG23	2.09	0.53
1:7B:122:GLN:OE1	1:7B:122:GLN:N	2.38	0.53
1:BA:78:LEU:HD22	1:BB:78:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DC:107:VAL:O	1:DC:111:VAL:HG23	2.09	0.53
1:RC:107:VAL:O	1:RC:111:VAL:HG23	2.09	0.53
1:aB:122:GLN:OE1	1:aB:122:GLN:N	2.38	0.53
1:bC:107:VAL:O	1:bC:111:VAL:HG23	2.08	0.53
1:cA:78:LEU:HD22	1:cB:78:LEU:HD23	1.91	0.53
1:dA:78:LEU:HD22	1:dB:78:LEU:HD23	1.91	0.53
1:kC:107:VAL:O	1:kC:111:VAL:HG23	2.09	0.53
1:qA:78:LEU:HD22	1:qB:78:LEU:HD23	1.91	0.53
1:4A:78:LEU:HD22	1:4B:78:LEU:HD23	1.91	0.53
1:FA:78:LEU:HD22	1:FB:78:LEU:HD23	1.91	0.53
1:MA:78:LEU:HD22	1:MB:78:LEU:HD23	1.91	0.53
1:SA:78:LEU:HD22	1:SB:78:LEU:HD23	1.91	0.53
1:UA:78:LEU:HD22	1:UB:78:LEU:HD23	1.91	0.53
1:iA:78:LEU:HD22	1:iB:78:LEU:HD23	1.91	0.53
1:tA:78:LEU:HD22	1:tB:78:LEU:HD23	1.91	0.53
1:1A:78:LEU:HD22	1:1B:78:LEU:HD23	1.91	0.53
1:IA:78:LEU:HD22	1:IB:78:LEU:HD23	1.91	0.53
1:WA:78:LEU:HD22	1:WB:78:LEU:HD23	1.91	0.53
1:YB:122:GLN:OE1	1:YB:122:GLN:N	2.38	0.53
1:aA:78:LEU:HD22	1:aB:78:LEU:HD23	1.91	0.53
1:2A:78:LEU:HD22	1:2B:78:LEU:HD23	1.91	0.53
1:fA:78:LEU:HD22	1:fB:78:LEU:HD23	1.91	0.53
1:oA:78:LEU:HD22	1:oB:78:LEU:HD23	1.91	0.53
1:rC:107:VAL:O	1:rC:111:VAL:HG23	2.09	0.53
1:xA:78:LEU:HD22	1:xB:78:LEU:HD23	1.91	0.53
1:CC:107:VAL:O	1:CC:111:VAL:HG23	2.08	0.52
1:DA:78:LEU:HD22	1:DB:78:LEU:HD23	1.91	0.52
1:GC:107:VAL:O	1:GC:111:VAL:HG23	2.09	0.52
1:LA:78:LEU:HD22	1:LB:78:LEU:HD23	1.91	0.52
1:OC:107:VAL:O	1:OC:111:VAL:HG23	2.09	0.52
1:TB:122:GLN:OE1	1:TB:122:GLN:N	2.38	0.52
1:eC:107:VAL:O	1:eC:111:VAL:HG23	2.09	0.52
1:6C:107:VAL:O	1:6C:111:VAL:HG23	2.09	0.52
1:pC:12:GLY:O	1:5C:43:HIS:ND1	2.42	0.52
1:wA:78:LEU:HD22	1:wB:78:LEU:HD23	1.91	0.52
1:3A:78:LEU:HD22	1:3B:78:LEU:HD23	1.91	0.52
1:XC:107:VAL:O	1:XC:111:VAL:HG23	2.08	0.52
1:YA:78:LEU:HD22	1:YB:78:LEU:HD23	1.91	0.52
1:lC:107:VAL:O	1:lC:111:VAL:HG23	2.08	0.52
1:8A:78:LEU:HD22	1:8B:78:LEU:HD23	1.91	0.52
1:PA:78:LEU:HD22	1:PB:78:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HA:78:LEU:HD22	1:HB:78:LEU:HD23	1.91	0.52
1:LC:107:VAL:O	1:LC:111:VAL:HG23	2.08	0.52
1:NC:107:VAL:O	1:NC:111:VAL:HG23	2.08	0.52
1:SC:107:VAL:O	1:SC:111:VAL:HG23	2.09	0.52
1:mB:122:GLN:OE1	1:mB:122:GLN:N	2.38	0.52
1:nA:78:LEU:HD22	1:nB:78:LEU:HD23	1.91	0.52
1:sA:78:LEU:HD22	1:sB:78:LEU:HD23	1.91	0.52
1:8C:107:VAL:O	1:8C:111:VAL:HG23	2.08	0.52
1:hA:78:LEU:HD22	1:hB:78:LEU:HD23	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	2.08	0.52
1:HC:107:VAL:O	1:HC:111:VAL:HG23	2.08	0.52
1:ZA:78:LEU:HD22	1:ZB:78:LEU:HD23	1.91	0.52
1:sC:107:VAL:O	1:sC:111:VAL:HG23	2.09	0.52
1:OB:122:GLN:N	1:OB:122:GLN:OE1	2.38	0.52
1:QA:78:LEU:HD22	1:QB:78:LEU:HD23	1.91	0.52
1:bA:78:LEU:HD22	1:bB:78:LEU:HD23	1.91	0.52
1:jA:78:LEU:HD22	1:jB:78:LEU:HD23	1.91	0.52
1:5C:107:VAL:O	1:5C:111:VAL:HG23	2.09	0.52
1:EC:3:PHE:HE2	1:SC:58:LEU:CD1	2.23	0.52
1:JA:78:LEU:HD22	1:JB:78:LEU:HD23	1.91	0.52
1:eA:78:LEU:HD22	1:eB:78:LEU:HD23	1.91	0.52
1:pA:78:LEU:HD22	1:pB:78:LEU:HD23	1.91	0.52
1:zA:78:LEU:HD22	1:zB:78:LEU:HD23	1.91	0.52
1:1B:122:GLN:N	1:1B:122:GLN:OE1	2.38	0.51
1:vA:78:LEU:HD22	1:vB:78:LEU:HD23	1.91	0.51
1:NA:78:LEU:HD22	1:NB:78:LEU:HD23	1.91	0.51
1:TA:78:LEU:HD22	1:TB:78:LEU:HD23	1.91	0.51
1:mA:78:LEU:HD22	1:mB:78:LEU:HD23	1.91	0.51
1:VA:78:LEU:HD22	1:VB:78:LEU:HD23	1.91	0.51
1:6B:122:GLN:N	1:6B:122:GLN:OE1	2.38	0.51
1:7C:107:VAL:O	1:7C:111:VAL:HG23	2.09	0.51
1:KC:107:VAL:O	1:KC:111:VAL:HG23	2.09	0.51
1:nC:87:LEU:O	1:nC:90:THR:OG1	2.27	0.51
1:rC:12:GLY:O	1:8C:43:HIS:ND1	2.43	0.51
1:AA:78:LEU:HD22	1:AB:78:LEU:HD23	1.91	0.51
1:CA:78:LEU:HD22	1:CB:78:LEU:HD23	1.91	0.51
1:bC:74:GLU:OE2	1:eC:74:GLU:OE2	2.29	0.51
1:5A:78:LEU:HD22	1:5B:78:LEU:HD23	1.91	0.51
1:7C:87:LEU:O	1:7C:90:THR:OG1	2.27	0.51
1:AB:122:GLN:OE1	1:AB:122:GLN:N	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:VB:122:GLN:N	1:VB:122:GLN:OE1	2.38	0.51
1:mC:87:LEU:O	1:mC:90:THR:OG1	2.27	0.51
1:KC:87:LEU:O	1:KC:90:THR:OG1	2.27	0.51
1:cC:87:LEU:O	1:cC:90:THR:OG1	2.27	0.51
1:4C:87:LEU:O	1:4C:90:THR:OG1	2.27	0.51
1:PC:87:LEU:O	1:PC:90:THR:OG1	2.27	0.51
1:TC:87:LEU:O	1:TC:90:THR:OG1	2.27	0.51
1:XA:78:LEU:HD22	1:XB:78:LEU:HD23	1.91	0.51
1:gC:87:LEU:O	1:gC:90:THR:OG1	2.27	0.51
1:FC:87:LEU:O	1:FC:90:THR:OG1	2.27	0.51
1:JC:87:LEU:O	1:JC:90:THR:OG1	2.27	0.51
1:aC:87:LEU:O	1:aC:90:THR:OG1	2.27	0.51
1:2C:87:LEU:O	1:2C:90:THR:OG1	2.27	0.51
1:xC:87:LEU:O	1:xC:90:THR:OG1	2.27	0.51
1:MC:87:LEU:O	1:MC:90:THR:OG1	2.27	0.51
1:QC:87:LEU:O	1:QC:90:THR:OG1	2.27	0.51
1:jC:87:LEU:O	1:jC:90:THR:OG1	2.27	0.51
1:qC:87:LEU:O	1:qC:90:THR:OG1	2.27	0.51
1:EC:3:PHE:CE2	1:SC:58:LEU:CD1	2.94	0.50
1:IC:87:LEU:O	1:IC:90:THR:OG1	2.27	0.50
1:iC:87:LEU:O	1:iC:90:THR:OG1	2.27	0.50
1:yB:122:GLN:OE1	1:yB:122:GLN:N	2.38	0.50
1:EC:87:LEU:O	1:EC:90:THR:OG1	2.27	0.50
1:HC:87:LEU:O	1:HC:90:THR:OG1	2.27	0.50
1:XC:116:LEU:CD2	1:FB:102:TYR:OH	2.60	0.50
1:dC:87:LEU:O	1:dC:90:THR:OG1	2.27	0.50
1:oC:87:LEU:O	1:oC:90:THR:OG1	2.27	0.50
1:pC:43:HIS:ND1	1:5C:12:GLY:O	2.43	0.50
1:vC:87:LEU:O	1:vC:90:THR:OG1	2.27	0.50
1:sC:87:LEU:O	1:sC:90:THR:OG1	2.27	0.50
1:zC:87:LEU:O	1:zC:90:THR:OG1	2.27	0.50
1:lC:87:LEU:O	1:lC:90:THR:OG1	2.27	0.50
1:pC:87:LEU:O	1:pC:90:THR:OG1	2.27	0.50
1:EC:43:HIS:CD2	1:SC:7:VAL:HG13	2.46	0.50
1:uC:87:LEU:O	1:uC:90:THR:OG1	2.27	0.50
1:rC:87:LEU:O	1:rC:90:THR:OG1	2.27	0.50
1:yC:87:LEU:O	1:yC:90:THR:OG1	2.27	0.50
1:DC:74:GLU:OE2	1:TC:74:GLU:OE2	2.30	0.50
1:SC:87:LEU:O	1:SC:90:THR:OG1	2.27	0.50
1:wC:87:LEU:O	1:wC:90:THR:OG1	2.27	0.50
1:1C:87:LEU:O	1:1C:90:THR:OG1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DC:87:LEU:O	1:DC:90:THR:OG1	2.27	0.50
1:GC:87:LEU:O	1:GC:90:THR:OG1	2.27	0.50
1:VC:87:LEU:O	1:VC:90:THR:OG1	2.27	0.50
1:AC:87:LEU:O	1:AC:90:THR:OG1	2.27	0.49
1:RC:87:LEU:O	1:RC:90:THR:OG1	2.27	0.49
1:YC:87:LEU:O	1:YC:90:THR:OG1	2.27	0.49
1:BC:87:LEU:O	1:BC:90:THR:OG1	2.27	0.49
1:tC:87:LEU:O	1:tC:90:THR:OG1	2.27	0.49
1:3C:87:LEU:O	1:3C:90:THR:OG1	2.27	0.49
1:WC:87:LEU:O	1:WC:90:THR:OG1	2.27	0.49
1:kC:87:LEU:O	1:kC:90:THR:OG1	2.27	0.49
1:XC:87:LEU:O	1:XC:90:THR:OG1	2.27	0.49
1:CC:87:LEU:O	1:CC:90:THR:OG1	2.27	0.49
1:dC:43:HIS:ND1	1:hC:12:GLY:O	2.46	0.49
1:bC:87:LEU:O	1:bC:90:THR:OG1	2.27	0.49
1:eC:87:LEU:O	1:eC:90:THR:OG1	2.27	0.48
1:ZC:87:LEU:O	1:ZC:90:THR:OG1	2.27	0.48
1:hC:87:LEU:O	1:hC:90:THR:OG1	2.27	0.48
1:8C:87:LEU:O	1:8C:90:THR:OG1	2.27	0.48
1:LC:87:LEU:O	1:LC:90:THR:OG1	2.27	0.48
1:NA:56:GLN:O	1:NA:60:HIS:ND1	2.41	0.47
1:5A:56:GLN:O	1:5A:60:HIS:ND1	2.41	0.47
1:YC:43:HIS:ND1	1:mC:12:GLY:O	2.48	0.47
1:lA:56:GLN:O	1:lA:60:HIS:ND1	2.41	0.47
1:UA:56:GLN:O	1:UA:60:HIS:ND1	2.41	0.47
1:AA:56:GLN:O	1:AA:60:HIS:ND1	2.41	0.47
1:EA:56:GLN:O	1:EA:60:HIS:ND1	2.41	0.47
1:SA:56:GLN:O	1:SA:60:HIS:ND1	2.41	0.46
1:VA:56:GLN:O	1:VA:60:HIS:ND1	2.41	0.46
1:eA:56:GLN:O	1:eA:60:HIS:ND1	2.41	0.46
1:EC:43:HIS:HD2	1:SC:7:VAL:HG13	1.81	0.46
1:5C:87:LEU:O	1:5C:90:THR:OG1	2.27	0.46
1:UA:78:LEU:C	1:UA:78:LEU:HD23	2.41	0.46
1:wA:78:LEU:C	1:wA:78:LEU:HD23	2.41	0.46
1:QA:78:LEU:C	1:QA:78:LEU:HD23	2.41	0.46
1:jA:78:LEU:HD23	1:jA:78:LEU:C	2.41	0.46
1:vA:78:LEU:HD23	1:vA:78:LEU:C	2.41	0.46
1:EC:43:HIS:CD2	1:SC:7:VAL:CG1	2.99	0.46
1:KA:78:LEU:C	1:KA:78:LEU:HD23	2.41	0.46
1:NC:87:LEU:O	1:NC:90:THR:OG1	2.27	0.46
1:OA:78:LEU:HD23	1:OA:78:LEU:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PA:56:GLN:O	1:PA:60:HIS:ND1	2.41	0.46
1:bA:78:LEU:C	1:bA:78:LEU:HD23	2.41	0.46
1:eA:78:LEU:HD23	1:eA:78:LEU:C	2.41	0.46
1:zA:78:LEU:C	1:zA:78:LEU:HD23	2.41	0.46
1:7A:78:LEU:HD23	1:7A:78:LEU:C	2.41	0.46
1:1A:78:LEU:C	1:1A:78:LEU:HD23	2.41	0.45
1:EA:78:LEU:C	1:EA:78:LEU:HD23	2.41	0.45
1:MA:78:LEU:HD23	1:MA:78:LEU:C	2.41	0.45
1:SA:78:LEU:C	1:SA:78:LEU:HD23	2.41	0.45
1:TA:78:LEU:HD23	1:TA:78:LEU:C	2.41	0.45
1:XA:78:LEU:C	1:XA:78:LEU:HD23	2.41	0.45
1:YA:78:LEU:HD23	1:YA:78:LEU:C	2.41	0.45
1:uA:78:LEU:C	1:uA:78:LEU:HD23	2.41	0.45
1:yA:78:LEU:C	1:yA:78:LEU:HD23	2.41	0.45
1:3A:78:LEU:C	1:3A:78:LEU:HD23	2.41	0.45
1:CA:78:LEU:HD23	1:CA:78:LEU:C	2.41	0.45
1:bA:56:GLN:O	1:bA:60:HIS:ND1	2.41	0.45
1:fA:78:LEU:C	1:fA:78:LEU:HD23	2.41	0.45
1:mA:78:LEU:C	1:mA:78:LEU:HD23	2.41	0.45
1:rA:78:LEU:C	1:rA:78:LEU:HD23	2.41	0.45
1:tA:78:LEU:HD23	1:tA:78:LEU:C	2.41	0.45
1:6A:78:LEU:C	1:6A:78:LEU:HD23	2.41	0.45
1:GA:78:LEU:C	1:GA:78:LEU:HD23	2.41	0.45
1:4A:78:LEU:C	1:4A:78:LEU:HD23	2.41	0.45
1:DA:78:LEU:C	1:DA:78:LEU:HD23	2.41	0.45
1:OC:87:LEU:O	1:OC:90:THR:OG1	2.27	0.45
1:iA:78:LEU:C	1:iA:78:LEU:HD23	2.41	0.45
1:lA:78:LEU:C	1:lA:78:LEU:HD23	2.41	0.45
1:nA:56:GLN:O	1:nA:60:HIS:ND1	2.41	0.45
1:FA:78:LEU:C	1:FA:78:LEU:HD23	2.41	0.45
1:aA:78:LEU:C	1:aA:78:LEU:HD23	2.41	0.45
1:qA:78:LEU:HD23	1:qA:78:LEU:C	2.41	0.45
1:HA:78:LEU:HD23	1:HA:78:LEU:C	2.41	0.45
1:WA:78:LEU:C	1:WA:78:LEU:HD23	2.41	0.45
1:oA:78:LEU:HD23	1:oA:78:LEU:C	2.41	0.45
1:6C:87:LEU:O	1:6C:90:THR:OG1	2.27	0.45
1:8A:56:GLN:O	1:8A:60:HIS:ND1	2.41	0.45
1:IA:78:LEU:C	1:IA:78:LEU:HD23	2.41	0.45
1:RA:78:LEU:HD23	1:RA:78:LEU:C	2.41	0.45
1:VA:78:LEU:C	1:VA:78:LEU:HD23	2.41	0.45
1:cA:78:LEU:HD23	1:cA:78:LEU:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:sA:78:LEU:C	1:sA:78:LEU:HD23	2.41	0.45
1:AA:78:LEU:HD23	1:AA:78:LEU:C	2.41	0.45
1:LA:56:GLN:O	1:LA:60:HIS:ND1	2.41	0.45
1:LA:78:LEU:C	1:LA:78:LEU:HD23	2.41	0.45
1:gA:78:LEU:C	1:gA:78:LEU:HD23	2.41	0.45
1:kA:78:LEU:C	1:kA:78:LEU:HD23	2.41	0.45
1:BA:78:LEU:C	1:BA:78:LEU:HD23	2.41	0.45
1:OA:56:GLN:O	1:OA:60:HIS:ND1	2.41	0.45
1:dA:78:LEU:C	1:dA:78:LEU:HD23	2.41	0.45
1:nA:78:LEU:C	1:nA:78:LEU:HD23	2.41	0.45
1:pA:78:LEU:C	1:pA:78:LEU:HD23	2.41	0.45
1:wA:56:GLN:O	1:wA:60:HIS:ND1	2.41	0.45
1:PA:78:LEU:C	1:PA:78:LEU:HD23	2.41	0.45
1:8A:78:LEU:C	1:8A:78:LEU:HD23	2.41	0.45
1:QA:56:GLN:O	1:QA:60:HIS:ND1	2.41	0.44
1:gA:56:GLN:O	1:gA:60:HIS:ND1	2.41	0.44
1:vC:41:LYS:O	1:yC:10:MET:HE1	2.16	0.44
1:JA:78:LEU:C	1:JA:78:LEU:HD23	2.41	0.44
1:NA:78:LEU:C	1:NA:78:LEU:HD23	2.41	0.44
1:5A:78:LEU:C	1:5A:78:LEU:HD23	2.41	0.44
1:2A:78:LEU:HD23	1:2A:78:LEU:C	2.41	0.44
1:dA:56:GLN:O	1:dA:60:HIS:ND1	2.41	0.44
1:jA:56:GLN:O	1:jA:60:HIS:ND1	2.41	0.44
1:mA:56:GLN:O	1:mA:60:HIS:ND1	2.41	0.44
1:tA:56:GLN:O	1:tA:60:HIS:ND1	2.41	0.44
1:3A:56:GLN:O	1:3A:60:HIS:ND1	2.41	0.44
1:4A:56:GLN:O	1:4A:60:HIS:ND1	2.41	0.44
1:XC:9:ASN:HA	1:FB:41:LYS:HD2	2.00	0.44
1:ZA:78:LEU:C	1:ZA:78:LEU:HD23	2.41	0.44
1:xA:78:LEU:C	1:xA:78:LEU:HD23	2.41	0.44
1:MA:56:GLN:O	1:MA:60:HIS:ND1	2.41	0.44
1:YA:56:GLN:O	1:YA:60:HIS:ND1	2.41	0.44
1:hA:78:LEU:C	1:hA:78:LEU:HD23	2.41	0.44
1:6A:56:GLN:O	1:6A:60:HIS:ND1	2.41	0.44
1:fC:87:LEU:O	1:fC:90:THR:OG1	2.27	0.44
1:TA:56:GLN:O	1:TA:60:HIS:ND1	2.41	0.44
1:1A:56:GLN:O	1:1A:60:HIS:ND1	2.41	0.44
1:DB:41:LYS:HD2	1:6C:9:ASN:HA	1.99	0.43
1:JC:12:GLY:O	1:NC:43:HIS:ND1	2.50	0.43
1:qC:12:GLY:O	1:4C:43:HIS:ND1	2.50	0.43
1:DA:56:GLN:O	1:DA:60:HIS:ND1	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:uA:56:GLN:O	1:uA:60:HIS:ND1	2.41	0.43
1:HC:43:HIS:ND1	1:KC:12:GLY:O	2.52	0.43
1:UC:87:LEU:O	1:UC:90:THR:OG1	2.27	0.43
1:BC:116:LEU:CD2	1:1B:102:TYR:OH	2.67	0.43
1:CA:56:GLN:O	1:CA:60:HIS:ND1	2.41	0.43
1:XA:56:GLN:O	1:XA:60:HIS:ND1	2.41	0.43
1:yA:56:GLN:O	1:yA:60:HIS:ND1	2.41	0.43
1:GA:56:GLN:O	1:GA:60:HIS:ND1	2.41	0.42
1:cC:116:LEU:CD2	1:kB:102:TYR:OH	2.68	0.42
1:rA:56:GLN:O	1:rA:60:HIS:ND1	2.41	0.42
1:HC:12:GLY:O	1:KC:43:HIS:ND1	2.52	0.42
1:BC:124:PHE:CD2	1:1B:22:MET:HE2	2.54	0.42
1:GC:43:HIS:ND1	1:LC:12:GLY:O	2.52	0.42
1:zA:56:GLN:O	1:zA:60:HIS:ND1	2.41	0.41
1:NC:43:HIS:HE2	1:NC:48:THR:HG1	1.68	0.41
1:vA:56:GLN:O	1:vA:60:HIS:ND1	2.41	0.41
1:aA:56:GLN:O	1:aA:60:HIS:ND1	2.41	0.41
1:pA:56:GLN:O	1:pA:60:HIS:ND1	2.41	0.41
1:JC:74:GLU:OE2	1:NC:74:GLU:OE2	2.37	0.41
1:AB:26:PRO:O	1:AB:28:VAL:N	2.54	0.41
1:HA:56:GLN:O	1:HA:60:HIS:ND1	2.41	0.41
1:VB:26:PRO:O	1:VB:28:VAL:N	2.54	0.41
1:OC:43:HIS:HE2	1:OC:48:THR:HG1	1.67	0.41
1:YB:26:PRO:O	1:YB:28:VAL:N	2.54	0.41
1:DB:26:PRO:O	1:DB:28:VAL:N	2.54	0.41
1:DC:79:ILE:HG12	1:TC:78:LEU:HD21	2.03	0.41
1:GB:26:PRO:O	1:GB:28:VAL:N	2.54	0.41
1:JA:56:GLN:O	1:JA:60:HIS:ND1	2.41	0.41
1:KB:26:PRO:O	1:KB:28:VAL:N	2.54	0.41
1:iA:56:GLN:O	1:iA:60:HIS:ND1	2.41	0.41
1:rB:26:PRO:O	1:rB:28:VAL:N	2.54	0.41
1:uB:26:PRO:O	1:uB:28:VAL:N	2.54	0.41
1:yB:26:PRO:O	1:yB:28:VAL:N	2.54	0.41
1:3C:43:HIS:HE2	1:3C:48:THR:HG1	1.69	0.41
1:5C:43:HIS:HE2	1:5C:48:THR:HG1	1.69	0.41
1:7B:26:PRO:O	1:7B:28:VAL:N	2.54	0.41
1:EC:43:HIS:HE2	1:EC:48:THR:HG1	1.68	0.41
1:cC:12:GLY:O	1:iC:43:HIS:ND1	2.54	0.41
1:tC:43:HIS:HE2	1:tC:48:THR:HG1	1.69	0.41
1:ZA:56:GLN:O	1:ZA:60:HIS:ND1	2.41	0.40
1:sA:56:GLN:O	1:sA:60:HIS:ND1	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:56:GLN:O	1:BA:60:HIS:ND1	2.41	0.40
1:NB:26:PRO:O	1:NB:28:VAL:N	2.54	0.40
1:2C:43:HIS:HE2	1:2C:48:THR:HG1	1.69	0.40
1:sC:41:LYS:O	1:7C:10:MET:HE1	2.20	0.40
1:4B:26:PRO:O	1:4B:28:VAL:N	2.54	0.40
1:5B:26:PRO:O	1:5B:28:VAL:N	2.54	0.40
1:7A:56:GLN:O	1:7A:60:HIS:ND1	2.41	0.40
1:MB:26:PRO:O	1:MB:28:VAL:N	2.54	0.40
1:cB:26:PRO:O	1:cB:28:VAL:N	2.54	0.40
1:vB:26:PRO:O	1:vB:28:VAL:N	2.54	0.40
1:hA:56:GLN:O	1:hA:60:HIS:ND1	2.41	0.40
1:iB:26:PRO:O	1:iB:28:VAL:N	2.54	0.40
1:HB:26:PRO:O	1:HB:28:VAL:N	2.54	0.40
1:aB:26:PRO:O	1:aB:28:VAL:N	2.54	0.40
1:fB:26:PRO:O	1:fB:28:VAL:N	2.54	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	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	1B	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	1C	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	2A	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	2B	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	2C	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	3A	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	3B	122/175 (70%)	118 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3C	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	4A	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	4B	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	4C	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	5A	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	5B	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	5C	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	6A	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	6B	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	6C	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	7A	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	7B	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	7C	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	8A	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	8B	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	8C	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	AA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	AB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	AC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	BA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	BB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	BC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	CA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	CB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	CC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	DA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	DB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	DC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	EA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	EB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	EC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	FA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	FB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	FC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	GA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	GB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	GC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	HA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	HB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	HC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	IA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	IB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	IC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	JA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	JB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	JC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	KA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	KB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	KC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	LA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	LB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	LC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	MA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	MB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	MC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	NA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	NB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	NC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	OA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	OB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	OC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	PA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	PB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	PC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	QA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	QB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	QC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	RA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	RB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	RC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	SA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	SB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	SC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	TA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	TB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	TC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	UA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	UB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	UC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	VA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	VB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	VC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	WA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	WB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	WC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	XA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	XB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	XC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	YA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	YB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	YC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	ZA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	ZB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	ZC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	aA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	aB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	aC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	bA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	bB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	bC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	cA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	cB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	cC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	dA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	dB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	dC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	eA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	eB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	eC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	fA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	fB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	fC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	gA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	gB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	gC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	hA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	hB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	hC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	iA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	iB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	iC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	jA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	jB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	jC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	kA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	kB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	kC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	lA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	lB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	lC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	mA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	mB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	mC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	nA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	nB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	nC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	oA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	oB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	oC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	pA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	pB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	pC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	qA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	qB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	qC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	rA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	rB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	rC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	sA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	sB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	sC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	tA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	tB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	tC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	uA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	uB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	uC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	vA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	vB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	vC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	wA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	wB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	wC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	xA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	xB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	xC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	yA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	yB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	yC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
1	zA	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
1	zB	122/175 (70%)	118 (97%)	4 (3%)	0	100	100
1	zC	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
All	All	22080/31500 (70%)	21540 (98%)	540 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	114/148 (77%)	114 (100%)	0	100	100
1	1B	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	1C	114/148 (77%)	114 (100%)	0	100	100
1	2A	114/148 (77%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2B	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	2C	114/148 (77%)	114 (100%)	0	100	100
1	3A	114/148 (77%)	114 (100%)	0	100	100
1	3B	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	3C	114/148 (77%)	114 (100%)	0	100	100
1	4A	114/148 (77%)	114 (100%)	0	100	100
1	4B	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	4C	114/148 (77%)	114 (100%)	0	100	100
1	5A	114/148 (77%)	114 (100%)	0	100	100
1	5B	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	5C	114/148 (77%)	114 (100%)	0	100	100
1	6A	114/148 (77%)	114 (100%)	0	100	100
1	6B	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	6C	114/148 (77%)	114 (100%)	0	100	100
1	7A	114/148 (77%)	114 (100%)	0	100	100
1	7B	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	7C	114/148 (77%)	114 (100%)	0	100	100
1	8A	114/148 (77%)	114 (100%)	0	100	100
1	8B	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	8C	114/148 (77%)	114 (100%)	0	100	100
1	AA	114/148 (77%)	114 (100%)	0	100	100
1	AB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	AC	114/148 (77%)	114 (100%)	0	100	100
1	BA	114/148 (77%)	114 (100%)	0	100	100
1	BB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	BC	114/148 (77%)	114 (100%)	0	100	100
1	CA	114/148 (77%)	114 (100%)	0	100	100
1	CB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	CC	114/148 (77%)	114 (100%)	0	100	100
1	DA	114/148 (77%)	114 (100%)	0	100	100
1	DB	113/148 (76%)	112 (99%)	1 (1%)	70	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DC	114/148 (77%)	114 (100%)	0	100	100
1	EA	114/148 (77%)	114 (100%)	0	100	100
1	EB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	EC	114/148 (77%)	114 (100%)	0	100	100
1	FA	114/148 (77%)	114 (100%)	0	100	100
1	FB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	FC	114/148 (77%)	114 (100%)	0	100	100
1	GA	114/148 (77%)	114 (100%)	0	100	100
1	GB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	GC	114/148 (77%)	114 (100%)	0	100	100
1	HA	114/148 (77%)	114 (100%)	0	100	100
1	HB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	HC	114/148 (77%)	114 (100%)	0	100	100
1	IA	114/148 (77%)	114 (100%)	0	100	100
1	IB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	IC	114/148 (77%)	114 (100%)	0	100	100
1	JA	114/148 (77%)	114 (100%)	0	100	100
1	JB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	JC	114/148 (77%)	114 (100%)	0	100	100
1	KA	114/148 (77%)	114 (100%)	0	100	100
1	KB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	KC	114/148 (77%)	114 (100%)	0	100	100
1	LA	114/148 (77%)	114 (100%)	0	100	100
1	LB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	LC	114/148 (77%)	114 (100%)	0	100	100
1	MA	114/148 (77%)	114 (100%)	0	100	100
1	MB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	MC	114/148 (77%)	114 (100%)	0	100	100
1	NA	114/148 (77%)	114 (100%)	0	100	100
1	NB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	NC	114/148 (77%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	OA	114/148 (77%)	114 (100%)	0	100	100
1	OB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	OC	114/148 (77%)	114 (100%)	0	100	100
1	PA	114/148 (77%)	114 (100%)	0	100	100
1	PB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	PC	114/148 (77%)	114 (100%)	0	100	100
1	QA	114/148 (77%)	114 (100%)	0	100	100
1	QB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	QC	114/148 (77%)	114 (100%)	0	100	100
1	RA	114/148 (77%)	114 (100%)	0	100	100
1	RB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	RC	114/148 (77%)	114 (100%)	0	100	100
1	SA	114/148 (77%)	114 (100%)	0	100	100
1	SB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	SC	114/148 (77%)	114 (100%)	0	100	100
1	TA	114/148 (77%)	114 (100%)	0	100	100
1	TB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	TC	114/148 (77%)	114 (100%)	0	100	100
1	UA	114/148 (77%)	114 (100%)	0	100	100
1	UB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	UC	114/148 (77%)	114 (100%)	0	100	100
1	VA	114/148 (77%)	114 (100%)	0	100	100
1	VB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	VC	114/148 (77%)	114 (100%)	0	100	100
1	WA	114/148 (77%)	114 (100%)	0	100	100
1	WB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	WC	114/148 (77%)	114 (100%)	0	100	100
1	XA	114/148 (77%)	114 (100%)	0	100	100
1	XB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	XC	114/148 (77%)	114 (100%)	0	100	100
1	YA	114/148 (77%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	YB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	YC	114/148 (77%)	114 (100%)	0	100	100
1	ZA	114/148 (77%)	114 (100%)	0	100	100
1	ZB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	ZC	114/148 (77%)	114 (100%)	0	100	100
1	aA	114/148 (77%)	114 (100%)	0	100	100
1	aB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	aC	114/148 (77%)	114 (100%)	0	100	100
1	bA	114/148 (77%)	114 (100%)	0	100	100
1	bB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	bC	114/148 (77%)	114 (100%)	0	100	100
1	cA	114/148 (77%)	114 (100%)	0	100	100
1	cB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	cC	114/148 (77%)	114 (100%)	0	100	100
1	dA	114/148 (77%)	114 (100%)	0	100	100
1	dB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	dC	114/148 (77%)	114 (100%)	0	100	100
1	eA	114/148 (77%)	114 (100%)	0	100	100
1	eB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	eC	114/148 (77%)	114 (100%)	0	100	100
1	fA	114/148 (77%)	114 (100%)	0	100	100
1	fB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	fC	114/148 (77%)	114 (100%)	0	100	100
1	gA	114/148 (77%)	114 (100%)	0	100	100
1	gB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	gC	114/148 (77%)	114 (100%)	0	100	100
1	hA	114/148 (77%)	114 (100%)	0	100	100
1	hB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	hC	114/148 (77%)	114 (100%)	0	100	100
1	iA	114/148 (77%)	114 (100%)	0	100	100
1	iB	113/148 (76%)	112 (99%)	1 (1%)	70	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	iC	114/148 (77%)	114 (100%)	0	100	100
1	jA	114/148 (77%)	114 (100%)	0	100	100
1	jB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	jC	114/148 (77%)	114 (100%)	0	100	100
1	kA	114/148 (77%)	114 (100%)	0	100	100
1	kB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	kC	114/148 (77%)	114 (100%)	0	100	100
1	lA	114/148 (77%)	114 (100%)	0	100	100
1	lB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	lC	114/148 (77%)	114 (100%)	0	100	100
1	mA	114/148 (77%)	114 (100%)	0	100	100
1	mB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	mC	114/148 (77%)	114 (100%)	0	100	100
1	nA	114/148 (77%)	114 (100%)	0	100	100
1	nB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	nC	114/148 (77%)	114 (100%)	0	100	100
1	oA	114/148 (77%)	114 (100%)	0	100	100
1	oB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	oC	114/148 (77%)	114 (100%)	0	100	100
1	pA	114/148 (77%)	114 (100%)	0	100	100
1	pB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	pC	114/148 (77%)	114 (100%)	0	100	100
1	qA	114/148 (77%)	114 (100%)	0	100	100
1	qB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	qC	114/148 (77%)	114 (100%)	0	100	100
1	rA	114/148 (77%)	114 (100%)	0	100	100
1	rB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	rC	114/148 (77%)	114 (100%)	0	100	100
1	sA	114/148 (77%)	114 (100%)	0	100	100
1	sB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	sC	114/148 (77%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	tA	114/148 (77%)	114 (100%)	0	100	100
1	tB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	tC	114/148 (77%)	114 (100%)	0	100	100
1	uA	114/148 (77%)	114 (100%)	0	100	100
1	uB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	uC	114/148 (77%)	114 (100%)	0	100	100
1	vA	114/148 (77%)	114 (100%)	0	100	100
1	vB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	vC	114/148 (77%)	114 (100%)	0	100	100
1	wA	114/148 (77%)	114 (100%)	0	100	100
1	wB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	wC	114/148 (77%)	114 (100%)	0	100	100
1	xA	114/148 (77%)	114 (100%)	0	100	100
1	xB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	xC	114/148 (77%)	114 (100%)	0	100	100
1	yA	114/148 (77%)	114 (100%)	0	100	100
1	yB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	yC	114/148 (77%)	114 (100%)	0	100	100
1	zA	114/148 (77%)	114 (100%)	0	100	100
1	zB	113/148 (76%)	112 (99%)	1 (1%)	70	75
1	zC	114/148 (77%)	114 (100%)	0	100	100
All	All	20460/26640 (77%)	20400 (100%)	60 (0%)	84	83

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BB	93	LEU
1	CB	93	LEU
1	DB	93	LEU
1	EB	93	LEU
1	FB	93	LEU
1	GB	93	LEU
1	HB	93	LEU
1	IB	93	LEU
1	1B	93	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	JB	93	LEU
1	KB	93	LEU
1	LB	93	LEU
1	MB	93	LEU
1	NB	93	LEU
1	OB	93	LEU
1	PB	93	LEU
1	QB	93	LEU
1	RB	93	LEU
1	SB	93	LEU
1	TB	93	LEU
1	UB	93	LEU
1	VB	93	LEU
1	WB	93	LEU
1	XB	93	LEU
1	YB	93	LEU
1	ZB	93	LEU
1	aB	93	LEU
1	bB	93	LEU
1	cB	93	LEU
1	dB	93	LEU
1	eB	93	LEU
1	fB	93	LEU
1	gB	93	LEU
1	hB	93	LEU
1	iB	93	LEU
1	2B	93	LEU
1	jB	93	LEU
1	kB	93	LEU
1	lB	93	LEU
1	mB	93	LEU
1	nB	93	LEU
1	oB	93	LEU
1	pB	93	LEU
1	qB	93	LEU
1	rB	93	LEU
1	sB	93	LEU
1	tB	93	LEU
1	uB	93	LEU
1	vB	93	LEU
1	wB	93	LEU
1	xB	93	LEU

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Mol	Chain	Res	Type
1	yB	93	LEU
1	zB	93	LEU
1	3B	93	LEU
1	4B	93	LEU
1	5B	93	LEU
1	6B	93	LEU
1	7B	93	LEU
1	8B	93	LEU
1	AB	93	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (514) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	56	GLN
1	1A	84	GLN
1	1A	100	HIS
1	1A	101	HIS
1	1A	122	GLN
1	AC	113	GLN
1	BA	56	GLN
1	BA	84	GLN
1	BA	100	HIS
1	BA	101	HIS
1	BA	122	GLN
1	BB	56	GLN
1	BB	100	HIS
1	BC	40	GLN
1	BC	60	HIS
1	BC	113	GLN
1	CA	56	GLN
1	CA	84	GLN
1	CA	100	HIS
1	CA	101	HIS
1	CA	122	GLN
1	CB	56	GLN
1	CB	100	HIS
1	CC	40	GLN
1	CC	60	HIS
1	CC	113	GLN
1	DA	56	GLN
1	DA	84	GLN
1	DA	100	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	DA	101	HIS
1	DA	122	GLN
1	DB	56	GLN
1	DB	100	HIS
1	DC	113	GLN
1	EA	56	GLN
1	EA	84	GLN
1	EA	100	HIS
1	EA	101	HIS
1	EA	113	GLN
1	EA	122	GLN
1	EA	128	GLN
1	EB	56	GLN
1	EB	100	HIS
1	EC	40	GLN
1	EC	113	GLN
1	FA	56	GLN
1	FA	84	GLN
1	FA	100	HIS
1	FA	101	HIS
1	FA	113	GLN
1	FA	122	GLN
1	FB	56	GLN
1	FB	100	HIS
1	FC	113	GLN
1	GA	56	GLN
1	GA	84	GLN
1	GA	100	HIS
1	GA	101	HIS
1	GA	122	GLN
1	GA	128	GLN
1	GB	56	GLN
1	GB	100	HIS
1	GC	40	GLN
1	GC	60	HIS
1	GC	113	GLN
1	HA	56	GLN
1	HA	84	GLN
1	HA	100	HIS
1	HA	101	HIS
1	HA	122	GLN
1	HB	56	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	HB	100	HIS
1	HC	60	HIS
1	HC	113	GLN
1	IA	56	GLN
1	IA	84	GLN
1	IA	100	HIS
1	IA	101	HIS
1	IA	122	GLN
1	IB	56	GLN
1	IB	100	HIS
1	IC	113	GLN
1	JA	56	GLN
1	JA	84	GLN
1	JA	100	HIS
1	JA	101	HIS
1	JA	122	GLN
1	1B	56	GLN
1	1B	100	HIS
1	JB	56	GLN
1	JB	100	HIS
1	JC	40	GLN
1	JC	113	GLN
1	KA	56	GLN
1	KA	84	GLN
1	KA	100	HIS
1	KA	101	HIS
1	KA	122	GLN
1	KB	56	GLN
1	KB	100	HIS
1	KC	40	GLN
1	KC	113	GLN
1	LA	56	GLN
1	LA	84	GLN
1	LA	101	HIS
1	LA	122	GLN
1	LB	56	GLN
1	LB	100	HIS
1	LC	113	GLN
1	MA	56	GLN
1	MA	84	GLN
1	MA	101	HIS
1	MA	122	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	MB	56	GLN
1	MB	100	HIS
1	MC	40	GLN
1	MC	113	GLN
1	NA	56	GLN
1	NA	84	GLN
1	NA	101	HIS
1	NA	122	GLN
1	NB	56	GLN
1	NB	100	HIS
1	NC	40	GLN
1	NC	113	GLN
1	OA	56	GLN
1	OA	84	GLN
1	OA	100	HIS
1	OA	101	HIS
1	OA	122	GLN
1	OB	56	GLN
1	OB	100	HIS
1	OC	40	GLN
1	OC	113	GLN
1	PA	56	GLN
1	PA	84	GLN
1	PA	122	GLN
1	PB	56	GLN
1	PB	100	HIS
1	PC	40	GLN
1	PC	60	HIS
1	PC	113	GLN
1	QA	56	GLN
1	QA	84	GLN
1	QA	100	HIS
1	QA	101	HIS
1	QA	122	GLN
1	QB	56	GLN
1	QB	100	HIS
1	QC	40	GLN
1	QC	113	GLN
1	RA	56	GLN
1	RA	84	GLN
1	RA	100	HIS
1	RA	101	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	RA	122	GLN
1	RB	56	GLN
1	RB	100	HIS
1	RC	40	GLN
1	RC	113	GLN
1	1C	40	GLN
1	1C	60	HIS
1	1C	113	GLN
1	SA	56	GLN
1	SA	84	GLN
1	SA	122	GLN
1	SA	128	GLN
1	SB	56	GLN
1	SB	100	HIS
1	SC	40	GLN
1	SC	113	GLN
1	TA	56	GLN
1	TA	84	GLN
1	TA	122	GLN
1	TA	128	GLN
1	TB	56	GLN
1	TB	100	HIS
1	TC	113	GLN
1	UA	56	GLN
1	UA	84	GLN
1	UA	100	HIS
1	UA	101	HIS
1	UA	122	GLN
1	UB	56	GLN
1	UB	100	HIS
1	UC	113	GLN
1	VA	56	GLN
1	VA	84	GLN
1	VA	100	HIS
1	VA	101	HIS
1	VA	122	GLN
1	VB	56	GLN
1	VB	100	HIS
1	VC	113	GLN
1	WA	56	GLN
1	WA	84	GLN
1	WA	100	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	WA	101	HIS
1	WA	122	GLN
1	WB	56	GLN
1	WB	100	HIS
1	WC	60	HIS
1	WC	113	GLN
1	XA	56	GLN
1	XA	84	GLN
1	XA	101	HIS
1	XA	122	GLN
1	XB	56	GLN
1	XB	100	HIS
1	XC	113	GLN
1	YA	56	GLN
1	YA	84	GLN
1	YA	100	HIS
1	YA	101	HIS
1	YA	122	GLN
1	YA	128	GLN
1	YB	56	GLN
1	YB	100	HIS
1	YC	113	GLN
1	ZA	56	GLN
1	ZA	84	GLN
1	ZA	100	HIS
1	ZA	101	HIS
1	ZA	122	GLN
1	ZB	56	GLN
1	ZB	100	HIS
1	ZC	40	GLN
1	ZC	113	GLN
1	aA	56	GLN
1	aA	84	GLN
1	aA	100	HIS
1	aA	101	HIS
1	aA	122	GLN
1	aB	56	GLN
1	aB	100	HIS
1	2A	56	GLN
1	2A	84	GLN
1	2A	100	HIS
1	2A	101	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	122	GLN
1	2A	128	GLN
1	aC	60	HIS
1	aC	113	GLN
1	bA	56	GLN
1	bA	84	GLN
1	bA	100	HIS
1	bA	101	HIS
1	bA	122	GLN
1	bB	56	GLN
1	bB	100	HIS
1	bC	113	GLN
1	cA	56	GLN
1	cA	84	GLN
1	cA	101	HIS
1	cA	122	GLN
1	cB	56	GLN
1	cB	100	HIS
1	cC	113	GLN
1	dA	56	GLN
1	dA	84	GLN
1	dA	101	HIS
1	dA	122	GLN
1	dB	56	GLN
1	dB	100	HIS
1	dC	113	GLN
1	eA	56	GLN
1	eA	84	GLN
1	eA	100	HIS
1	eA	122	GLN
1	eB	56	GLN
1	eB	100	HIS
1	eC	113	GLN
1	fA	56	GLN
1	fA	84	GLN
1	fA	100	HIS
1	fA	101	HIS
1	fA	122	GLN
1	fB	56	GLN
1	fB	100	HIS
1	fC	40	GLN
1	fC	113	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	gA	56	GLN
1	gA	84	GLN
1	gA	101	HIS
1	gA	122	GLN
1	gB	56	GLN
1	gB	100	HIS
1	gC	113	GLN
1	hA	56	GLN
1	hA	84	GLN
1	hA	100	HIS
1	hA	101	HIS
1	hA	122	GLN
1	hB	56	GLN
1	hB	100	HIS
1	hC	113	GLN
1	iA	56	GLN
1	iA	84	GLN
1	iA	100	HIS
1	iA	101	HIS
1	iA	122	GLN
1	iB	56	GLN
1	iB	100	HIS
1	iC	60	HIS
1	iC	113	GLN
1	jA	56	GLN
1	jA	84	GLN
1	jA	100	HIS
1	jA	101	HIS
1	jA	122	GLN
1	2B	56	GLN
1	2B	100	HIS
1	jB	56	GLN
1	jB	100	HIS
1	jC	40	GLN
1	jC	113	GLN
1	kA	56	GLN
1	kA	84	GLN
1	kA	100	HIS
1	kA	101	HIS
1	kA	122	GLN
1	kB	56	GLN
1	kB	100	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	kC	60	HIS
1	kC	113	GLN
1	lA	56	GLN
1	lA	84	GLN
1	lA	122	GLN
1	lA	128	GLN
1	lB	56	GLN
1	lB	100	HIS
1	lC	113	GLN
1	mA	56	GLN
1	mA	84	GLN
1	mA	101	HIS
1	mA	122	GLN
1	mB	56	GLN
1	mB	100	HIS
1	mC	40	GLN
1	mC	113	GLN
1	nA	56	GLN
1	nA	84	GLN
1	nA	122	GLN
1	nA	128	GLN
1	nB	56	GLN
1	nB	100	HIS
1	nC	40	GLN
1	nC	113	GLN
1	oA	56	GLN
1	oA	84	GLN
1	oA	122	GLN
1	oA	128	GLN
1	oB	56	GLN
1	oB	100	HIS
1	oC	60	HIS
1	oC	113	GLN
1	pA	56	GLN
1	pA	84	GLN
1	pA	100	HIS
1	pA	101	HIS
1	pA	122	GLN
1	pB	56	GLN
1	pB	100	HIS
1	pC	40	GLN
1	pC	113	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	qA	56	GLN
1	qA	84	GLN
1	qA	100	HIS
1	qA	101	HIS
1	qA	113	GLN
1	qA	122	GLN
1	qB	56	GLN
1	qB	100	HIS
1	qC	60	HIS
1	qC	113	GLN
1	rA	56	GLN
1	rA	84	GLN
1	rA	100	HIS
1	rA	101	HIS
1	rA	122	GLN
1	rB	56	GLN
1	rB	100	HIS
1	rC	40	GLN
1	rC	113	GLN
1	2C	113	GLN
1	sA	56	GLN
1	sA	84	GLN
1	sA	100	HIS
1	sA	101	HIS
1	sA	122	GLN
1	sB	56	GLN
1	sB	100	HIS
1	sC	113	GLN
1	tA	56	GLN
1	tA	84	GLN
1	tA	100	HIS
1	tA	101	HIS
1	tA	122	GLN
1	tB	56	GLN
1	tB	100	HIS
1	tC	40	GLN
1	tC	60	HIS
1	tC	113	GLN
1	uA	56	GLN
1	uA	84	GLN
1	uA	100	HIS
1	uA	101	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	uA	122	GLN
1	uB	56	GLN
1	uB	100	HIS
1	uC	113	GLN
1	vA	9	ASN
1	vA	56	GLN
1	vA	84	GLN
1	vA	100	HIS
1	vA	101	HIS
1	vA	122	GLN
1	vA	128	GLN
1	vB	56	GLN
1	vB	100	HIS
1	vC	113	GLN
1	wA	56	GLN
1	wA	84	GLN
1	wA	100	HIS
1	wA	101	HIS
1	wA	122	GLN
1	wB	56	GLN
1	wB	100	HIS
1	wC	113	GLN
1	xA	56	GLN
1	xA	84	GLN
1	xA	100	HIS
1	xA	101	HIS
1	xA	122	GLN
1	xB	56	GLN
1	xB	100	HIS
1	xC	60	HIS
1	xC	113	GLN
1	yA	56	GLN
1	yA	84	GLN
1	yA	100	HIS
1	yA	101	HIS
1	yA	122	GLN
1	yB	56	GLN
1	yB	100	HIS
1	yC	60	HIS
1	yC	113	GLN
1	zA	56	GLN
1	zA	84	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	zA	100	HIS
1	zA	101	HIS
1	zA	122	GLN
1	zB	56	GLN
1	zB	100	HIS
1	zC	113	GLN
1	3A	56	GLN
1	3A	84	GLN
1	3A	101	HIS
1	3A	122	GLN
1	3B	56	GLN
1	3B	100	HIS
1	3C	40	GLN
1	3C	113	GLN
1	4A	56	GLN
1	4A	84	GLN
1	4A	101	HIS
1	4A	122	GLN
1	4A	128	GLN
1	4B	56	GLN
1	4B	100	HIS
1	4C	40	GLN
1	4C	113	GLN
1	5A	56	GLN
1	5A	84	GLN
1	5A	101	HIS
1	5A	122	GLN
1	5B	56	GLN
1	5B	100	HIS
1	5C	40	GLN
1	5C	60	HIS
1	5C	113	GLN
1	6A	56	GLN
1	6A	84	GLN
1	6A	100	HIS
1	6A	101	HIS
1	6A	122	GLN
1	6B	56	GLN
1	6B	100	HIS
1	6C	40	GLN
1	6C	60	HIS
1	6C	113	GLN

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Mol	Chain	Res	Type
1	7A	56	GLN
1	7A	84	GLN
1	7A	100	HIS
1	7A	101	HIS
1	7A	122	GLN
1	7B	56	GLN
1	7B	100	HIS
1	7C	40	GLN
1	7C	113	GLN
1	8A	56	GLN
1	8A	84	GLN
1	8A	101	HIS
1	8A	122	GLN
1	8B	56	GLN
1	8B	100	HIS
1	8C	113	GLN
1	AA	56	GLN
1	AA	84	GLN
1	AA	100	HIS
1	AA	101	HIS
1	AA	122	GLN
1	AB	56	GLN
1	AB	100	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

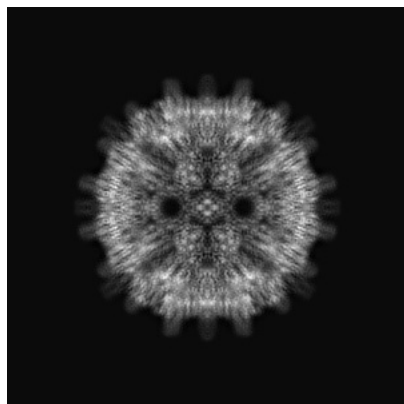
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15295. These allow visual inspection of the internal detail of the map and identification of artifacts.

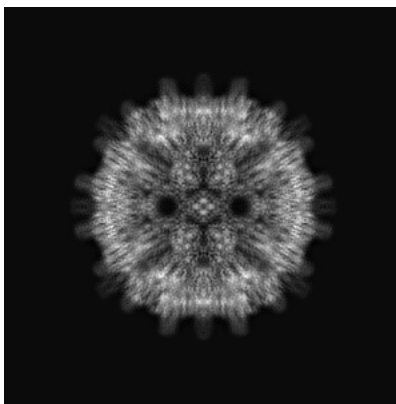
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

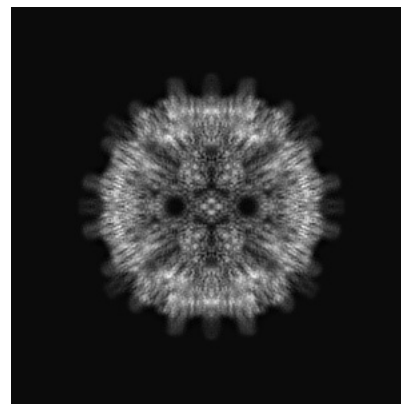
#### 6.1.1 Primary map



X

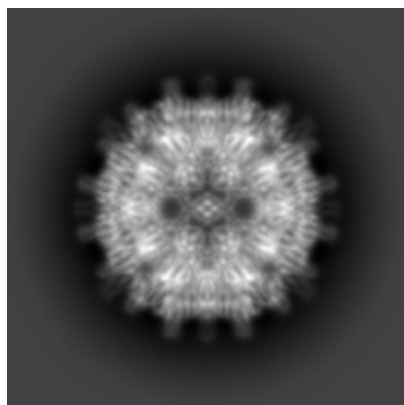


Y

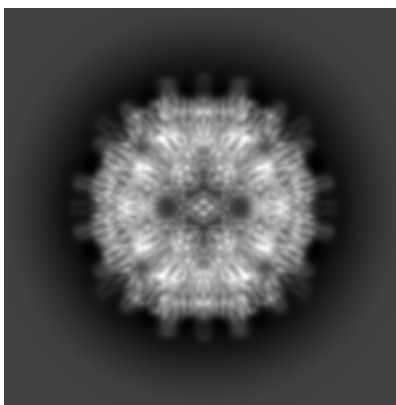


Z

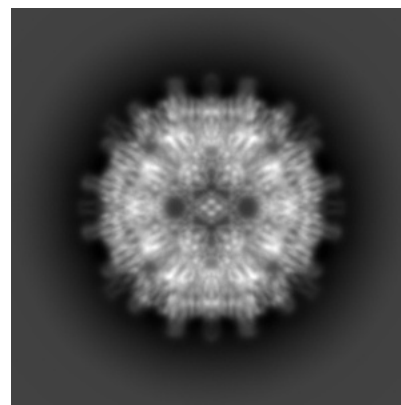
#### 6.1.2 Raw map



X



Y

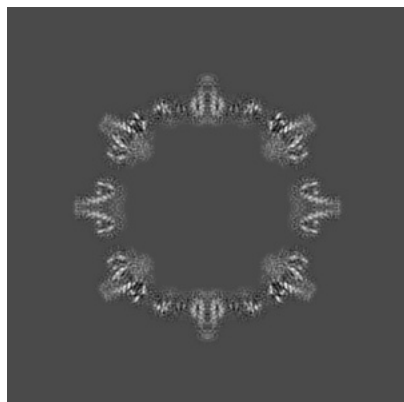


Z

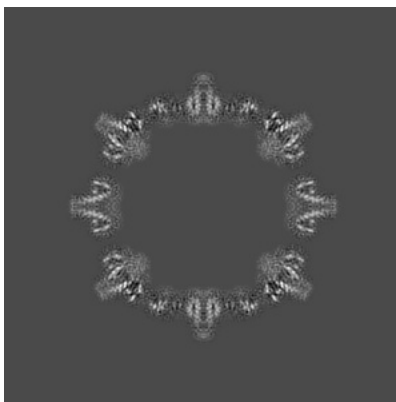
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

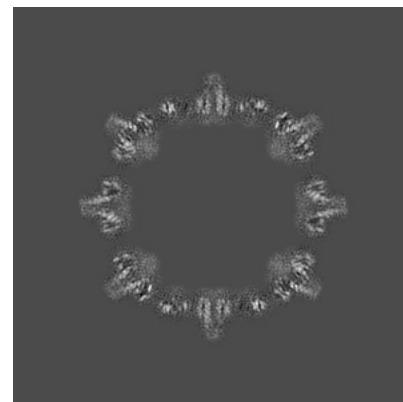
### 6.2.1 Primary map



X Index: 216

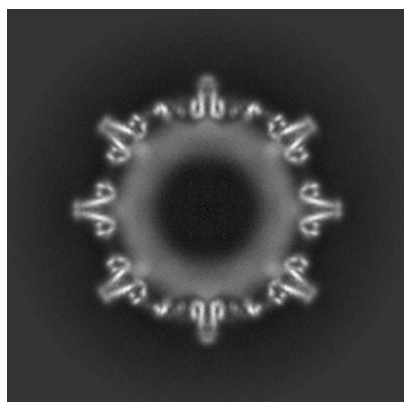


Y Index: 216

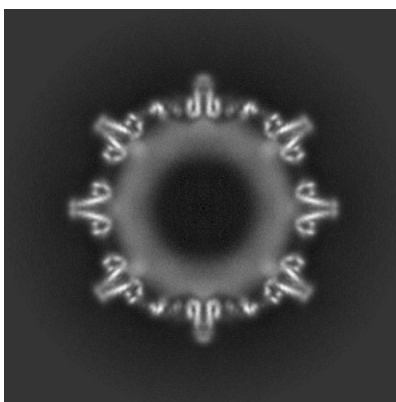


Z Index: 216

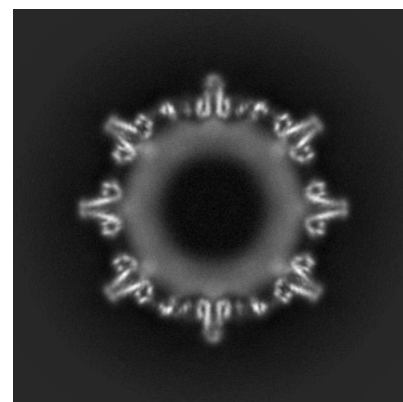
### 6.2.2 Raw map



X Index: 216



Y Index: 216

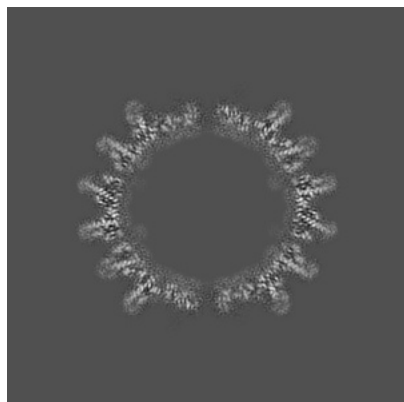


Z Index: 216

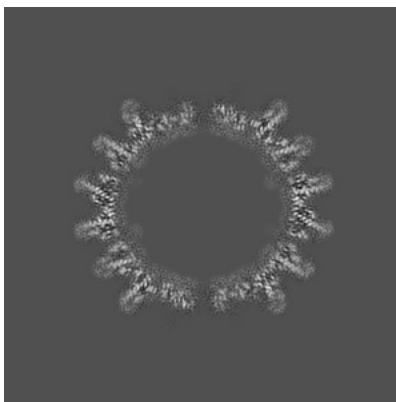
The images above show central slices of the map in three orthogonal directions.

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

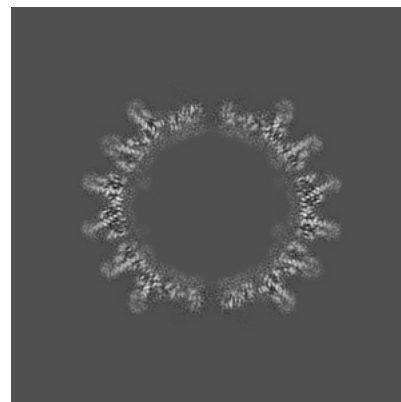
### 6.3.1 Primary map



X Index: 173

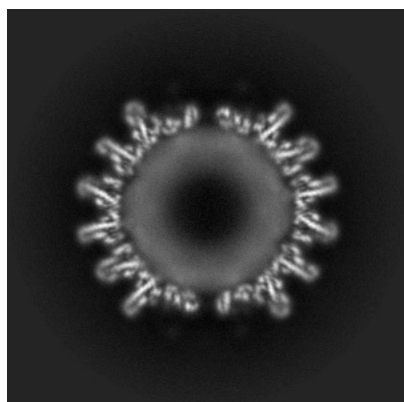


Y Index: 173

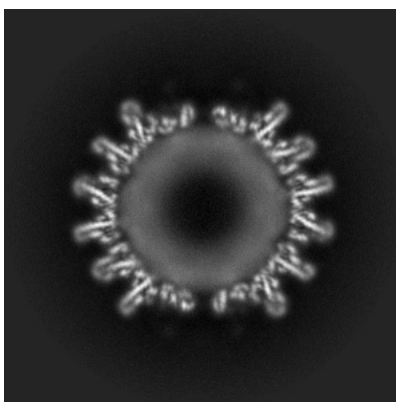


Z Index: 258

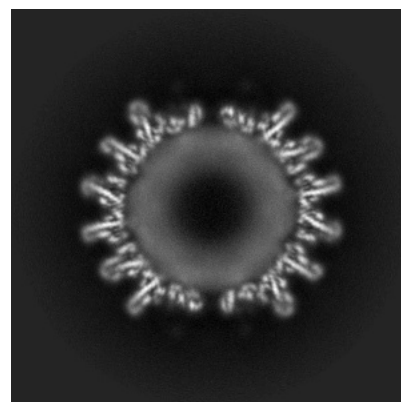
### 6.3.2 Raw map



X Index: 174



Y Index: 174

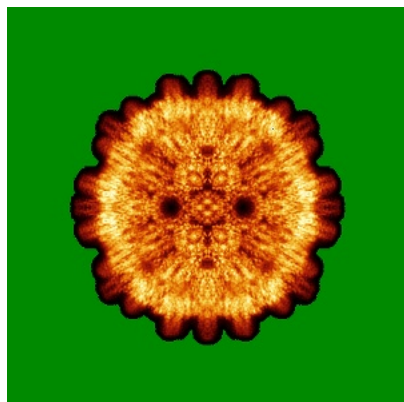


Z Index: 173

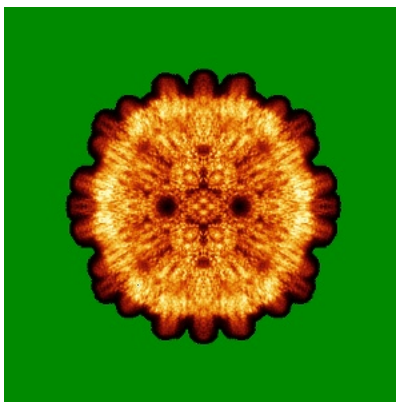
The images above show the largest variance slices of the map in three orthogonal directions.

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

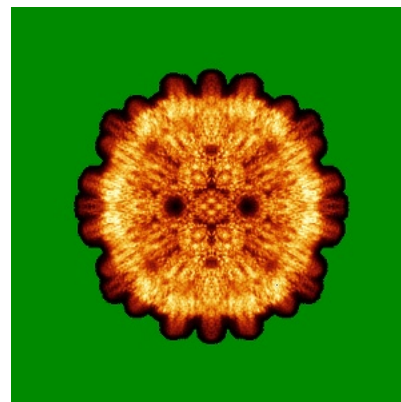
### 6.4.1 Primary map



X

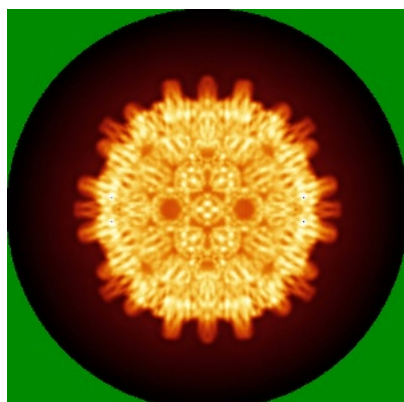


Y



Z

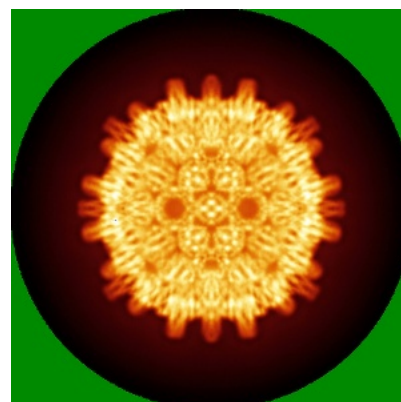
### 6.4.2 Raw map



X



Y

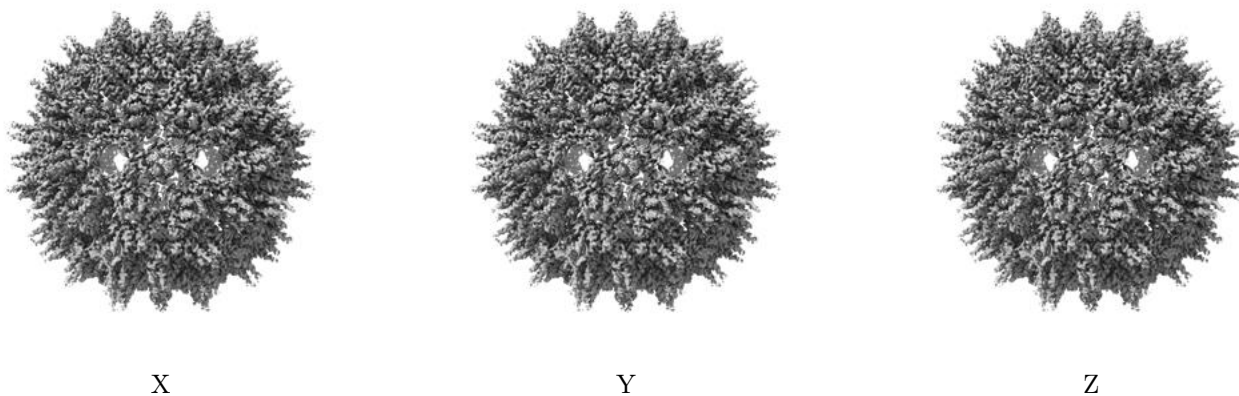


Z

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.

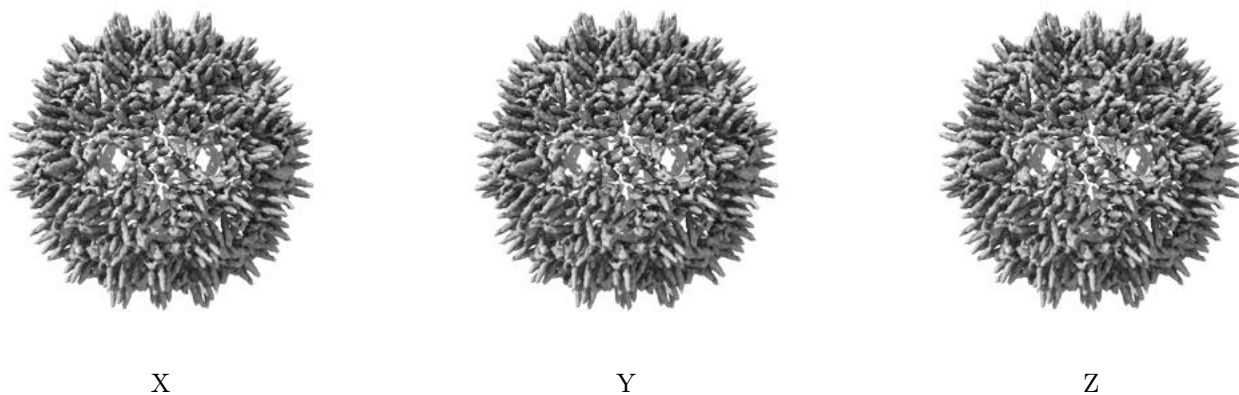
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0103. 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.

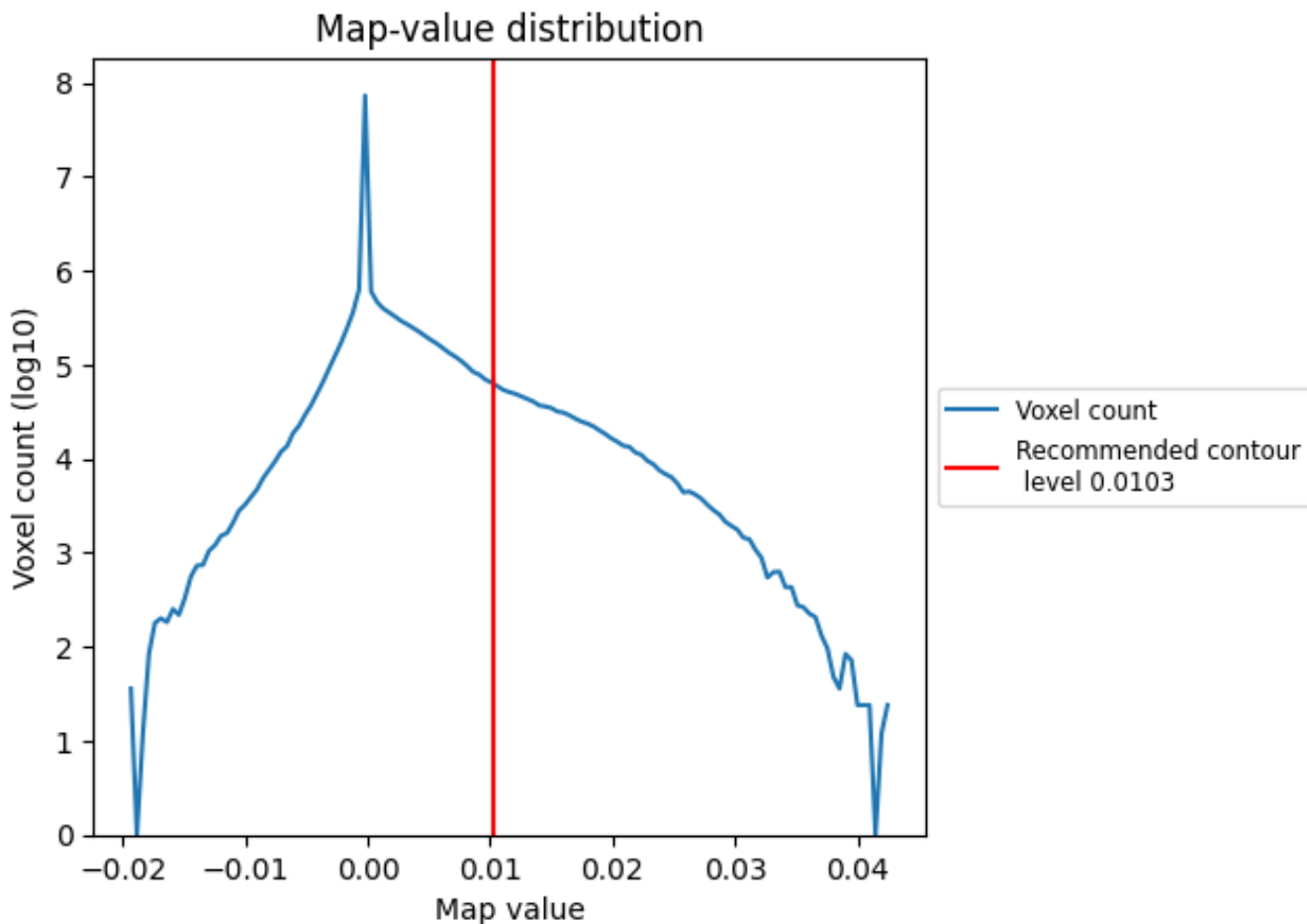
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

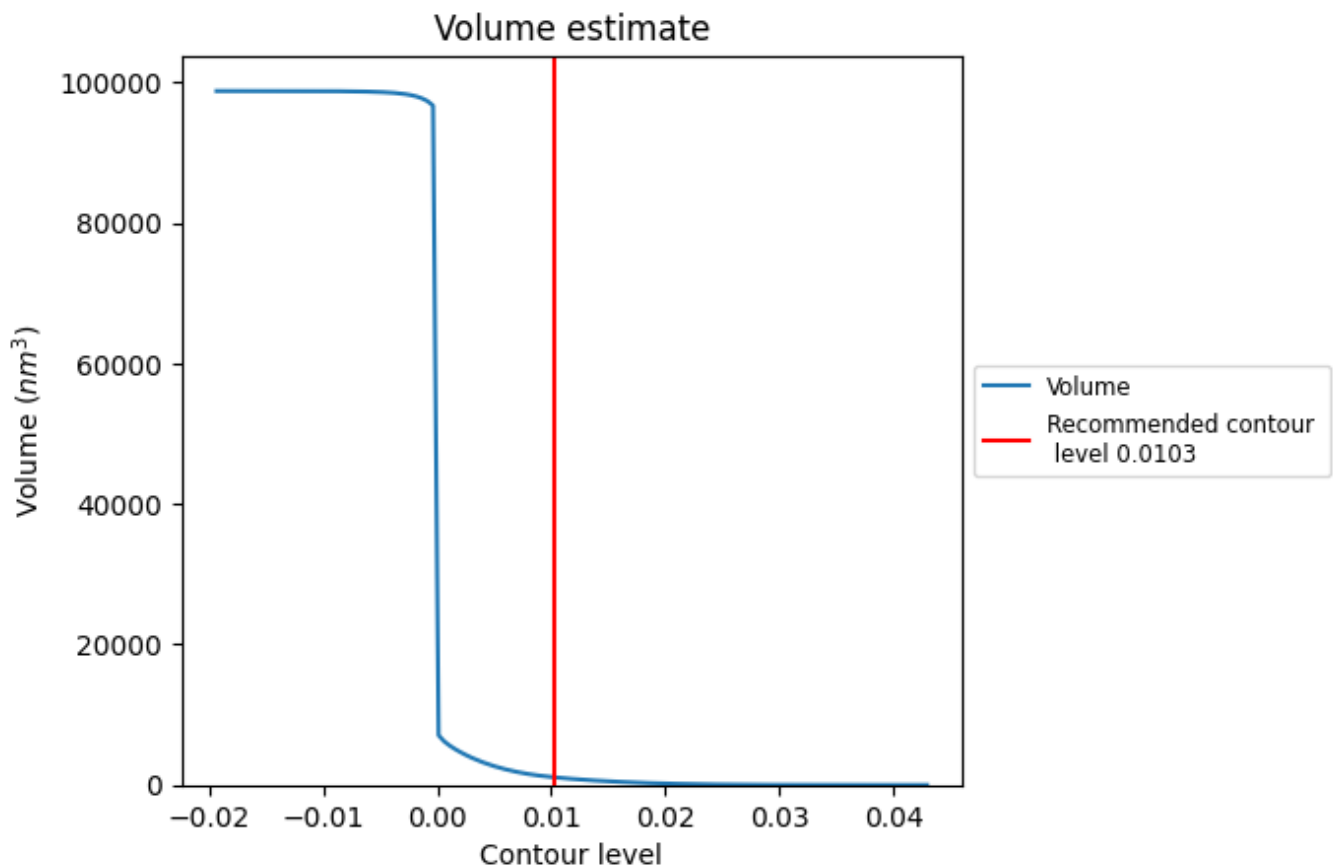
This section contains the results of statistical analysis of the map.

### 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.

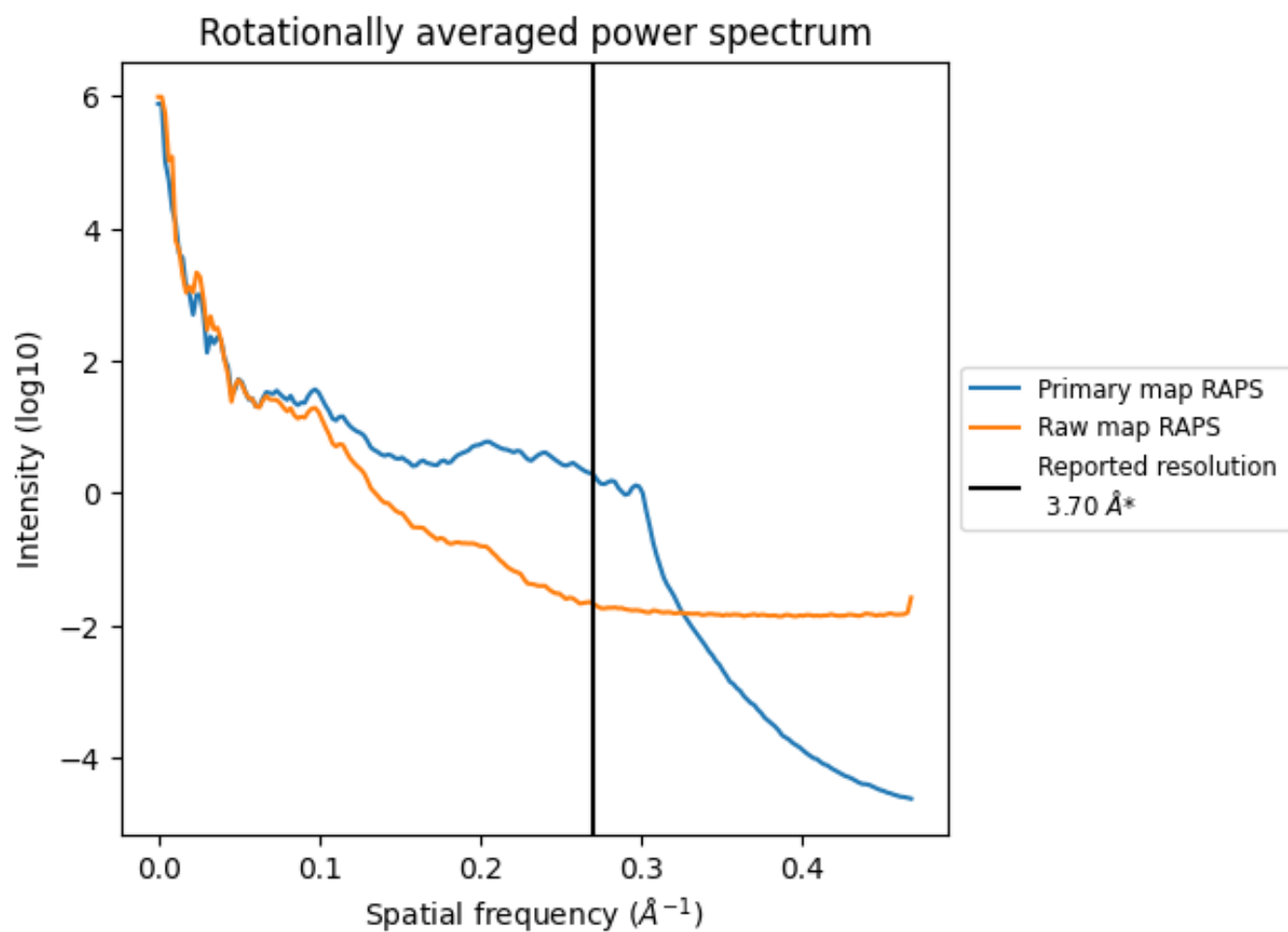
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1083  $\text{nm}^3$ ; this corresponds to an approximate mass of 978 kDa.

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

### 7.3 Rotationally averaged power spectrum i

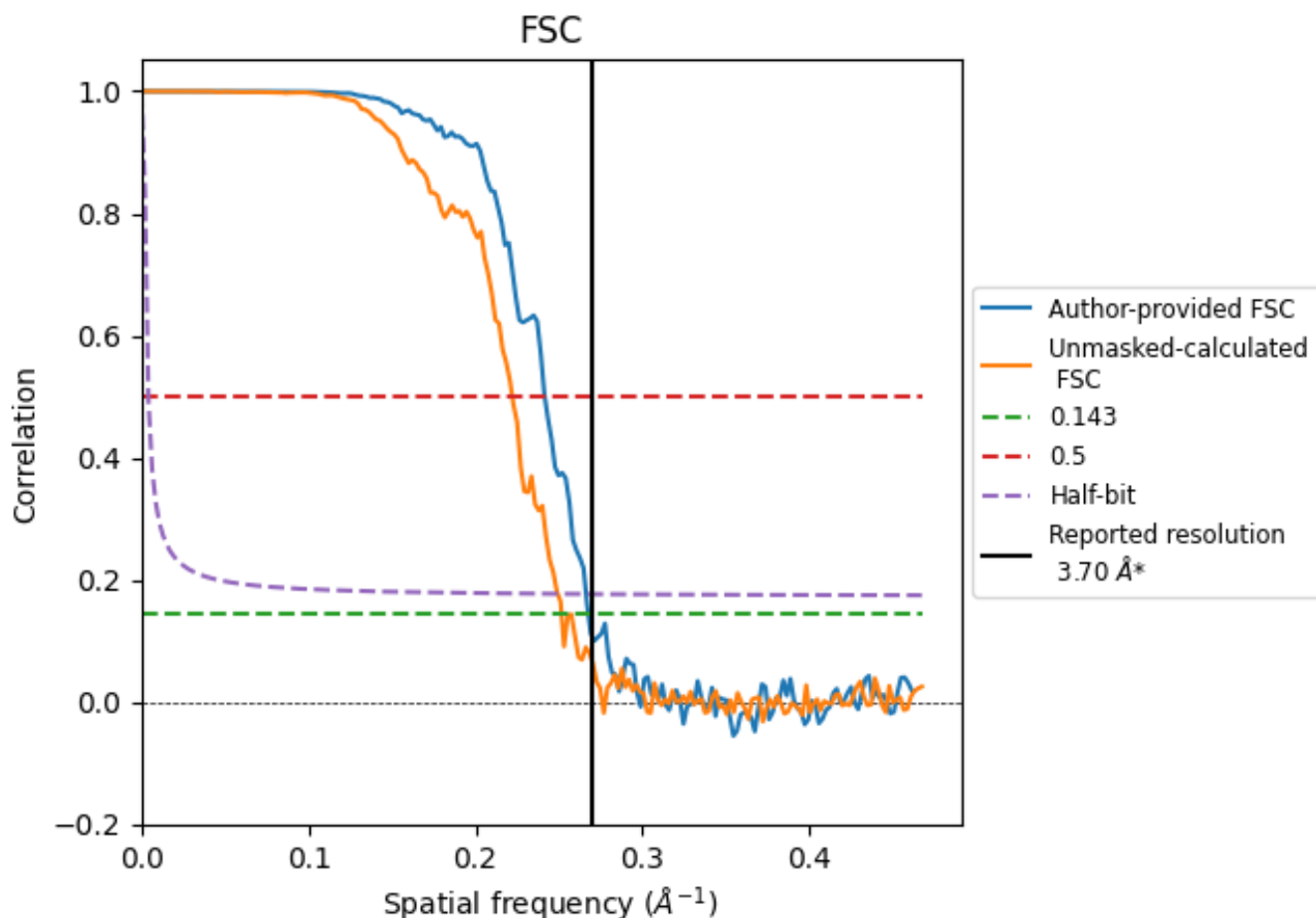


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

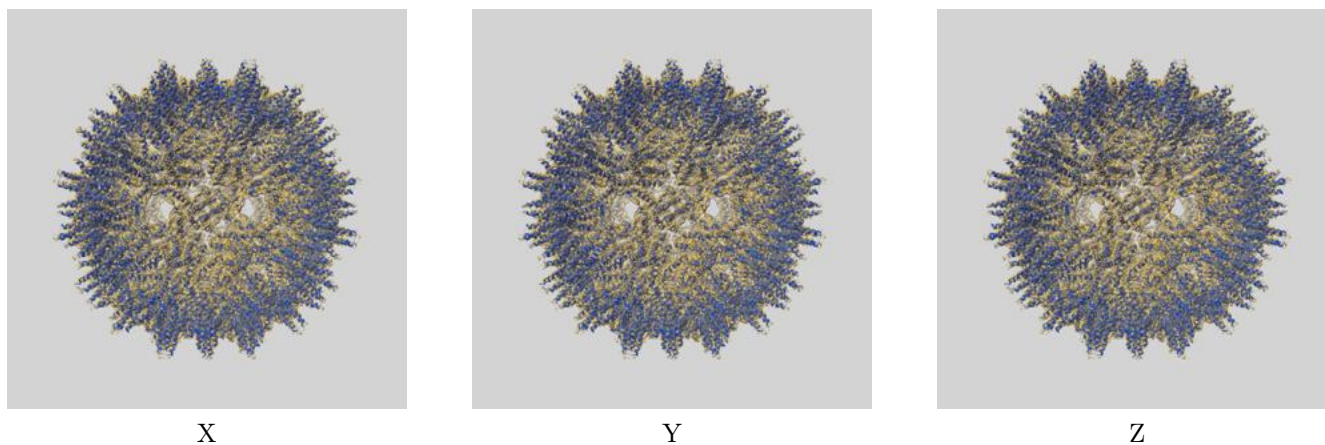
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	4.14	3.76
Unmasked-calculated*	3.97	4.50	4.01

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

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

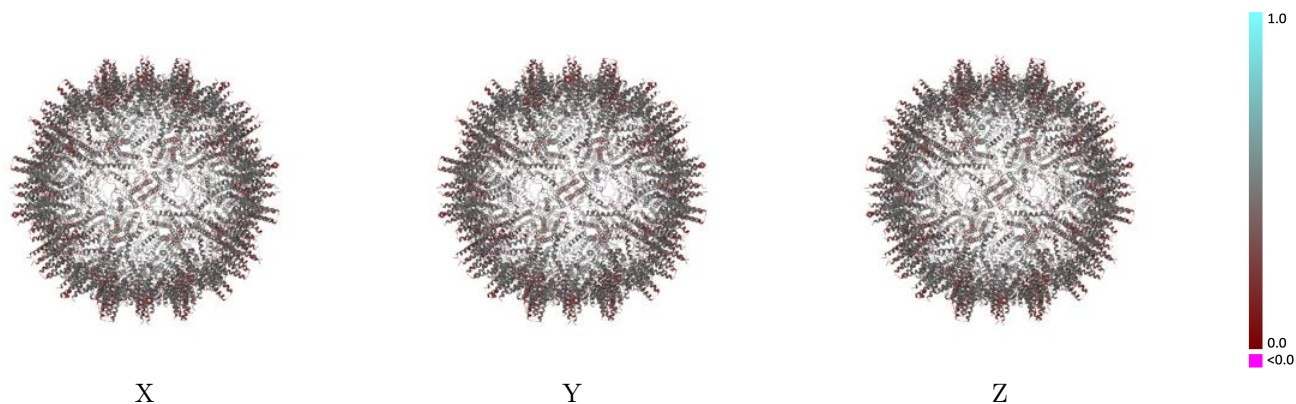
This section contains information regarding the fit between EMDB map EMD-15295 and PDB model 8AAC. Per-residue inclusion information can be found in section 3 on page 29.

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



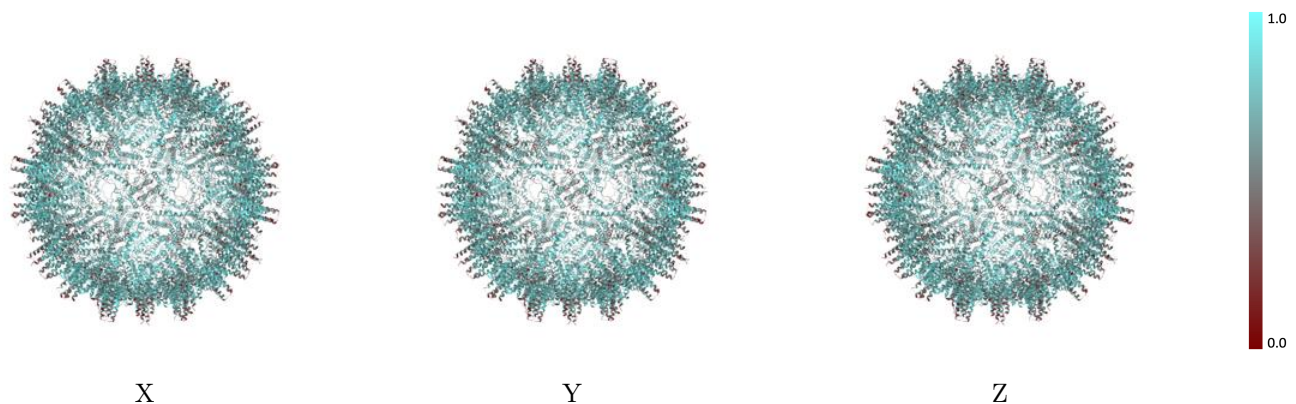
The images above show the 3D surface view of the map at the recommended contour level 0.0103 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



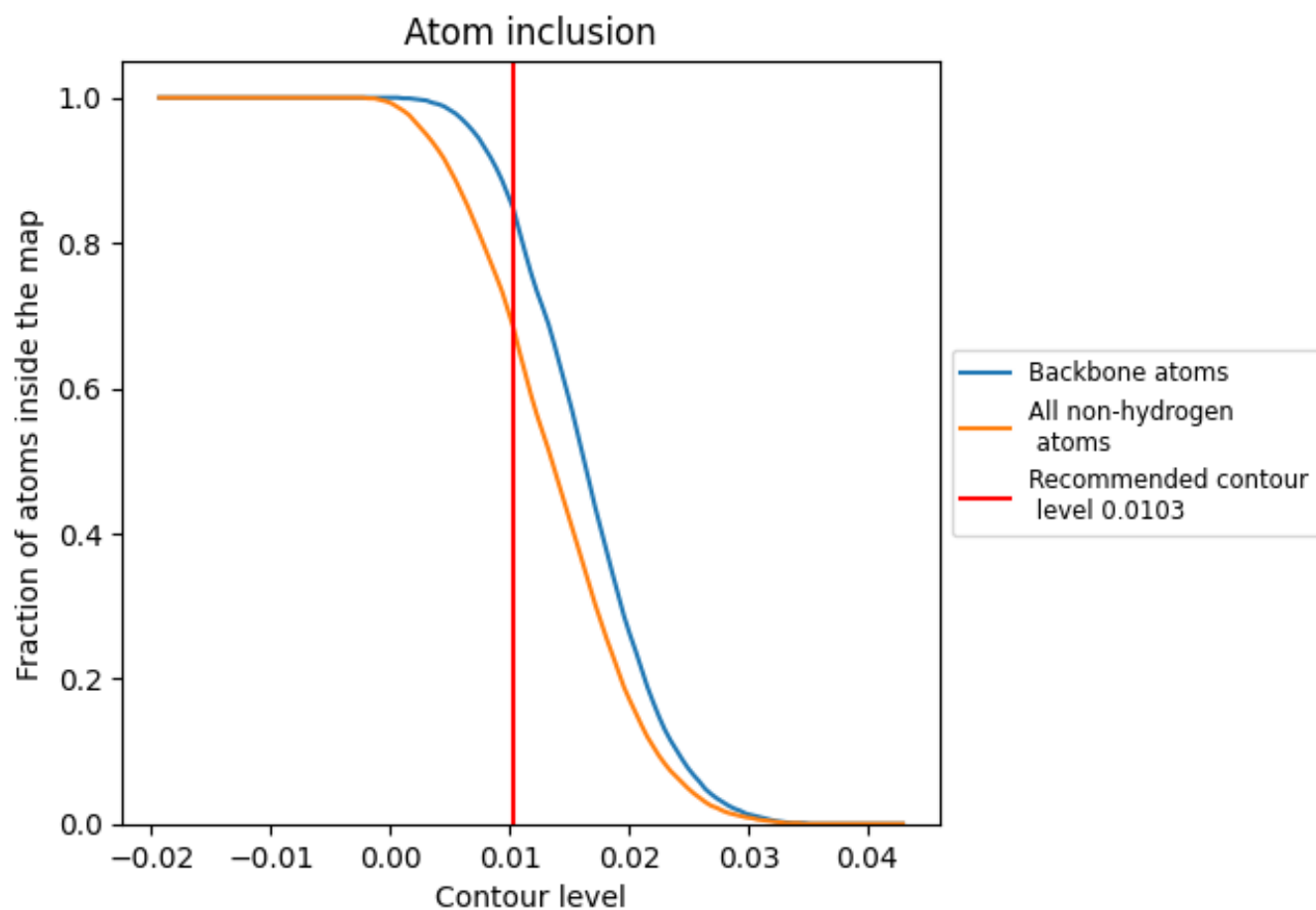
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0103).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 68% 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 (0.0103) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6850	 0.4060
1A	 0.7290	 0.4270
1B	 0.6930	 0.4080
1C	 0.6070	 0.3630
2A	 0.7280	 0.4230
2B	 0.6980	 0.4140
2C	 0.6150	 0.3800
3A	 0.7320	 0.4280
3B	 0.7050	 0.4190
3C	 0.6290	 0.3820
4A	 0.7390	 0.4280
4B	 0.7020	 0.4170
4C	 0.6290	 0.3810
5A	 0.7340	 0.4300
5B	 0.7080	 0.4190
5C	 0.6320	 0.3840
6A	 0.7280	 0.4250
6B	 0.7000	 0.4050
6C	 0.5980	 0.3600
7A	 0.7240	 0.4220
7B	 0.7000	 0.4180
7C	 0.6100	 0.3710
8A	 0.7370	 0.4290
8B	 0.7060	 0.4150
8C	 0.6180	 0.3790
AA	 0.7360	 0.4310
AB	 0.7020	 0.4150
AC	 0.6300	 0.3840
BA	 0.7360	 0.4290
BB	 0.7070	 0.4170
BC	 0.6300	 0.3810
CA	 0.7170	 0.4250
CB	 0.6930	 0.4060
CC	 0.5890	 0.3510
DA	 0.7280	 0.4200























































































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Chain	Atom inclusion	Q-score
DB	 0.6950	 0.4110
DC	 0.6070	 0.3630
EA	 0.7240	 0.4250
EB	 0.6930	 0.4020
EC	 0.6050	 0.3620
FA	 0.7360	 0.4300
FB	 0.7040	 0.4170
FC	 0.6190	 0.3810
GA	 0.7320	 0.4280
GB	 0.7000	 0.4160
GC	 0.6300	 0.3800
HA	 0.7380	 0.4300
HB	 0.7080	 0.4170
HC	 0.6380	 0.3850
IA	 0.7270	 0.4240
IB	 0.7000	 0.4140
IC	 0.6130	 0.3690
JA	 0.7320	 0.4290
JB	 0.7030	 0.4190
JC	 0.6280	 0.3820
KA	 0.7280	 0.4270
KB	 0.7050	 0.4150
KC	 0.6270	 0.3790
LA	 0.7320	 0.4230
LB	 0.7060	 0.4090
LC	 0.6230	 0.3760
MA	 0.7390	 0.4280
MB	 0.7010	 0.4170
MC	 0.6320	 0.3830
NA	 0.7350	 0.4310
NB	 0.7040	 0.4170
NC	 0.6330	 0.3860
OA	 0.7300	 0.4250
OB	 0.7030	 0.4140
OC	 0.6210	 0.3800
PA	 0.7240	 0.4260
PB	 0.7040	 0.4130
PC	 0.6140	 0.3780
QA	 0.7270	 0.4220
QB	 0.6940	 0.4080
QC	 0.6190	 0.3590
RA	 0.7390	 0.4300





















































































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Chain	Atom inclusion	Q-score
RB	 0.7060	 0.4160
RC	 0.6090	 0.3840
SA	 0.7320	 0.4300
SB	 0.7030	 0.4160
SC	 0.6200	 0.3760
TA	 0.7350	 0.4300
TB	 0.7060	 0.4170
TC	 0.6340	 0.3820
UA	 0.7360	 0.4280
UB	 0.7050	 0.4160
UC	 0.6210	 0.3840
VA	 0.7340	 0.4300
VB	 0.7020	 0.4170
VC	 0.6280	 0.3830
WA	 0.7380	 0.4320
WB	 0.7030	 0.4160
WC	 0.6400	 0.3830
XA	 0.7280	 0.4260
XB	 0.6960	 0.4150
XC	 0.6180	 0.3720
YA	 0.7340	 0.4250
YB	 0.6980	 0.4150
YC	 0.6240	 0.3770
ZA	 0.7330	 0.4280
ZB	 0.6990	 0.4140
ZC	 0.6260	 0.3820
aA	 0.7340	 0.4280
aB	 0.7060	 0.4160
aC	 0.6400	 0.3860
bA	 0.7250	 0.4220
bB	 0.6890	 0.4160
bC	 0.6060	 0.3730
cA	 0.7250	 0.4250
cB	 0.6970	 0.4120
cC	 0.6240	 0.3760
dA	 0.7370	 0.4300
dB	 0.7050	 0.4150
dC	 0.6170	 0.3800
eA	 0.7320	 0.4260
eB	 0.7030	 0.4150
eC	 0.6260	 0.3850
fA	 0.7310	 0.4270









































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Chain	Atom inclusion	Q-score
fB	 0.6970	 0.4100
fC	 0.6050	 0.3640
gA	 0.7340	 0.4290
gB	 0.7040	 0.4180
gC	 0.6140	 0.3810
hA	 0.7360	 0.4300
hB	 0.6970	 0.4180
hC	 0.6340	 0.3800
iA	 0.7360	 0.4280
iB	 0.7010	 0.4140
iC	 0.6280	 0.3810
jA	 0.7310	 0.4220
jB	 0.7030	 0.4130
jC	 0.6240	 0.3760
kA	 0.7340	 0.4270
kB	 0.7000	 0.4160
kC	 0.6090	 0.3750
lA	 0.7390	 0.4310
lB	 0.6990	 0.4170
lC	 0.6290	 0.3850
mA	 0.7330	 0.4320
mB	 0.7040	 0.4180
mC	 0.6330	 0.3840
nA	 0.7290	 0.4270
nB	 0.7010	 0.4140
nC	 0.6180	 0.3730
oA	 0.7280	 0.4240
oB	 0.6960	 0.4090
oC	 0.6030	 0.3660
pA	 0.7340	 0.4300
pB	 0.7050	 0.4160
pC	 0.6300	 0.3830
qA	 0.7360	 0.4270
qB	 0.7010	 0.4140
qC	 0.6160	 0.3760
rA	 0.7360	 0.4280
rB	 0.7000	 0.4190
rC	 0.6300	 0.3830
sA	 0.7370	 0.4310
sB	 0.7060	 0.4150
sC	 0.6370	 0.3850
tA	 0.7280	 0.4270

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Chain	Atom inclusion	Q-score
tB	 0.6960	 0.4100
tC	 0.5970	 0.3620
uA	 0.7360	 0.4290
uB	 0.7060	 0.4160
uC	 0.6150	 0.3810
vA	 0.7280	 0.4270
vB	 0.6980	 0.4150
vC	 0.6250	 0.3780
wA	 0.7350	 0.4280
wB	 0.7040	 0.4150
wC	 0.6300	 0.3840
xA	 0.7360	 0.4280
xB	 0.7030	 0.4150
xC	 0.6260	 0.3820
yA	 0.7350	 0.4270
yB	 0.7010	 0.4190
yC	 0.6150	 0.3790
zA	 0.7360	 0.4310
zB	 0.6990	 0.4170
zC	 0.6270	 0.3820