



Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 01:01 pm GMT

PDB ID : 6QN1
EMDB ID : EMD-4595
Title : T=4 quasi-symmetric bacterial microcompartment particle
Authors : Kalnins, G.
Deposited on : 2019-02-08
Resolution : 3.28 Å(reported)
Based on initial models : 4N8X, 4QIV

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

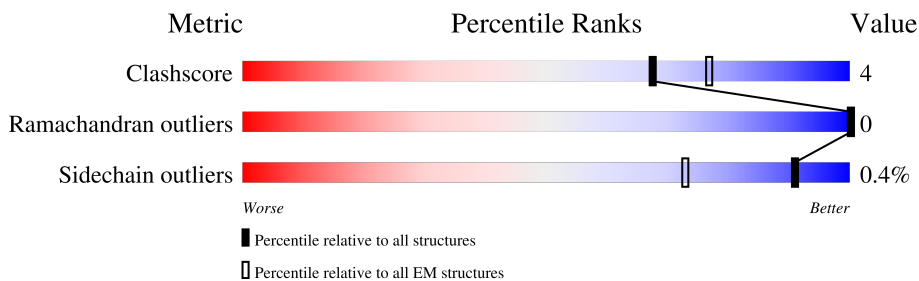
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.28 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	AA	88	
1	AE	88	
1	AI	88	
1	AM	88	
1	AQ	88	
1	AU	88	
1	AY	88	
1	BC	88	

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Mol	Chain	Length	Quality of chain
1	BG	88	18% 83% 9% 8%
1	BK	88	18% 82% 10% 8%
1	BO	88	17% 80% 13% 8%
1	BS	88	18% 82% 10% 8%
1	BW	88	17% 84% 8% 8%
1	CA	88	18% 82% 10% 8%
1	CE	88	15% 83% 9% 8%
1	CI	88	19% 83% 9% 8%
1	CM	88	17% 80% 13% 8%
1	CQ	88	16% 83% 9% 8%
1	CU	88	20% 83% 9% 8%
1	CY	88	17% 83% 9% 8%
1	DC	88	18% 83% 9% 8%
1	DG	88	18% 84% 8% 8%
1	DK	88	16% 83% 9% 8%
1	DO	88	18% 81% 11% 8%
1	DS	88	17% 80% 13% 8%
1	DW	88	18% 82% 10% 8%
1	EA	88	16% 83% 9% 8%
1	EE	88	18% 80% 13% 8%
1	EI	88	18% 83% 9% 8%
1	EM	88	15% 83% 9% 8%
1	EQ	88	14% 80% 13% 8%
1	EU	88	19% 83% 9% 8%
1	EY	88	18% 78% 14% 8%

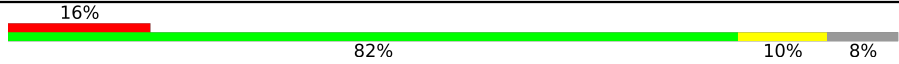

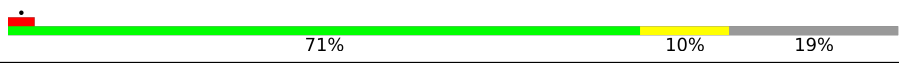

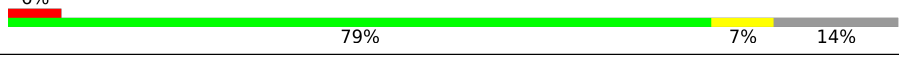
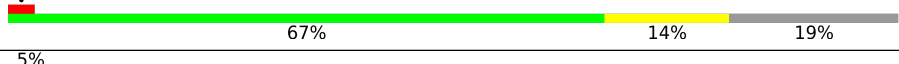
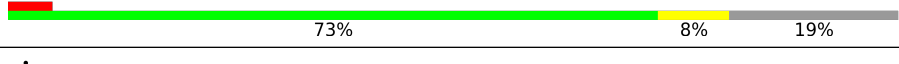

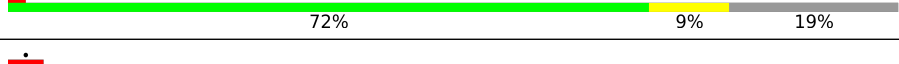


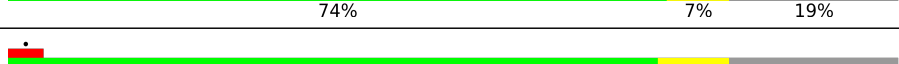
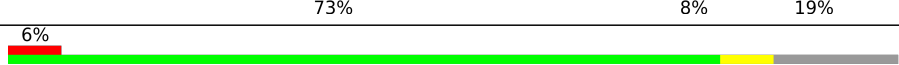
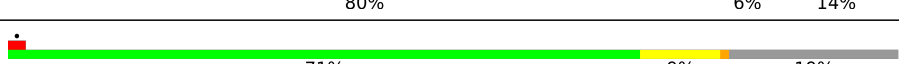

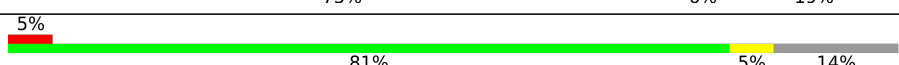
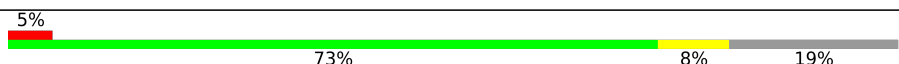
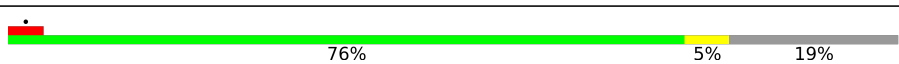
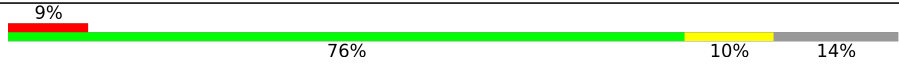


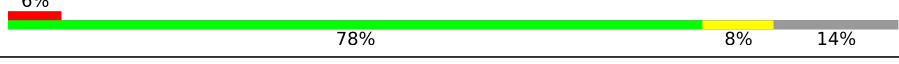
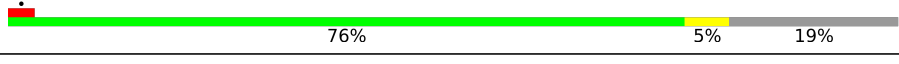


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Mol	Chain	Length	Quality of chain
1	FC	88	16% 83% 9% 8%
1	FG	88	15% 77% 15% 8%
1	FK	88	17% 80% 13% 8%
1	FO	88	17% 83% 9% 8%
1	FS	88	15% 86% 6% 8%
1	FW	88	17% 83% 9% 8%
1	GA	88	19% 80% 13% 8%
1	GE	88	18% 83% 9% 8%
1	GI	88	19% 80% 13% 8%
1	GM	88	18% 83% 9% 8%
1	GQ	88	16% 78% 14% 8%
1	GU	88	17% 82% 10% 8%
1	GY	88	18% 84% 8% 8%
1	HC	88	19% 83% 9% 8%
1	HG	88	17% 82% 10% 8%
1	HK	88	18% 83% 9% 8%
1	HO	88	17% 83% 9% 8%
1	HS	88	19% 83% 9% 8%
1	HW	88	18% 82% 10% 8%
1	IA	88	17% 85% 7% 8%
1	IE	88	17% 83% 9% 8%
1	II	88	19% 83% 9% 8%
1	IM	88	17% 82% 10% 8%
1	IQ	88	17% 83% 9% 8%
1	IU	88	18% 83% 9% 8%

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Mol	Chain	Length	Quality of chain
1	IY	88	
1	JC	88	
2	AB	100	
2	AC	100	
2	AD	100	
2	AF	100	
2	AG	100	
2	AH	100	
2	AJ	100	
2	AK	100	
2	AL	100	
2	AN	100	
2	AO	100	
2	AP	100	
2	AR	100	
2	AS	100	
2	AT	100	
2	AV	100	
2	AW	100	
2	AX	100	
2	AZ	100	
2	BA	100	
2	BB	100	
2	BD	100	
2	BE	100	

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Mol	Chain	Length	Quality of chain
2	BF	100	 5% 79% 7% 14%
2	BH	100	 73% 8% 19%
2	BI	100	 72% 9% 19%
2	BJ	100	 5% 80% 6% 14%
2	BL	100	 73% 8% 19%
2	BM	100	 76% 5% 19%
2	BN	100	 9% 77% 9% 14%
2	BP	100	 5% 72% 9% 19%
2	BQ	100	 79% 19%
2	BR	100	 8% 75% 11% 14%
2	BT	100	 69% 12% 19%
2	BU	100	 5% 73% 8% 19%
2	BV	100	 82% 14%
2	BX	100	 76% 5% 19%
2	BY	100	 5% 73% 8% 19%
2	BZ	100	 5% 83% 14%
2	CB	100	 72% 9% 19%
2	CC	100	 76% 5% 19%
2	CD	100	 7% 79% 7% 14%
2	CF	100	 5% 72% 9% 19%
2	CG	100	 77% 19%
2	CH	100	 8% 78% 8% 14%
2	CJ	100	 73% 8% 19%
2	CK	100	 73% 8% 19%
2	CL	100	 5% 80% 6% 14%

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Mol	Chain	Length	Quality of chain
2	CN	100	69% 12% 19%
2	CO	100	5% 74% 7% 19%
2	CP	100	81% 5% 14%
2	CR	100	74% 7% 19%
2	CS	100	5% 73% 8% 19%
2	CT	100	6% 82% 14%
2	CV	100	5% 73% 8% 19%
2	CW	100	74% 7% 19%
2	CX	100	8% 78% 8% 14%
2	CZ	100	72% 9% 19%
2	DA	100	73% 8% 19%
2	DB	100	5% 80% 6% 14%
2	DD	100	67% 14% 19%
2	DE	100	5% 74% 7% 19%
2	DF	100	82% 14%
2	DH	100	5% 70% 11% 19%
2	DI	100	76% 5% 19%
2	DJ	100	7% 78% 8% 14%
2	DL	100	74% 7% 19%
2	DM	100	73% 8% 19%
2	DN	100	79% 7% 14%
2	DP	100	75% 6% 19%
2	DQ	100	75% 6% 19%
2	DR	100	7% 81% 5% 14%
2	DT	100	70% 11% 19%

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Mol	Chain	Length	Quality of chain
2	DU	100	5% 74% 7% 19%
2	DV	100	5% 82% 14%
2	DX	100	5% 71% 10% 19%
2	DY	100	5% 77% 19%
2	DZ	100	9% 74% 11% 14%
2	EB	100	5% 71% 10% 19%
2	EC	100	5% 74% 7% 19%
2	ED	100	7% 81% 5% 14%
2	EF	100	5% 71% 10% 19%
2	EG	100	5% 75% 6% 19%
2	EH	100	5% 82% 14%
2	EJ	100	5% 72% 9% 19%
2	EK	100	5% 73% 8% 19%
2	EL	100	8% 80% 6% 14%
2	EN	100	5% 74% 7% 19%
2	EO	100	5% 73% 8% 19%
2	EP	100	5% 79% 7% 14%
2	ER	100	5% 74% 7% 19%
2	ES	100	5% 74% 7% 19%
2	ET	100	6% 82% 14%
2	EV	100	5% 73% 8% 19%
2	EW	100	5% 74% 7% 19%
2	EX	100	8% 83% 14%
2	EZ	100	5% 69% 12% 19%
2	FA	100	5% 71% 10% 19%

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Mol	Chain	Length	Quality of chain
2	FB	100	5% 79% 7% 14%
2	FD	100	5% 71% 10% 19%
2	FE	100	5% 72% 9% 19%
2	FF	100	6% 80% 6% 14%
2	FH	100	5% 72% 9% 19%
2	FI	100	5% 73% 8% 19%
2	FJ	100	7% 77% 9% 14%
2	FL	100	5% 72% 9% 19%
2	FM	100	5% 72% 9% 19%
2	FN	100	5% 80% 6% 14%
2	FP	100	5% 71% 10% 19%
2	FQ	100	5% 73% 8% 19%
2	FR	100	5% 81% 5% 14%
2	FT	100	5% 72% 9% 19%
2	FU	100	5% 76% 5% 19%
2	FV	100	5% 78% 8% 14%
2	FX	100	5% 72% 9% 19%
2	FY	100	5% 75% 6% 19%
2	FZ	100	8% 77% 9% 14%
2	GB	100	5% 68% 13% 19%
2	GC	100	6% 75% 6% 19%
2	GD	100	5% 81% 5% 14%
2	GF	100	5% 74% 7% 19%
2	GG	100	5% 72% 9% 19%
2	GH	100	5% 82% 14%

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Mol	Chain	Length	Quality of chain
2	GJ	100	70% 11% 19%
2	GK	100	75% 6% 19%
2	GL	100	8% 80% 6% 14%
2	GN	100	5% 71% 10% 19%
2	GO	100	79% 19%
2	GP	100	9% 77% 9% 14%
2	GR	100	72% 9% 19%
2	GS	100	5% 74% 7% 19%
2	GT	100	81% 5% 14%
2	GV	100	74% 7% 19%
2	GW	100	71% 10% 19%
2	GX	100	6% 78% 8% 14%
2	GZ	100	5% 70% 11% 19%
2	HA	100	74% 7% 19%
2	HB	100	8% 77% 9% 14%
2	HD	100	73% 8% 19%
2	HE	100	73% 8% 19%
2	HF	100	8% 78% 8% 14%
2	HH	100	76% 5% 19%
2	HI	100	74% 7% 19%
2	HJ	100	6% 81% 5% 14%
2	HL	100	73% 8% 19%
2	HM	100	73% 8% 19%
2	HN	100	6% 80% 6% 14%
2	HP	100	70% 11% 19%

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Mol	Chain	Length	Quality of chain
2	HQ	100	76% 5% 19%
2	HR	100	79% 7% 14%
2	HT	100	73% 8% 19%
2	HU	100	73% 8% 19%
2	HV	100	79% 7% 14%
2	HX	100	74% 7% 19%
2	HY	100	75% 6% 19%
2	HZ	100	82% 14%
2	IB	100	71% 10% 19%
2	IC	100	73% 8% 19%
2	ID	100	78% 8% 14%
2	IF	100	67% 14% 19%
2	IG	100	73% 8% 19%
2	IH	100	81% 5% 14%
2	IJ	100	73% 8% 19%
2	IK	100	77% 19%
2	IL	100	79% 7% 14%
2	IN	100	74% 7% 19%
2	IO	100	73% 8% 19%
2	IP	100	81% 5% 14%
2	IR	100	72% 9% 19%
2	IS	100	76% 5% 19%
2	IT	100	76% 10% 14%
2	IV	100	72% 9% 19%
2	IW	100	75% 6% 19%

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Mol	Chain	Length	Quality of chain
2	IX	100	<p>7% 82% 14%</p>
2	IZ	100	<p>6% 67% 14% 19%</p>
2	JA	100	<p>5% 76% 5% 19%</p>
2	JB	100	<p>6% 80% 6% 14%</p>
2	JD	100	<p>5% 71% 10% 19%</p>
2	JE	100	<p>6% 74% 7% 19%</p>
2	JF	100	<p>8% 75% 11% 14%</p>

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 141480 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 Carbon dioxide concentrating mechanism protein CcmL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	81	616	389	106	116	5	0	0
1	AE	81	616	389	106	116	5	0	0
1	AI	81	616	389	106	116	5	0	0
1	AM	81	616	389	106	116	5	0	0
1	AQ	81	616	389	106	116	5	0	0
1	AU	81	616	389	106	116	5	0	0
1	AY	81	616	389	106	116	5	0	0
1	BC	81	616	389	106	116	5	0	0
1	BG	81	616	389	106	116	5	0	0
1	BK	81	616	389	106	116	5	0	0
1	BO	81	616	389	106	116	5	0	0
1	BS	81	616	389	106	116	5	0	0
1	BW	81	616	389	106	116	5	0	0
1	CA	81	616	389	106	116	5	0	0
1	CE	81	616	389	106	116	5	0	0
1	CI	81	616	389	106	116	5	0	0
1	CM	81	616	389	106	116	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	CQ	81	616	389	106	116	5	0	0
1	CU	81	616	389	106	116	5	0	0
1	CY	81	616	389	106	116	5	0	0
1	DC	81	616	389	106	116	5	0	0
1	DG	81	616	389	106	116	5	0	0
1	DK	81	616	389	106	116	5	0	0
1	DO	81	616	389	106	116	5	0	0
1	DS	81	616	389	106	116	5	0	0
1	DW	81	616	389	106	116	5	0	0
1	EA	81	616	389	106	116	5	0	0
1	EE	81	616	389	106	116	5	0	0
1	EI	81	616	389	106	116	5	0	0
1	EM	81	616	389	106	116	5	0	0
1	EQ	81	616	389	106	116	5	0	0
1	EU	81	616	389	106	116	5	0	0
1	EY	81	616	389	106	116	5	0	0
1	FC	81	616	389	106	116	5	0	0
1	FG	81	616	389	106	116	5	0	0
1	FK	81	616	389	106	116	5	0	0
1	FO	81	616	389	106	116	5	0	0
1	FS	81	616	389	106	116	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	FW	81	616	389	106	116	5	0	0
1	GA	81	616	389	106	116	5	0	0
1	GE	81	616	389	106	116	5	0	0
1	GI	81	616	389	106	116	5	0	0
1	GM	81	616	389	106	116	5	0	0
1	GQ	81	616	389	106	116	5	0	0
1	GU	81	616	389	106	116	5	0	0
1	GY	81	616	389	106	116	5	0	0
1	HC	81	616	389	106	116	5	0	0
1	HG	81	616	389	106	116	5	0	0
1	HK	81	616	389	106	116	5	0	0
1	HO	81	616	389	106	116	5	0	0
1	HS	81	616	389	106	116	5	0	0
1	HW	81	616	389	106	116	5	0	0
1	IA	81	616	389	106	116	5	0	0
1	IE	81	616	389	106	116	5	0	0
1	II	81	616	389	106	116	5	0	0
1	IM	81	616	389	106	116	5	0	0
1	IQ	81	616	389	106	116	5	0	0
1	IU	81	616	389	106	116	5	0	0
1	IY	81	616	389	106	116	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	JC	81	616	389	106	116	5	0	0

- Molecule 2 is a protein called BMC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AB	81	569	352	101	112	4	0	0
2	AC	81	569	352	101	112	4	0	0
2	AD	86	604	374	107	119	4	0	0
2	AF	81	569	352	101	112	4	0	0
2	AG	81	569	352	101	112	4	0	0
2	AH	86	604	374	107	119	4	0	0
2	AJ	81	569	352	101	112	4	0	0
2	AK	81	569	352	101	112	4	0	0
2	AL	86	604	374	107	119	4	0	0
2	AN	81	569	352	101	112	4	0	0
2	AO	81	569	352	101	112	4	0	0
2	AP	86	604	374	107	119	4	0	0
2	AR	81	569	352	101	112	4	0	0
2	AS	81	569	352	101	112	4	0	0
2	AT	86	604	374	107	119	4	0	0
2	AV	81	569	352	101	112	4	0	0
2	AW	81	569	352	101	112	4	0	0
2	AX	86	604	374	107	119	4	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O	S		
2	AZ	81	569	352	101	112	4	0	0
2	BA	81	569	352	101	112	4	0	0
2	BB	86	604	374	107	119	4	0	0
2	BD	81	569	352	101	112	4	0	0
2	BE	81	569	352	101	112	4	0	0
2	BF	86	604	374	107	119	4	0	0
2	BH	81	569	352	101	112	4	0	0
2	BI	81	569	352	101	112	4	0	0
2	BJ	86	604	374	107	119	4	0	0
2	BL	81	569	352	101	112	4	0	0
2	BM	81	569	352	101	112	4	0	0
2	BN	86	604	374	107	119	4	0	0
2	BP	81	569	352	101	112	4	0	0
2	BQ	81	569	352	101	112	4	0	0
2	BR	86	604	374	107	119	4	0	0
2	BT	81	569	352	101	112	4	0	0
2	BU	81	569	352	101	112	4	0	0
2	BV	86	604	374	107	119	4	0	0
2	BX	81	569	352	101	112	4	0	0
2	BY	81	569	352	101	112	4	0	0
2	BZ	86	604	374	107	119	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	CB	81	569	352	101	112	4	0	0
2	CC	81	569	352	101	112	4	0	0
2	CD	86	604	374	107	119	4	0	0
2	CF	81	569	352	101	112	4	0	0
2	CG	81	569	352	101	112	4	0	0
2	CH	86	604	374	107	119	4	0	0
2	CJ	81	569	352	101	112	4	0	0
2	CK	81	569	352	101	112	4	0	0
2	CL	86	604	374	107	119	4	0	0
2	CN	81	569	352	101	112	4	0	0
2	CO	81	569	352	101	112	4	0	0
2	CP	86	604	374	107	119	4	0	0
2	CR	81	569	352	101	112	4	0	0
2	CS	81	569	352	101	112	4	0	0
2	CT	86	604	374	107	119	4	0	0
2	CV	81	569	352	101	112	4	0	0
2	CW	81	569	352	101	112	4	0	0
2	CX	86	604	374	107	119	4	0	0
2	CZ	81	569	352	101	112	4	0	0
2	DA	81	569	352	101	112	4	0	0
2	DB	86	604	374	107	119	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	DD	81	569	352	101	112	4	0	0
2	DE	81	569	352	101	112	4	0	0
2	DF	86	604	374	107	119	4	0	0
2	DH	81	569	352	101	112	4	0	0
2	DI	81	569	352	101	112	4	0	0
2	DJ	86	604	374	107	119	4	0	0
2	DL	81	569	352	101	112	4	0	0
2	DM	81	569	352	101	112	4	0	0
2	DN	86	604	374	107	119	4	0	0
2	DP	81	569	352	101	112	4	0	0
2	DQ	81	569	352	101	112	4	0	0
2	DR	86	604	374	107	119	4	0	0
2	DT	81	569	352	101	112	4	0	0
2	DU	81	569	352	101	112	4	0	0
2	DV	86	604	374	107	119	4	0	0
2	DX	81	569	352	101	112	4	0	0
2	DY	81	569	352	101	112	4	0	0
2	DZ	86	604	374	107	119	4	0	0
2	EB	81	569	352	101	112	4	0	0
2	EC	81	569	352	101	112	4	0	0
2	ED	86	604	374	107	119	4	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O	S		
2	EF	81	569	352	101	112	4	0	0
2	EG	81	569	352	101	112	4	0	0
2	EH	86	604	374	107	119	4	0	0
2	EJ	81	569	352	101	112	4	0	0
2	EK	81	569	352	101	112	4	0	0
2	EL	86	604	374	107	119	4	0	0
2	EN	81	569	352	101	112	4	0	0
2	EO	81	569	352	101	112	4	0	0
2	EP	86	604	374	107	119	4	0	0
2	ER	81	569	352	101	112	4	0	0
2	ES	81	569	352	101	112	4	0	0
2	ET	86	604	374	107	119	4	0	0
2	EV	81	569	352	101	112	4	0	0
2	EW	81	569	352	101	112	4	0	0
2	EX	86	604	374	107	119	4	0	0
2	EZ	81	569	352	101	112	4	0	0
2	FA	81	569	352	101	112	4	0	0
2	FB	86	604	374	107	119	4	0	0
2	FD	81	569	352	101	112	4	0	0
2	FE	81	569	352	101	112	4	0	0
2	FF	86	604	374	107	119	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	FH	81	569	352	101	112	4	0	0
2	FI	81	569	352	101	112	4	0	0
2	FJ	86	604	374	107	119	4	0	0
2	FL	81	569	352	101	112	4	0	0
2	FM	81	569	352	101	112	4	0	0
2	FN	86	604	374	107	119	4	0	0
2	FP	81	569	352	101	112	4	0	0
2	FQ	81	569	352	101	112	4	0	0
2	FR	86	604	374	107	119	4	0	0
2	FT	81	569	352	101	112	4	0	0
2	FU	81	569	352	101	112	4	0	0
2	FV	86	604	374	107	119	4	0	0
2	FX	81	569	352	101	112	4	0	0
2	FY	81	569	352	101	112	4	0	0
2	FZ	86	604	374	107	119	4	0	0
2	GB	81	569	352	101	112	4	0	0
2	GC	81	569	352	101	112	4	0	0
2	GD	86	604	374	107	119	4	0	0
2	GF	81	569	352	101	112	4	0	0
2	GG	81	569	352	101	112	4	0	0
2	GH	86	604	374	107	119	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	GJ	81	569	352	101	112	4	0	0
2	GK	81	569	352	101	112	4	0	0
2	GL	86	604	374	107	119	4	0	0
2	GN	81	569	352	101	112	4	0	0
2	GO	81	569	352	101	112	4	0	0
2	GP	86	604	374	107	119	4	0	0
2	GR	81	569	352	101	112	4	0	0
2	GS	81	569	352	101	112	4	0	0
2	GT	86	604	374	107	119	4	0	0
2	GV	81	569	352	101	112	4	0	0
2	GW	81	569	352	101	112	4	0	0
2	GX	86	604	374	107	119	4	0	0
2	GZ	81	569	352	101	112	4	0	0
2	HA	81	569	352	101	112	4	0	0
2	HB	86	604	374	107	119	4	0	0
2	HD	81	569	352	101	112	4	0	0
2	HE	81	569	352	101	112	4	0	0
2	HF	86	604	374	107	119	4	0	0
2	HH	81	569	352	101	112	4	0	0
2	HI	81	569	352	101	112	4	0	0
2	HJ	86	604	374	107	119	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	HL	81	569	352	101	112	4	0	0
2	HM	81	569	352	101	112	4	0	0
2	HN	86	604	374	107	119	4	0	0
2	HP	81	569	352	101	112	4	0	0
2	HQ	81	569	352	101	112	4	0	0
2	HR	86	604	374	107	119	4	0	0
2	HT	81	569	352	101	112	4	0	0
2	HU	81	569	352	101	112	4	0	0
2	HV	86	604	374	107	119	4	0	0
2	HX	81	569	352	101	112	4	0	0
2	HY	81	569	352	101	112	4	0	0
2	HZ	86	604	374	107	119	4	0	0
2	IB	81	569	352	101	112	4	0	0
2	IC	81	569	352	101	112	4	0	0
2	ID	86	604	374	107	119	4	0	0
2	IF	81	569	352	101	112	4	0	0
2	IG	81	569	352	101	112	4	0	0
2	IH	86	604	374	107	119	4	0	0
2	IJ	81	569	352	101	112	4	0	0
2	IK	81	569	352	101	112	4	0	0
2	IL	86	604	374	107	119	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	IN	81	Total 569	C 352	N 101	O 112	S 4	0	0
2	IO	81	Total 569	C 352	N 101	O 112	S 4	0	0
2	IP	86	Total 604	C 374	N 107	O 119	S 4	0	0
2	IR	81	Total 569	C 352	N 101	O 112	S 4	0	0
2	IS	81	Total 569	C 352	N 101	O 112	S 4	0	0
2	IT	86	Total 604	C 374	N 107	O 119	S 4	0	0
2	IV	81	Total 569	C 352	N 101	O 112	S 4	0	0
2	IW	81	Total 569	C 352	N 101	O 112	S 4	0	0
2	IX	86	Total 604	C 374	N 107	O 119	S 4	0	0
2	IZ	81	Total 569	C 352	N 101	O 112	S 4	0	0
2	JA	81	Total 569	C 352	N 101	O 112	S 4	0	0
2	JB	86	Total 604	C 374	N 107	O 119	S 4	0	0
2	JD	81	Total 569	C 352	N 101	O 112	S 4	0	0
2	JE	81	Total 569	C 352	N 101	O 112	S 4	0	0
2	JF	86	Total 604	C 374	N 107	O 119	S 4	0	0

There are 2520 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AB	88	GLY	-	expression tag	UNP A0A0J4R4X1
AB	89	SER	-	expression tag	UNP A0A0J4R4X1
AB	90	THR	-	expression tag	UNP A0A0J4R4X1
AB	91	LYS	-	expression tag	UNP A0A0J4R4X1
AB	92	HIS	-	expression tag	UNP A0A0J4R4X1
AB	93	LYS	-	expression tag	UNP A0A0J4R4X1
AB	94	SER	-	expression tag	UNP A0A0J4R4X1
AB	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
AB	96	ARG	-	expression tag	UNP A0A0J4R4X1
AB	97	PRO	-	expression tag	UNP A0A0J4R4X1
AB	98	HIS	-	expression tag	UNP A0A0J4R4X1
AB	99	ASN	-	expression tag	UNP A0A0J4R4X1
AB	100	ALA	-	expression tag	UNP A0A0J4R4X1
AC	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AC	88	GLY	-	expression tag	UNP A0A0J4R4X1
AC	89	SER	-	expression tag	UNP A0A0J4R4X1
AC	90	THR	-	expression tag	UNP A0A0J4R4X1
AC	91	LYS	-	expression tag	UNP A0A0J4R4X1
AC	92	HIS	-	expression tag	UNP A0A0J4R4X1
AC	93	LYS	-	expression tag	UNP A0A0J4R4X1
AC	94	SER	-	expression tag	UNP A0A0J4R4X1
AC	95	LEU	-	expression tag	UNP A0A0J4R4X1
AC	96	ARG	-	expression tag	UNP A0A0J4R4X1
AC	97	PRO	-	expression tag	UNP A0A0J4R4X1
AC	98	HIS	-	expression tag	UNP A0A0J4R4X1
AC	99	ASN	-	expression tag	UNP A0A0J4R4X1
AC	100	ALA	-	expression tag	UNP A0A0J4R4X1
AD	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AD	88	GLY	-	expression tag	UNP A0A0J4R4X1
AD	89	SER	-	expression tag	UNP A0A0J4R4X1
AD	90	THR	-	expression tag	UNP A0A0J4R4X1
AD	91	LYS	-	expression tag	UNP A0A0J4R4X1
AD	92	HIS	-	expression tag	UNP A0A0J4R4X1
AD	93	LYS	-	expression tag	UNP A0A0J4R4X1
AD	94	SER	-	expression tag	UNP A0A0J4R4X1
AD	95	LEU	-	expression tag	UNP A0A0J4R4X1
AD	96	ARG	-	expression tag	UNP A0A0J4R4X1
AD	97	PRO	-	expression tag	UNP A0A0J4R4X1
AD	98	HIS	-	expression tag	UNP A0A0J4R4X1
AD	99	ASN	-	expression tag	UNP A0A0J4R4X1
AD	100	ALA	-	expression tag	UNP A0A0J4R4X1
AF	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AF	88	GLY	-	expression tag	UNP A0A0J4R4X1
AF	89	SER	-	expression tag	UNP A0A0J4R4X1
AF	90	THR	-	expression tag	UNP A0A0J4R4X1
AF	91	LYS	-	expression tag	UNP A0A0J4R4X1
AF	92	HIS	-	expression tag	UNP A0A0J4R4X1
AF	93	LYS	-	expression tag	UNP A0A0J4R4X1
AF	94	SER	-	expression tag	UNP A0A0J4R4X1
AF	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
AF	96	ARG	-	expression tag	UNP A0A0J4R4X1
AF	97	PRO	-	expression tag	UNP A0A0J4R4X1
AF	98	HIS	-	expression tag	UNP A0A0J4R4X1
AF	99	ASN	-	expression tag	UNP A0A0J4R4X1
AF	100	ALA	-	expression tag	UNP A0A0J4R4X1
AG	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AG	88	GLY	-	expression tag	UNP A0A0J4R4X1
AG	89	SER	-	expression tag	UNP A0A0J4R4X1
AG	90	THR	-	expression tag	UNP A0A0J4R4X1
AG	91	LYS	-	expression tag	UNP A0A0J4R4X1
AG	92	HIS	-	expression tag	UNP A0A0J4R4X1
AG	93	LYS	-	expression tag	UNP A0A0J4R4X1
AG	94	SER	-	expression tag	UNP A0A0J4R4X1
AG	95	LEU	-	expression tag	UNP A0A0J4R4X1
AG	96	ARG	-	expression tag	UNP A0A0J4R4X1
AG	97	PRO	-	expression tag	UNP A0A0J4R4X1
AG	98	HIS	-	expression tag	UNP A0A0J4R4X1
AG	99	ASN	-	expression tag	UNP A0A0J4R4X1
AG	100	ALA	-	expression tag	UNP A0A0J4R4X1
AH	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AH	88	GLY	-	expression tag	UNP A0A0J4R4X1
AH	89	SER	-	expression tag	UNP A0A0J4R4X1
AH	90	THR	-	expression tag	UNP A0A0J4R4X1
AH	91	LYS	-	expression tag	UNP A0A0J4R4X1
AH	92	HIS	-	expression tag	UNP A0A0J4R4X1
AH	93	LYS	-	expression tag	UNP A0A0J4R4X1
AH	94	SER	-	expression tag	UNP A0A0J4R4X1
AH	95	LEU	-	expression tag	UNP A0A0J4R4X1
AH	96	ARG	-	expression tag	UNP A0A0J4R4X1
AH	97	PRO	-	expression tag	UNP A0A0J4R4X1
AH	98	HIS	-	expression tag	UNP A0A0J4R4X1
AH	99	ASN	-	expression tag	UNP A0A0J4R4X1
AH	100	ALA	-	expression tag	UNP A0A0J4R4X1
AJ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AJ	88	GLY	-	expression tag	UNP A0A0J4R4X1
AJ	89	SER	-	expression tag	UNP A0A0J4R4X1
AJ	90	THR	-	expression tag	UNP A0A0J4R4X1
AJ	91	LYS	-	expression tag	UNP A0A0J4R4X1
AJ	92	HIS	-	expression tag	UNP A0A0J4R4X1
AJ	93	LYS	-	expression tag	UNP A0A0J4R4X1
AJ	94	SER	-	expression tag	UNP A0A0J4R4X1
AJ	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
AJ	96	ARG	-	expression tag	UNP A0A0J4R4X1
AJ	97	PRO	-	expression tag	UNP A0A0J4R4X1
AJ	98	HIS	-	expression tag	UNP A0A0J4R4X1
AJ	99	ASN	-	expression tag	UNP A0A0J4R4X1
AJ	100	ALA	-	expression tag	UNP A0A0J4R4X1
AK	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AK	88	GLY	-	expression tag	UNP A0A0J4R4X1
AK	89	SER	-	expression tag	UNP A0A0J4R4X1
AK	90	THR	-	expression tag	UNP A0A0J4R4X1
AK	91	LYS	-	expression tag	UNP A0A0J4R4X1
AK	92	HIS	-	expression tag	UNP A0A0J4R4X1
AK	93	LYS	-	expression tag	UNP A0A0J4R4X1
AK	94	SER	-	expression tag	UNP A0A0J4R4X1
AK	95	LEU	-	expression tag	UNP A0A0J4R4X1
AK	96	ARG	-	expression tag	UNP A0A0J4R4X1
AK	97	PRO	-	expression tag	UNP A0A0J4R4X1
AK	98	HIS	-	expression tag	UNP A0A0J4R4X1
AK	99	ASN	-	expression tag	UNP A0A0J4R4X1
AK	100	ALA	-	expression tag	UNP A0A0J4R4X1
AL	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AL	88	GLY	-	expression tag	UNP A0A0J4R4X1
AL	89	SER	-	expression tag	UNP A0A0J4R4X1
AL	90	THR	-	expression tag	UNP A0A0J4R4X1
AL	91	LYS	-	expression tag	UNP A0A0J4R4X1
AL	92	HIS	-	expression tag	UNP A0A0J4R4X1
AL	93	LYS	-	expression tag	UNP A0A0J4R4X1
AL	94	SER	-	expression tag	UNP A0A0J4R4X1
AL	95	LEU	-	expression tag	UNP A0A0J4R4X1
AL	96	ARG	-	expression tag	UNP A0A0J4R4X1
AL	97	PRO	-	expression tag	UNP A0A0J4R4X1
AL	98	HIS	-	expression tag	UNP A0A0J4R4X1
AL	99	ASN	-	expression tag	UNP A0A0J4R4X1
AL	100	ALA	-	expression tag	UNP A0A0J4R4X1
AN	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AN	88	GLY	-	expression tag	UNP A0A0J4R4X1
AN	89	SER	-	expression tag	UNP A0A0J4R4X1
AN	90	THR	-	expression tag	UNP A0A0J4R4X1
AN	91	LYS	-	expression tag	UNP A0A0J4R4X1
AN	92	HIS	-	expression tag	UNP A0A0J4R4X1
AN	93	LYS	-	expression tag	UNP A0A0J4R4X1
AN	94	SER	-	expression tag	UNP A0A0J4R4X1
AN	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
AN	96	ARG	-	expression tag	UNP A0A0J4R4X1
AN	97	PRO	-	expression tag	UNP A0A0J4R4X1
AN	98	HIS	-	expression tag	UNP A0A0J4R4X1
AN	99	ASN	-	expression tag	UNP A0A0J4R4X1
AN	100	ALA	-	expression tag	UNP A0A0J4R4X1
AO	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AO	88	GLY	-	expression tag	UNP A0A0J4R4X1
AO	89	SER	-	expression tag	UNP A0A0J4R4X1
AO	90	THR	-	expression tag	UNP A0A0J4R4X1
AO	91	LYS	-	expression tag	UNP A0A0J4R4X1
AO	92	HIS	-	expression tag	UNP A0A0J4R4X1
AO	93	LYS	-	expression tag	UNP A0A0J4R4X1
AO	94	SER	-	expression tag	UNP A0A0J4R4X1
AO	95	LEU	-	expression tag	UNP A0A0J4R4X1
AO	96	ARG	-	expression tag	UNP A0A0J4R4X1
AO	97	PRO	-	expression tag	UNP A0A0J4R4X1
AO	98	HIS	-	expression tag	UNP A0A0J4R4X1
AO	99	ASN	-	expression tag	UNP A0A0J4R4X1
AO	100	ALA	-	expression tag	UNP A0A0J4R4X1
AP	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AP	88	GLY	-	expression tag	UNP A0A0J4R4X1
AP	89	SER	-	expression tag	UNP A0A0J4R4X1
AP	90	THR	-	expression tag	UNP A0A0J4R4X1
AP	91	LYS	-	expression tag	UNP A0A0J4R4X1
AP	92	HIS	-	expression tag	UNP A0A0J4R4X1
AP	93	LYS	-	expression tag	UNP A0A0J4R4X1
AP	94	SER	-	expression tag	UNP A0A0J4R4X1
AP	95	LEU	-	expression tag	UNP A0A0J4R4X1
AP	96	ARG	-	expression tag	UNP A0A0J4R4X1
AP	97	PRO	-	expression tag	UNP A0A0J4R4X1
AP	98	HIS	-	expression tag	UNP A0A0J4R4X1
AP	99	ASN	-	expression tag	UNP A0A0J4R4X1
AP	100	ALA	-	expression tag	UNP A0A0J4R4X1
AR	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AR	88	GLY	-	expression tag	UNP A0A0J4R4X1
AR	89	SER	-	expression tag	UNP A0A0J4R4X1
AR	90	THR	-	expression tag	UNP A0A0J4R4X1
AR	91	LYS	-	expression tag	UNP A0A0J4R4X1
AR	92	HIS	-	expression tag	UNP A0A0J4R4X1
AR	93	LYS	-	expression tag	UNP A0A0J4R4X1
AR	94	SER	-	expression tag	UNP A0A0J4R4X1
AR	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
AR	96	ARG	-	expression tag	UNP A0A0J4R4X1
AR	97	PRO	-	expression tag	UNP A0A0J4R4X1
AR	98	HIS	-	expression tag	UNP A0A0J4R4X1
AR	99	ASN	-	expression tag	UNP A0A0J4R4X1
AR	100	ALA	-	expression tag	UNP A0A0J4R4X1
AS	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AS	88	GLY	-	expression tag	UNP A0A0J4R4X1
AS	89	SER	-	expression tag	UNP A0A0J4R4X1
AS	90	THR	-	expression tag	UNP A0A0J4R4X1
AS	91	LYS	-	expression tag	UNP A0A0J4R4X1
AS	92	HIS	-	expression tag	UNP A0A0J4R4X1
AS	93	LYS	-	expression tag	UNP A0A0J4R4X1
AS	94	SER	-	expression tag	UNP A0A0J4R4X1
AS	95	LEU	-	expression tag	UNP A0A0J4R4X1
AS	96	ARG	-	expression tag	UNP A0A0J4R4X1
AS	97	PRO	-	expression tag	UNP A0A0J4R4X1
AS	98	HIS	-	expression tag	UNP A0A0J4R4X1
AS	99	ASN	-	expression tag	UNP A0A0J4R4X1
AS	100	ALA	-	expression tag	UNP A0A0J4R4X1
AT	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AT	88	GLY	-	expression tag	UNP A0A0J4R4X1
AT	89	SER	-	expression tag	UNP A0A0J4R4X1
AT	90	THR	-	expression tag	UNP A0A0J4R4X1
AT	91	LYS	-	expression tag	UNP A0A0J4R4X1
AT	92	HIS	-	expression tag	UNP A0A0J4R4X1
AT	93	LYS	-	expression tag	UNP A0A0J4R4X1
AT	94	SER	-	expression tag	UNP A0A0J4R4X1
AT	95	LEU	-	expression tag	UNP A0A0J4R4X1
AT	96	ARG	-	expression tag	UNP A0A0J4R4X1
AT	97	PRO	-	expression tag	UNP A0A0J4R4X1
AT	98	HIS	-	expression tag	UNP A0A0J4R4X1
AT	99	ASN	-	expression tag	UNP A0A0J4R4X1
AT	100	ALA	-	expression tag	UNP A0A0J4R4X1
AV	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AV	88	GLY	-	expression tag	UNP A0A0J4R4X1
AV	89	SER	-	expression tag	UNP A0A0J4R4X1
AV	90	THR	-	expression tag	UNP A0A0J4R4X1
AV	91	LYS	-	expression tag	UNP A0A0J4R4X1
AV	92	HIS	-	expression tag	UNP A0A0J4R4X1
AV	93	LYS	-	expression tag	UNP A0A0J4R4X1
AV	94	SER	-	expression tag	UNP A0A0J4R4X1
AV	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
AV	96	ARG	-	expression tag	UNP A0A0J4R4X1
AV	97	PRO	-	expression tag	UNP A0A0J4R4X1
AV	98	HIS	-	expression tag	UNP A0A0J4R4X1
AV	99	ASN	-	expression tag	UNP A0A0J4R4X1
AV	100	ALA	-	expression tag	UNP A0A0J4R4X1
AW	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AW	88	GLY	-	expression tag	UNP A0A0J4R4X1
AW	89	SER	-	expression tag	UNP A0A0J4R4X1
AW	90	THR	-	expression tag	UNP A0A0J4R4X1
AW	91	LYS	-	expression tag	UNP A0A0J4R4X1
AW	92	HIS	-	expression tag	UNP A0A0J4R4X1
AW	93	LYS	-	expression tag	UNP A0A0J4R4X1
AW	94	SER	-	expression tag	UNP A0A0J4R4X1
AW	95	LEU	-	expression tag	UNP A0A0J4R4X1
AW	96	ARG	-	expression tag	UNP A0A0J4R4X1
AW	97	PRO	-	expression tag	UNP A0A0J4R4X1
AW	98	HIS	-	expression tag	UNP A0A0J4R4X1
AW	99	ASN	-	expression tag	UNP A0A0J4R4X1
AW	100	ALA	-	expression tag	UNP A0A0J4R4X1
AX	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AX	88	GLY	-	expression tag	UNP A0A0J4R4X1
AX	89	SER	-	expression tag	UNP A0A0J4R4X1
AX	90	THR	-	expression tag	UNP A0A0J4R4X1
AX	91	LYS	-	expression tag	UNP A0A0J4R4X1
AX	92	HIS	-	expression tag	UNP A0A0J4R4X1
AX	93	LYS	-	expression tag	UNP A0A0J4R4X1
AX	94	SER	-	expression tag	UNP A0A0J4R4X1
AX	95	LEU	-	expression tag	UNP A0A0J4R4X1
AX	96	ARG	-	expression tag	UNP A0A0J4R4X1
AX	97	PRO	-	expression tag	UNP A0A0J4R4X1
AX	98	HIS	-	expression tag	UNP A0A0J4R4X1
AX	99	ASN	-	expression tag	UNP A0A0J4R4X1
AX	100	ALA	-	expression tag	UNP A0A0J4R4X1
AZ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
AZ	88	GLY	-	expression tag	UNP A0A0J4R4X1
AZ	89	SER	-	expression tag	UNP A0A0J4R4X1
AZ	90	THR	-	expression tag	UNP A0A0J4R4X1
AZ	91	LYS	-	expression tag	UNP A0A0J4R4X1
AZ	92	HIS	-	expression tag	UNP A0A0J4R4X1
AZ	93	LYS	-	expression tag	UNP A0A0J4R4X1
AZ	94	SER	-	expression tag	UNP A0A0J4R4X1
AZ	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
AZ	96	ARG	-	expression tag	UNP A0A0J4R4X1
AZ	97	PRO	-	expression tag	UNP A0A0J4R4X1
AZ	98	HIS	-	expression tag	UNP A0A0J4R4X1
AZ	99	ASN	-	expression tag	UNP A0A0J4R4X1
AZ	100	ALA	-	expression tag	UNP A0A0J4R4X1
BA	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BA	88	GLY	-	expression tag	UNP A0A0J4R4X1
BA	89	SER	-	expression tag	UNP A0A0J4R4X1
BA	90	THR	-	expression tag	UNP A0A0J4R4X1
BA	91	LYS	-	expression tag	UNP A0A0J4R4X1
BA	92	HIS	-	expression tag	UNP A0A0J4R4X1
BA	93	LYS	-	expression tag	UNP A0A0J4R4X1
BA	94	SER	-	expression tag	UNP A0A0J4R4X1
BA	95	LEU	-	expression tag	UNP A0A0J4R4X1
BA	96	ARG	-	expression tag	UNP A0A0J4R4X1
BA	97	PRO	-	expression tag	UNP A0A0J4R4X1
BA	98	HIS	-	expression tag	UNP A0A0J4R4X1
BA	99	ASN	-	expression tag	UNP A0A0J4R4X1
BA	100	ALA	-	expression tag	UNP A0A0J4R4X1
BB	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BB	88	GLY	-	expression tag	UNP A0A0J4R4X1
BB	89	SER	-	expression tag	UNP A0A0J4R4X1
BB	90	THR	-	expression tag	UNP A0A0J4R4X1
BB	91	LYS	-	expression tag	UNP A0A0J4R4X1
BB	92	HIS	-	expression tag	UNP A0A0J4R4X1
BB	93	LYS	-	expression tag	UNP A0A0J4R4X1
BB	94	SER	-	expression tag	UNP A0A0J4R4X1
BB	95	LEU	-	expression tag	UNP A0A0J4R4X1
BB	96	ARG	-	expression tag	UNP A0A0J4R4X1
BB	97	PRO	-	expression tag	UNP A0A0J4R4X1
BB	98	HIS	-	expression tag	UNP A0A0J4R4X1
BB	99	ASN	-	expression tag	UNP A0A0J4R4X1
BB	100	ALA	-	expression tag	UNP A0A0J4R4X1
BD	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BD	88	GLY	-	expression tag	UNP A0A0J4R4X1
BD	89	SER	-	expression tag	UNP A0A0J4R4X1
BD	90	THR	-	expression tag	UNP A0A0J4R4X1
BD	91	LYS	-	expression tag	UNP A0A0J4R4X1
BD	92	HIS	-	expression tag	UNP A0A0J4R4X1
BD	93	LYS	-	expression tag	UNP A0A0J4R4X1
BD	94	SER	-	expression tag	UNP A0A0J4R4X1
BD	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
BD	96	ARG	-	expression tag	UNP A0A0J4R4X1
BD	97	PRO	-	expression tag	UNP A0A0J4R4X1
BD	98	HIS	-	expression tag	UNP A0A0J4R4X1
BD	99	ASN	-	expression tag	UNP A0A0J4R4X1
BD	100	ALA	-	expression tag	UNP A0A0J4R4X1
BE	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BE	88	GLY	-	expression tag	UNP A0A0J4R4X1
BE	89	SER	-	expression tag	UNP A0A0J4R4X1
BE	90	THR	-	expression tag	UNP A0A0J4R4X1
BE	91	LYS	-	expression tag	UNP A0A0J4R4X1
BE	92	HIS	-	expression tag	UNP A0A0J4R4X1
BE	93	LYS	-	expression tag	UNP A0A0J4R4X1
BE	94	SER	-	expression tag	UNP A0A0J4R4X1
BE	95	LEU	-	expression tag	UNP A0A0J4R4X1
BE	96	ARG	-	expression tag	UNP A0A0J4R4X1
BE	97	PRO	-	expression tag	UNP A0A0J4R4X1
BE	98	HIS	-	expression tag	UNP A0A0J4R4X1
BE	99	ASN	-	expression tag	UNP A0A0J4R4X1
BE	100	ALA	-	expression tag	UNP A0A0J4R4X1
BF	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BF	88	GLY	-	expression tag	UNP A0A0J4R4X1
BF	89	SER	-	expression tag	UNP A0A0J4R4X1
BF	90	THR	-	expression tag	UNP A0A0J4R4X1
BF	91	LYS	-	expression tag	UNP A0A0J4R4X1
BF	92	HIS	-	expression tag	UNP A0A0J4R4X1
BF	93	LYS	-	expression tag	UNP A0A0J4R4X1
BF	94	SER	-	expression tag	UNP A0A0J4R4X1
BF	95	LEU	-	expression tag	UNP A0A0J4R4X1
BF	96	ARG	-	expression tag	UNP A0A0J4R4X1
BF	97	PRO	-	expression tag	UNP A0A0J4R4X1
BF	98	HIS	-	expression tag	UNP A0A0J4R4X1
BF	99	ASN	-	expression tag	UNP A0A0J4R4X1
BF	100	ALA	-	expression tag	UNP A0A0J4R4X1
BH	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BH	88	GLY	-	expression tag	UNP A0A0J4R4X1
BH	89	SER	-	expression tag	UNP A0A0J4R4X1
BH	90	THR	-	expression tag	UNP A0A0J4R4X1
BH	91	LYS	-	expression tag	UNP A0A0J4R4X1
BH	92	HIS	-	expression tag	UNP A0A0J4R4X1
BH	93	LYS	-	expression tag	UNP A0A0J4R4X1
BH	94	SER	-	expression tag	UNP A0A0J4R4X1
BH	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
BH	96	ARG	-	expression tag	UNP A0A0J4R4X1
BH	97	PRO	-	expression tag	UNP A0A0J4R4X1
BH	98	HIS	-	expression tag	UNP A0A0J4R4X1
BH	99	ASN	-	expression tag	UNP A0A0J4R4X1
BH	100	ALA	-	expression tag	UNP A0A0J4R4X1
BI	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BI	88	GLY	-	expression tag	UNP A0A0J4R4X1
BI	89	SER	-	expression tag	UNP A0A0J4R4X1
BI	90	THR	-	expression tag	UNP A0A0J4R4X1
BI	91	LYS	-	expression tag	UNP A0A0J4R4X1
BI	92	HIS	-	expression tag	UNP A0A0J4R4X1
BI	93	LYS	-	expression tag	UNP A0A0J4R4X1
BI	94	SER	-	expression tag	UNP A0A0J4R4X1
BI	95	LEU	-	expression tag	UNP A0A0J4R4X1
BI	96	ARG	-	expression tag	UNP A0A0J4R4X1
BI	97	PRO	-	expression tag	UNP A0A0J4R4X1
BI	98	HIS	-	expression tag	UNP A0A0J4R4X1
BI	99	ASN	-	expression tag	UNP A0A0J4R4X1
BI	100	ALA	-	expression tag	UNP A0A0J4R4X1
BJ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BJ	88	GLY	-	expression tag	UNP A0A0J4R4X1
BJ	89	SER	-	expression tag	UNP A0A0J4R4X1
BJ	90	THR	-	expression tag	UNP A0A0J4R4X1
BJ	91	LYS	-	expression tag	UNP A0A0J4R4X1
BJ	92	HIS	-	expression tag	UNP A0A0J4R4X1
BJ	93	LYS	-	expression tag	UNP A0A0J4R4X1
BJ	94	SER	-	expression tag	UNP A0A0J4R4X1
BJ	95	LEU	-	expression tag	UNP A0A0J4R4X1
BJ	96	ARG	-	expression tag	UNP A0A0J4R4X1
BJ	97	PRO	-	expression tag	UNP A0A0J4R4X1
BJ	98	HIS	-	expression tag	UNP A0A0J4R4X1
BJ	99	ASN	-	expression tag	UNP A0A0J4R4X1
BJ	100	ALA	-	expression tag	UNP A0A0J4R4X1
BL	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BL	88	GLY	-	expression tag	UNP A0A0J4R4X1
BL	89	SER	-	expression tag	UNP A0A0J4R4X1
BL	90	THR	-	expression tag	UNP A0A0J4R4X1
BL	91	LYS	-	expression tag	UNP A0A0J4R4X1
BL	92	HIS	-	expression tag	UNP A0A0J4R4X1
BL	93	LYS	-	expression tag	UNP A0A0J4R4X1
BL	94	SER	-	expression tag	UNP A0A0J4R4X1
BL	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
BL	96	ARG	-	expression tag	UNP A0A0J4R4X1
BL	97	PRO	-	expression tag	UNP A0A0J4R4X1
BL	98	HIS	-	expression tag	UNP A0A0J4R4X1
BL	99	ASN	-	expression tag	UNP A0A0J4R4X1
BL	100	ALA	-	expression tag	UNP A0A0J4R4X1
BM	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BM	88	GLY	-	expression tag	UNP A0A0J4R4X1
BM	89	SER	-	expression tag	UNP A0A0J4R4X1
BM	90	THR	-	expression tag	UNP A0A0J4R4X1
BM	91	LYS	-	expression tag	UNP A0A0J4R4X1
BM	92	HIS	-	expression tag	UNP A0A0J4R4X1
BM	93	LYS	-	expression tag	UNP A0A0J4R4X1
BM	94	SER	-	expression tag	UNP A0A0J4R4X1
BM	95	LEU	-	expression tag	UNP A0A0J4R4X1
BM	96	ARG	-	expression tag	UNP A0A0J4R4X1
BM	97	PRO	-	expression tag	UNP A0A0J4R4X1
BM	98	HIS	-	expression tag	UNP A0A0J4R4X1
BM	99	ASN	-	expression tag	UNP A0A0J4R4X1
BM	100	ALA	-	expression tag	UNP A0A0J4R4X1
BN	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BN	88	GLY	-	expression tag	UNP A0A0J4R4X1
BN	89	SER	-	expression tag	UNP A0A0J4R4X1
BN	90	THR	-	expression tag	UNP A0A0J4R4X1
BN	91	LYS	-	expression tag	UNP A0A0J4R4X1
BN	92	HIS	-	expression tag	UNP A0A0J4R4X1
BN	93	LYS	-	expression tag	UNP A0A0J4R4X1
BN	94	SER	-	expression tag	UNP A0A0J4R4X1
BN	95	LEU	-	expression tag	UNP A0A0J4R4X1
BN	96	ARG	-	expression tag	UNP A0A0J4R4X1
BN	97	PRO	-	expression tag	UNP A0A0J4R4X1
BN	98	HIS	-	expression tag	UNP A0A0J4R4X1
BN	99	ASN	-	expression tag	UNP A0A0J4R4X1
BN	100	ALA	-	expression tag	UNP A0A0J4R4X1
BP	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BP	88	GLY	-	expression tag	UNP A0A0J4R4X1
BP	89	SER	-	expression tag	UNP A0A0J4R4X1
BP	90	THR	-	expression tag	UNP A0A0J4R4X1
BP	91	LYS	-	expression tag	UNP A0A0J4R4X1
BP	92	HIS	-	expression tag	UNP A0A0J4R4X1
BP	93	LYS	-	expression tag	UNP A0A0J4R4X1
BP	94	SER	-	expression tag	UNP A0A0J4R4X1
BP	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
BP	96	ARG	-	expression tag	UNP A0A0J4R4X1
BP	97	PRO	-	expression tag	UNP A0A0J4R4X1
BP	98	HIS	-	expression tag	UNP A0A0J4R4X1
BP	99	ASN	-	expression tag	UNP A0A0J4R4X1
BP	100	ALA	-	expression tag	UNP A0A0J4R4X1
BQ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BQ	88	GLY	-	expression tag	UNP A0A0J4R4X1
BQ	89	SER	-	expression tag	UNP A0A0J4R4X1
BQ	90	THR	-	expression tag	UNP A0A0J4R4X1
BQ	91	LYS	-	expression tag	UNP A0A0J4R4X1
BQ	92	HIS	-	expression tag	UNP A0A0J4R4X1
BQ	93	LYS	-	expression tag	UNP A0A0J4R4X1
BQ	94	SER	-	expression tag	UNP A0A0J4R4X1
BQ	95	LEU	-	expression tag	UNP A0A0J4R4X1
BQ	96	ARG	-	expression tag	UNP A0A0J4R4X1
BQ	97	PRO	-	expression tag	UNP A0A0J4R4X1
BQ	98	HIS	-	expression tag	UNP A0A0J4R4X1
BQ	99	ASN	-	expression tag	UNP A0A0J4R4X1
BQ	100	ALA	-	expression tag	UNP A0A0J4R4X1
BR	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BR	88	GLY	-	expression tag	UNP A0A0J4R4X1
BR	89	SER	-	expression tag	UNP A0A0J4R4X1
BR	90	THR	-	expression tag	UNP A0A0J4R4X1
BR	91	LYS	-	expression tag	UNP A0A0J4R4X1
BR	92	HIS	-	expression tag	UNP A0A0J4R4X1
BR	93	LYS	-	expression tag	UNP A0A0J4R4X1
BR	94	SER	-	expression tag	UNP A0A0J4R4X1
BR	95	LEU	-	expression tag	UNP A0A0J4R4X1
BR	96	ARG	-	expression tag	UNP A0A0J4R4X1
BR	97	PRO	-	expression tag	UNP A0A0J4R4X1
BR	98	HIS	-	expression tag	UNP A0A0J4R4X1
BR	99	ASN	-	expression tag	UNP A0A0J4R4X1
BR	100	ALA	-	expression tag	UNP A0A0J4R4X1
BT	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BT	88	GLY	-	expression tag	UNP A0A0J4R4X1
BT	89	SER	-	expression tag	UNP A0A0J4R4X1
BT	90	THR	-	expression tag	UNP A0A0J4R4X1
BT	91	LYS	-	expression tag	UNP A0A0J4R4X1
BT	92	HIS	-	expression tag	UNP A0A0J4R4X1
BT	93	LYS	-	expression tag	UNP A0A0J4R4X1
BT	94	SER	-	expression tag	UNP A0A0J4R4X1
BT	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
BT	96	ARG	-	expression tag	UNP A0A0J4R4X1
BT	97	PRO	-	expression tag	UNP A0A0J4R4X1
BT	98	HIS	-	expression tag	UNP A0A0J4R4X1
BT	99	ASN	-	expression tag	UNP A0A0J4R4X1
BT	100	ALA	-	expression tag	UNP A0A0J4R4X1
BU	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BU	88	GLY	-	expression tag	UNP A0A0J4R4X1
BU	89	SER	-	expression tag	UNP A0A0J4R4X1
BU	90	THR	-	expression tag	UNP A0A0J4R4X1
BU	91	LYS	-	expression tag	UNP A0A0J4R4X1
BU	92	HIS	-	expression tag	UNP A0A0J4R4X1
BU	93	LYS	-	expression tag	UNP A0A0J4R4X1
BU	94	SER	-	expression tag	UNP A0A0J4R4X1
BU	95	LEU	-	expression tag	UNP A0A0J4R4X1
BU	96	ARG	-	expression tag	UNP A0A0J4R4X1
BU	97	PRO	-	expression tag	UNP A0A0J4R4X1
BU	98	HIS	-	expression tag	UNP A0A0J4R4X1
BU	99	ASN	-	expression tag	UNP A0A0J4R4X1
BU	100	ALA	-	expression tag	UNP A0A0J4R4X1
BV	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BV	88	GLY	-	expression tag	UNP A0A0J4R4X1
BV	89	SER	-	expression tag	UNP A0A0J4R4X1
BV	90	THR	-	expression tag	UNP A0A0J4R4X1
BV	91	LYS	-	expression tag	UNP A0A0J4R4X1
BV	92	HIS	-	expression tag	UNP A0A0J4R4X1
BV	93	LYS	-	expression tag	UNP A0A0J4R4X1
BV	94	SER	-	expression tag	UNP A0A0J4R4X1
BV	95	LEU	-	expression tag	UNP A0A0J4R4X1
BV	96	ARG	-	expression tag	UNP A0A0J4R4X1
BV	97	PRO	-	expression tag	UNP A0A0J4R4X1
BV	98	HIS	-	expression tag	UNP A0A0J4R4X1
BV	99	ASN	-	expression tag	UNP A0A0J4R4X1
BV	100	ALA	-	expression tag	UNP A0A0J4R4X1
BX	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BX	88	GLY	-	expression tag	UNP A0A0J4R4X1
BX	89	SER	-	expression tag	UNP A0A0J4R4X1
BX	90	THR	-	expression tag	UNP A0A0J4R4X1
BX	91	LYS	-	expression tag	UNP A0A0J4R4X1
BX	92	HIS	-	expression tag	UNP A0A0J4R4X1
BX	93	LYS	-	expression tag	UNP A0A0J4R4X1
BX	94	SER	-	expression tag	UNP A0A0J4R4X1
BX	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
BX	96	ARG	-	expression tag	UNP A0A0J4R4X1
BX	97	PRO	-	expression tag	UNP A0A0J4R4X1
BX	98	HIS	-	expression tag	UNP A0A0J4R4X1
BX	99	ASN	-	expression tag	UNP A0A0J4R4X1
BX	100	ALA	-	expression tag	UNP A0A0J4R4X1
BY	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BY	88	GLY	-	expression tag	UNP A0A0J4R4X1
BY	89	SER	-	expression tag	UNP A0A0J4R4X1
BY	90	THR	-	expression tag	UNP A0A0J4R4X1
BY	91	LYS	-	expression tag	UNP A0A0J4R4X1
BY	92	HIS	-	expression tag	UNP A0A0J4R4X1
BY	93	LYS	-	expression tag	UNP A0A0J4R4X1
BY	94	SER	-	expression tag	UNP A0A0J4R4X1
BY	95	LEU	-	expression tag	UNP A0A0J4R4X1
BY	96	ARG	-	expression tag	UNP A0A0J4R4X1
BY	97	PRO	-	expression tag	UNP A0A0J4R4X1
BY	98	HIS	-	expression tag	UNP A0A0J4R4X1
BY	99	ASN	-	expression tag	UNP A0A0J4R4X1
BY	100	ALA	-	expression tag	UNP A0A0J4R4X1
BZ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
BZ	88	GLY	-	expression tag	UNP A0A0J4R4X1
BZ	89	SER	-	expression tag	UNP A0A0J4R4X1
BZ	90	THR	-	expression tag	UNP A0A0J4R4X1
BZ	91	LYS	-	expression tag	UNP A0A0J4R4X1
BZ	92	HIS	-	expression tag	UNP A0A0J4R4X1
BZ	93	LYS	-	expression tag	UNP A0A0J4R4X1
BZ	94	SER	-	expression tag	UNP A0A0J4R4X1
BZ	95	LEU	-	expression tag	UNP A0A0J4R4X1
BZ	96	ARG	-	expression tag	UNP A0A0J4R4X1
BZ	97	PRO	-	expression tag	UNP A0A0J4R4X1
BZ	98	HIS	-	expression tag	UNP A0A0J4R4X1
BZ	99	ASN	-	expression tag	UNP A0A0J4R4X1
BZ	100	ALA	-	expression tag	UNP A0A0J4R4X1
CB	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CB	88	GLY	-	expression tag	UNP A0A0J4R4X1
CB	89	SER	-	expression tag	UNP A0A0J4R4X1
CB	90	THR	-	expression tag	UNP A0A0J4R4X1
CB	91	LYS	-	expression tag	UNP A0A0J4R4X1
CB	92	HIS	-	expression tag	UNP A0A0J4R4X1
CB	93	LYS	-	expression tag	UNP A0A0J4R4X1
CB	94	SER	-	expression tag	UNP A0A0J4R4X1
CB	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
CB	96	ARG	-	expression tag	UNP A0A0J4R4X1
CB	97	PRO	-	expression tag	UNP A0A0J4R4X1
CB	98	HIS	-	expression tag	UNP A0A0J4R4X1
CB	99	ASN	-	expression tag	UNP A0A0J4R4X1
CB	100	ALA	-	expression tag	UNP A0A0J4R4X1
CC	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CC	88	GLY	-	expression tag	UNP A0A0J4R4X1
CC	89	SER	-	expression tag	UNP A0A0J4R4X1
CC	90	THR	-	expression tag	UNP A0A0J4R4X1
CC	91	LYS	-	expression tag	UNP A0A0J4R4X1
CC	92	HIS	-	expression tag	UNP A0A0J4R4X1
CC	93	LYS	-	expression tag	UNP A0A0J4R4X1
CC	94	SER	-	expression tag	UNP A0A0J4R4X1
CC	95	LEU	-	expression tag	UNP A0A0J4R4X1
CC	96	ARG	-	expression tag	UNP A0A0J4R4X1
CC	97	PRO	-	expression tag	UNP A0A0J4R4X1
CC	98	HIS	-	expression tag	UNP A0A0J4R4X1
CC	99	ASN	-	expression tag	UNP A0A0J4R4X1
CC	100	ALA	-	expression tag	UNP A0A0J4R4X1
CD	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CD	88	GLY	-	expression tag	UNP A0A0J4R4X1
CD	89	SER	-	expression tag	UNP A0A0J4R4X1
CD	90	THR	-	expression tag	UNP A0A0J4R4X1
CD	91	LYS	-	expression tag	UNP A0A0J4R4X1
CD	92	HIS	-	expression tag	UNP A0A0J4R4X1
CD	93	LYS	-	expression tag	UNP A0A0J4R4X1
CD	94	SER	-	expression tag	UNP A0A0J4R4X1
CD	95	LEU	-	expression tag	UNP A0A0J4R4X1
CD	96	ARG	-	expression tag	UNP A0A0J4R4X1
CD	97	PRO	-	expression tag	UNP A0A0J4R4X1
CD	98	HIS	-	expression tag	UNP A0A0J4R4X1
CD	99	ASN	-	expression tag	UNP A0A0J4R4X1
CD	100	ALA	-	expression tag	UNP A0A0J4R4X1
CF	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CF	88	GLY	-	expression tag	UNP A0A0J4R4X1
CF	89	SER	-	expression tag	UNP A0A0J4R4X1
CF	90	THR	-	expression tag	UNP A0A0J4R4X1
CF	91	LYS	-	expression tag	UNP A0A0J4R4X1
CF	92	HIS	-	expression tag	UNP A0A0J4R4X1
CF	93	LYS	-	expression tag	UNP A0A0J4R4X1
CF	94	SER	-	expression tag	UNP A0A0J4R4X1
CF	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
CF	96	ARG	-	expression tag	UNP A0A0J4R4X1
CF	97	PRO	-	expression tag	UNP A0A0J4R4X1
CF	98	HIS	-	expression tag	UNP A0A0J4R4X1
CF	99	ASN	-	expression tag	UNP A0A0J4R4X1
CF	100	ALA	-	expression tag	UNP A0A0J4R4X1
CG	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CG	88	GLY	-	expression tag	UNP A0A0J4R4X1
CG	89	SER	-	expression tag	UNP A0A0J4R4X1
CG	90	THR	-	expression tag	UNP A0A0J4R4X1
CG	91	LYS	-	expression tag	UNP A0A0J4R4X1
CG	92	HIS	-	expression tag	UNP A0A0J4R4X1
CG	93	LYS	-	expression tag	UNP A0A0J4R4X1
CG	94	SER	-	expression tag	UNP A0A0J4R4X1
CG	95	LEU	-	expression tag	UNP A0A0J4R4X1
CG	96	ARG	-	expression tag	UNP A0A0J4R4X1
CG	97	PRO	-	expression tag	UNP A0A0J4R4X1
CG	98	HIS	-	expression tag	UNP A0A0J4R4X1
CG	99	ASN	-	expression tag	UNP A0A0J4R4X1
CG	100	ALA	-	expression tag	UNP A0A0J4R4X1
CH	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CH	88	GLY	-	expression tag	UNP A0A0J4R4X1
CH	89	SER	-	expression tag	UNP A0A0J4R4X1
CH	90	THR	-	expression tag	UNP A0A0J4R4X1
CH	91	LYS	-	expression tag	UNP A0A0J4R4X1
CH	92	HIS	-	expression tag	UNP A0A0J4R4X1
CH	93	LYS	-	expression tag	UNP A0A0J4R4X1
CH	94	SER	-	expression tag	UNP A0A0J4R4X1
CH	95	LEU	-	expression tag	UNP A0A0J4R4X1
CH	96	ARG	-	expression tag	UNP A0A0J4R4X1
CH	97	PRO	-	expression tag	UNP A0A0J4R4X1
CH	98	HIS	-	expression tag	UNP A0A0J4R4X1
CH	99	ASN	-	expression tag	UNP A0A0J4R4X1
CH	100	ALA	-	expression tag	UNP A0A0J4R4X1
CJ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CJ	88	GLY	-	expression tag	UNP A0A0J4R4X1
CJ	89	SER	-	expression tag	UNP A0A0J4R4X1
CJ	90	THR	-	expression tag	UNP A0A0J4R4X1
CJ	91	LYS	-	expression tag	UNP A0A0J4R4X1
CJ	92	HIS	-	expression tag	UNP A0A0J4R4X1
CJ	93	LYS	-	expression tag	UNP A0A0J4R4X1
CJ	94	SER	-	expression tag	UNP A0A0J4R4X1
CJ	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
CJ	96	ARG	-	expression tag	UNP A0A0J4R4X1
CJ	97	PRO	-	expression tag	UNP A0A0J4R4X1
CJ	98	HIS	-	expression tag	UNP A0A0J4R4X1
CJ	99	ASN	-	expression tag	UNP A0A0J4R4X1
CJ	100	ALA	-	expression tag	UNP A0A0J4R4X1
CK	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CK	88	GLY	-	expression tag	UNP A0A0J4R4X1
CK	89	SER	-	expression tag	UNP A0A0J4R4X1
CK	90	THR	-	expression tag	UNP A0A0J4R4X1
CK	91	LYS	-	expression tag	UNP A0A0J4R4X1
CK	92	HIS	-	expression tag	UNP A0A0J4R4X1
CK	93	LYS	-	expression tag	UNP A0A0J4R4X1
CK	94	SER	-	expression tag	UNP A0A0J4R4X1
CK	95	LEU	-	expression tag	UNP A0A0J4R4X1
CK	96	ARG	-	expression tag	UNP A0A0J4R4X1
CK	97	PRO	-	expression tag	UNP A0A0J4R4X1
CK	98	HIS	-	expression tag	UNP A0A0J4R4X1
CK	99	ASN	-	expression tag	UNP A0A0J4R4X1
CK	100	ALA	-	expression tag	UNP A0A0J4R4X1
CL	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CL	88	GLY	-	expression tag	UNP A0A0J4R4X1
CL	89	SER	-	expression tag	UNP A0A0J4R4X1
CL	90	THR	-	expression tag	UNP A0A0J4R4X1
CL	91	LYS	-	expression tag	UNP A0A0J4R4X1
CL	92	HIS	-	expression tag	UNP A0A0J4R4X1
CL	93	LYS	-	expression tag	UNP A0A0J4R4X1
CL	94	SER	-	expression tag	UNP A0A0J4R4X1
CL	95	LEU	-	expression tag	UNP A0A0J4R4X1
CL	96	ARG	-	expression tag	UNP A0A0J4R4X1
CL	97	PRO	-	expression tag	UNP A0A0J4R4X1
CL	98	HIS	-	expression tag	UNP A0A0J4R4X1
CL	99	ASN	-	expression tag	UNP A0A0J4R4X1
CL	100	ALA	-	expression tag	UNP A0A0J4R4X1
CN	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CN	88	GLY	-	expression tag	UNP A0A0J4R4X1
CN	89	SER	-	expression tag	UNP A0A0J4R4X1
CN	90	THR	-	expression tag	UNP A0A0J4R4X1
CN	91	LYS	-	expression tag	UNP A0A0J4R4X1
CN	92	HIS	-	expression tag	UNP A0A0J4R4X1
CN	93	LYS	-	expression tag	UNP A0A0J4R4X1
CN	94	SER	-	expression tag	UNP A0A0J4R4X1
CN	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
CN	96	ARG	-	expression tag	UNP A0A0J4R4X1
CN	97	PRO	-	expression tag	UNP A0A0J4R4X1
CN	98	HIS	-	expression tag	UNP A0A0J4R4X1
CN	99	ASN	-	expression tag	UNP A0A0J4R4X1
CN	100	ALA	-	expression tag	UNP A0A0J4R4X1
CO	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CO	88	GLY	-	expression tag	UNP A0A0J4R4X1
CO	89	SER	-	expression tag	UNP A0A0J4R4X1
CO	90	THR	-	expression tag	UNP A0A0J4R4X1
CO	91	LYS	-	expression tag	UNP A0A0J4R4X1
CO	92	HIS	-	expression tag	UNP A0A0J4R4X1
CO	93	LYS	-	expression tag	UNP A0A0J4R4X1
CO	94	SER	-	expression tag	UNP A0A0J4R4X1
CO	95	LEU	-	expression tag	UNP A0A0J4R4X1
CO	96	ARG	-	expression tag	UNP A0A0J4R4X1
CO	97	PRO	-	expression tag	UNP A0A0J4R4X1
CO	98	HIS	-	expression tag	UNP A0A0J4R4X1
CO	99	ASN	-	expression tag	UNP A0A0J4R4X1
CO	100	ALA	-	expression tag	UNP A0A0J4R4X1
CP	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CP	88	GLY	-	expression tag	UNP A0A0J4R4X1
CP	89	SER	-	expression tag	UNP A0A0J4R4X1
CP	90	THR	-	expression tag	UNP A0A0J4R4X1
CP	91	LYS	-	expression tag	UNP A0A0J4R4X1
CP	92	HIS	-	expression tag	UNP A0A0J4R4X1
CP	93	LYS	-	expression tag	UNP A0A0J4R4X1
CP	94	SER	-	expression tag	UNP A0A0J4R4X1
CP	95	LEU	-	expression tag	UNP A0A0J4R4X1
CP	96	ARG	-	expression tag	UNP A0A0J4R4X1
CP	97	PRO	-	expression tag	UNP A0A0J4R4X1
CP	98	HIS	-	expression tag	UNP A0A0J4R4X1
CP	99	ASN	-	expression tag	UNP A0A0J4R4X1
CP	100	ALA	-	expression tag	UNP A0A0J4R4X1
CR	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CR	88	GLY	-	expression tag	UNP A0A0J4R4X1
CR	89	SER	-	expression tag	UNP A0A0J4R4X1
CR	90	THR	-	expression tag	UNP A0A0J4R4X1
CR	91	LYS	-	expression tag	UNP A0A0J4R4X1
CR	92	HIS	-	expression tag	UNP A0A0J4R4X1
CR	93	LYS	-	expression tag	UNP A0A0J4R4X1
CR	94	SER	-	expression tag	UNP A0A0J4R4X1
CR	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
CR	96	ARG	-	expression tag	UNP A0A0J4R4X1
CR	97	PRO	-	expression tag	UNP A0A0J4R4X1
CR	98	HIS	-	expression tag	UNP A0A0J4R4X1
CR	99	ASN	-	expression tag	UNP A0A0J4R4X1
CR	100	ALA	-	expression tag	UNP A0A0J4R4X1
CS	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CS	88	GLY	-	expression tag	UNP A0A0J4R4X1
CS	89	SER	-	expression tag	UNP A0A0J4R4X1
CS	90	THR	-	expression tag	UNP A0A0J4R4X1
CS	91	LYS	-	expression tag	UNP A0A0J4R4X1
CS	92	HIS	-	expression tag	UNP A0A0J4R4X1
CS	93	LYS	-	expression tag	UNP A0A0J4R4X1
CS	94	SER	-	expression tag	UNP A0A0J4R4X1
CS	95	LEU	-	expression tag	UNP A0A0J4R4X1
CS	96	ARG	-	expression tag	UNP A0A0J4R4X1
CS	97	PRO	-	expression tag	UNP A0A0J4R4X1
CS	98	HIS	-	expression tag	UNP A0A0J4R4X1
CS	99	ASN	-	expression tag	UNP A0A0J4R4X1
CS	100	ALA	-	expression tag	UNP A0A0J4R4X1
CT	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CT	88	GLY	-	expression tag	UNP A0A0J4R4X1
CT	89	SER	-	expression tag	UNP A0A0J4R4X1
CT	90	THR	-	expression tag	UNP A0A0J4R4X1
CT	91	LYS	-	expression tag	UNP A0A0J4R4X1
CT	92	HIS	-	expression tag	UNP A0A0J4R4X1
CT	93	LYS	-	expression tag	UNP A0A0J4R4X1
CT	94	SER	-	expression tag	UNP A0A0J4R4X1
CT	95	LEU	-	expression tag	UNP A0A0J4R4X1
CT	96	ARG	-	expression tag	UNP A0A0J4R4X1
CT	97	PRO	-	expression tag	UNP A0A0J4R4X1
CT	98	HIS	-	expression tag	UNP A0A0J4R4X1
CT	99	ASN	-	expression tag	UNP A0A0J4R4X1
CT	100	ALA	-	expression tag	UNP A0A0J4R4X1
CV	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CV	88	GLY	-	expression tag	UNP A0A0J4R4X1
CV	89	SER	-	expression tag	UNP A0A0J4R4X1
CV	90	THR	-	expression tag	UNP A0A0J4R4X1
CV	91	LYS	-	expression tag	UNP A0A0J4R4X1
CV	92	HIS	-	expression tag	UNP A0A0J4R4X1
CV	93	LYS	-	expression tag	UNP A0A0J4R4X1
CV	94	SER	-	expression tag	UNP A0A0J4R4X1
CV	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
CV	96	ARG	-	expression tag	UNP A0A0J4R4X1
CV	97	PRO	-	expression tag	UNP A0A0J4R4X1
CV	98	HIS	-	expression tag	UNP A0A0J4R4X1
CV	99	ASN	-	expression tag	UNP A0A0J4R4X1
CV	100	ALA	-	expression tag	UNP A0A0J4R4X1
CW	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CW	88	GLY	-	expression tag	UNP A0A0J4R4X1
CW	89	SER	-	expression tag	UNP A0A0J4R4X1
CW	90	THR	-	expression tag	UNP A0A0J4R4X1
CW	91	LYS	-	expression tag	UNP A0A0J4R4X1
CW	92	HIS	-	expression tag	UNP A0A0J4R4X1
CW	93	LYS	-	expression tag	UNP A0A0J4R4X1
CW	94	SER	-	expression tag	UNP A0A0J4R4X1
CW	95	LEU	-	expression tag	UNP A0A0J4R4X1
CW	96	ARG	-	expression tag	UNP A0A0J4R4X1
CW	97	PRO	-	expression tag	UNP A0A0J4R4X1
CW	98	HIS	-	expression tag	UNP A0A0J4R4X1
CW	99	ASN	-	expression tag	UNP A0A0J4R4X1
CW	100	ALA	-	expression tag	UNP A0A0J4R4X1
CX	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CX	88	GLY	-	expression tag	UNP A0A0J4R4X1
CX	89	SER	-	expression tag	UNP A0A0J4R4X1
CX	90	THR	-	expression tag	UNP A0A0J4R4X1
CX	91	LYS	-	expression tag	UNP A0A0J4R4X1
CX	92	HIS	-	expression tag	UNP A0A0J4R4X1
CX	93	LYS	-	expression tag	UNP A0A0J4R4X1
CX	94	SER	-	expression tag	UNP A0A0J4R4X1
CX	95	LEU	-	expression tag	UNP A0A0J4R4X1
CX	96	ARG	-	expression tag	UNP A0A0J4R4X1
CX	97	PRO	-	expression tag	UNP A0A0J4R4X1
CX	98	HIS	-	expression tag	UNP A0A0J4R4X1
CX	99	ASN	-	expression tag	UNP A0A0J4R4X1
CX	100	ALA	-	expression tag	UNP A0A0J4R4X1
CZ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
CZ	88	GLY	-	expression tag	UNP A0A0J4R4X1
CZ	89	SER	-	expression tag	UNP A0A0J4R4X1
CZ	90	THR	-	expression tag	UNP A0A0J4R4X1
CZ	91	LYS	-	expression tag	UNP A0A0J4R4X1
CZ	92	HIS	-	expression tag	UNP A0A0J4R4X1
CZ	93	LYS	-	expression tag	UNP A0A0J4R4X1
CZ	94	SER	-	expression tag	UNP A0A0J4R4X1
CZ	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
CZ	96	ARG	-	expression tag	UNP A0A0J4R4X1
CZ	97	PRO	-	expression tag	UNP A0A0J4R4X1
CZ	98	HIS	-	expression tag	UNP A0A0J4R4X1
CZ	99	ASN	-	expression tag	UNP A0A0J4R4X1
CZ	100	ALA	-	expression tag	UNP A0A0J4R4X1
DA	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DA	88	GLY	-	expression tag	UNP A0A0J4R4X1
DA	89	SER	-	expression tag	UNP A0A0J4R4X1
DA	90	THR	-	expression tag	UNP A0A0J4R4X1
DA	91	LYS	-	expression tag	UNP A0A0J4R4X1
DA	92	HIS	-	expression tag	UNP A0A0J4R4X1
DA	93	LYS	-	expression tag	UNP A0A0J4R4X1
DA	94	SER	-	expression tag	UNP A0A0J4R4X1
DA	95	LEU	-	expression tag	UNP A0A0J4R4X1
DA	96	ARG	-	expression tag	UNP A0A0J4R4X1
DA	97	PRO	-	expression tag	UNP A0A0J4R4X1
DA	98	HIS	-	expression tag	UNP A0A0J4R4X1
DA	99	ASN	-	expression tag	UNP A0A0J4R4X1
DA	100	ALA	-	expression tag	UNP A0A0J4R4X1
DB	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DB	88	GLY	-	expression tag	UNP A0A0J4R4X1
DB	89	SER	-	expression tag	UNP A0A0J4R4X1
DB	90	THR	-	expression tag	UNP A0A0J4R4X1
DB	91	LYS	-	expression tag	UNP A0A0J4R4X1
DB	92	HIS	-	expression tag	UNP A0A0J4R4X1
DB	93	LYS	-	expression tag	UNP A0A0J4R4X1
DB	94	SER	-	expression tag	UNP A0A0J4R4X1
DB	95	LEU	-	expression tag	UNP A0A0J4R4X1
DB	96	ARG	-	expression tag	UNP A0A0J4R4X1
DB	97	PRO	-	expression tag	UNP A0A0J4R4X1
DB	98	HIS	-	expression tag	UNP A0A0J4R4X1
DB	99	ASN	-	expression tag	UNP A0A0J4R4X1
DB	100	ALA	-	expression tag	UNP A0A0J4R4X1
DD	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DD	88	GLY	-	expression tag	UNP A0A0J4R4X1
DD	89	SER	-	expression tag	UNP A0A0J4R4X1
DD	90	THR	-	expression tag	UNP A0A0J4R4X1
DD	91	LYS	-	expression tag	UNP A0A0J4R4X1
DD	92	HIS	-	expression tag	UNP A0A0J4R4X1
DD	93	LYS	-	expression tag	UNP A0A0J4R4X1
DD	94	SER	-	expression tag	UNP A0A0J4R4X1
DD	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
DD	96	ARG	-	expression tag	UNP A0A0J4R4X1
DD	97	PRO	-	expression tag	UNP A0A0J4R4X1
DD	98	HIS	-	expression tag	UNP A0A0J4R4X1
DD	99	ASN	-	expression tag	UNP A0A0J4R4X1
DD	100	ALA	-	expression tag	UNP A0A0J4R4X1
DE	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DE	88	GLY	-	expression tag	UNP A0A0J4R4X1
DE	89	SER	-	expression tag	UNP A0A0J4R4X1
DE	90	THR	-	expression tag	UNP A0A0J4R4X1
DE	91	LYS	-	expression tag	UNP A0A0J4R4X1
DE	92	HIS	-	expression tag	UNP A0A0J4R4X1
DE	93	LYS	-	expression tag	UNP A0A0J4R4X1
DE	94	SER	-	expression tag	UNP A0A0J4R4X1
DE	95	LEU	-	expression tag	UNP A0A0J4R4X1
DE	96	ARG	-	expression tag	UNP A0A0J4R4X1
DE	97	PRO	-	expression tag	UNP A0A0J4R4X1
DE	98	HIS	-	expression tag	UNP A0A0J4R4X1
DE	99	ASN	-	expression tag	UNP A0A0J4R4X1
DE	100	ALA	-	expression tag	UNP A0A0J4R4X1
DF	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DF	88	GLY	-	expression tag	UNP A0A0J4R4X1
DF	89	SER	-	expression tag	UNP A0A0J4R4X1
DF	90	THR	-	expression tag	UNP A0A0J4R4X1
DF	91	LYS	-	expression tag	UNP A0A0J4R4X1
DF	92	HIS	-	expression tag	UNP A0A0J4R4X1
DF	93	LYS	-	expression tag	UNP A0A0J4R4X1
DF	94	SER	-	expression tag	UNP A0A0J4R4X1
DF	95	LEU	-	expression tag	UNP A0A0J4R4X1
DF	96	ARG	-	expression tag	UNP A0A0J4R4X1
DF	97	PRO	-	expression tag	UNP A0A0J4R4X1
DF	98	HIS	-	expression tag	UNP A0A0J4R4X1
DF	99	ASN	-	expression tag	UNP A0A0J4R4X1
DF	100	ALA	-	expression tag	UNP A0A0J4R4X1
DH	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DH	88	GLY	-	expression tag	UNP A0A0J4R4X1
DH	89	SER	-	expression tag	UNP A0A0J4R4X1
DH	90	THR	-	expression tag	UNP A0A0J4R4X1
DH	91	LYS	-	expression tag	UNP A0A0J4R4X1
DH	92	HIS	-	expression tag	UNP A0A0J4R4X1
DH	93	LYS	-	expression tag	UNP A0A0J4R4X1
DH	94	SER	-	expression tag	UNP A0A0J4R4X1
DH	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
DH	96	ARG	-	expression tag	UNP A0A0J4R4X1
DH	97	PRO	-	expression tag	UNP A0A0J4R4X1
DH	98	HIS	-	expression tag	UNP A0A0J4R4X1
DH	99	ASN	-	expression tag	UNP A0A0J4R4X1
DH	100	ALA	-	expression tag	UNP A0A0J4R4X1
DI	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DI	88	GLY	-	expression tag	UNP A0A0J4R4X1
DI	89	SER	-	expression tag	UNP A0A0J4R4X1
DI	90	THR	-	expression tag	UNP A0A0J4R4X1
DI	91	LYS	-	expression tag	UNP A0A0J4R4X1
DI	92	HIS	-	expression tag	UNP A0A0J4R4X1
DI	93	LYS	-	expression tag	UNP A0A0J4R4X1
DI	94	SER	-	expression tag	UNP A0A0J4R4X1
DI	95	LEU	-	expression tag	UNP A0A0J4R4X1
DI	96	ARG	-	expression tag	UNP A0A0J4R4X1
DI	97	PRO	-	expression tag	UNP A0A0J4R4X1
DI	98	HIS	-	expression tag	UNP A0A0J4R4X1
DI	99	ASN	-	expression tag	UNP A0A0J4R4X1
DI	100	ALA	-	expression tag	UNP A0A0J4R4X1
DJ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DJ	88	GLY	-	expression tag	UNP A0A0J4R4X1
DJ	89	SER	-	expression tag	UNP A0A0J4R4X1
DJ	90	THR	-	expression tag	UNP A0A0J4R4X1
DJ	91	LYS	-	expression tag	UNP A0A0J4R4X1
DJ	92	HIS	-	expression tag	UNP A0A0J4R4X1
DJ	93	LYS	-	expression tag	UNP A0A0J4R4X1
DJ	94	SER	-	expression tag	UNP A0A0J4R4X1
DJ	95	LEU	-	expression tag	UNP A0A0J4R4X1
DJ	96	ARG	-	expression tag	UNP A0A0J4R4X1
DJ	97	PRO	-	expression tag	UNP A0A0J4R4X1
DJ	98	HIS	-	expression tag	UNP A0A0J4R4X1
DJ	99	ASN	-	expression tag	UNP A0A0J4R4X1
DJ	100	ALA	-	expression tag	UNP A0A0J4R4X1
DL	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DL	88	GLY	-	expression tag	UNP A0A0J4R4X1
DL	89	SER	-	expression tag	UNP A0A0J4R4X1
DL	90	THR	-	expression tag	UNP A0A0J4R4X1
DL	91	LYS	-	expression tag	UNP A0A0J4R4X1
DL	92	HIS	-	expression tag	UNP A0A0J4R4X1
DL	93	LYS	-	expression tag	UNP A0A0J4R4X1
DL	94	SER	-	expression tag	UNP A0A0J4R4X1
DL	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
DL	96	ARG	-	expression tag	UNP A0A0J4R4X1
DL	97	PRO	-	expression tag	UNP A0A0J4R4X1
DL	98	HIS	-	expression tag	UNP A0A0J4R4X1
DL	99	ASN	-	expression tag	UNP A0A0J4R4X1
DL	100	ALA	-	expression tag	UNP A0A0J4R4X1
DM	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DM	88	GLY	-	expression tag	UNP A0A0J4R4X1
DM	89	SER	-	expression tag	UNP A0A0J4R4X1
DM	90	THR	-	expression tag	UNP A0A0J4R4X1
DM	91	LYS	-	expression tag	UNP A0A0J4R4X1
DM	92	HIS	-	expression tag	UNP A0A0J4R4X1
DM	93	LYS	-	expression tag	UNP A0A0J4R4X1
DM	94	SER	-	expression tag	UNP A0A0J4R4X1
DM	95	LEU	-	expression tag	UNP A0A0J4R4X1
DM	96	ARG	-	expression tag	UNP A0A0J4R4X1
DM	97	PRO	-	expression tag	UNP A0A0J4R4X1
DM	98	HIS	-	expression tag	UNP A0A0J4R4X1
DM	99	ASN	-	expression tag	UNP A0A0J4R4X1
DM	100	ALA	-	expression tag	UNP A0A0J4R4X1
DN	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DN	88	GLY	-	expression tag	UNP A0A0J4R4X1
DN	89	SER	-	expression tag	UNP A0A0J4R4X1
DN	90	THR	-	expression tag	UNP A0A0J4R4X1
DN	91	LYS	-	expression tag	UNP A0A0J4R4X1
DN	92	HIS	-	expression tag	UNP A0A0J4R4X1
DN	93	LYS	-	expression tag	UNP A0A0J4R4X1
DN	94	SER	-	expression tag	UNP A0A0J4R4X1
DN	95	LEU	-	expression tag	UNP A0A0J4R4X1
DN	96	ARG	-	expression tag	UNP A0A0J4R4X1
DN	97	PRO	-	expression tag	UNP A0A0J4R4X1
DN	98	HIS	-	expression tag	UNP A0A0J4R4X1
DN	99	ASN	-	expression tag	UNP A0A0J4R4X1
DN	100	ALA	-	expression tag	UNP A0A0J4R4X1
DP	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DP	88	GLY	-	expression tag	UNP A0A0J4R4X1
DP	89	SER	-	expression tag	UNP A0A0J4R4X1
DP	90	THR	-	expression tag	UNP A0A0J4R4X1
DP	91	LYS	-	expression tag	UNP A0A0J4R4X1
DP	92	HIS	-	expression tag	UNP A0A0J4R4X1
DP	93	LYS	-	expression tag	UNP A0A0J4R4X1
DP	94	SER	-	expression tag	UNP A0A0J4R4X1
DP	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
DP	96	ARG	-	expression tag	UNP A0A0J4R4X1
DP	97	PRO	-	expression tag	UNP A0A0J4R4X1
DP	98	HIS	-	expression tag	UNP A0A0J4R4X1
DP	99	ASN	-	expression tag	UNP A0A0J4R4X1
DP	100	ALA	-	expression tag	UNP A0A0J4R4X1
DQ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DQ	88	GLY	-	expression tag	UNP A0A0J4R4X1
DQ	89	SER	-	expression tag	UNP A0A0J4R4X1
DQ	90	THR	-	expression tag	UNP A0A0J4R4X1
DQ	91	LYS	-	expression tag	UNP A0A0J4R4X1
DQ	92	HIS	-	expression tag	UNP A0A0J4R4X1
DQ	93	LYS	-	expression tag	UNP A0A0J4R4X1
DQ	94	SER	-	expression tag	UNP A0A0J4R4X1
DQ	95	LEU	-	expression tag	UNP A0A0J4R4X1
DQ	96	ARG	-	expression tag	UNP A0A0J4R4X1
DQ	97	PRO	-	expression tag	UNP A0A0J4R4X1
DQ	98	HIS	-	expression tag	UNP A0A0J4R4X1
DQ	99	ASN	-	expression tag	UNP A0A0J4R4X1
DQ	100	ALA	-	expression tag	UNP A0A0J4R4X1
DR	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DR	88	GLY	-	expression tag	UNP A0A0J4R4X1
DR	89	SER	-	expression tag	UNP A0A0J4R4X1
DR	90	THR	-	expression tag	UNP A0A0J4R4X1
DR	91	LYS	-	expression tag	UNP A0A0J4R4X1
DR	92	HIS	-	expression tag	UNP A0A0J4R4X1
DR	93	LYS	-	expression tag	UNP A0A0J4R4X1
DR	94	SER	-	expression tag	UNP A0A0J4R4X1
DR	95	LEU	-	expression tag	UNP A0A0J4R4X1
DR	96	ARG	-	expression tag	UNP A0A0J4R4X1
DR	97	PRO	-	expression tag	UNP A0A0J4R4X1
DR	98	HIS	-	expression tag	UNP A0A0J4R4X1
DR	99	ASN	-	expression tag	UNP A0A0J4R4X1
DR	100	ALA	-	expression tag	UNP A0A0J4R4X1
DT	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DT	88	GLY	-	expression tag	UNP A0A0J4R4X1
DT	89	SER	-	expression tag	UNP A0A0J4R4X1
DT	90	THR	-	expression tag	UNP A0A0J4R4X1
DT	91	LYS	-	expression tag	UNP A0A0J4R4X1
DT	92	HIS	-	expression tag	UNP A0A0J4R4X1
DT	93	LYS	-	expression tag	UNP A0A0J4R4X1
DT	94	SER	-	expression tag	UNP A0A0J4R4X1
DT	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
DT	96	ARG	-	expression tag	UNP A0A0J4R4X1
DT	97	PRO	-	expression tag	UNP A0A0J4R4X1
DT	98	HIS	-	expression tag	UNP A0A0J4R4X1
DT	99	ASN	-	expression tag	UNP A0A0J4R4X1
DT	100	ALA	-	expression tag	UNP A0A0J4R4X1
DU	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DU	88	GLY	-	expression tag	UNP A0A0J4R4X1
DU	89	SER	-	expression tag	UNP A0A0J4R4X1
DU	90	THR	-	expression tag	UNP A0A0J4R4X1
DU	91	LYS	-	expression tag	UNP A0A0J4R4X1
DU	92	HIS	-	expression tag	UNP A0A0J4R4X1
DU	93	LYS	-	expression tag	UNP A0A0J4R4X1
DU	94	SER	-	expression tag	UNP A0A0J4R4X1
DU	95	LEU	-	expression tag	UNP A0A0J4R4X1
DU	96	ARG	-	expression tag	UNP A0A0J4R4X1
DU	97	PRO	-	expression tag	UNP A0A0J4R4X1
DU	98	HIS	-	expression tag	UNP A0A0J4R4X1
DU	99	ASN	-	expression tag	UNP A0A0J4R4X1
DU	100	ALA	-	expression tag	UNP A0A0J4R4X1
DV	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DV	88	GLY	-	expression tag	UNP A0A0J4R4X1
DV	89	SER	-	expression tag	UNP A0A0J4R4X1
DV	90	THR	-	expression tag	UNP A0A0J4R4X1
DV	91	LYS	-	expression tag	UNP A0A0J4R4X1
DV	92	HIS	-	expression tag	UNP A0A0J4R4X1
DV	93	LYS	-	expression tag	UNP A0A0J4R4X1
DV	94	SER	-	expression tag	UNP A0A0J4R4X1
DV	95	LEU	-	expression tag	UNP A0A0J4R4X1
DV	96	ARG	-	expression tag	UNP A0A0J4R4X1
DV	97	PRO	-	expression tag	UNP A0A0J4R4X1
DV	98	HIS	-	expression tag	UNP A0A0J4R4X1
DV	99	ASN	-	expression tag	UNP A0A0J4R4X1
DV	100	ALA	-	expression tag	UNP A0A0J4R4X1
DX	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DX	88	GLY	-	expression tag	UNP A0A0J4R4X1
DX	89	SER	-	expression tag	UNP A0A0J4R4X1
DX	90	THR	-	expression tag	UNP A0A0J4R4X1
DX	91	LYS	-	expression tag	UNP A0A0J4R4X1
DX	92	HIS	-	expression tag	UNP A0A0J4R4X1
DX	93	LYS	-	expression tag	UNP A0A0J4R4X1
DX	94	SER	-	expression tag	UNP A0A0J4R4X1
DX	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
DX	96	ARG	-	expression tag	UNP A0A0J4R4X1
DX	97	PRO	-	expression tag	UNP A0A0J4R4X1
DX	98	HIS	-	expression tag	UNP A0A0J4R4X1
DX	99	ASN	-	expression tag	UNP A0A0J4R4X1
DX	100	ALA	-	expression tag	UNP A0A0J4R4X1
DY	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DY	88	GLY	-	expression tag	UNP A0A0J4R4X1
DY	89	SER	-	expression tag	UNP A0A0J4R4X1
DY	90	THR	-	expression tag	UNP A0A0J4R4X1
DY	91	LYS	-	expression tag	UNP A0A0J4R4X1
DY	92	HIS	-	expression tag	UNP A0A0J4R4X1
DY	93	LYS	-	expression tag	UNP A0A0J4R4X1
DY	94	SER	-	expression tag	UNP A0A0J4R4X1
DY	95	LEU	-	expression tag	UNP A0A0J4R4X1
DY	96	ARG	-	expression tag	UNP A0A0J4R4X1
DY	97	PRO	-	expression tag	UNP A0A0J4R4X1
DY	98	HIS	-	expression tag	UNP A0A0J4R4X1
DY	99	ASN	-	expression tag	UNP A0A0J4R4X1
DY	100	ALA	-	expression tag	UNP A0A0J4R4X1
DZ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
DZ	88	GLY	-	expression tag	UNP A0A0J4R4X1
DZ	89	SER	-	expression tag	UNP A0A0J4R4X1
DZ	90	THR	-	expression tag	UNP A0A0J4R4X1
DZ	91	LYS	-	expression tag	UNP A0A0J4R4X1
DZ	92	HIS	-	expression tag	UNP A0A0J4R4X1
DZ	93	LYS	-	expression tag	UNP A0A0J4R4X1
DZ	94	SER	-	expression tag	UNP A0A0J4R4X1
DZ	95	LEU	-	expression tag	UNP A0A0J4R4X1
DZ	96	ARG	-	expression tag	UNP A0A0J4R4X1
DZ	97	PRO	-	expression tag	UNP A0A0J4R4X1
DZ	98	HIS	-	expression tag	UNP A0A0J4R4X1
DZ	99	ASN	-	expression tag	UNP A0A0J4R4X1
DZ	100	ALA	-	expression tag	UNP A0A0J4R4X1
EB	69	LYS	GLU	conflict	UNP A0A0J4R4X1
EB	88	GLY	-	expression tag	UNP A0A0J4R4X1
EB	89	SER	-	expression tag	UNP A0A0J4R4X1
EB	90	THR	-	expression tag	UNP A0A0J4R4X1
EB	91	LYS	-	expression tag	UNP A0A0J4R4X1
EB	92	HIS	-	expression tag	UNP A0A0J4R4X1
EB	93	LYS	-	expression tag	UNP A0A0J4R4X1
EB	94	SER	-	expression tag	UNP A0A0J4R4X1
EB	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
EB	96	ARG	-	expression tag	UNP A0A0J4R4X1
EB	97	PRO	-	expression tag	UNP A0A0J4R4X1
EB	98	HIS	-	expression tag	UNP A0A0J4R4X1
EB	99	ASN	-	expression tag	UNP A0A0J4R4X1
EB	100	ALA	-	expression tag	UNP A0A0J4R4X1
EC	69	LYS	GLU	conflict	UNP A0A0J4R4X1
EC	88	GLY	-	expression tag	UNP A0A0J4R4X1
EC	89	SER	-	expression tag	UNP A0A0J4R4X1
EC	90	THR	-	expression tag	UNP A0A0J4R4X1
EC	91	LYS	-	expression tag	UNP A0A0J4R4X1
EC	92	HIS	-	expression tag	UNP A0A0J4R4X1
EC	93	LYS	-	expression tag	UNP A0A0J4R4X1
EC	94	SER	-	expression tag	UNP A0A0J4R4X1
EC	95	LEU	-	expression tag	UNP A0A0J4R4X1
EC	96	ARG	-	expression tag	UNP A0A0J4R4X1
EC	97	PRO	-	expression tag	UNP A0A0J4R4X1
EC	98	HIS	-	expression tag	UNP A0A0J4R4X1
EC	99	ASN	-	expression tag	UNP A0A0J4R4X1
EC	100	ALA	-	expression tag	UNP A0A0J4R4X1
ED	69	LYS	GLU	conflict	UNP A0A0J4R4X1
ED	88	GLY	-	expression tag	UNP A0A0J4R4X1
ED	89	SER	-	expression tag	UNP A0A0J4R4X1
ED	90	THR	-	expression tag	UNP A0A0J4R4X1
ED	91	LYS	-	expression tag	UNP A0A0J4R4X1
ED	92	HIS	-	expression tag	UNP A0A0J4R4X1
ED	93	LYS	-	expression tag	UNP A0A0J4R4X1
ED	94	SER	-	expression tag	UNP A0A0J4R4X1
ED	95	LEU	-	expression tag	UNP A0A0J4R4X1
ED	96	ARG	-	expression tag	UNP A0A0J4R4X1
ED	97	PRO	-	expression tag	UNP A0A0J4R4X1
ED	98	HIS	-	expression tag	UNP A0A0J4R4X1
ED	99	ASN	-	expression tag	UNP A0A0J4R4X1
ED	100	ALA	-	expression tag	UNP A0A0J4R4X1
EF	69	LYS	GLU	conflict	UNP A0A0J4R4X1
EF	88	GLY	-	expression tag	UNP A0A0J4R4X1
EF	89	SER	-	expression tag	UNP A0A0J4R4X1
EF	90	THR	-	expression tag	UNP A0A0J4R4X1
EF	91	LYS	-	expression tag	UNP A0A0J4R4X1
EF	92	HIS	-	expression tag	UNP A0A0J4R4X1
EF	93	LYS	-	expression tag	UNP A0A0J4R4X1
EF	94	SER	-	expression tag	UNP A0A0J4R4X1
EF	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
EF	96	ARG	-	expression tag	UNP A0A0J4R4X1
EF	97	PRO	-	expression tag	UNP A0A0J4R4X1
EF	98	HIS	-	expression tag	UNP A0A0J4R4X1
EF	99	ASN	-	expression tag	UNP A0A0J4R4X1
EF	100	ALA	-	expression tag	UNP A0A0J4R4X1
EG	69	LYS	GLU	conflict	UNP A0A0J4R4X1
EG	88	GLY	-	expression tag	UNP A0A0J4R4X1
EG	89	SER	-	expression tag	UNP A0A0J4R4X1
EG	90	THR	-	expression tag	UNP A0A0J4R4X1
EG	91	LYS	-	expression tag	UNP A0A0J4R4X1
EG	92	HIS	-	expression tag	UNP A0A0J4R4X1
EG	93	LYS	-	expression tag	UNP A0A0J4R4X1
EG	94	SER	-	expression tag	UNP A0A0J4R4X1
EG	95	LEU	-	expression tag	UNP A0A0J4R4X1
EG	96	ARG	-	expression tag	UNP A0A0J4R4X1
EG	97	PRO	-	expression tag	UNP A0A0J4R4X1
EG	98	HIS	-	expression tag	UNP A0A0J4R4X1
EG	99	ASN	-	expression tag	UNP A0A0J4R4X1
EG	100	ALA	-	expression tag	UNP A0A0J4R4X1
EH	69	LYS	GLU	conflict	UNP A0A0J4R4X1
EH	88	GLY	-	expression tag	UNP A0A0J4R4X1
EH	89	SER	-	expression tag	UNP A0A0J4R4X1
EH	90	THR	-	expression tag	UNP A0A0J4R4X1
EH	91	LYS	-	expression tag	UNP A0A0J4R4X1
EH	92	HIS	-	expression tag	UNP A0A0J4R4X1
EH	93	LYS	-	expression tag	UNP A0A0J4R4X1
EH	94	SER	-	expression tag	UNP A0A0J4R4X1
EH	95	LEU	-	expression tag	UNP A0A0J4R4X1
EH	96	ARG	-	expression tag	UNP A0A0J4R4X1
EH	97	PRO	-	expression tag	UNP A0A0J4R4X1
EH	98	HIS	-	expression tag	UNP A0A0J4R4X1
EH	99	ASN	-	expression tag	UNP A0A0J4R4X1
EH	100	ALA	-	expression tag	UNP A0A0J4R4X1
EJ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
EJ	88	GLY	-	expression tag	UNP A0A0J4R4X1
EJ	89	SER	-	expression tag	UNP A0A0J4R4X1
EJ	90	THR	-	expression tag	UNP A0A0J4R4X1
EJ	91	LYS	-	expression tag	UNP A0A0J4R4X1
EJ	92	HIS	-	expression tag	UNP A0A0J4R4X1
EJ	93	LYS	-	expression tag	UNP A0A0J4R4X1
EJ	94	SER	-	expression tag	UNP A0A0J4R4X1
EJ	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
EJ	96	ARG	-	expression tag	UNP A0A0J4R4X1
EJ	97	PRO	-	expression tag	UNP A0A0J4R4X1
EJ	98	HIS	-	expression tag	UNP A0A0J4R4X1
EJ	99	ASN	-	expression tag	UNP A0A0J4R4X1
EJ	100	ALA	-	expression tag	UNP A0A0J4R4X1
EK	69	LYS	GLU	conflict	UNP A0A0J4R4X1
EK	88	GLY	-	expression tag	UNP A0A0J4R4X1
EK	89	SER	-	expression tag	UNP A0A0J4R4X1
EK	90	THR	-	expression tag	UNP A0A0J4R4X1
EK	91	LYS	-	expression tag	UNP A0A0J4R4X1
EK	92	HIS	-	expression tag	UNP A0A0J4R4X1
EK	93	LYS	-	expression tag	UNP A0A0J4R4X1
EK	94	SER	-	expression tag	UNP A0A0J4R4X1
EK	95	LEU	-	expression tag	UNP A0A0J4R4X1
EK	96	ARG	-	expression tag	UNP A0A0J4R4X1
EK	97	PRO	-	expression tag	UNP A0A0J4R4X1
EK	98	HIS	-	expression tag	UNP A0A0J4R4X1
EK	99	ASN	-	expression tag	UNP A0A0J4R4X1
EK	100	ALA	-	expression tag	UNP A0A0J4R4X1
EL	69	LYS	GLU	conflict	UNP A0A0J4R4X1
EL	88	GLY	-	expression tag	UNP A0A0J4R4X1
EL	89	SER	-	expression tag	UNP A0A0J4R4X1
EL	90	THR	-	expression tag	UNP A0A0J4R4X1
EL	91	LYS	-	expression tag	UNP A0A0J4R4X1
EL	92	HIS	-	expression tag	UNP A0A0J4R4X1
EL	93	LYS	-	expression tag	UNP A0A0J4R4X1
EL	94	SER	-	expression tag	UNP A0A0J4R4X1
EL	95	LEU	-	expression tag	UNP A0A0J4R4X1
EL	96	ARG	-	expression tag	UNP A0A0J4R4X1
EL	97	PRO	-	expression tag	UNP A0A0J4R4X1
EL	98	HIS	-	expression tag	UNP A0A0J4R4X1
EL	99	ASN	-	expression tag	UNP A0A0J4R4X1
EL	100	ALA	-	expression tag	UNP A0A0J4R4X1
EN	69	LYS	GLU	conflict	UNP A0A0J4R4X1
EN	88	GLY	-	expression tag	UNP A0A0J4R4X1
EN	89	SER	-	expression tag	UNP A0A0J4R4X1
EN	90	THR	-	expression tag	UNP A0A0J4R4X1
EN	91	LYS	-	expression tag	UNP A0A0J4R4X1
EN	92	HIS	-	expression tag	UNP A0A0J4R4X1
EN	93	LYS	-	expression tag	UNP A0A0J4R4X1
EN	94	SER	-	expression tag	UNP A0A0J4R4X1
EN	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
EN	96	ARG	-	expression tag	UNP A0A0J4R4X1
EN	97	PRO	-	expression tag	UNP A0A0J4R4X1
EN	98	HIS	-	expression tag	UNP A0A0J4R4X1
EN	99	ASN	-	expression tag	UNP A0A0J4R4X1
EN	100	ALA	-	expression tag	UNP A0A0J4R4X1
EO	69	LYS	GLU	conflict	UNP A0A0J4R4X1
EO	88	GLY	-	expression tag	UNP A0A0J4R4X1
EO	89	SER	-	expression tag	UNP A0A0J4R4X1
EO	90	THR	-	expression tag	UNP A0A0J4R4X1
EO	91	LYS	-	expression tag	UNP A0A0J4R4X1
EO	92	HIS	-	expression tag	UNP A0A0J4R4X1
EO	93	LYS	-	expression tag	UNP A0A0J4R4X1
EO	94	SER	-	expression tag	UNP A0A0J4R4X1
EO	95	LEU	-	expression tag	UNP A0A0J4R4X1
EO	96	ARG	-	expression tag	UNP A0A0J4R4X1
EO	97	PRO	-	expression tag	UNP A0A0J4R4X1
EO	98	HIS	-	expression tag	UNP A0A0J4R4X1
EO	99	ASN	-	expression tag	UNP A0A0J4R4X1
EO	100	ALA	-	expression tag	UNP A0A0J4R4X1
EP	69	LYS	GLU	conflict	UNP A0A0J4R4X1
EP	88	GLY	-	expression tag	UNP A0A0J4R4X1
EP	89	SER	-	expression tag	UNP A0A0J4R4X1
EP	90	THR	-	expression tag	UNP A0A0J4R4X1
EP	91	LYS	-	expression tag	UNP A0A0J4R4X1
EP	92	HIS	-	expression tag	UNP A0A0J4R4X1
EP	93	LYS	-	expression tag	UNP A0A0J4R4X1
EP	94	SER	-	expression tag	UNP A0A0J4R4X1
EP	95	LEU	-	expression tag	UNP A0A0J4R4X1
EP	96	ARG	-	expression tag	UNP A0A0J4R4X1
EP	97	PRO	-	expression tag	UNP A0A0J4R4X1
EP	98	HIS	-	expression tag	UNP A0A0J4R4X1
EP	99	ASN	-	expression tag	UNP A0A0J4R4X1
EP	100	ALA	-	expression tag	UNP A0A0J4R4X1
ER	69	LYS	GLU	conflict	UNP A0A0J4R4X1
ER	88	GLY	-	expression tag	UNP A0A0J4R4X1
ER	89	SER	-	expression tag	UNP A0A0J4R4X1
ER	90	THR	-	expression tag	UNP A0A0J4R4X1
ER	91	LYS	-	expression tag	UNP A0A0J4R4X1
ER	92	HIS	-	expression tag	UNP A0A0J4R4X1
ER	93	LYS	-	expression tag	UNP A0A0J4R4X1
ER	94	SER	-	expression tag	UNP A0A0J4R4X1
ER	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
ER	96	ARG	-	expression tag	UNP A0A0J4R4X1
ER	97	PRO	-	expression tag	UNP A0A0J4R4X1
ER	98	HIS	-	expression tag	UNP A0A0J4R4X1
ER	99	ASN	-	expression tag	UNP A0A0J4R4X1
ER	100	ALA	-	expression tag	UNP A0A0J4R4X1
ES	69	LYS	GLU	conflict	UNP A0A0J4R4X1
ES	88	GLY	-	expression tag	UNP A0A0J4R4X1
ES	89	SER	-	expression tag	UNP A0A0J4R4X1
ES	90	THR	-	expression tag	UNP A0A0J4R4X1
ES	91	LYS	-	expression tag	UNP A0A0J4R4X1
ES	92	HIS	-	expression tag	UNP A0A0J4R4X1
ES	93	LYS	-	expression tag	UNP A0A0J4R4X1
ES	94	SER	-	expression tag	UNP A0A0J4R4X1
ES	95	LEU	-	expression tag	UNP A0A0J4R4X1
ES	96	ARG	-	expression tag	UNP A0A0J4R4X1
ES	97	PRO	-	expression tag	UNP A0A0J4R4X1
ES	98	HIS	-	expression tag	UNP A0A0J4R4X1
ES	99	ASN	-	expression tag	UNP A0A0J4R4X1
ES	100	ALA	-	expression tag	UNP A0A0J4R4X1
ET	69	LYS	GLU	conflict	UNP A0A0J4R4X1
ET	88	GLY	-	expression tag	UNP A0A0J4R4X1
ET	89	SER	-	expression tag	UNP A0A0J4R4X1
ET	90	THR	-	expression tag	UNP A0A0J4R4X1
ET	91	LYS	-	expression tag	UNP A0A0J4R4X1
ET	92	HIS	-	expression tag	UNP A0A0J4R4X1
ET	93	LYS	-	expression tag	UNP A0A0J4R4X1
ET	94	SER	-	expression tag	UNP A0A0J4R4X1
ET	95	LEU	-	expression tag	UNP A0A0J4R4X1
ET	96	ARG	-	expression tag	UNP A0A0J4R4X1
ET	97	PRO	-	expression tag	UNP A0A0J4R4X1
ET	98	HIS	-	expression tag	UNP A0A0J4R4X1
ET	99	ASN	-	expression tag	UNP A0A0J4R4X1
ET	100	ALA	-	expression tag	UNP A0A0J4R4X1
EV	69	LYS	GLU	conflict	UNP A0A0J4R4X1
EV	88	GLY	-	expression tag	UNP A0A0J4R4X1
EV	89	SER	-	expression tag	UNP A0A0J4R4X1
EV	90	THR	-	expression tag	UNP A0A0J4R4X1
EV	91	LYS	-	expression tag	UNP A0A0J4R4X1
EV	92	HIS	-	expression tag	UNP A0A0J4R4X1
EV	93	LYS	-	expression tag	UNP A0A0J4R4X1
EV	94	SER	-	expression tag	UNP A0A0J4R4X1
EV	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
EV	96	ARG	-	expression tag	UNP A0A0J4R4X1
EV	97	PRO	-	expression tag	UNP A0A0J4R4X1
EV	98	HIS	-	expression tag	UNP A0A0J4R4X1
EV	99	ASN	-	expression tag	UNP A0A0J4R4X1
EV	100	ALA	-	expression tag	UNP A0A0J4R4X1
EW	69	LYS	GLU	conflict	UNP A0A0J4R4X1
EW	88	GLY	-	expression tag	UNP A0A0J4R4X1
EW	89	SER	-	expression tag	UNP A0A0J4R4X1
EW	90	THR	-	expression tag	UNP A0A0J4R4X1
EW	91	LYS	-	expression tag	UNP A0A0J4R4X1
EW	92	HIS	-	expression tag	UNP A0A0J4R4X1
EW	93	LYS	-	expression tag	UNP A0A0J4R4X1
EW	94	SER	-	expression tag	UNP A0A0J4R4X1
EW	95	LEU	-	expression tag	UNP A0A0J4R4X1
EW	96	ARG	-	expression tag	UNP A0A0J4R4X1
EW	97	PRO	-	expression tag	UNP A0A0J4R4X1
EW	98	HIS	-	expression tag	UNP A0A0J4R4X1
EW	99	ASN	-	expression tag	UNP A0A0J4R4X1
EW	100	ALA	-	expression tag	UNP A0A0J4R4X1
EX	69	LYS	GLU	conflict	UNP A0A0J4R4X1
EX	88	GLY	-	expression tag	UNP A0A0J4R4X1
EX	89	SER	-	expression tag	UNP A0A0J4R4X1
EX	90	THR	-	expression tag	UNP A0A0J4R4X1
EX	91	LYS	-	expression tag	UNP A0A0J4R4X1
EX	92	HIS	-	expression tag	UNP A0A0J4R4X1
EX	93	LYS	-	expression tag	UNP A0A0J4R4X1
EX	94	SER	-	expression tag	UNP A0A0J4R4X1
EX	95	LEU	-	expression tag	UNP A0A0J4R4X1
EX	96	ARG	-	expression tag	UNP A0A0J4R4X1
EX	97	PRO	-	expression tag	UNP A0A0J4R4X1
EX	98	HIS	-	expression tag	UNP A0A0J4R4X1
EX	99	ASN	-	expression tag	UNP A0A0J4R4X1
EX	100	ALA	-	expression tag	UNP A0A0J4R4X1
EZ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
EZ	88	GLY	-	expression tag	UNP A0A0J4R4X1
EZ	89	SER	-	expression tag	UNP A0A0J4R4X1
EZ	90	THR	-	expression tag	UNP A0A0J4R4X1
EZ	91	LYS	-	expression tag	UNP A0A0J4R4X1
EZ	92	HIS	-	expression tag	UNP A0A0J4R4X1
EZ	93	LYS	-	expression tag	UNP A0A0J4R4X1
EZ	94	SER	-	expression tag	UNP A0A0J4R4X1
EZ	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
EZ	96	ARG	-	expression tag	UNP A0A0J4R4X1
EZ	97	PRO	-	expression tag	UNP A0A0J4R4X1
EZ	98	HIS	-	expression tag	UNP A0A0J4R4X1
EZ	99	ASN	-	expression tag	UNP A0A0J4R4X1
EZ	100	ALA	-	expression tag	UNP A0A0J4R4X1
FA	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FA	88	GLY	-	expression tag	UNP A0A0J4R4X1
FA	89	SER	-	expression tag	UNP A0A0J4R4X1
FA	90	THR	-	expression tag	UNP A0A0J4R4X1
FA	91	LYS	-	expression tag	UNP A0A0J4R4X1
FA	92	HIS	-	expression tag	UNP A0A0J4R4X1
FA	93	LYS	-	expression tag	UNP A0A0J4R4X1
FA	94	SER	-	expression tag	UNP A0A0J4R4X1
FA	95	LEU	-	expression tag	UNP A0A0J4R4X1
FA	96	ARG	-	expression tag	UNP A0A0J4R4X1
FA	97	PRO	-	expression tag	UNP A0A0J4R4X1
FA	98	HIS	-	expression tag	UNP A0A0J4R4X1
FA	99	ASN	-	expression tag	UNP A0A0J4R4X1
FA	100	ALA	-	expression tag	UNP A0A0J4R4X1
FB	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FB	88	GLY	-	expression tag	UNP A0A0J4R4X1
FB	89	SER	-	expression tag	UNP A0A0J4R4X1
FB	90	THR	-	expression tag	UNP A0A0J4R4X1
FB	91	LYS	-	expression tag	UNP A0A0J4R4X1
FB	92	HIS	-	expression tag	UNP A0A0J4R4X1
FB	93	LYS	-	expression tag	UNP A0A0J4R4X1
FB	94	SER	-	expression tag	UNP A0A0J4R4X1
FB	95	LEU	-	expression tag	UNP A0A0J4R4X1
FB	96	ARG	-	expression tag	UNP A0A0J4R4X1
FB	97	PRO	-	expression tag	UNP A0A0J4R4X1
FB	98	HIS	-	expression tag	UNP A0A0J4R4X1
FB	99	ASN	-	expression tag	UNP A0A0J4R4X1
FB	100	ALA	-	expression tag	UNP A0A0J4R4X1
FD	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FD	88	GLY	-	expression tag	UNP A0A0J4R4X1
FD	89	SER	-	expression tag	UNP A0A0J4R4X1
FD	90	THR	-	expression tag	UNP A0A0J4R4X1
FD	91	LYS	-	expression tag	UNP A0A0J4R4X1
FD	92	HIS	-	expression tag	UNP A0A0J4R4X1
FD	93	LYS	-	expression tag	UNP A0A0J4R4X1
FD	94	SER	-	expression tag	UNP A0A0J4R4X1
FD	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
FD	96	ARG	-	expression tag	UNP A0A0J4R4X1
FD	97	PRO	-	expression tag	UNP A0A0J4R4X1
FD	98	HIS	-	expression tag	UNP A0A0J4R4X1
FD	99	ASN	-	expression tag	UNP A0A0J4R4X1
FD	100	ALA	-	expression tag	UNP A0A0J4R4X1
FE	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FE	88	GLY	-	expression tag	UNP A0A0J4R4X1
FE	89	SER	-	expression tag	UNP A0A0J4R4X1
FE	90	THR	-	expression tag	UNP A0A0J4R4X1
FE	91	LYS	-	expression tag	UNP A0A0J4R4X1
FE	92	HIS	-	expression tag	UNP A0A0J4R4X1
FE	93	LYS	-	expression tag	UNP A0A0J4R4X1
FE	94	SER	-	expression tag	UNP A0A0J4R4X1
FE	95	LEU	-	expression tag	UNP A0A0J4R4X1
FE	96	ARG	-	expression tag	UNP A0A0J4R4X1
FE	97	PRO	-	expression tag	UNP A0A0J4R4X1
FE	98	HIS	-	expression tag	UNP A0A0J4R4X1
FE	99	ASN	-	expression tag	UNP A0A0J4R4X1
FE	100	ALA	-	expression tag	UNP A0A0J4R4X1
FF	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FF	88	GLY	-	expression tag	UNP A0A0J4R4X1
FF	89	SER	-	expression tag	UNP A0A0J4R4X1
FF	90	THR	-	expression tag	UNP A0A0J4R4X1
FF	91	LYS	-	expression tag	UNP A0A0J4R4X1
FF	92	HIS	-	expression tag	UNP A0A0J4R4X1
FF	93	LYS	-	expression tag	UNP A0A0J4R4X1
FF	94	SER	-	expression tag	UNP A0A0J4R4X1
FF	95	LEU	-	expression tag	UNP A0A0J4R4X1
FF	96	ARG	-	expression tag	UNP A0A0J4R4X1
FF	97	PRO	-	expression tag	UNP A0A0J4R4X1
FF	98	HIS	-	expression tag	UNP A0A0J4R4X1
FF	99	ASN	-	expression tag	UNP A0A0J4R4X1
FF	100	ALA	-	expression tag	UNP A0A0J4R4X1
FH	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FH	88	GLY	-	expression tag	UNP A0A0J4R4X1
FH	89	SER	-	expression tag	UNP A0A0J4R4X1
FH	90	THR	-	expression tag	UNP A0A0J4R4X1
FH	91	LYS	-	expression tag	UNP A0A0J4R4X1
FH	92	HIS	-	expression tag	UNP A0A0J4R4X1
FH	93	LYS	-	expression tag	UNP A0A0J4R4X1
FH	94	SER	-	expression tag	UNP A0A0J4R4X1
FH	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
FH	96	ARG	-	expression tag	UNP A0A0J4R4X1
FH	97	PRO	-	expression tag	UNP A0A0J4R4X1
FH	98	HIS	-	expression tag	UNP A0A0J4R4X1
FH	99	ASN	-	expression tag	UNP A0A0J4R4X1
FH	100	ALA	-	expression tag	UNP A0A0J4R4X1
FI	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FI	88	GLY	-	expression tag	UNP A0A0J4R4X1
FI	89	SER	-	expression tag	UNP A0A0J4R4X1
FI	90	THR	-	expression tag	UNP A0A0J4R4X1
FI	91	LYS	-	expression tag	UNP A0A0J4R4X1
FI	92	HIS	-	expression tag	UNP A0A0J4R4X1
FI	93	LYS	-	expression tag	UNP A0A0J4R4X1
FI	94	SER	-	expression tag	UNP A0A0J4R4X1
FI	95	LEU	-	expression tag	UNP A0A0J4R4X1
FI	96	ARG	-	expression tag	UNP A0A0J4R4X1
FI	97	PRO	-	expression tag	UNP A0A0J4R4X1
FI	98	HIS	-	expression tag	UNP A0A0J4R4X1
FI	99	ASN	-	expression tag	UNP A0A0J4R4X1
FI	100	ALA	-	expression tag	UNP A0A0J4R4X1
FJ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FJ	88	GLY	-	expression tag	UNP A0A0J4R4X1
FJ	89	SER	-	expression tag	UNP A0A0J4R4X1
FJ	90	THR	-	expression tag	UNP A0A0J4R4X1
FJ	91	LYS	-	expression tag	UNP A0A0J4R4X1
FJ	92	HIS	-	expression tag	UNP A0A0J4R4X1
FJ	93	LYS	-	expression tag	UNP A0A0J4R4X1
FJ	94	SER	-	expression tag	UNP A0A0J4R4X1
FJ	95	LEU	-	expression tag	UNP A0A0J4R4X1
FJ	96	ARG	-	expression tag	UNP A0A0J4R4X1
FJ	97	PRO	-	expression tag	UNP A0A0J4R4X1
FJ	98	HIS	-	expression tag	UNP A0A0J4R4X1
FJ	99	ASN	-	expression tag	UNP A0A0J4R4X1
FJ	100	ALA	-	expression tag	UNP A0A0J4R4X1
FL	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FL	88	GLY	-	expression tag	UNP A0A0J4R4X1
FL	89	SER	-	expression tag	UNP A0A0J4R4X1
FL	90	THR	-	expression tag	UNP A0A0J4R4X1
FL	91	LYS	-	expression tag	UNP A0A0J4R4X1
FL	92	HIS	-	expression tag	UNP A0A0J4R4X1
FL	93	LYS	-	expression tag	UNP A0A0J4R4X1
FL	94	SER	-	expression tag	UNP A0A0J4R4X1
FL	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
FL	96	ARG	-	expression tag	UNP A0A0J4R4X1
FL	97	PRO	-	expression tag	UNP A0A0J4R4X1
FL	98	HIS	-	expression tag	UNP A0A0J4R4X1
FL	99	ASN	-	expression tag	UNP A0A0J4R4X1
FL	100	ALA	-	expression tag	UNP A0A0J4R4X1
FM	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FM	88	GLY	-	expression tag	UNP A0A0J4R4X1
FM	89	SER	-	expression tag	UNP A0A0J4R4X1
FM	90	THR	-	expression tag	UNP A0A0J4R4X1
FM	91	LYS	-	expression tag	UNP A0A0J4R4X1
FM	92	HIS	-	expression tag	UNP A0A0J4R4X1
FM	93	LYS	-	expression tag	UNP A0A0J4R4X1
FM	94	SER	-	expression tag	UNP A0A0J4R4X1
FM	95	LEU	-	expression tag	UNP A0A0J4R4X1
FM	96	ARG	-	expression tag	UNP A0A0J4R4X1
FM	97	PRO	-	expression tag	UNP A0A0J4R4X1
FM	98	HIS	-	expression tag	UNP A0A0J4R4X1
FM	99	ASN	-	expression tag	UNP A0A0J4R4X1
FM	100	ALA	-	expression tag	UNP A0A0J4R4X1
FN	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FN	88	GLY	-	expression tag	UNP A0A0J4R4X1
FN	89	SER	-	expression tag	UNP A0A0J4R4X1
FN	90	THR	-	expression tag	UNP A0A0J4R4X1
FN	91	LYS	-	expression tag	UNP A0A0J4R4X1
FN	92	HIS	-	expression tag	UNP A0A0J4R4X1
FN	93	LYS	-	expression tag	UNP A0A0J4R4X1
FN	94	SER	-	expression tag	UNP A0A0J4R4X1
FN	95	LEU	-	expression tag	UNP A0A0J4R4X1
FN	96	ARG	-	expression tag	UNP A0A0J4R4X1
FN	97	PRO	-	expression tag	UNP A0A0J4R4X1
FN	98	HIS	-	expression tag	UNP A0A0J4R4X1
FN	99	ASN	-	expression tag	UNP A0A0J4R4X1
FN	100	ALA	-	expression tag	UNP A0A0J4R4X1
FP	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FP	88	GLY	-	expression tag	UNP A0A0J4R4X1
FP	89	SER	-	expression tag	UNP A0A0J4R4X1
FP	90	THR	-	expression tag	UNP A0A0J4R4X1
FP	91	LYS	-	expression tag	UNP A0A0J4R4X1
FP	92	HIS	-	expression tag	UNP A0A0J4R4X1
FP	93	LYS	-	expression tag	UNP A0A0J4R4X1
FP	94	SER	-	expression tag	UNP A0A0J4R4X1
FP	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
FP	96	ARG	-	expression tag	UNP A0A0J4R4X1
FP	97	PRO	-	expression tag	UNP A0A0J4R4X1
FP	98	HIS	-	expression tag	UNP A0A0J4R4X1
FP	99	ASN	-	expression tag	UNP A0A0J4R4X1
FP	100	ALA	-	expression tag	UNP A0A0J4R4X1
FQ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FQ	88	GLY	-	expression tag	UNP A0A0J4R4X1
FQ	89	SER	-	expression tag	UNP A0A0J4R4X1
FQ	90	THR	-	expression tag	UNP A0A0J4R4X1
FQ	91	LYS	-	expression tag	UNP A0A0J4R4X1
FQ	92	HIS	-	expression tag	UNP A0A0J4R4X1
FQ	93	LYS	-	expression tag	UNP A0A0J4R4X1
FQ	94	SER	-	expression tag	UNP A0A0J4R4X1
FQ	95	LEU	-	expression tag	UNP A0A0J4R4X1
FQ	96	ARG	-	expression tag	UNP A0A0J4R4X1
FQ	97	PRO	-	expression tag	UNP A0A0J4R4X1
FQ	98	HIS	-	expression tag	UNP A0A0J4R4X1
FQ	99	ASN	-	expression tag	UNP A0A0J4R4X1
FQ	100	ALA	-	expression tag	UNP A0A0J4R4X1
FR	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FR	88	GLY	-	expression tag	UNP A0A0J4R4X1
FR	89	SER	-	expression tag	UNP A0A0J4R4X1
FR	90	THR	-	expression tag	UNP A0A0J4R4X1
FR	91	LYS	-	expression tag	UNP A0A0J4R4X1
FR	92	HIS	-	expression tag	UNP A0A0J4R4X1
FR	93	LYS	-	expression tag	UNP A0A0J4R4X1
FR	94	SER	-	expression tag	UNP A0A0J4R4X1
FR	95	LEU	-	expression tag	UNP A0A0J4R4X1
FR	96	ARG	-	expression tag	UNP A0A0J4R4X1
FR	97	PRO	-	expression tag	UNP A0A0J4R4X1
FR	98	HIS	-	expression tag	UNP A0A0J4R4X1
FR	99	ASN	-	expression tag	UNP A0A0J4R4X1
FR	100	ALA	-	expression tag	UNP A0A0J4R4X1
FT	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FT	88	GLY	-	expression tag	UNP A0A0J4R4X1
FT	89	SER	-	expression tag	UNP A0A0J4R4X1
FT	90	THR	-	expression tag	UNP A0A0J4R4X1
FT	91	LYS	-	expression tag	UNP A0A0J4R4X1
FT	92	HIS	-	expression tag	UNP A0A0J4R4X1
FT	93	LYS	-	expression tag	UNP A0A0J4R4X1
FT	94	SER	-	expression tag	UNP A0A0J4R4X1
FT	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
FT	96	ARG	-	expression tag	UNP A0A0J4R4X1
FT	97	PRO	-	expression tag	UNP A0A0J4R4X1
FT	98	HIS	-	expression tag	UNP A0A0J4R4X1
FT	99	ASN	-	expression tag	UNP A0A0J4R4X1
FT	100	ALA	-	expression tag	UNP A0A0J4R4X1
FU	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FU	88	GLY	-	expression tag	UNP A0A0J4R4X1
FU	89	SER	-	expression tag	UNP A0A0J4R4X1
FU	90	THR	-	expression tag	UNP A0A0J4R4X1
FU	91	LYS	-	expression tag	UNP A0A0J4R4X1
FU	92	HIS	-	expression tag	UNP A0A0J4R4X1
FU	93	LYS	-	expression tag	UNP A0A0J4R4X1
FU	94	SER	-	expression tag	UNP A0A0J4R4X1
FU	95	LEU	-	expression tag	UNP A0A0J4R4X1
FU	96	ARG	-	expression tag	UNP A0A0J4R4X1
FU	97	PRO	-	expression tag	UNP A0A0J4R4X1
FU	98	HIS	-	expression tag	UNP A0A0J4R4X1
FU	99	ASN	-	expression tag	UNP A0A0J4R4X1
FU	100	ALA	-	expression tag	UNP A0A0J4R4X1
FV	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FV	88	GLY	-	expression tag	UNP A0A0J4R4X1
FV	89	SER	-	expression tag	UNP A0A0J4R4X1
FV	90	THR	-	expression tag	UNP A0A0J4R4X1
FV	91	LYS	-	expression tag	UNP A0A0J4R4X1
FV	92	HIS	-	expression tag	UNP A0A0J4R4X1
FV	93	LYS	-	expression tag	UNP A0A0J4R4X1
FV	94	SER	-	expression tag	UNP A0A0J4R4X1
FV	95	LEU	-	expression tag	UNP A0A0J4R4X1
FV	96	ARG	-	expression tag	UNP A0A0J4R4X1
FV	97	PRO	-	expression tag	UNP A0A0J4R4X1
FV	98	HIS	-	expression tag	UNP A0A0J4R4X1
FV	99	ASN	-	expression tag	UNP A0A0J4R4X1
FV	100	ALA	-	expression tag	UNP A0A0J4R4X1
FX	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FX	88	GLY	-	expression tag	UNP A0A0J4R4X1
FX	89	SER	-	expression tag	UNP A0A0J4R4X1
FX	90	THR	-	expression tag	UNP A0A0J4R4X1
FX	91	LYS	-	expression tag	UNP A0A0J4R4X1
FX	92	HIS	-	expression tag	UNP A0A0J4R4X1
FX	93	LYS	-	expression tag	UNP A0A0J4R4X1
FX	94	SER	-	expression tag	UNP A0A0J4R4X1
FX	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
FX	96	ARG	-	expression tag	UNP A0A0J4R4X1
FX	97	PRO	-	expression tag	UNP A0A0J4R4X1
FX	98	HIS	-	expression tag	UNP A0A0J4R4X1
FX	99	ASN	-	expression tag	UNP A0A0J4R4X1
FX	100	ALA	-	expression tag	UNP A0A0J4R4X1
FY	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FY	88	GLY	-	expression tag	UNP A0A0J4R4X1
FY	89	SER	-	expression tag	UNP A0A0J4R4X1
FY	90	THR	-	expression tag	UNP A0A0J4R4X1
FY	91	LYS	-	expression tag	UNP A0A0J4R4X1
FY	92	HIS	-	expression tag	UNP A0A0J4R4X1
FY	93	LYS	-	expression tag	UNP A0A0J4R4X1
FY	94	SER	-	expression tag	UNP A0A0J4R4X1
FY	95	LEU	-	expression tag	UNP A0A0J4R4X1
FY	96	ARG	-	expression tag	UNP A0A0J4R4X1
FY	97	PRO	-	expression tag	UNP A0A0J4R4X1
FY	98	HIS	-	expression tag	UNP A0A0J4R4X1
FY	99	ASN	-	expression tag	UNP A0A0J4R4X1
FY	100	ALA	-	expression tag	UNP A0A0J4R4X1
FZ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
FZ	88	GLY	-	expression tag	UNP A0A0J4R4X1
FZ	89	SER	-	expression tag	UNP A0A0J4R4X1
FZ	90	THR	-	expression tag	UNP A0A0J4R4X1
FZ	91	LYS	-	expression tag	UNP A0A0J4R4X1
FZ	92	HIS	-	expression tag	UNP A0A0J4R4X1
FZ	93	LYS	-	expression tag	UNP A0A0J4R4X1
FZ	94	SER	-	expression tag	UNP A0A0J4R4X1
FZ	95	LEU	-	expression tag	UNP A0A0J4R4X1
FZ	96	ARG	-	expression tag	UNP A0A0J4R4X1
FZ	97	PRO	-	expression tag	UNP A0A0J4R4X1
FZ	98	HIS	-	expression tag	UNP A0A0J4R4X1
FZ	99	ASN	-	expression tag	UNP A0A0J4R4X1
FZ	100	ALA	-	expression tag	UNP A0A0J4R4X1
GB	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GB	88	GLY	-	expression tag	UNP A0A0J4R4X1
GB	89	SER	-	expression tag	UNP A0A0J4R4X1
GB	90	THR	-	expression tag	UNP A0A0J4R4X1
GB	91	LYS	-	expression tag	UNP A0A0J4R4X1
GB	92	HIS	-	expression tag	UNP A0A0J4R4X1
GB	93	LYS	-	expression tag	UNP A0A0J4R4X1
GB	94	SER	-	expression tag	UNP A0A0J4R4X1
GB	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
GB	96	ARG	-	expression tag	UNP A0A0J4R4X1
GB	97	PRO	-	expression tag	UNP A0A0J4R4X1
GB	98	HIS	-	expression tag	UNP A0A0J4R4X1
GB	99	ASN	-	expression tag	UNP A0A0J4R4X1
GB	100	ALA	-	expression tag	UNP A0A0J4R4X1
GC	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GC	88	GLY	-	expression tag	UNP A0A0J4R4X1
GC	89	SER	-	expression tag	UNP A0A0J4R4X1
GC	90	THR	-	expression tag	UNP A0A0J4R4X1
GC	91	LYS	-	expression tag	UNP A0A0J4R4X1
GC	92	HIS	-	expression tag	UNP A0A0J4R4X1
GC	93	LYS	-	expression tag	UNP A0A0J4R4X1
GC	94	SER	-	expression tag	UNP A0A0J4R4X1
GC	95	LEU	-	expression tag	UNP A0A0J4R4X1
GC	96	ARG	-	expression tag	UNP A0A0J4R4X1
GC	97	PRO	-	expression tag	UNP A0A0J4R4X1
GC	98	HIS	-	expression tag	UNP A0A0J4R4X1
GC	99	ASN	-	expression tag	UNP A0A0J4R4X1
GC	100	ALA	-	expression tag	UNP A0A0J4R4X1
GD	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GD	88	GLY	-	expression tag	UNP A0A0J4R4X1
GD	89	SER	-	expression tag	UNP A0A0J4R4X1
GD	90	THR	-	expression tag	UNP A0A0J4R4X1
GD	91	LYS	-	expression tag	UNP A0A0J4R4X1
GD	92	HIS	-	expression tag	UNP A0A0J4R4X1
GD	93	LYS	-	expression tag	UNP A0A0J4R4X1
GD	94	SER	-	expression tag	UNP A0A0J4R4X1
GD	95	LEU	-	expression tag	UNP A0A0J4R4X1
GD	96	ARG	-	expression tag	UNP A0A0J4R4X1
GD	97	PRO	-	expression tag	UNP A0A0J4R4X1
GD	98	HIS	-	expression tag	UNP A0A0J4R4X1
GD	99	ASN	-	expression tag	UNP A0A0J4R4X1
GD	100	ALA	-	expression tag	UNP A0A0J4R4X1
GF	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GF	88	GLY	-	expression tag	UNP A0A0J4R4X1
GF	89	SER	-	expression tag	UNP A0A0J4R4X1
GF	90	THR	-	expression tag	UNP A0A0J4R4X1
GF	91	LYS	-	expression tag	UNP A0A0J4R4X1
GF	92	HIS	-	expression tag	UNP A0A0J4R4X1
GF	93	LYS	-	expression tag	UNP A0A0J4R4X1
GF	94	SER	-	expression tag	UNP A0A0J4R4X1
GF	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
GF	96	ARG	-	expression tag	UNP A0A0J4R4X1
GF	97	PRO	-	expression tag	UNP A0A0J4R4X1
GF	98	HIS	-	expression tag	UNP A0A0J4R4X1
GF	99	ASN	-	expression tag	UNP A0A0J4R4X1
GF	100	ALA	-	expression tag	UNP A0A0J4R4X1
GG	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GG	88	GLY	-	expression tag	UNP A0A0J4R4X1
GG	89	SER	-	expression tag	UNP A0A0J4R4X1
GG	90	THR	-	expression tag	UNP A0A0J4R4X1
GG	91	LYS	-	expression tag	UNP A0A0J4R4X1
GG	92	HIS	-	expression tag	UNP A0A0J4R4X1
GG	93	LYS	-	expression tag	UNP A0A0J4R4X1
GG	94	SER	-	expression tag	UNP A0A0J4R4X1
GG	95	LEU	-	expression tag	UNP A0A0J4R4X1
GG	96	ARG	-	expression tag	UNP A0A0J4R4X1
GG	97	PRO	-	expression tag	UNP A0A0J4R4X1
GG	98	HIS	-	expression tag	UNP A0A0J4R4X1
GG	99	ASN	-	expression tag	UNP A0A0J4R4X1
GG	100	ALA	-	expression tag	UNP A0A0J4R4X1
GH	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GH	88	GLY	-	expression tag	UNP A0A0J4R4X1
GH	89	SER	-	expression tag	UNP A0A0J4R4X1
GH	90	THR	-	expression tag	UNP A0A0J4R4X1
GH	91	LYS	-	expression tag	UNP A0A0J4R4X1
GH	92	HIS	-	expression tag	UNP A0A0J4R4X1
GH	93	LYS	-	expression tag	UNP A0A0J4R4X1
GH	94	SER	-	expression tag	UNP A0A0J4R4X1
GH	95	LEU	-	expression tag	UNP A0A0J4R4X1
GH	96	ARG	-	expression tag	UNP A0A0J4R4X1
GH	97	PRO	-	expression tag	UNP A0A0J4R4X1
GH	98	HIS	-	expression tag	UNP A0A0J4R4X1
GH	99	ASN	-	expression tag	UNP A0A0J4R4X1
GH	100	ALA	-	expression tag	UNP A0A0J4R4X1
GJ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GJ	88	GLY	-	expression tag	UNP A0A0J4R4X1
GJ	89	SER	-	expression tag	UNP A0A0J4R4X1
GJ	90	THR	-	expression tag	UNP A0A0J4R4X1
GJ	91	LYS	-	expression tag	UNP A0A0J4R4X1
GJ	92	HIS	-	expression tag	UNP A0A0J4R4X1
GJ	93	LYS	-	expression tag	UNP A0A0J4R4X1
GJ	94	SER	-	expression tag	UNP A0A0J4R4X1
GJ	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
GJ	96	ARG	-	expression tag	UNP A0A0J4R4X1
GJ	97	PRO	-	expression tag	UNP A0A0J4R4X1
GJ	98	HIS	-	expression tag	UNP A0A0J4R4X1
GJ	99	ASN	-	expression tag	UNP A0A0J4R4X1
GJ	100	ALA	-	expression tag	UNP A0A0J4R4X1
GK	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GK	88	GLY	-	expression tag	UNP A0A0J4R4X1
GK	89	SER	-	expression tag	UNP A0A0J4R4X1
GK	90	THR	-	expression tag	UNP A0A0J4R4X1
GK	91	LYS	-	expression tag	UNP A0A0J4R4X1
GK	92	HIS	-	expression tag	UNP A0A0J4R4X1
GK	93	LYS	-	expression tag	UNP A0A0J4R4X1
GK	94	SER	-	expression tag	UNP A0A0J4R4X1
GK	95	LEU	-	expression tag	UNP A0A0J4R4X1
GK	96	ARG	-	expression tag	UNP A0A0J4R4X1
GK	97	PRO	-	expression tag	UNP A0A0J4R4X1
GK	98	HIS	-	expression tag	UNP A0A0J4R4X1
GK	99	ASN	-	expression tag	UNP A0A0J4R4X1
GK	100	ALA	-	expression tag	UNP A0A0J4R4X1
GL	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GL	88	GLY	-	expression tag	UNP A0A0J4R4X1
GL	89	SER	-	expression tag	UNP A0A0J4R4X1
GL	90	THR	-	expression tag	UNP A0A0J4R4X1
GL	91	LYS	-	expression tag	UNP A0A0J4R4X1
GL	92	HIS	-	expression tag	UNP A0A0J4R4X1
GL	93	LYS	-	expression tag	UNP A0A0J4R4X1
GL	94	SER	-	expression tag	UNP A0A0J4R4X1
GL	95	LEU	-	expression tag	UNP A0A0J4R4X1
GL	96	ARG	-	expression tag	UNP A0A0J4R4X1
GL	97	PRO	-	expression tag	UNP A0A0J4R4X1
GL	98	HIS	-	expression tag	UNP A0A0J4R4X1
GL	99	ASN	-	expression tag	UNP A0A0J4R4X1
GL	100	ALA	-	expression tag	UNP A0A0J4R4X1
GN	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GN	88	GLY	-	expression tag	UNP A0A0J4R4X1
GN	89	SER	-	expression tag	UNP A0A0J4R4X1
GN	90	THR	-	expression tag	UNP A0A0J4R4X1
GN	91	LYS	-	expression tag	UNP A0A0J4R4X1
GN	92	HIS	-	expression tag	UNP A0A0J4R4X1
GN	93	LYS	-	expression tag	UNP A0A0J4R4X1
GN	94	SER	-	expression tag	UNP A0A0J4R4X1
GN	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
GN	96	ARG	-	expression tag	UNP A0A0J4R4X1
GN	97	PRO	-	expression tag	UNP A0A0J4R4X1
GN	98	HIS	-	expression tag	UNP A0A0J4R4X1
GN	99	ASN	-	expression tag	UNP A0A0J4R4X1
GN	100	ALA	-	expression tag	UNP A0A0J4R4X1
GO	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GO	88	GLY	-	expression tag	UNP A0A0J4R4X1
GO	89	SER	-	expression tag	UNP A0A0J4R4X1
GO	90	THR	-	expression tag	UNP A0A0J4R4X1
GO	91	LYS	-	expression tag	UNP A0A0J4R4X1
GO	92	HIS	-	expression tag	UNP A0A0J4R4X1
GO	93	LYS	-	expression tag	UNP A0A0J4R4X1
GO	94	SER	-	expression tag	UNP A0A0J4R4X1
GO	95	LEU	-	expression tag	UNP A0A0J4R4X1
GO	96	ARG	-	expression tag	UNP A0A0J4R4X1
GO	97	PRO	-	expression tag	UNP A0A0J4R4X1
GO	98	HIS	-	expression tag	UNP A0A0J4R4X1
GO	99	ASN	-	expression tag	UNP A0A0J4R4X1
GO	100	ALA	-	expression tag	UNP A0A0J4R4X1
GP	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GP	88	GLY	-	expression tag	UNP A0A0J4R4X1
GP	89	SER	-	expression tag	UNP A0A0J4R4X1
GP	90	THR	-	expression tag	UNP A0A0J4R4X1
GP	91	LYS	-	expression tag	UNP A0A0J4R4X1
GP	92	HIS	-	expression tag	UNP A0A0J4R4X1
GP	93	LYS	-	expression tag	UNP A0A0J4R4X1
GP	94	SER	-	expression tag	UNP A0A0J4R4X1
GP	95	LEU	-	expression tag	UNP A0A0J4R4X1
GP	96	ARG	-	expression tag	UNP A0A0J4R4X1
GP	97	PRO	-	expression tag	UNP A0A0J4R4X1
GP	98	HIS	-	expression tag	UNP A0A0J4R4X1
GP	99	ASN	-	expression tag	UNP A0A0J4R4X1
GP	100	ALA	-	expression tag	UNP A0A0J4R4X1
GR	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GR	88	GLY	-	expression tag	UNP A0A0J4R4X1
GR	89	SER	-	expression tag	UNP A0A0J4R4X1
GR	90	THR	-	expression tag	UNP A0A0J4R4X1
GR	91	LYS	-	expression tag	UNP A0A0J4R4X1
GR	92	HIS	-	expression tag	UNP A0A0J4R4X1
GR	93	LYS	-	expression tag	UNP A0A0J4R4X1
GR	94	SER	-	expression tag	UNP A0A0J4R4X1
GR	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
GR	96	ARG	-	expression tag	UNP A0A0J4R4X1
GR	97	PRO	-	expression tag	UNP A0A0J4R4X1
GR	98	HIS	-	expression tag	UNP A0A0J4R4X1
GR	99	ASN	-	expression tag	UNP A0A0J4R4X1
GR	100	ALA	-	expression tag	UNP A0A0J4R4X1
GS	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GS	88	GLY	-	expression tag	UNP A0A0J4R4X1
GS	89	SER	-	expression tag	UNP A0A0J4R4X1
GS	90	THR	-	expression tag	UNP A0A0J4R4X1
GS	91	LYS	-	expression tag	UNP A0A0J4R4X1
GS	92	HIS	-	expression tag	UNP A0A0J4R4X1
GS	93	LYS	-	expression tag	UNP A0A0J4R4X1
GS	94	SER	-	expression tag	UNP A0A0J4R4X1
GS	95	LEU	-	expression tag	UNP A0A0J4R4X1
GS	96	ARG	-	expression tag	UNP A0A0J4R4X1
GS	97	PRO	-	expression tag	UNP A0A0J4R4X1
GS	98	HIS	-	expression tag	UNP A0A0J4R4X1
GS	99	ASN	-	expression tag	UNP A0A0J4R4X1
GS	100	ALA	-	expression tag	UNP A0A0J4R4X1
GT	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GT	88	GLY	-	expression tag	UNP A0A0J4R4X1
GT	89	SER	-	expression tag	UNP A0A0J4R4X1
GT	90	THR	-	expression tag	UNP A0A0J4R4X1
GT	91	LYS	-	expression tag	UNP A0A0J4R4X1
GT	92	HIS	-	expression tag	UNP A0A0J4R4X1
GT	93	LYS	-	expression tag	UNP A0A0J4R4X1
GT	94	SER	-	expression tag	UNP A0A0J4R4X1
GT	95	LEU	-	expression tag	UNP A0A0J4R4X1
GT	96	ARG	-	expression tag	UNP A0A0J4R4X1
GT	97	PRO	-	expression tag	UNP A0A0J4R4X1
GT	98	HIS	-	expression tag	UNP A0A0J4R4X1
GT	99	ASN	-	expression tag	UNP A0A0J4R4X1
GT	100	ALA	-	expression tag	UNP A0A0J4R4X1
GV	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GV	88	GLY	-	expression tag	UNP A0A0J4R4X1
GV	89	SER	-	expression tag	UNP A0A0J4R4X1
GV	90	THR	-	expression tag	UNP A0A0J4R4X1
GV	91	LYS	-	expression tag	UNP A0A0J4R4X1
GV	92	HIS	-	expression tag	UNP A0A0J4R4X1
GV	93	LYS	-	expression tag	UNP A0A0J4R4X1
GV	94	SER	-	expression tag	UNP A0A0J4R4X1
GV	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
GV	96	ARG	-	expression tag	UNP A0A0J4R4X1
GV	97	PRO	-	expression tag	UNP A0A0J4R4X1
GV	98	HIS	-	expression tag	UNP A0A0J4R4X1
GV	99	ASN	-	expression tag	UNP A0A0J4R4X1
GV	100	ALA	-	expression tag	UNP A0A0J4R4X1
GW	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GW	88	GLY	-	expression tag	UNP A0A0J4R4X1
GW	89	SER	-	expression tag	UNP A0A0J4R4X1
GW	90	THR	-	expression tag	UNP A0A0J4R4X1
GW	91	LYS	-	expression tag	UNP A0A0J4R4X1
GW	92	HIS	-	expression tag	UNP A0A0J4R4X1
GW	93	LYS	-	expression tag	UNP A0A0J4R4X1
GW	94	SER	-	expression tag	UNP A0A0J4R4X1
GW	95	LEU	-	expression tag	UNP A0A0J4R4X1
GW	96	ARG	-	expression tag	UNP A0A0J4R4X1
GW	97	PRO	-	expression tag	UNP A0A0J4R4X1
GW	98	HIS	-	expression tag	UNP A0A0J4R4X1
GW	99	ASN	-	expression tag	UNP A0A0J4R4X1
GW	100	ALA	-	expression tag	UNP A0A0J4R4X1
GX	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GX	88	GLY	-	expression tag	UNP A0A0J4R4X1
GX	89	SER	-	expression tag	UNP A0A0J4R4X1
GX	90	THR	-	expression tag	UNP A0A0J4R4X1
GX	91	LYS	-	expression tag	UNP A0A0J4R4X1
GX	92	HIS	-	expression tag	UNP A0A0J4R4X1
GX	93	LYS	-	expression tag	UNP A0A0J4R4X1
GX	94	SER	-	expression tag	UNP A0A0J4R4X1
GX	95	LEU	-	expression tag	UNP A0A0J4R4X1
GX	96	ARG	-	expression tag	UNP A0A0J4R4X1
GX	97	PRO	-	expression tag	UNP A0A0J4R4X1
GX	98	HIS	-	expression tag	UNP A0A0J4R4X1
GX	99	ASN	-	expression tag	UNP A0A0J4R4X1
GX	100	ALA	-	expression tag	UNP A0A0J4R4X1
GZ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
GZ	88	GLY	-	expression tag	UNP A0A0J4R4X1
GZ	89	SER	-	expression tag	UNP A0A0J4R4X1
GZ	90	THR	-	expression tag	UNP A0A0J4R4X1
GZ	91	LYS	-	expression tag	UNP A0A0J4R4X1
GZ	92	HIS	-	expression tag	UNP A0A0J4R4X1
GZ	93	LYS	-	expression tag	UNP A0A0J4R4X1
GZ	94	SER	-	expression tag	UNP A0A0J4R4X1
GZ	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
GZ	96	ARG	-	expression tag	UNP A0A0J4R4X1
GZ	97	PRO	-	expression tag	UNP A0A0J4R4X1
GZ	98	HIS	-	expression tag	UNP A0A0J4R4X1
GZ	99	ASN	-	expression tag	UNP A0A0J4R4X1
GZ	100	ALA	-	expression tag	UNP A0A0J4R4X1
HA	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HA	88	GLY	-	expression tag	UNP A0A0J4R4X1
HA	89	SER	-	expression tag	UNP A0A0J4R4X1
HA	90	THR	-	expression tag	UNP A0A0J4R4X1
HA	91	LYS	-	expression tag	UNP A0A0J4R4X1
HA	92	HIS	-	expression tag	UNP A0A0J4R4X1
HA	93	LYS	-	expression tag	UNP A0A0J4R4X1
HA	94	SER	-	expression tag	UNP A0A0J4R4X1
HA	95	LEU	-	expression tag	UNP A0A0J4R4X1
HA	96	ARG	-	expression tag	UNP A0A0J4R4X1
HA	97	PRO	-	expression tag	UNP A0A0J4R4X1
HA	98	HIS	-	expression tag	UNP A0A0J4R4X1
HA	99	ASN	-	expression tag	UNP A0A0J4R4X1
HA	100	ALA	-	expression tag	UNP A0A0J4R4X1
HB	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HB	88	GLY	-	expression tag	UNP A0A0J4R4X1
HB	89	SER	-	expression tag	UNP A0A0J4R4X1
HB	90	THR	-	expression tag	UNP A0A0J4R4X1
HB	91	LYS	-	expression tag	UNP A0A0J4R4X1
HB	92	HIS	-	expression tag	UNP A0A0J4R4X1
HB	93	LYS	-	expression tag	UNP A0A0J4R4X1
HB	94	SER	-	expression tag	UNP A0A0J4R4X1
HB	95	LEU	-	expression tag	UNP A0A0J4R4X1
HB	96	ARG	-	expression tag	UNP A0A0J4R4X1
HB	97	PRO	-	expression tag	UNP A0A0J4R4X1
HB	98	HIS	-	expression tag	UNP A0A0J4R4X1
HB	99	ASN	-	expression tag	UNP A0A0J4R4X1
HB	100	ALA	-	expression tag	UNP A0A0J4R4X1
HD	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HD	88	GLY	-	expression tag	UNP A0A0J4R4X1
HD	89	SER	-	expression tag	UNP A0A0J4R4X1
HD	90	THR	-	expression tag	UNP A0A0J4R4X1
HD	91	LYS	-	expression tag	UNP A0A0J4R4X1
HD	92	HIS	-	expression tag	UNP A0A0J4R4X1
HD	93	LYS	-	expression tag	UNP A0A0J4R4X1
HD	94	SER	-	expression tag	UNP A0A0J4R4X1
HD	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
HD	96	ARG	-	expression tag	UNP A0A0J4R4X1
HD	97	PRO	-	expression tag	UNP A0A0J4R4X1
HD	98	HIS	-	expression tag	UNP A0A0J4R4X1
HD	99	ASN	-	expression tag	UNP A0A0J4R4X1
HD	100	ALA	-	expression tag	UNP A0A0J4R4X1
HE	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HE	88	GLY	-	expression tag	UNP A0A0J4R4X1
HE	89	SER	-	expression tag	UNP A0A0J4R4X1
HE	90	THR	-	expression tag	UNP A0A0J4R4X1
HE	91	LYS	-	expression tag	UNP A0A0J4R4X1
HE	92	HIS	-	expression tag	UNP A0A0J4R4X1
HE	93	LYS	-	expression tag	UNP A0A0J4R4X1
HE	94	SER	-	expression tag	UNP A0A0J4R4X1
HE	95	LEU	-	expression tag	UNP A0A0J4R4X1
HE	96	ARG	-	expression tag	UNP A0A0J4R4X1
HE	97	PRO	-	expression tag	UNP A0A0J4R4X1
HE	98	HIS	-	expression tag	UNP A0A0J4R4X1
HE	99	ASN	-	expression tag	UNP A0A0J4R4X1
HE	100	ALA	-	expression tag	UNP A0A0J4R4X1
HF	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HF	88	GLY	-	expression tag	UNP A0A0J4R4X1
HF	89	SER	-	expression tag	UNP A0A0J4R4X1
HF	90	THR	-	expression tag	UNP A0A0J4R4X1
HF	91	LYS	-	expression tag	UNP A0A0J4R4X1
HF	92	HIS	-	expression tag	UNP A0A0J4R4X1
HF	93	LYS	-	expression tag	UNP A0A0J4R4X1
HF	94	SER	-	expression tag	UNP A0A0J4R4X1
HF	95	LEU	-	expression tag	UNP A0A0J4R4X1
HF	96	ARG	-	expression tag	UNP A0A0J4R4X1
HF	97	PRO	-	expression tag	UNP A0A0J4R4X1
HF	98	HIS	-	expression tag	UNP A0A0J4R4X1
HF	99	ASN	-	expression tag	UNP A0A0J4R4X1
HF	100	ALA	-	expression tag	UNP A0A0J4R4X1
HH	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HH	88	GLY	-	expression tag	UNP A0A0J4R4X1
HH	89	SER	-	expression tag	UNP A0A0J4R4X1
HH	90	THR	-	expression tag	UNP A0A0J4R4X1
HH	91	LYS	-	expression tag	UNP A0A0J4R4X1
HH	92	HIS	-	expression tag	UNP A0A0J4R4X1
HH	93	LYS	-	expression tag	UNP A0A0J4R4X1
HH	94	SER	-	expression tag	UNP A0A0J4R4X1
HH	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
HH	96	ARG	-	expression tag	UNP A0A0J4R4X1
HH	97	PRO	-	expression tag	UNP A0A0J4R4X1
HH	98	HIS	-	expression tag	UNP A0A0J4R4X1
HH	99	ASN	-	expression tag	UNP A0A0J4R4X1
HH	100	ALA	-	expression tag	UNP A0A0J4R4X1
HI	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HI	88	GLY	-	expression tag	UNP A0A0J4R4X1
HI	89	SER	-	expression tag	UNP A0A0J4R4X1
HI	90	THR	-	expression tag	UNP A0A0J4R4X1
HI	91	LYS	-	expression tag	UNP A0A0J4R4X1
HI	92	HIS	-	expression tag	UNP A0A0J4R4X1
HI	93	LYS	-	expression tag	UNP A0A0J4R4X1
HI	94	SER	-	expression tag	UNP A0A0J4R4X1
HI	95	LEU	-	expression tag	UNP A0A0J4R4X1
HI	96	ARG	-	expression tag	UNP A0A0J4R4X1
HI	97	PRO	-	expression tag	UNP A0A0J4R4X1
HI	98	HIS	-	expression tag	UNP A0A0J4R4X1
HI	99	ASN	-	expression tag	UNP A0A0J4R4X1
HI	100	ALA	-	expression tag	UNP A0A0J4R4X1
HJ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HJ	88	GLY	-	expression tag	UNP A0A0J4R4X1
HJ	89	SER	-	expression tag	UNP A0A0J4R4X1
HJ	90	THR	-	expression tag	UNP A0A0J4R4X1
HJ	91	LYS	-	expression tag	UNP A0A0J4R4X1
HJ	92	HIS	-	expression tag	UNP A0A0J4R4X1
HJ	93	LYS	-	expression tag	UNP A0A0J4R4X1
HJ	94	SER	-	expression tag	UNP A0A0J4R4X1
HJ	95	LEU	-	expression tag	UNP A0A0J4R4X1
HJ	96	ARG	-	expression tag	UNP A0A0J4R4X1
HJ	97	PRO	-	expression tag	UNP A0A0J4R4X1
HJ	98	HIS	-	expression tag	UNP A0A0J4R4X1
HJ	99	ASN	-	expression tag	UNP A0A0J4R4X1
HJ	100	ALA	-	expression tag	UNP A0A0J4R4X1
HL	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HL	88	GLY	-	expression tag	UNP A0A0J4R4X1
HL	89	SER	-	expression tag	UNP A0A0J4R4X1
HL	90	THR	-	expression tag	UNP A0A0J4R4X1
HL	91	LYS	-	expression tag	UNP A0A0J4R4X1
HL	92	HIS	-	expression tag	UNP A0A0J4R4X1
HL	93	LYS	-	expression tag	UNP A0A0J4R4X1
HL	94	SER	-	expression tag	UNP A0A0J4R4X1
HL	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
HL	96	ARG	-	expression tag	UNP A0A0J4R4X1
HL	97	PRO	-	expression tag	UNP A0A0J4R4X1
HL	98	HIS	-	expression tag	UNP A0A0J4R4X1
HL	99	ASN	-	expression tag	UNP A0A0J4R4X1
HL	100	ALA	-	expression tag	UNP A0A0J4R4X1
HM	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HM	88	GLY	-	expression tag	UNP A0A0J4R4X1
HM	89	SER	-	expression tag	UNP A0A0J4R4X1
HM	90	THR	-	expression tag	UNP A0A0J4R4X1
HM	91	LYS	-	expression tag	UNP A0A0J4R4X1
HM	92	HIS	-	expression tag	UNP A0A0J4R4X1
HM	93	LYS	-	expression tag	UNP A0A0J4R4X1
HM	94	SER	-	expression tag	UNP A0A0J4R4X1
HM	95	LEU	-	expression tag	UNP A0A0J4R4X1
HM	96	ARG	-	expression tag	UNP A0A0J4R4X1
HM	97	PRO	-	expression tag	UNP A0A0J4R4X1
HM	98	HIS	-	expression tag	UNP A0A0J4R4X1
HM	99	ASN	-	expression tag	UNP A0A0J4R4X1
HM	100	ALA	-	expression tag	UNP A0A0J4R4X1
HN	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HN	88	GLY	-	expression tag	UNP A0A0J4R4X1
HN	89	SER	-	expression tag	UNP A0A0J4R4X1
HN	90	THR	-	expression tag	UNP A0A0J4R4X1
HN	91	LYS	-	expression tag	UNP A0A0J4R4X1
HN	92	HIS	-	expression tag	UNP A0A0J4R4X1
HN	93	LYS	-	expression tag	UNP A0A0J4R4X1
HN	94	SER	-	expression tag	UNP A0A0J4R4X1
HN	95	LEU	-	expression tag	UNP A0A0J4R4X1
HN	96	ARG	-	expression tag	UNP A0A0J4R4X1
HN	97	PRO	-	expression tag	UNP A0A0J4R4X1
HN	98	HIS	-	expression tag	UNP A0A0J4R4X1
HN	99	ASN	-	expression tag	UNP A0A0J4R4X1
HN	100	ALA	-	expression tag	UNP A0A0J4R4X1
HP	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HP	88	GLY	-	expression tag	UNP A0A0J4R4X1
HP	89	SER	-	expression tag	UNP A0A0J4R4X1
HP	90	THR	-	expression tag	UNP A0A0J4R4X1
HP	91	LYS	-	expression tag	UNP A0A0J4R4X1
HP	92	HIS	-	expression tag	UNP A0A0J4R4X1
HP	93	LYS	-	expression tag	UNP A0A0J4R4X1
HP	94	SER	-	expression tag	UNP A0A0J4R4X1
HP	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
HP	96	ARG	-	expression tag	UNP A0A0J4R4X1
HP	97	PRO	-	expression tag	UNP A0A0J4R4X1
HP	98	HIS	-	expression tag	UNP A0A0J4R4X1
HP	99	ASN	-	expression tag	UNP A0A0J4R4X1
HP	100	ALA	-	expression tag	UNP A0A0J4R4X1
HQ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HQ	88	GLY	-	expression tag	UNP A0A0J4R4X1
HQ	89	SER	-	expression tag	UNP A0A0J4R4X1
HQ	90	THR	-	expression tag	UNP A0A0J4R4X1
HQ	91	LYS	-	expression tag	UNP A0A0J4R4X1
HQ	92	HIS	-	expression tag	UNP A0A0J4R4X1
HQ	93	LYS	-	expression tag	UNP A0A0J4R4X1
HQ	94	SER	-	expression tag	UNP A0A0J4R4X1
HQ	95	LEU	-	expression tag	UNP A0A0J4R4X1
HQ	96	ARG	-	expression tag	UNP A0A0J4R4X1
HQ	97	PRO	-	expression tag	UNP A0A0J4R4X1
HQ	98	HIS	-	expression tag	UNP A0A0J4R4X1
HQ	99	ASN	-	expression tag	UNP A0A0J4R4X1
HQ	100	ALA	-	expression tag	UNP A0A0J4R4X1
HR	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HR	88	GLY	-	expression tag	UNP A0A0J4R4X1
HR	89	SER	-	expression tag	UNP A0A0J4R4X1
HR	90	THR	-	expression tag	UNP A0A0J4R4X1
HR	91	LYS	-	expression tag	UNP A0A0J4R4X1
HR	92	HIS	-	expression tag	UNP A0A0J4R4X1
HR	93	LYS	-	expression tag	UNP A0A0J4R4X1
HR	94	SER	-	expression tag	UNP A0A0J4R4X1
HR	95	LEU	-	expression tag	UNP A0A0J4R4X1
HR	96	ARG	-	expression tag	UNP A0A0J4R4X1
HR	97	PRO	-	expression tag	UNP A0A0J4R4X1
HR	98	HIS	-	expression tag	UNP A0A0J4R4X1
HR	99	ASN	-	expression tag	UNP A0A0J4R4X1
HR	100	ALA	-	expression tag	UNP A0A0J4R4X1
HT	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HT	88	GLY	-	expression tag	UNP A0A0J4R4X1
HT	89	SER	-	expression tag	UNP A0A0J4R4X1
HT	90	THR	-	expression tag	UNP A0A0J4R4X1
HT	91	LYS	-	expression tag	UNP A0A0J4R4X1
HT	92	HIS	-	expression tag	UNP A0A0J4R4X1
HT	93	LYS	-	expression tag	UNP A0A0J4R4X1
HT	94	SER	-	expression tag	UNP A0A0J4R4X1
HT	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
HT	96	ARG	-	expression tag	UNP A0A0J4R4X1
HT	97	PRO	-	expression tag	UNP A0A0J4R4X1
HT	98	HIS	-	expression tag	UNP A0A0J4R4X1
HT	99	ASN	-	expression tag	UNP A0A0J4R4X1
HT	100	ALA	-	expression tag	UNP A0A0J4R4X1
HU	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HU	88	GLY	-	expression tag	UNP A0A0J4R4X1
HU	89	SER	-	expression tag	UNP A0A0J4R4X1
HU	90	THR	-	expression tag	UNP A0A0J4R4X1
HU	91	LYS	-	expression tag	UNP A0A0J4R4X1
HU	92	HIS	-	expression tag	UNP A0A0J4R4X1
HU	93	LYS	-	expression tag	UNP A0A0J4R4X1
HU	94	SER	-	expression tag	UNP A0A0J4R4X1
HU	95	LEU	-	expression tag	UNP A0A0J4R4X1
HU	96	ARG	-	expression tag	UNP A0A0J4R4X1
HU	97	PRO	-	expression tag	UNP A0A0J4R4X1
HU	98	HIS	-	expression tag	UNP A0A0J4R4X1
HU	99	ASN	-	expression tag	UNP A0A0J4R4X1
HU	100	ALA	-	expression tag	UNP A0A0J4R4X1
HV	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HV	88	GLY	-	expression tag	UNP A0A0J4R4X1
HV	89	SER	-	expression tag	UNP A0A0J4R4X1
HV	90	THR	-	expression tag	UNP A0A0J4R4X1
HV	91	LYS	-	expression tag	UNP A0A0J4R4X1
HV	92	HIS	-	expression tag	UNP A0A0J4R4X1
HV	93	LYS	-	expression tag	UNP A0A0J4R4X1
HV	94	SER	-	expression tag	UNP A0A0J4R4X1
HV	95	LEU	-	expression tag	UNP A0A0J4R4X1
HV	96	ARG	-	expression tag	UNP A0A0J4R4X1
HV	97	PRO	-	expression tag	UNP A0A0J4R4X1
HV	98	HIS	-	expression tag	UNP A0A0J4R4X1
HV	99	ASN	-	expression tag	UNP A0A0J4R4X1
HV	100	ALA	-	expression tag	UNP A0A0J4R4X1
HX	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HX	88	GLY	-	expression tag	UNP A0A0J4R4X1
HX	89	SER	-	expression tag	UNP A0A0J4R4X1
HX	90	THR	-	expression tag	UNP A0A0J4R4X1
HX	91	LYS	-	expression tag	UNP A0A0J4R4X1
HX	92	HIS	-	expression tag	UNP A0A0J4R4X1
HX	93	LYS	-	expression tag	UNP A0A0J4R4X1
HX	94	SER	-	expression tag	UNP A0A0J4R4X1
HX	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
HX	96	ARG	-	expression tag	UNP A0A0J4R4X1
HX	97	PRO	-	expression tag	UNP A0A0J4R4X1
HX	98	HIS	-	expression tag	UNP A0A0J4R4X1
HX	99	ASN	-	expression tag	UNP A0A0J4R4X1
HX	100	ALA	-	expression tag	UNP A0A0J4R4X1
HY	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HY	88	GLY	-	expression tag	UNP A0A0J4R4X1
HY	89	SER	-	expression tag	UNP A0A0J4R4X1
HY	90	THR	-	expression tag	UNP A0A0J4R4X1
HY	91	LYS	-	expression tag	UNP A0A0J4R4X1
HY	92	HIS	-	expression tag	UNP A0A0J4R4X1
HY	93	LYS	-	expression tag	UNP A0A0J4R4X1
HY	94	SER	-	expression tag	UNP A0A0J4R4X1
HY	95	LEU	-	expression tag	UNP A0A0J4R4X1
HY	96	ARG	-	expression tag	UNP A0A0J4R4X1
HY	97	PRO	-	expression tag	UNP A0A0J4R4X1
HY	98	HIS	-	expression tag	UNP A0A0J4R4X1
HY	99	ASN	-	expression tag	UNP A0A0J4R4X1
HY	100	ALA	-	expression tag	UNP A0A0J4R4X1
HZ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
HZ	88	GLY	-	expression tag	UNP A0A0J4R4X1
HZ	89	SER	-	expression tag	UNP A0A0J4R4X1
HZ	90	THR	-	expression tag	UNP A0A0J4R4X1
HZ	91	LYS	-	expression tag	UNP A0A0J4R4X1
HZ	92	HIS	-	expression tag	UNP A0A0J4R4X1
HZ	93	LYS	-	expression tag	UNP A0A0J4R4X1
HZ	94	SER	-	expression tag	UNP A0A0J4R4X1
HZ	95	LEU	-	expression tag	UNP A0A0J4R4X1
HZ	96	ARG	-	expression tag	UNP A0A0J4R4X1
HZ	97	PRO	-	expression tag	UNP A0A0J4R4X1
HZ	98	HIS	-	expression tag	UNP A0A0J4R4X1
HZ	99	ASN	-	expression tag	UNP A0A0J4R4X1
HZ	100	ALA	-	expression tag	UNP A0A0J4R4X1
IB	69	LYS	GLU	conflict	UNP A0A0J4R4X1
IB	88	GLY	-	expression tag	UNP A0A0J4R4X1
IB	89	SER	-	expression tag	UNP A0A0J4R4X1
IB	90	THR	-	expression tag	UNP A0A0J4R4X1
IB	91	LYS	-	expression tag	UNP A0A0J4R4X1
IB	92	HIS	-	expression tag	UNP A0A0J4R4X1
IB	93	LYS	-	expression tag	UNP A0A0J4R4X1
IB	94	SER	-	expression tag	UNP A0A0J4R4X1
IB	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
IB	96	ARG	-	expression tag	UNP A0A0J4R4X1
IB	97	PRO	-	expression tag	UNP A0A0J4R4X1
IB	98	HIS	-	expression tag	UNP A0A0J4R4X1
IB	99	ASN	-	expression tag	UNP A0A0J4R4X1
IB	100	ALA	-	expression tag	UNP A0A0J4R4X1
IC	69	LYS	GLU	conflict	UNP A0A0J4R4X1
IC	88	GLY	-	expression tag	UNP A0A0J4R4X1
IC	89	SER	-	expression tag	UNP A0A0J4R4X1
IC	90	THR	-	expression tag	UNP A0A0J4R4X1
IC	91	LYS	-	expression tag	UNP A0A0J4R4X1
IC	92	HIS	-	expression tag	UNP A0A0J4R4X1
IC	93	LYS	-	expression tag	UNP A0A0J4R4X1
IC	94	SER	-	expression tag	UNP A0A0J4R4X1
IC	95	LEU	-	expression tag	UNP A0A0J4R4X1
IC	96	ARG	-	expression tag	UNP A0A0J4R4X1
IC	97	PRO	-	expression tag	UNP A0A0J4R4X1
IC	98	HIS	-	expression tag	UNP A0A0J4R4X1
IC	99	ASN	-	expression tag	UNP A0A0J4R4X1
IC	100	ALA	-	expression tag	UNP A0A0J4R4X1
ID	69	LYS	GLU	conflict	UNP A0A0J4R4X1
ID	88	GLY	-	expression tag	UNP A0A0J4R4X1
ID	89	SER	-	expression tag	UNP A0A0J4R4X1
ID	90	THR	-	expression tag	UNP A0A0J4R4X1
ID	91	LYS	-	expression tag	UNP A0A0J4R4X1
ID	92	HIS	-	expression tag	UNP A0A0J4R4X1
ID	93	LYS	-	expression tag	UNP A0A0J4R4X1
ID	94	SER	-	expression tag	UNP A0A0J4R4X1
ID	95	LEU	-	expression tag	UNP A0A0J4R4X1
ID	96	ARG	-	expression tag	UNP A0A0J4R4X1
ID	97	PRO	-	expression tag	UNP A0A0J4R4X1
ID	98	HIS	-	expression tag	UNP A0A0J4R4X1
ID	99	ASN	-	expression tag	UNP A0A0J4R4X1
ID	100	ALA	-	expression tag	UNP A0A0J4R4X1
IF	69	LYS	GLU	conflict	UNP A0A0J4R4X1
IF	88	GLY	-	expression tag	UNP A0A0J4R4X1
IF	89	SER	-	expression tag	UNP A0A0J4R4X1
IF	90	THR	-	expression tag	UNP A0A0J4R4X1
IF	91	LYS	-	expression tag	UNP A0A0J4R4X1
IF	92	HIS	-	expression tag	UNP A0A0J4R4X1
IF	93	LYS	-	expression tag	UNP A0A0J4R4X1
IF	94	SER	-	expression tag	UNP A0A0J4R4X1
IF	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
IF	96	ARG	-	expression tag	UNP A0A0J4R4X1
IF	97	PRO	-	expression tag	UNP A0A0J4R4X1
IF	98	HIS	-	expression tag	UNP A0A0J4R4X1
IF	99	ASN	-	expression tag	UNP A0A0J4R4X1
IF	100	ALA	-	expression tag	UNP A0A0J4R4X1
IG	69	LYS	GLU	conflict	UNP A0A0J4R4X1
IG	88	GLY	-	expression tag	UNP A0A0J4R4X1
IG	89	SER	-	expression tag	UNP A0A0J4R4X1
IG	90	THR	-	expression tag	UNP A0A0J4R4X1
IG	91	LYS	-	expression tag	UNP A0A0J4R4X1
IG	92	HIS	-	expression tag	UNP A0A0J4R4X1
IG	93	LYS	-	expression tag	UNP A0A0J4R4X1
IG	94	SER	-	expression tag	UNP A0A0J4R4X1
IG	95	LEU	-	expression tag	UNP A0A0J4R4X1
IG	96	ARG	-	expression tag	UNP A0A0J4R4X1
IG	97	PRO	-	expression tag	UNP A0A0J4R4X1
IG	98	HIS	-	expression tag	UNP A0A0J4R4X1
IG	99	ASN	-	expression tag	UNP A0A0J4R4X1
IG	100	ALA	-	expression tag	UNP A0A0J4R4X1
IH	69	LYS	GLU	conflict	UNP A0A0J4R4X1
IH	88	GLY	-	expression tag	UNP A0A0J4R4X1
IH	89	SER	-	expression tag	UNP A0A0J4R4X1
IH	90	THR	-	expression tag	UNP A0A0J4R4X1
IH	91	LYS	-	expression tag	UNP A0A0J4R4X1
IH	92	HIS	-	expression tag	UNP A0A0J4R4X1
IH	93	LYS	-	expression tag	UNP A0A0J4R4X1
IH	94	SER	-	expression tag	UNP A0A0J4R4X1
IH	95	LEU	-	expression tag	UNP A0A0J4R4X1
IH	96	ARG	-	expression tag	UNP A0A0J4R4X1
IH	97	PRO	-	expression tag	UNP A0A0J4R4X1
IH	98	HIS	-	expression tag	UNP A0A0J4R4X1
IH	99	ASN	-	expression tag	UNP A0A0J4R4X1
IH	100	ALA	-	expression tag	UNP A0A0J4R4X1
IJ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
IJ	88	GLY	-	expression tag	UNP A0A0J4R4X1
IJ	89	SER	-	expression tag	UNP A0A0J4R4X1
IJ	90	THR	-	expression tag	UNP A0A0J4R4X1
IJ	91	LYS	-	expression tag	UNP A0A0J4R4X1
IJ	92	HIS	-	expression tag	UNP A0A0J4R4X1
IJ	93	LYS	-	expression tag	UNP A0A0J4R4X1
IJ	94	SER	-	expression tag	UNP A0A0J4R4X1
IJ	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
IJ	96	ARG	-	expression tag	UNP A0A0J4R4X1
IJ	97	PRO	-	expression tag	UNP A0A0J4R4X1
IJ	98	HIS	-	expression tag	UNP A0A0J4R4X1
IJ	99	ASN	-	expression tag	UNP A0A0J4R4X1
IJ	100	ALA	-	expression tag	UNP A0A0J4R4X1
IK	69	LYS	GLU	conflict	UNP A0A0J4R4X1
IK	88	GLY	-	expression tag	UNP A0A0J4R4X1
IK	89	SER	-	expression tag	UNP A0A0J4R4X1
IK	90	THR	-	expression tag	UNP A0A0J4R4X1
IK	91	LYS	-	expression tag	UNP A0A0J4R4X1
IK	92	HIS	-	expression tag	UNP A0A0J4R4X1
IK	93	LYS	-	expression tag	UNP A0A0J4R4X1
IK	94	SER	-	expression tag	UNP A0A0J4R4X1
IK	95	LEU	-	expression tag	UNP A0A0J4R4X1
IK	96	ARG	-	expression tag	UNP A0A0J4R4X1
IK	97	PRO	-	expression tag	UNP A0A0J4R4X1
IK	98	HIS	-	expression tag	UNP A0A0J4R4X1
IK	99	ASN	-	expression tag	UNP A0A0J4R4X1
IK	100	ALA	-	expression tag	UNP A0A0J4R4X1
IL	69	LYS	GLU	conflict	UNP A0A0J4R4X1
IL	88	GLY	-	expression tag	UNP A0A0J4R4X1
IL	89	SER	-	expression tag	UNP A0A0J4R4X1
IL	90	THR	-	expression tag	UNP A0A0J4R4X1
IL	91	LYS	-	expression tag	UNP A0A0J4R4X1
IL	92	HIS	-	expression tag	UNP A0A0J4R4X1
IL	93	LYS	-	expression tag	UNP A0A0J4R4X1
IL	94	SER	-	expression tag	UNP A0A0J4R4X1
IL	95	LEU	-	expression tag	UNP A0A0J4R4X1
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IL	97	PRO	-	expression tag	UNP A0A0J4R4X1
IL	98	HIS	-	expression tag	UNP A0A0J4R4X1
IL	99	ASN	-	expression tag	UNP A0A0J4R4X1
IL	100	ALA	-	expression tag	UNP A0A0J4R4X1
IN	69	LYS	GLU	conflict	UNP A0A0J4R4X1
IN	88	GLY	-	expression tag	UNP A0A0J4R4X1
IN	89	SER	-	expression tag	UNP A0A0J4R4X1
IN	90	THR	-	expression tag	UNP A0A0J4R4X1
IN	91	LYS	-	expression tag	UNP A0A0J4R4X1
IN	92	HIS	-	expression tag	UNP A0A0J4R4X1
IN	93	LYS	-	expression tag	UNP A0A0J4R4X1
IN	94	SER	-	expression tag	UNP A0A0J4R4X1
IN	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
IN	96	ARG	-	expression tag	UNP A0A0J4R4X1
IN	97	PRO	-	expression tag	UNP A0A0J4R4X1
IN	98	HIS	-	expression tag	UNP A0A0J4R4X1
IN	99	ASN	-	expression tag	UNP A0A0J4R4X1
IN	100	ALA	-	expression tag	UNP A0A0J4R4X1
IO	69	LYS	GLU	conflict	UNP A0A0J4R4X1
IO	88	GLY	-	expression tag	UNP A0A0J4R4X1
IO	89	SER	-	expression tag	UNP A0A0J4R4X1
IO	90	THR	-	expression tag	UNP A0A0J4R4X1
IO	91	LYS	-	expression tag	UNP A0A0J4R4X1
IO	92	HIS	-	expression tag	UNP A0A0J4R4X1
IO	93	LYS	-	expression tag	UNP A0A0J4R4X1
IO	94	SER	-	expression tag	UNP A0A0J4R4X1
IO	95	LEU	-	expression tag	UNP A0A0J4R4X1
IO	96	ARG	-	expression tag	UNP A0A0J4R4X1
IO	97	PRO	-	expression tag	UNP A0A0J4R4X1
IO	98	HIS	-	expression tag	UNP A0A0J4R4X1
IO	99	ASN	-	expression tag	UNP A0A0J4R4X1
IO	100	ALA	-	expression tag	UNP A0A0J4R4X1
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IP	88	GLY	-	expression tag	UNP A0A0J4R4X1
IP	89	SER	-	expression tag	UNP A0A0J4R4X1
IP	90	THR	-	expression tag	UNP A0A0J4R4X1
IP	91	LYS	-	expression tag	UNP A0A0J4R4X1
IP	92	HIS	-	expression tag	UNP A0A0J4R4X1
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IP	95	LEU	-	expression tag	UNP A0A0J4R4X1
IP	96	ARG	-	expression tag	UNP A0A0J4R4X1
IP	97	PRO	-	expression tag	UNP A0A0J4R4X1
IP	98	HIS	-	expression tag	UNP A0A0J4R4X1
IP	99	ASN	-	expression tag	UNP A0A0J4R4X1
IP	100	ALA	-	expression tag	UNP A0A0J4R4X1
IR	69	LYS	GLU	conflict	UNP A0A0J4R4X1
IR	88	GLY	-	expression tag	UNP A0A0J4R4X1
IR	89	SER	-	expression tag	UNP A0A0J4R4X1
IR	90	THR	-	expression tag	UNP A0A0J4R4X1
IR	91	LYS	-	expression tag	UNP A0A0J4R4X1
IR	92	HIS	-	expression tag	UNP A0A0J4R4X1
IR	93	LYS	-	expression tag	UNP A0A0J4R4X1
IR	94	SER	-	expression tag	UNP A0A0J4R4X1
IR	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
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IR	97	PRO	-	expression tag	UNP A0A0J4R4X1
IR	98	HIS	-	expression tag	UNP A0A0J4R4X1
IR	99	ASN	-	expression tag	UNP A0A0J4R4X1
IR	100	ALA	-	expression tag	UNP A0A0J4R4X1
IS	69	LYS	GLU	conflict	UNP A0A0J4R4X1
IS	88	GLY	-	expression tag	UNP A0A0J4R4X1
IS	89	SER	-	expression tag	UNP A0A0J4R4X1
IS	90	THR	-	expression tag	UNP A0A0J4R4X1
IS	91	LYS	-	expression tag	UNP A0A0J4R4X1
IS	92	HIS	-	expression tag	UNP A0A0J4R4X1
IS	93	LYS	-	expression tag	UNP A0A0J4R4X1
IS	94	SER	-	expression tag	UNP A0A0J4R4X1
IS	95	LEU	-	expression tag	UNP A0A0J4R4X1
IS	96	ARG	-	expression tag	UNP A0A0J4R4X1
IS	97	PRO	-	expression tag	UNP A0A0J4R4X1
IS	98	HIS	-	expression tag	UNP A0A0J4R4X1
IS	99	ASN	-	expression tag	UNP A0A0J4R4X1
IS	100	ALA	-	expression tag	UNP A0A0J4R4X1
IT	69	LYS	GLU	conflict	UNP A0A0J4R4X1
IT	88	GLY	-	expression tag	UNP A0A0J4R4X1
IT	89	SER	-	expression tag	UNP A0A0J4R4X1
IT	90	THR	-	expression tag	UNP A0A0J4R4X1
IT	91	LYS	-	expression tag	UNP A0A0J4R4X1
IT	92	HIS	-	expression tag	UNP A0A0J4R4X1
IT	93	LYS	-	expression tag	UNP A0A0J4R4X1
IT	94	SER	-	expression tag	UNP A0A0J4R4X1
IT	95	LEU	-	expression tag	UNP A0A0J4R4X1
IT	96	ARG	-	expression tag	UNP A0A0J4R4X1
IT	97	PRO	-	expression tag	UNP A0A0J4R4X1
IT	98	HIS	-	expression tag	UNP A0A0J4R4X1
IT	99	ASN	-	expression tag	UNP A0A0J4R4X1
IT	100	ALA	-	expression tag	UNP A0A0J4R4X1
IV	69	LYS	GLU	conflict	UNP A0A0J4R4X1
IV	88	GLY	-	expression tag	UNP A0A0J4R4X1
IV	89	SER	-	expression tag	UNP A0A0J4R4X1
IV	90	THR	-	expression tag	UNP A0A0J4R4X1
IV	91	LYS	-	expression tag	UNP A0A0J4R4X1
IV	92	HIS	-	expression tag	UNP A0A0J4R4X1
IV	93	LYS	-	expression tag	UNP A0A0J4R4X1
IV	94	SER	-	expression tag	UNP A0A0J4R4X1
IV	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
IV	96	ARG	-	expression tag	UNP A0A0J4R4X1
IV	97	PRO	-	expression tag	UNP A0A0J4R4X1
IV	98	HIS	-	expression tag	UNP A0A0J4R4X1
IV	99	ASN	-	expression tag	UNP A0A0J4R4X1
IV	100	ALA	-	expression tag	UNP A0A0J4R4X1
IW	69	LYS	GLU	conflict	UNP A0A0J4R4X1
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IW	89	SER	-	expression tag	UNP A0A0J4R4X1
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IW	91	LYS	-	expression tag	UNP A0A0J4R4X1
IW	92	HIS	-	expression tag	UNP A0A0J4R4X1
IW	93	LYS	-	expression tag	UNP A0A0J4R4X1
IW	94	SER	-	expression tag	UNP A0A0J4R4X1
IW	95	LEU	-	expression tag	UNP A0A0J4R4X1
IW	96	ARG	-	expression tag	UNP A0A0J4R4X1
IW	97	PRO	-	expression tag	UNP A0A0J4R4X1
IW	98	HIS	-	expression tag	UNP A0A0J4R4X1
IW	99	ASN	-	expression tag	UNP A0A0J4R4X1
IW	100	ALA	-	expression tag	UNP A0A0J4R4X1
IX	69	LYS	GLU	conflict	UNP A0A0J4R4X1
IX	88	GLY	-	expression tag	UNP A0A0J4R4X1
IX	89	SER	-	expression tag	UNP A0A0J4R4X1
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IX	91	LYS	-	expression tag	UNP A0A0J4R4X1
IX	92	HIS	-	expression tag	UNP A0A0J4R4X1
IX	93	LYS	-	expression tag	UNP A0A0J4R4X1
IX	94	SER	-	expression tag	UNP A0A0J4R4X1
IX	95	LEU	-	expression tag	UNP A0A0J4R4X1
IX	96	ARG	-	expression tag	UNP A0A0J4R4X1
IX	97	PRO	-	expression tag	UNP A0A0J4R4X1
IX	98	HIS	-	expression tag	UNP A0A0J4R4X1
IX	99	ASN	-	expression tag	UNP A0A0J4R4X1
IX	100	ALA	-	expression tag	UNP A0A0J4R4X1
IZ	69	LYS	GLU	conflict	UNP A0A0J4R4X1
IZ	88	GLY	-	expression tag	UNP A0A0J4R4X1
IZ	89	SER	-	expression tag	UNP A0A0J4R4X1
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IZ	91	LYS	-	expression tag	UNP A0A0J4R4X1
IZ	92	HIS	-	expression tag	UNP A0A0J4R4X1
IZ	93	LYS	-	expression tag	UNP A0A0J4R4X1
IZ	94	SER	-	expression tag	UNP A0A0J4R4X1
IZ	95	LEU	-	expression tag	UNP A0A0J4R4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
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IZ	97	PRO	-	expression tag	UNP A0A0J4R4X1
IZ	98	HIS	-	expression tag	UNP A0A0J4R4X1
IZ	99	ASN	-	expression tag	UNP A0A0J4R4X1
IZ	100	ALA	-	expression tag	UNP A0A0J4R4X1
JA	69	LYS	GLU	conflict	UNP A0A0J4R4X1
JA	88	GLY	-	expression tag	UNP A0A0J4R4X1
JA	89	SER	-	expression tag	UNP A0A0J4R4X1
JA	90	THR	-	expression tag	UNP A0A0J4R4X1
JA	91	LYS	-	expression tag	UNP A0A0J4R4X1
JA	92	HIS	-	expression tag	UNP A0A0J4R4X1
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JA	95	LEU	-	expression tag	UNP A0A0J4R4X1
JA	96	ARG	-	expression tag	UNP A0A0J4R4X1
JA	97	PRO	-	expression tag	UNP A0A0J4R4X1
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JA	99	ASN	-	expression tag	UNP A0A0J4R4X1
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JB	89	SER	-	expression tag	UNP A0A0J4R4X1
JB	90	THR	-	expression tag	UNP A0A0J4R4X1
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JB	92	HIS	-	expression tag	UNP A0A0J4R4X1
JB	93	LYS	-	expression tag	UNP A0A0J4R4X1
JB	94	SER	-	expression tag	UNP A0A0J4R4X1
JB	95	LEU	-	expression tag	UNP A0A0J4R4X1
JB	96	ARG	-	expression tag	UNP A0A0J4R4X1
JB	97	PRO	-	expression tag	UNP A0A0J4R4X1
JB	98	HIS	-	expression tag	UNP A0A0J4R4X1
JB	99	ASN	-	expression tag	UNP A0A0J4R4X1
JB	100	ALA	-	expression tag	UNP A0A0J4R4X1
JD	69	LYS	GLU	conflict	UNP A0A0J4R4X1
JD	88	GLY	-	expression tag	UNP A0A0J4R4X1
JD	89	SER	-	expression tag	UNP A0A0J4R4X1
JD	90	THR	-	expression tag	UNP A0A0J4R4X1
JD	91	LYS	-	expression tag	UNP A0A0J4R4X1
JD	92	HIS	-	expression tag	UNP A0A0J4R4X1
JD	93	LYS	-	expression tag	UNP A0A0J4R4X1
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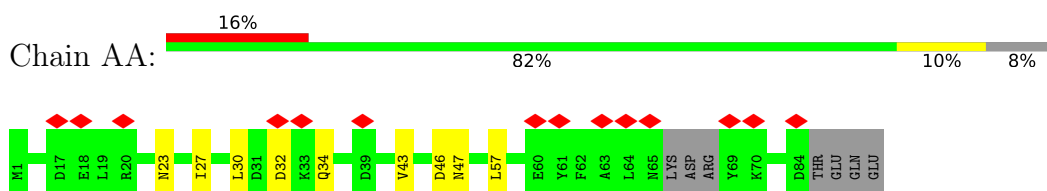
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Chain	Residue	Modelled	Actual	Comment	Reference
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JD	97	PRO	-	expression tag	UNP A0A0J4R4X1
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JD	99	ASN	-	expression tag	UNP A0A0J4R4X1
JD	100	ALA	-	expression tag	UNP A0A0J4R4X1
JE	69	LYS	GLU	conflict	UNP A0A0J4R4X1
JE	88	GLY	-	expression tag	UNP A0A0J4R4X1
JE	89	SER	-	expression tag	UNP A0A0J4R4X1
JE	90	THR	-	expression tag	UNP A0A0J4R4X1
JE	91	LYS	-	expression tag	UNP A0A0J4R4X1
JE	92	HIS	-	expression tag	UNP A0A0J4R4X1
JE	93	LYS	-	expression tag	UNP A0A0J4R4X1
JE	94	SER	-	expression tag	UNP A0A0J4R4X1
JE	95	LEU	-	expression tag	UNP A0A0J4R4X1
JE	96	ARG	-	expression tag	UNP A0A0J4R4X1
JE	97	PRO	-	expression tag	UNP A0A0J4R4X1
JE	98	HIS	-	expression tag	UNP A0A0J4R4X1
JE	99	ASN	-	expression tag	UNP A0A0J4R4X1
JE	100	ALA	-	expression tag	UNP A0A0J4R4X1
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JF	88	GLY	-	expression tag	UNP A0A0J4R4X1
JF	89	SER	-	expression tag	UNP A0A0J4R4X1
JF	90	THR	-	expression tag	UNP A0A0J4R4X1
JF	91	LYS	-	expression tag	UNP A0A0J4R4X1
JF	92	HIS	-	expression tag	UNP A0A0J4R4X1
JF	93	LYS	-	expression tag	UNP A0A0J4R4X1
JF	94	SER	-	expression tag	UNP A0A0J4R4X1
JF	95	LEU	-	expression tag	UNP A0A0J4R4X1
JF	96	ARG	-	expression tag	UNP A0A0J4R4X1
JF	97	PRO	-	expression tag	UNP A0A0J4R4X1
JF	98	HIS	-	expression tag	UNP A0A0J4R4X1
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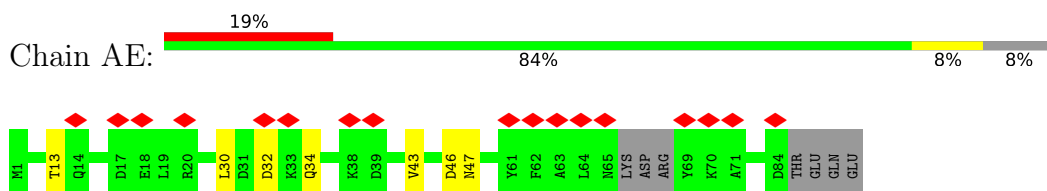
3 Residue-property plots [i](#)

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

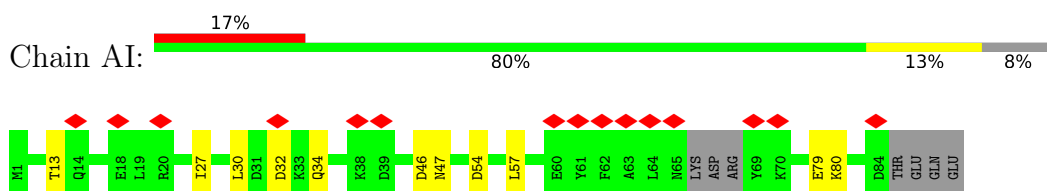
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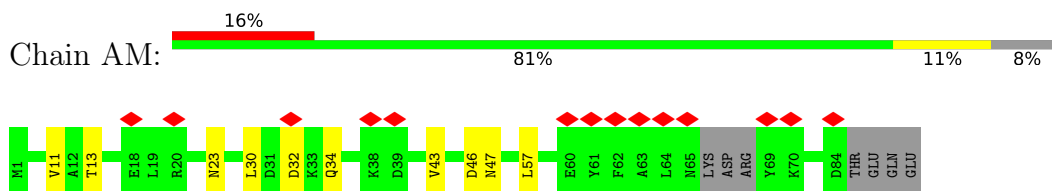
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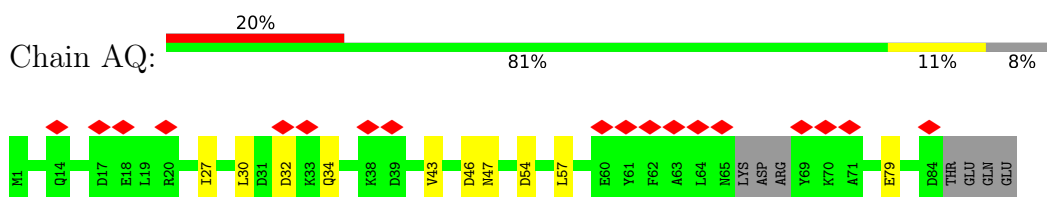
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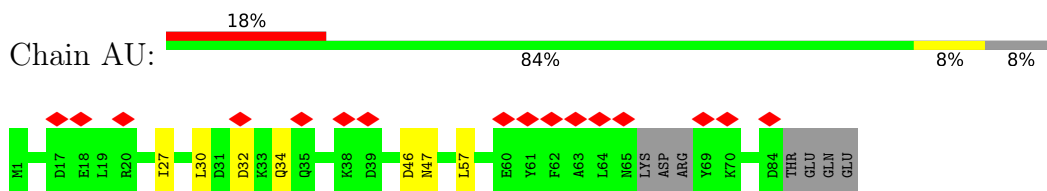
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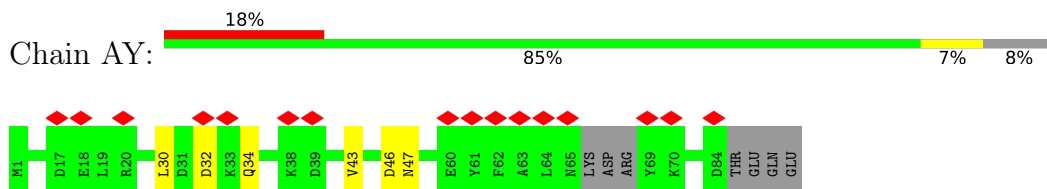
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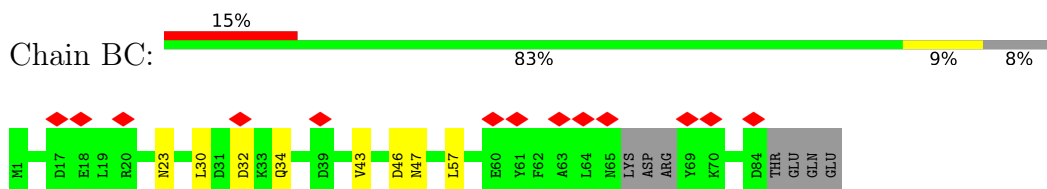
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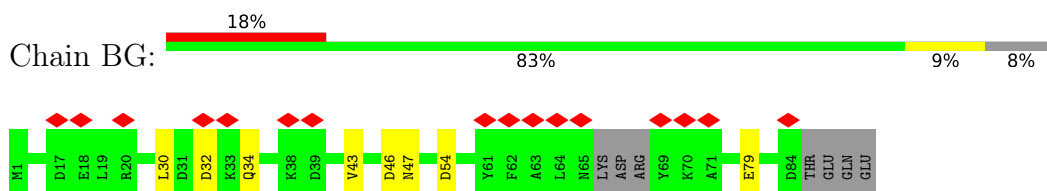
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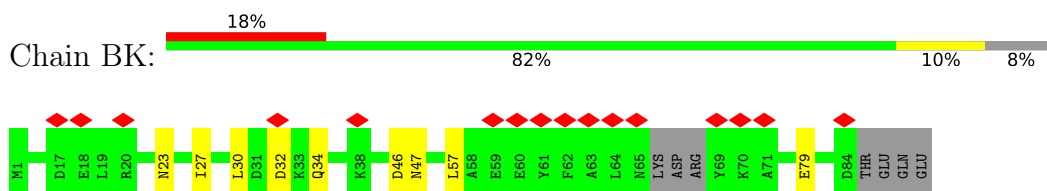
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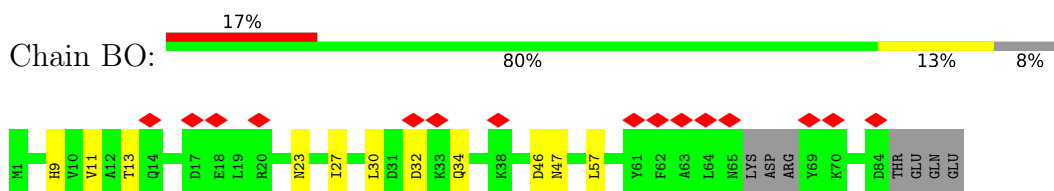
- Molecule 1: Carbon dioxide concentrating mechanism protein CcmL



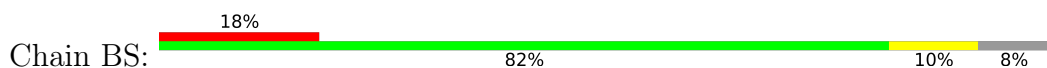
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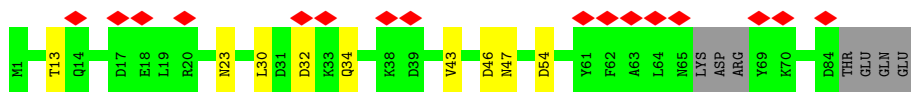


- Molecule 1: Carbon dioxide concentrating mechanism protein CcmL

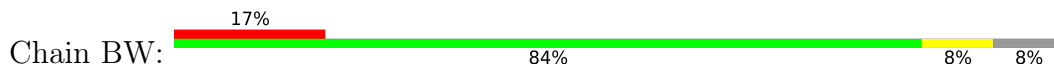


- Molecule 1: Carbon dioxide concentrating mechanism protein CcmL

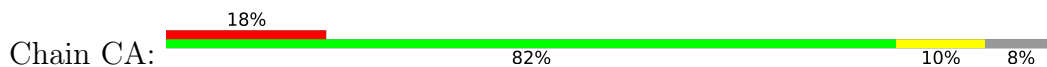




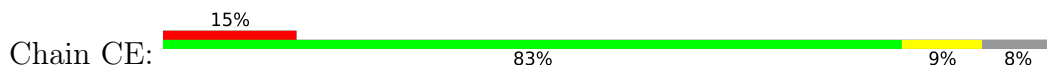
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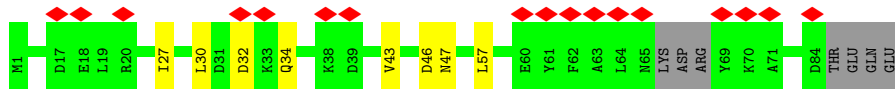
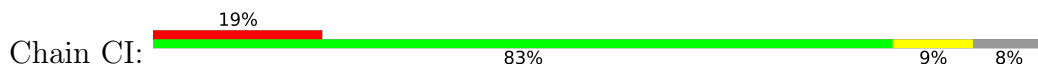
- Molecule 1: Carbon dioxide concentrating mechanism protein CcmL



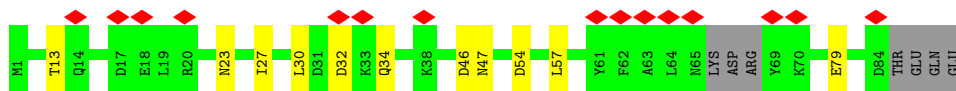
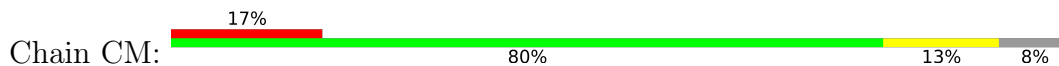
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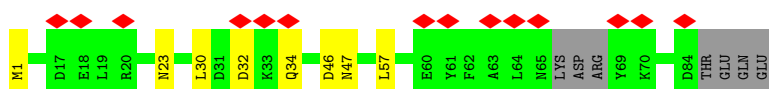
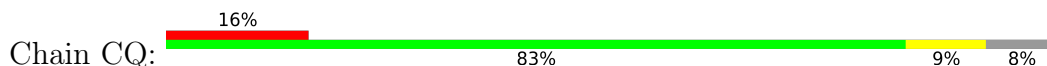
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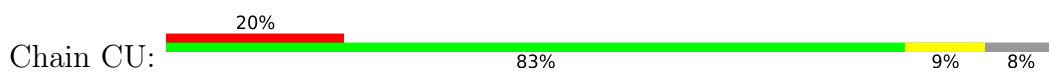
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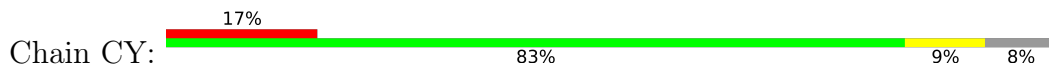
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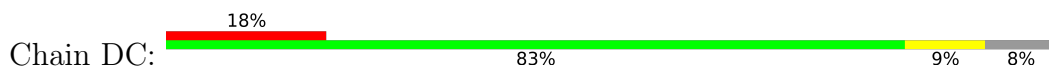
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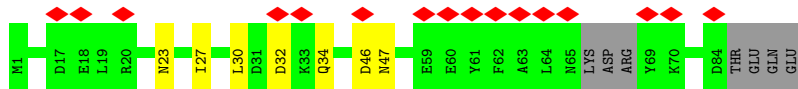
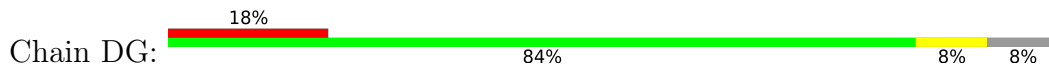
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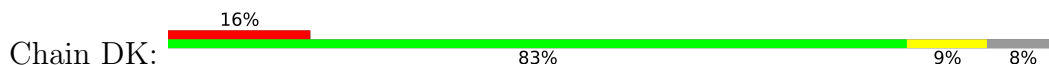
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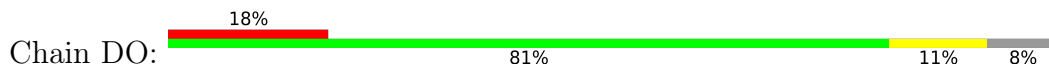
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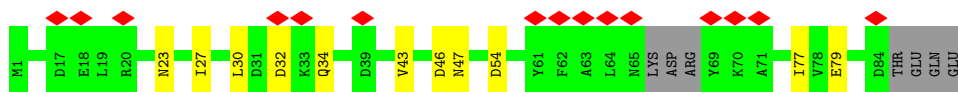
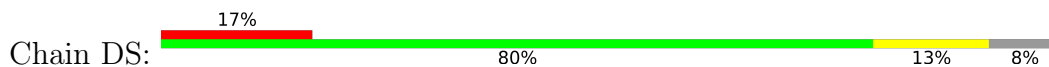
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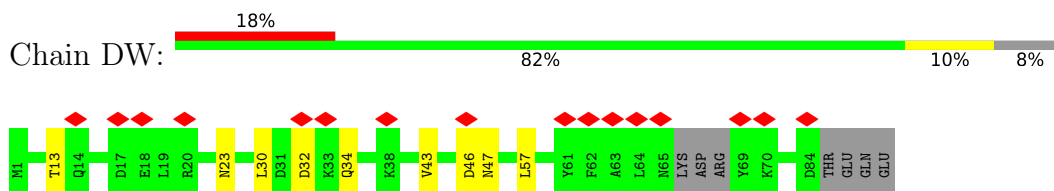
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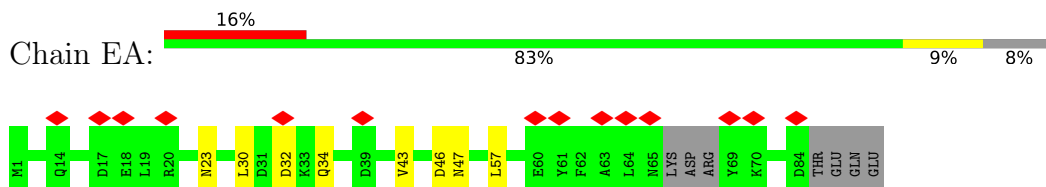
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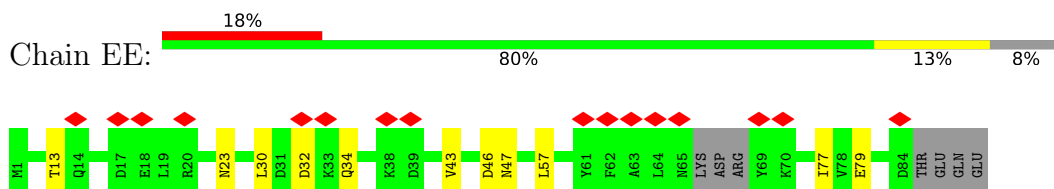
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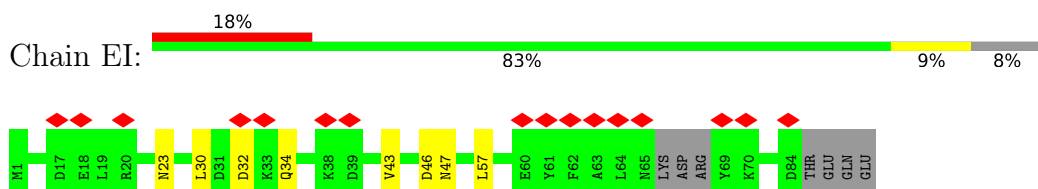
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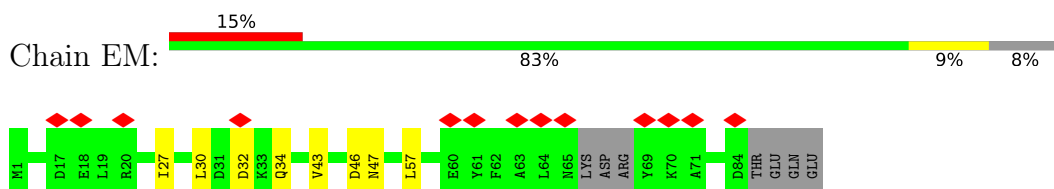
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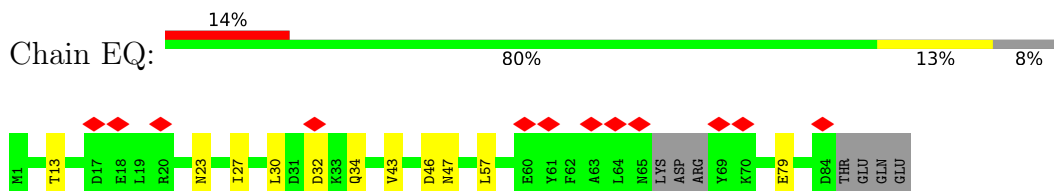
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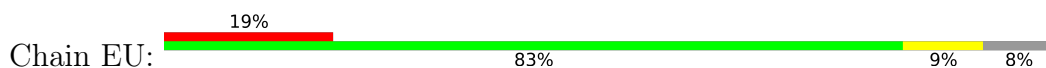
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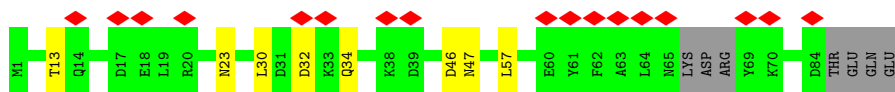


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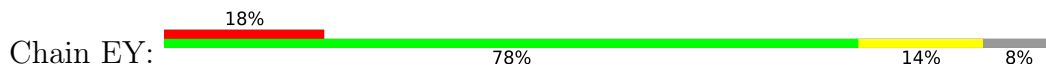


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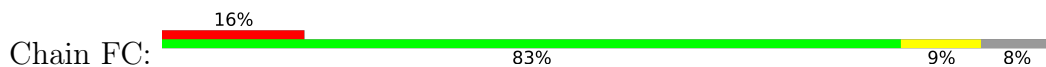




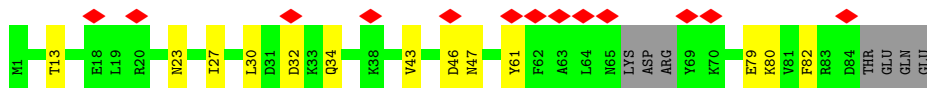
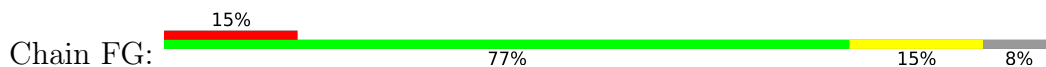
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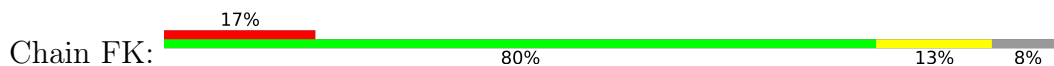
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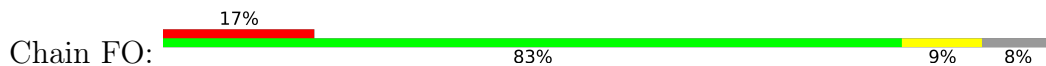
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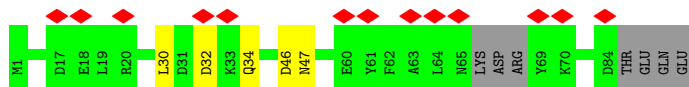
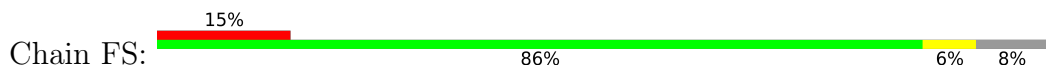
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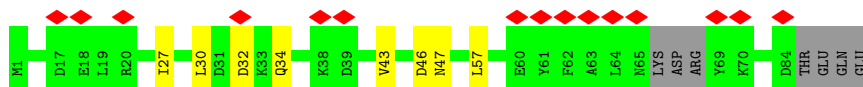
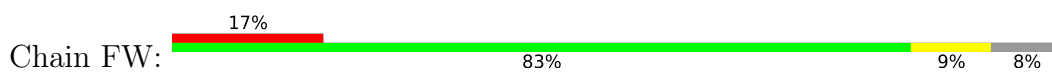
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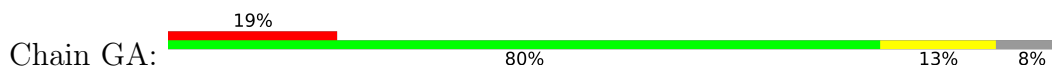
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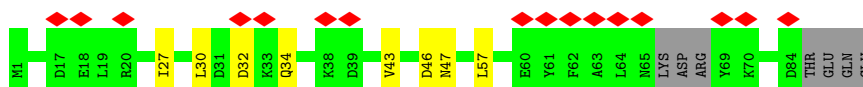
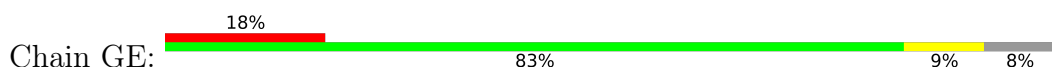
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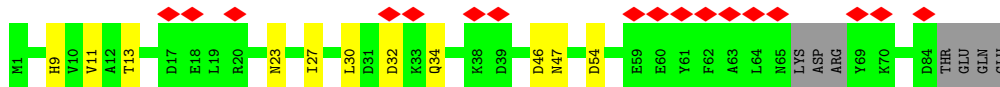
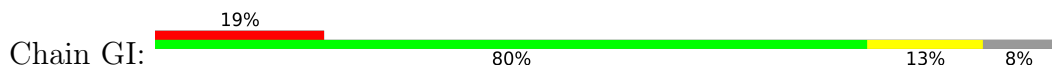
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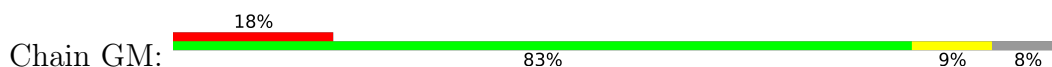
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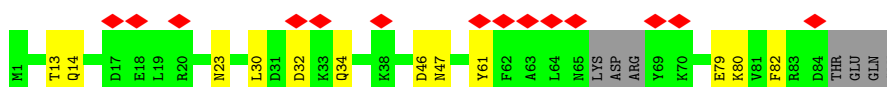
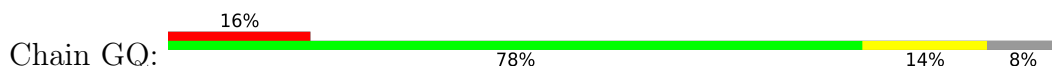
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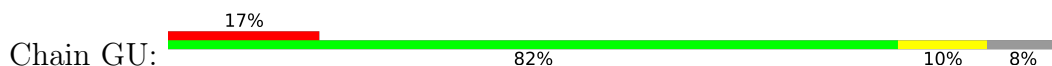
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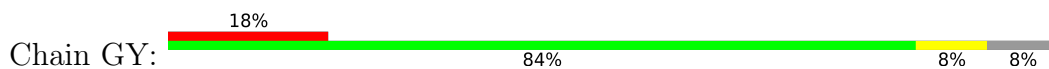
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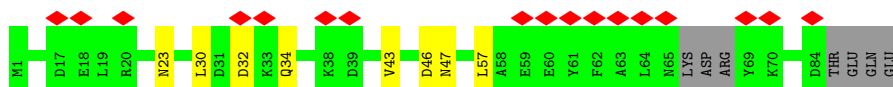
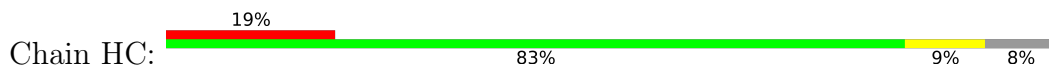
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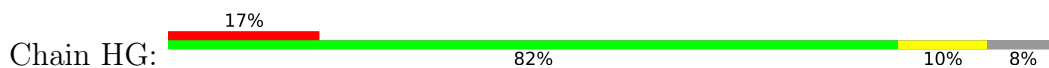
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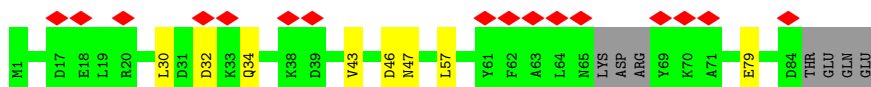
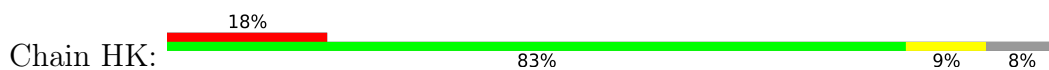
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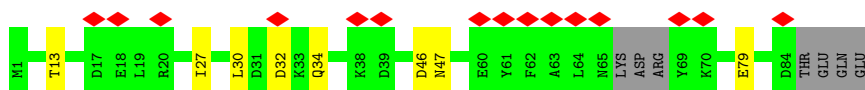
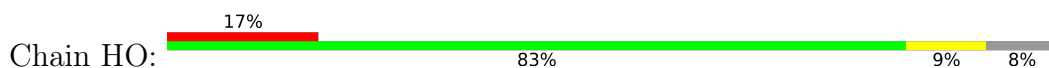
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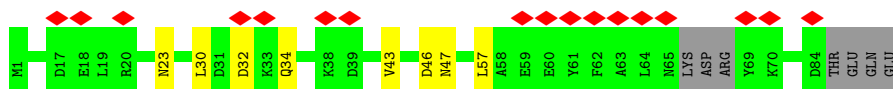
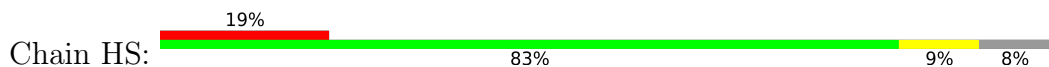
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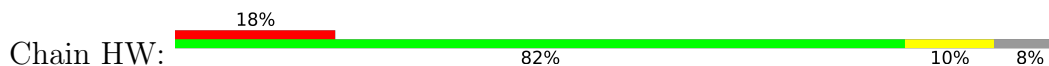
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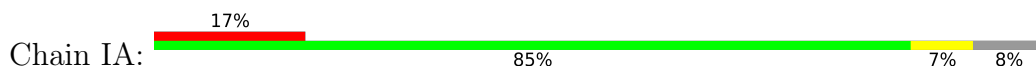


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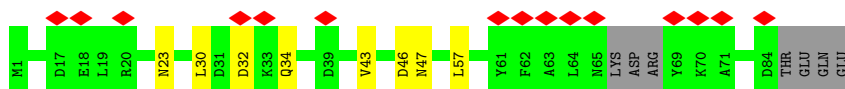
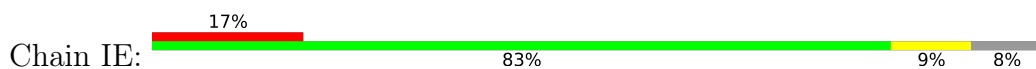




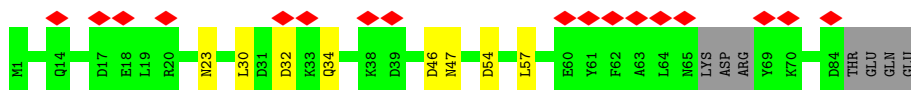
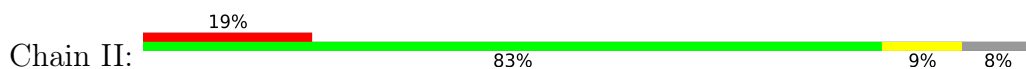
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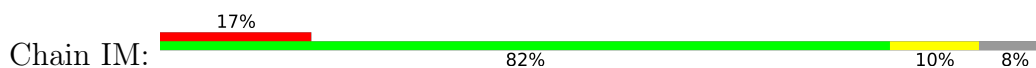
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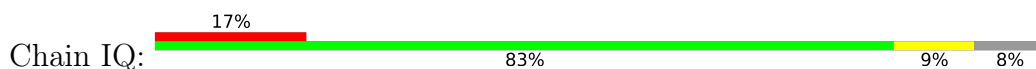
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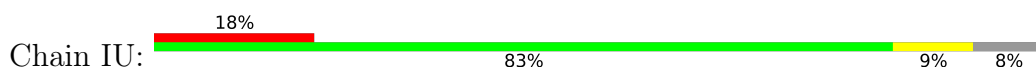
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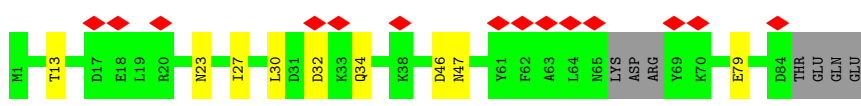
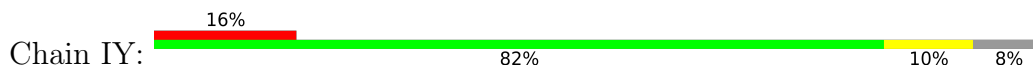
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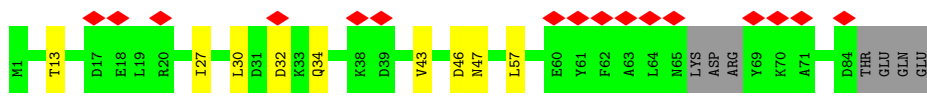
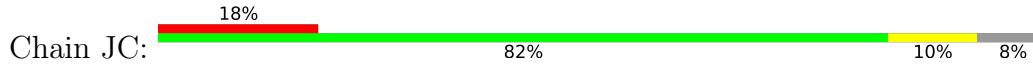
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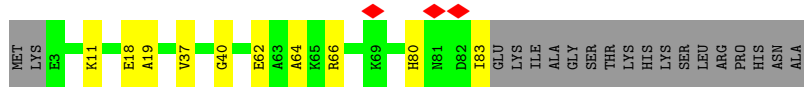
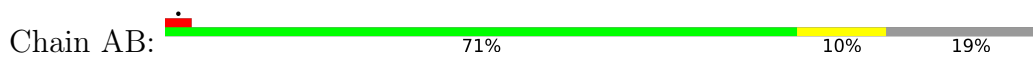
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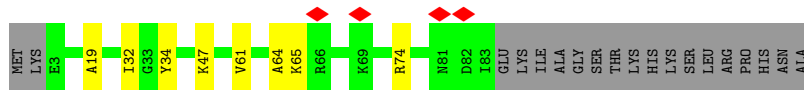
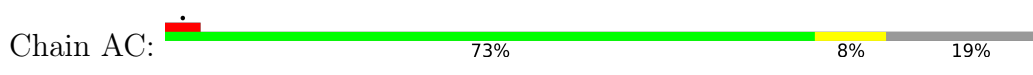
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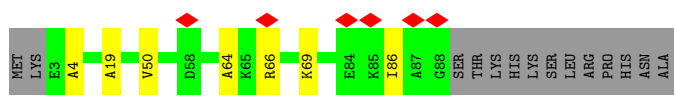
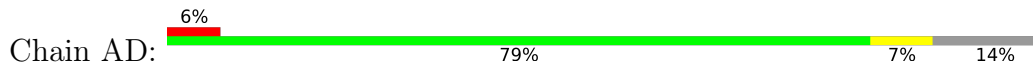
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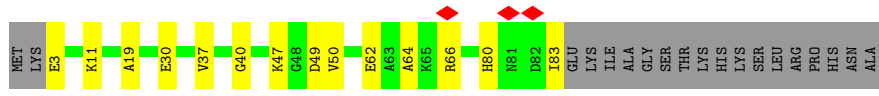
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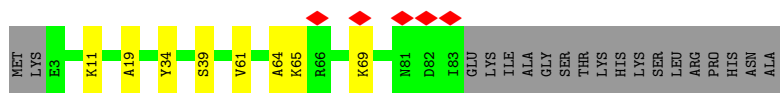
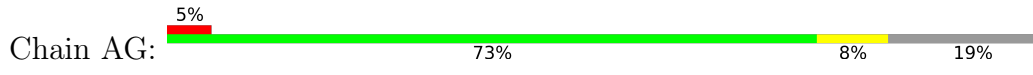
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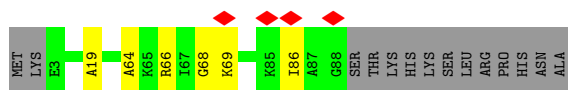
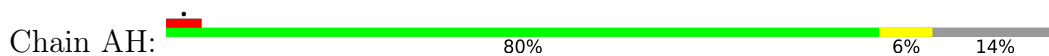
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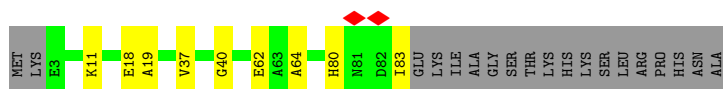
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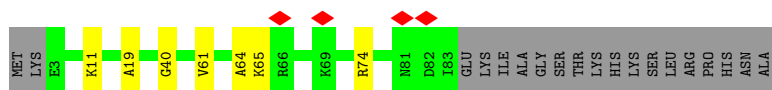
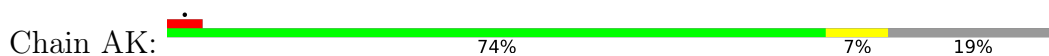
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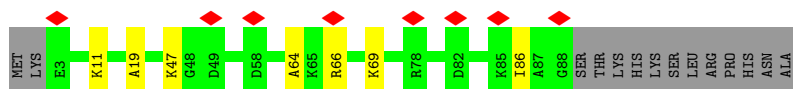
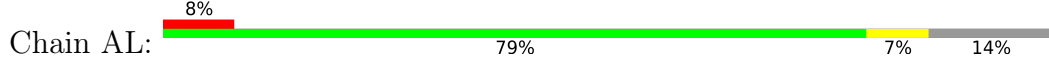
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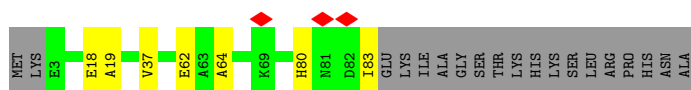
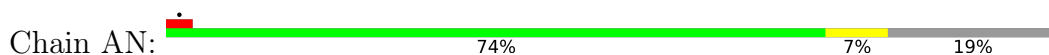
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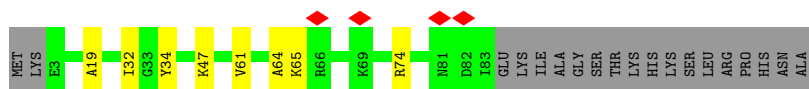
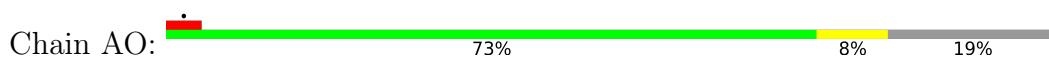
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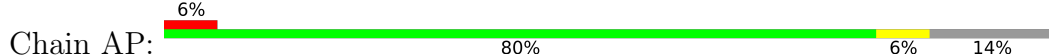
• Molecule 2: BMC domain-containing protein

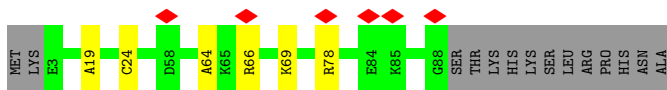


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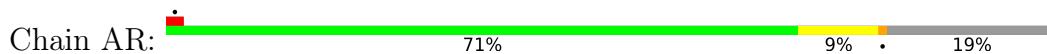


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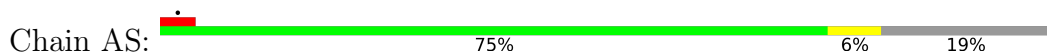




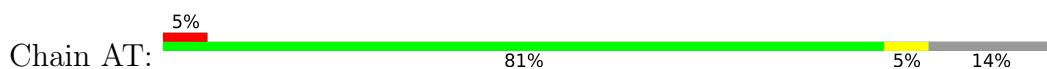
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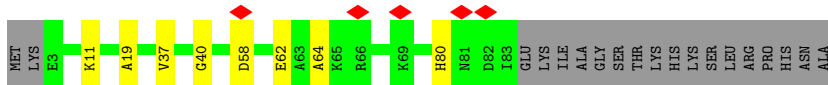
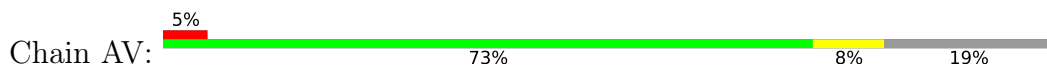
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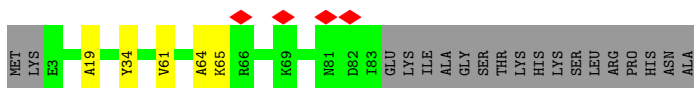
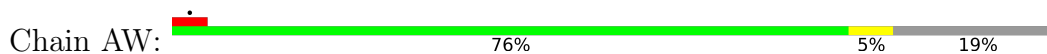
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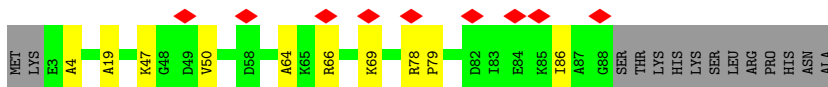
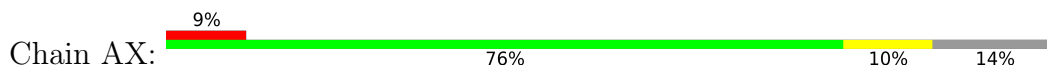
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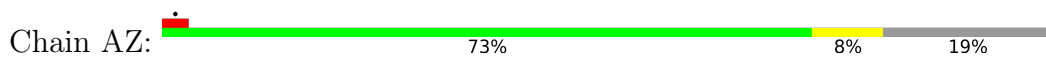
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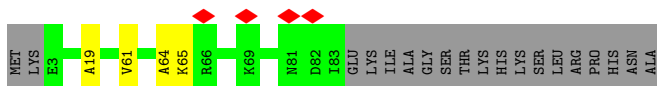
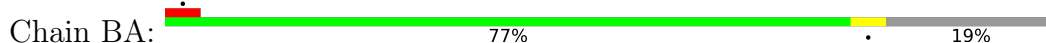
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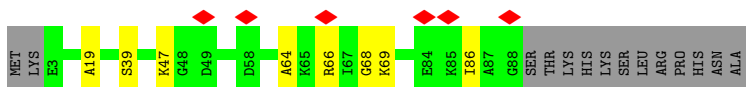
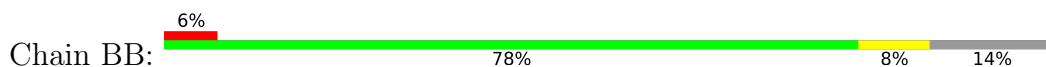
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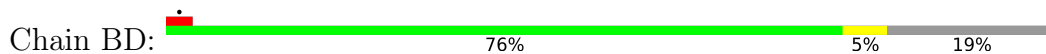
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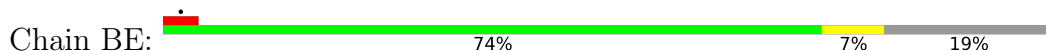
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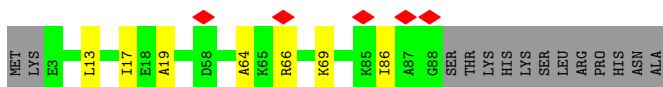
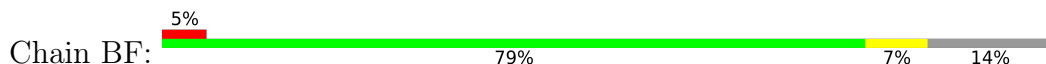
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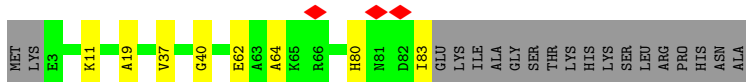
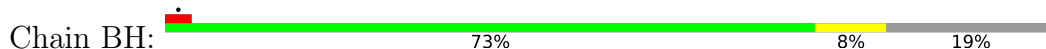
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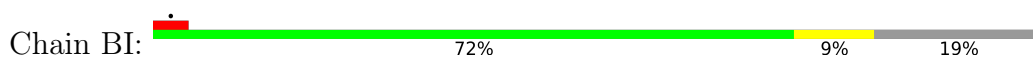
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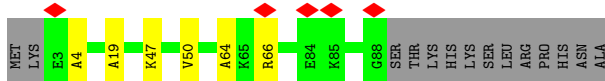
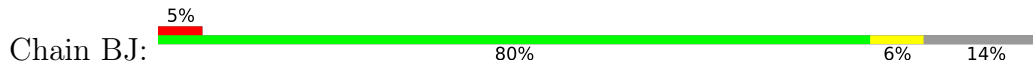
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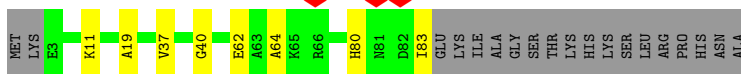
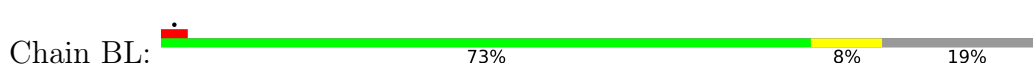
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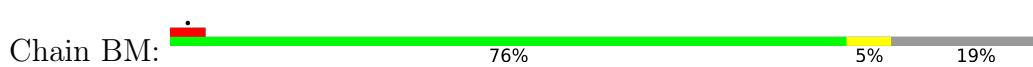
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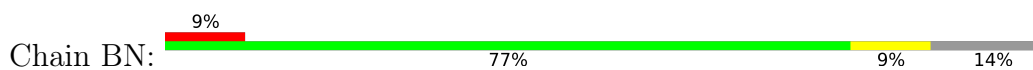
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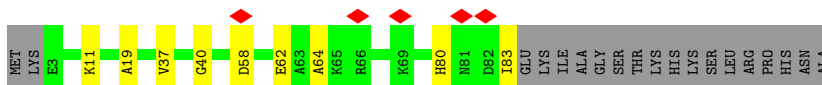
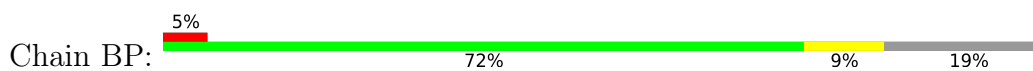
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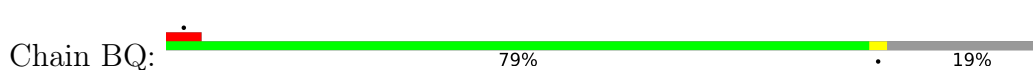
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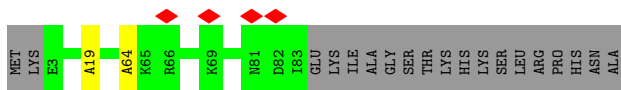


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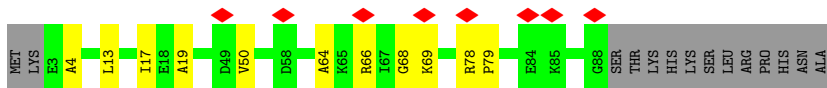
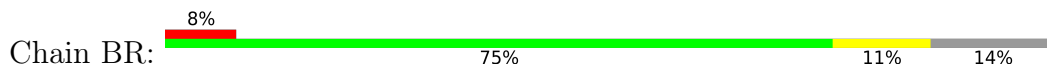


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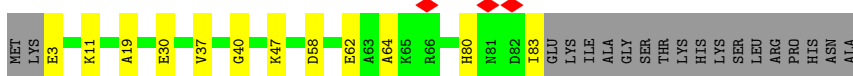




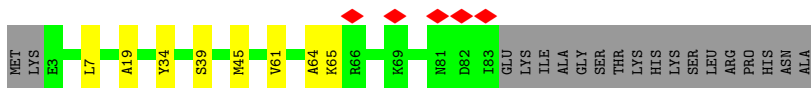
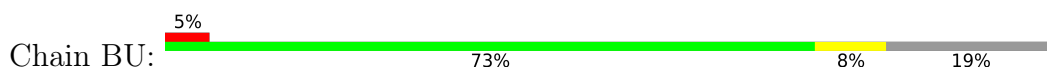
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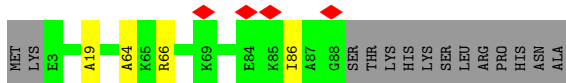
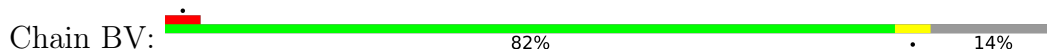
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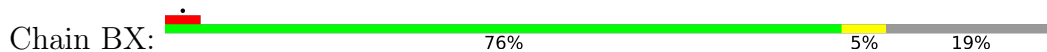
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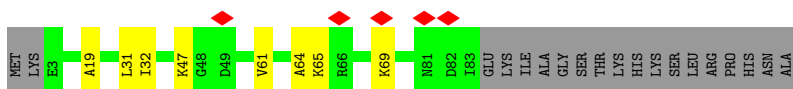
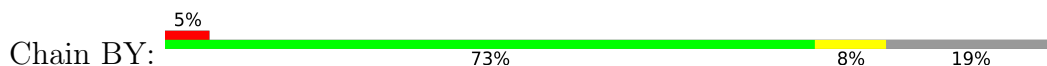
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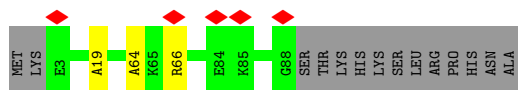
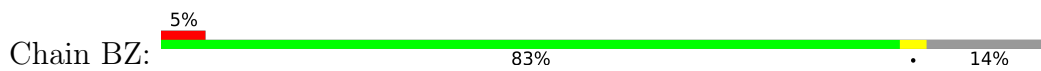
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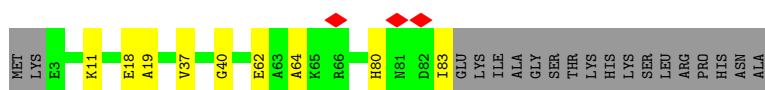
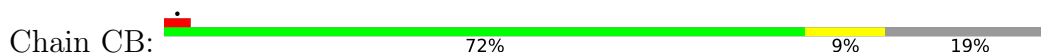
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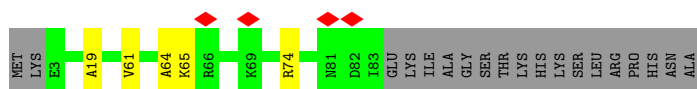
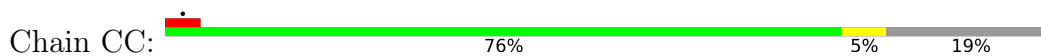
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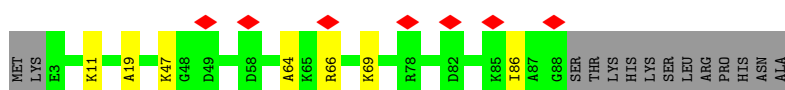
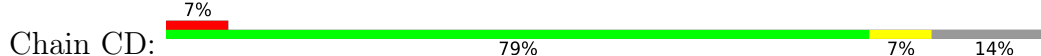
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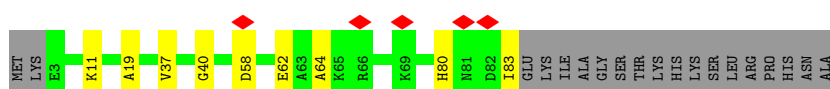
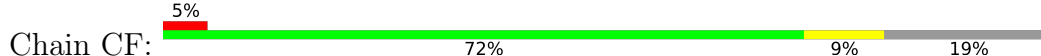
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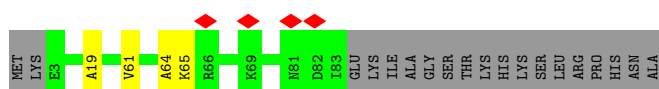
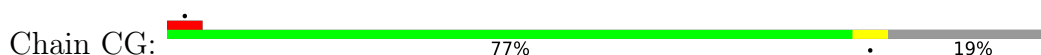
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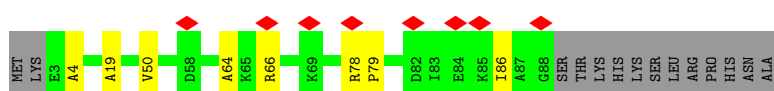
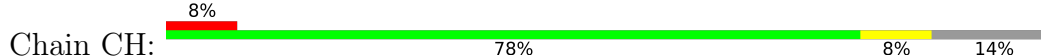
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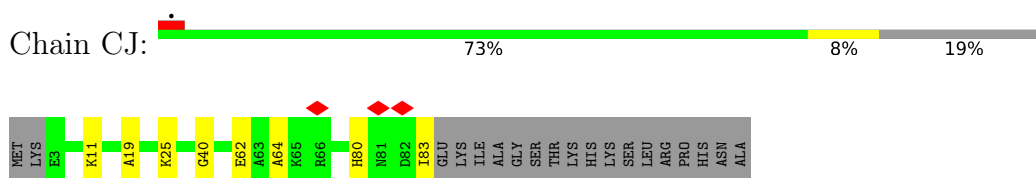
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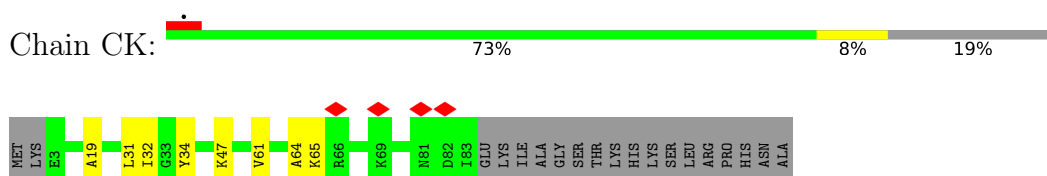
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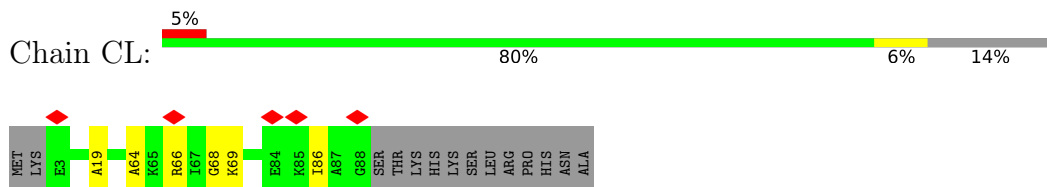
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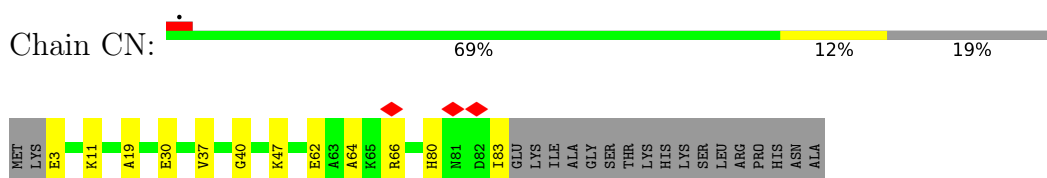
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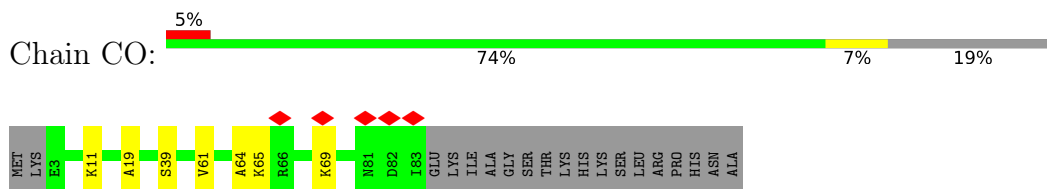
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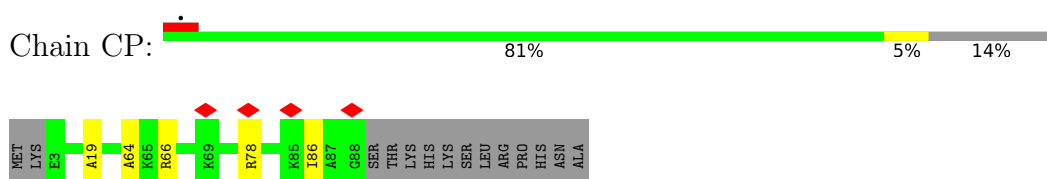
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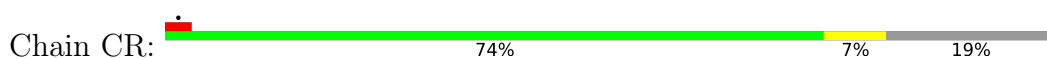
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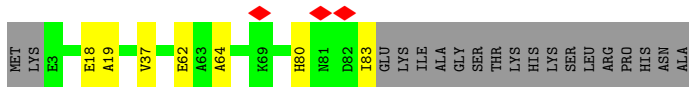


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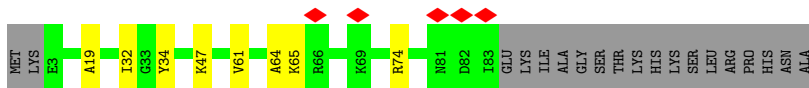
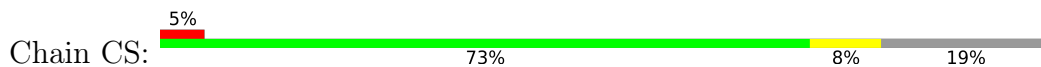


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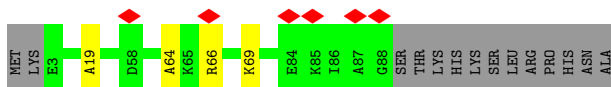
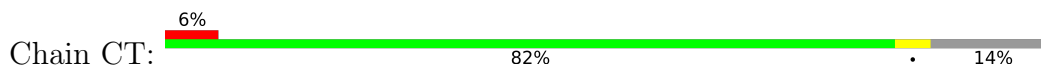




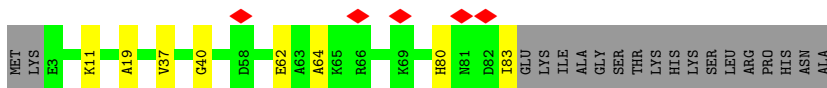
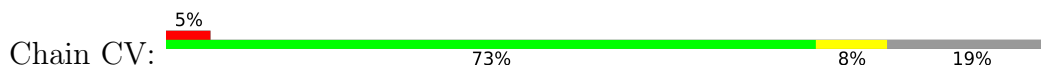
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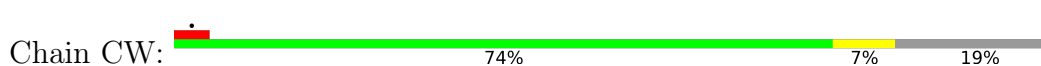
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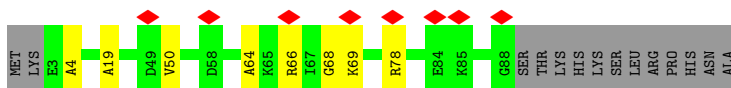
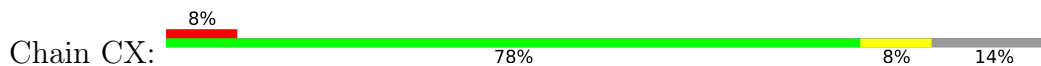
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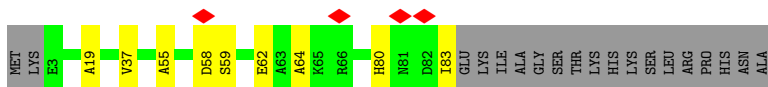
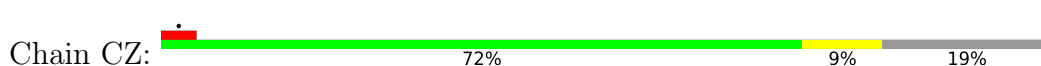
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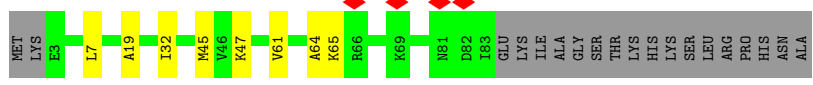
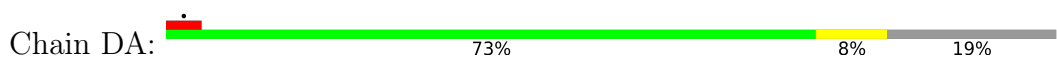
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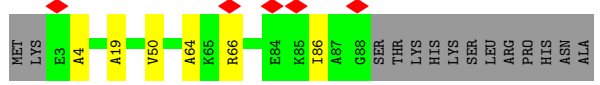
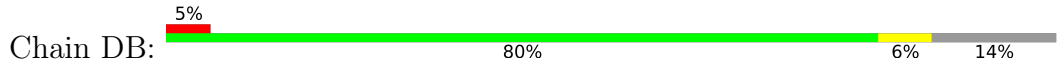
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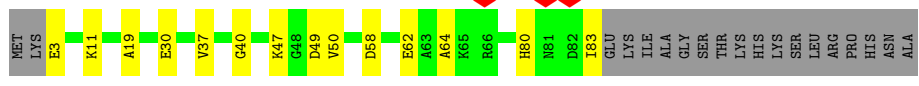
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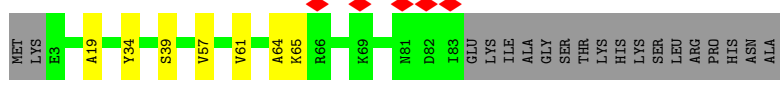
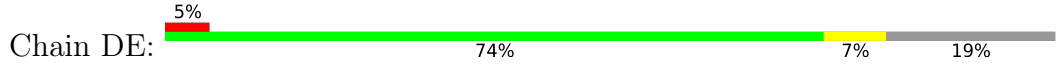
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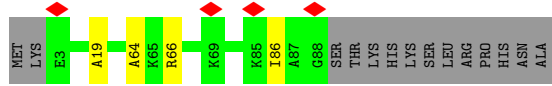
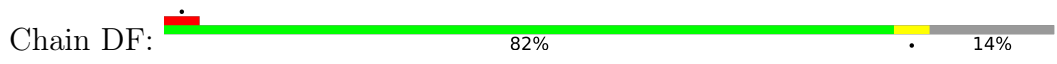
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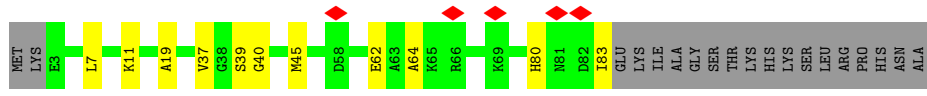
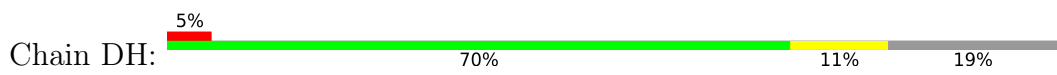
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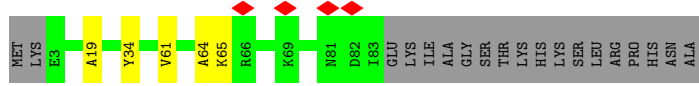
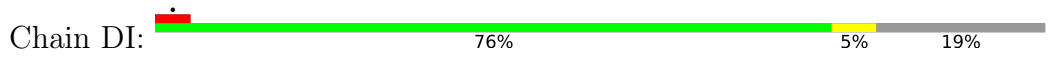
● Molecule 2: BMC domain-containing protein



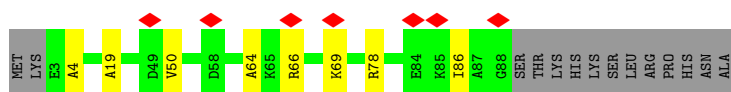
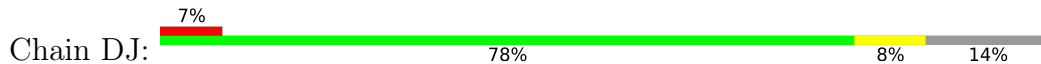
● Molecule 2: BMC domain-containing protein



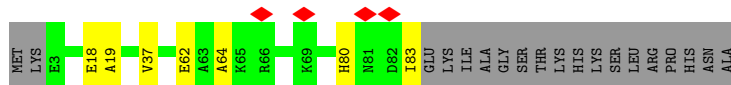
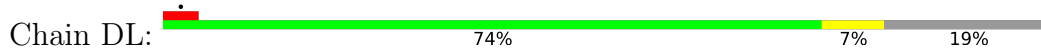
● Molecule 2: BMC domain-containing protein



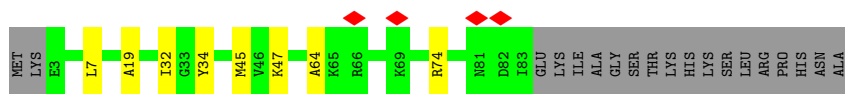
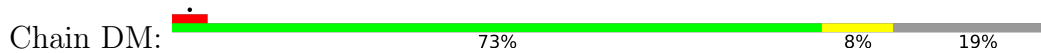
• Molecule 2: BMC domain-containing protein



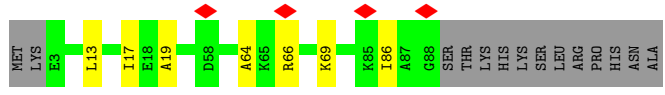
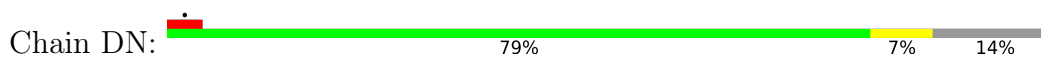
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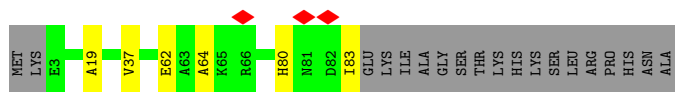
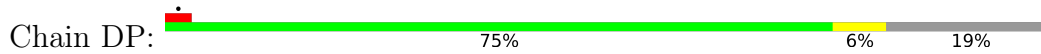
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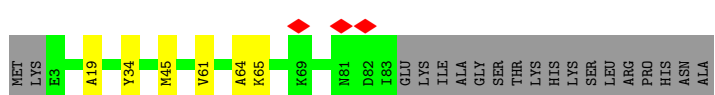
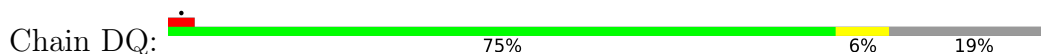
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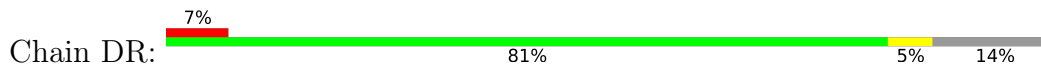
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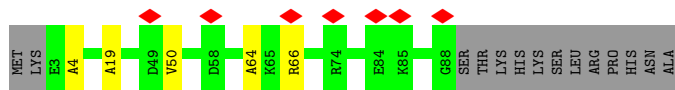


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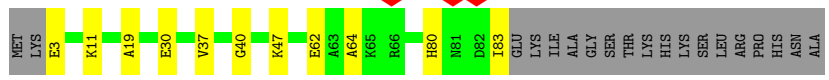


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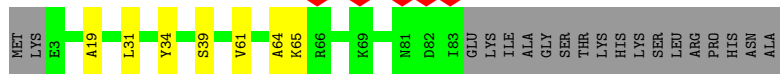
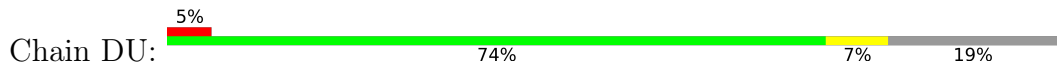




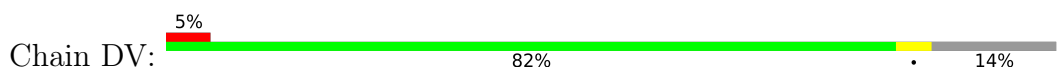
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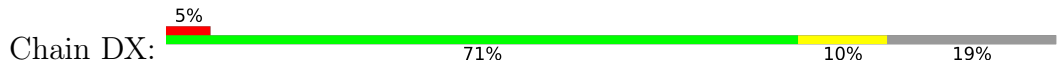
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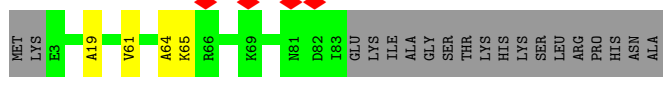
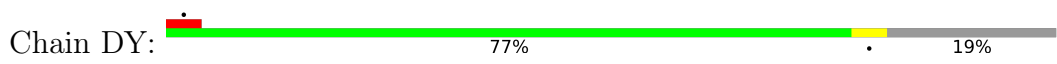
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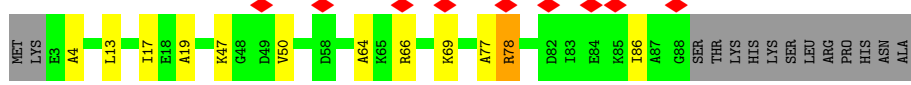
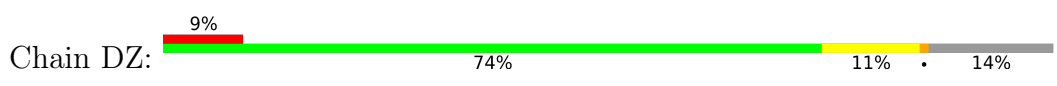
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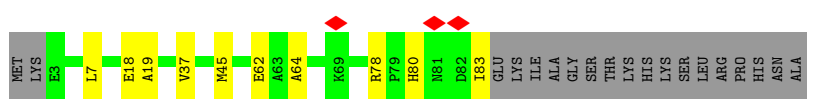
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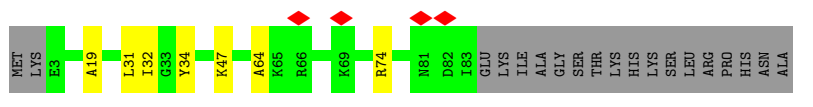
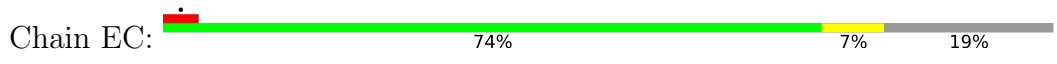
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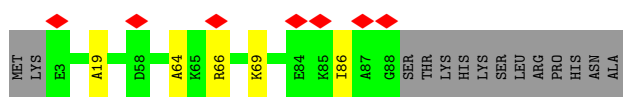
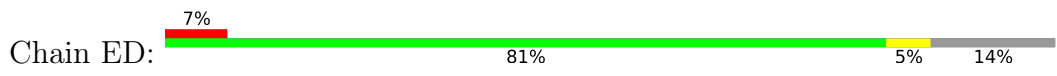
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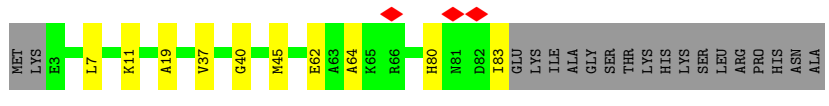
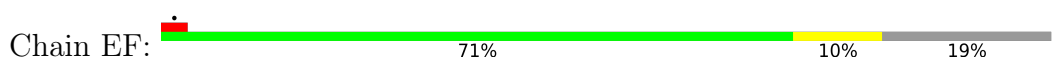
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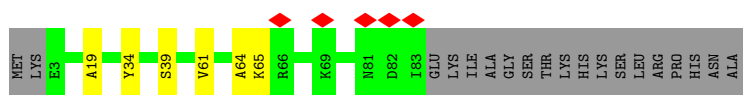
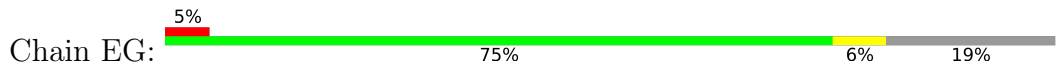
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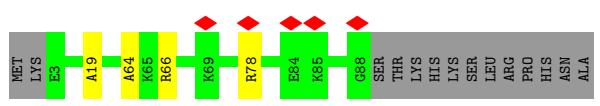
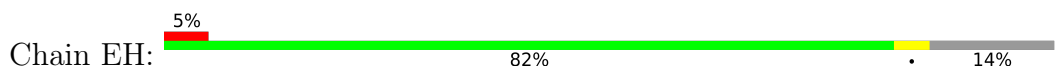
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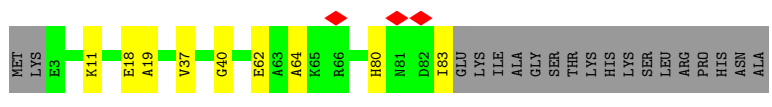
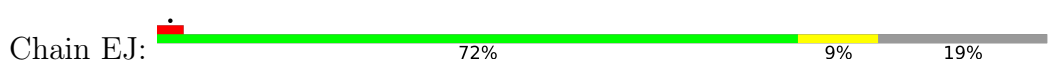
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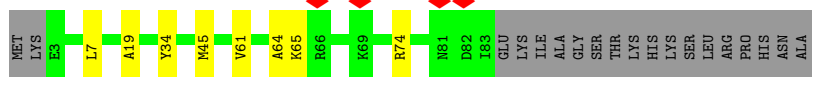
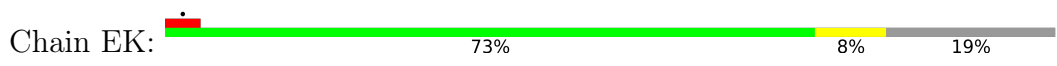
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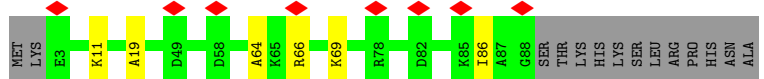
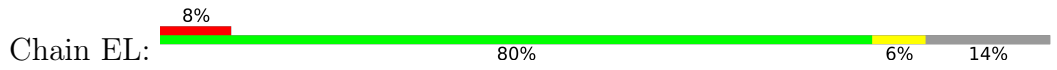
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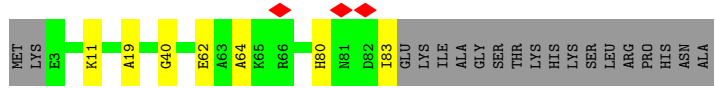
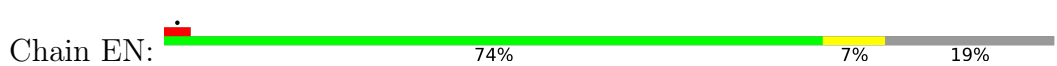
• Molecule 2: BMC domain-containing protein



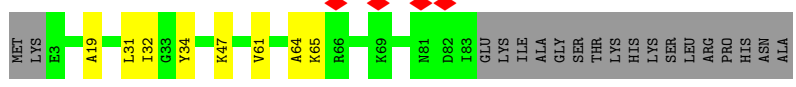
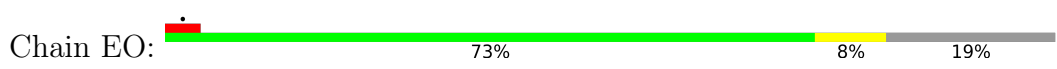
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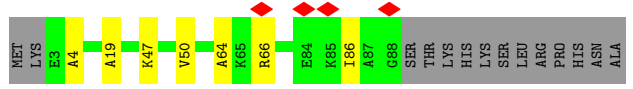
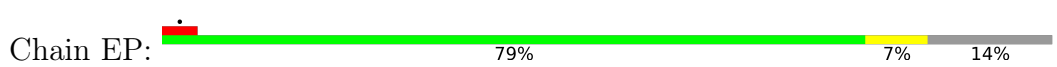
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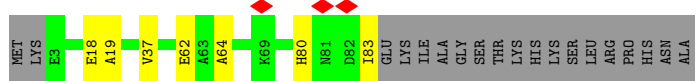
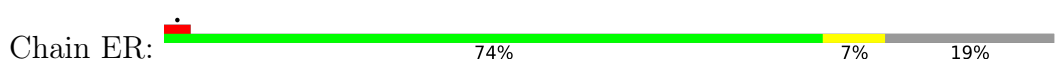
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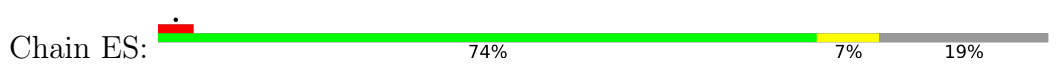
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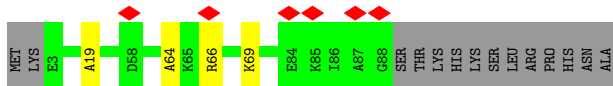
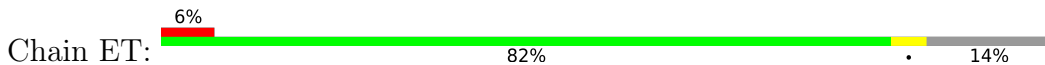


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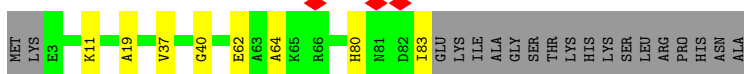
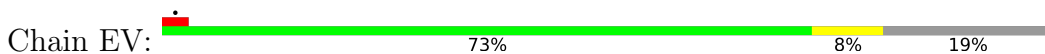




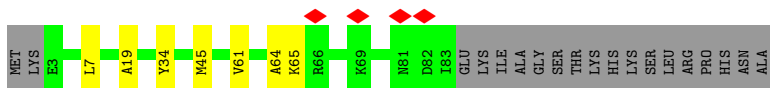
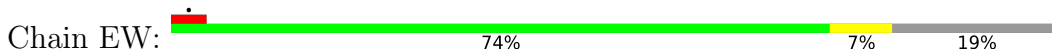
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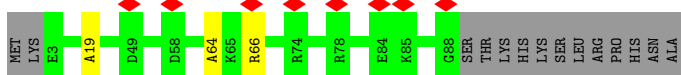
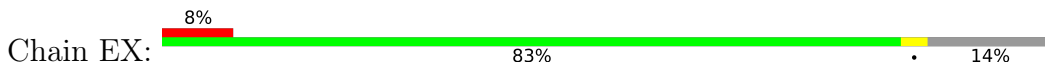
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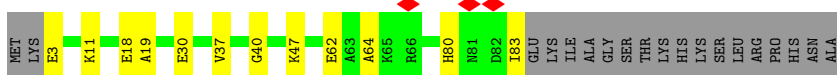
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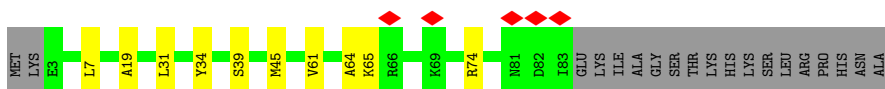
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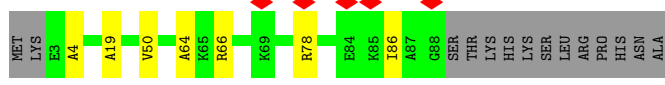
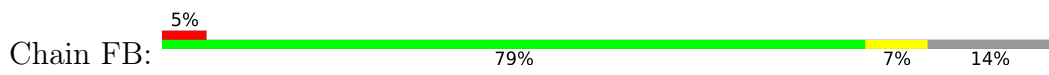
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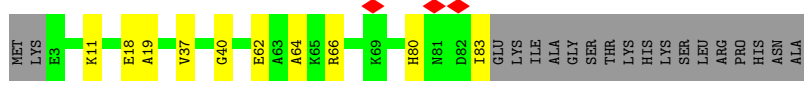
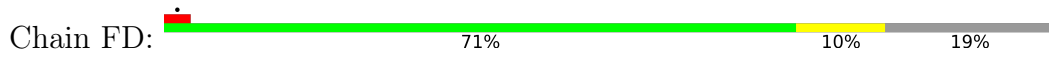
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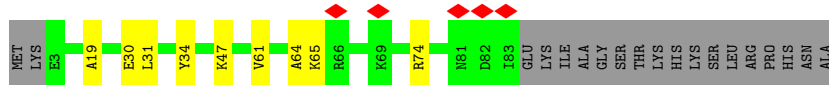
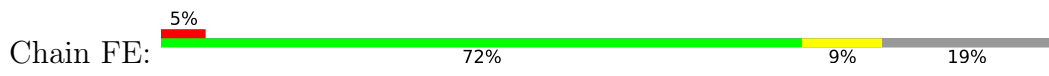
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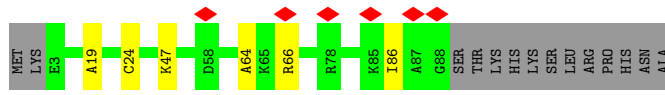
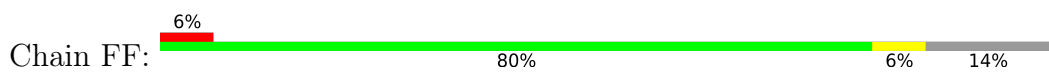
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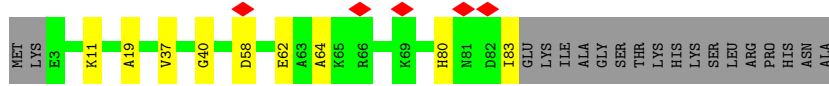
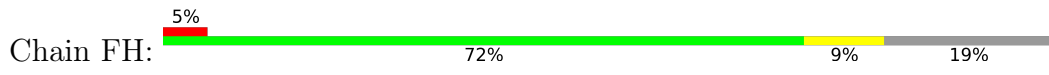
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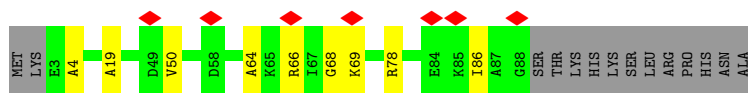
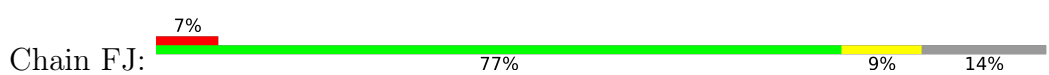
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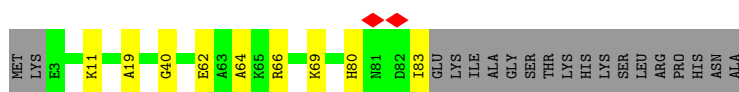
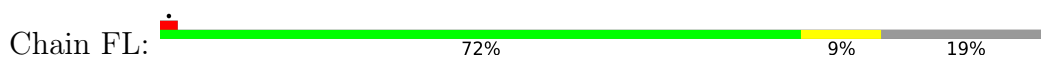
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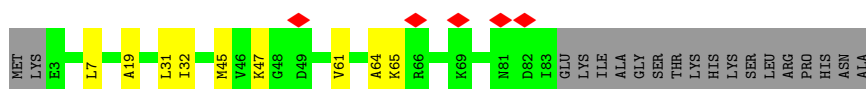
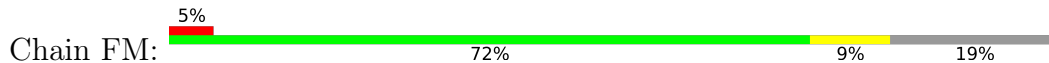
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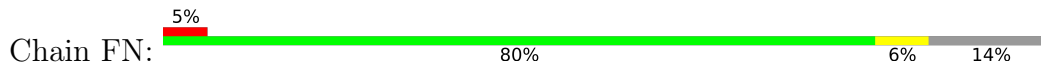
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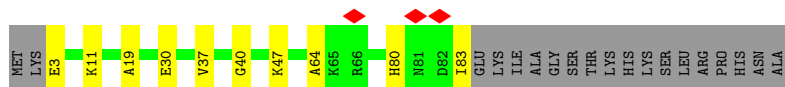
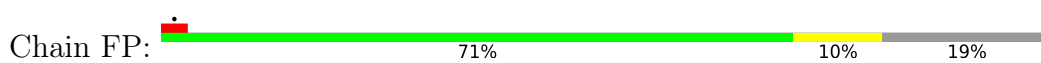
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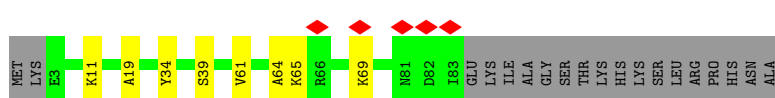
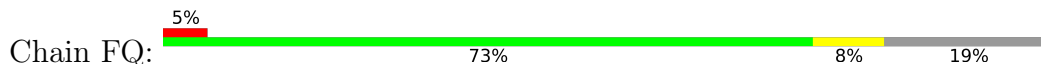
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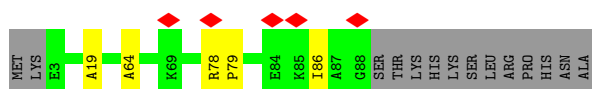
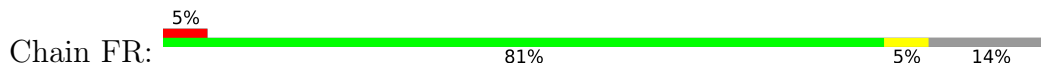
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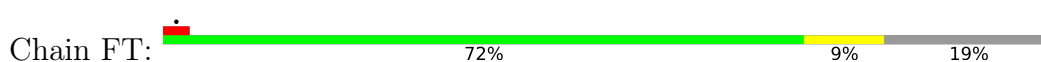
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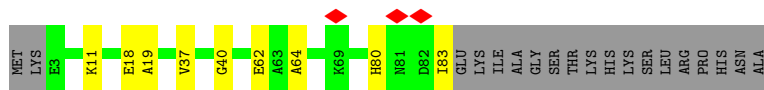


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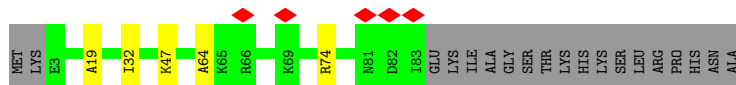
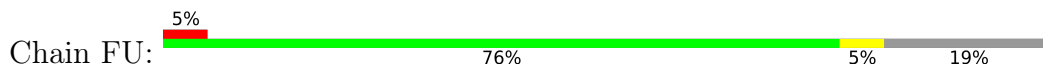


• Molecule 2: BMC domain-containing protein

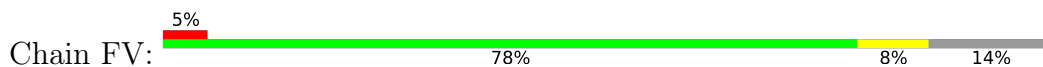




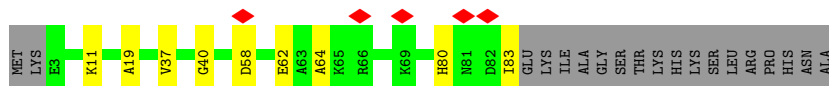
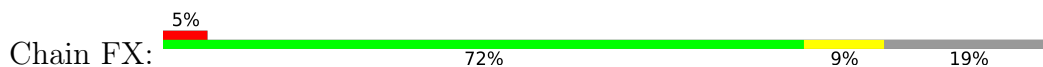
- Molecule 2: BMC domain-containing protein



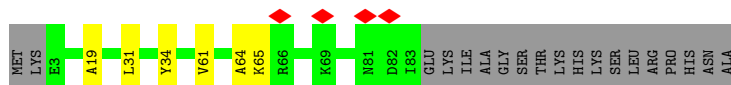
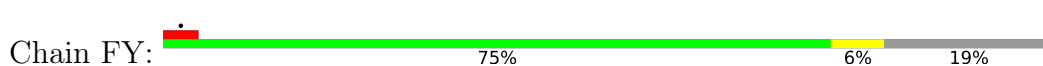
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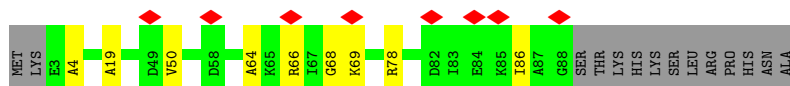
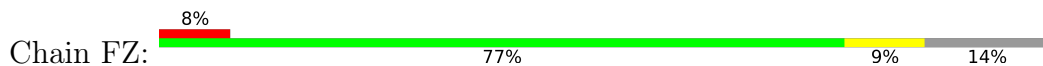
- Molecule 2: BMC domain-containing protein



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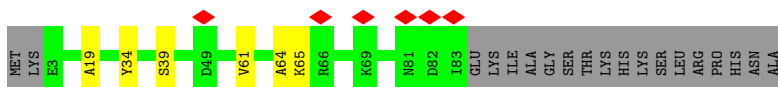
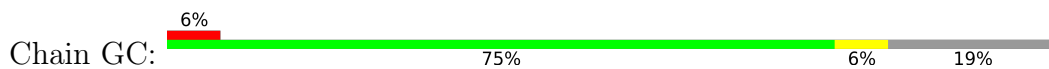
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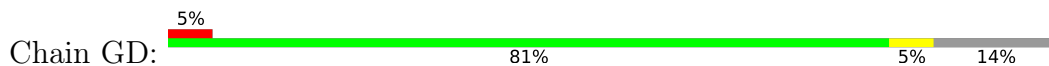
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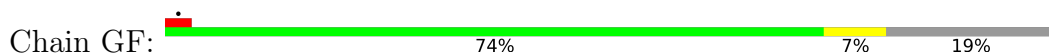
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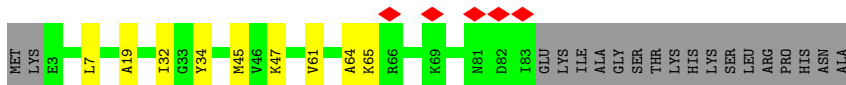
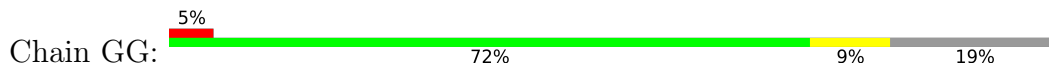
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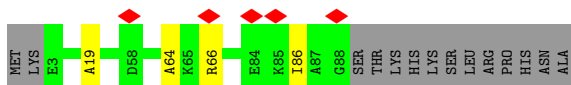
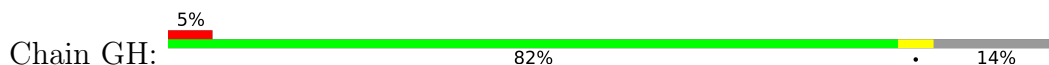
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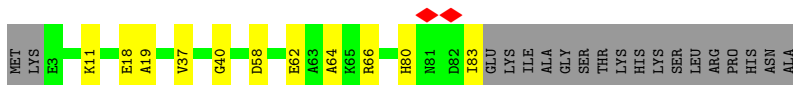
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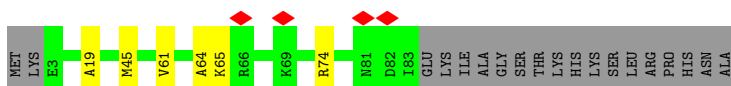
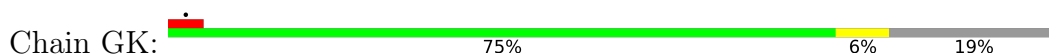
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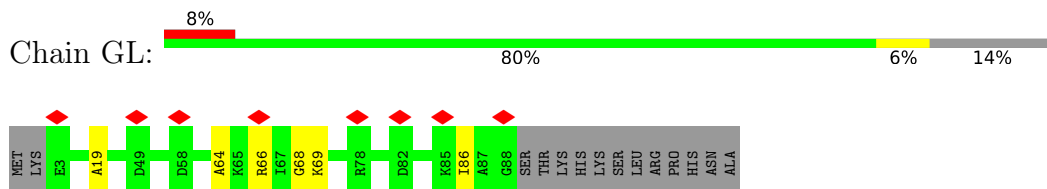
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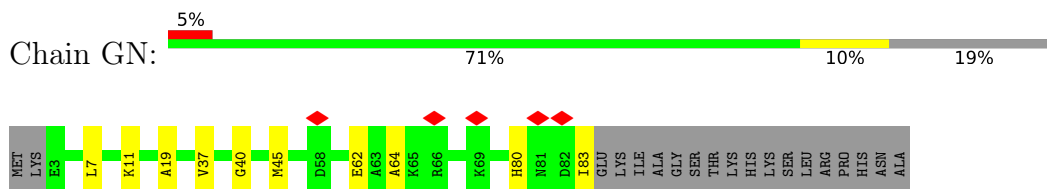
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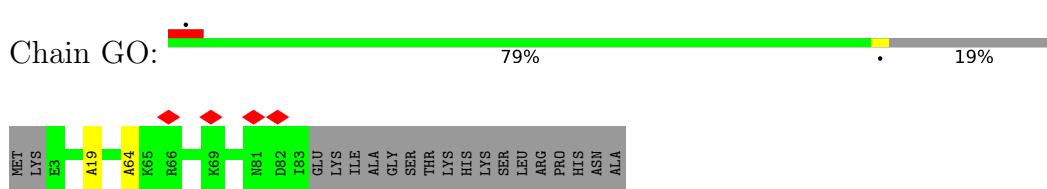
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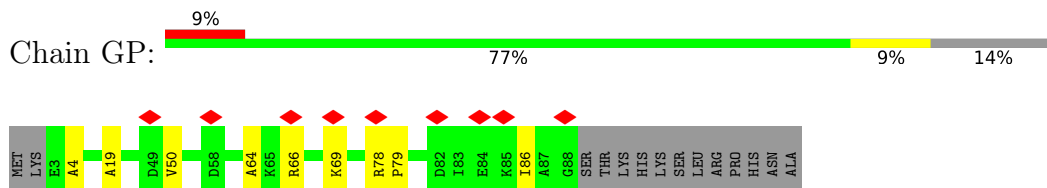
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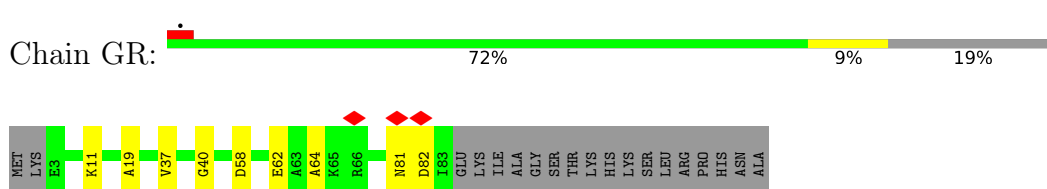
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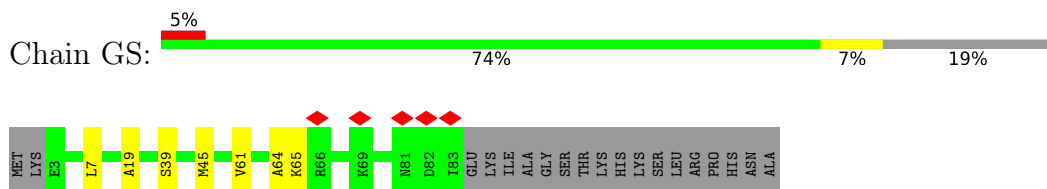
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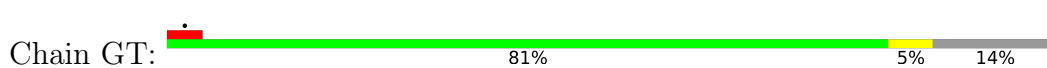
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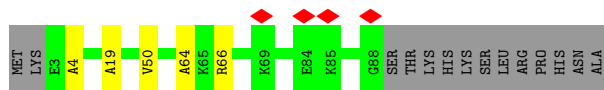


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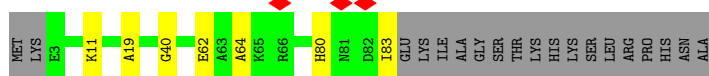
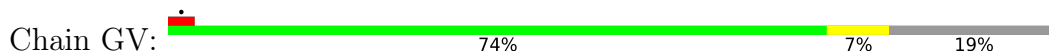


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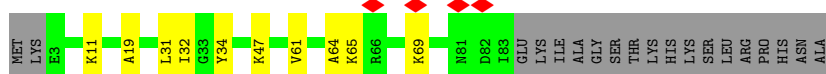
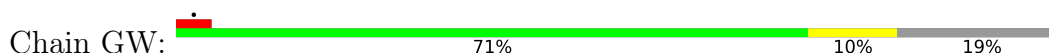




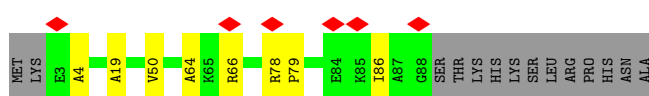
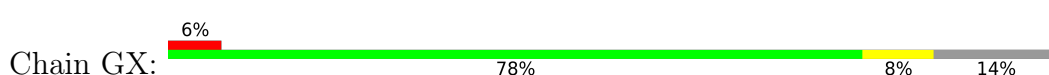
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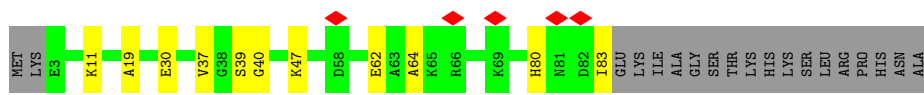
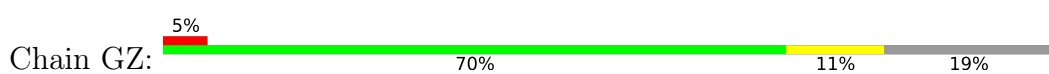
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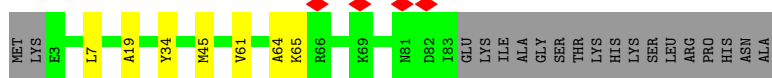
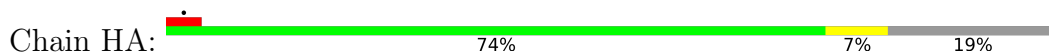
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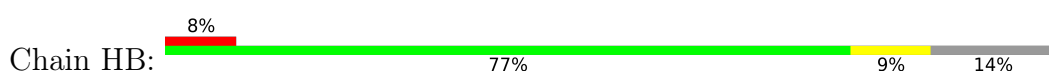
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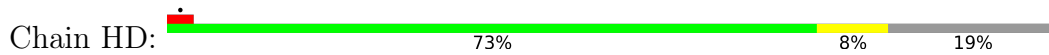
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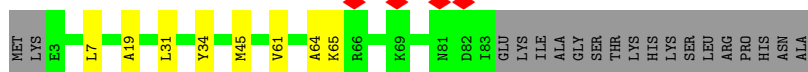
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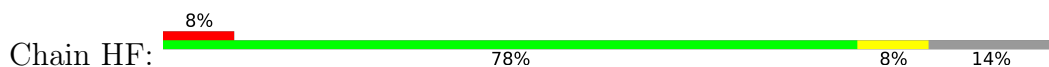
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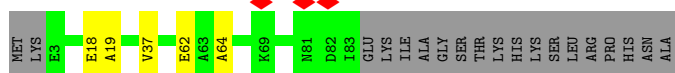
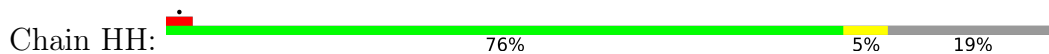
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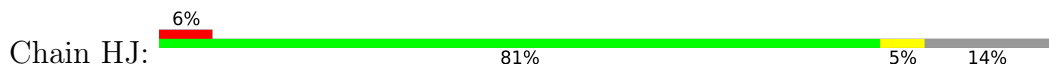
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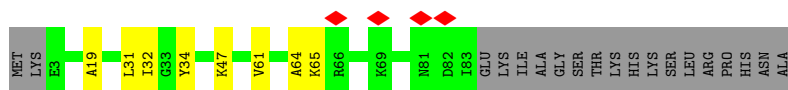
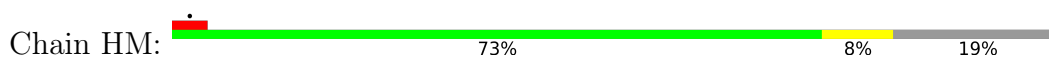
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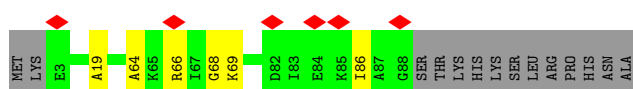
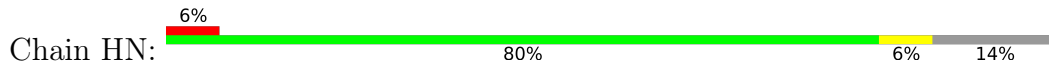
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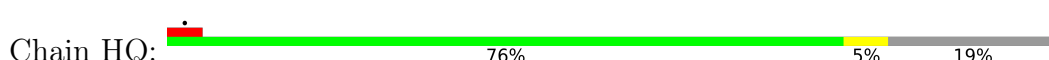
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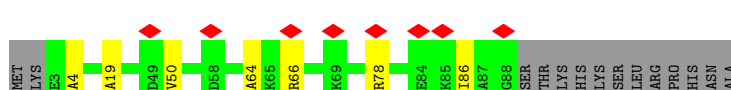
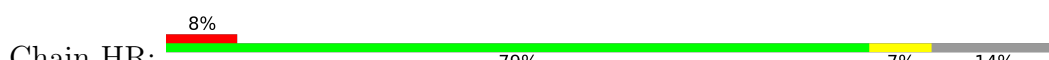
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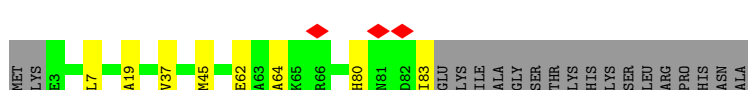
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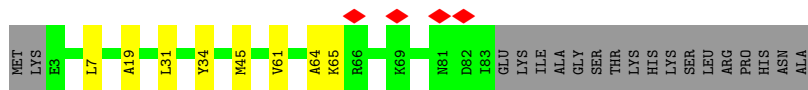


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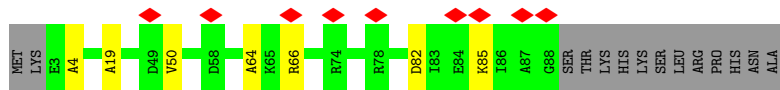
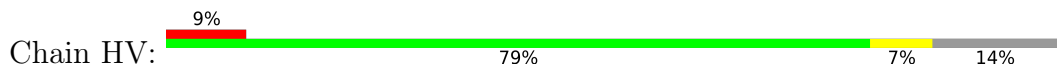


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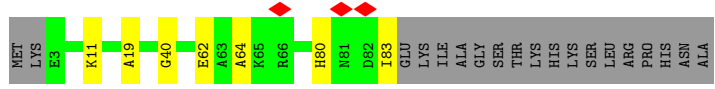
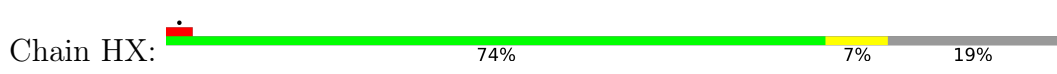




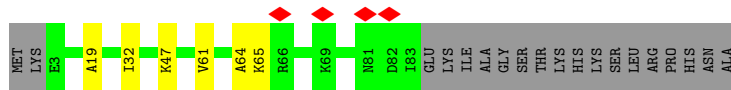
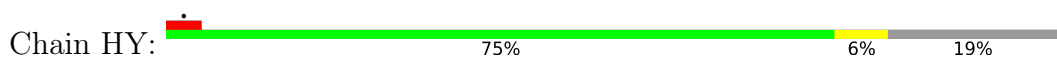
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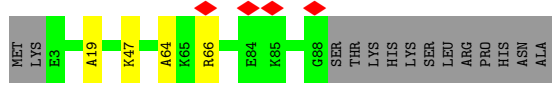
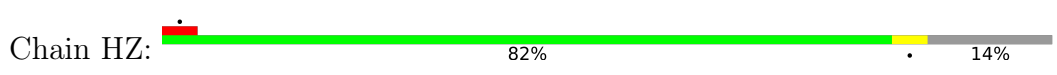
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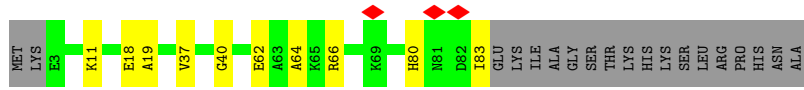
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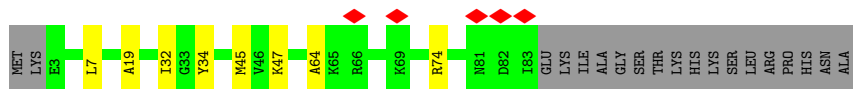
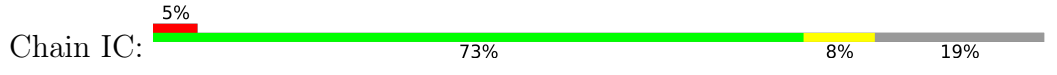
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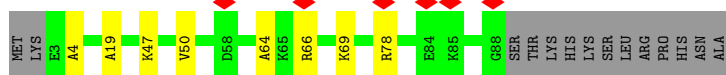
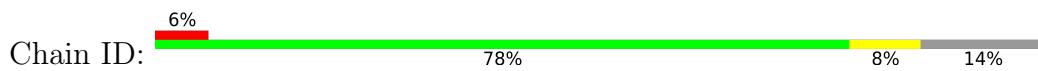
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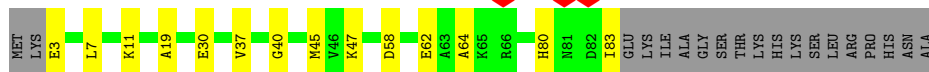
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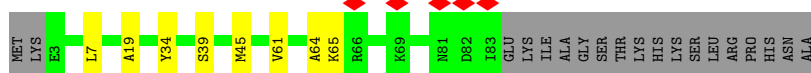
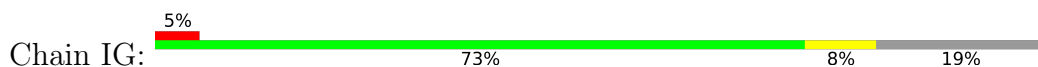
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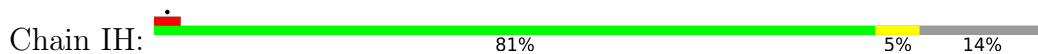
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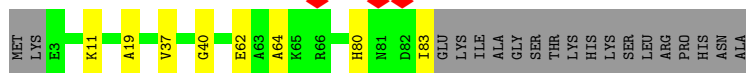
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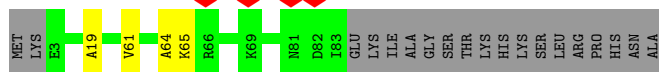
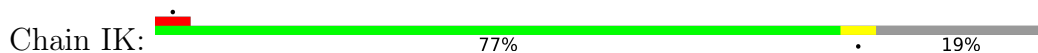
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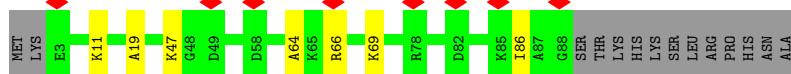
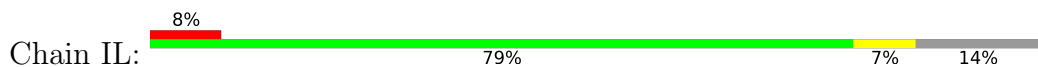
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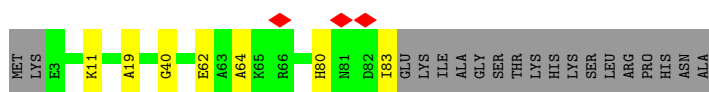
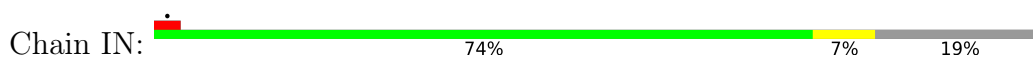
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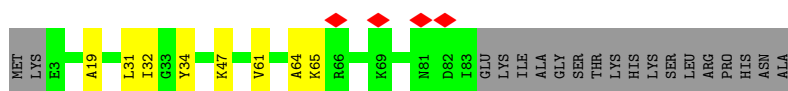
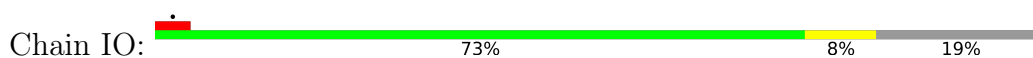
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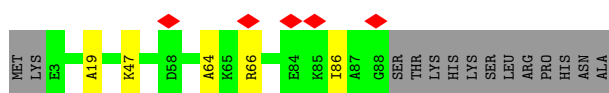
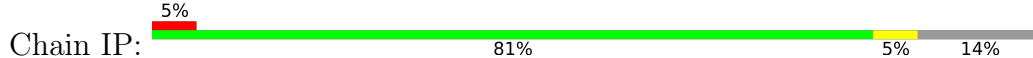
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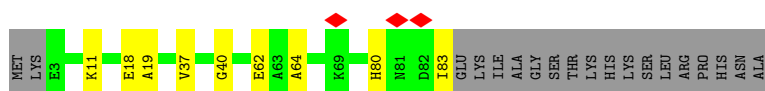
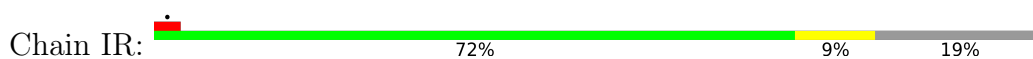
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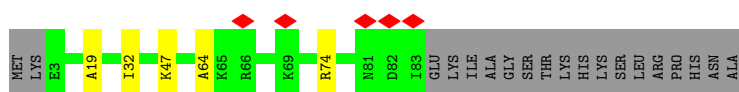
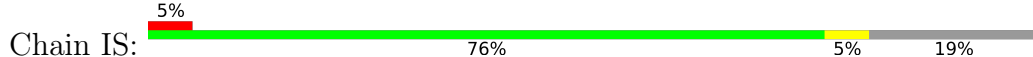
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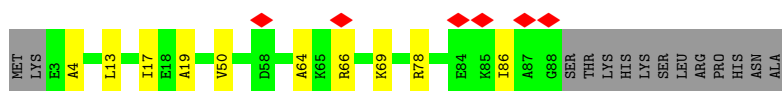
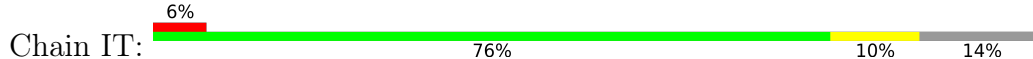
• Molecule 2: BMC domain-containing protein



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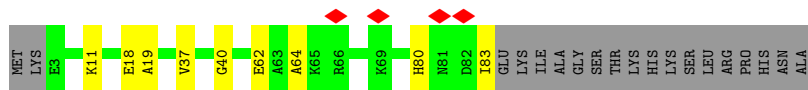


• Molecule 2: BMC domain-containing protein

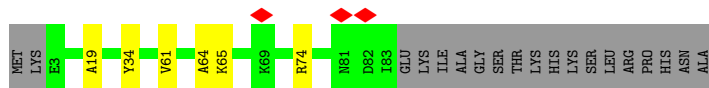
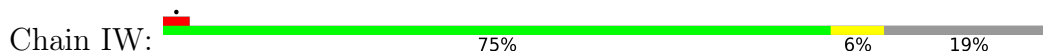


• Molecule 2: BMC domain-containing protein

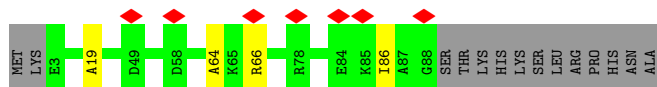
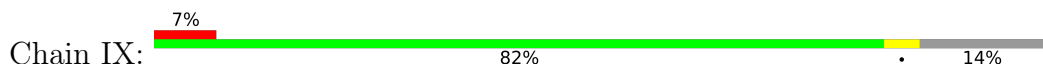




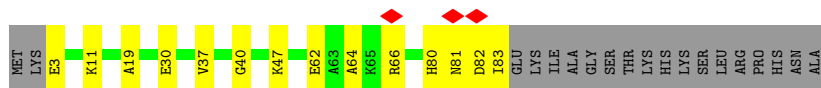
• Molecule 2: BMC domain-containing protein



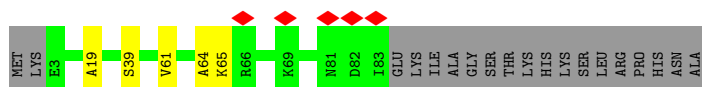
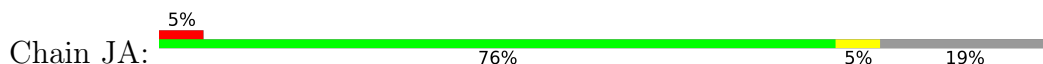
• Molecule 2: BMC domain-containing protein



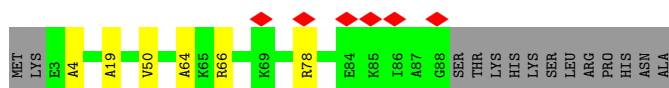
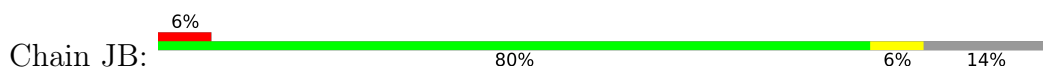
• Molecule 2: BMC domain-containing protein



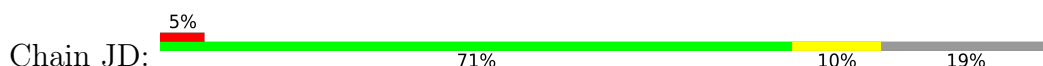
• Molecule 2: BMC domain-containing protein



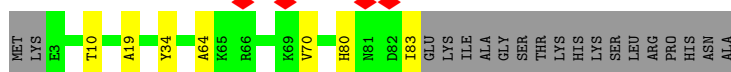
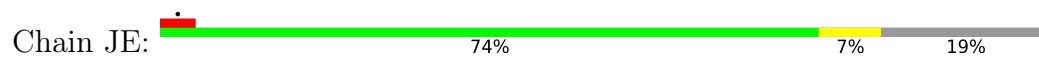
• Molecule 2: BMC domain-containing protein



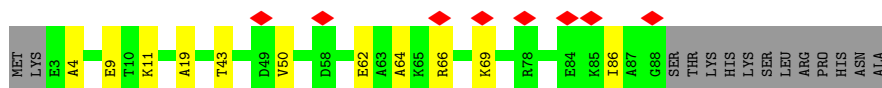
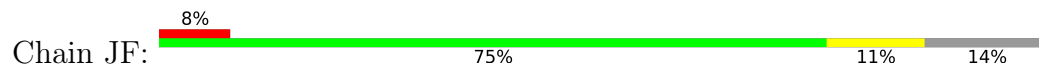
• Molecule 2: BMC domain-containing protein



• Molecule 2: BMC domain-containing protein



- Molecule 2: BMC domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	45915	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	-1400	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.281	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.0759	Depositor
Map size (Å)	393.6, 393.6, 393.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	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	AA	0.39	0/622	0.51	0/840
1	AE	0.39	0/622	0.51	0/840
1	AI	0.39	0/622	0.51	0/840
1	AM	0.39	0/622	0.51	0/840
1	AQ	0.39	0/622	0.51	0/840
1	AU	0.39	0/622	0.51	0/840
1	AY	0.39	0/622	0.51	0/840
1	BC	0.39	0/622	0.51	0/840
1	BG	0.39	0/622	0.51	0/840
1	BK	0.39	0/622	0.51	0/840
1	BO	0.39	0/622	0.51	0/840
1	BS	0.39	0/622	0.51	0/840
1	BW	0.39	0/622	0.51	0/840
1	CA	0.39	0/622	0.51	0/840
1	CE	0.39	0/622	0.51	0/840
1	CI	0.39	0/622	0.51	0/840
1	CM	0.39	0/622	0.51	0/840
1	CQ	0.39	0/622	0.51	0/840
1	CU	0.39	0/622	0.51	0/840
1	CY	0.39	0/622	0.51	0/840
1	DC	0.39	0/622	0.51	0/840
1	DG	0.39	0/622	0.51	0/840
1	DK	0.39	0/622	0.51	0/840
1	DO	0.39	0/622	0.51	0/840
1	DS	0.39	0/622	0.51	0/840
1	DW	0.39	0/622	0.51	0/840
1	EA	0.39	0/622	0.51	0/840
1	EE	0.39	0/622	0.51	0/840
1	EI	0.39	0/622	0.51	0/840
1	EM	0.39	0/622	0.51	0/840
1	EQ	0.39	0/622	0.51	0/840
1	EU	0.39	0/622	0.51	0/840
1	EY	0.39	0/622	0.51	0/840
1	FC	0.39	0/622	0.51	0/840

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	FG	0.39	0/622	0.51	0/840
1	FK	0.39	0/622	0.51	0/840
1	FO	0.39	0/622	0.51	0/840
1	FS	0.39	0/622	0.51	0/840
1	FW	0.39	0/622	0.51	0/840
1	GA	0.39	0/622	0.51	0/840
1	GE	0.39	0/622	0.51	0/840
1	GI	0.39	0/622	0.51	0/840
1	GM	0.39	0/622	0.51	0/840
1	GQ	0.39	0/622	0.51	0/840
1	GU	0.39	0/622	0.51	0/840
1	GY	0.39	0/622	0.51	0/840
1	HC	0.39	0/622	0.51	0/840
1	HG	0.39	0/622	0.51	0/840
1	HK	0.39	0/622	0.51	0/840
1	HO	0.39	0/622	0.51	0/840
1	HS	0.39	0/622	0.51	0/840
1	HW	0.39	0/622	0.51	0/840
1	IA	0.39	0/622	0.51	0/840
1	IE	0.39	0/622	0.51	0/840
1	II	0.39	0/622	0.51	0/840
1	IM	0.39	0/622	0.51	0/840
1	IQ	0.39	0/622	0.51	0/840
1	IU	0.39	0/622	0.51	0/840
1	IY	0.39	0/622	0.51	0/840
1	JC	0.39	0/622	0.51	0/840
2	AB	0.38	0/571	0.48	0/771
2	AC	0.37	0/571	0.49	0/771
2	AD	0.38	0/606	0.49	0/817
2	AF	0.39	0/571	0.50	0/771
2	AG	0.37	0/571	0.50	0/771
2	AH	0.38	0/606	0.49	0/817
2	AJ	0.37	0/571	0.48	0/771
2	AK	0.37	0/571	0.48	0/771
2	AL	0.37	0/606	0.48	0/817
2	AN	0.38	0/571	0.48	0/771
2	AO	0.37	0/571	0.49	0/771
2	AP	0.39	0/606	0.49	0/817
2	AR	0.40	0/571	0.53	1/771 (0.1%)
2	AS	0.37	0/571	0.50	0/771
2	AT	0.38	0/606	0.48	0/817
2	AV	0.37	0/571	0.48	0/771
2	AW	0.37	0/571	0.48	0/771

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	AX	0.37	0/606	0.49	0/817
2	AZ	0.37	0/571	0.48	0/771
2	BA	0.37	0/571	0.49	0/771
2	BB	0.38	0/606	0.49	0/817
2	BD	0.38	0/571	0.48	0/771
2	BE	0.37	0/571	0.49	0/771
2	BF	0.38	0/606	0.49	0/817
2	BH	0.37	0/571	0.49	0/771
2	BI	0.38	0/571	0.52	0/771
2	BJ	0.37	0/606	0.48	0/817
2	BL	0.37	0/571	0.49	0/771
2	BM	0.37	0/571	0.48	0/771
2	BN	0.36	0/606	0.50	0/817
2	BP	0.37	0/571	0.49	0/771
2	BQ	0.37	0/571	0.49	0/771
2	BR	0.37	0/606	0.49	0/817
2	BT	0.37	0/571	0.49	0/771
2	BU	0.37	0/571	0.49	0/771
2	BV	0.36	0/606	0.48	0/817
2	BX	0.37	0/571	0.47	0/771
2	BY	0.37	0/571	0.50	0/771
2	BZ	0.37	0/606	0.48	0/817
2	CB	0.37	0/571	0.48	0/771
2	CC	0.37	0/571	0.49	0/771
2	CD	0.36	0/606	0.48	0/817
2	CF	0.39	0/571	0.49	0/771
2	CG	0.37	0/571	0.50	0/771
2	CH	0.38	0/606	0.49	0/817
2	CJ	0.37	0/571	0.48	0/771
2	CK	0.38	0/571	0.51	0/771
2	CL	0.38	0/606	0.48	0/817
2	CN	0.39	0/571	0.49	0/771
2	CO	0.37	0/571	0.50	0/771
2	CP	0.38	0/606	0.49	0/817
2	CR	0.37	0/571	0.48	0/771
2	CS	0.37	0/571	0.49	0/771
2	CT	0.38	0/606	0.49	0/817
2	CV	0.38	0/571	0.49	0/771
2	CW	0.37	0/571	0.48	0/771
2	CX	0.38	0/606	0.49	0/817
2	CZ	0.38	0/571	0.52	0/771
2	DA	0.38	0/571	0.52	0/771
2	DB	0.38	0/606	0.48	0/817

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	DD	0.38	0/571	0.49	0/771
2	DE	0.38	0/571	0.51	0/771
2	DF	0.37	0/606	0.49	0/817
2	DH	0.37	0/571	0.49	0/771
2	DI	0.37	0/571	0.48	0/771
2	DJ	0.37	0/606	0.48	0/817
2	DL	0.37	0/571	0.48	0/771
2	DM	0.37	0/571	0.49	0/771
2	DN	0.37	0/606	0.49	0/817
2	DP	0.37	0/571	0.49	0/771
2	DQ	0.37	0/571	0.49	0/771
2	DR	0.37	0/606	0.49	0/817
2	DT	0.37	0/571	0.49	0/771
2	DU	0.37	0/571	0.50	0/771
2	DV	0.38	0/606	0.49	0/817
2	DX	0.37	0/571	0.48	0/771
2	DY	0.37	0/571	0.49	0/771
2	DZ	0.37	0/606	0.57	1/817 (0.1%)
2	EB	0.37	0/571	0.48	0/771
2	EC	0.37	0/571	0.50	0/771
2	ED	0.38	0/606	0.49	0/817
2	EF	0.37	0/571	0.48	0/771
2	EG	0.37	0/571	0.50	0/771
2	EH	0.37	0/606	0.48	0/817
2	EJ	0.38	0/571	0.48	0/771
2	EK	0.37	0/571	0.48	0/771
2	EL	0.36	0/606	0.48	0/817
2	EN	0.37	0/571	0.47	0/771
2	EO	0.37	0/571	0.50	0/771
2	EP	0.37	0/606	0.48	0/817
2	ER	0.38	0/571	0.48	0/771
2	ES	0.37	0/571	0.50	0/771
2	ET	0.38	0/606	0.49	0/817
2	EV	0.37	0/571	0.48	0/771
2	EW	0.37	0/571	0.48	0/771
2	EX	0.36	0/606	0.49	0/817
2	EZ	0.37	0/571	0.49	0/771
2	FA	0.37	0/571	0.49	0/771
2	FB	0.37	0/606	0.48	0/817
2	FD	0.38	0/571	0.48	0/771
2	FE	0.38	0/571	0.50	0/771
2	FF	0.40	0/606	0.49	0/817
2	FH	0.37	0/571	0.48	0/771

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	FI	0.38	0/571	0.49	0/771
2	FJ	0.37	0/606	0.49	0/817
2	FL	0.39	0/571	0.48	0/771
2	FM	0.38	0/571	0.52	0/771
2	FN	0.38	0/606	0.48	0/817
2	FP	0.37	0/571	0.49	0/771
2	FQ	0.37	0/571	0.50	0/771
2	FR	0.36	0/606	0.48	0/817
2	FT	0.38	0/571	0.48	0/771
2	FU	0.37	0/571	0.49	0/771
2	FV	0.38	0/606	0.49	0/817
2	FX	0.37	0/571	0.48	0/771
2	FY	0.37	0/571	0.49	0/771
2	FZ	0.37	0/606	0.49	0/817
2	GB	0.39	0/571	0.50	0/771
2	GC	0.37	0/571	0.50	0/771
2	GD	0.38	0/606	0.49	0/817
2	GF	0.37	0/571	0.48	0/771
2	GG	0.38	0/571	0.51	0/771
2	GH	0.38	0/606	0.48	0/817
2	GJ	0.37	0/571	0.48	0/771
2	GK	0.37	0/571	0.50	0/771
2	GL	0.36	0/606	0.49	0/817
2	GN	0.38	0/571	0.48	0/771
2	GO	0.38	0/571	0.50	0/771
2	GP	0.37	0/606	0.48	0/817
2	GR	0.37	0/571	0.48	0/771
2	GS	0.37	0/571	0.50	0/771
2	GT	0.37	0/606	0.48	0/817
2	GV	0.37	0/571	0.47	0/771
2	GW	0.37	0/571	0.49	0/771
2	GX	0.37	0/606	0.48	0/817
2	GZ	0.38	0/571	0.49	0/771
2	HA	0.37	0/571	0.49	0/771
2	HB	0.37	0/606	0.49	0/817
2	HD	0.37	0/571	0.48	0/771
2	HE	0.37	0/571	0.49	0/771
2	HF	0.36	0/606	0.49	0/817
2	HH	0.38	0/571	0.48	0/771
2	HI	0.37	0/571	0.49	0/771
2	HJ	0.38	0/606	0.50	0/817
2	HL	0.39	0/571	0.48	0/771
2	HM	0.37	0/571	0.50	0/771

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	HN	0.38	0/606	0.49	0/817
2	HP	0.37	0/571	0.48	0/771
2	HQ	0.37	0/571	0.49	0/771
2	HR	0.37	0/606	0.48	0/817
2	HT	0.37	0/571	0.48	0/771
2	HU	0.37	0/571	0.49	0/771
2	HV	0.35	0/606	0.49	0/817
2	HX	0.37	0/571	0.48	0/771
2	HY	0.37	0/571	0.49	0/771
2	HZ	0.38	0/606	0.48	0/817
2	IB	0.38	0/571	0.48	0/771
2	IC	0.37	0/571	0.49	0/771
2	ID	0.39	0/606	0.49	0/817
2	IF	0.37	0/571	0.49	0/771
2	IG	0.37	0/571	0.50	0/771
2	IH	0.36	0/606	0.48	0/817
2	IJ	0.37	0/571	0.49	0/771
2	IK	0.37	0/571	0.48	0/771
2	IL	0.36	0/606	0.48	0/817
2	IN	0.37	0/571	0.48	0/771
2	IO	0.37	0/571	0.50	0/771
2	IP	0.37	0/606	0.47	0/817
2	IR	0.38	0/571	0.49	0/771
2	IS	0.37	0/571	0.49	0/771
2	IT	0.38	0/606	0.49	0/817
2	IV	0.37	0/571	0.48	0/771
2	IW	0.37	0/571	0.47	0/771
2	IX	0.36	0/606	0.48	0/817
2	IZ	0.37	0/571	0.49	0/771
2	JA	0.37	0/571	0.50	0/771
2	JB	0.37	0/606	0.49	0/817
2	JD	0.42	0/571	0.51	0/771
2	JE	0.40	0/571	0.57	0/771
2	JF	0.43	0/606	0.54	0/817
All	All	0.38	0/142200	0.50	2/191940 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DZ	78	ARG	NE-CZ-NH1	-7.09	116.76	120.30
2	AR	7	LEU	CB-CG-CD2	-5.83	101.09	111.00

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	AA	616	0	618	6	0
1	AE	616	0	618	4	0
1	AI	616	0	618	8	0
1	AM	616	0	618	7	0
1	AQ	616	0	618	7	0
1	AU	616	0	618	4	0
1	AY	616	0	618	3	0
1	BC	616	0	618	5	0
1	BG	616	0	618	5	0
1	BK	616	0	618	6	0
1	BO	616	0	618	8	0
1	BS	616	0	618	6	0
1	BW	616	0	618	4	0
1	CA	616	0	618	6	0
1	CE	616	0	618	5	0
1	CI	616	0	618	5	0
1	CM	616	0	618	8	0
1	CQ	616	0	618	5	0
1	CU	616	0	618	5	0
1	CY	616	0	618	6	0
1	DC	616	0	618	5	0
1	DG	616	0	618	4	0
1	DK	616	0	618	5	0
1	DO	616	0	618	7	0
1	DS	616	0	618	8	0
1	DW	616	0	618	6	0
1	EA	616	0	618	5	0
1	EE	616	0	618	8	0
1	EI	616	0	618	5	0
1	EM	616	0	618	5	0
1	EQ	616	0	618	8	0
1	EU	616	0	618	5	0
1	EY	616	0	618	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FC	616	0	618	5	0
1	FG	616	0	618	11	0
1	FK	616	0	618	8	0
1	FO	616	0	618	5	0
1	FS	616	0	618	2	0
1	FW	616	0	618	5	0
1	GA	616	0	618	8	0
1	GE	616	0	618	5	0
1	GI	616	0	618	8	0
1	GM	616	0	618	5	0
1	GQ	616	0	618	9	0
1	GU	616	0	618	6	0
1	GY	616	0	618	4	0
1	HC	616	0	618	5	0
1	HG	616	0	618	6	0
1	HK	616	0	618	5	0
1	HO	616	0	618	5	0
1	HS	616	0	618	5	0
1	HW	616	0	618	6	0
1	IA	616	0	618	3	0
1	IE	616	0	618	5	0
1	II	616	0	618	5	0
1	IM	616	0	618	6	0
1	IQ	616	0	618	5	0
1	IU	616	0	618	5	0
1	IY	616	0	618	6	0
1	JC	616	0	618	6	0
2	AB	569	0	590	8	0
2	AC	569	0	590	5	0
2	AD	604	0	628	8	0
2	AF	569	0	590	11	0
2	AG	569	0	590	5	0
2	AH	604	0	628	8	0
2	AJ	569	0	590	7	0
2	AK	569	0	590	4	0
2	AL	604	0	628	5	0
2	AN	569	0	590	6	0
2	AO	569	0	590	5	0
2	AP	604	0	628	7	0
2	AR	569	0	590	7	0
2	AS	569	0	590	3	0
2	AT	604	0	628	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AV	569	0	590	8	0
2	AW	569	0	590	3	0
2	AX	604	0	628	8	0
2	AZ	569	0	590	6	0
2	BA	569	0	590	2	0
2	BB	604	0	628	7	0
2	BD	569	0	590	4	0
2	BE	569	0	590	5	0
2	BF	604	0	628	7	0
2	BH	569	0	590	6	0
2	BI	569	0	590	5	0
2	BJ	604	0	628	4	0
2	BL	569	0	590	6	0
2	BM	569	0	590	3	0
2	BN	604	0	628	5	0
2	BP	569	0	590	8	0
2	BQ	569	0	590	1	0
2	BR	604	0	628	6	0
2	BT	569	0	590	10	0
2	BU	569	0	590	5	0
2	BV	604	0	628	4	0
2	BX	569	0	590	3	0
2	BY	569	0	590	5	0
2	BZ	604	0	628	2	0
2	CB	569	0	590	8	0
2	CC	569	0	590	3	0
2	CD	604	0	628	6	0
2	CF	569	0	590	6	0
2	CG	569	0	590	2	0
2	CH	604	0	628	5	0
2	CJ	569	0	590	6	0
2	CK	569	0	590	6	0
2	CL	604	0	628	5	0
2	CN	569	0	590	10	0
2	CO	569	0	590	4	0
2	CP	604	0	628	5	0
2	CR	569	0	590	5	0
2	CS	569	0	590	5	0
2	CT	604	0	628	4	0
2	CV	569	0	590	7	0
2	CW	569	0	590	4	0
2	CX	604	0	628	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CZ	569	0	590	6	0
2	DA	569	0	590	4	0
2	DB	604	0	628	4	0
2	DD	569	0	590	11	0
2	DE	569	0	590	5	0
2	DF	604	0	628	5	0
2	DH	569	0	590	8	0
2	DI	569	0	590	3	0
2	DJ	604	0	628	6	0
2	DL	569	0	590	6	0
2	DM	569	0	590	5	0
2	DN	604	0	628	6	0
2	DP	569	0	590	5	0
2	DQ	569	0	590	4	0
2	DR	604	0	628	3	0
2	DT	569	0	590	9	0
2	DU	569	0	590	5	0
2	DV	604	0	628	5	0
2	DX	569	0	590	8	0
2	DY	569	0	590	2	0
2	DZ	604	0	628	11	0
2	EB	569	0	590	8	0
2	EC	569	0	590	5	0
2	ED	604	0	628	5	0
2	EF	569	0	590	8	0
2	EG	569	0	590	4	0
2	EH	604	0	628	3	0
2	EJ	569	0	590	8	0
2	EK	569	0	590	5	0
2	EL	604	0	628	4	0
2	EN	569	0	590	6	0
2	EO	569	0	590	6	0
2	EP	604	0	628	5	0
2	ER	569	0	590	6	0
2	ES	569	0	590	4	0
2	ET	604	0	628	4	0
2	EV	569	0	590	6	0
2	EW	569	0	590	4	0
2	EX	604	0	628	2	0
2	EZ	569	0	590	10	0
2	FA	569	0	590	7	0
2	FB	604	0	628	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	FD	569	0	590	8	0
2	FE	569	0	590	6	0
2	FF	604	0	628	8	0
2	FH	569	0	590	11	0
2	FI	569	0	590	5	0
2	FJ	604	0	628	7	0
2	FL	569	0	590	8	0
2	FM	569	0	590	5	0
2	FN	604	0	628	5	0
2	FP	569	0	590	8	0
2	FQ	569	0	590	5	0
2	FR	604	0	628	3	0
2	FT	569	0	590	7	0
2	FU	569	0	590	3	0
2	FV	604	0	628	6	0
2	FX	569	0	590	7	0
2	FY	569	0	590	4	0
2	FZ	604	0	628	7	0
2	GB	569	0	590	11	0
2	GC	569	0	590	4	0
2	GD	604	0	628	5	0
2	GF	569	0	590	6	0
2	GG	569	0	590	5	0
2	GH	604	0	628	4	0
2	GJ	569	0	590	10	0
2	GK	569	0	590	4	0
2	GL	604	0	628	6	0
2	GN	569	0	590	6	0
2	GO	569	0	590	1	0
2	GP	604	0	628	7	0
2	GR	569	0	590	7	0
2	GS	569	0	590	4	0
2	GT	604	0	628	3	0
2	GV	569	0	590	6	0
2	GW	569	0	590	6	0
2	GX	604	0	628	5	0
2	GZ	569	0	590	7	0
2	HA	569	0	590	4	0
2	HB	604	0	628	6	0
2	HD	569	0	590	6	0
2	HE	569	0	590	5	0
2	HF	604	0	628	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	HH	569	0	590	4	0
2	HI	569	0	590	4	0
2	HJ	604	0	628	5	0
2	HL	569	0	590	7	0
2	HM	569	0	590	6	0
2	HN	604	0	628	6	0
2	HP	569	0	590	9	0
2	HQ	569	0	590	3	0
2	HR	604	0	628	7	0
2	HT	569	0	590	6	0
2	HU	569	0	590	5	0
2	HV	604	0	628	4	0
2	HX	569	0	590	6	0
2	HY	569	0	590	3	0
2	HZ	604	0	628	3	0
2	IB	569	0	590	8	0
2	IC	569	0	590	5	0
2	ID	604	0	628	8	0
2	IF	569	0	590	11	0
2	IG	569	0	590	5	0
2	IH	604	0	628	7	0
2	IJ	569	0	590	6	0
2	IK	569	0	590	2	0
2	IL	604	0	628	5	0
2	IN	569	0	590	6	0
2	IO	569	0	590	7	0
2	IP	604	0	628	4	0
2	IR	569	0	590	7	0
2	IS	569	0	590	3	0
2	IT	604	0	628	8	0
2	IV	569	0	590	7	0
2	IW	569	0	590	4	0
2	IX	604	0	628	3	0
2	IZ	569	0	590	10	0
2	JA	569	0	590	3	0
2	JB	604	0	628	5	0
2	JD	569	0	590	10	0
2	JE	569	0	590	5	0
2	JF	604	0	628	8	0
All	All	141480	0	145560	1120	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 4.

All (1120) 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:BO:13:THR:OG1	1:GQ:79:GLU:OE1	1.90	0.90
1:AI:79:GLU:OE1	1:AM:13:THR:OG1	1.96	0.83
1:FG:79:GLU:OE1	1:GI:13:THR:OG1	1.98	0.81
2:JD:66:ARG:HD3	2:JF:62:GLU:OE2	1.79	0.81
2:AJ:19:ALA:HB2	2:AJ:64:ALA:HB2	1.68	0.76
2:CB:19:ALA:HB2	2:CB:64:ALA:HB2	1.69	0.75
2:AZ:19:ALA:HB2	2:AZ:64:ALA:HB2	1.70	0.74
2:GJ:19:ALA:HB2	2:GJ:64:ALA:HB2	1.68	0.74
2:HT:19:ALA:HB2	2:HT:64:ALA:HB2	1.70	0.74
2:IJ:19:ALA:HB2	2:IJ:64:ALA:HB2	1.69	0.74
2:BL:19:ALA:HB2	2:BL:64:ALA:HB2	1.70	0.73
2:AH:19:ALA:HB2	2:AH:64:ALA:HB2	1.71	0.73
2:IB:11:LYS:HD2	2:IB:40:GLY:O	1.88	0.73
2:FT:11:LYS:HD2	2:FT:40:GLY:O	1.88	0.73
2:HL:19:ALA:HB2	2:HL:64:ALA:HB2	1.71	0.73
2:IR:11:LYS:HD2	2:IR:40:GLY:O	1.88	0.73
2:IN:11:LYS:HD2	2:IN:40:GLY:O	1.89	0.73
2:HX:11:LYS:HD2	2:HX:40:GLY:O	1.89	0.73
2:CJ:19:ALA:HB2	2:CJ:64:ALA:HB2	1.72	0.72
2:AB:11:LYS:HD2	2:AB:40:GLY:O	1.88	0.72
2:EV:19:ALA:HB2	2:EV:64:ALA:HB2	1.71	0.72
2:FD:11:LYS:HD2	2:FD:40:GLY:O	1.88	0.72
2:IV:19:ALA:HB2	2:IV:64:ALA:HB2	1.72	0.71
2:BH:19:ALA:HB2	2:BH:64:ALA:HB2	1.72	0.71
2:DF:19:ALA:HB2	2:DF:64:ALA:HB2	1.73	0.71
2:EJ:19:ALA:HB2	2:EJ:64:ALA:HB2	1.71	0.71
2:FL:19:ALA:HB2	2:FL:64:ALA:HB2	1.71	0.71
2:AF:19:ALA:HB2	2:AF:64:ALA:HB2	1.72	0.71
2:FB:19:ALA:HB2	2:FB:64:ALA:HB2	1.73	0.71
2:HX:19:ALA:HB2	2:HX:64:ALA:HB2	1.72	0.71
2:AR:19:ALA:HB2	2:AR:64:ALA:HB2	1.71	0.71
2:CN:19:ALA:HB2	2:CN:64:ALA:HB2	1.73	0.71
2:DP:19:ALA:HB2	2:DP:64:ALA:HB2	1.70	0.71
1:GQ:13:THR:OG1	1:HW:79:GLU:OE1	2.08	0.71
2:DV:19:ALA:HB2	2:DV:64:ALA:HB2	1.71	0.71
2:GD:19:ALA:HB2	2:GD:64:ALA:HB2	1.72	0.71
2:FT:19:ALA:HB2	2:FT:64:ALA:HB2	1.73	0.71
2:IN:19:ALA:HB2	2:IN:64:ALA:HB2	1.73	0.71
2:JD:11:LYS:HD2	2:JD:40:GLY:O	1.91	0.71
2:HD:19:ALA:HB2	2:HD:64:ALA:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BX:19:ALA:HB2	2:BX:64:ALA:HB2	1.72	0.70
2:CP:19:ALA:HB2	2:CP:64:ALA:HB2	1.71	0.70
2:GB:19:ALA:HB2	2:GB:64:ALA:HB2	1.72	0.70
2:IR:19:ALA:HB2	2:IR:64:ALA:HB2	1.73	0.70
2:ER:19:ALA:HB2	2:ER:64:ALA:HB2	1.73	0.70
2:GT:19:ALA:HB2	2:GT:64:ALA:HB2	1.73	0.70
2:GV:19:ALA:HB2	2:GV:64:ALA:HB2	1.73	0.70
2:IZ:19:ALA:HB2	2:IZ:64:ALA:HB2	1.74	0.70
2:AB:19:ALA:HB2	2:AB:64:ALA:HB2	1.73	0.70
2:AN:19:ALA:HB2	2:AN:64:ALA:HB2	1.73	0.70
2:DD:19:ALA:HB2	2:DD:64:ALA:HB2	1.73	0.70
2:BV:19:ALA:HB2	2:BV:64:ALA:HB2	1.73	0.70
2:HF:19:ALA:HB2	2:HF:64:ALA:HB2	1.73	0.70
2:BB:19:ALA:HB2	2:BB:64:ALA:HB2	1.74	0.70
2:DT:19:ALA:HB2	2:DT:64:ALA:HB2	1.73	0.70
2:EB:19:ALA:HB2	2:EB:64:ALA:HB2	1.73	0.70
2:EZ:19:ALA:HB2	2:EZ:64:ALA:HB2	1.73	0.70
2:FD:19:ALA:HB2	2:FD:64:ALA:HB2	1.73	0.70
2:IB:19:ALA:HB2	2:IB:64:ALA:HB2	1.73	0.70
2:CZ:19:ALA:HB2	2:CZ:64:ALA:HB2	1.72	0.70
2:DX:19:ALA:HB2	2:DX:64:ALA:HB2	1.74	0.70
2:DL:19:ALA:HB2	2:DL:64:ALA:HB2	1.73	0.70
2:EF:19:ALA:HB2	2:EF:64:ALA:HB2	1.73	0.69
2:BD:19:ALA:HB2	2:BD:64:ALA:HB2	1.73	0.69
2:IF:19:ALA:HB2	2:IF:64:ALA:HB2	1.73	0.69
2:JB:19:ALA:HB2	2:JB:64:ALA:HB2	1.73	0.69
2:EH:19:ALA:HB2	2:EH:64:ALA:HB2	1.73	0.69
2:EX:19:ALA:HB2	2:EX:64:ALA:HB2	1.74	0.69
2:AX:19:ALA:HB2	2:AX:64:ALA:HB2	1.75	0.69
2:HV:19:ALA:HB2	2:HV:64:ALA:HB2	1.75	0.69
2:FX:19:ALA:HB2	2:FX:64:ALA:HB2	1.75	0.69
2:IL:19:ALA:HB2	2:IL:64:ALA:HB2	1.75	0.69
2:JD:19:ALA:HB2	2:JD:64:ALA:HB2	1.75	0.69
2:BN:19:ALA:HB2	2:BN:64:ALA:HB2	1.75	0.69
2:CH:19:ALA:HB2	2:CH:64:ALA:HB2	1.75	0.69
2:DZ:19:ALA:HB2	2:DZ:64:ALA:HB2	1.75	0.69
2:GR:19:ALA:HB2	2:GR:64:ALA:HB2	1.74	0.69
2:DR:19:ALA:HB2	2:DR:64:ALA:HB2	1.74	0.69
1:EY:79:GLU:OE1	1:FG:13:THR:OG1	2.10	0.69
2:BT:19:ALA:HB2	2:BT:64:ALA:HB2	1.74	0.69
2:IH:19:ALA:HB2	2:IH:64:ALA:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AL:19:ALA:HB2	2:AL:64:ALA:HB2	1.75	0.68
2:GF:19:ALA:HB2	2:GF:64:ALA:HB2	1.73	0.68
2:HB:19:ALA:HB2	2:HB:64:ALA:HB2	1.75	0.68
2:BR:19:ALA:HB2	2:BR:64:ALA:HB2	1.75	0.68
2:CX:19:ALA:HB2	2:CX:64:ALA:HB2	1.75	0.68
2:IX:19:ALA:HB2	2:IX:64:ALA:HB2	1.76	0.68
2:HH:19:ALA:HB2	2:HH:64:ALA:HB2	1.73	0.68
2:FP:19:ALA:HB2	2:FP:64:ALA:HB2	1.74	0.68
2:BJ:19:ALA:HB2	2:BJ:64:ALA:HB2	1.76	0.68
1:CQ:30:LEU:HD13	1:CQ:34:GLN:HA	1.76	0.68
1:GE:30:LEU:HD13	1:GE:34:GLN:HA	1.76	0.68
1:HG:30:LEU:HD13	1:HG:34:GLN:HA	1.76	0.68
2:CF:19:ALA:HB2	2:CF:64:ALA:HB2	1.75	0.68
1:BG:30:LEU:HD13	1:BG:34:GLN:HA	1.76	0.68
1:CY:30:LEU:HD13	1:CY:34:GLN:HA	1.76	0.68
2:FJ:19:ALA:HB2	2:FJ:64:ALA:HB2	1.75	0.68
2:GL:19:ALA:HB2	2:GL:64:ALA:HB2	1.75	0.68
1:AQ:30:LEU:HD13	1:AQ:34:GLN:HA	1.76	0.68
1:AY:30:LEU:HD13	1:AY:34:GLN:HA	1.76	0.68
2:DH:19:ALA:HB2	2:DH:64:ALA:HB2	1.75	0.68
1:DS:30:LEU:HD13	1:DS:34:GLN:HA	1.76	0.68
2:FR:19:ALA:HB2	2:FR:64:ALA:HB2	1.74	0.68
2:GN:19:ALA:HB2	2:GN:64:ALA:HB2	1.75	0.68
1:IU:30:LEU:HD13	1:IU:34:GLN:HA	1.76	0.68
2:EN:19:ALA:HB2	2:EN:64:ALA:HB2	1.74	0.68
1:EU:30:LEU:HD13	1:EU:34:GLN:HA	1.76	0.68
2:FV:19:ALA:HB2	2:FV:64:ALA:HB2	1.76	0.68
1:GA:30:LEU:HD13	1:GA:34:GLN:HA	1.76	0.68
1:HS:30:LEU:HD13	1:HS:34:GLN:HA	1.76	0.68
2:JF:19:ALA:HB2	2:JF:64:ALA:HB2	1.76	0.68
2:AV:19:ALA:HB2	2:AV:64:ALA:HB2	1.76	0.68
2:CD:19:ALA:HB2	2:CD:64:ALA:HB2	1.75	0.68
2:CG:19:ALA:HB2	2:CG:64:ALA:HB2	1.76	0.68
2:DY:19:ALA:HB2	2:DY:64:ALA:HB2	1.76	0.68
2:FN:19:ALA:HB2	2:FN:64:ALA:HB2	1.76	0.68
2:AT:19:ALA:HB2	2:AT:64:ALA:HB2	1.76	0.67
2:GP:19:ALA:HB2	2:GP:64:ALA:HB2	1.75	0.67
1:GY:30:LEU:HD13	1:GY:34:GLN:HA	1.76	0.67
2:CR:19:ALA:HB2	2:CR:64:ALA:HB2	1.74	0.67
2:GH:19:ALA:HB2	2:GH:64:ALA:HB2	1.76	0.67
2:IT:19:ALA:HB2	2:IT:64:ALA:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AU:30:LEU:HD13	1:AU:34:GLN:HA	1.76	0.67
2:BZ:19:ALA:HB2	2:BZ:64:ALA:HB2	1.75	0.67
1:CU:30:LEU:HD13	1:CU:34:GLN:HA	1.76	0.67
2:DB:19:ALA:HB2	2:DB:64:ALA:HB2	1.77	0.67
1:EA:30:LEU:HD13	1:EA:34:GLN:HA	1.76	0.67
2:GX:19:ALA:HB2	2:GX:64:ALA:HB2	1.76	0.67
1:BC:30:LEU:HD13	1:BC:34:GLN:HA	1.76	0.67
1:CM:30:LEU:HD13	1:CM:34:GLN:HA	1.76	0.67
1:EM:30:LEU:HD13	1:EM:34:GLN:HA	1.76	0.67
1:FK:30:LEU:HD13	1:FK:34:GLN:HA	1.76	0.67
2:HR:19:ALA:HB2	2:HR:64:ALA:HB2	1.75	0.67
1:JC:30:LEU:HD13	1:JC:34:GLN:HA	1.76	0.67
2:AR:7:LEU:CD2	2:AR:45:MET:HG2	2.25	0.67
1:CA:30:LEU:HD13	1:CA:34:GLN:HA	1.76	0.67
2:CV:19:ALA:HB2	2:CV:64:ALA:HB2	1.74	0.67
2:FF:19:ALA:HB2	2:FF:64:ALA:HB2	1.75	0.67
1:GQ:30:LEU:HD13	1:GQ:34:GLN:HA	1.76	0.67
1:IY:30:LEU:HD13	1:IY:34:GLN:HA	1.76	0.67
2:DI:19:ALA:HB2	2:DI:64:ALA:HB2	1.77	0.67
2:DJ:19:ALA:HB2	2:DJ:64:ALA:HB2	1.75	0.67
1:DW:30:LEU:HD13	1:DW:34:GLN:HA	1.76	0.67
1:EE:30:LEU:HD13	1:EE:34:GLN:HA	1.76	0.67
2:GZ:19:ALA:HB2	2:GZ:64:ALA:HB2	1.75	0.67
1:CE:30:LEU:HD13	1:CE:34:GLN:HA	1.76	0.67
2:EL:19:ALA:HB2	2:EL:64:ALA:HB2	1.76	0.67
1:FO:30:LEU:HD13	1:FO:34:GLN:HA	1.76	0.67
2:ID:19:ALA:HB2	2:ID:64:ALA:HB2	1.75	0.67
1:EY:30:LEU:HD13	1:EY:34:GLN:HA	1.76	0.67
2:FZ:19:ALA:HB2	2:FZ:64:ALA:HB2	1.76	0.67
1:GU:30:LEU:HD13	1:GU:34:GLN:HA	1.76	0.67
1:HK:30:LEU:HD13	1:HK:34:GLN:HA	1.76	0.67
1:IM:30:LEU:HD13	1:IM:34:GLN:HA	1.76	0.67
1:IQ:30:LEU:HD13	1:IQ:34:GLN:HA	1.76	0.67
1:DC:30:LEU:HD13	1:DC:34:GLN:HA	1.76	0.67
1:DO:30:LEU:HD13	1:DO:34:GLN:HA	1.76	0.67
1:FG:30:LEU:HD13	1:FG:34:GLN:HA	1.76	0.67
2:FH:19:ALA:HB2	2:FH:64:ALA:HB2	1.74	0.67
2:FI:19:ALA:HB2	2:FI:64:ALA:HB2	1.77	0.67
1:FS:30:LEU:HD13	1:FS:34:GLN:HA	1.76	0.67
1:GI:30:LEU:HD13	1:GI:34:GLN:HA	1.76	0.67
2:HZ:19:ALA:HB2	2:HZ:64:ALA:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JD:62:GLU:OE2	2:JF:66:ARG:HD3	1.95	0.67
1:DK:30:LEU:HD13	1:DK:34:GLN:HA	1.76	0.66
1:HO:30:LEU:HD13	1:HO:34:GLN:HA	1.76	0.66
1:IA:30:LEU:HD13	1:IA:34:GLN:HA	1.76	0.66
1:AI:13:THR:OG1	1:HO:79:GLU:OE1	2.10	0.66
1:AI:30:LEU:HD13	1:AI:34:GLN:HA	1.76	0.66
1:FW:30:LEU:HD13	1:FW:34:GLN:HA	1.76	0.66
2:ED:19:ALA:HB2	2:ED:64:ALA:HB2	1.77	0.66
2:GO:19:ALA:HB2	2:GO:64:ALA:HB2	1.78	0.66
1:IE:30:LEU:HD13	1:IE:34:GLN:HA	1.76	0.66
1:AE:30:LEU:HD13	1:AE:34:GLN:HA	1.76	0.66
1:BO:30:LEU:HD13	1:BO:34:GLN:HA	1.76	0.66
1:CI:30:LEU:HD13	1:CI:34:GLN:HA	1.76	0.66
2:AP:19:ALA:HB2	2:AP:64:ALA:HB2	1.76	0.66
1:BS:30:LEU:HD13	1:BS:34:GLN:HA	1.76	0.66
1:EI:30:LEU:HD13	1:EI:34:GLN:HA	1.76	0.66
1:HC:30:LEU:HD13	1:HC:34:GLN:HA	1.76	0.66
1:BK:30:LEU:HD13	1:BK:34:GLN:HA	1.76	0.66
2:BQ:19:ALA:HB2	2:BQ:64:ALA:HB2	1.78	0.66
1:DG:30:LEU:HD13	1:DG:34:GLN:HA	1.76	0.66
2:EP:19:ALA:HB2	2:EP:64:ALA:HB2	1.78	0.66
1:II:30:LEU:HD13	1:II:34:GLN:HA	1.76	0.66
2:IP:19:ALA:HB2	2:IP:64:ALA:HB2	1.77	0.66
1:AA:30:LEU:HD13	1:AA:34:GLN:HA	1.76	0.66
1:FC:30:LEU:HD13	1:FC:34:GLN:HA	1.76	0.66
2:HA:19:ALA:HB2	2:HA:64:ALA:HB2	1.78	0.66
1:GM:30:LEU:HD13	1:GM:34:GLN:HA	1.76	0.66
2:CW:19:ALA:HB2	2:CW:64:ALA:HB2	1.78	0.65
2:AK:19:ALA:HB2	2:AK:64:ALA:HB2	1.78	0.65
1:HW:30:LEU:HD13	1:HW:34:GLN:HA	1.76	0.65
1:BW:30:LEU:HD13	1:BW:34:GLN:HA	1.76	0.65
2:CT:19:ALA:HB2	2:CT:64:ALA:HB2	1.77	0.65
2:HN:19:ALA:HB2	2:HN:64:ALA:HB2	1.76	0.65
2:DN:19:ALA:HB2	2:DN:64:ALA:HB2	1.77	0.65
2:AD:19:ALA:HB2	2:AD:64:ALA:HB2	1.76	0.65
2:AO:19:ALA:HB2	2:AO:64:ALA:HB2	1.79	0.65
2:BF:19:ALA:HB2	2:BF:64:ALA:HB2	1.79	0.65
2:HP:19:ALA:HB2	2:HP:64:ALA:HB2	1.79	0.65
2:HQ:19:ALA:HB2	2:HQ:64:ALA:HB2	1.77	0.65
2:HE:19:ALA:HB2	2:HE:64:ALA:HB2	1.79	0.65
1:AM:30:LEU:HD13	1:AM:34:GLN:HA	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BP:19:ALA:HB2	2:BP:64:ALA:HB2	1.77	0.65
2:EK:19:ALA:HB2	2:EK:64:ALA:HB2	1.79	0.65
1:EQ:30:LEU:HD13	1:EQ:34:GLN:HA	1.76	0.65
2:CL:19:ALA:HB2	2:CL:64:ALA:HB2	1.76	0.65
2:HU:19:ALA:HB2	2:HU:64:ALA:HB2	1.79	0.64
2:BA:19:ALA:HB2	2:BA:64:ALA:HB2	1.79	0.64
2:DD:49:ASP:OD1	2:DD:50:VAL:N	2.31	0.64
2:GK:19:ALA:HB2	2:GK:64:ALA:HB2	1.79	0.64
2:HJ:19:ALA:HB2	2:HJ:64:ALA:HB2	1.79	0.64
2:FY:19:ALA:HB2	2:FY:64:ALA:HB2	1.79	0.64
2:CC:19:ALA:HB2	2:CC:64:ALA:HB2	1.80	0.64
2:ES:19:ALA:HB2	2:ES:64:ALA:HB2	1.80	0.64
2:DZ:77:ALA:C	2:DZ:78:ARG:HD2	2.17	0.64
2:JE:19:ALA:HB2	2:JE:64:ALA:HB2	1.80	0.64
1:CM:79:GLU:OE1	1:CU:13:THR:OG1	2.13	0.64
1:GY:13:THR:OG1	1:IY:79:GLU:OE1	2.14	0.63
2:HI:19:ALA:HB2	2:HI:64:ALA:HB2	1.81	0.63
2:FE:19:ALA:HB2	2:FE:64:ALA:HB2	1.81	0.63
2:IH:86:ILE:HD11	2:IO:31:LEU:HD21	1.78	0.63
2:IW:19:ALA:HB2	2:IW:64:ALA:HB2	1.80	0.63
2:ET:19:ALA:HB2	2:ET:64:ALA:HB2	1.79	0.63
2:AW:19:ALA:HB2	2:AW:64:ALA:HB2	1.79	0.63
2:CS:19:ALA:HB2	2:CS:64:ALA:HB2	1.81	0.63
1:CY:79:GLU:OE1	1:IY:13:THR:OG1	2.15	0.63
2:FQ:19:ALA:HB2	2:FQ:64:ALA:HB2	1.80	0.63
2:IC:19:ALA:HB2	2:IC:64:ALA:HB2	1.80	0.63
2:EW:19:ALA:HB2	2:EW:64:ALA:HB2	1.81	0.63
2:IK:19:ALA:HB2	2:IK:64:ALA:HB2	1.79	0.63
2:DM:19:ALA:HB2	2:DM:64:ALA:HB2	1.80	0.62
2:EC:19:ALA:HB2	2:EC:64:ALA:HB2	1.80	0.62
2:BM:19:ALA:HB2	2:BM:64:ALA:HB2	1.81	0.62
2:DQ:19:ALA:HB2	2:DQ:64:ALA:HB2	1.81	0.62
2:IG:19:ALA:HB2	2:IG:64:ALA:HB2	1.82	0.62
2:AC:19:ALA:HB2	2:AC:64:ALA:HB2	1.82	0.62
2:BD:62:GLU:OE2	2:BF:66:ARG:HD3	1.99	0.62
2:FA:19:ALA:HB2	2:FA:64:ALA:HB2	1.81	0.61
2:BR:78:ARG:NH1	2:BR:79:PRO:O	2.33	0.61
2:CK:19:ALA:HB2	2:CK:64:ALA:HB2	1.82	0.61
2:EG:19:ALA:HB2	2:EG:64:ALA:HB2	1.82	0.61
2:CO:19:ALA:HB2	2:CO:64:ALA:HB2	1.82	0.61
2:GS:19:ALA:HB2	2:GS:64:ALA:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JA:19:ALA:HB2	2:JA:64:ALA:HB2	1.82	0.61
2:BU:19:ALA:HB2	2:BU:64:ALA:HB2	1.83	0.61
2:GC:19:ALA:HB2	2:GC:64:ALA:HB2	1.82	0.61
2:HB:78:ARG:NH1	2:HB:79:PRO:O	2.34	0.61
2:BE:19:ALA:HB2	2:BE:64:ALA:HB2	1.81	0.60
2:FU:19:ALA:HB2	2:FU:64:ALA:HB2	1.81	0.60
2:EO:19:ALA:HB2	2:EO:64:ALA:HB2	1.83	0.60
2:FM:19:ALA:HB2	2:FM:64:ALA:HB2	1.83	0.60
2:AF:11:LYS:HD3	2:AF:40:GLY:O	2.01	0.60
2:CF:62:GLU:OE2	2:CH:66:ARG:HD3	2.02	0.60
2:GW:19:ALA:HB2	2:GW:64:ALA:HB2	1.84	0.60
2:AB:62:GLU:OE2	2:AD:66:ARG:HD3	2.02	0.60
2:BY:19:ALA:HB2	2:BY:64:ALA:HB2	1.84	0.60
2:IS:19:ALA:HB2	2:IS:64:ALA:HB2	1.82	0.60
2:HH:62:GLU:OE2	2:HJ:66:ARG:HD3	2.02	0.60
2:BI:19:ALA:HB2	2:BI:64:ALA:HB2	1.83	0.60
2:DE:19:ALA:HB2	2:DE:64:ALA:HB2	1.83	0.60
2:ER:62:GLU:OE2	2:ET:66:ARG:HD3	2.00	0.60
2:AN:62:GLU:OE2	2:AP:66:ARG:HD3	2.02	0.60
2:DH:11:LYS:HD3	2:DH:40:GLY:O	2.02	0.60
2:FL:62:GLU:OE2	2:FN:66:ARG:HD3	2.01	0.60
2:HM:19:ALA:HB2	2:HM:64:ALA:HB2	1.83	0.60
2:AG:19:ALA:HB2	2:AG:64:ALA:HB2	1.83	0.59
2:AF:49:ASP:OD1	2:AF:50:VAL:N	2.30	0.59
2:AS:19:ALA:HB2	2:AS:64:ALA:HB2	1.84	0.59
2:BI:31:LEU:HD21	2:CP:86:ILE:HD11	1.82	0.59
2:EZ:11:LYS:HD3	2:EZ:40:GLY:O	2.02	0.59
2:DU:19:ALA:HB2	2:DU:64:ALA:HB2	1.83	0.59
2:IR:62:GLU:OE2	2:IT:66:ARG:HD3	2.03	0.59
2:GP:78:ARG:NH1	2:GP:79:PRO:O	2.35	0.59
2:DA:19:ALA:HB2	2:DA:64:ALA:HB2	1.84	0.59
2:EB:62:GLU:OE2	2:ED:66:ARG:HD3	2.03	0.59
2:HY:19:ALA:HB2	2:HY:64:ALA:HB2	1.85	0.59
2:IO:19:ALA:HB2	2:IO:64:ALA:HB2	1.85	0.59
2:AX:78:ARG:NH1	2:AX:79:PRO:O	2.36	0.58
2:IZ:11:LYS:HD3	2:IZ:40:GLY:O	2.03	0.58
2:GG:19:ALA:HB2	2:GG:64:ALA:HB2	1.86	0.58
2:BP:11:LYS:HD3	2:BP:40:GLY:O	2.02	0.58
2:DD:62:GLU:OE2	2:DF:66:ARG:HD3	2.04	0.58
2:IF:62:GLU:OE2	2:IH:66:ARG:HD3	2.04	0.58
2:AF:62:GLU:OE2	2:AH:66:ARG:HD3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CN:62:GLU:OE2	2:CP:66:ARG:HD3	2.03	0.57
2:IB:62:GLU:OE2	2:ID:66:ARG:HD3	2.03	0.57
2:CR:62:GLU:OE2	2:CT:66:ARG:HD3	2.04	0.57
2:CN:11:LYS:HD3	2:CN:40:GLY:O	2.04	0.57
1:EA:43:VAL:HG21	1:EI:57:LEU:HD11	1.87	0.57
1:CQ:57:LEU:HD11	1:CY:43:VAL:HG21	1.86	0.57
2:DD:11:LYS:HD3	2:DD:40:GLY:O	2.05	0.57
1:BC:43:VAL:HG21	1:HC:57:LEU:HD11	1.87	0.57
2:FD:62:GLU:OE2	2:FF:66:ARG:HD3	2.04	0.57
2:BP:62:GLU:OE2	2:BR:66:ARG:HD3	2.05	0.57
2:HP:11:LYS:HD3	2:HP:40:GLY:O	2.05	0.56
2:FT:62:GLU:OE2	2:FV:66:ARG:HD3	2.05	0.56
2:GJ:62:GLU:OE2	2:GL:66:ARG:HD3	2.06	0.56
2:HL:62:GLU:OE2	2:HN:66:ARG:HD3	2.05	0.56
2:GN:62:GLU:OE2	2:GP:66:ARG:HD3	2.06	0.56
2:FX:11:LYS:HD2	2:FX:40:GLY:O	2.06	0.56
1:CE:13:THR:OG1	1:FO:79:GLU:OE1	2.19	0.56
2:FH:62:GLU:OE2	2:FJ:66:ARG:HD3	2.06	0.55
2:FP:11:LYS:HD3	2:FP:40:GLY:O	2.06	0.55
2:BN:82:ASP:O	2:BN:85:LYS:HG2	2.07	0.55
2:CB:62:GLU:OE2	2:CD:66:ARG:HD3	2.07	0.55
1:DW:13:THR:OG1	1:EE:79:GLU:OE1	2.21	0.55
2:DX:62:GLU:OE2	2:DZ:66:ARG:HD3	2.06	0.55
2:FM:31:LEU:HD21	2:GD:86:ILE:HD11	1.87	0.55
2:IF:11:LYS:HD3	2:IF:40:GLY:O	2.05	0.55
2:GB:11:LYS:HD3	2:GB:40:GLY:O	2.07	0.55
1:IE:43:VAL:HG21	1:IM:57:LEU:HD11	1.88	0.55
2:CZ:62:GLU:OE2	2:DB:66:ARG:HD3	2.07	0.55
1:DC:79:GLU:OE1	1:JC:13:THR:OG1	2.24	0.55
2:BX:62:GLU:OE2	2:BZ:66:ARG:HD3	2.07	0.55
2:DH:62:GLU:OE2	2:DJ:66:ARG:HD3	2.07	0.55
2:EF:62:GLU:OE2	2:EH:66:ARG:HD3	2.07	0.55
2:FX:62:GLU:OE2	2:FZ:66:ARG:HD3	2.06	0.55
2:IZ:62:GLU:OE2	2:JB:66:ARG:HD3	2.07	0.55
2:IV:11:LYS:HD2	2:IV:40:GLY:O	2.06	0.54
2:AZ:11:LYS:HD2	2:AZ:40:GLY:O	2.06	0.54
2:BH:62:GLU:OE2	2:BJ:66:ARG:HD3	2.07	0.54
2:CH:78:ARG:NH1	2:CH:79:PRO:O	2.40	0.54
2:AR:11:LYS:HD2	2:AR:40:GLY:O	2.07	0.54
2:AV:62:GLU:OE2	2:AX:66:ARG:HD3	2.07	0.54
2:AZ:62:GLU:OE2	2:BB:66:ARG:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FE:30:GLU:OE2	2:FE:47:LYS:HG2	2.07	0.54
2:GB:62:GLU:OE2	2:GD:66:ARG:HD3	2.07	0.54
2:BL:62:GLU:OE2	2:BN:66:ARG:HD3	2.07	0.54
2:DT:62:GLU:OE2	2:DV:66:ARG:HD3	2.08	0.54
2:GF:11:LYS:HD2	2:GF:40:GLY:O	2.07	0.54
1:CM:54:ASP:OD1	2:CX:78:ARG:NH1	2.41	0.54
2:HX:62:GLU:OE2	2:HZ:66:ARG:HD3	2.07	0.54
1:AA:57:LEU:HD11	1:AQ:43:VAL:HG21	1.90	0.54
2:EZ:62:GLU:OE2	2:FB:66:ARG:HD3	2.07	0.54
2:GZ:62:GLU:OE2	2:HB:66:ARG:HD3	2.07	0.54
2:HV:82:ASP:O	2:HV:85:LYS:HG2	2.08	0.54
2:AJ:62:GLU:OE2	2:AL:66:ARG:HD3	2.07	0.54
2:EJ:62:GLU:OE2	2:EL:66:ARG:HD3	2.06	0.54
2:AR:62:GLU:OE2	2:AT:66:ARG:HD3	2.08	0.54
2:HF:82:ASP:O	2:HF:85:LYS:HG2	2.08	0.54
1:BG:79:GLU:OE1	1:CM:13:THR:OG1	2.26	0.53
2:CJ:62:GLU:OE2	2:CL:66:ARG:HD3	2.08	0.53
2:FR:78:ARG:NH1	2:FR:79:PRO:O	2.41	0.53
2:IV:62:GLU:OE2	2:IX:66:ARG:HD3	2.09	0.53
1:AE:13:THR:OG1	1:HK:79:GLU:OE1	2.25	0.53
2:DL:62:GLU:OE2	2:DN:66:ARG:HD3	2.09	0.53
2:HP:62:GLU:OE2	2:HR:66:ARG:HD3	2.07	0.53
2:DP:62:GLU:OE2	2:DR:66:ARG:HD3	2.08	0.53
2:HT:62:GLU:OE2	2:HV:66:ARG:HD3	2.07	0.53
2:DV:86:ILE:HD11	2:EO:31:LEU:HD21	1.89	0.53
2:EJ:18:GLU:OE1	2:EK:74:ARG:NE	2.42	0.53
1:FK:54:ASP:OD1	2:GD:78:ARG:NH1	2.42	0.53
2:HD:62:GLU:OE2	2:HF:66:ARG:HD3	2.09	0.53
1:CA:79:GLU:OE1	1:EQ:13:THR:OG1	2.24	0.52
2:CD:11:LYS:HE3	2:CD:69:LYS:HG2	1.91	0.52
2:CV:62:GLU:OE2	2:CX:66:ARG:HD3	2.09	0.52
2:GV:62:GLU:OE2	2:GX:66:ARG:HD3	2.08	0.52
2:IJ:62:GLU:OE2	2:IL:66:ARG:HD3	2.09	0.52
1:BG:43:VAL:HG21	1:HG:57:LEU:HD11	1.91	0.52
2:GR:81:ASN:OD1	2:GR:82:ASP:N	2.43	0.52
2:GX:78:ARG:NH1	2:GX:79:PRO:O	2.42	0.52
2:EN:62:GLU:OE2	2:EP:66:ARG:HD3	2.08	0.52
2:BT:62:GLU:OE2	2:BV:66:ARG:HD3	2.09	0.52
1:HW:43:VAL:HG21	1:IQ:57:LEU:HD11	1.90	0.52
2:CB:18:GLU:OE1	2:CC:74:ARG:NE	2.42	0.52
2:IV:18:GLU:OE1	2:IW:74:ARG:NE	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:18:GLU:OE1	2:AC:74:ARG:NE	2.42	0.52
2:AH:86:ILE:HD11	2:HM:31:LEU:HD21	1.92	0.52
2:GR:62:GLU:OE2	2:GT:66:ARG:HD3	2.10	0.52
1:IA:43:VAL:HG21	1:II:57:LEU:HD11	1.92	0.52
2:FP:3:GLU:HB2	2:FP:47:LYS:HE2	1.92	0.51
1:EA:57:LEU:HD11	1:HK:43:VAL:HG21	1.93	0.51
2:IZ:30:GLU:OE2	2:IZ:47:LYS:HG2	2.10	0.51
2:IZ:81:ASN:OD1	2:IZ:82:ASP:N	2.42	0.51
1:DK:46:ASP:OD1	1:DK:47:ASN:N	2.44	0.51
1:EY:46:ASP:OD1	1:EY:47:ASN:N	2.44	0.51
1:GQ:46:ASP:OD1	1:GQ:47:ASN:N	2.44	0.51
1:GU:46:ASP:OD1	1:GU:47:ASN:N	2.44	0.51
1:AQ:46:ASP:OD1	1:AQ:47:ASN:N	2.44	0.51
1:DS:46:ASP:OD1	1:DS:47:ASN:N	2.44	0.51
1:GA:46:ASP:OD1	1:GA:47:ASN:N	2.44	0.51
1:GE:46:ASP:OD1	1:GE:47:ASN:N	2.44	0.51
1:IM:46:ASP:OD1	1:IM:47:ASN:N	2.44	0.51
1:AQ:54:ASP:OD1	2:EH:78:ARG:NH1	2.44	0.51
1:BG:54:ASP:OD1	2:CP:78:ARG:NH1	2.44	0.51
1:EI:46:ASP:OD1	1:EI:47:ASN:N	2.44	0.51
1:EM:46:ASP:OD1	1:EM:47:ASN:N	2.44	0.51
1:FK:46:ASP:OD1	1:FK:47:ASN:N	2.44	0.51
1:HC:46:ASP:OD1	1:HC:47:ASN:N	2.44	0.51
1:IA:46:ASP:OD1	1:IA:47:ASN:N	2.44	0.51
1:AA:46:ASP:OD1	1:AA:47:ASN:N	2.44	0.51
2:AF:3:GLU:HB2	2:AF:47:LYS:HE2	1.92	0.51
1:BC:46:ASP:OD1	1:BC:47:ASN:N	2.44	0.51
1:BK:46:ASP:OD1	1:BK:47:ASN:N	2.44	0.51
1:BW:46:ASP:OD1	1:BW:47:ASN:N	2.44	0.51
1:CY:46:ASP:OD1	1:CY:47:ASN:N	2.44	0.51
2:DD:3:GLU:HB2	2:DD:47:LYS:HE2	1.93	0.51
1:HW:46:ASP:OD1	1:HW:47:ASN:N	2.44	0.51
1:II:46:ASP:OD1	1:II:47:ASN:N	2.44	0.51
1:IU:46:ASP:OD1	1:IU:47:ASN:N	2.44	0.51
2:JF:4:ALA:HB2	2:JF:50:VAL:HG22	1.93	0.51
1:AU:46:ASP:OD1	1:AU:47:ASN:N	2.44	0.50
1:AY:46:ASP:OD1	1:AY:47:ASN:N	2.44	0.50
1:BG:46:ASP:OD1	1:BG:47:ASN:N	2.44	0.50
1:CE:46:ASP:OD1	1:CE:47:ASN:N	2.44	0.50
2:CN:30:GLU:OE2	2:CN:47:LYS:HG2	2.11	0.50
1:DW:46:ASP:OD1	1:DW:47:ASN:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FC:46:ASP:OD1	1:FC:47:ASN:N	2.44	0.50
1:FG:46:ASP:OD1	1:FG:47:ASN:N	2.44	0.50
1:FS:46:ASP:OD1	1:FS:47:ASN:N	2.44	0.50
1:GY:46:ASP:OD1	1:GY:47:ASN:N	2.44	0.50
1:IQ:46:ASP:OD1	1:IQ:47:ASN:N	2.44	0.50
1:JC:46:ASP:OD1	1:JC:47:ASN:N	2.44	0.50
1:AM:46:ASP:OD1	1:AM:47:ASN:N	2.44	0.50
1:BO:46:ASP:OD1	1:BO:47:ASN:N	2.44	0.50
1:CI:46:ASP:OD1	1:CI:47:ASN:N	2.44	0.50
1:EA:46:ASP:OD1	1:EA:47:ASN:N	2.44	0.50
1:EQ:46:ASP:OD1	1:EQ:47:ASN:N	2.44	0.50
2:CK:31:LEU:HD21	2:DF:86:ILE:HD11	1.93	0.50
1:CU:46:ASP:OD1	1:CU:47:ASN:N	2.44	0.50
1:DG:46:ASP:OD1	1:DG:47:ASN:N	2.44	0.50
1:EU:46:ASP:OD1	1:EU:47:ASN:N	2.44	0.50
2:GF:62:GLU:OE2	2:GH:66:ARG:HD3	2.11	0.50
1:GM:46:ASP:OD1	1:GM:47:ASN:N	2.44	0.50
1:HK:46:ASP:OD1	1:HK:47:ASN:N	2.44	0.50
1:AE:46:ASP:OD1	1:AE:47:ASN:N	2.44	0.50
1:AI:46:ASP:OD1	1:AI:47:ASN:N	2.44	0.50
1:CM:46:ASP:OD1	1:CM:47:ASN:N	2.44	0.50
2:CR:18:GLU:OE1	2:CS:74:ARG:NE	2.45	0.50
2:EZ:30:GLU:OE2	2:EZ:47:LYS:HG2	2.12	0.50
1:FO:46:ASP:OD1	1:FO:47:ASN:N	2.44	0.50
1:HS:46:ASP:OD1	1:HS:47:ASN:N	2.44	0.50
1:EE:46:ASP:OD1	1:EE:47:ASN:N	2.44	0.50
2:IF:3:GLU:HB2	2:IF:47:LYS:HE2	1.93	0.50
1:DC:46:ASP:OD1	1:DC:47:ASN:N	2.44	0.50
1:IY:46:ASP:OD1	1:IY:47:ASN:N	2.44	0.50
1:BK:79:GLU:OE1	1:DK:13:THR:OG1	2.30	0.50
2:BT:3:GLU:HB2	2:BT:47:LYS:HE2	1.93	0.50
1:BW:57:LEU:HD11	1:EY:43:VAL:HG21	1.94	0.50
2:EV:62:GLU:OE2	2:EX:66:ARG:HD3	2.11	0.50
1:FW:46:ASP:OD1	1:FW:47:ASN:N	2.44	0.50
1:CE:79:GLU:OE1	1:EU:13:THR:OG1	2.29	0.50
1:DC:57:LEU:HD11	1:JC:43:VAL:HG21	1.94	0.50
2:GB:30:GLU:OE2	2:GB:47:LYS:HG2	2.11	0.50
1:HO:46:ASP:OD1	1:HO:47:ASN:N	2.44	0.50
1:CA:46:ASP:OD1	1:CA:47:ASN:N	2.44	0.49
1:DO:46:ASP:OD1	1:DO:47:ASN:N	2.44	0.49
1:HG:46:ASP:OD1	1:HG:47:ASN:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IE:46:ASP:OD1	1:IE:47:ASN:N	2.44	0.49
2:BN:77:ALA:C	2:BN:78:ARG:HD2	2.32	0.49
1:BS:46:ASP:OD1	1:BS:47:ASN:N	2.44	0.49
1:CQ:46:ASP:OD1	1:CQ:47:ASN:N	2.44	0.49
1:GI:46:ASP:OD1	1:GI:47:ASN:N	2.44	0.49
2:IR:18:GLU:OE1	2:IS:74:ARG:NE	2.44	0.49
1:FK:79:GLU:OE1	1:GA:13:THR:OG1	2.29	0.49
2:IN:62:GLU:OE2	2:IP:66:ARG:HD3	2.11	0.49
2:JF:11:LYS:HE3	2:JF:69:LYS:HG2	1.95	0.49
1:BO:9:HIS:CE1	1:GQ:82:PHE:CD2	3.01	0.49
2:DD:30:GLU:OE2	2:DD:47:LYS:HG2	2.12	0.49
2:CN:3:GLU:HB2	2:CN:47:LYS:HE2	1.95	0.49
2:EZ:18:GLU:OE1	2:FA:74:ARG:NE	2.45	0.49
2:FP:30:GLU:OE2	2:FP:47:LYS:HG2	2.13	0.49
2:GJ:18:GLU:OE1	2:GK:74:ARG:NE	2.44	0.49
1:CU:57:LEU:HD11	1:IU:43:VAL:HG21	1.95	0.49
2:JD:39:SER:O	2:JD:39:SER:OG	2.30	0.49
2:IG:39:SER:O	2:IG:39:SER:OG	2.31	0.49
2:AF:30:GLU:OE2	2:AF:47:LYS:HG2	2.13	0.49
2:BT:30:GLU:OE2	2:BT:47:LYS:HG2	2.12	0.49
1:FC:57:LEU:HD11	1:GE:43:VAL:HG21	1.95	0.48
2:CD:86:ILE:HG21	2:FY:34:TYR:CE2	2.47	0.48
2:BI:7:LEU:CD2	2:BI:45:MET:HG2	2.44	0.48
2:AJ:18:GLU:OE1	2:AK:74:ARG:NE	2.45	0.48
1:DO:57:LEU:HD11	1:IQ:43:VAL:HG21	1.95	0.48
2:HJ:86:ILE:HG21	2:IW:34:TYR:CE2	2.48	0.48
2:DA:7:LEU:CD2	2:DA:45:MET:HG2	2.44	0.48
2:DT:30:GLU:OE2	2:DT:47:LYS:HG2	2.12	0.48
2:HF:86:ILE:HD13	2:JE:34:TYR:HE1	1.78	0.48
2:FM:7:LEU:CD2	2:FM:45:MET:HG2	2.43	0.48
1:CI:57:LEU:HD11	1:DC:43:VAL:HG21	1.94	0.48
2:DT:3:GLU:HB2	2:DT:47:LYS:HE2	1.94	0.48
1:GM:43:VAL:HG21	1:IE:57:LEU:HD11	1.96	0.48
2:EZ:3:GLU:HB2	2:EZ:47:LYS:HE2	1.95	0.48
1:CA:43:VAL:HG21	1:FW:57:LEU:HD11	1.96	0.47
1:EU:57:LEU:HD11	1:FC:43:VAL:HG21	1.94	0.47
2:IZ:3:GLU:HB2	2:IZ:47:LYS:HE2	1.96	0.47
1:FG:82:PHE:CD2	1:GI:9:HIS:CE1	3.01	0.47
2:FT:18:GLU:OE1	2:FU:74:ARG:NE	2.46	0.47
2:IF:30:GLU:OE2	2:IF:47:LYS:HG2	2.14	0.47
2:BB:39:SER:O	2:BB:39:SER:OG	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:3:GLU:HB2	2:GB:47:LYS:HE2	1.95	0.47
2:CD:86:ILE:HD11	2:FY:31:LEU:HD21	1.96	0.47
1:DS:43:VAL:HG21	1:EM:57:LEU:HD11	1.96	0.47
2:BF:86:ILE:HG21	2:HE:34:TYR:CE2	2.50	0.47
1:EQ:79:GLU:OE1	1:FK:13:THR:OG1	2.30	0.47
2:GG:7:LEU:CD2	2:GG:45:MET:HG2	2.44	0.47
2:HB:69:LYS:HE3	2:HB:69:LYS:HA	1.97	0.47
2:ID:78:ARG:HD2	1:II:54:ASP:OD1	2.14	0.47
2:IF:11:LYS:HA	2:IF:40:GLY:O	2.15	0.47
2:DE:57:VAL:O	2:DE:61:VAL:HG23	2.13	0.47
1:FO:43:VAL:HG21	1:GE:57:LEU:HD11	1.97	0.47
2:FP:11:LYS:HA	2:FP:40:GLY:O	2.15	0.47
2:AD:86:ILE:HG21	2:HU:34:TYR:CE2	2.49	0.47
2:AH:69:LYS:HE3	2:AH:69:LYS:HA	1.97	0.47
2:CK:34:TYR:CE1	2:DF:86:ILE:HD13	2.50	0.47
2:EF:11:LYS:HD3	2:EF:40:GLY:O	2.14	0.47
2:IH:86:ILE:HG21	2:IO:34:TYR:CE2	2.50	0.47
2:CX:69:LYS:HE3	2:CX:69:LYS:HA	1.97	0.46
2:DX:39:SER:O	2:DX:39:SER:OG	2.30	0.46
2:FA:39:SER:O	2:FA:39:SER:OG	2.31	0.46
2:FE:34:TYR:CE2	2:GH:86:ILE:HG21	2.50	0.46
2:GZ:30:GLU:OE2	2:GZ:47:LYS:HG2	2.14	0.46
1:HC:43:VAL:HG21	1:JC:57:LEU:HD11	1.97	0.46
2:JA:39:SER:O	2:JA:39:SER:OG	2.31	0.46
1:AE:43:VAL:HG21	1:HK:57:LEU:HD11	1.96	0.46
2:AF:66:ARG:NH2	2:AH:66:ARG:HH22	2.14	0.46
2:AP:24:CYS:HG	2:AV:80:HIS:CE1	2.31	0.46
2:DU:31:LEU:HD21	2:HR:86:ILE:HD11	1.97	0.46
2:HE:7:LEU:HD21	2:HE:45:MET:HE3	1.97	0.46
1:DS:54:ASP:OD1	2:HR:78:ARG:NH1	2.48	0.46
2:FV:78:ARG:HD2	1:GI:54:ASP:OD1	2.15	0.46
2:DD:11:LYS:HA	2:DD:40:GLY:O	2.15	0.46
1:AY:43:VAL:HG21	1:GY:57:LEU:HD11	1.97	0.46
2:GS:39:SER:O	2:GS:39:SER:OG	2.31	0.46
1:HG:43:VAL:HG21	1:IU:57:LEU:HD11	1.97	0.46
1:CY:54:ASP:OD1	2:JB:78:ARG:NH1	2.49	0.46
2:FV:69:LYS:HE3	2:FV:69:LYS:HA	1.97	0.46
2:IB:18:GLU:OE1	2:IC:74:ARG:NE	2.47	0.46
1:BS:13:THR:OG1	1:GU:79:GLU:OE1	2.33	0.46
2:EW:34:TYR:CE2	2:FF:86:ILE:HG21	2.51	0.46
2:GR:11:LYS:HD3	2:GR:40:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AQ:79:GLU:OE1	1:EE:13:THR:OG1	2.32	0.46
2:AR:80:HIS:HB3	2:AR:83:ILE:HD13	1.98	0.46
2:CN:11:LYS:HA	2:CN:40:GLY:O	2.16	0.46
2:EB:18:GLU:OE1	2:EC:74:ARG:NE	2.48	0.46
2:FF:24:CYS:SG	2:FH:80:HIS:CE1	3.09	0.46
1:FK:57:LEU:HD11	1:GA:43:VAL:HG21	1.98	0.46
1:BS:43:VAL:HG21	1:GU:57:LEU:HD11	1.98	0.45
1:BW:54:ASP:OD1	2:FB:78:ARG:NH1	2.49	0.45
2:CL:68:GLY:O	2:CL:69:LYS:HE2	2.16	0.45
2:CO:39:SER:O	2:CO:39:SER:OG	2.31	0.45
2:BI:32:ILE:HD11	2:BI:47:LYS:HD2	1.98	0.45
1:BC:57:LEU:HD11	1:CI:43:VAL:HG21	1.98	0.45
2:CZ:58:ASP:OD1	2:CZ:59:SER:N	2.48	0.45
2:HN:68:GLY:O	2:HN:69:LYS:HE2	2.16	0.45
2:AH:86:ILE:HG21	2:HM:34:TYR:CE2	2.52	0.45
1:AU:57:LEU:HD11	1:EI:43:VAL:HG21	1.98	0.45
2:EK:7:LEU:HD21	2:EK:45:MET:HE3	1.98	0.45
2:FF:24:CYS:HG	2:FH:80:HIS:CE1	2.34	0.45
2:JD:66:ARG:NH2	2:JF:66:ARG:HH22	2.14	0.45
2:AF:11:LYS:HA	2:AF:40:GLY:O	2.16	0.45
2:DQ:61:VAL:O	2:DQ:65:LYS:HB2	2.17	0.45
2:FI:34:TYR:CE2	2:GL:86:ILE:HG21	2.51	0.45
2:GR:11:LYS:HA	2:GR:40:GLY:O	2.16	0.45
2:HU:7:LEU:HD21	2:HU:45:MET:HE2	1.99	0.45
2:AP:24:CYS:SG	2:AV:80:HIS:CE1	3.09	0.45
2:DX:11:LYS:HD2	2:DX:40:GLY:O	2.17	0.45
1:EY:57:LEU:HD11	1:FG:43:VAL:HG21	1.99	0.45
2:FD:18:GLU:OE1	2:FE:74:ARG:NE	2.48	0.45
2:FP:80:HIS:HB3	2:FP:83:ILE:HD13	1.99	0.45
2:FQ:39:SER:O	2:FQ:39:SER:OG	2.30	0.45
2:GB:11:LYS:HA	2:GB:40:GLY:O	2.16	0.45
2:HP:39:SER:O	2:HP:39:SER:OG	2.32	0.45
2:IZ:11:LYS:HA	2:IZ:40:GLY:O	2.16	0.45
2:BT:37:VAL:HG23	2:BT:37:VAL:O	2.17	0.45
2:FE:31:LEU:HD21	2:GH:86:ILE:HD11	1.98	0.45
2:CR:37:VAL:HG23	2:CR:37:VAL:O	2.17	0.45
2:EZ:11:LYS:HA	2:EZ:40:GLY:O	2.17	0.45
2:HH:37:VAL:O	2:HH:37:VAL:HG23	2.17	0.45
2:AL:86:ILE:HG21	2:HQ:34:TYR:CE2	2.52	0.45
2:BL:80:HIS:HB3	2:BL:83:ILE:HD13	1.99	0.45
1:DK:57:LEU:HD11	1:IM:43:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EG:39:SER:O	2:EG:39:SER:OG	2.31	0.45
2:EW:7:LEU:HD21	2:EW:45:MET:HE2	1.99	0.45
2:CB:80:HIS:HB3	2:CB:83:ILE:HD13	1.99	0.44
2:DZ:4:ALA:HB2	2:DZ:50:VAL:HG22	1.99	0.44
2:EB:37:VAL:HG23	2:EB:37:VAL:O	2.17	0.44
2:FX:37:VAL:O	2:FX:37:VAL:HG23	2.17	0.44
2:FZ:78:ARG:HD2	1:GA:54:ASP:OD1	2.17	0.44
2:GB:37:VAL:O	2:GB:37:VAL:HG23	2.17	0.44
2:GJ:80:HIS:HB3	2:GJ:83:ILE:HD13	2.00	0.44
2:AZ:37:VAL:HG23	2:AZ:37:VAL:O	2.17	0.44
2:BD:37:VAL:HG23	2:BD:37:VAL:O	2.17	0.44
2:DL:37:VAL:HG23	2:DL:37:VAL:O	2.17	0.44
2:DT:37:VAL:HG23	2:DT:37:VAL:O	2.17	0.44
2:IB:37:VAL:HG23	2:IB:37:VAL:O	2.17	0.44
2:IV:37:VAL:HG23	2:IV:37:VAL:O	2.18	0.44
2:JF:9:GLU:HB2	2:JF:43:THR:OG1	2.18	0.44
2:AD:86:ILE:HD11	2:HU:31:LEU:HD21	1.99	0.44
2:AV:37:VAL:HG23	2:AV:37:VAL:O	2.17	0.44
2:DD:80:HIS:HB3	2:DD:83:ILE:HD13	1.99	0.44
2:DL:18:GLU:OE1	2:DM:74:ARG:NE	2.49	0.44
2:DU:61:VAL:O	2:DU:65:LYS:HB2	2.17	0.44
2:HA:7:LEU:HD21	2:HA:45:MET:HE3	1.99	0.44
2:HP:7:LEU:CD2	2:HP:45:MET:HG2	2.48	0.44
2:IJ:80:HIS:HB3	2:IJ:83:ILE:HD13	2.00	0.44
2:IR:37:VAL:HG23	2:IR:37:VAL:O	2.17	0.44
2:JD:37:VAL:HG23	2:JD:37:VAL:O	2.18	0.44
2:AW:34:TYR:CE2	2:EL:86:ILE:HG21	2.52	0.44
2:BP:37:VAL:HG23	2:BP:37:VAL:O	2.18	0.44
2:BV:86:ILE:HG21	2:GW:34:TYR:CE2	2.53	0.44
2:FT:37:VAL:O	2:FT:37:VAL:HG23	2.17	0.44
2:FZ:69:LYS:HE3	2:FZ:69:LYS:HA	1.98	0.44
2:AF:37:VAL:HG23	2:AF:37:VAL:O	2.18	0.44
2:AJ:80:HIS:HB3	2:AJ:83:ILE:HD13	2.00	0.44
2:CF:37:VAL:HG23	2:CF:37:VAL:O	2.17	0.44
2:DP:37:VAL:HG23	2:DP:37:VAL:O	2.18	0.44
2:DT:11:LYS:HD2	2:DT:40:GLY:O	2.17	0.44
2:DU:39:SER:O	2:DU:39:SER:OG	2.31	0.44
2:GF:80:HIS:HB3	2:GF:83:ILE:HD13	2.00	0.44
2:GR:37:VAL:O	2:GR:37:VAL:HG23	2.18	0.44
2:IZ:37:VAL:HG23	2:IZ:37:VAL:O	2.17	0.44
1:AI:27:ILE:HD13	1:AI:27:ILE:HA	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CZ:37:VAL:HG23	2:CZ:37:VAL:O	2.17	0.44
2:ER:18:GLU:OE1	2:ES:74:ARG:NE	2.51	0.44
2:EZ:37:VAL:O	2:EZ:37:VAL:HG23	2.18	0.44
2:GG:61:VAL:O	2:GG:65:LYS:HB2	2.18	0.44
2:IL:11:LYS:HE3	2:IL:69:LYS:HG2	2.00	0.44
2:JE:10:THR:HG22	2:JE:70:VAL:HA	1.98	0.44
1:AI:80:LYS:HB2	1:AM:11:VAL:HB	2.00	0.44
2:BT:11:LYS:HA	2:BT:40:GLY:O	2.18	0.44
2:CN:37:VAL:HG23	2:CN:37:VAL:O	2.17	0.44
2:HD:37:VAL:O	2:HD:37:VAL:HG23	2.18	0.44
2:HY:61:VAL:O	2:HY:65:LYS:HB2	2.18	0.44
2:IF:80:HIS:HB3	2:IF:83:ILE:HD13	2.00	0.44
2:IH:86:ILE:HD13	2:IO:34:TYR:CZ	2.53	0.44
2:IO:61:VAL:O	2:IO:65:LYS:HB2	2.18	0.44
2:AJ:37:VAL:HG23	2:AJ:37:VAL:O	2.18	0.44
2:AL:11:LYS:HE3	2:AL:69:LYS:HG2	2.00	0.44
2:BF:86:ILE:HD11	2:HE:31:LEU:HD21	1.98	0.44
2:BH:37:VAL:HG23	2:BH:37:VAL:O	2.18	0.44
1:BK:27:ILE:HD13	1:BK:27:ILE:HA	1.90	0.44
2:CT:69:LYS:HE3	2:CT:69:LYS:HA	2.00	0.44
2:DX:37:VAL:HG23	2:DX:37:VAL:O	2.18	0.44
2:EF:11:LYS:HA	2:EF:40:GLY:O	2.17	0.44
2:ER:37:VAL:HG23	2:ER:37:VAL:O	2.17	0.44
2:GB:66:ARG:NH2	2:GD:66:ARG:HH22	2.16	0.44
2:GJ:11:LYS:HD2	2:GJ:40:GLY:O	2.18	0.44
2:GJ:37:VAL:O	2:GJ:37:VAL:HG23	2.18	0.44
2:AN:37:VAL:HG23	2:AN:37:VAL:O	2.17	0.44
2:BP:80:HIS:HB3	2:BP:83:ILE:CD1	2.48	0.44
1:CI:27:ILE:HD13	1:CI:27:ILE:HA	1.89	0.44
2:CN:66:ARG:NH2	2:CP:66:ARG:HH22	2.16	0.44
2:DH:7:LEU:CD2	2:DH:45:MET:HG2	2.47	0.44
2:EJ:37:VAL:HG23	2:EJ:37:VAL:O	2.18	0.44
2:EL:11:LYS:HE3	2:EL:69:LYS:HG2	2.00	0.44
2:GZ:37:VAL:O	2:GZ:37:VAL:HG23	2.18	0.44
2:HM:61:VAL:O	2:HM:65:LYS:HB2	2.18	0.44
2:BY:32:ILE:HD11	2:BY:47:LYS:HD2	2.00	0.43
2:BY:61:VAL:O	2:BY:65:LYS:HB2	2.18	0.43
2:CB:37:VAL:HG23	2:CB:37:VAL:O	2.18	0.43
2:CV:37:VAL:HG23	2:CV:37:VAL:O	2.17	0.43
2:DH:39:SER:O	2:DH:39:SER:OG	2.33	0.43
2:FH:37:VAL:HG23	2:FH:37:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GC:39:SER:O	2:GC:39:SER:OG	2.31	0.43
2:GW:61:VAL:O	2:GW:65:LYS:HB2	2.18	0.43
2:HX:80:HIS:HB3	2:HX:83:ILE:HD13	2.00	0.43
2:HY:32:ILE:HD11	2:HY:47:LYS:HD2	2.00	0.43
2:AF:80:HIS:HB3	2:AF:83:ILE:HD13	2.00	0.43
2:AH:68:GLY:C	2:AH:69:LYS:HD2	2.38	0.43
2:CO:11:LYS:HD3	2:CO:69:LYS:HE2	2.01	0.43
2:CX:4:ALA:HB2	2:CX:50:VAL:HG22	1.99	0.43
2:DP:80:HIS:HB3	2:DP:83:ILE:HD13	2.01	0.43
2:DT:11:LYS:HA	2:DT:40:GLY:O	2.18	0.43
2:DV:86:ILE:HG21	2:EO:34:TYR:CE2	2.53	0.43
2:DZ:69:LYS:HE3	2:DZ:69:LYS:HA	2.01	0.43
2:DZ:77:ALA:O	2:DZ:78:ARG:HD2	2.17	0.43
2:EJ:80:HIS:HB3	2:EJ:83:ILE:HD13	2.00	0.43
2:EK:61:VAL:O	2:EK:65:LYS:HB2	2.18	0.43
2:FM:32:ILE:HD11	2:FM:47:LYS:HD2	2.00	0.43
2:GL:68:GLY:O	2:GL:69:LYS:HE2	2.18	0.43
2:GN:7:LEU:CD2	2:GN:45:MET:HG2	2.48	0.43
1:GQ:61:TYR:HE1	1:HW:60:GLU:HG3	1.82	0.43
2:HT:37:VAL:HG23	2:HT:37:VAL:O	2.18	0.43
2:IG:7:LEU:HD21	2:IG:45:MET:HE3	2.00	0.43
2:JA:61:VAL:O	2:JA:65:LYS:HB2	2.18	0.43
2:AS:61:VAL:O	2:AS:65:LYS:HB2	2.18	0.43
2:AT:47:LYS:HE2	2:AT:47:LYS:HB3	1.91	0.43
2:BE:34:TYR:CE2	2:CL:86:ILE:HG21	2.53	0.43
2:BL:37:VAL:HG23	2:BL:37:VAL:O	2.18	0.43
2:CC:61:VAL:O	2:CC:65:LYS:HB2	2.18	0.43
2:IJ:37:VAL:HG23	2:IJ:37:VAL:O	2.17	0.43
1:IY:27:ILE:HD13	1:IY:27:ILE:HA	1.90	0.43
2:AB:37:VAL:HG23	2:AB:37:VAL:O	2.17	0.43
2:BD:18:GLU:OE1	2:BE:74:ARG:NE	2.50	0.43
2:BP:80:HIS:HB3	2:BP:83:ILE:HD13	2.01	0.43
2:FA:34:TYR:CE2	2:FJ:86:ILE:HG21	2.53	0.43
2:FZ:4:ALA:HB2	2:FZ:50:VAL:HG22	2.00	0.43
2:BM:34:TYR:CE2	2:DN:86:ILE:HG21	2.54	0.43
2:BV:86:ILE:HD11	2:GW:31:LEU:HD21	1.99	0.43
2:CJ:80:HIS:HB3	2:CJ:83:ILE:HD13	1.99	0.43
2:DQ:34:TYR:CE2	2:IT:86:ILE:HG21	2.54	0.43
2:EV:37:VAL:HG23	2:EV:37:VAL:O	2.18	0.43
2:FA:61:VAL:O	2:FA:65:LYS:HB2	2.18	0.43
2:FD:37:VAL:O	2:FD:37:VAL:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HB:4:ALA:HB2	2:HB:50:VAL:HG22	2.00	0.43
2:HP:37:VAL:HG23	2:HP:37:VAL:O	2.18	0.43
2:IF:37:VAL:HG23	2:IF:37:VAL:O	2.18	0.43
2:IH:86:ILE:HD13	2:IO:34:TYR:CE1	2.53	0.43
2:AX:69:LYS:HE3	2:AX:69:LYS:HA	2.00	0.43
2:BB:69:LYS:HE3	2:BB:69:LYS:HA	2.00	0.43
2:BH:80:HIS:HB3	2:BH:83:ILE:HD13	2.00	0.43
1:BO:11:VAL:HB	1:GQ:80:LYS:HB2	2.00	0.43
2:BT:80:HIS:HB3	2:BT:83:ILE:HD13	2.01	0.43
2:DH:37:VAL:HG23	2:DH:37:VAL:O	2.18	0.43
2:GN:37:VAL:O	2:GN:37:VAL:HG23	2.18	0.43
1:AQ:57:LEU:HD11	1:EE:43:VAL:HG21	2.00	0.43
1:BS:54:ASP:OD1	2:DJ:78:ARG:HD2	2.19	0.43
2:DD:37:VAL:HG23	2:DD:37:VAL:O	2.18	0.43
2:DL:80:HIS:HB3	2:DL:83:ILE:HD13	2.01	0.43
1:DS:79:GLU:OE1	1:HO:13:THR:OG1	2.33	0.43
2:HD:80:HIS:HB3	2:HD:83:ILE:HD13	2.00	0.43
2:HP:80:HIS:HB3	2:HP:83:ILE:CD1	2.49	0.43
2:AG:11:LYS:HD3	2:AG:69:LYS:HE2	2.01	0.43
2:AK:11:LYS:NZ	2:AK:40:GLY:HA3	2.34	0.43
2:AL:47:LYS:HE2	2:AL:47:LYS:HB3	1.91	0.43
1:AQ:27:ILE:HD13	1:AQ:27:ILE:HA	1.89	0.43
2:BR:4:ALA:HB2	2:BR:50:VAL:HG22	2.00	0.43
2:BT:11:LYS:HD2	2:BT:40:GLY:O	2.18	0.43
2:DE:61:VAL:O	2:DE:65:LYS:HB2	2.19	0.43
2:DN:69:LYS:HE3	2:DN:69:LYS:HA	2.01	0.43
2:EF:37:VAL:HG23	2:EF:37:VAL:O	2.18	0.43
2:EO:61:VAL:O	2:EO:65:LYS:HB2	2.18	0.43
1:FG:27:ILE:HD13	1:FG:27:ILE:HA	1.90	0.43
1:FK:27:ILE:HD13	1:FK:27:ILE:HA	1.89	0.43
2:FP:37:VAL:O	2:FP:37:VAL:HG23	2.18	0.43
2:FX:80:HIS:HB3	2:FX:83:ILE:CD1	2.49	0.43
2:GP:69:LYS:HE3	2:GP:69:LYS:HA	2.01	0.43
2:HH:18:GLU:OE1	2:HI:74:ARG:NE	2.49	0.43
2:HP:11:LYS:HA	2:HP:40:GLY:O	2.19	0.43
2:IB:80:HIS:HB3	2:IB:83:ILE:HD13	2.01	0.43
2:IH:47:LYS:HE2	2:IH:47:LYS:HB3	1.88	0.43
1:AA:43:VAL:HG21	1:HS:57:LEU:HD11	2.00	0.43
1:AI:54:ASP:OD1	2:AP:78:ARG:HD2	2.18	0.43
2:BU:61:VAL:O	2:BU:65:LYS:HB2	2.19	0.43
2:CN:80:HIS:HB3	2:CN:83:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DD:80:HIS:HB3	2:DD:83:ILE:CD1	2.49	0.43
1:FC:27:ILE:HD13	1:FC:27:ILE:HA	1.90	0.43
2:FT:80:HIS:HB3	2:FT:83:ILE:HD13	2.01	0.43
2:GK:61:VAL:O	2:GK:65:LYS:HB2	2.19	0.43
2:HL:66:ARG:NH2	2:HN:66:ARG:HH22	2.17	0.43
2:HL:80:HIS:HB3	2:HL:83:ILE:HD13	2.00	0.43
2:ID:69:LYS:HA	2:ID:69:LYS:HE3	2.01	0.43
2:IR:80:HIS:HB3	2:IR:83:ILE:HD13	2.01	0.43
2:AR:80:HIS:HB3	2:AR:83:ILE:CD1	2.49	0.43
2:AZ:80:HIS:HB3	2:AZ:83:ILE:HD13	2.01	0.43
1:CM:27:ILE:HD13	1:CM:27:ILE:HA	1.89	0.43
2:CS:34:TYR:CE2	2:DB:86:ILE:HG21	2.54	0.43
2:ED:69:LYS:HE3	2:ED:69:LYS:HA	2.01	0.43
2:EJ:11:LYS:HD2	2:EJ:40:GLY:O	2.19	0.43
2:EV:80:HIS:HB3	2:EV:83:ILE:HD13	2.00	0.43
2:FA:31:LEU:HD21	2:FJ:86:ILE:HD11	2.01	0.43
2:FD:80:HIS:HB3	2:FD:83:ILE:HD13	2.01	0.43
2:FL:66:ARG:NH2	2:FN:66:ARG:HH22	2.17	0.43
2:FZ:68:GLY:C	2:FZ:69:LYS:HD2	2.40	0.43
2:GN:11:LYS:HD3	2:GN:40:GLY:O	2.19	0.43
2:GV:80:HIS:HB3	2:GV:83:ILE:HD13	2.01	0.43
2:IV:80:HIS:HB3	2:IV:83:ILE:HD13	2.01	0.43
2:AH:86:ILE:HD13	2:HM:34:TYR:CE1	2.54	0.42
1:AM:57:LEU:HD11	1:EM:43:VAL:HG21	2.01	0.42
2:BF:69:LYS:HE3	2:BF:69:LYS:HA	2.01	0.42
1:CA:27:ILE:HD13	1:CA:27:ILE:HA	1.89	0.42
1:CA:57:LEU:HD11	1:EQ:43:VAL:HG21	2.01	0.42
2:CK:61:VAL:O	2:CK:65:LYS:HB2	2.19	0.42
2:DX:80:HIS:HB3	2:DX:83:ILE:CD1	2.49	0.42
2:ED:86:ILE:HG21	2:EK:34:TYR:CE2	2.54	0.42
1:EM:27:ILE:HD13	1:EM:27:ILE:HA	1.90	0.42
2:EO:32:ILE:HD11	2:EO:47:LYS:HD2	2.01	0.42
2:FM:61:VAL:O	2:FM:65:LYS:HB2	2.19	0.42
1:GQ:14:GLN:HG2	1:HW:77:ILE:HD12	2.01	0.42
2:HJ:69:LYS:HA	2:HJ:69:LYS:HE3	2.01	0.42
2:HM:32:ILE:HD11	2:HM:47:LYS:HD2	2.01	0.42
2:IG:61:VAL:O	2:IG:65:LYS:HB2	2.19	0.42
2:AP:69:LYS:HE3	2:AP:69:LYS:HA	2.01	0.42
2:CK:32:ILE:HD11	2:CK:47:LYS:HD2	2.01	0.42
2:EC:34:TYR:CE2	2:HN:86:ILE:HG21	2.54	0.42
2:EF:7:LEU:HD21	2:EF:45:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EG:61:VAL:O	2:EG:65:LYS:HB2	2.19	0.42
2:ET:69:LYS:CE	2:ET:69:LYS:HA	2.50	0.42
2:FQ:61:VAL:O	2:FQ:65:LYS:HB2	2.19	0.42
2:HF:86:ILE:HD13	2:JE:34:TYR:CE1	2.54	0.42
2:IK:61:VAL:O	2:IK:65:LYS:HB2	2.19	0.42
2:IN:80:HIS:HB3	2:IN:83:ILE:HD13	2.01	0.42
1:AA:27:ILE:HD13	1:AA:27:ILE:HA	1.90	0.42
2:AB:80:HIS:HB3	2:AB:83:ILE:HD13	2.01	0.42
2:CB:80:HIS:HB3	2:CB:83:ILE:CD1	2.49	0.42
2:CX:68:GLY:C	2:CX:69:LYS:HD2	2.39	0.42
1:DO:54:ASP:OD1	2:IT:78:ARG:HD2	2.19	0.42
2:DT:80:HIS:HB3	2:DT:83:ILE:HD13	2.02	0.42
2:GG:32:ILE:HD11	2:GG:47:LYS:HD2	2.01	0.42
1:GM:27:ILE:HD13	1:GM:27:ILE:HA	1.89	0.42
2:GS:61:VAL:O	2:GS:65:LYS:HB2	2.19	0.42
2:HJ:69:LYS:HA	2:HJ:69:LYS:CE	2.50	0.42
2:HP:80:HIS:HB3	2:HP:83:ILE:HD13	2.02	0.42
2:HR:4:ALA:HB2	2:HR:50:VAL:HG22	2.01	0.42
2:IS:32:ILE:HD11	2:IS:47:LYS:HD2	2.02	0.42
2:AP:69:LYS:HA	2:AP:69:LYS:CE	2.50	0.42
2:BH:80:HIS:HB3	2:BH:83:ILE:CD1	2.49	0.42
2:CH:86:ILE:HG21	2:FQ:34:TYR:CE2	2.54	0.42
2:CK:34:TYR:CE2	2:DF:86:ILE:HG21	2.54	0.42
1:CM:57:LEU:HD11	1:CU:43:VAL:HG21	2.00	0.42
2:DJ:4:ALA:HB2	2:DJ:50:VAL:HG22	2.00	0.42
1:DS:77:ILE:HG21	2:HR:78:ARG:HE	1.83	0.42
2:ET:69:LYS:HA	2:ET:69:LYS:HE3	2.01	0.42
2:FA:7:LEU:HD21	2:FA:45:MET:HE2	2.01	0.42
2:GC:61:VAL:O	2:GC:65:LYS:HB2	2.20	0.42
2:AG:61:VAL:O	2:AG:65:LYS:HB2	2.19	0.42
2:AS:32:ILE:HD11	2:AS:47:LYS:HD2	2.01	0.42
2:AX:4:ALA:HB2	2:AX:50:VAL:HG22	2.00	0.42
2:DP:80:HIS:HB3	2:DP:83:ILE:CD1	2.49	0.42
2:DU:34:TYR:CE2	2:HR:86:ILE:HG21	2.54	0.42
2:EJ:80:HIS:HB3	2:EJ:83:ILE:CD1	2.50	0.42
2:EW:61:VAL:O	2:EW:65:LYS:HB2	2.19	0.42
2:GW:11:LYS:HD3	2:GW:69:LYS:HE2	2.00	0.42
2:HB:68:GLY:C	2:HB:69:LYS:HD2	2.39	0.42
2:HD:80:HIS:HB3	2:HD:83:ILE:CD1	2.49	0.42
1:IM:27:ILE:HD13	1:IM:27:ILE:HA	1.90	0.42
2:AJ:80:HIS:HB3	2:AJ:83:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BM:61:VAL:O	2:BM:65:LYS:HB2	2.20	0.42
2:CB:11:LYS:HA	2:CB:40:GLY:O	2.20	0.42
2:CH:4:ALA:HB2	2:CH:50:VAL:HG22	2.02	0.42
1:CQ:1:MET:HB2	1:CY:43:VAL:HB	2.02	0.42
2:FF:47:LYS:HE2	2:FF:47:LYS:HB3	1.90	0.42
2:FH:80:HIS:HB3	2:FH:83:ILE:CD1	2.50	0.42
2:FU:32:ILE:HD11	2:FU:47:LYS:HD2	2.02	0.42
2:HX:80:HIS:HB3	2:HX:83:ILE:CD1	2.50	0.42
2:CJ:80:HIS:HB3	2:CJ:83:ILE:CD1	2.50	0.42
2:FI:61:VAL:O	2:FI:65:LYS:HB2	2.19	0.42
2:FV:68:GLY:C	2:FV:69:LYS:HD2	2.40	0.42
1:FW:43:VAL:HG21	1:GA:57:LEU:HD11	2.02	0.42
2:FX:80:HIS:HB3	2:FX:83:ILE:HD13	2.02	0.42
2:HL:80:HIS:HB3	2:HL:83:ILE:CD1	2.50	0.42
2:IB:80:HIS:HB3	2:IB:83:ILE:CD1	2.50	0.42
2:AG:34:TYR:CE2	2:AX:86:ILE:HG21	2.54	0.42
2:AK:61:VAL:O	2:AK:65:LYS:HB2	2.19	0.42
2:AR:66:ARG:NH2	2:AT:66:ARG:HH22	2.17	0.42
2:AZ:80:HIS:HB3	2:AZ:83:ILE:CD1	2.49	0.42
2:BI:61:VAL:O	2:BI:65:LYS:HB2	2.19	0.42
2:CB:11:LYS:HD2	2:CB:40:GLY:O	2.19	0.42
2:CT:69:LYS:HA	2:CT:69:LYS:CE	2.50	0.42
2:CV:80:HIS:HB3	2:CV:83:ILE:CD1	2.50	0.42
2:DA:32:ILE:HD11	2:DA:47:LYS:HD2	2.01	0.42
2:DM:32:ILE:HD11	2:DM:47:LYS:HD2	2.02	0.42
2:DR:4:ALA:HB2	2:DR:50:VAL:HG22	2.02	0.42
2:FH:11:LYS:HE2	2:FH:40:GLY:HA3	2.02	0.42
2:FL:80:HIS:HB3	2:FL:83:ILE:CD1	2.50	0.42
2:FR:86:ILE:HG21	2:GG:34:TYR:CE2	2.55	0.42
1:HG:13:THR:OG1	1:IU:79:GLU:OE1	2.35	0.42
2:HQ:61:VAL:O	2:HQ:65:LYS:HB2	2.20	0.42
2:IT:69:LYS:HA	2:IT:69:LYS:HE3	2.01	0.42
2:AC:32:ILE:HD11	2:AC:47:LYS:HD2	2.02	0.42
2:CN:80:HIS:HB3	2:CN:83:ILE:HD13	2.01	0.42
2:DL:80:HIS:HB3	2:DL:83:ILE:CD1	2.50	0.42
2:DN:69:LYS:HA	2:DN:69:LYS:CE	2.50	0.42
1:DW:43:VAL:HG21	1:EE:57:LEU:HD11	2.02	0.42
2:EP:4:ALA:HB2	2:EP:50:VAL:HG22	2.02	0.42
1:FG:80:LYS:HB2	1:GI:11:VAL:HB	2.02	0.42
2:FI:31:LEU:HD21	2:GL:86:ILE:HD11	2.01	0.42
2:FL:11:LYS:HD2	2:FL:40:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FT:80:HIS:HB3	2:FT:83:ILE:CD1	2.50	0.42
1:GU:27:ILE:HD13	1:GU:27:ILE:HA	1.90	0.42
1:HO:27:ILE:HD13	1:HO:27:ILE:HA	1.90	0.42
2:ID:69:LYS:HA	2:ID:69:LYS:CE	2.50	0.42
2:IR:80:HIS:HB3	2:IR:83:ILE:CD1	2.50	0.42
2:AF:80:HIS:HB3	2:AF:83:ILE:CD1	2.50	0.42
2:DA:61:VAL:O	2:DA:65:LYS:HB2	2.19	0.42
2:DH:11:LYS:HA	2:DH:40:GLY:O	2.19	0.42
2:DZ:47:LYS:HE2	2:DZ:47:LYS:HB3	1.96	0.42
2:EJ:11:LYS:HA	2:EJ:40:GLY:O	2.20	0.42
2:FD:66:ARG:NH2	2:FF:66:ARG:HH22	2.18	0.42
2:FJ:4:ALA:HB2	2:FJ:50:VAL:HG22	2.01	0.42
2:FZ:86:ILE:HG21	2:GC:34:TYR:CE2	2.54	0.42
2:GJ:80:HIS:HB3	2:GJ:83:ILE:CD1	2.49	0.42
2:IJ:80:HIS:HB3	2:IJ:83:ILE:CD1	2.49	0.42
2:IV:80:HIS:HB3	2:IV:83:ILE:CD1	2.49	0.42
2:AN:80:HIS:HB3	2:AN:83:ILE:HD13	2.01	0.41
2:BB:68:GLY:C	2:BB:69:LYS:HD2	2.41	0.41
2:BL:80:HIS:HB3	2:BL:83:ILE:CD1	2.49	0.41
2:BP:11:LYS:HA	2:BP:40:GLY:O	2.19	0.41
2:CD:47:LYS:HE2	2:CD:47:LYS:HB3	1.93	0.41
2:CO:61:VAL:O	2:CO:65:LYS:HB2	2.20	0.41
2:CS:32:ILE:HD11	2:CS:47:LYS:HD2	2.02	0.41
2:CW:34:TYR:CE2	2:IX:86:ILE:HG21	2.55	0.41
1:DG:27:ILE:HD13	1:DG:27:ILE:HA	1.90	0.41
1:DW:57:LEU:HD11	1:HS:43:VAL:HG21	2.01	0.41
2:EN:11:LYS:HE2	2:EN:40:GLY:HA3	2.02	0.41
2:ES:61:VAL:O	2:ES:65:LYS:HB2	2.20	0.41
2:FH:80:HIS:HB3	2:FH:83:ILE:HD13	2.02	0.41
2:FL:80:HIS:HB3	2:FL:83:ILE:HD13	2.01	0.41
2:FP:80:HIS:HB3	2:FP:83:ILE:CD1	2.49	0.41
2:FQ:11:LYS:HD3	2:FQ:69:LYS:HE2	2.01	0.41
2:HF:4:ALA:HB2	2:HF:50:VAL:HG22	2.02	0.41
2:HT:80:HIS:HB3	2:HT:83:ILE:CD1	2.49	0.41
2:HT:80:HIS:HB3	2:HT:83:ILE:HD13	2.01	0.41
2:HV:4:ALA:HB2	2:HV:50:VAL:HG22	2.01	0.41
2:ID:47:LYS:HE2	2:ID:47:LYS:HB3	1.94	0.41
2:JB:4:ALA:HB2	2:JB:50:VAL:HG22	2.02	0.41
2:AV:11:LYS:HD2	2:AV:40:GLY:O	2.20	0.41
2:BF:69:LYS:HA	2:BF:69:LYS:CE	2.50	0.41
2:BU:7:LEU:HD21	2:BU:45:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DI:61:VAL:O	2:DI:65:LYS:HB2	2.21	0.41
2:DN:13:LEU:O	2:DN:17:ILE:HG13	2.20	0.41
1:DO:79:GLU:OE1	1:IQ:13:THR:OG1	2.36	0.41
2:DZ:78:ARG:NH1	1:EE:77:ILE:HG21	2.34	0.41
2:DZ:86:ILE:HG21	2:EG:34:TYR:CE2	2.55	0.41
2:ER:80:HIS:HB3	2:ER:83:ILE:HD13	2.01	0.41
2:EV:80:HIS:HB3	2:EV:83:ILE:CD1	2.49	0.41
2:FJ:68:GLY:O	2:FJ:69:LYS:HD2	2.20	0.41
2:IL:47:LYS:HE2	2:IL:47:LYS:HB3	1.92	0.41
2:IT:4:ALA:HB2	2:IT:50:VAL:HG22	2.02	0.41
2:AO:34:TYR:CE2	2:EP:86:ILE:HG21	2.56	0.41
2:BB:47:LYS:HE2	2:BB:47:LYS:HB3	1.95	0.41
1:BO:27:ILE:HD13	1:BO:27:ILE:HA	1.89	0.41
2:BR:68:GLY:O	2:BR:69:LYS:HD2	2.20	0.41
2:DE:39:SER:O	2:DE:39:SER:OG	2.31	0.41
2:FE:61:VAL:O	2:FE:65:LYS:HB2	2.20	0.41
2:GB:80:HIS:HB3	2:GB:83:ILE:CD1	2.50	0.41
2:GX:4:ALA:HB2	2:GX:50:VAL:HG22	2.01	0.41
2:GZ:11:LYS:HA	2:GZ:40:GLY:O	2.20	0.41
2:HE:61:VAL:O	2:HE:65:LYS:HB2	2.20	0.41
2:IC:7:LEU:HD21	2:IC:45:MET:HE3	2.02	0.41
2:CJ:11:LYS:HD2	2:CJ:40:GLY:O	2.20	0.41
2:DV:86:ILE:HD13	2:EO:34:TYR:CE1	2.55	0.41
2:DZ:69:LYS:HA	2:DZ:69:LYS:CE	2.50	0.41
2:EB:80:HIS:HB3	2:EB:83:ILE:HD13	2.01	0.41
2:ED:69:LYS:HA	2:ED:69:LYS:CE	2.50	0.41
2:EN:80:HIS:HB3	2:EN:83:ILE:CD1	2.51	0.41
2:FL:11:LYS:HA	2:FL:40:GLY:O	2.20	0.41
1:FW:27:ILE:HD13	1:FW:27:ILE:HA	1.90	0.41
2:GF:80:HIS:HB3	2:GF:83:ILE:CD1	2.50	0.41
2:GJ:11:LYS:HA	2:GJ:40:GLY:O	2.20	0.41
2:GP:4:ALA:HB2	2:GP:50:VAL:HG22	2.01	0.41
2:IT:69:LYS:HA	2:IT:69:LYS:CE	2.50	0.41
2:IW:61:VAL:O	2:IW:65:LYS:HB2	2.19	0.41
1:JC:27:ILE:HD13	1:JC:27:ILE:HA	1.89	0.41
2:JE:80:HIS:HB3	2:JE:83:ILE:HG12	2.03	0.41
2:AD:69:LYS:HE3	2:AD:69:LYS:HA	2.01	0.41
2:BX:11:LYS:HA	2:BX:40:GLY:O	2.21	0.41
2:DM:34:TYR:CE2	2:IP:86:ILE:HG21	2.56	0.41
2:EF:80:HIS:HB3	2:EF:83:ILE:HD13	2.03	0.41
2:FF:24:CYS:SG	2:FH:80:HIS:ND1	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FH:11:LYS:HA	2:FH:40:GLY:O	2.21	0.41
2:FL:69:LYS:HB3	2:FL:69:LYS:HE2	1.86	0.41
2:GK:45:MET:HE2	2:GK:45:MET:HB3	1.93	0.41
2:IT:13:LEU:O	2:IT:17:ILE:HG13	2.20	0.41
2:BU:34:TYR:CE2	2:DJ:86:ILE:HG21	2.56	0.41
2:CG:61:VAL:O	2:CG:65:LYS:HB2	2.20	0.41
1:DS:23:ASN:HB2	1:DS:46:ASP:HB3	2.03	0.41
1:EA:23:ASN:HB2	1:EA:46:ASP:HB3	2.03	0.41
1:EI:23:ASN:HB2	1:EI:46:ASP:HB3	2.03	0.41
2:EZ:80:HIS:HB3	2:EZ:83:ILE:CD1	2.50	0.41
2:FX:58:ASP:OD1	2:FX:58:ASP:N	2.54	0.41
2:GB:80:HIS:HB3	2:GB:83:ILE:HD13	2.03	0.41
2:GP:86:ILE:HG21	2:IG:34:TYR:CE2	2.56	0.41
1:HC:23:ASN:HB2	1:HC:46:ASP:HB3	2.03	0.41
2:HX:11:LYS:HA	2:HX:40:GLY:O	2.21	0.41
1:IE:23:ASN:HB2	1:IE:46:ASP:HB3	2.03	0.41
2:IF:7:LEU:HD21	2:IF:45:MET:HE2	2.02	0.41
2:JD:80:HIS:HB3	2:JD:83:ILE:CD1	2.50	0.41
2:AB:80:HIS:HB3	2:AB:83:ILE:CD1	2.50	0.41
2:AO:61:VAL:O	2:AO:65:LYS:HB2	2.21	0.41
2:AV:11:LYS:HA	2:AV:40:GLY:O	2.20	0.41
1:BC:23:ASN:HB2	1:BC:46:ASP:HB3	2.03	0.41
1:BS:23:ASN:HB2	1:BS:46:ASP:HB3	2.03	0.41
1:CE:23:ASN:HB2	1:CE:46:ASP:HB3	2.03	0.41
2:CF:11:LYS:HA	2:CF:40:GLY:O	2.20	0.41
2:CS:61:VAL:O	2:CS:65:LYS:HB2	2.21	0.41
1:DO:27:ILE:HD13	1:DO:27:ILE:HA	1.90	0.41
2:DT:80:HIS:HB3	2:DT:83:ILE:CD1	2.50	0.41
1:DW:23:ASN:HB2	1:DW:46:ASP:HB3	2.03	0.41
2:DX:80:HIS:HB3	2:DX:83:ILE:HD13	2.02	0.41
2:FB:4:ALA:HB2	2:FB:50:VAL:HG22	2.03	0.41
2:FD:80:HIS:HB3	2:FD:83:ILE:CD1	2.50	0.41
1:FG:23:ASN:HB2	1:FG:46:ASP:HB3	2.03	0.41
2:FN:4:ALA:HB2	2:FN:50:VAL:HG22	2.03	0.41
1:GA:23:ASN:HB2	1:GA:46:ASP:HB3	2.03	0.41
1:GI:27:ILE:HD13	1:GI:27:ILE:HA	1.90	0.41
2:HD:11:LYS:HA	2:HD:40:GLY:O	2.21	0.41
2:HL:11:LYS:HD2	2:HL:40:GLY:O	2.20	0.41
2:ID:4:ALA:HB2	2:ID:50:VAL:HG22	2.02	0.41
2:AN:80:HIS:HB3	2:AN:83:ILE:CD1	2.50	0.41
2:CJ:25:LYS:O	2:EB:78:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:80:HIS:HB3	2:EB:83:ILE:CD1	2.51	0.41
2:EF:80:HIS:HB3	2:EF:83:ILE:CD1	2.50	0.41
2:ER:80:HIS:HB3	2:ER:83:ILE:CD1	2.50	0.41
1:EU:23:ASN:HB2	1:EU:46:ASP:HB3	2.03	0.41
2:FV:13:LEU:O	2:FV:17:ILE:HG13	2.20	0.41
1:GE:27:ILE:HD13	1:GE:27:ILE:HA	1.90	0.41
2:GR:58:ASP:OD1	2:GR:58:ASP:N	2.54	0.41
2:GV:11:LYS:HA	2:GV:40:GLY:O	2.20	0.41
2:IN:11:LYS:HA	2:IN:40:GLY:O	2.21	0.41
2:IP:47:LYS:HE2	2:IP:47:LYS:HB3	1.90	0.41
2:AB:66:ARG:NH2	2:AD:66:ARG:HH22	2.19	0.41
2:AD:4:ALA:HB2	2:AD:50:VAL:HG22	2.02	0.41
1:AM:23:ASN:HB2	1:AM:46:ASP:HB3	2.03	0.41
2:AV:58:ASP:OD1	2:AV:58:ASP:N	2.54	0.41
2:BF:13:LEU:O	2:BF:17:ILE:HG13	2.21	0.41
1:BK:23:ASN:HB2	1:BK:46:ASP:HB3	2.03	0.41
1:BO:23:ASN:HB2	1:BO:46:ASP:HB3	2.03	0.41
2:DD:58:ASP:OD1	2:DD:58:ASP:N	2.54	0.41
2:DE:34:TYR:CE2	2:JF:86:ILE:HG21	2.56	0.41
2:DM:7:LEU:HD21	2:DM:45:MET:HE3	2.03	0.41
1:EE:23:ASN:HB2	1:EE:46:ASP:HB3	2.03	0.41
2:EN:80:HIS:HB3	2:EN:83:ILE:HD13	2.02	0.41
2:ES:7:LEU:HD21	2:ES:45:MET:HE3	2.02	0.41
1:EY:61:TYR:CE2	1:FG:61:TYR:CE2	3.09	0.41
2:FI:80:HIS:HB3	2:FI:83:ILE:HG12	2.02	0.41
1:FO:23:ASN:HB2	1:FO:46:ASP:HB3	2.03	0.41
2:GJ:58:ASP:OD1	2:GJ:58:ASP:N	2.54	0.41
1:GQ:23:ASN:HB2	1:GQ:46:ASP:HB3	2.03	0.41
2:GV:11:LYS:HE2	2:GV:40:GLY:HA3	2.02	0.41
1:HG:23:ASN:HB2	1:HG:46:ASP:HB3	2.03	0.41
2:HI:32:ILE:HD11	2:HI:47:LYS:HD2	2.03	0.41
1:HS:23:ASN:HB2	1:HS:46:ASP:HB3	2.03	0.41
2:HU:61:VAL:O	2:HU:65:LYS:HB2	2.20	0.41
2:HZ:47:LYS:HE2	2:HZ:47:LYS:HB3	1.90	0.41
2:JD:80:HIS:HB3	2:JD:83:ILE:HD13	2.02	0.41
2:AC:34:TYR:CE2	2:AT:86:ILE:HG21	2.56	0.41
2:AX:69:LYS:HA	2:AX:69:LYS:CE	2.50	0.41
2:BA:61:VAL:O	2:BA:65:LYS:HB2	2.20	0.41
2:BE:32:ILE:HD11	2:BE:47:LYS:HD2	2.03	0.41
2:BJ:4:ALA:HB2	2:BJ:50:VAL:HG22	2.03	0.41
2:BN:4:ALA:HB2	2:BN:50:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BT:58:ASP:OD1	2:BT:58:ASP:N	2.54	0.41
2:BU:39:SER:O	2:BU:39:SER:OG	2.31	0.41
2:CF:80:HIS:HB3	2:CF:83:ILE:CD1	2.51	0.41
2:CV:11:LYS:HA	2:CV:40:GLY:O	2.21	0.41
2:CW:61:VAL:O	2:CW:65:LYS:HB2	2.21	0.41
2:DB:4:ALA:HB2	2:DB:50:VAL:HG22	2.03	0.41
2:DH:80:HIS:HB3	2:DH:83:ILE:CD1	2.50	0.41
2:DZ:13:LEU:O	2:DZ:17:ILE:HG13	2.22	0.41
2:EB:7:LEU:HD21	2:EB:45:MET:HE2	2.03	0.41
1:EQ:23:ASN:HB2	1:EQ:46:ASP:HB3	2.03	0.41
2:EV:11:LYS:HA	2:EV:40:GLY:O	2.21	0.41
1:EY:23:ASN:HB2	1:EY:46:ASP:HB3	2.03	0.41
1:EY:60:GLU:HB2	1:FG:61:TYR:CE1	2.56	0.41
1:GU:23:ASN:HB2	1:GU:46:ASP:HB3	2.03	0.41
1:IM:23:ASN:HB2	1:IM:46:ASP:HB3	2.03	0.41
2:AJ:11:LYS:HA	2:AJ:40:GLY:O	2.21	0.40
1:AU:27:ILE:HD13	1:AU:27:ILE:HA	1.89	0.40
1:BK:57:LEU:HD11	1:DK:43:VAL:HG21	2.03	0.40
1:BO:57:LEU:HD11	1:DO:43:VAL:HG21	2.01	0.40
2:BY:31:LEU:HD21	2:FB:86:ILE:HD11	2.03	0.40
2:BY:69:LYS:HB3	2:BY:69:LYS:HE2	1.84	0.40
2:CF:58:ASP:OD1	2:CF:58:ASP:N	2.54	0.40
1:CQ:23:ASN:HB2	1:CQ:46:ASP:HB3	2.03	0.40
2:CZ:55:ALA:O	2:CZ:58:ASP:OD1	2.39	0.40
2:CZ:80:HIS:HB3	2:CZ:83:ILE:CD1	2.51	0.40
1:EQ:57:LEU:HD11	1:FK:43:VAL:HG21	2.02	0.40
1:EY:77:ILE:HG21	2:FJ:78:ARG:HH21	1.85	0.40
2:FH:58:ASP:OD1	2:FH:58:ASP:N	2.54	0.40
2:GT:4:ALA:HB2	2:GT:50:VAL:HG22	2.03	0.40
2:GZ:39:SER:O	2:GZ:39:SER:OG	2.30	0.40
2:HL:11:LYS:HA	2:HL:40:GLY:O	2.20	0.40
2:IO:32:ILE:HD11	2:IO:47:LYS:HD2	2.01	0.40
2:IZ:80:HIS:HB3	2:IZ:83:ILE:CD1	2.51	0.40
2:JD:11:LYS:HA	2:JD:40:GLY:O	2.21	0.40
2:BL:11:LYS:HA	2:BL:40:GLY:O	2.20	0.40
2:CV:11:LYS:HE2	2:CV:40:GLY:HA3	2.02	0.40
2:EC:31:LEU:HD21	2:HN:86:ILE:HD11	2.02	0.40
2:FN:47:LYS:HE2	2:FN:47:LYS:HB3	1.93	0.40
2:GJ:66:ARG:NH2	2:GL:66:ARG:HH22	2.19	0.40
2:GV:80:HIS:HB3	2:GV:83:ILE:CD1	2.50	0.40
2:GW:32:ILE:HD11	2:GW:47:LYS:HD2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IF:80:HIS:HB3	2:IF:83:ILE:CD1	2.50	0.40
1:II:23:ASN:HB2	1:II:46:ASP:HB3	2.03	0.40
1:IY:23:ASN:HB2	1:IY:46:ASP:HB3	2.03	0.40
2:AG:39:SER:O	2:AG:39:SER:OG	2.31	0.40
2:AN:18:GLU:OE1	2:AO:74:ARG:NE	2.49	0.40
2:AO:32:ILE:HD11	2:AO:47:LYS:HD2	2.03	0.40
2:AX:47:LYS:HE2	2:AX:47:LYS:HB3	1.94	0.40
2:BB:86:ILE:HG21	2:HA:34:TYR:CE2	2.56	0.40
2:BJ:47:LYS:HE2	2:BJ:47:LYS:HB3	1.90	0.40
2:BP:58:ASP:N	2:BP:58:ASP:OD1	2.54	0.40
2:BT:80:HIS:HB3	2:BT:83:ILE:CD1	2.50	0.40
2:CV:80:HIS:HB3	2:CV:83:ILE:HD13	2.02	0.40
1:DG:23:ASN:HB2	1:DG:46:ASP:HB3	2.03	0.40
2:DQ:45:MET:HB3	2:DQ:45:MET:HE2	1.92	0.40
2:DY:61:VAL:O	2:DY:65:LYS:HB2	2.21	0.40
2:EN:11:LYS:HA	2:EN:40:GLY:O	2.21	0.40
2:GN:80:HIS:HB3	2:GN:83:ILE:CD1	2.50	0.40
2:GP:69:LYS:HA	2:GP:69:LYS:CE	2.50	0.40
2:GS:7:LEU:HD21	2:GS:45:MET:HE3	2.03	0.40
2:GZ:80:HIS:HB3	2:GZ:83:ILE:CD1	2.51	0.40
2:HI:61:VAL:O	2:HI:65:LYS:HB2	2.22	0.40
1:AA:23:ASN:HB2	1:AA:46:ASP:HB3	2.03	0.40
2:AC:61:VAL:O	2:AC:65:LYS:HB2	2.21	0.40
1:AI:57:LEU:HD11	1:AM:43:VAL:HG21	2.02	0.40
2:AW:61:VAL:O	2:AW:65:LYS:HB2	2.22	0.40
2:BE:31:LEU:HD21	2:CL:86:ILE:HD11	2.02	0.40
2:BH:11:LYS:HA	2:BH:40:GLY:O	2.22	0.40
1:CM:23:ASN:HB2	1:CM:46:ASP:HB3	2.03	0.40
2:CR:80:HIS:HB3	2:CR:83:ILE:CD1	2.50	0.40
2:CW:80:HIS:HB3	2:CW:83:ILE:HG12	2.03	0.40
2:EC:32:ILE:HD11	2:EC:47:LYS:HD2	2.04	0.40
2:EP:47:LYS:HE2	2:EP:47:LYS:HB3	1.92	0.40
1:EQ:27:ILE:HD13	1:EQ:27:ILE:HA	1.89	0.40
2:EZ:80:HIS:HB3	2:EZ:83:ILE:HD13	2.02	0.40
1:GA:27:ILE:HD13	1:GA:27:ILE:HA	1.89	0.40
2:GF:11:LYS:HA	2:GF:40:GLY:O	2.21	0.40
2:GX:86:ILE:HG21	2:IC:34:TYR:CE2	2.57	0.40
2:IB:66:ARG:NH2	2:ID:66:ARG:HH22	2.19	0.40
2:IF:58:ASP:OD1	2:IF:58:ASP:N	2.54	0.40
2:IN:80:HIS:HB3	2:IN:83:ILE:CD1	2.50	0.40
2:AD:69:LYS:HA	2:AD:69:LYS:CE	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BR:13:LEU:O	2:BR:17:ILE:HG13	2.21	0.40
2:DI:34:TYR:CE2	2:IL:86:ILE:HG21	2.56	0.40
2:DJ:69:LYS:HA	2:DJ:69:LYS:HD3	1.78	0.40
1:DS:27:ILE:HD13	1:DS:27:ILE:HA	1.89	0.40
2:DX:58:ASP:N	2:DX:58:ASP:OD1	2.53	0.40
2:FY:61:VAL:O	2:FY:65:LYS:HB2	2.22	0.40
2:GB:58:ASP:OD1	2:GB:58:ASP:N	2.54	0.40
1:GI:23:ASN:HB2	1:GI:46:ASP:HB3	2.03	0.40
1:GM:23:ASN:HB2	1:GM:46:ASP:HB3	2.03	0.40
2:HA:61:VAL:O	2:HA:65:LYS:HB2	2.22	0.40
2:HT:7:LEU:HD21	2:HT:45:MET:HE2	2.03	0.40
2:IC:32:ILE:HD11	2:IC:47:LYS:HD2	2.04	0.40
2:IJ:11:LYS:HA	2:IJ:40:GLY:O	2.21	0.40
2:IZ:66:ARG:NH2	2:JB:66:ARG:HH22	2.20	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	AA	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	AE	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	AI	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	AM	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	AQ	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	AU	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	AY	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	BC	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	BG	77/88 (88%)	71 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BK	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	BO	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	BS	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	BW	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	CA	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	CE	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	CI	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	CM	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	CQ	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	CU	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	CY	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	DC	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	DG	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	DK	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	DO	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	DS	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	DW	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	EA	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	EE	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	EI	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	EM	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	EQ	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	EU	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	EY	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	FC	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	FG	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	FK	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	FO	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	FS	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	FW	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	GA	77/88 (88%)	71 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GE	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	GI	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	GM	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	GQ	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	GU	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	GY	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	HC	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	HG	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	HK	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	HO	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	HS	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	HW	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	IA	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	IE	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	II	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	IM	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	IQ	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	IU	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	IY	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
1	JC	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
2	AB	79/100 (79%)	76 (96%)	3 (4%)	0	100	100
2	AC	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	AD	84/100 (84%)	80 (95%)	4 (5%)	0	100	100
2	AF	79/100 (79%)	76 (96%)	3 (4%)	0	100	100
2	AG	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	AH	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	AJ	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	AK	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	AL	84/100 (84%)	81 (96%)	3 (4%)	0	100	100
2	AN	79/100 (79%)	76 (96%)	3 (4%)	0	100	100
2	AO	79/100 (79%)	77 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AP	84/100 (84%)	80 (95%)	4 (5%)	0	100	100
2	AR	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	AS	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	AT	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	AV	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	AW	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	AX	84/100 (84%)	80 (95%)	4 (5%)	0	100	100
2	AZ	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	BA	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	BB	84/100 (84%)	80 (95%)	4 (5%)	0	100	100
2	BD	79/100 (79%)	76 (96%)	3 (4%)	0	100	100
2	BE	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	BF	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	BH	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	BI	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	BJ	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	BL	79/100 (79%)	74 (94%)	5 (6%)	0	100	100
2	BM	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	BN	84/100 (84%)	81 (96%)	3 (4%)	0	100	100
2	BP	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	BQ	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	BR	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	BT	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	BU	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	BV	84/100 (84%)	78 (93%)	6 (7%)	0	100	100
2	BX	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	BY	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	BZ	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	CB	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	CC	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	CD	84/100 (84%)	80 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CF	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	CG	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	CH	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	CJ	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	CK	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	CL	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	CN	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	CO	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	CP	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	CR	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	CS	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	CT	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	CV	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	CW	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	CX	84/100 (84%)	80 (95%)	4 (5%)	0	100	100
2	CZ	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	DA	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	DB	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	DD	79/100 (79%)	74 (94%)	5 (6%)	0	100	100
2	DE	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	DF	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	DH	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	DI	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	DJ	84/100 (84%)	80 (95%)	4 (5%)	0	100	100
2	DL	79/100 (79%)	76 (96%)	3 (4%)	0	100	100
2	DM	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	DN	84/100 (84%)	80 (95%)	4 (5%)	0	100	100
2	DP	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	DQ	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	DR	84/100 (84%)	81 (96%)	3 (4%)	0	100	100
2	DT	79/100 (79%)	75 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	DU	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	DV	84/100 (84%)	78 (93%)	6 (7%)	0	100	100
2	DX	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	DY	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	DZ	84/100 (84%)	80 (95%)	4 (5%)	0	100	100
2	EB	79/100 (79%)	76 (96%)	3 (4%)	0	100	100
2	EC	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	ED	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	EF	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	EG	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	EH	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	EJ	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	EK	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	EL	84/100 (84%)	80 (95%)	4 (5%)	0	100	100
2	EN	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	EO	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	EP	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	ER	79/100 (79%)	76 (96%)	3 (4%)	0	100	100
2	ES	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	ET	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	EV	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	EW	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	EX	84/100 (84%)	81 (96%)	3 (4%)	0	100	100
2	EZ	79/100 (79%)	76 (96%)	3 (4%)	0	100	100
2	FA	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	FB	84/100 (84%)	78 (93%)	6 (7%)	0	100	100
2	FD	79/100 (79%)	76 (96%)	3 (4%)	0	100	100
2	FE	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	FF	84/100 (84%)	80 (95%)	4 (5%)	0	100	100
2	FH	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	FI	79/100 (79%)	77 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	FJ	84/100 (84%)	80 (95%)	4 (5%)	0	100	100
2	FL	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	FM	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	FN	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	FP	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	FQ	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	FR	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	FT	79/100 (79%)	76 (96%)	3 (4%)	0	100	100
2	FU	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	FV	84/100 (84%)	81 (96%)	3 (4%)	0	100	100
2	FX	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	FY	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	FZ	84/100 (84%)	80 (95%)	4 (5%)	0	100	100
2	GB	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	GC	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	GD	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	GF	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	GG	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	GH	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	GJ	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	GK	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	GL	84/100 (84%)	81 (96%)	3 (4%)	0	100	100
2	GN	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	GO	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	GP	84/100 (84%)	80 (95%)	4 (5%)	0	100	100
2	GR	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	GS	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	GT	84/100 (84%)	78 (93%)	6 (7%)	0	100	100
2	GV	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	GW	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	GX	84/100 (84%)	79 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	GZ	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	HA	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	HB	84/100 (84%)	80 (95%)	4 (5%)	0	100	100
2	HD	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	HE	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	HF	84/100 (84%)	81 (96%)	3 (4%)	0	100	100
2	HH	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	HI	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	HJ	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	HL	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	HM	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	HN	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	HP	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	HQ	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	HR	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	HT	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	HU	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	HV	84/100 (84%)	81 (96%)	3 (4%)	0	100	100
2	HX	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	HY	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	HZ	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	IB	79/100 (79%)	76 (96%)	3 (4%)	0	100	100
2	IC	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	ID	84/100 (84%)	81 (96%)	3 (4%)	0	100	100
2	IF	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	IG	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	IH	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	IJ	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	IK	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	IL	84/100 (84%)	81 (96%)	3 (4%)	0	100	100
2	IN	79/100 (79%)	75 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	IO	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	IP	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	IR	79/100 (79%)	76 (96%)	3 (4%)	0	100	100
2	IS	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	IT	84/100 (84%)	80 (95%)	4 (5%)	0	100	100
2	IV	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	IW	79/100 (79%)	77 (98%)	2 (2%)	0	100	100
2	IX	84/100 (84%)	80 (95%)	4 (5%)	0	100	100
2	IZ	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	JA	79/100 (79%)	78 (99%)	1 (1%)	0	100	100
2	JB	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
2	JD	79/100 (79%)	75 (95%)	4 (5%)	0	100	100
2	JE	79/100 (79%)	79 (100%)	0	0	100	100
2	JF	84/100 (84%)	83 (99%)	1 (1%)	0	100	100
All	All	19140/23280 (82%)	18195 (95%)	945 (5%)	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	AA	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	AE	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	AI	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	AM	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	AQ	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	AU	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	AY	65/76 (86%)	64 (98%)	1 (2%)	65	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BC	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	BG	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	BK	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	BO	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	BS	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	BW	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	CA	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	CE	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	CI	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	CM	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	CQ	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	CU	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	CY	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	DC	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	DG	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	DK	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	DO	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	DS	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	DW	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	EA	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	EE	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	EI	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	EM	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	EQ	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	EU	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	EY	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	FC	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	FG	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	FK	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	FO	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	FS	65/76 (86%)	64 (98%)	1 (2%)	65	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FW	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	GA	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	GE	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	GI	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	GM	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	GQ	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	GU	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	GY	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	HC	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	HG	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	HK	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	HO	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	HS	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	HW	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	IA	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	IE	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	II	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	IM	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	IQ	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	IU	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	IY	65/76 (86%)	64 (98%)	1 (2%)	65	81
1	JC	65/76 (86%)	64 (98%)	1 (2%)	65	81
2	AB	58/74 (78%)	58 (100%)	0	100	100
2	AC	58/74 (78%)	58 (100%)	0	100	100
2	AD	61/74 (82%)	61 (100%)	0	100	100
2	AF	58/74 (78%)	58 (100%)	0	100	100
2	AG	58/74 (78%)	58 (100%)	0	100	100
2	AH	61/74 (82%)	61 (100%)	0	100	100
2	AJ	58/74 (78%)	58 (100%)	0	100	100
2	AK	58/74 (78%)	58 (100%)	0	100	100
2	AL	61/74 (82%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AN	58/74 (78%)	58 (100%)	0	100	100
2	AO	58/74 (78%)	58 (100%)	0	100	100
2	AP	61/74 (82%)	61 (100%)	0	100	100
2	AR	58/74 (78%)	58 (100%)	0	100	100
2	AS	58/74 (78%)	58 (100%)	0	100	100
2	AT	61/74 (82%)	61 (100%)	0	100	100
2	AV	58/74 (78%)	58 (100%)	0	100	100
2	AW	58/74 (78%)	58 (100%)	0	100	100
2	AX	61/74 (82%)	61 (100%)	0	100	100
2	AZ	58/74 (78%)	58 (100%)	0	100	100
2	BA	58/74 (78%)	58 (100%)	0	100	100
2	BB	61/74 (82%)	61 (100%)	0	100	100
2	BD	58/74 (78%)	58 (100%)	0	100	100
2	BE	58/74 (78%)	58 (100%)	0	100	100
2	BF	61/74 (82%)	61 (100%)	0	100	100
2	BH	58/74 (78%)	58 (100%)	0	100	100
2	BI	58/74 (78%)	58 (100%)	0	100	100
2	BJ	61/74 (82%)	61 (100%)	0	100	100
2	BL	58/74 (78%)	58 (100%)	0	100	100
2	BM	58/74 (78%)	58 (100%)	0	100	100
2	BN	61/74 (82%)	61 (100%)	0	100	100
2	BP	58/74 (78%)	58 (100%)	0	100	100
2	BQ	58/74 (78%)	58 (100%)	0	100	100
2	BR	61/74 (82%)	61 (100%)	0	100	100
2	BT	58/74 (78%)	58 (100%)	0	100	100
2	BU	58/74 (78%)	58 (100%)	0	100	100
2	BV	61/74 (82%)	61 (100%)	0	100	100
2	BX	58/74 (78%)	58 (100%)	0	100	100
2	BY	58/74 (78%)	58 (100%)	0	100	100
2	BZ	61/74 (82%)	61 (100%)	0	100	100
2	CB	58/74 (78%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	CC	58/74 (78%)	58 (100%)	0	100	100
2	CD	61/74 (82%)	61 (100%)	0	100	100
2	CF	58/74 (78%)	58 (100%)	0	100	100
2	CG	58/74 (78%)	58 (100%)	0	100	100
2	CH	61/74 (82%)	61 (100%)	0	100	100
2	CJ	58/74 (78%)	58 (100%)	0	100	100
2	CK	58/74 (78%)	58 (100%)	0	100	100
2	CL	61/74 (82%)	61 (100%)	0	100	100
2	CN	58/74 (78%)	58 (100%)	0	100	100
2	CO	58/74 (78%)	58 (100%)	0	100	100
2	CP	61/74 (82%)	61 (100%)	0	100	100
2	CR	58/74 (78%)	58 (100%)	0	100	100
2	CS	58/74 (78%)	58 (100%)	0	100	100
2	CT	61/74 (82%)	61 (100%)	0	100	100
2	CV	58/74 (78%)	58 (100%)	0	100	100
2	CW	58/74 (78%)	58 (100%)	0	100	100
2	CX	61/74 (82%)	61 (100%)	0	100	100
2	CZ	58/74 (78%)	58 (100%)	0	100	100
2	DA	58/74 (78%)	58 (100%)	0	100	100
2	DB	61/74 (82%)	61 (100%)	0	100	100
2	DD	58/74 (78%)	58 (100%)	0	100	100
2	DE	58/74 (78%)	58 (100%)	0	100	100
2	DF	61/74 (82%)	61 (100%)	0	100	100
2	DH	58/74 (78%)	58 (100%)	0	100	100
2	DI	58/74 (78%)	58 (100%)	0	100	100
2	DJ	61/74 (82%)	61 (100%)	0	100	100
2	DL	58/74 (78%)	58 (100%)	0	100	100
2	DM	58/74 (78%)	58 (100%)	0	100	100
2	DN	61/74 (82%)	61 (100%)	0	100	100
2	DP	58/74 (78%)	58 (100%)	0	100	100
2	DQ	58/74 (78%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	DR	61/74 (82%)	61 (100%)	0	100	100
2	DT	58/74 (78%)	58 (100%)	0	100	100
2	DU	58/74 (78%)	58 (100%)	0	100	100
2	DV	61/74 (82%)	61 (100%)	0	100	100
2	DX	58/74 (78%)	58 (100%)	0	100	100
2	DY	58/74 (78%)	58 (100%)	0	100	100
2	DZ	61/74 (82%)	61 (100%)	0	100	100
2	EB	58/74 (78%)	58 (100%)	0	100	100
2	EC	58/74 (78%)	58 (100%)	0	100	100
2	ED	61/74 (82%)	61 (100%)	0	100	100
2	EF	58/74 (78%)	58 (100%)	0	100	100
2	EG	58/74 (78%)	58 (100%)	0	100	100
2	EH	61/74 (82%)	61 (100%)	0	100	100
2	EJ	58/74 (78%)	58 (100%)	0	100	100
2	EK	58/74 (78%)	58 (100%)	0	100	100
2	EL	61/74 (82%)	61 (100%)	0	100	100
2	EN	58/74 (78%)	58 (100%)	0	100	100
2	EO	58/74 (78%)	58 (100%)	0	100	100
2	EP	61/74 (82%)	61 (100%)	0	100	100
2	ER	58/74 (78%)	58 (100%)	0	100	100
2	ES	58/74 (78%)	58 (100%)	0	100	100
2	ET	61/74 (82%)	61 (100%)	0	100	100
2	EV	58/74 (78%)	58 (100%)	0	100	100
2	EW	58/74 (78%)	58 (100%)	0	100	100
2	EX	61/74 (82%)	61 (100%)	0	100	100
2	EZ	58/74 (78%)	58 (100%)	0	100	100
2	FA	58/74 (78%)	58 (100%)	0	100	100
2	FB	61/74 (82%)	61 (100%)	0	100	100
2	FD	58/74 (78%)	58 (100%)	0	100	100
2	FE	58/74 (78%)	58 (100%)	0	100	100
2	FF	61/74 (82%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	FH	58/74 (78%)	58 (100%)	0	100	100
2	FI	58/74 (78%)	58 (100%)	0	100	100
2	FJ	61/74 (82%)	61 (100%)	0	100	100
2	FL	58/74 (78%)	58 (100%)	0	100	100
2	FM	58/74 (78%)	58 (100%)	0	100	100
2	FN	61/74 (82%)	61 (100%)	0	100	100
2	FP	58/74 (78%)	58 (100%)	0	100	100
2	FQ	58/74 (78%)	58 (100%)	0	100	100
2	FR	61/74 (82%)	61 (100%)	0	100	100
2	FT	58/74 (78%)	58 (100%)	0	100	100
2	FU	58/74 (78%)	58 (100%)	0	100	100
2	FV	61/74 (82%)	61 (100%)	0	100	100
2	FX	58/74 (78%)	58 (100%)	0	100	100
2	FY	58/74 (78%)	58 (100%)	0	100	100
2	FZ	61/74 (82%)	61 (100%)	0	100	100
2	GB	58/74 (78%)	58 (100%)	0	100	100
2	GC	58/74 (78%)	58 (100%)	0	100	100
2	GD	61/74 (82%)	61 (100%)	0	100	100
2	GF	58/74 (78%)	58 (100%)	0	100	100
2	GG	58/74 (78%)	58 (100%)	0	100	100
2	GH	61/74 (82%)	61 (100%)	0	100	100
2	GJ	58/74 (78%)	58 (100%)	0	100	100
2	GK	58/74 (78%)	58 (100%)	0	100	100
2	GL	61/74 (82%)	61 (100%)	0	100	100
2	GN	58/74 (78%)	58 (100%)	0	100	100
2	GO	58/74 (78%)	58 (100%)	0	100	100
2	GP	61/74 (82%)	61 (100%)	0	100	100
2	GR	58/74 (78%)	58 (100%)	0	100	100
2	GS	58/74 (78%)	58 (100%)	0	100	100
2	GT	61/74 (82%)	61 (100%)	0	100	100
2	GV	58/74 (78%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	GW	58/74 (78%)	58 (100%)	0	100	100
2	GX	61/74 (82%)	61 (100%)	0	100	100
2	GZ	58/74 (78%)	58 (100%)	0	100	100
2	HA	58/74 (78%)	58 (100%)	0	100	100
2	HB	61/74 (82%)	61 (100%)	0	100	100
2	HD	58/74 (78%)	58 (100%)	0	100	100
2	HE	58/74 (78%)	58 (100%)	0	100	100
2	HF	61/74 (82%)	61 (100%)	0	100	100
2	HH	58/74 (78%)	58 (100%)	0	100	100
2	HI	58/74 (78%)	58 (100%)	0	100	100
2	HJ	61/74 (82%)	61 (100%)	0	100	100
2	HL	58/74 (78%)	58 (100%)	0	100	100
2	HM	58/74 (78%)	58 (100%)	0	100	100
2	HN	61/74 (82%)	61 (100%)	0	100	100
2	HP	58/74 (78%)	58 (100%)	0	100	100
2	HQ	58/74 (78%)	58 (100%)	0	100	100
2	HR	61/74 (82%)	61 (100%)	0	100	100
2	HT	58/74 (78%)	58 (100%)	0	100	100
2	HU	58/74 (78%)	58 (100%)	0	100	100
2	HV	61/74 (82%)	61 (100%)	0	100	100
2	HX	58/74 (78%)	58 (100%)	0	100	100
2	HY	58/74 (78%)	58 (100%)	0	100	100
2	HZ	61/74 (82%)	61 (100%)	0	100	100
2	IB	58/74 (78%)	58 (100%)	0	100	100
2	IC	58/74 (78%)	58 (100%)	0	100	100
2	ID	61/74 (82%)	61 (100%)	0	100	100
2	IF	58/74 (78%)	58 (100%)	0	100	100
2	IG	58/74 (78%)	58 (100%)	0	100	100
2	IH	61/74 (82%)	61 (100%)	0	100	100
2	IJ	58/74 (78%)	58 (100%)	0	100	100
2	IK	58/74 (78%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	IL	61/74 (82%)	61 (100%)	0	100	100
2	IN	58/74 (78%)	58 (100%)	0	100	100
2	IO	58/74 (78%)	58 (100%)	0	100	100
2	IP	61/74 (82%)	61 (100%)	0	100	100
2	IR	58/74 (78%)	58 (100%)	0	100	100
2	IS	58/74 (78%)	58 (100%)	0	100	100
2	IT	61/74 (82%)	61 (100%)	0	100	100
2	IV	58/74 (78%)	58 (100%)	0	100	100
2	IW	58/74 (78%)	58 (100%)	0	100	100
2	IX	61/74 (82%)	61 (100%)	0	100	100
2	IZ	58/74 (78%)	58 (100%)	0	100	100
2	JA	58/74 (78%)	58 (100%)	0	100	100
2	JB	61/74 (82%)	61 (100%)	0	100	100
2	JD	58/74 (78%)	58 (100%)	0	100	100
2	JE	58/74 (78%)	58 (100%)	0	100	100
2	JF	61/74 (82%)	61 (100%)	0	100	100
All	All	14520/17880 (81%)	14460 (100%)	60 (0%)	91	95

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

Mol	Chain	Res	Type
1	AA	32	ASP
1	AE	32	ASP
1	AI	32	ASP
1	AM	32	ASP
1	AQ	32	ASP
1	AU	32	ASP
1	AY	32	ASP
1	BC	32	ASP
1	BG	32	ASP
1	BK	32	ASP
1	BO	32	ASP
1	BS	32	ASP
1	BW	32	ASP
1	CA	32	ASP
1	CE	32	ASP

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Mol	Chain	Res	Type
1	CI	32	ASP
1	CM	32	ASP
1	CQ	32	ASP
1	CU	32	ASP
1	CY	32	ASP
1	DC	32	ASP
1	DG	32	ASP
1	DK	32	ASP
1	DO	32	ASP
1	DS	32	ASP
1	DW	32	ASP
1	EA	32	ASP
1	EE	32	ASP
1	EI	32	ASP
1	EM	32	ASP
1	EQ	32	ASP
1	EU	32	ASP
1	EY	32	ASP
1	FC	32	ASP
1	FG	32	ASP
1	FK	32	ASP
1	FO	32	ASP
1	FS	32	ASP
1	FW	32	ASP
1	GA	32	ASP
1	GE	32	ASP
1	GI	32	ASP
1	GM	32	ASP
1	GQ	32	ASP
1	GU	32	ASP
1	GY	32	ASP
1	HC	32	ASP
1	HG	32	ASP
1	HK	32	ASP
1	HO	32	ASP
1	HS	32	ASP
1	HW	32	ASP
1	IA	32	ASP
1	IE	32	ASP
1	II	32	ASP
1	IM	32	ASP
1	IQ	32	ASP

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Mol	Chain	Res	Type
1	IU	32	ASP
1	IY	32	ASP
1	JC	32	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	AI	9	HIS
1	AM	9	HIS
1	BO	9	HIS
1	CU	9	HIS
1	DG	9	HIS
1	GI	9	HIS
1	GY	9	HIS
1	HO	9	HIS
1	IU	9	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

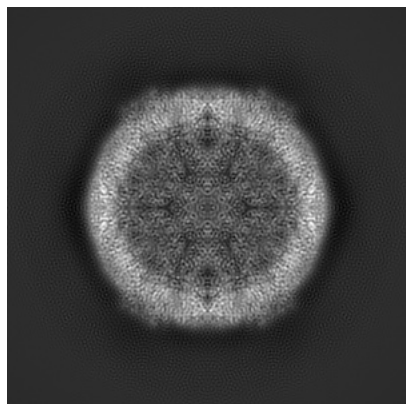
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4595. These allow visual inspection of the internal detail of the map and identification of artifacts.

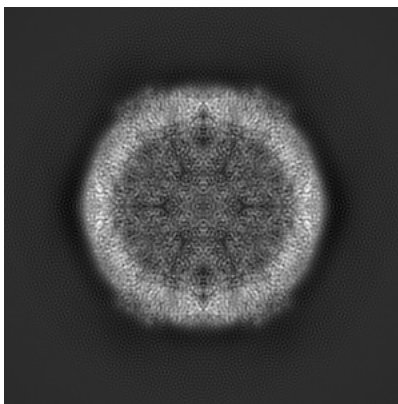
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

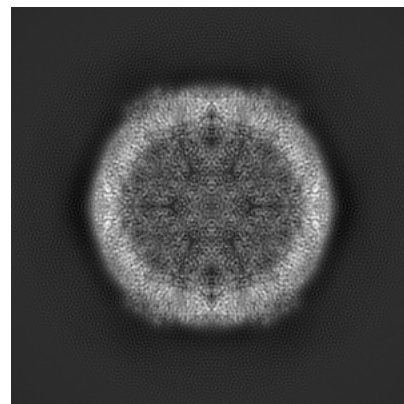
6.1.1 Primary map



X

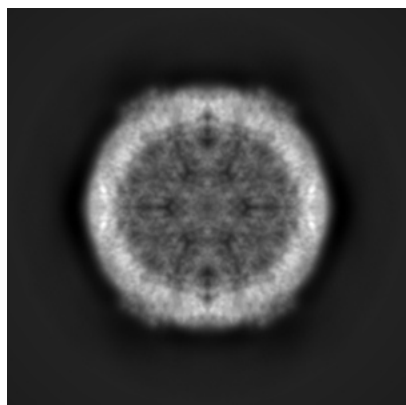


Y

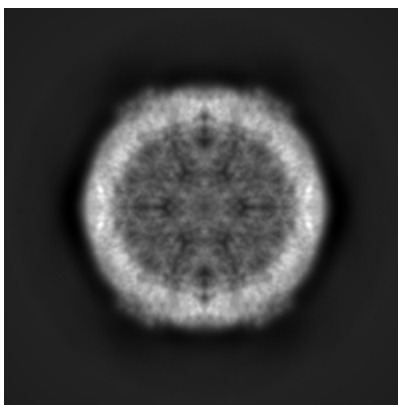


Z

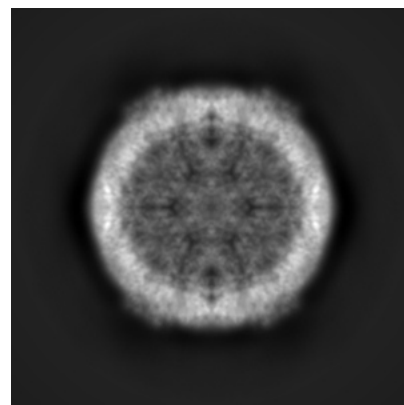
6.1.2 Raw map



X



Y

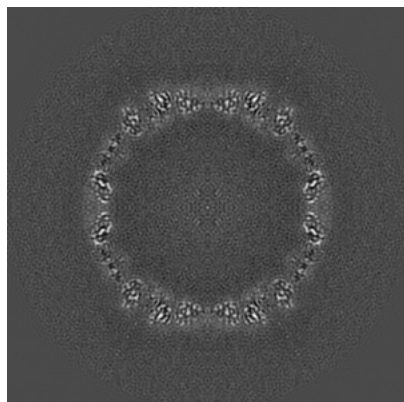


Z

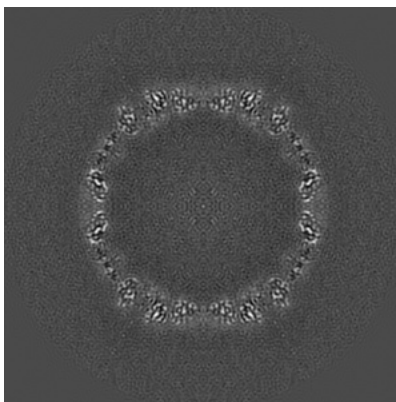
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

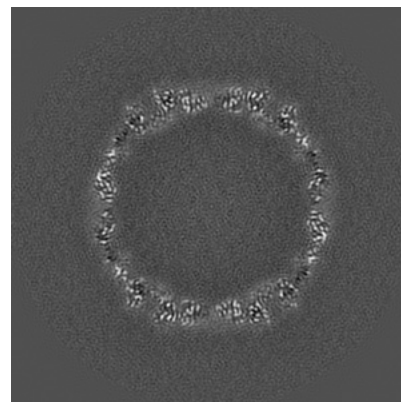
6.2.1 Primary map



X Index: 160

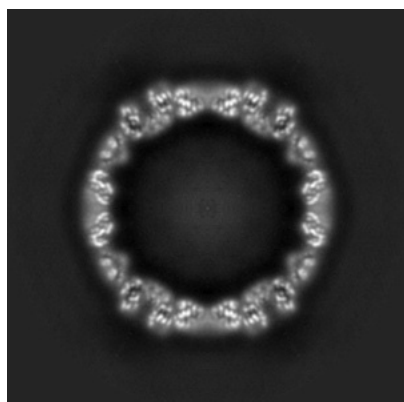


Y Index: 160

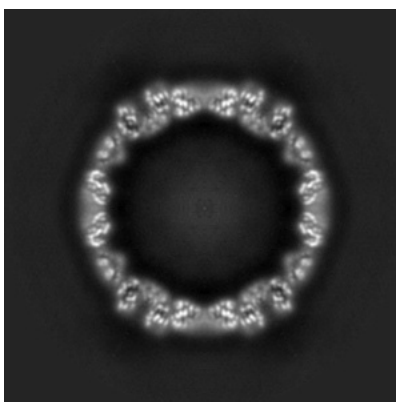


Z Index: 160

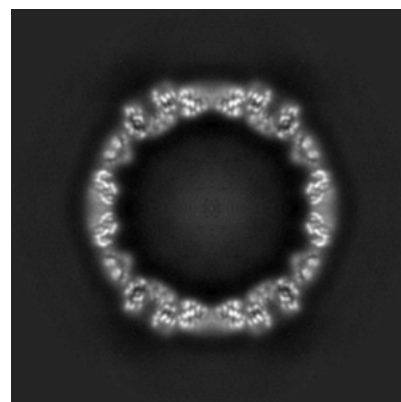
6.2.2 Raw map



X Index: 160



Y Index: 160

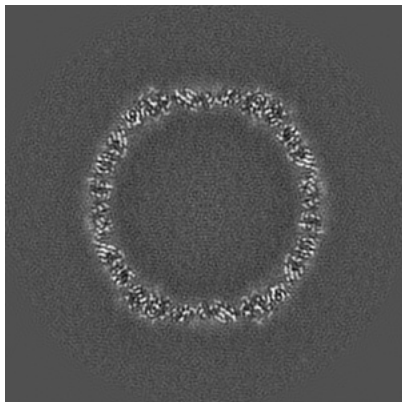


Z Index: 160

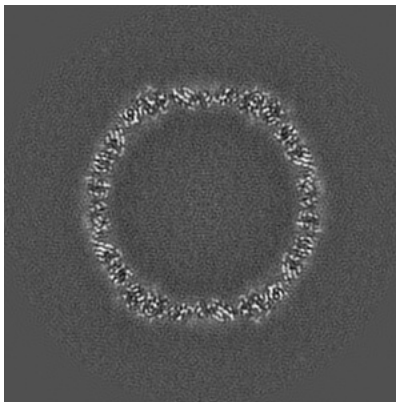
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

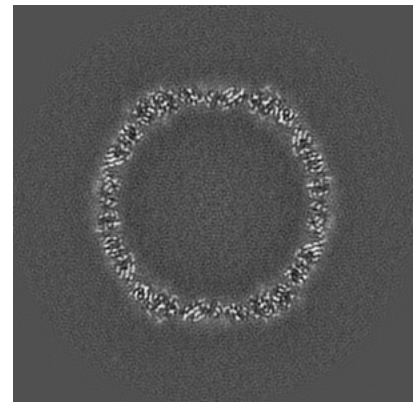
6.3.1 Primary map



X Index: 150

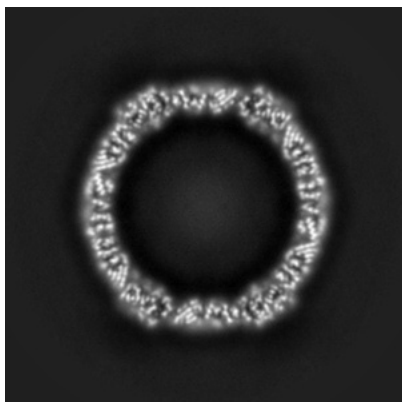


Y Index: 150

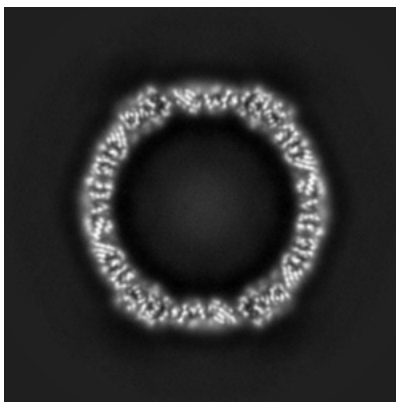


Z Index: 169

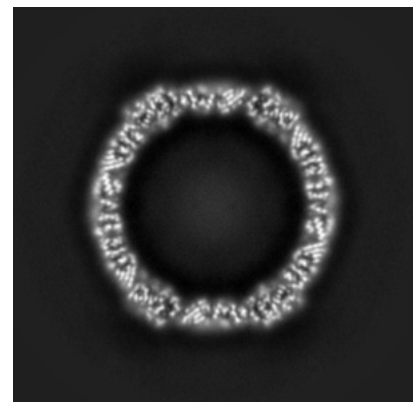
6.3.2 Raw map



X Index: 150



Y Index: 170

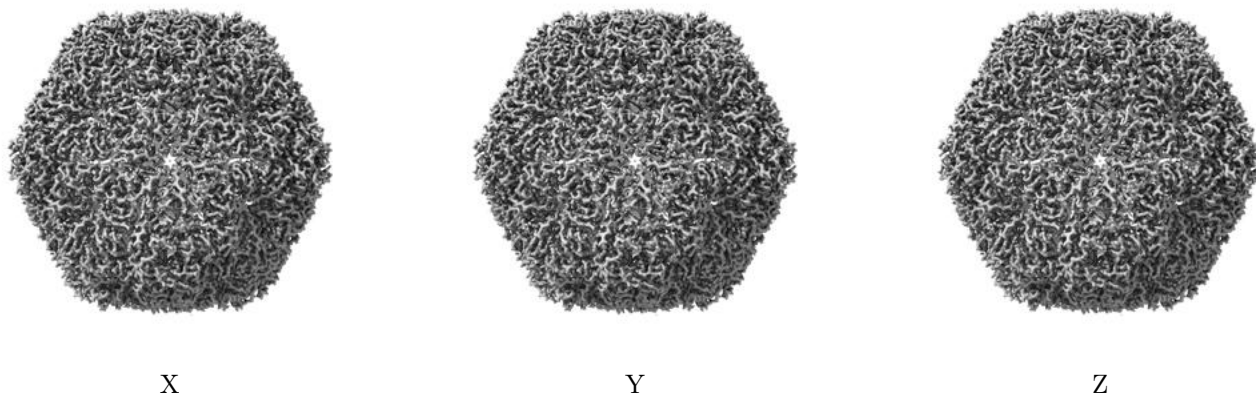


Z Index: 150

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

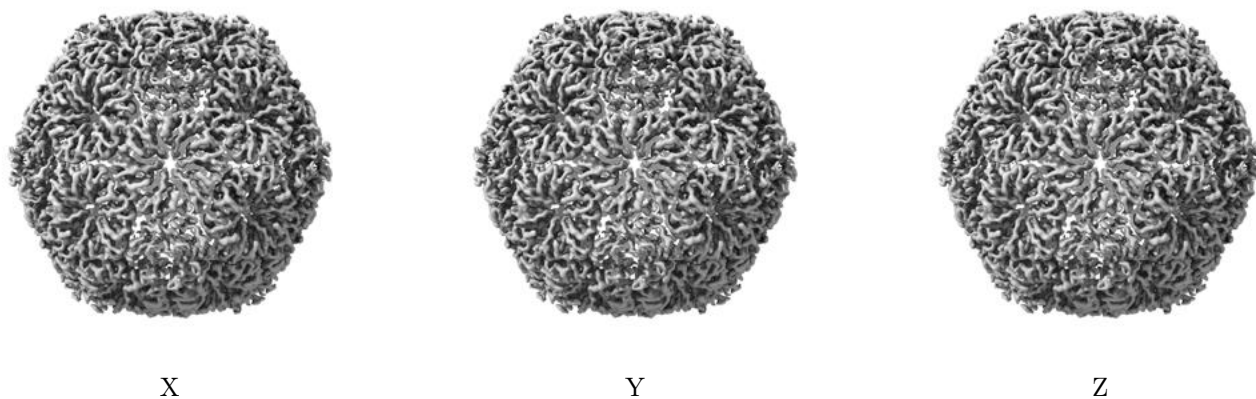
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0759. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

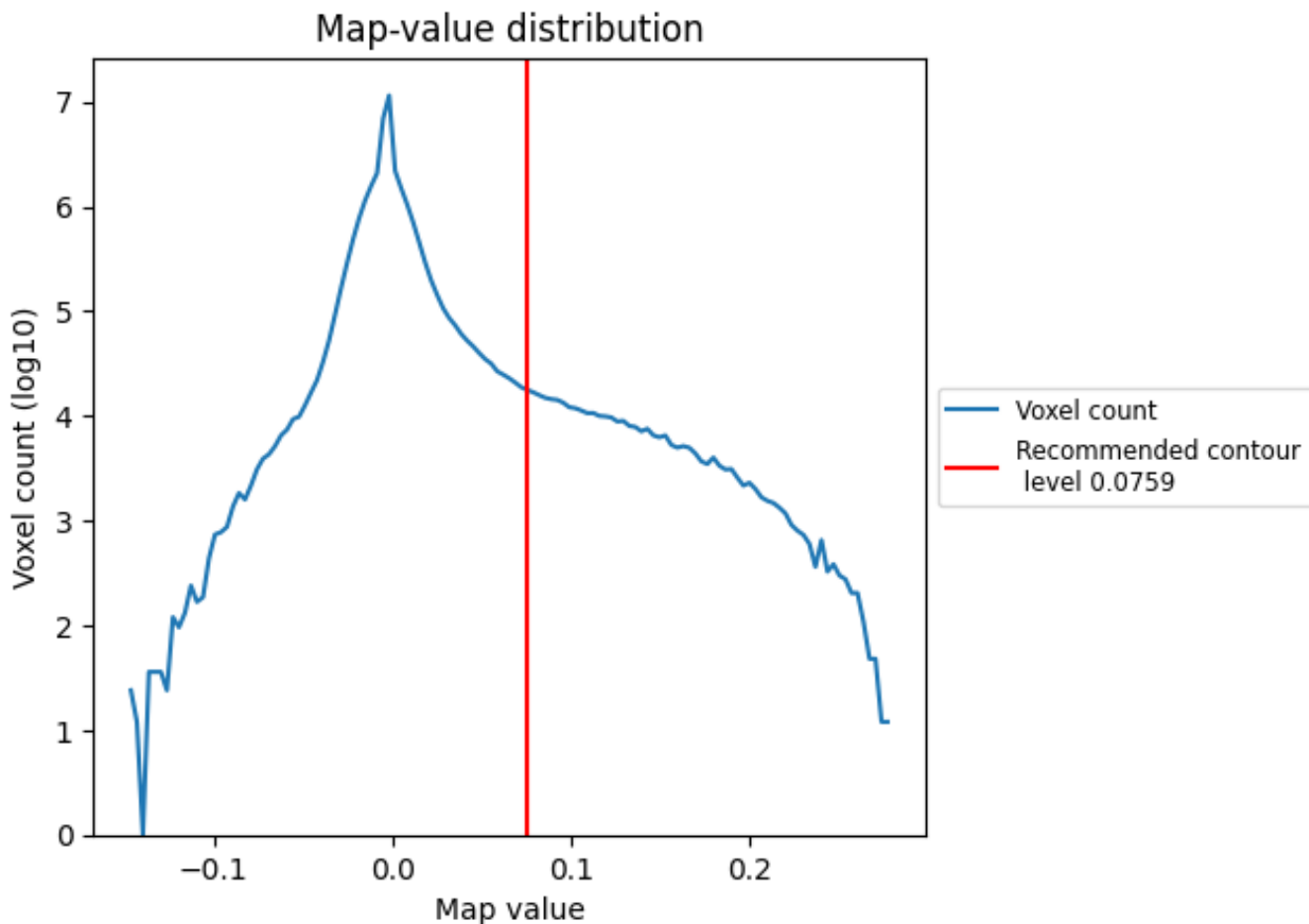
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

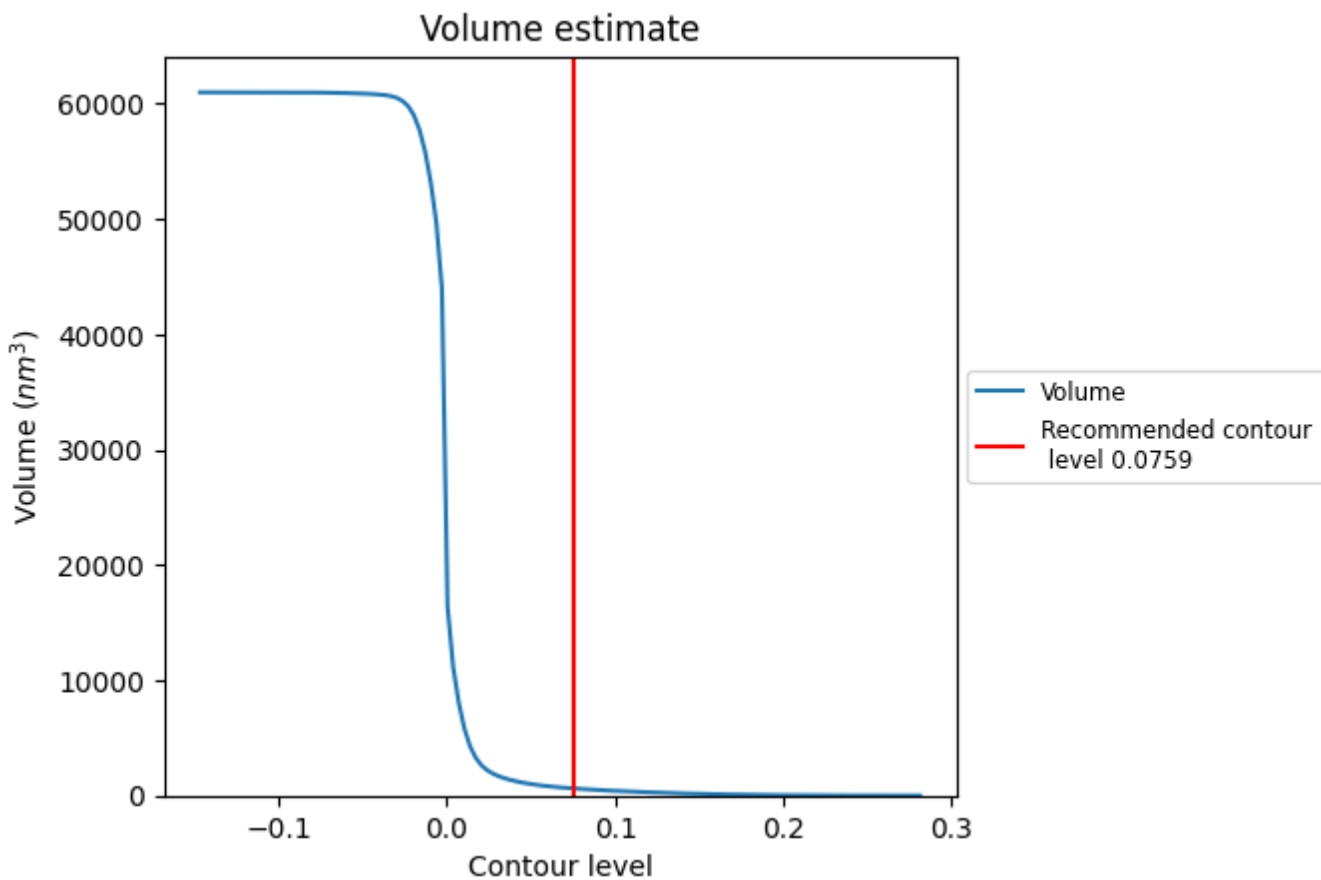
This section contains the results of statistical analysis of the map.

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.

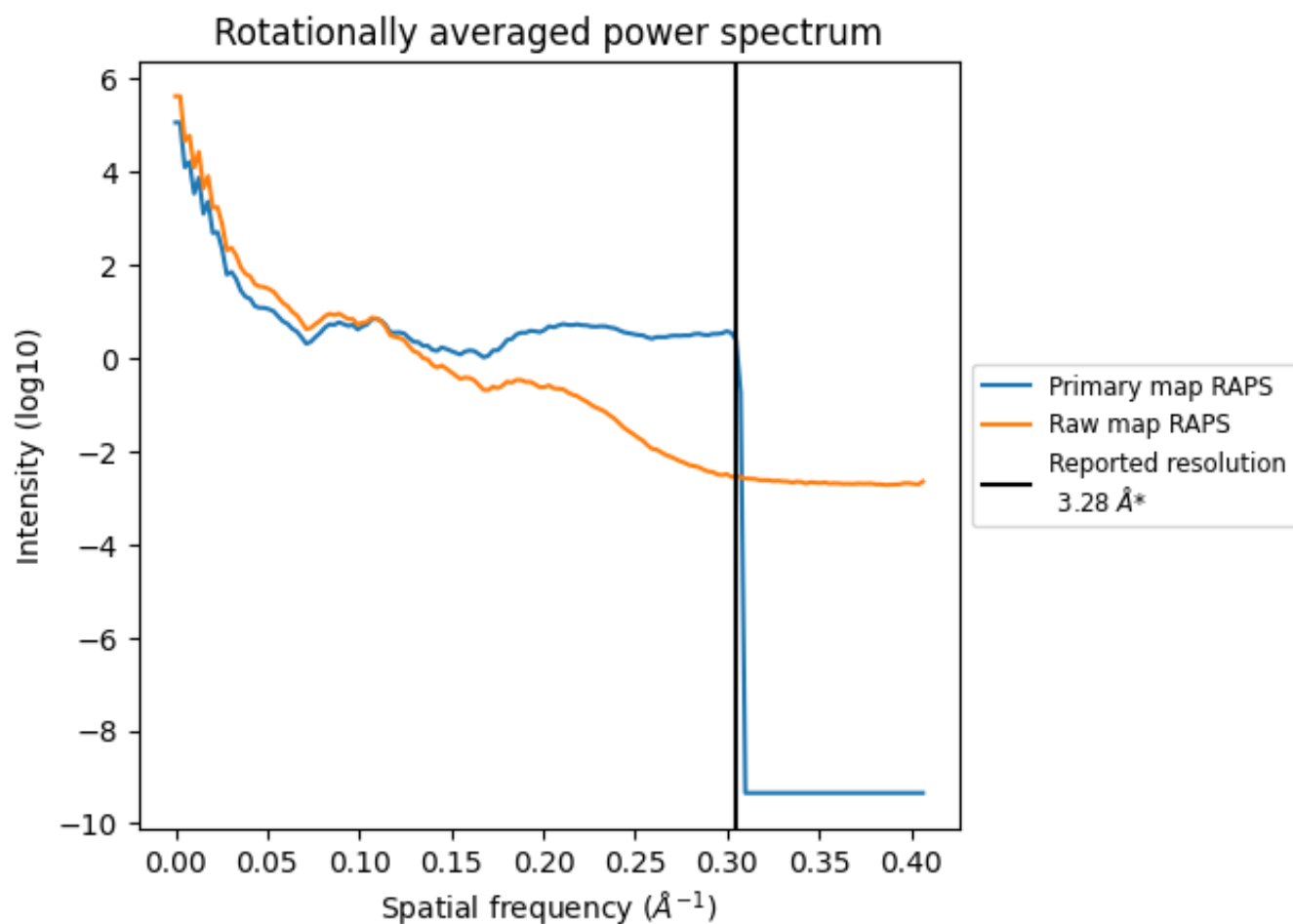
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 612 nm³; this corresponds to an approximate mass of 553 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](#)

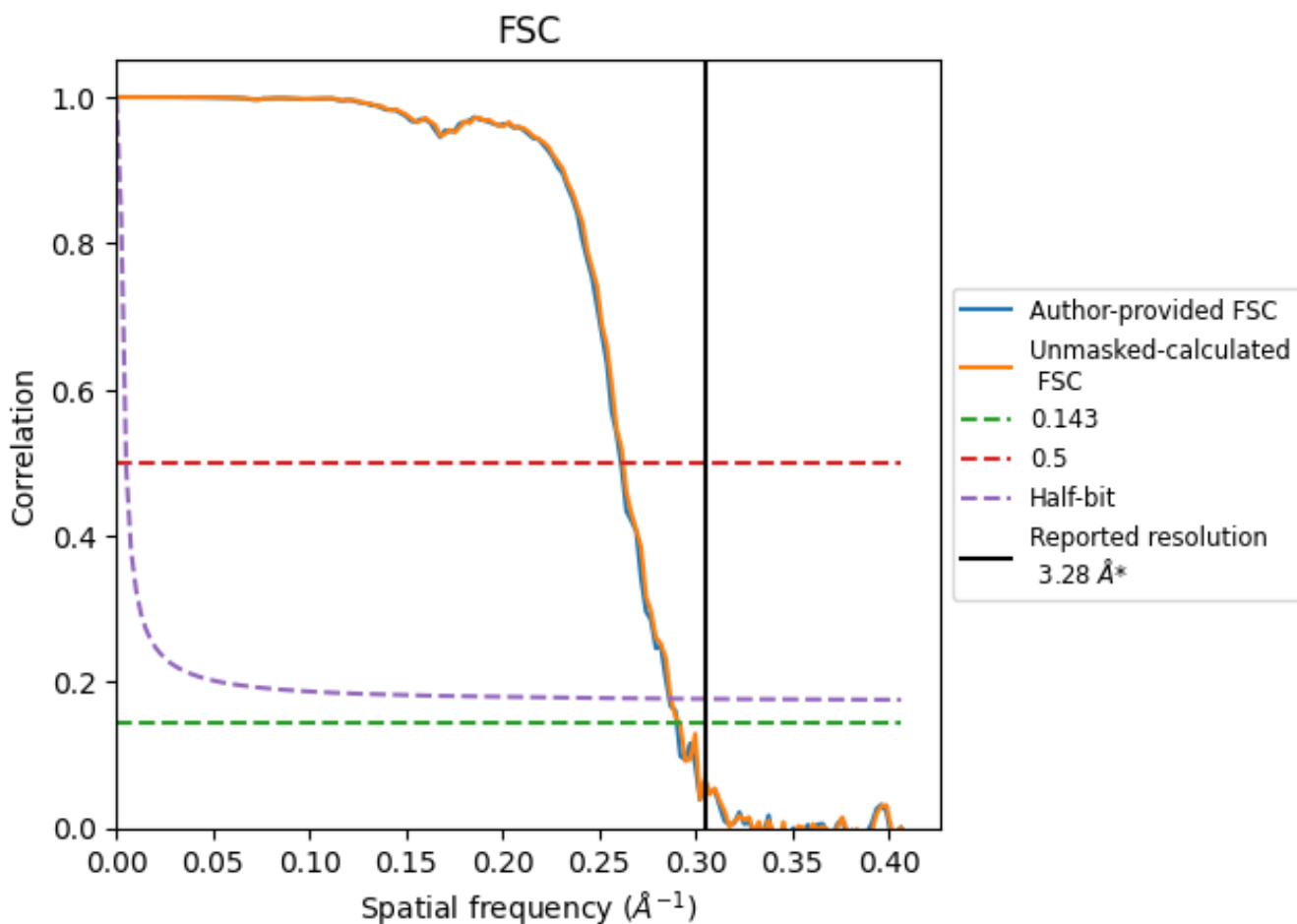


*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

8.2 Resolution estimates [i](#)

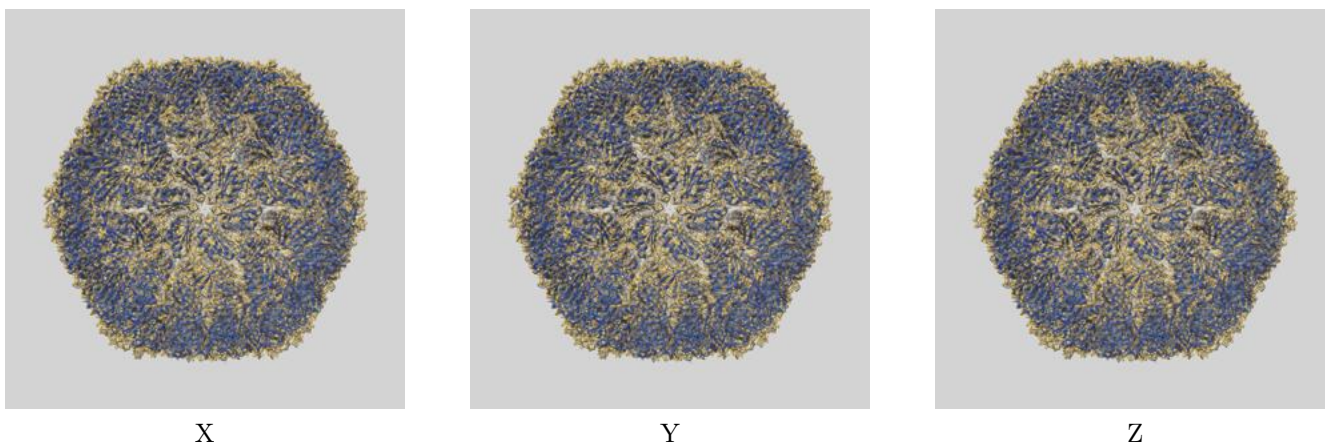
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.44	3.83	3.49
Unmasked-calculated*	3.43	3.81	3.48

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

9 Map-model fit [i](#)

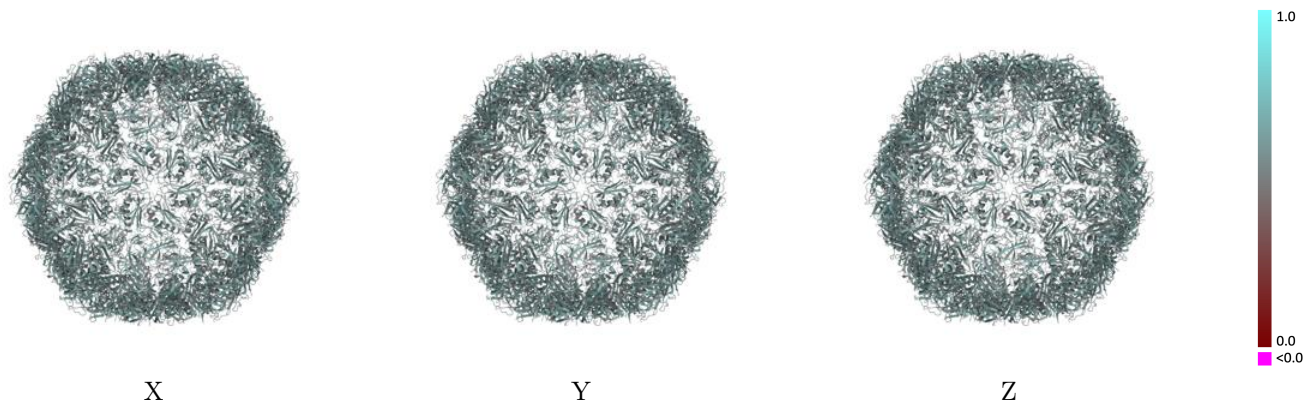
This section contains information regarding the fit between EMDB map EMD-4595 and PDB model 6QN1. Per-residue inclusion information can be found in section 3 on page 85.

9.1 Map-model overlay [i](#)



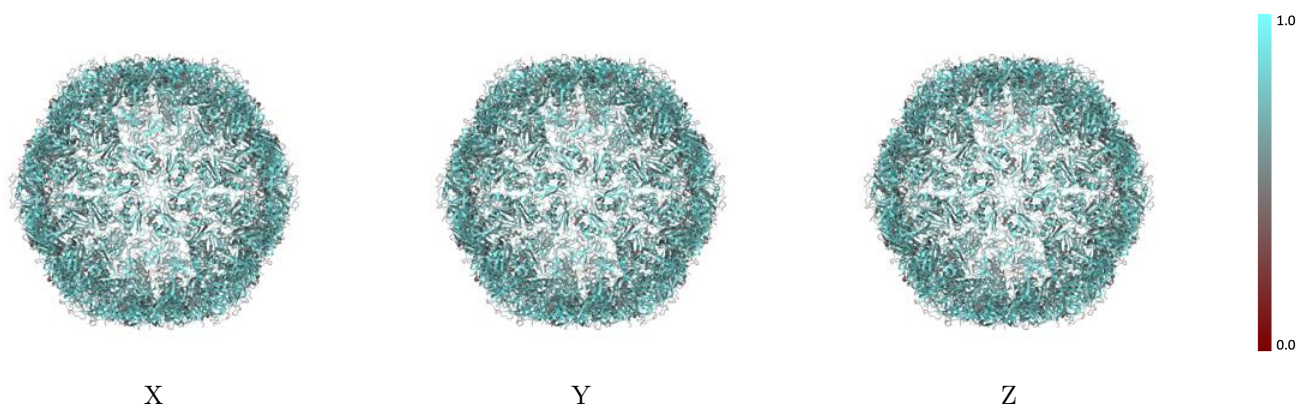
The images above show the 3D surface view of the map at the recommended contour level 0.0759 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



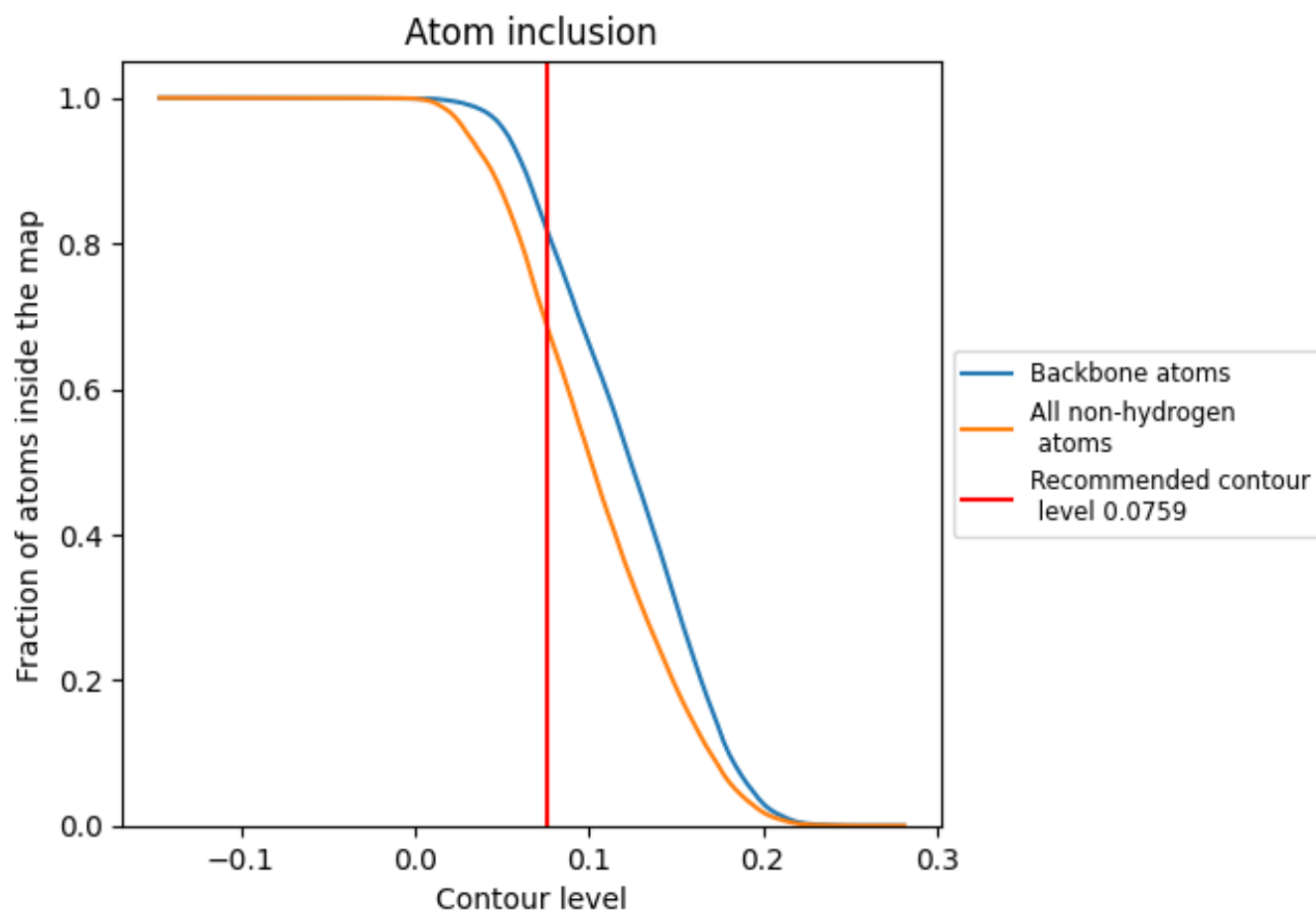
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0759).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 69% 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 (0.0759) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6869	 0.5510
AA	 0.6612	 0.5500
AB	 0.7206	 0.5490
AC	 0.7011	 0.5520
AD	 0.6884	 0.5460
AE	 0.6365	 0.5460
AF	 0.7242	 0.5550
AG	 0.7046	 0.5560
AH	 0.6985	 0.5480
AI	 0.6414	 0.5470
AJ	 0.7171	 0.5500
AK	 0.6940	 0.5510
AL	 0.6817	 0.5490
AM	 0.6480	 0.5470
AN	 0.7206	 0.5510
AO	 0.7064	 0.5570
AP	 0.6918	 0.5450
AQ	 0.6414	 0.5520
AR	 0.7295	 0.5500
AS	 0.7028	 0.5540
AT	 0.6801	 0.5460
AU	 0.6464	 0.5510
AV	 0.7100	 0.5490
AW	 0.7046	 0.5520
AX	 0.6784	 0.5470
AY	 0.6480	 0.5510
AZ	 0.7171	 0.5530
BA	 0.6940	 0.5510
BB	 0.6834	 0.5460
BC	 0.6612	 0.5480
BD	 0.7206	 0.5560
BE	 0.7011	 0.5570
BF	 0.6918	 0.5480
BG	 0.6299	 0.5520
BH	 0.7242	 0.5580























































































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Chain	Atom inclusion	Q-score
BI	 0.6975	 0.5560
BJ	 0.6817	 0.5470
BK	 0.6480	 0.5440
BL	 0.7117	 0.5540
BM	 0.6975	 0.5530
BN	 0.6734	 0.5450
BO	 0.6349	 0.5480
BP	 0.7171	 0.5500
BQ	 0.7011	 0.5540
BR	 0.6851	 0.5470
BS	 0.6480	 0.5500
BT	 0.7153	 0.5570
BU	 0.7028	 0.5550
BV	 0.7018	 0.5500
BW	 0.6398	 0.5540
BX	 0.7206	 0.5530
BY	 0.6993	 0.5580
BZ	 0.6801	 0.5520
CA	 0.6431	 0.5500
CB	 0.7189	 0.5520
CC	 0.6957	 0.5530
CD	 0.6784	 0.5500
CE	 0.6447	 0.5460
CF	 0.7135	 0.5490
CG	 0.7011	 0.5550
CH	 0.6834	 0.5480
CI	 0.6365	 0.5500
CJ	 0.7295	 0.5550
CK	 0.7064	 0.5520
CL	 0.6868	 0.5470
CM	 0.6464	 0.5480
CN	 0.7189	 0.5560
CO	 0.6993	 0.5530
CP	 0.7002	 0.5460
CQ	 0.6480	 0.5430
CR	 0.7242	 0.5510
CS	 0.6975	 0.5550
CT	 0.6901	 0.5420
CU	 0.6398	 0.5480
CV	 0.7153	 0.5540
CW	 0.7064	 0.5550
CX	 0.6868	 0.5470





















































































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Chain	Atom inclusion	Q-score
CY	 0.6431	 0.5540
CZ	 0.7206	 0.5530
DA	 0.7064	 0.5530
DB	 0.6801	 0.5490
DC	 0.6382	 0.5460
DD	 0.7153	 0.5580
DE	 0.7028	 0.5540
DF	 0.6951	 0.5480
DG	 0.6349	 0.5340
DH	 0.7135	 0.5560
DI	 0.7082	 0.5530
DJ	 0.6817	 0.5510
DK	 0.6579	 0.5540
DL	 0.7171	 0.5550
DM	 0.6975	 0.5540
DN	 0.6951	 0.5490
DO	 0.6480	 0.5510
DP	 0.7189	 0.5550
DQ	 0.7011	 0.5500
DR	 0.6817	 0.5470
DS	 0.6464	 0.5480
DT	 0.7189	 0.5540
DU	 0.7028	 0.5560
DV	 0.6935	 0.5480
DW	 0.6464	 0.5470
DX	 0.7117	 0.5510
DY	 0.7028	 0.5570
DZ	 0.6784	 0.5450
EA	 0.6595	 0.5530
EB	 0.7171	 0.5560
EC	 0.7011	 0.5540
ED	 0.6918	 0.5480
EE	 0.6398	 0.5460
EF	 0.7206	 0.5560
EG	 0.7046	 0.5520
EH	 0.6985	 0.5510
EI	 0.6431	 0.5540
EJ	 0.7135	 0.5510
EK	 0.6993	 0.5530
EL	 0.6851	 0.5530
EM	 0.6513	 0.5480
EN	 0.7278	 0.5520

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Chain	Atom inclusion	Q-score
EO	 0.6993	 0.5540
EP	 0.6817	 0.5460
EQ	 0.6464	 0.5510
ER	 0.7206	 0.5530
ES	 0.6993	 0.5560
ET	 0.6935	 0.5460
EU	 0.6382	 0.5510
EV	 0.7171	 0.5560
EW	 0.6957	 0.5490
EX	 0.6734	 0.5500
EY	 0.6480	 0.5500
EZ	 0.7117	 0.5530
FA	 0.7028	 0.5540
FB	 0.6951	 0.5480
FC	 0.6562	 0.5490
FD	 0.7206	 0.5500
FE	 0.6993	 0.5560
FF	 0.6951	 0.5470
FG	 0.6431	 0.5440
FH	 0.7117	 0.5520
FI	 0.7135	 0.5550
FJ	 0.6868	 0.5500
FK	 0.6464	 0.5520
FL	 0.7242	 0.5530
FM	 0.6975	 0.5520
FN	 0.6784	 0.5480
FO	 0.6414	 0.5460
FP	 0.7153	 0.5540
FQ	 0.7011	 0.5500
FR	 0.7002	 0.5480
FS	 0.6579	 0.5540
FT	 0.7189	 0.5540
FU	 0.6993	 0.5560
FV	 0.6918	 0.5490
FW	 0.6480	 0.5480
FX	 0.7117	 0.5540
FY	 0.7046	 0.5540
FZ	 0.6834	 0.5490
GA	 0.6447	 0.5510
GB	 0.7224	 0.5570
GC	 0.6993	 0.5560
GD	 0.6968	 0.5470













































































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Chain	Atom inclusion	Q-score
GE	0.6382	0.5500
GF	0.7278	0.5520
GG	0.6993	0.5470
GH	0.6884	0.5460
GI	0.6464	0.5460
GJ	0.7135	0.5550
GK	0.6940	0.5540
GL	0.6817	0.5490
GM	0.6464	0.5510
GN	0.7135	0.5540
GO	0.7046	0.5570
GP	0.6801	0.5490
GQ	0.6349	0.5420
GR	0.7117	0.5530
GS	0.7011	0.5520
GT	0.7035	0.5480
GU	0.6447	0.5520
GV	0.7278	0.5570
GW	0.6993	0.5570
GX	0.6767	0.5490
GY	0.6349	0.5470
GZ	0.7153	0.5540
HA	0.7028	0.5580
HB	0.6834	0.5480
HC	0.6382	0.5520
HD	0.7206	0.5530
HE	0.6975	0.5510
HF	0.6801	0.5480
HG	0.6579	0.5560
HH	0.7206	0.5530
HI	0.7011	0.5530
HJ	0.6968	0.5490
HK	0.6365	0.5520
HL	0.7260	0.5530
HM	0.6993	0.5570
HN	0.6784	0.5500
HO	0.6513	0.5470
HP	0.7171	0.5550
HQ	0.7082	0.5500
HR	0.6834	0.5470
HS	0.6414	0.5460
HT	0.7189	0.5560

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Chain	Atom inclusion	Q-score
HU	 0.6957	 0.5520
HV	 0.6717	 0.5440
HW	 0.6382	 0.5490
HX	 0.7242	 0.5580
HY	 0.6993	 0.5560
HZ	 0.6851	 0.5470
IA	 0.6562	 0.5520
IB	 0.7206	 0.5520
IC	 0.6993	 0.5590
ID	 0.6935	 0.5500
IE	 0.6447	 0.5450
IF	 0.7171	 0.5570
IG	 0.7046	 0.5540
IH	 0.7018	 0.5510
II	 0.6431	 0.5500
IJ	 0.7189	 0.5520
IK	 0.6940	 0.5490
IL	 0.6817	 0.5530
IM	 0.6398	 0.5510
IN	 0.7206	 0.5580
IO	 0.6940	 0.5570
IP	 0.6868	 0.5490
IQ	 0.6530	 0.5500
IR	 0.7189	 0.5560
IS	 0.6993	 0.5540
IT	 0.6935	 0.5510
IU	 0.6464	 0.5520
IV	 0.7153	 0.5530
IW	 0.7028	 0.5510
IX	 0.6817	 0.5450
IY	 0.6398	 0.5450
IZ	 0.7117	 0.5560
JA	 0.7011	 0.5550
JB	 0.6868	 0.5480
JC	 0.6497	 0.5520
JD	 0.7117	 0.5510
JE	 0.6904	 0.5500
JF	 0.6767	 0.5450