



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 09:12 PM UTC

PDB ID : 7PE1 / pdb_00007pe1
EMDB ID : EMD-13344
Title : Cryo-EM structure of BMV-derived VLP expressed in E. coli and assembled in the presence of tRNA (tVLP)
Authors : Ruszkowski, M.; Strugala, A.; Indyka, P.; Urbanowicz, A.
Deposited on : 2021-08-09
Resolution : 3.00 Å(reported)
Based on initial model : 6VOC

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

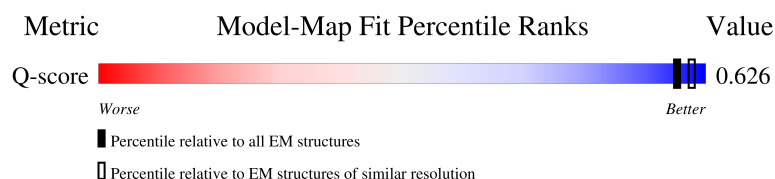
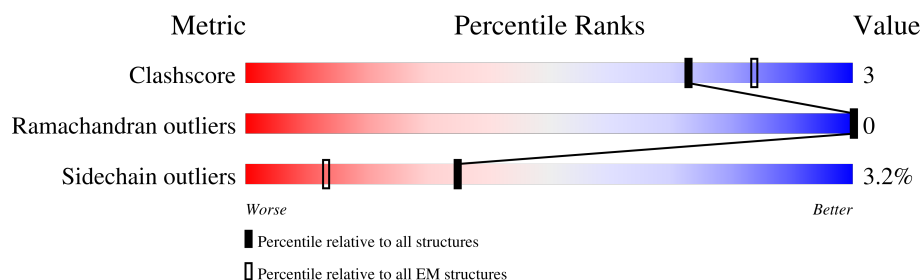
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	A	192	9% 67% 9% 22%
1	AA	192	9% 78% 7% 15%
1	AB	192	9% 67% 10% 22%
1	AC	192	9% 76% 8% 15%

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Mol	Chain	Length	Quality of chain
1	AD	192	
1	AE	192	
1	AF	192	
1	B	192	
1	BA	192	
1	BB	192	
1	BC	192	
1	BD	192	
1	BE	192	
1	BF	192	
1	C	192	
1	CA	192	
1	CB	192	
1	CC	192	
1	CD	192	
1	CE	192	
1	CF	192	
1	D	192	
1	DA	192	
1	DB	192	
1	DC	192	
1	DD	192	
1	DE	192	
1	DF	192	
1	E	192	

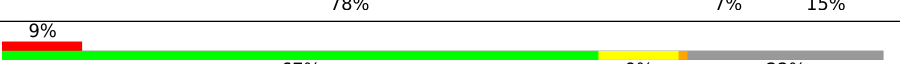
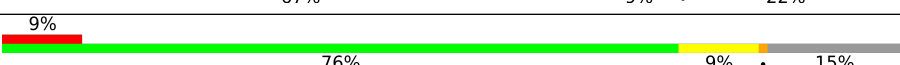
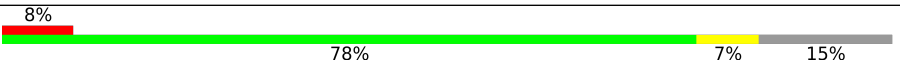
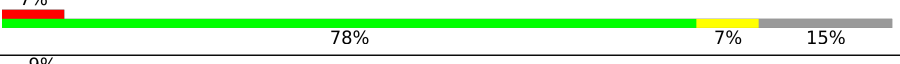
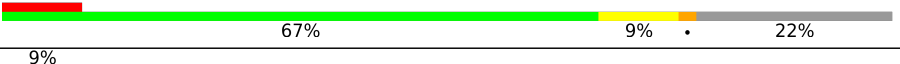
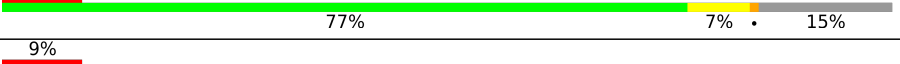
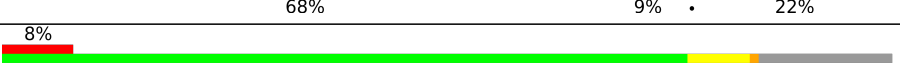
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Mol	Chain	Length	Quality of chain
1	EA	192	
1	EB	192	
1	EC	192	
1	ED	192	
1	EE	192	
1	EF	192	
1	F	192	
1	FA	192	
1	FB	192	
1	FC	192	
1	FD	192	
1	FE	192	
1	FF	192	
1	G	192	
1	GA	192	
1	GB	192	
1	GC	192	
1	GD	192	
1	GE	192	
1	GF	192	
1	H	192	
1	HA	192	
1	HB	192	
1	HC	192	
1	HD	192	

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Mol	Chain	Length	Quality of chain
1	HE	192	
1	HF	192	
1	I	192	
1	IA	192	
1	IB	192	
1	IC	192	
1	ID	192	
1	IE	192	
1	IF	192	
1	J	192	
1	JA	192	
1	JB	192	
1	JC	192	
1	JD	192	
1	JE	192	
1	JF	192	
1	K	192	
1	KA	192	
1	KB	192	
1	KC	192	
1	KD	192	
1	KE	192	
1	KF	192	
1	L	192	
1	LA	192	

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Mol	Chain	Length	Quality of chain
1	LB	192	
1	LC	192	
1	LD	192	
1	LE	192	
1	LF	192	
1	M	192	
1	MA	192	
1	MB	192	
1	MC	192	
1	MD	192	
1	ME	192	
1	MF	192	
1	N	192	
1	NA	192	
1	NB	192	
1	NC	192	
1	ND	192	
1	NE	192	
1	NF	192	
1	O	192	
1	OA	192	
1	OB	192	
1	OC	192	
1	OD	192	
1	OE	192	

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Mol	Chain	Length	Quality of chain
1	OF	192	
1	P	192	
1	PA	192	
1	PB	192	
1	PC	192	
1	PD	192	
1	PE	192	
1	PF	192	
1	Q	192	
1	QA	192	
1	QB	192	
1	QC	192	
1	QD	192	
1	QE	192	
1	QF	192	
1	R	192	
1	RA	192	
1	RB	192	
1	RC	192	
1	RD	192	
1	RE	192	
1	RF	192	
1	S	192	
1	SA	192	
1	SB	192	

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Mol	Chain	Length	Quality of chain
1	SC	192	
1	SD	192	
1	SE	192	
1	SF	192	
1	T	192	
1	TA	192	
1	TB	192	
1	TC	192	
1	TD	192	
1	TE	192	
1	TF	192	
1	UA	192	
1	UB	192	
1	UC	192	
1	UD	192	
1	UE	192	
1	UF	192	
1	V	192	
1	VA	192	
1	VB	192	
1	VC	192	
1	VD	192	
1	VE	192	
1	VF	192	
1	W	192	

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Mol	Chain	Length	Quality of chain
1	WA	192	
1	WB	192	
1	WC	192	
1	WD	192	
1	WE	192	
1	WF	192	
1	X	192	
1	XA	192	
1	XB	192	
1	XC	192	
1	XD	192	
1	XE	192	
1	XF	192	
1	Y	192	
1	YA	192	
1	YB	192	
1	YC	192	
1	YD	192	
1	YE	192	
1	YF	192	
1	Z	192	
1	ZA	192	
1	ZB	192	
1	ZC	192	
1	ZD	192	

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Mol	Chain	Length	Quality of chain
1	ZE	192	 7% 78% 7% 15%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 215160 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 Coat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	B	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	C	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	D	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	E	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	F	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	G	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	H	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	I	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	J	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	K	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	L	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	M	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	N	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	O	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	P	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	Q	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	S	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	T	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	V	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	W	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	X	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	Y	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	Z	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	AA	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	BA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	CA	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	DA	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	EA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	FA	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	GA	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	HA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	IA	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	JA	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	KA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	LA	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	MA	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	NA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	OA	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	PA	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	QA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	RA	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	SA	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	TA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	UA	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	VA	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	WA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	XA	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	YA	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	ZA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	AB	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	BB	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	CB	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	DB	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	EB	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	FB	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	GB	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	HB	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	IB	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	JB	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	KB	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	LB	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	MB	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	NB	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	OB	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	PB	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	QB	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	RB	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	SB	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	TB	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	UB	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	VB	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	WB	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	XB	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	YB	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	ZB	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	AC	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	BC	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	CC	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DC	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	EC	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	FC	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	GC	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	HC	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	IC	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	JC	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	KC	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	LC	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	MC	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	NC	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	OC	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	PC	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	QC	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	RC	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	SC	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	TC	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	UC	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	VC	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	WC	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	XC	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	YC	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	ZC	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	AD	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	BD	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	CD	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	DD	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	ED	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	FD	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	GD	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	HD	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	ID	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	JD	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	KD	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	LD	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	MD	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	ND	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	OD	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	PD	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	QD	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	RD	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	SD	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	TD	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	UD	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	VD	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	WD	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	XD	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	YD	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	ZD	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	AE	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	BE	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	CE	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	DE	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	EE	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	FE	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	GE	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	HE	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	IE	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	JE	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	KE	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	LE	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	ME	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	NE	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	OE	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	PE	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	QE	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	RE	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	SE	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	TE	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	UE	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	VE	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	WE	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	XE	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	YE	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	ZE	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	AF	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	BF	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	CF	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	DF	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	EF	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	FF	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	GF	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	HF	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	IF	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	JF	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	KF	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	LF	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	MF	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	NF	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	OF	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	PF	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	QF	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	RF	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	SF	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	TF	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	UF	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	VF	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	WF	149	Total	C	N	O	S	0	0
			1131	728	188	212	3		
1	XF	163	Total	C	N	O	S	0	0
			1221	786	203	229	3		
1	YF	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		

There are 720 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9QCJ1
A	-1	ASN	-	expression tag	UNP Q9QCJ1
A	0	ILE	-	expression tag	UNP Q9QCJ1
A	189	LYS	-	expression tag	UNP Q9QCJ1
B	-2	SER	-	expression tag	UNP Q9QCJ1
B	-1	ASN	-	expression tag	UNP Q9QCJ1
B	0	ILE	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	189	LYS	-	expression tag	UNP Q9QCJ1
C	-2	SER	-	expression tag	UNP Q9QCJ1
C	-1	ASN	-	expression tag	UNP Q9QCJ1
C	0	ILE	-	expression tag	UNP Q9QCJ1
C	189	LYS	-	expression tag	UNP Q9QCJ1
D	-2	SER	-	expression tag	UNP Q9QCJ1
D	-1	ASN	-	expression tag	UNP Q9QCJ1
D	0	ILE	-	expression tag	UNP Q9QCJ1
D	189	LYS	-	expression tag	UNP Q9QCJ1
E	-2	SER	-	expression tag	UNP Q9QCJ1
E	-1	ASN	-	expression tag	UNP Q9QCJ1
E	0	ILE	-	expression tag	UNP Q9QCJ1
E	189	LYS	-	expression tag	UNP Q9QCJ1
F	-2	SER	-	expression tag	UNP Q9QCJ1
F	-1	ASN	-	expression tag	UNP Q9QCJ1
F	0	ILE	-	expression tag	UNP Q9QCJ1
F	189	LYS	-	expression tag	UNP Q9QCJ1
G	-2	SER	-	expression tag	UNP Q9QCJ1
G	-1	ASN	-	expression tag	UNP Q9QCJ1
G	0	ILE	-	expression tag	UNP Q9QCJ1
G	189	LYS	-	expression tag	UNP Q9QCJ1
H	-2	SER	-	expression tag	UNP Q9QCJ1
H	-1	ASN	-	expression tag	UNP Q9QCJ1
H	0	ILE	-	expression tag	UNP Q9QCJ1
H	189	LYS	-	expression tag	UNP Q9QCJ1
I	-2	SER	-	expression tag	UNP Q9QCJ1
I	-1	ASN	-	expression tag	UNP Q9QCJ1
I	0	ILE	-	expression tag	UNP Q9QCJ1
I	189	LYS	-	expression tag	UNP Q9QCJ1
J	-2	SER	-	expression tag	UNP Q9QCJ1
J	-1	ASN	-	expression tag	UNP Q9QCJ1
J	0	ILE	-	expression tag	UNP Q9QCJ1
J	189	LYS	-	expression tag	UNP Q9QCJ1
K	-2	SER	-	expression tag	UNP Q9QCJ1
K	-1	ASN	-	expression tag	UNP Q9QCJ1
K	0	ILE	-	expression tag	UNP Q9QCJ1
K	189	LYS	-	expression tag	UNP Q9QCJ1
L	-2	SER	-	expression tag	UNP Q9QCJ1
L	-1	ASN	-	expression tag	UNP Q9QCJ1
L	0	ILE	-	expression tag	UNP Q9QCJ1
L	189	LYS	-	expression tag	UNP Q9QCJ1
M	-2	SER	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-1	ASN	-	expression tag	UNP Q9QCJ1
M	0	ILE	-	expression tag	UNP Q9QCJ1
M	189	LYS	-	expression tag	UNP Q9QCJ1
N	-2	SER	-	expression tag	UNP Q9QCJ1
N	-1	ASN	-	expression tag	UNP Q9QCJ1
N	0	ILE	-	expression tag	UNP Q9QCJ1
N	189	LYS	-	expression tag	UNP Q9QCJ1
O	-2	SER	-	expression tag	UNP Q9QCJ1
O	-1	ASN	-	expression tag	UNP Q9QCJ1
O	0	ILE	-	expression tag	UNP Q9QCJ1
O	189	LYS	-	expression tag	UNP Q9QCJ1
P	-2	SER	-	expression tag	UNP Q9QCJ1
P	-1	ASN	-	expression tag	UNP Q9QCJ1
P	0	ILE	-	expression tag	UNP Q9QCJ1
P	189	LYS	-	expression tag	UNP Q9QCJ1
Q	-2	SER	-	expression tag	UNP Q9QCJ1
Q	-1	ASN	-	expression tag	UNP Q9QCJ1
Q	0	ILE	-	expression tag	UNP Q9QCJ1
Q	189	LYS	-	expression tag	UNP Q9QCJ1
R	-2	SER	-	expression tag	UNP Q9QCJ1
R	-1	ASN	-	expression tag	UNP Q9QCJ1
R	0	ILE	-	expression tag	UNP Q9QCJ1
R	189	LYS	-	expression tag	UNP Q9QCJ1
S	-2	SER	-	expression tag	UNP Q9QCJ1
S	-1	ASN	-	expression tag	UNP Q9QCJ1
S	0	ILE	-	expression tag	UNP Q9QCJ1
S	189	LYS	-	expression tag	UNP Q9QCJ1
T	-2	SER	-	expression tag	UNP Q9QCJ1
T	-1	ASN	-	expression tag	UNP Q9QCJ1
T	0	ILE	-	expression tag	UNP Q9QCJ1
T	189	LYS	-	expression tag	UNP Q9QCJ1
V	-2	SER	-	expression tag	UNP Q9QCJ1
V	-1	ASN	-	expression tag	UNP Q9QCJ1
V	0	ILE	-	expression tag	UNP Q9QCJ1
V	189	LYS	-	expression tag	UNP Q9QCJ1
W	-2	SER	-	expression tag	UNP Q9QCJ1
W	-1	ASN	-	expression tag	UNP Q9QCJ1
W	0	ILE	-	expression tag	UNP Q9QCJ1
W	189	LYS	-	expression tag	UNP Q9QCJ1
X	-2	SER	-	expression tag	UNP Q9QCJ1
X	-1	ASN	-	expression tag	UNP Q9QCJ1
X	0	ILE	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
X	189	LYS	-	expression tag	UNP Q9QCJ1
Y	-2	SER	-	expression tag	UNP Q9QCJ1
Y	-1	ASN	-	expression tag	UNP Q9QCJ1
Y	0	ILE	-	expression tag	UNP Q9QCJ1
Y	189	LYS	-	expression tag	UNP Q9QCJ1
Z	-2	SER	-	expression tag	UNP Q9QCJ1
Z	-1	ASN	-	expression tag	UNP Q9QCJ1
Z	0	ILE	-	expression tag	UNP Q9QCJ1
Z	189	LYS	-	expression tag	UNP Q9QCJ1
AA	-2	SER	-	expression tag	UNP Q9QCJ1
AA	-1	ASN	-	expression tag	UNP Q9QCJ1
AA	0	ILE	-	expression tag	UNP Q9QCJ1
AA	189	LYS	-	expression tag	UNP Q9QCJ1
BA	-2	SER	-	expression tag	UNP Q9QCJ1
BA	-1	ASN	-	expression tag	UNP Q9QCJ1
BA	0	ILE	-	expression tag	UNP Q9QCJ1
BA	189	LYS	-	expression tag	UNP Q9QCJ1
CA	-2	SER	-	expression tag	UNP Q9QCJ1
CA	-1	ASN	-	expression tag	UNP Q9QCJ1
CA	0	ILE	-	expression tag	UNP Q9QCJ1
CA	189	LYS	-	expression tag	UNP Q9QCJ1
DA	-2	SER	-	expression tag	UNP Q9QCJ1
DA	-1	ASN	-	expression tag	UNP Q9QCJ1
DA	0	ILE	-	expression tag	UNP Q9QCJ1
DA	189	LYS	-	expression tag	UNP Q9QCJ1
EA	-2	SER	-	expression tag	UNP Q9QCJ1
EA	-1	ASN	-	expression tag	UNP Q9QCJ1
EA	0	ILE	-	expression tag	UNP Q9QCJ1
EA	189	LYS	-	expression tag	UNP Q9QCJ1
FA	-2	SER	-	expression tag	UNP Q9QCJ1
FA	-1	ASN	-	expression tag	UNP Q9QCJ1
FA	0	ILE	-	expression tag	UNP Q9QCJ1
FA	189	LYS	-	expression tag	UNP Q9QCJ1
GA	-2	SER	-	expression tag	UNP Q9QCJ1
GA	-1	ASN	-	expression tag	UNP Q9QCJ1
GA	0	ILE	-	expression tag	UNP Q9QCJ1
GA	189	LYS	-	expression tag	UNP Q9QCJ1
HA	-2	SER	-	expression tag	UNP Q9QCJ1
HA	-1	ASN	-	expression tag	UNP Q9QCJ1
HA	0	ILE	-	expression tag	UNP Q9QCJ1
HA	189	LYS	-	expression tag	UNP Q9QCJ1
IA	-2	SER	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
IA	-1	ASN	-	expression tag	UNP Q9QCJ1
IA	0	ILE	-	expression tag	UNP Q9QCJ1
IA	189	LYS	-	expression tag	UNP Q9QCJ1
JA	-2	SER	-	expression tag	UNP Q9QCJ1
JA	-1	ASN	-	expression tag	UNP Q9QCJ1
JA	0	ILE	-	expression tag	UNP Q9QCJ1
JA	189	LYS	-	expression tag	UNP Q9QCJ1
KA	-2	SER	-	expression tag	UNP Q9QCJ1
KA	-1	ASN	-	expression tag	UNP Q9QCJ1
KA	0	ILE	-	expression tag	UNP Q9QCJ1
KA	189	LYS	-	expression tag	UNP Q9QCJ1
LA	-2	SER	-	expression tag	UNP Q9QCJ1
LA	-1	ASN	-	expression tag	UNP Q9QCJ1
LA	0	ILE	-	expression tag	UNP Q9QCJ1
LA	189	LYS	-	expression tag	UNP Q9QCJ1
MA	-2	SER	-	expression tag	UNP Q9QCJ1
MA	-1	ASN	-	expression tag	UNP Q9QCJ1
MA	0	ILE	-	expression tag	UNP Q9QCJ1
MA	189	LYS	-	expression tag	UNP Q9QCJ1
NA	-2	SER	-	expression tag	UNP Q9QCJ1
NA	-1	ASN	-	expression tag	UNP Q9QCJ1
NA	0	ILE	-	expression tag	UNP Q9QCJ1
NA	189	LYS	-	expression tag	UNP Q9QCJ1
OA	-2	SER	-	expression tag	UNP Q9QCJ1
OA	-1	ASN	-	expression tag	UNP Q9QCJ1
OA	0	ILE	-	expression tag	UNP Q9QCJ1
OA	189	LYS	-	expression tag	UNP Q9QCJ1
PA	-2	SER	-	expression tag	UNP Q9QCJ1
PA	-1	ASN	-	expression tag	UNP Q9QCJ1
PA	0	ILE	-	expression tag	UNP Q9QCJ1
PA	189	LYS	-	expression tag	UNP Q9QCJ1
QA	-2	SER	-	expression tag	UNP Q9QCJ1
QA	-1	ASN	-	expression tag	UNP Q9QCJ1
QA	0	ILE	-	expression tag	UNP Q9QCJ1
QA	189	LYS	-	expression tag	UNP Q9QCJ1
RA	-2	SER	-	expression tag	UNP Q9QCJ1
RA	-1	ASN	-	expression tag	UNP Q9QCJ1
RA	0	ILE	-	expression tag	UNP Q9QCJ1
RA	189	LYS	-	expression tag	UNP Q9QCJ1
SA	-2	SER	-	expression tag	UNP Q9QCJ1
SA	-1	ASN	-	expression tag	UNP Q9QCJ1
SA	0	ILE	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
SA	189	LYS	-	expression tag	UNP Q9QCJ1
TA	-2	SER	-	expression tag	UNP Q9QCJ1
TA	-1	ASN	-	expression tag	UNP Q9QCJ1
TA	0	ILE	-	expression tag	UNP Q9QCJ1
TA	189	LYS	-	expression tag	UNP Q9QCJ1
UA	-2	SER	-	expression tag	UNP Q9QCJ1
UA	-1	ASN	-	expression tag	UNP Q9QCJ1
UA	0	ILE	-	expression tag	UNP Q9QCJ1
UA	189	LYS	-	expression tag	UNP Q9QCJ1
VA	-2	SER	-	expression tag	UNP Q9QCJ1
VA	-1	ASN	-	expression tag	UNP Q9QCJ1
VA	0	ILE	-	expression tag	UNP Q9QCJ1
VA	189	LYS	-	expression tag	UNP Q9QCJ1
WA	-2	SER	-	expression tag	UNP Q9QCJ1
WA	-1	ASN	-	expression tag	UNP Q9QCJ1
WA	0	ILE	-	expression tag	UNP Q9QCJ1
WA	189	LYS	-	expression tag	UNP Q9QCJ1
XA	-2	SER	-	expression tag	UNP Q9QCJ1
XA	-1	ASN	-	expression tag	UNP Q9QCJ1
XA	0	ILE	-	expression tag	UNP Q9QCJ1
XA	189	LYS	-	expression tag	UNP Q9QCJ1
YA	-2	SER	-	expression tag	UNP Q9QCJ1
YA	-1	ASN	-	expression tag	UNP Q9QCJ1
YA	0	ILE	-	expression tag	UNP Q9QCJ1
YA	189	LYS	-	expression tag	UNP Q9QCJ1
ZA	-2	SER	-	expression tag	UNP Q9QCJ1
ZA	-1	ASN	-	expression tag	UNP Q9QCJ1
ZA	0	ILE	-	expression tag	UNP Q9QCJ1
ZA	189	LYS	-	expression tag	UNP Q9QCJ1
AB	-2	SER	-	expression tag	UNP Q9QCJ1
AB	-1	ASN	-	expression tag	UNP Q9QCJ1
AB	0	ILE	-	expression tag	UNP Q9QCJ1
AB	189	LYS	-	expression tag	UNP Q9QCJ1
BB	-2	SER	-	expression tag	UNP Q9QCJ1
BB	-1	ASN	-	expression tag	UNP Q9QCJ1
BB	0	ILE	-	expression tag	UNP Q9QCJ1
BB	189	LYS	-	expression tag	UNP Q9QCJ1
CB	-2	SER	-	expression tag	UNP Q9QCJ1
CB	-1	ASN	-	expression tag	UNP Q9QCJ1
CB	0	ILE	-	expression tag	UNP Q9QCJ1
CB	189	LYS	-	expression tag	UNP Q9QCJ1
DB	-2	SER	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
DB	-1	ASN	-	expression tag	UNP Q9QCJ1
DB	0	ILE	-	expression tag	UNP Q9QCJ1
DB	189	LYS	-	expression tag	UNP Q9QCJ1
EB	-2	SER	-	expression tag	UNP Q9QCJ1
EB	-1	ASN	-	expression tag	UNP Q9QCJ1
EB	0	ILE	-	expression tag	UNP Q9QCJ1
EB	189	LYS	-	expression tag	UNP Q9QCJ1
FB	-2	SER	-	expression tag	UNP Q9QCJ1
FB	-1	ASN	-	expression tag	UNP Q9QCJ1
FB	0	ILE	-	expression tag	UNP Q9QCJ1
FB	189	LYS	-	expression tag	UNP Q9QCJ1
GB	-2	SER	-	expression tag	UNP Q9QCJ1
GB	-1	ASN	-	expression tag	UNP Q9QCJ1
GB	0	ILE	-	expression tag	UNP Q9QCJ1
GB	189	LYS	-	expression tag	UNP Q9QCJ1
HB	-2	SER	-	expression tag	UNP Q9QCJ1
HB	-1	ASN	-	expression tag	UNP Q9QCJ1
HB	0	ILE	-	expression tag	UNP Q9QCJ1
HB	189	LYS	-	expression tag	UNP Q9QCJ1
IB	-2	SER	-	expression tag	UNP Q9QCJ1
IB	-1	ASN	-	expression tag	UNP Q9QCJ1
IB	0	ILE	-	expression tag	UNP Q9QCJ1
IB	189	LYS	-	expression tag	UNP Q9QCJ1
JB	-2	SER	-	expression tag	UNP Q9QCJ1
JB	-1	ASN	-	expression tag	UNP Q9QCJ1
JB	0	ILE	-	expression tag	UNP Q9QCJ1
JB	189	LYS	-	expression tag	UNP Q9QCJ1
KB	-2	SER	-	expression tag	UNP Q9QCJ1
KB	-1	ASN	-	expression tag	UNP Q9QCJ1
KB	0	ILE	-	expression tag	UNP Q9QCJ1
KB	189	LYS	-	expression tag	UNP Q9QCJ1
LB	-2	SER	-	expression tag	UNP Q9QCJ1
LB	-1	ASN	-	expression tag	UNP Q9QCJ1
LB	0	ILE	-	expression tag	UNP Q9QCJ1
LB	189	LYS	-	expression tag	UNP Q9QCJ1
MB	-2	SER	-	expression tag	UNP Q9QCJ1
MB	-1	ASN	-	expression tag	UNP Q9QCJ1
MB	0	ILE	-	expression tag	UNP Q9QCJ1
MB	189	LYS	-	expression tag	UNP Q9QCJ1
NB	-2	SER	-	expression tag	UNP Q9QCJ1
NB	-1	ASN	-	expression tag	UNP Q9QCJ1
NB	0	ILE	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
NB	189	LYS	-	expression tag	UNP Q9QCJ1
OB	-2	SER	-	expression tag	UNP Q9QCJ1
OB	-1	ASN	-	expression tag	UNP Q9QCJ1
OB	0	ILE	-	expression tag	UNP Q9QCJ1
OB	189	LYS	-	expression tag	UNP Q9QCJ1
PB	-2	SER	-	expression tag	UNP Q9QCJ1
PB	-1	ASN	-	expression tag	UNP Q9QCJ1
PB	0	ILE	-	expression tag	UNP Q9QCJ1
PB	189	LYS	-	expression tag	UNP Q9QCJ1
QB	-2	SER	-	expression tag	UNP Q9QCJ1
QB	-1	ASN	-	expression tag	UNP Q9QCJ1
QB	0	ILE	-	expression tag	UNP Q9QCJ1
QB	189	LYS	-	expression tag	UNP Q9QCJ1
RB	-2	SER	-	expression tag	UNP Q9QCJ1
RB	-1	ASN	-	expression tag	UNP Q9QCJ1
RB	0	ILE	-	expression tag	UNP Q9QCJ1
RB	189	LYS	-	expression tag	UNP Q9QCJ1
SB	-2	SER	-	expression tag	UNP Q9QCJ1
SB	-1	ASN	-	expression tag	UNP Q9QCJ1
SB	0	ILE	-	expression tag	UNP Q9QCJ1
SB	189	LYS	-	expression tag	UNP Q9QCJ1
TB	-2	SER	-	expression tag	UNP Q9QCJ1
TB	-1	ASN	-	expression tag	UNP Q9QCJ1
TB	0	ILE	-	expression tag	UNP Q9QCJ1
TB	189	LYS	-	expression tag	UNP Q9QCJ1
UB	-2	SER	-	expression tag	UNP Q9QCJ1
UB	-1	ASN	-	expression tag	UNP Q9QCJ1
UB	0	ILE	-	expression tag	UNP Q9QCJ1
UB	189	LYS	-	expression tag	UNP Q9QCJ1
VB	-2	SER	-	expression tag	UNP Q9QCJ1
VB	-1	ASN	-	expression tag	UNP Q9QCJ1
VB	0	ILE	-	expression tag	UNP Q9QCJ1
VB	189	LYS	-	expression tag	UNP Q9QCJ1
WB	-2	SER	-	expression tag	UNP Q9QCJ1
WB	-1	ASN	-	expression tag	UNP Q9QCJ1
WB	0	ILE	-	expression tag	UNP Q9QCJ1
WB	189	LYS	-	expression tag	UNP Q9QCJ1
XB	-2	SER	-	expression tag	UNP Q9QCJ1
XB	-1	ASN	-	expression tag	UNP Q9QCJ1
XB	0	ILE	-	expression tag	UNP Q9QCJ1
XB	189	LYS	-	expression tag	UNP Q9QCJ1
YB	-2	SER	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
YB	-1	ASN	-	expression tag	UNP Q9QCJ1
YB	0	ILE	-	expression tag	UNP Q9QCJ1
YB	189	LYS	-	expression tag	UNP Q9QCJ1
ZB	-2	SER	-	expression tag	UNP Q9QCJ1
ZB	-1	ASN	-	expression tag	UNP Q9QCJ1
ZB	0	ILE	-	expression tag	UNP Q9QCJ1
ZB	189	LYS	-	expression tag	UNP Q9QCJ1
AC	-2	SER	-	expression tag	UNP Q9QCJ1
AC	-1	ASN	-	expression tag	UNP Q9QCJ1
AC	0	ILE	-	expression tag	UNP Q9QCJ1
AC	189	LYS	-	expression tag	UNP Q9QCJ1
BC	-2	SER	-	expression tag	UNP Q9QCJ1
BC	-1	ASN	-	expression tag	UNP Q9QCJ1
BC	0	ILE	-	expression tag	UNP Q9QCJ1
BC	189	LYS	-	expression tag	UNP Q9QCJ1
CC	-2	SER	-	expression tag	UNP Q9QCJ1
CC	-1	ASN	-	expression tag	UNP Q9QCJ1
CC	0	ILE	-	expression tag	UNP Q9QCJ1
CC	189	LYS	-	expression tag	UNP Q9QCJ1
DC	-2	SER	-	expression tag	UNP Q9QCJ1
DC	-1	ASN	-	expression tag	UNP Q9QCJ1
DC	0	ILE	-	expression tag	UNP Q9QCJ1
DC	189	LYS	-	expression tag	UNP Q9QCJ1
EC	-2	SER	-	expression tag	UNP Q9QCJ1
EC	-1	ASN	-	expression tag	UNP Q9QCJ1
EC	0	ILE	-	expression tag	UNP Q9QCJ1
EC	189	LYS	-	expression tag	UNP Q9QCJ1
FC	-2	SER	-	expression tag	UNP Q9QCJ1
FC	-1	ASN	-	expression tag	UNP Q9QCJ1
FC	0	ILE	-	expression tag	UNP Q9QCJ1
FC	189	LYS	-	expression tag	UNP Q9QCJ1
GC	-2	SER	-	expression tag	UNP Q9QCJ1
GC	-1	ASN	-	expression tag	UNP Q9QCJ1
GC	0	ILE	-	expression tag	UNP Q9QCJ1
GC	189	LYS	-	expression tag	UNP Q9QCJ1
HC	-2	SER	-	expression tag	UNP Q9QCJ1
HC	-1	ASN	-	expression tag	UNP Q9QCJ1
HC	0	ILE	-	expression tag	UNP Q9QCJ1
HC	189	LYS	-	expression tag	UNP Q9QCJ1
IC	-2	SER	-	expression tag	UNP Q9QCJ1
IC	-1	ASN	-	expression tag	UNP Q9QCJ1
IC	0	ILE	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
IC	189	LYS	-	expression tag	UNP Q9QCJ1
JC	-2	SER	-	expression tag	UNP Q9QCJ1
JC	-1	ASN	-	expression tag	UNP Q9QCJ1
JC	0	ILE	-	expression tag	UNP Q9QCJ1
JC	189	LYS	-	expression tag	UNP Q9QCJ1
KC	-2	SER	-	expression tag	UNP Q9QCJ1
KC	-1	ASN	-	expression tag	UNP Q9QCJ1
KC	0	ILE	-	expression tag	UNP Q9QCJ1
KC	189	LYS	-	expression tag	UNP Q9QCJ1
LC	-2	SER	-	expression tag	UNP Q9QCJ1
LC	-1	ASN	-	expression tag	UNP Q9QCJ1
LC	0	ILE	-	expression tag	UNP Q9QCJ1
LC	189	LYS	-	expression tag	UNP Q9QCJ1
MC	-2	SER	-	expression tag	UNP Q9QCJ1
MC	-1	ASN	-	expression tag	UNP Q9QCJ1
MC	0	ILE	-	expression tag	UNP Q9QCJ1
MC	189	LYS	-	expression tag	UNP Q9QCJ1
NC	-2	SER	-	expression tag	UNP Q9QCJ1
NC	-1	ASN	-	expression tag	UNP Q9QCJ1
NC	0	ILE	-	expression tag	UNP Q9QCJ1
NC	189	LYS	-	expression tag	UNP Q9QCJ1
OC	-2	SER	-	expression tag	UNP Q9QCJ1
OC	-1	ASN	-	expression tag	UNP Q9QCJ1
OC	0	ILE	-	expression tag	UNP Q9QCJ1
OC	189	LYS	-	expression tag	UNP Q9QCJ1
PC	-2	SER	-	expression tag	UNP Q9QCJ1
PC	-1	ASN	-	expression tag	UNP Q9QCJ1
PC	0	ILE	-	expression tag	UNP Q9QCJ1
PC	189	LYS	-	expression tag	UNP Q9QCJ1
QC	-2	SER	-	expression tag	UNP Q9QCJ1
QC	-1	ASN	-	expression tag	UNP Q9QCJ1
QC	0	ILE	-	expression tag	UNP Q9QCJ1
QC	189	LYS	-	expression tag	UNP Q9QCJ1
RC	-2	SER	-	expression tag	UNP Q9QCJ1
RC	-1	ASN	-	expression tag	UNP Q9QCJ1
RC	0	ILE	-	expression tag	UNP Q9QCJ1
RC	189	LYS	-	expression tag	UNP Q9QCJ1
SC	-2	SER	-	expression tag	UNP Q9QCJ1
SC	-1	ASN	-	expression tag	UNP Q9QCJ1
SC	0	ILE	-	expression tag	UNP Q9QCJ1
SC	189	LYS	-	expression tag	UNP Q9QCJ1
TC	-2	SER	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
TC	-1	ASN	-	expression tag	UNP Q9QCJ1
TC	0	ILE	-	expression tag	UNP Q9QCJ1
TC	189	LYS	-	expression tag	UNP Q9QCJ1
UC	-2	SER	-	expression tag	UNP Q9QCJ1
UC	-1	ASN	-	expression tag	UNP Q9QCJ1
UC	0	ILE	-	expression tag	UNP Q9QCJ1
UC	189	LYS	-	expression tag	UNP Q9QCJ1
VC	-2	SER	-	expression tag	UNP Q9QCJ1
VC	-1	ASN	-	expression tag	UNP Q9QCJ1
VC	0	ILE	-	expression tag	UNP Q9QCJ1
VC	189	LYS	-	expression tag	UNP Q9QCJ1
WC	-2	SER	-	expression tag	UNP Q9QCJ1
WC	-1	ASN	-	expression tag	UNP Q9QCJ1
WC	0	ILE	-	expression tag	UNP Q9QCJ1
WC	189	LYS	-	expression tag	UNP Q9QCJ1
XC	-2	SER	-	expression tag	UNP Q9QCJ1
XC	-1	ASN	-	expression tag	UNP Q9QCJ1
XC	0	ILE	-	expression tag	UNP Q9QCJ1
XC	189	LYS	-	expression tag	UNP Q9QCJ1
YC	-2	SER	-	expression tag	UNP Q9QCJ1
YC	-1	ASN	-	expression tag	UNP Q9QCJ1
YC	0	ILE	-	expression tag	UNP Q9QCJ1
YC	189	LYS	-	expression tag	UNP Q9QCJ1
ZC	-2	SER	-	expression tag	UNP Q9QCJ1
ZC	-1	ASN	-	expression tag	UNP Q9QCJ1
ZC	0	ILE	-	expression tag	UNP Q9QCJ1
ZC	189	LYS	-	expression tag	UNP Q9QCJ1
AD	-2	SER	-	expression tag	UNP Q9QCJ1
AD	-1	ASN	-	expression tag	UNP Q9QCJ1
AD	0	ILE	-	expression tag	UNP Q9QCJ1
AD	189	LYS	-	expression tag	UNP Q9QCJ1
BD	-2	SER	-	expression tag	UNP Q9QCJ1
BD	-1	ASN	-	expression tag	UNP Q9QCJ1
BD	0	ILE	-	expression tag	UNP Q9QCJ1
BD	189	LYS	-	expression tag	UNP Q9QCJ1
CD	-2	SER	-	expression tag	UNP Q9QCJ1
CD	-1	ASN	-	expression tag	UNP Q9QCJ1
CD	0	ILE	-	expression tag	UNP Q9QCJ1
CD	189	LYS	-	expression tag	UNP Q9QCJ1
DD	-2	SER	-	expression tag	UNP Q9QCJ1
DD	-1	ASN	-	expression tag	UNP Q9QCJ1
DD	0	ILE	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
DD	189	LYS	-	expression tag	UNP Q9QCJ1
ED	-2	SER	-	expression tag	UNP Q9QCJ1
ED	-1	ASN	-	expression tag	UNP Q9QCJ1
ED	0	ILE	-	expression tag	UNP Q9QCJ1
ED	189	LYS	-	expression tag	UNP Q9QCJ1
FD	-2	SER	-	expression tag	UNP Q9QCJ1
FD	-1	ASN	-	expression tag	UNP Q9QCJ1
FD	0	ILE	-	expression tag	UNP Q9QCJ1
FD	189	LYS	-	expression tag	UNP Q9QCJ1
GD	-2	SER	-	expression tag	UNP Q9QCJ1
GD	-1	ASN	-	expression tag	UNP Q9QCJ1
GD	0	ILE	-	expression tag	UNP Q9QCJ1
GD	189	LYS	-	expression tag	UNP Q9QCJ1
HD	-2	SER	-	expression tag	UNP Q9QCJ1
HD	-1	ASN	-	expression tag	UNP Q9QCJ1
HD	0	ILE	-	expression tag	UNP Q9QCJ1
HD	189	LYS	-	expression tag	UNP Q9QCJ1
ID	-2	SER	-	expression tag	UNP Q9QCJ1
ID	-1	ASN	-	expression tag	UNP Q9QCJ1
ID	0	ILE	-	expression tag	UNP Q9QCJ1
ID	189	LYS	-	expression tag	UNP Q9QCJ1
JD	-2	SER	-	expression tag	UNP Q9QCJ1
JD	-1	ASN	-	expression tag	UNP Q9QCJ1
JD	0	ILE	-	expression tag	UNP Q9QCJ1
JD	189	LYS	-	expression tag	UNP Q9QCJ1
KD	-2	SER	-	expression tag	UNP Q9QCJ1
KD	-1	ASN	-	expression tag	UNP Q9QCJ1
KD	0	ILE	-	expression tag	UNP Q9QCJ1
KD	189	LYS	-	expression tag	UNP Q9QCJ1
LD	-2	SER	-	expression tag	UNP Q9QCJ1
LD	-1	ASN	-	expression tag	UNP Q9QCJ1
LD	0	ILE	-	expression tag	UNP Q9QCJ1
LD	189	LYS	-	expression tag	UNP Q9QCJ1
MD	-2	SER	-	expression tag	UNP Q9QCJ1
MD	-1	ASN	-	expression tag	UNP Q9QCJ1
MD	0	ILE	-	expression tag	UNP Q9QCJ1
MD	189	LYS	-	expression tag	UNP Q9QCJ1
ND	-2	SER	-	expression tag	UNP Q9QCJ1
ND	-1	ASN	-	expression tag	UNP Q9QCJ1
ND	0	ILE	-	expression tag	UNP Q9QCJ1
ND	189	LYS	-	expression tag	UNP Q9QCJ1
OD	-2	SER	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
OD	-1	ASN	-	expression tag	UNP Q9QCJ1
OD	0	ILE	-	expression tag	UNP Q9QCJ1
OD	189	LYS	-	expression tag	UNP Q9QCJ1
PD	-2	SER	-	expression tag	UNP Q9QCJ1
PD	-1	ASN	-	expression tag	UNP Q9QCJ1
PD	0	ILE	-	expression tag	UNP Q9QCJ1
PD	189	LYS	-	expression tag	UNP Q9QCJ1
QD	-2	SER	-	expression tag	UNP Q9QCJ1
QD	-1	ASN	-	expression tag	UNP Q9QCJ1
QD	0	ILE	-	expression tag	UNP Q9QCJ1
QD	189	LYS	-	expression tag	UNP Q9QCJ1
RD	-2	SER	-	expression tag	UNP Q9QCJ1
RD	-1	ASN	-	expression tag	UNP Q9QCJ1
RD	0	ILE	-	expression tag	UNP Q9QCJ1
RD	189	LYS	-	expression tag	UNP Q9QCJ1
SD	-2	SER	-	expression tag	UNP Q9QCJ1
SD	-1	ASN	-	expression tag	UNP Q9QCJ1
SD	0	ILE	-	expression tag	UNP Q9QCJ1
SD	189	LYS	-	expression tag	UNP Q9QCJ1
TD	-2	SER	-	expression tag	UNP Q9QCJ1
TD	-1	ASN	-	expression tag	UNP Q9QCJ1
TD	0	ILE	-	expression tag	UNP Q9QCJ1
TD	189	LYS	-	expression tag	UNP Q9QCJ1
UD	-2	SER	-	expression tag	UNP Q9QCJ1
UD	-1	ASN	-	expression tag	UNP Q9QCJ1
UD	0	ILE	-	expression tag	UNP Q9QCJ1
UD	189	LYS	-	expression tag	UNP Q9QCJ1
VD	-2	SER	-	expression tag	UNP Q9QCJ1
VD	-1	ASN	-	expression tag	UNP Q9QCJ1
VD	0	ILE	-	expression tag	UNP Q9QCJ1
VD	189	LYS	-	expression tag	UNP Q9QCJ1
WD	-2	SER	-	expression tag	UNP Q9QCJ1
WD	-1	ASN	-	expression tag	UNP Q9QCJ1
WD	0	ILE	-	expression tag	UNP Q9QCJ1
WD	189	LYS	-	expression tag	UNP Q9QCJ1
XD	-2	SER	-	expression tag	UNP Q9QCJ1
XD	-1	ASN	-	expression tag	UNP Q9QCJ1
XD	0	ILE	-	expression tag	UNP Q9QCJ1
XD	189	LYS	-	expression tag	UNP Q9QCJ1
YD	-2	SER	-	expression tag	UNP Q9QCJ1
YD	-1	ASN	-	expression tag	UNP Q9QCJ1
YD	0	ILE	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
YD	189	LYS	-	expression tag	UNP Q9QCJ1
ZD	-2	SER	-	expression tag	UNP Q9QCJ1
ZD	-1	ASN	-	expression tag	UNP Q9QCJ1
ZD	0	ILE	-	expression tag	UNP Q9QCJ1
ZD	189	LYS	-	expression tag	UNP Q9QCJ1
AE	-2	SER	-	expression tag	UNP Q9QCJ1
AE	-1	ASN	-	expression tag	UNP Q9QCJ1
AE	0	ILE	-	expression tag	UNP Q9QCJ1
AE	189	LYS	-	expression tag	UNP Q9QCJ1
BE	-2	SER	-	expression tag	UNP Q9QCJ1
BE	-1	ASN	-	expression tag	UNP Q9QCJ1
BE	0	ILE	-	expression tag	UNP Q9QCJ1
BE	189	LYS	-	expression tag	UNP Q9QCJ1
CE	-2	SER	-	expression tag	UNP Q9QCJ1
CE	-1	ASN	-	expression tag	UNP Q9QCJ1
CE	0	ILE	-	expression tag	UNP Q9QCJ1
CE	189	LYS	-	expression tag	UNP Q9QCJ1
DE	-2	SER	-	expression tag	UNP Q9QCJ1
DE	-1	ASN	-	expression tag	UNP Q9QCJ1
DE	0	ILE	-	expression tag	UNP Q9QCJ1
DE	189	LYS	-	expression tag	UNP Q9QCJ1
EE	-2	SER	-	expression tag	UNP Q9QCJ1
EE	-1	ASN	-	expression tag	UNP Q9QCJ1
EE	0	ILE	-	expression tag	UNP Q9QCJ1
EE	189	LYS	-	expression tag	UNP Q9QCJ1
FE	-2	SER	-	expression tag	UNP Q9QCJ1
FE	-1	ASN	-	expression tag	UNP Q9QCJ1
FE	0	ILE	-	expression tag	UNP Q9QCJ1
FE	189	LYS	-	expression tag	UNP Q9QCJ1
GE	-2	SER	-	expression tag	UNP Q9QCJ1
GE	-1	ASN	-	expression tag	UNP Q9QCJ1
GE	0	ILE	-	expression tag	UNP Q9QCJ1
GE	189	LYS	-	expression tag	UNP Q9QCJ1
HE	-2	SER	-	expression tag	UNP Q9QCJ1
HE	-1	ASN	-	expression tag	UNP Q9QCJ1
HE	0	ILE	-	expression tag	UNP Q9QCJ1
HE	189	LYS	-	expression tag	UNP Q9QCJ1
IE	-2	SER	-	expression tag	UNP Q9QCJ1
IE	-1	ASN	-	expression tag	UNP Q9QCJ1
IE	0	ILE	-	expression tag	UNP Q9QCJ1
IE	189	LYS	-	expression tag	UNP Q9QCJ1
JE	-2	SER	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
JE	-1	ASN	-	expression tag	UNP Q9QCJ1
JE	0	ILE	-	expression tag	UNP Q9QCJ1
JE	189	LYS	-	expression tag	UNP Q9QCJ1
KE	-2	SER	-	expression tag	UNP Q9QCJ1
KE	-1	ASN	-	expression tag	UNP Q9QCJ1
KE	0	ILE	-	expression tag	UNP Q9QCJ1
KE	189	LYS	-	expression tag	UNP Q9QCJ1
LE	-2	SER	-	expression tag	UNP Q9QCJ1
LE	-1	ASN	-	expression tag	UNP Q9QCJ1
LE	0	ILE	-	expression tag	UNP Q9QCJ1
LE	189	LYS	-	expression tag	UNP Q9QCJ1
ME	-2	SER	-	expression tag	UNP Q9QCJ1
ME	-1	ASN	-	expression tag	UNP Q9QCJ1
ME	0	ILE	-	expression tag	UNP Q9QCJ1
ME	189	LYS	-	expression tag	UNP Q9QCJ1
NE	-2	SER	-	expression tag	UNP Q9QCJ1
NE	-1	ASN	-	expression tag	UNP Q9QCJ1
NE	0	ILE	-	expression tag	UNP Q9QCJ1
NE	189	LYS	-	expression tag	UNP Q9QCJ1
OE	-2	SER	-	expression tag	UNP Q9QCJ1
OE	-1	ASN	-	expression tag	UNP Q9QCJ1
OE	0	ILE	-	expression tag	UNP Q9QCJ1
OE	189	LYS	-	expression tag	UNP Q9QCJ1
PE	-2	SER	-	expression tag	UNP Q9QCJ1
PE	-1	ASN	-	expression tag	UNP Q9QCJ1
PE	0	ILE	-	expression tag	UNP Q9QCJ1
PE	189	LYS	-	expression tag	UNP Q9QCJ1
QE	-2	SER	-	expression tag	UNP Q9QCJ1
QE	-1	ASN	-	expression tag	UNP Q9QCJ1
QE	0	ILE	-	expression tag	UNP Q9QCJ1
QE	189	LYS	-	expression tag	UNP Q9QCJ1
RE	-2	SER	-	expression tag	UNP Q9QCJ1
RE	-1	ASN	-	expression tag	UNP Q9QCJ1
RE	0	ILE	-	expression tag	UNP Q9QCJ1
RE	189	LYS	-	expression tag	UNP Q9QCJ1
SE	-2	SER	-	expression tag	UNP Q9QCJ1
SE	-1	ASN	-	expression tag	UNP Q9QCJ1
SE	0	ILE	-	expression tag	UNP Q9QCJ1
SE	189	LYS	-	expression tag	UNP Q9QCJ1
TE	-2	SER	-	expression tag	UNP Q9QCJ1
TE	-1	ASN	-	expression tag	UNP Q9QCJ1
TE	0	ILE	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
TE	189	LYS	-	expression tag	UNP Q9QCJ1
UE	-2	SER	-	expression tag	UNP Q9QCJ1
UE	-1	ASN	-	expression tag	UNP Q9QCJ1
UE	0	ILE	-	expression tag	UNP Q9QCJ1
UE	189	LYS	-	expression tag	UNP Q9QCJ1
VE	-2	SER	-	expression tag	UNP Q9QCJ1
VE	-1	ASN	-	expression tag	UNP Q9QCJ1
VE	0	ILE	-	expression tag	UNP Q9QCJ1
VE	189	LYS	-	expression tag	UNP Q9QCJ1
WE	-2	SER	-	expression tag	UNP Q9QCJ1
WE	-1	ASN	-	expression tag	UNP Q9QCJ1
WE	0	ILE	-	expression tag	UNP Q9QCJ1
WE	189	LYS	-	expression tag	UNP Q9QCJ1
XE	-2	SER	-	expression tag	UNP Q9QCJ1
XE	-1	ASN	-	expression tag	UNP Q9QCJ1
XE	0	ILE	-	expression tag	UNP Q9QCJ1
XE	189	LYS	-	expression tag	UNP Q9QCJ1
YE	-2	SER	-	expression tag	UNP Q9QCJ1
YE	-1	ASN	-	expression tag	UNP Q9QCJ1
YE	0	ILE	-	expression tag	UNP Q9QCJ1
YE	189	LYS	-	expression tag	UNP Q9QCJ1
ZE	-2	SER	-	expression tag	UNP Q9QCJ1
ZE	-1	ASN	-	expression tag	UNP Q9QCJ1
ZE	0	ILE	-	expression tag	UNP Q9QCJ1
ZE	189	LYS	-	expression tag	UNP Q9QCJ1
AF	-2	SER	-	expression tag	UNP Q9QCJ1
AF	-1	ASN	-	expression tag	UNP Q9QCJ1
AF	0	ILE	-	expression tag	UNP Q9QCJ1
AF	189	LYS	-	expression tag	UNP Q9QCJ1
BF	-2	SER	-	expression tag	UNP Q9QCJ1
BF	-1	ASN	-	expression tag	UNP Q9QCJ1
BF	0	ILE	-	expression tag	UNP Q9QCJ1
BF	189	LYS	-	expression tag	UNP Q9QCJ1
CF	-2	SER	-	expression tag	UNP Q9QCJ1
CF	-1	ASN	-	expression tag	UNP Q9QCJ1
CF	0	ILE	-	expression tag	UNP Q9QCJ1
CF	189	LYS	-	expression tag	UNP Q9QCJ1
DF	-2	SER	-	expression tag	UNP Q9QCJ1
DF	-1	ASN	-	expression tag	UNP Q9QCJ1
DF	0	ILE	-	expression tag	UNP Q9QCJ1
DF	189	LYS	-	expression tag	UNP Q9QCJ1
EF	-2	SER	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
EF	-1	ASN	-	expression tag	UNP Q9QCJ1
EF	0	ILE	-	expression tag	UNP Q9QCJ1
EF	189	LYS	-	expression tag	UNP Q9QCJ1
FF	-2	SER	-	expression tag	UNP Q9QCJ1
FF	-1	ASN	-	expression tag	UNP Q9QCJ1
FF	0	ILE	-	expression tag	UNP Q9QCJ1
FF	189	LYS	-	expression tag	UNP Q9QCJ1
GF	-2	SER	-	expression tag	UNP Q9QCJ1
GF	-1	ASN	-	expression tag	UNP Q9QCJ1
GF	0	ILE	-	expression tag	UNP Q9QCJ1
GF	189	LYS	-	expression tag	UNP Q9QCJ1
HF	-2	SER	-	expression tag	UNP Q9QCJ1
HF	-1	ASN	-	expression tag	UNP Q9QCJ1
HF	0	ILE	-	expression tag	UNP Q9QCJ1
HF	189	LYS	-	expression tag	UNP Q9QCJ1
IF	-2	SER	-	expression tag	UNP Q9QCJ1
IF	-1	ASN	-	expression tag	UNP Q9QCJ1
IF	0	ILE	-	expression tag	UNP Q9QCJ1
IF	189	LYS	-	expression tag	UNP Q9QCJ1
JF	-2	SER	-	expression tag	UNP Q9QCJ1
JF	-1	ASN	-	expression tag	UNP Q9QCJ1
JF	0	ILE	-	expression tag	UNP Q9QCJ1
JF	189	LYS	-	expression tag	UNP Q9QCJ1
KF	-2	SER	-	expression tag	UNP Q9QCJ1
KF	-1	ASN	-	expression tag	UNP Q9QCJ1
KF	0	ILE	-	expression tag	UNP Q9QCJ1
KF	189	LYS	-	expression tag	UNP Q9QCJ1
LF	-2	SER	-	expression tag	UNP Q9QCJ1
LF	-1	ASN	-	expression tag	UNP Q9QCJ1
LF	0	ILE	-	expression tag	UNP Q9QCJ1
LF	189	LYS	-	expression tag	UNP Q9QCJ1
MF	-2	SER	-	expression tag	UNP Q9QCJ1
MF	-1	ASN	-	expression tag	UNP Q9QCJ1
MF	0	ILE	-	expression tag	UNP Q9QCJ1
MF	189	LYS	-	expression tag	UNP Q9QCJ1
NF	-2	SER	-	expression tag	UNP Q9QCJ1
NF	-1	ASN	-	expression tag	UNP Q9QCJ1
NF	0	ILE	-	expression tag	UNP Q9QCJ1
NF	189	LYS	-	expression tag	UNP Q9QCJ1
OF	-2	SER	-	expression tag	UNP Q9QCJ1
OF	-1	ASN	-	expression tag	UNP Q9QCJ1
OF	0	ILE	-	expression tag	UNP Q9QCJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
OF	189	LYS	-	expression tag	UNP Q9QCJ1
PF	-2	SER	-	expression tag	UNP Q9QCJ1
PF	-1	ASN	-	expression tag	UNP Q9QCJ1
PF	0	ILE	-	expression tag	UNP Q9QCJ1
PF	189	LYS	-	expression tag	UNP Q9QCJ1
QF	-2	SER	-	expression tag	UNP Q9QCJ1
QF	-1	ASN	-	expression tag	UNP Q9QCJ1
QF	0	ILE	-	expression tag	UNP Q9QCJ1
QF	189	LYS	-	expression tag	UNP Q9QCJ1
RF	-2	SER	-	expression tag	UNP Q9QCJ1
RF	-1	ASN	-	expression tag	UNP Q9QCJ1
RF	0	ILE	-	expression tag	UNP Q9QCJ1
RF	189	LYS	-	expression tag	UNP Q9QCJ1
SF	-2	SER	-	expression tag	UNP Q9QCJ1
SF	-1	ASN	-	expression tag	UNP Q9QCJ1
SF	0	ILE	-	expression tag	UNP Q9QCJ1
SF	189	LYS	-	expression tag	UNP Q9QCJ1
TF	-2	SER	-	expression tag	UNP Q9QCJ1
TF	-1	ASN	-	expression tag	UNP Q9QCJ1
TF	0	ILE	-	expression tag	UNP Q9QCJ1
TF	189	LYS	-	expression tag	UNP Q9QCJ1
UF	-2	SER	-	expression tag	UNP Q9QCJ1
UF	-1	ASN	-	expression tag	UNP Q9QCJ1
UF	0	ILE	-	expression tag	UNP Q9QCJ1
UF	189	LYS	-	expression tag	UNP Q9QCJ1
VF	-2	SER	-	expression tag	UNP Q9QCJ1
VF	-1	ASN	-	expression tag	UNP Q9QCJ1
VF	0	ILE	-	expression tag	UNP Q9QCJ1
VF	189	LYS	-	expression tag	UNP Q9QCJ1
WF	-2	SER	-	expression tag	UNP Q9QCJ1
WF	-1	ASN	-	expression tag	UNP Q9QCJ1
WF	0	ILE	-	expression tag	UNP Q9QCJ1
WF	189	LYS	-	expression tag	UNP Q9QCJ1
XF	-2	SER	-	expression tag	UNP Q9QCJ1
XF	-1	ASN	-	expression tag	UNP Q9QCJ1
XF	0	ILE	-	expression tag	UNP Q9QCJ1
XF	189	LYS	-	expression tag	UNP Q9QCJ1
YF	-2	SER	-	expression tag	UNP Q9QCJ1
YF	-1	ASN	-	expression tag	UNP Q9QCJ1
YF	0	ILE	-	expression tag	UNP Q9QCJ1
YF	189	LYS	-	expression tag	UNP Q9QCJ1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total O 1 1	0
2	B	1	Total O 1 1	0
2	C	1	Total O 1 1	0
2	D	1	Total O 1 1	0
2	E	1	Total O 1 1	0
2	F	1	Total O 1 1	0
2	G	1	Total O 1 1	0
2	H	1	Total O 1 1	0
2	I	1	Total O 1 1	0
2	J	1	Total O 1 1	0
2	K	1	Total O 1 1	0
2	L	1	Total O 1 1	0
2	M	1	Total O 1 1	0
2	N	1	Total O 1 1	0
2	O	1	Total O 1 1	0
2	P	1	Total O 1 1	0
2	Q	1	Total O 1 1	0
2	R	1	Total O 1 1	0
2	S	1	Total O 1 1	0
2	T	1	Total O 1 1	0
2	V	1	Total O 1 1	0
2	W	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
2	X	1	Total O 1 1	0
2	Y	1	Total O 1 1	0
2	Z	1	Total O 1 1	0
2	AA	1	Total O 1 1	0
2	BA	1	Total O 1 1	0
2	CA	1	Total O 1 1	0
2	DA	1	Total O 1 1	0
2	EA	1	Total O 1 1	0
2	FA	1	Total O 1 1	0
2	GA	1	Total O 1 1	0
2	HA	1	Total O 1 1	0
2	IA	1	Total O 1 1	0
2	JA	1	Total O 1 1	0
2	KA	1	Total O 1 1	0
2	LA	1	Total O 1 1	0
2	MA	1	Total O 1 1	0
2	NA	1	Total O 1 1	0
2	OA	1	Total O 1 1	0
2	PA	1	Total O 1 1	0
2	QA	1	Total O 1 1	0
2	RA	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
2	SA	1	Total O 1 1	0
2	TA	1	Total O 1 1	0
2	UA	1	Total O 1 1	0
2	VA	1	Total O 1 1	0
2	WA	1	Total O 1 1	0
2	XA	1	Total O 1 1	0
2	YA	1	Total O 1 1	0
2	ZA	1	Total O 1 1	0
2	AB	1	Total O 1 1	0
2	BB	1	Total O 1 1	0
2	CB	1	Total O 1 1	0
2	DB	1	Total O 1 1	0
2	EB	1	Total O 1 1	0
2	FB	1	Total O 1 1	0
2	GB	1	Total O 1 1	0
2	HB	1	Total O 1 1	0
2	IB	1	Total O 1 1	0
2	JB	1	Total O 1 1	0
2	KB	1	Total O 1 1	0
2	LB	1	Total O 1 1	0
2	MB	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
2	NB	1	Total O 1 1	0
2	OB	1	Total O 1 1	0
2	PB	1	Total O 1 1	0
2	QB	1	Total O 1 1	0
2	RB	1	Total O 1 1	0
2	SB	1	Total O 1 1	0
2	TB	1	Total O 1 1	0
2	UB	1	Total O 1 1	0
2	VB	1	Total O 1 1	0
2	WB	1	Total O 1 1	0
2	XB	1	Total O 1 1	0
2	YB	1	Total O 1 1	0
2	ZB	1	Total O 1 1	0
2	AC	1	Total O 1 1	0
2	BC	1	Total O 1 1	0
2	CC	1	Total O 1 1	0
2	DC	1	Total O 1 1	0
2	EC	1	Total O 1 1	0
2	FC	1	Total O 1 1	0
2	GC	1	Total O 1 1	0
2	HC	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
2	IC	1	Total O 1 1	0
2	JC	1	Total O 1 1	0
2	KC	1	Total O 1 1	0
2	LC	1	Total O 1 1	0
2	MC	1	Total O 1 1	0
2	NC	1	Total O 1 1	0
2	OC	1	Total O 1 1	0
2	PC	1	Total O 1 1	0
2	QC	1	Total O 1 1	0
2	RC	1	Total O 1 1	0
2	SC	1	Total O 1 1	0
2	TC	1	Total O 1 1	0
2	UC	1	Total O 1 1	0
2	VC	1	Total O 1 1	0
2	WC	1	Total O 1 1	0
2	XC	1	Total O 1 1	0
2	YC	1	Total O 1 1	0
2	ZC	1	Total O 1 1	0
2	AD	1	Total O 1 1	0
2	BD	1	Total O 1 1	0
2	CD	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
2	DD	1	Total O 1 1	0
2	ED	1	Total O 1 1	0
2	FD	1	Total O 1 1	0
2	GD	1	Total O 1 1	0
2	HD	1	Total O 1 1	0
2	ID	1	Total O 1 1	0
2	JD	1	Total O 1 1	0
2	KD	1	Total O 1 1	0
2	LD	1	Total O 1 1	0
2	MD	1	Total O 1 1	0
2	ND	1	Total O 1 1	0
2	OD	1	Total O 1 1	0
2	PD	1	Total O 1 1	0
2	QD	1	Total O 1 1	0
2	RD	1	Total O 1 1	0
2	SD	1	Total O 1 1	0
2	TD	1	Total O 1 1	0
2	UD	1	Total O 1 1	0
2	VD	1	Total O 1 1	0
2	WD	1	Total O 1 1	0
2	XD	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
2	YD	1	Total O 1 1	0
2	ZD	1	Total O 1 1	0
2	AE	1	Total O 1 1	0
2	BE	1	Total O 1 1	0
2	CE	1	Total O 1 1	0
2	DE	1	Total O 1 1	0
2	EE	1	Total O 1 1	0
2	FE	1	Total O 1 1	0
2	GE	1	Total O 1 1	0
2	HE	1	Total O 1 1	0
2	IE	1	Total O 1 1	0
2	JE	1	Total O 1 1	0
2	KE	1	Total O 1 1	0
2	LE	1	Total O 1 1	0
2	ME	1	Total O 1 1	0
2	NE	1	Total O 1 1	0
2	OE	1	Total O 1 1	0
2	PE	1	Total O 1 1	0
2	QE	1	Total O 1 1	0
2	RE	1	Total O 1 1	0
2	SE	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
2	TE	1	Total O 1 1	0
2	UE	1	Total O 1 1	0
2	VE	1	Total O 1 1	0
2	WE	1	Total O 1 1	0
2	XE	1	Total O 1 1	0
2	YE	1	Total O 1 1	0
2	ZE	1	Total O 1 1	0
2	AF	1	Total O 1 1	0
2	BF	1	Total O 1 1	0
2	CF	1	Total O 1 1	0
2	DF	1	Total O 1 1	0
2	EF	1	Total O 1 1	0
2	FF	1	Total O 1 1	0
2	GF	1	Total O 1 1	0
2	HF	1	Total O 1 1	0
2	IF	1	Total O 1 1	0
2	JF	1	Total O 1 1	0
2	KF	1	Total O 1 1	0
2	LF	1	Total O 1 1	0
2	MF	1	Total O 1 1	0
2	NF	1	Total O 1 1	0

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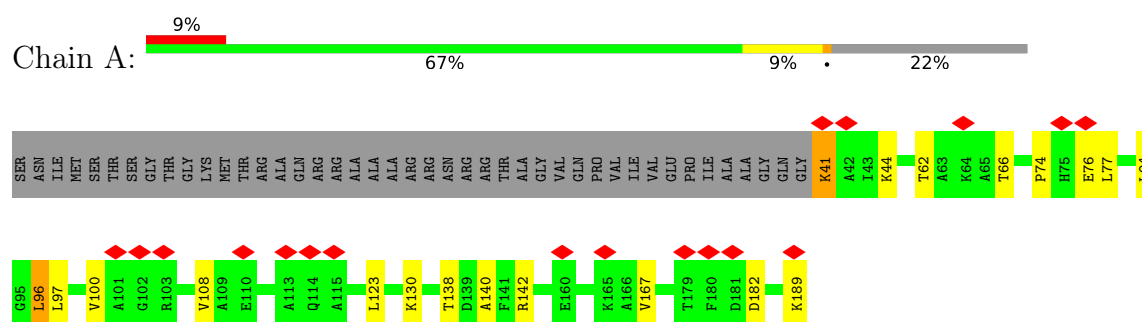
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Mol	Chain	Residues	Atoms		AltConf
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2	PF	1	Total 1	O 1	0
2	QF	1	Total 1	O 1	0
2	RF	1	Total 1	O 1	0
2	SF	1	Total 1	O 1	0
2	TF	1	Total 1	O 1	0
2	UF	1	Total 1	O 1	0
2	VF	1	Total 1	O 1	0
2	WF	1	Total 1	O 1	0
2	XF	1	Total 1	O 1	0
2	YF	1	Total 1	O 1	0

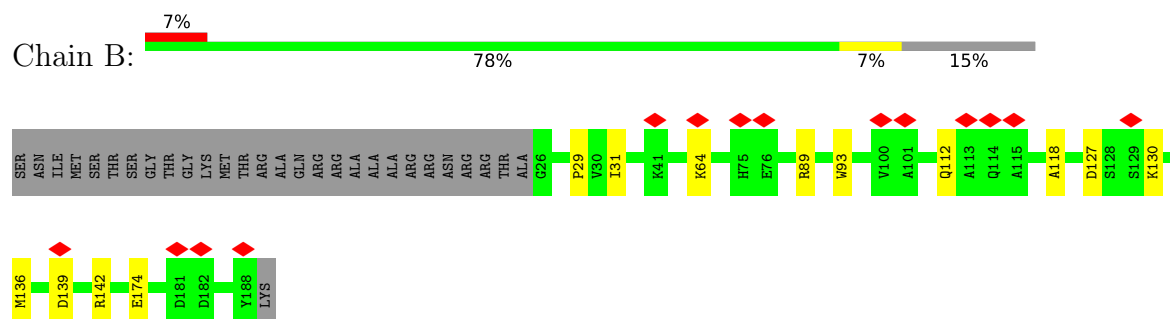
3 Residue-property plots [i](#)

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

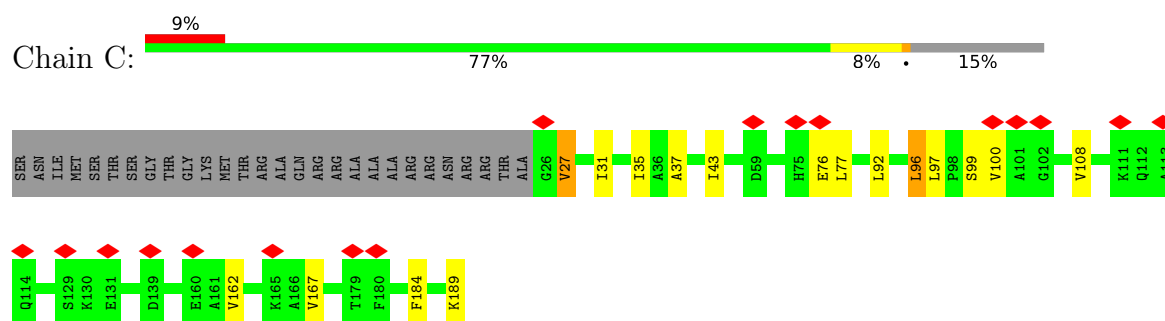
- Molecule 1: Coat protein



- Molecule 1: Coat protein

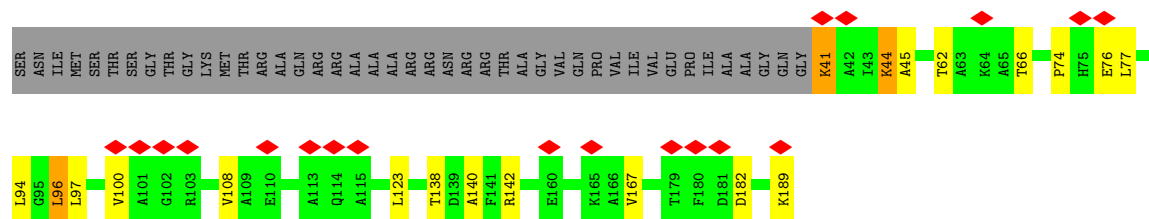


- Molecule 1: Coat protein

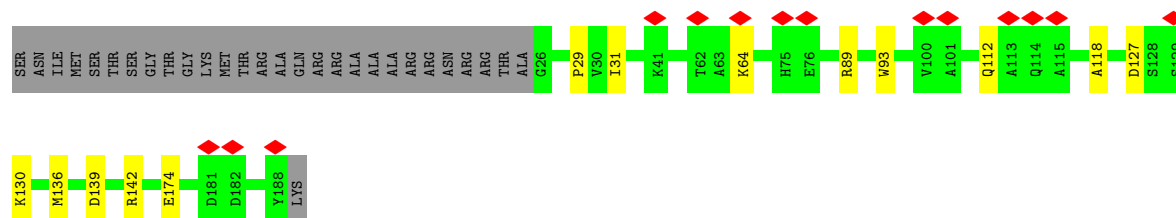
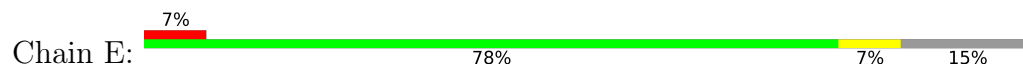


- Molecule 1: Coat protein

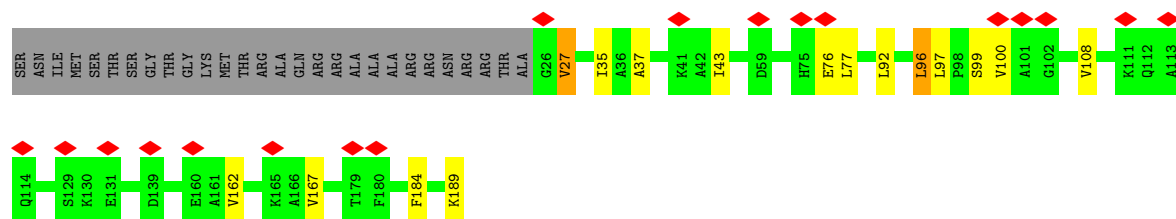
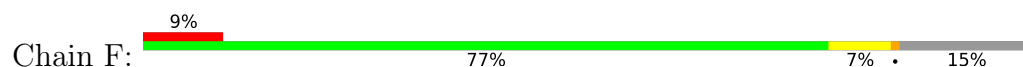




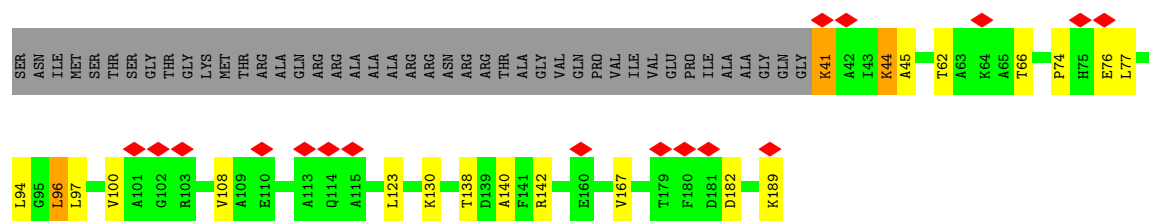
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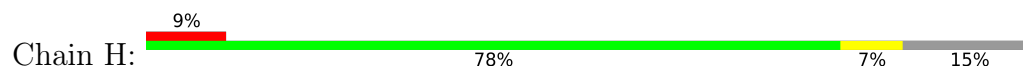
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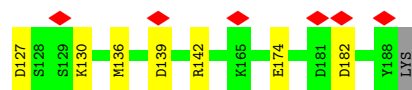


- Molecule 1: Coat protein

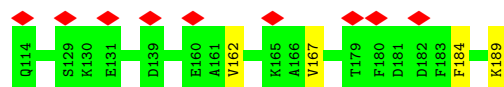
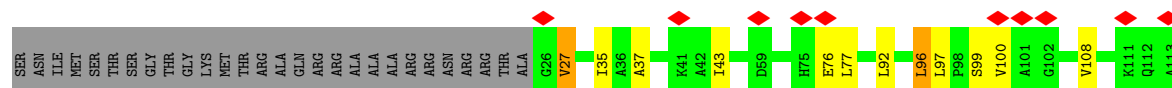
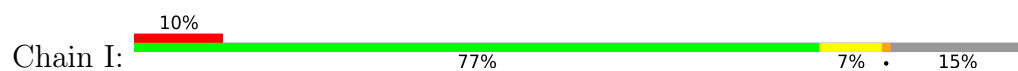


- Molecule 1: Coat protein

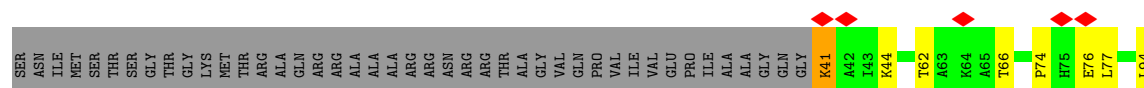




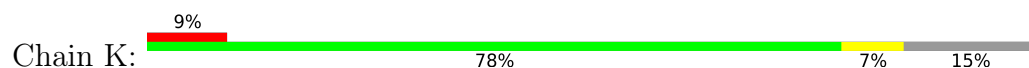
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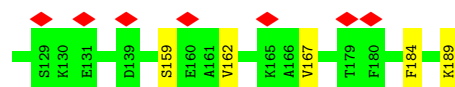
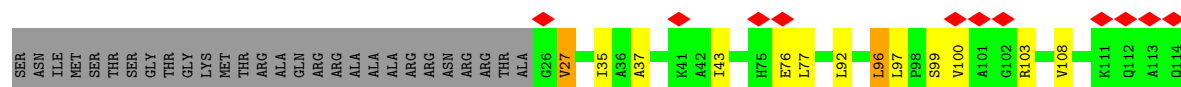
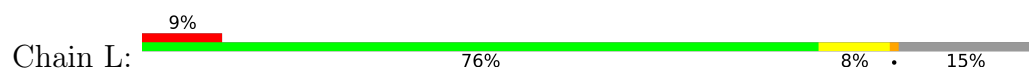
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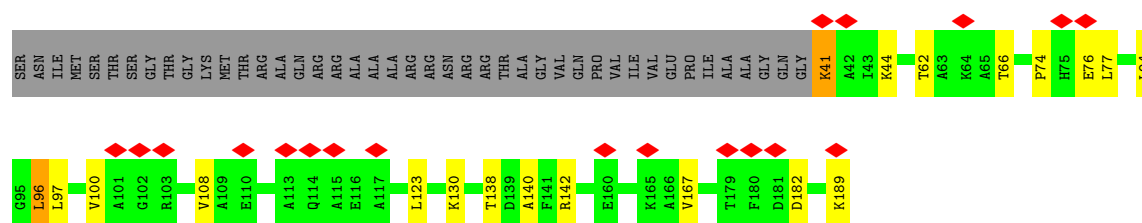
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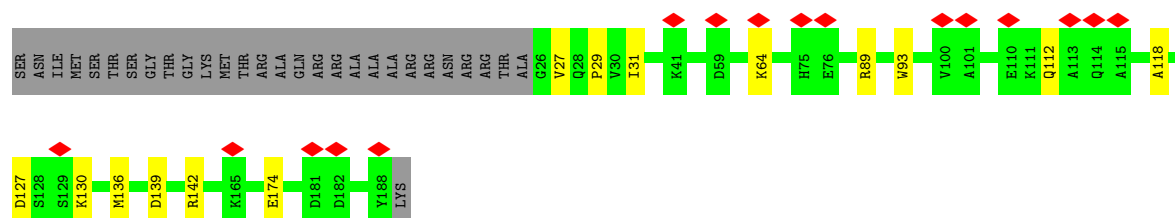
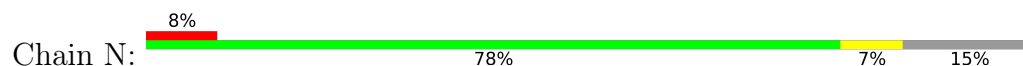
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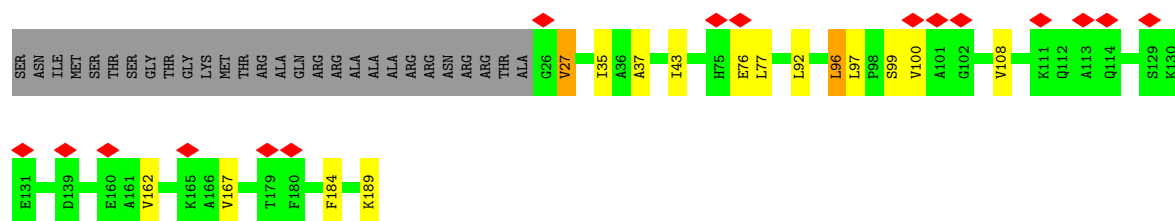
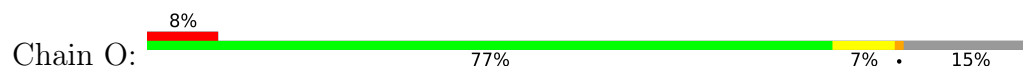
- Molecule 1: Coat protein



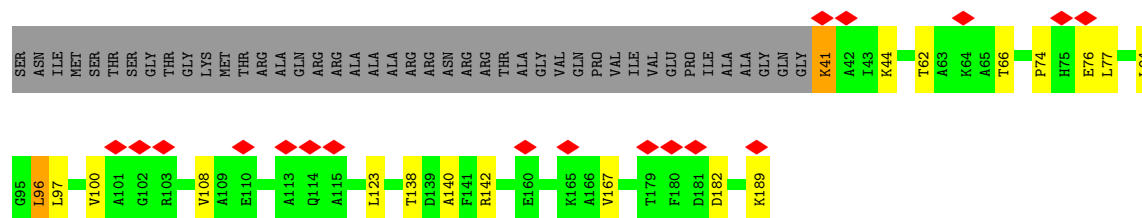
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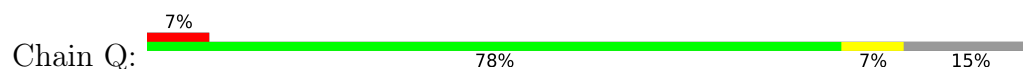
- Molecule 1: Coat protein

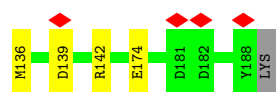


- Molecule 1: Coat protein

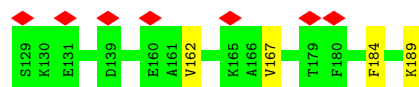
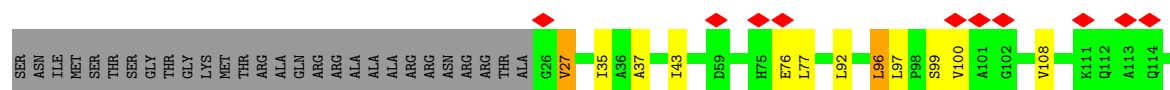
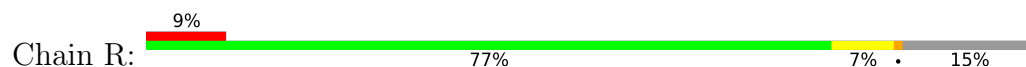


- Molecule 1: Coat protein

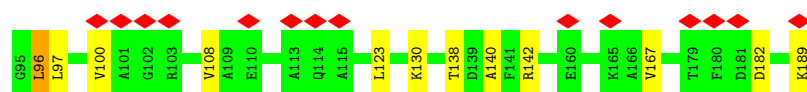
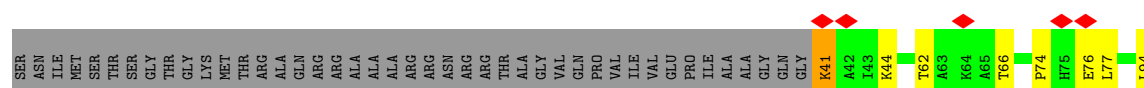




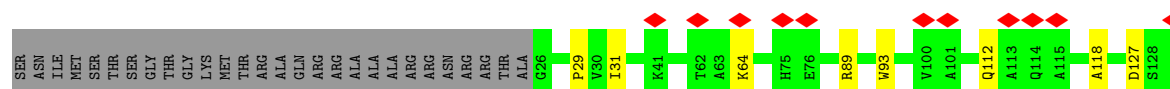
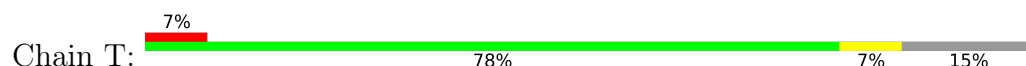
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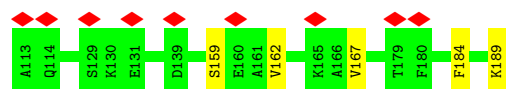
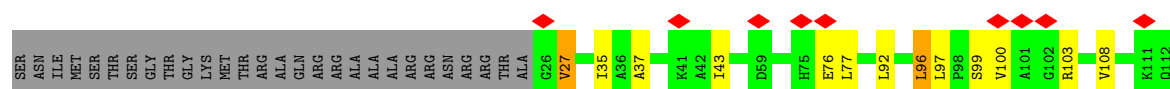
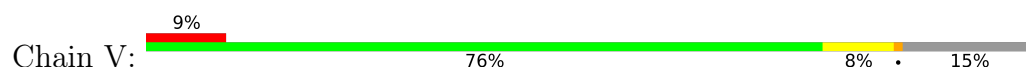
- Molecule 1: Coat protein



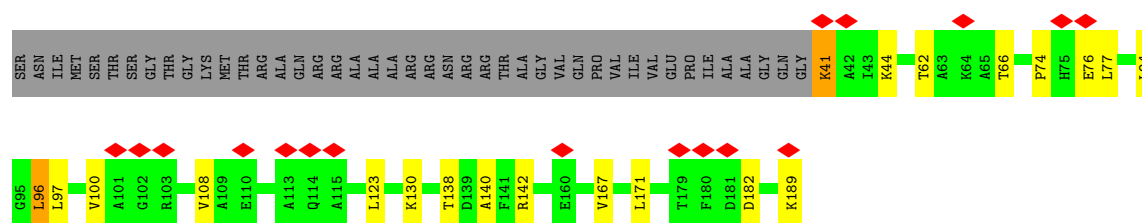
- Molecule 1: Coat protein



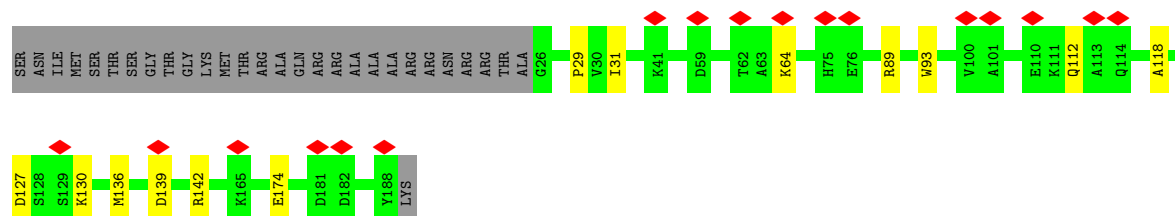
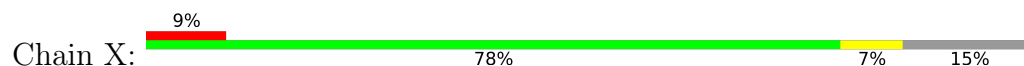
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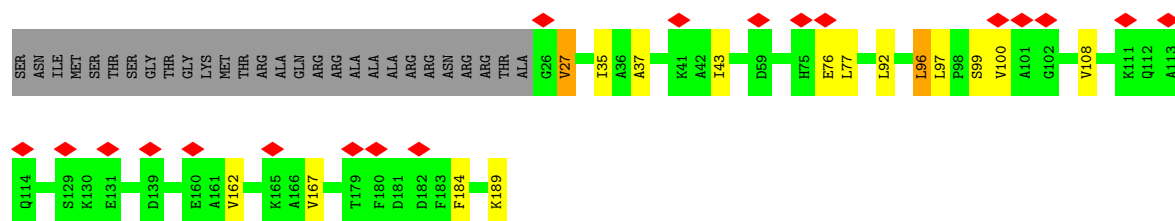
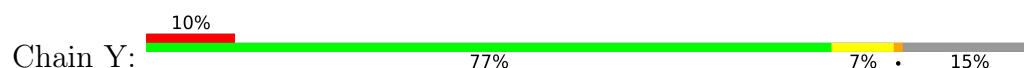
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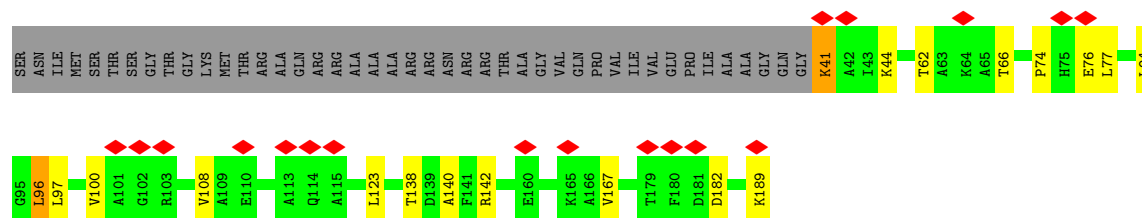
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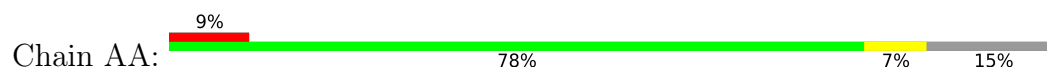
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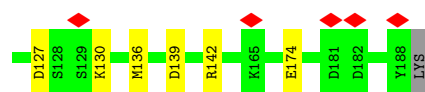


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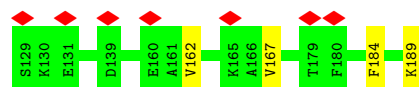
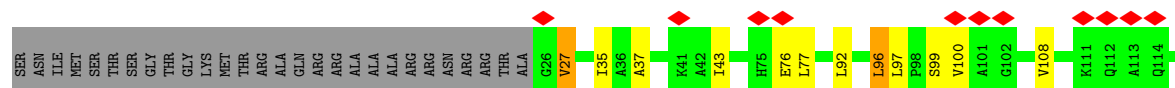
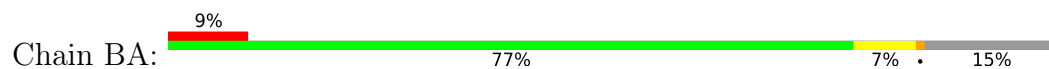


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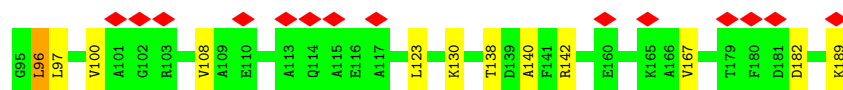
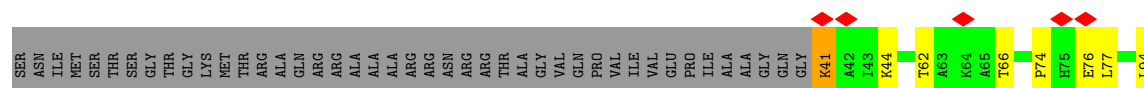




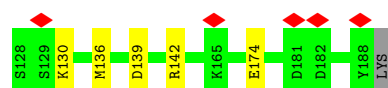
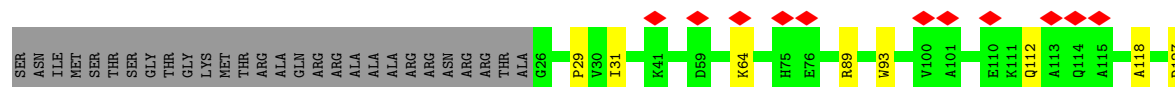
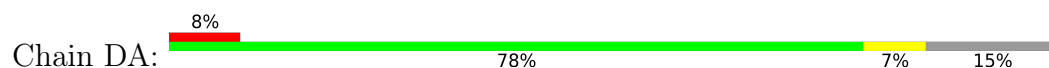
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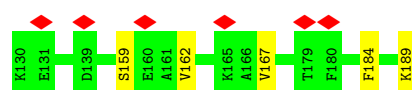
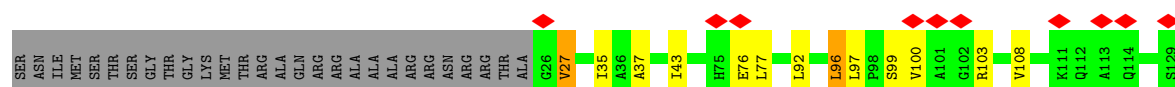
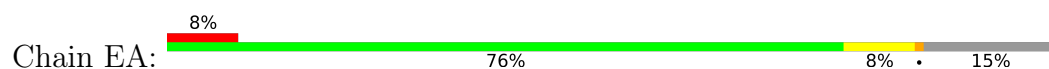
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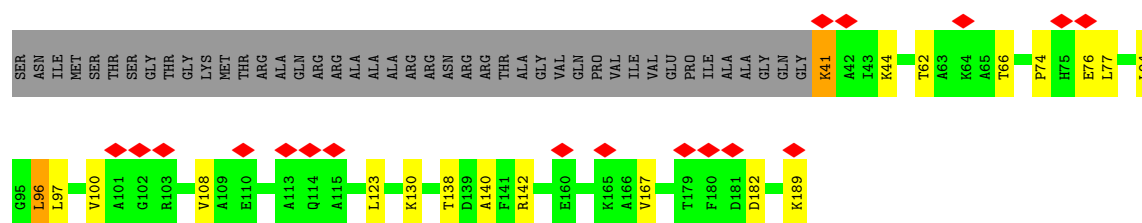
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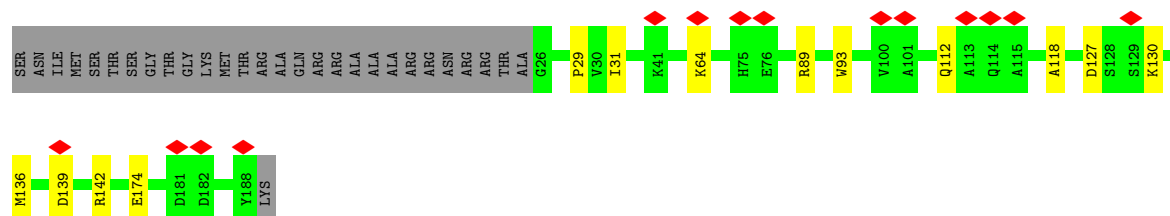
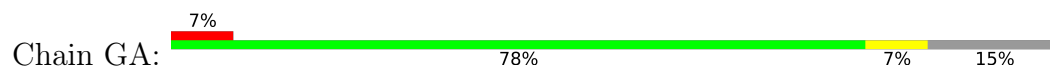
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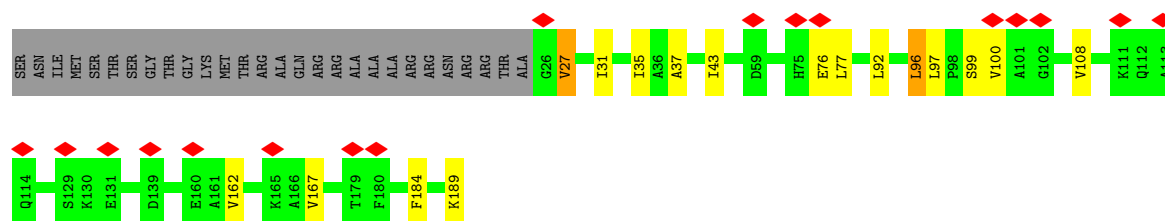
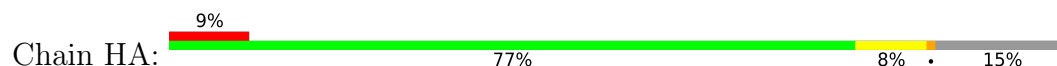
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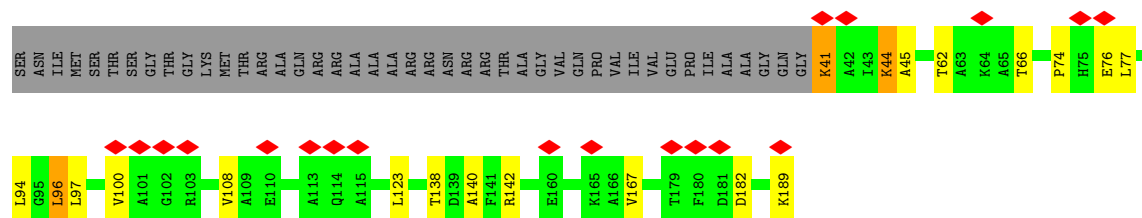
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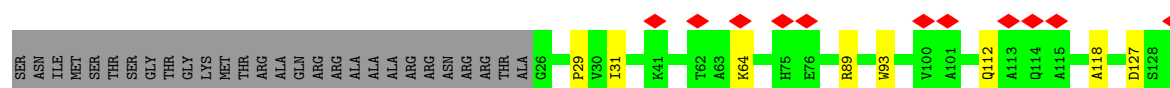
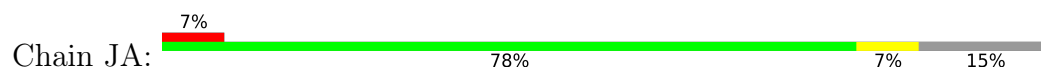
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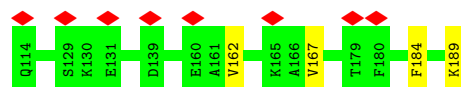
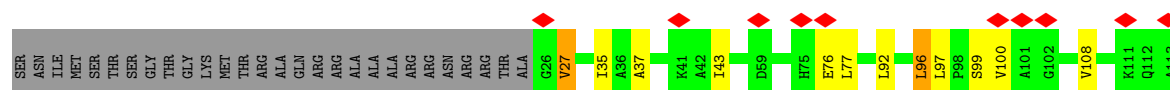
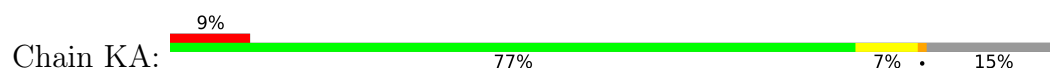


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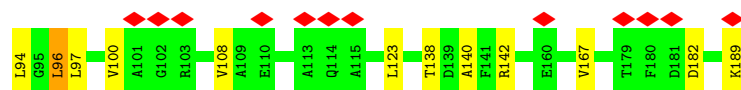
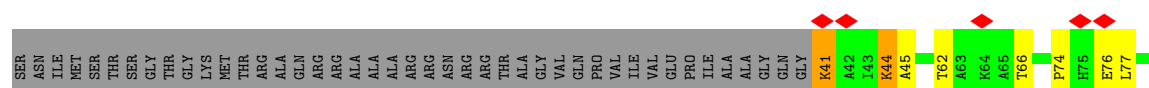




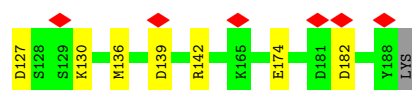
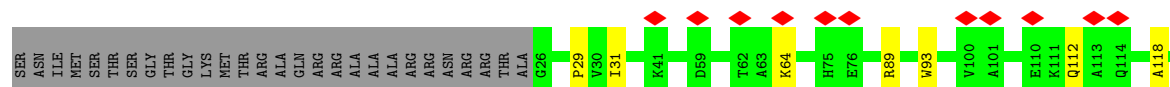
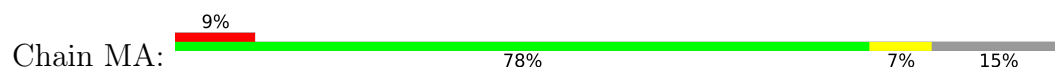
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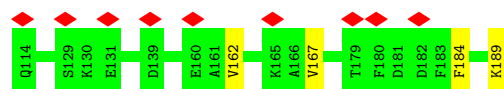
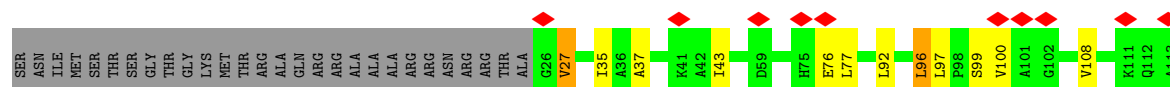
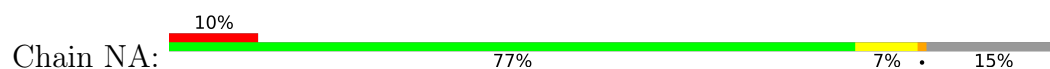
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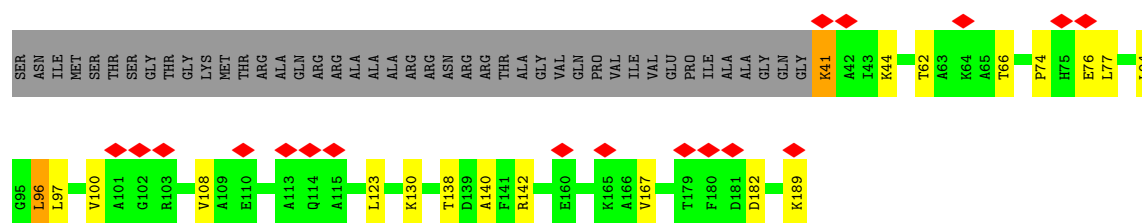
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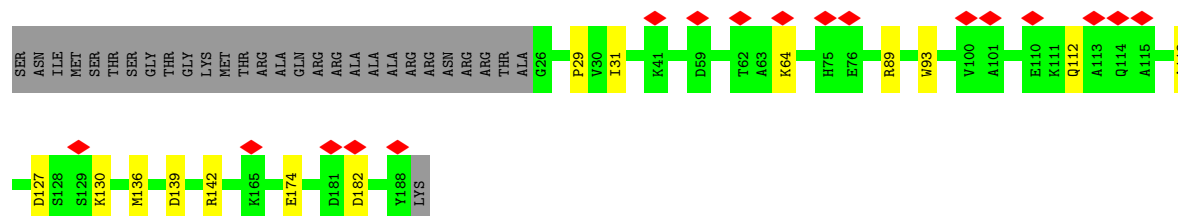
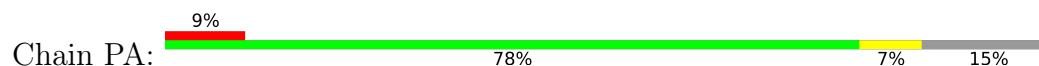
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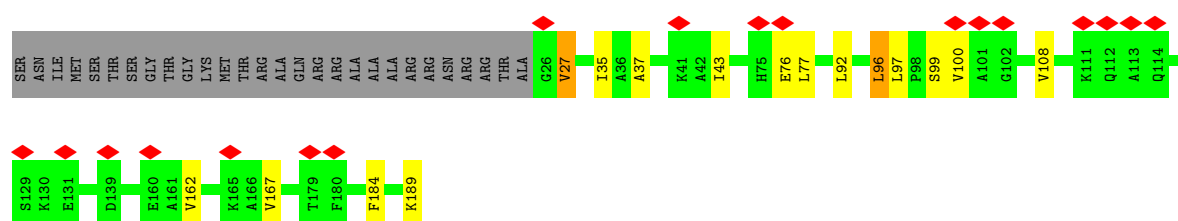
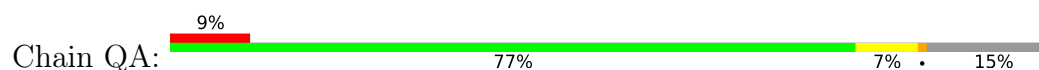
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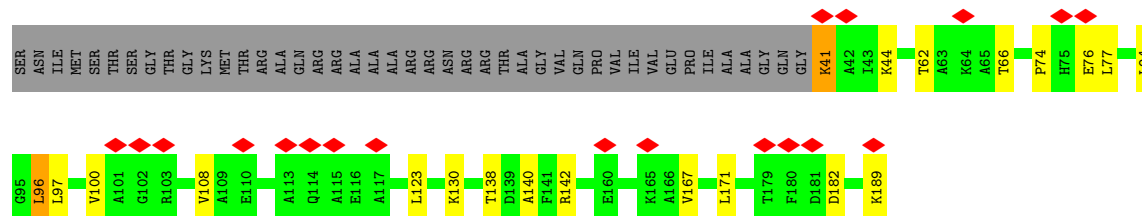
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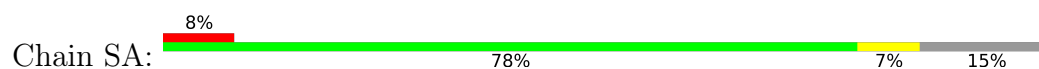
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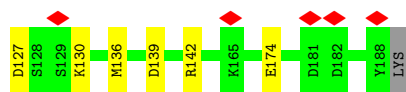


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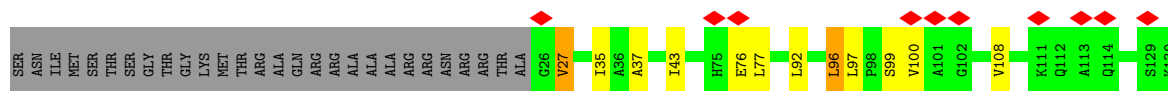
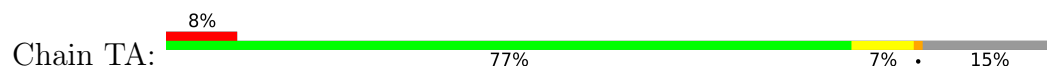


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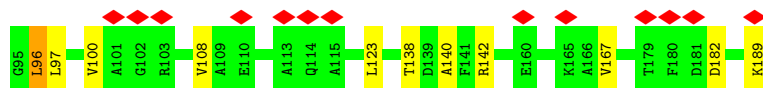
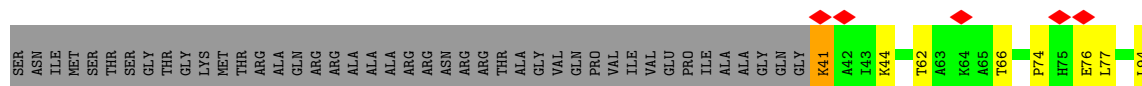




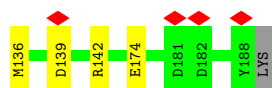
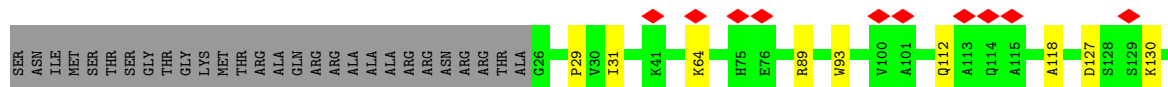
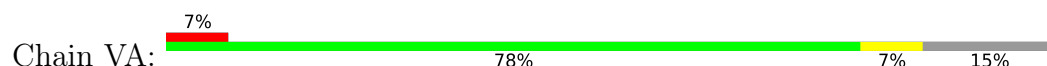
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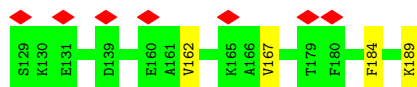
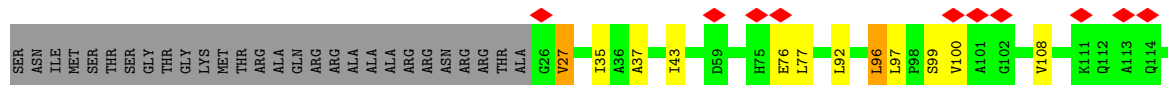
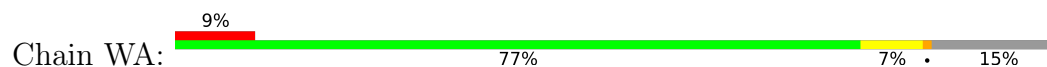
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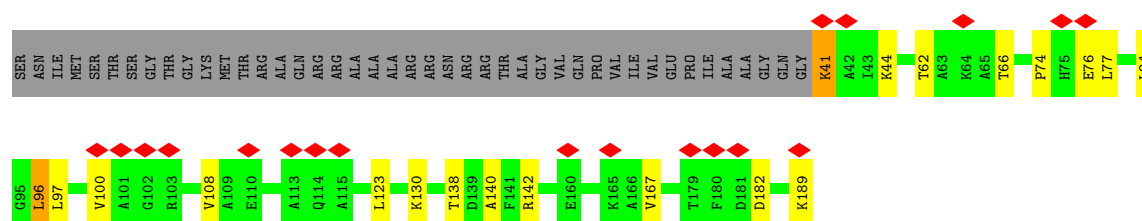
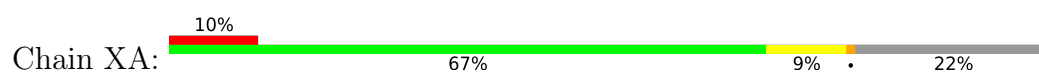
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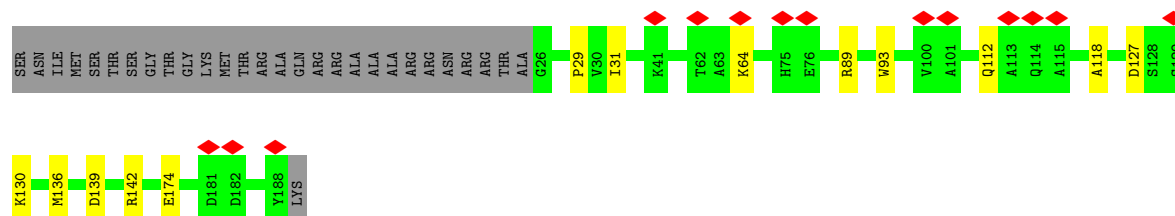
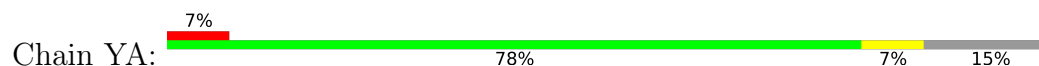
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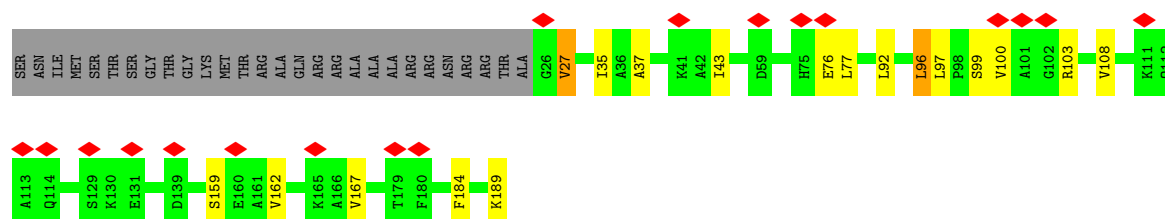
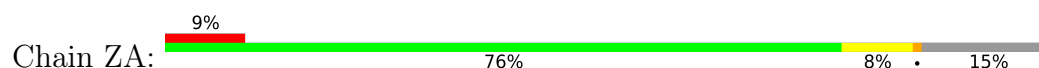
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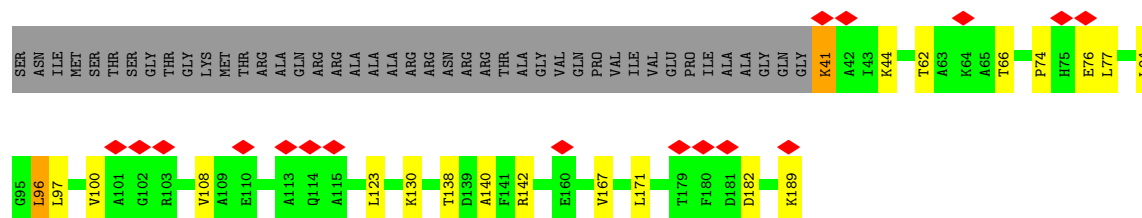
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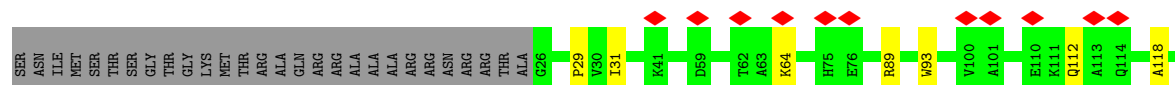
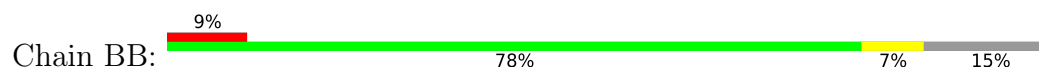
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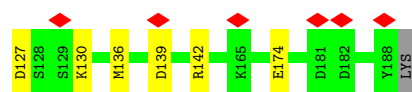


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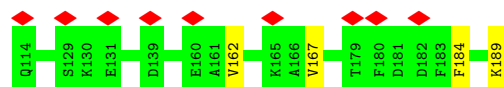
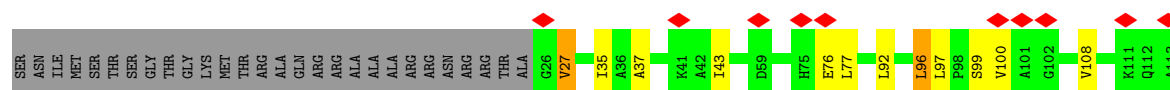
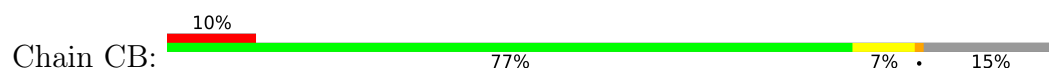


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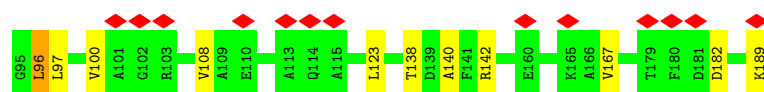
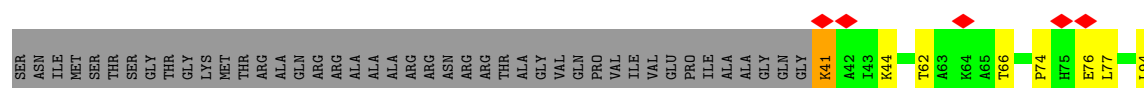




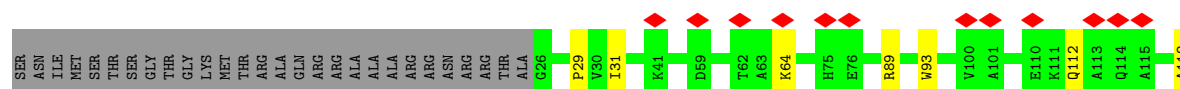
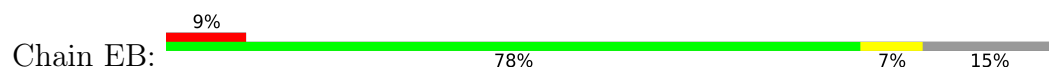
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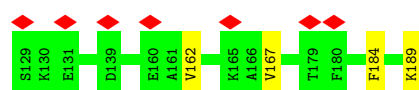
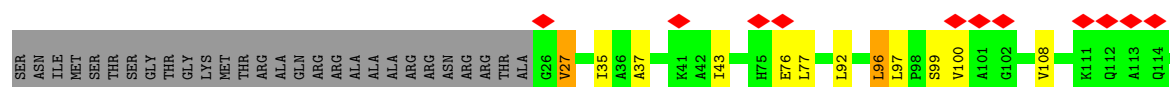
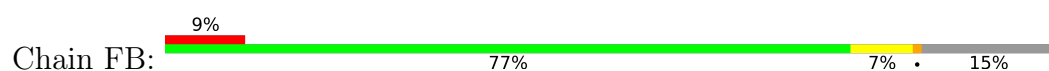
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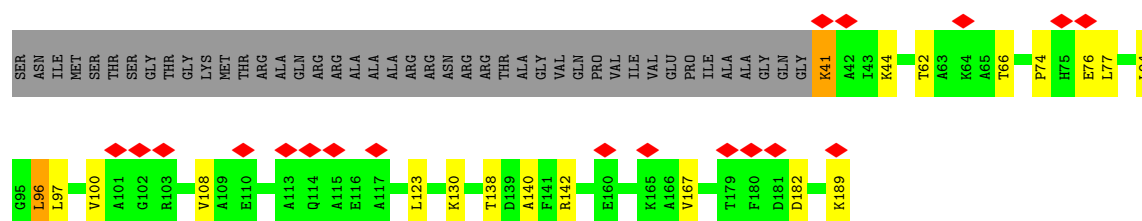
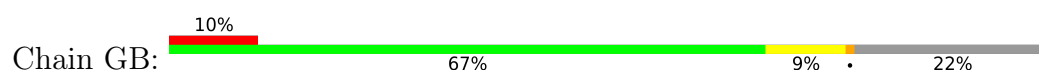
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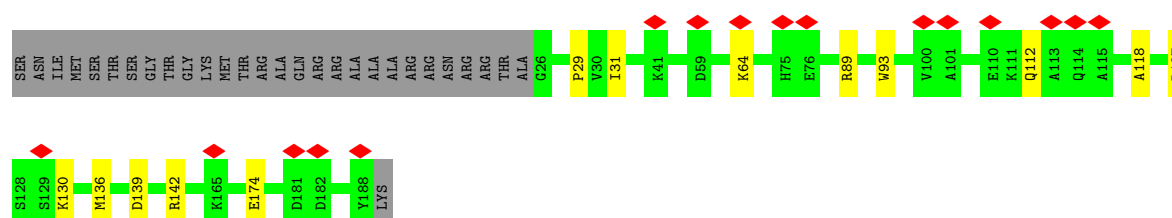
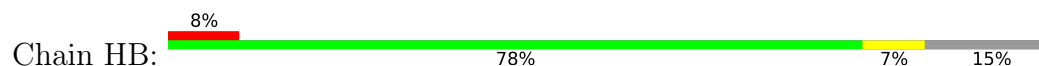
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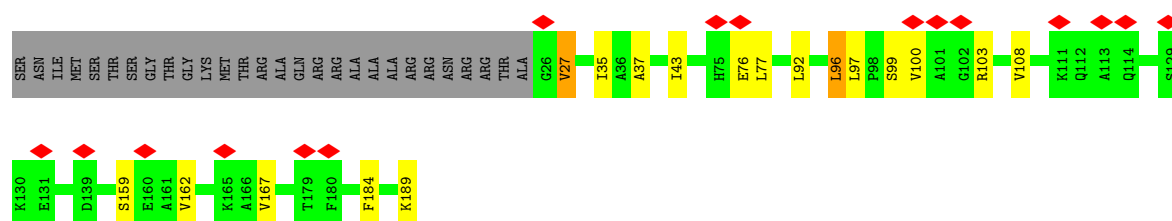
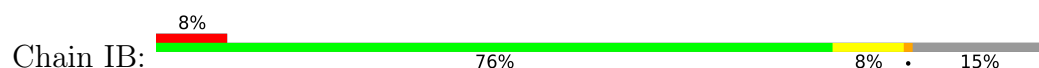
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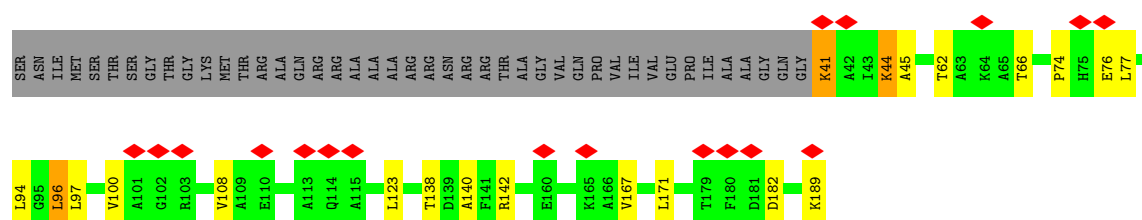
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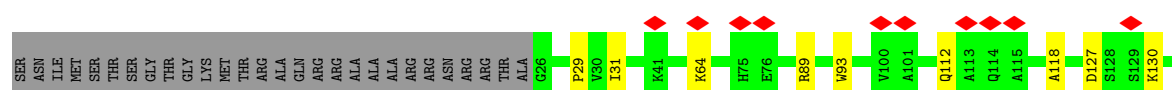
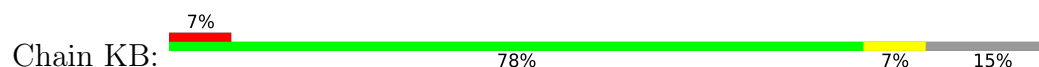
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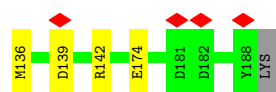


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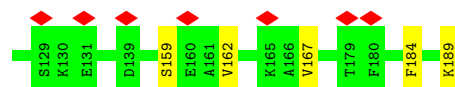
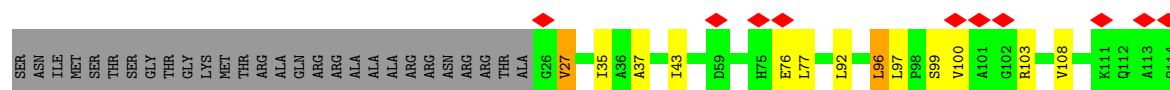
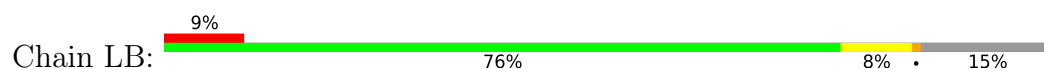


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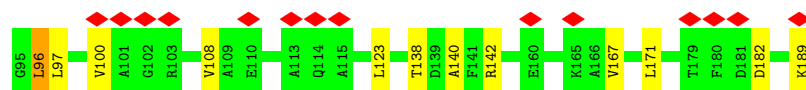
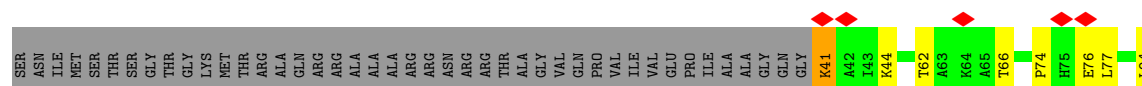




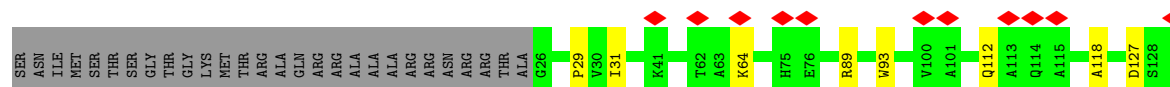
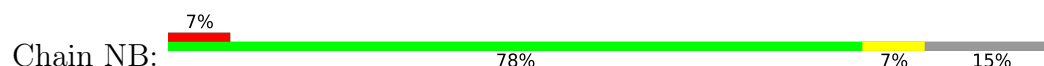
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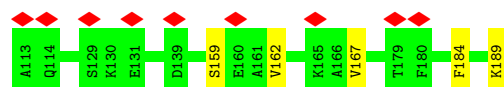
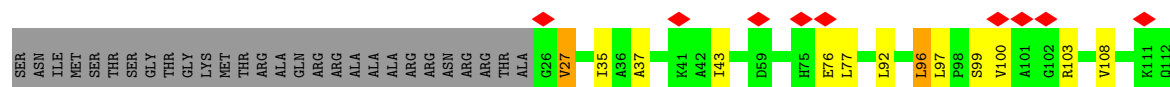
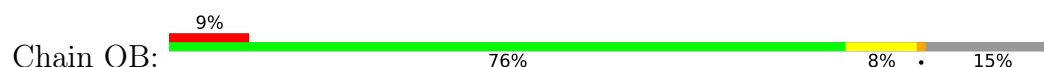
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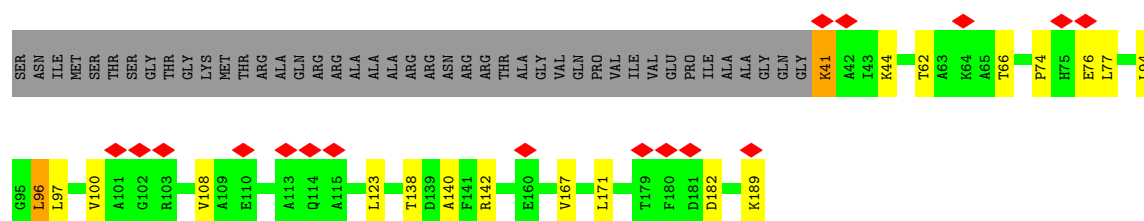
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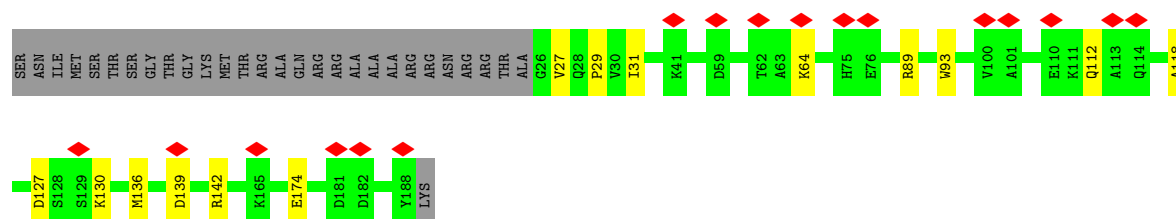
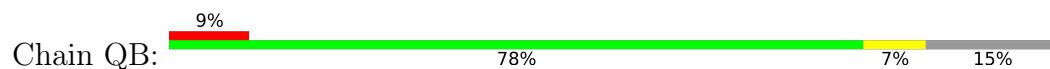
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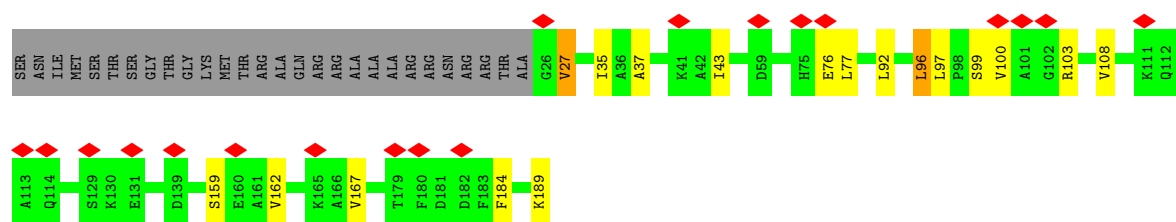
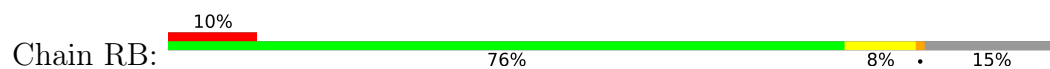
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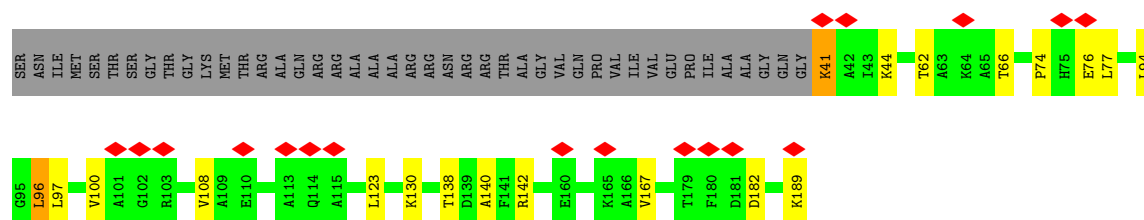
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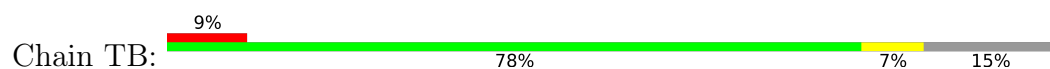
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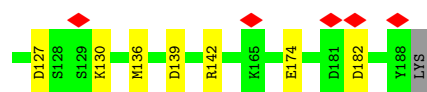


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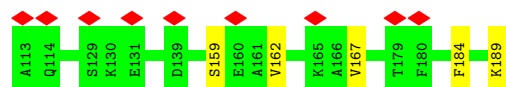
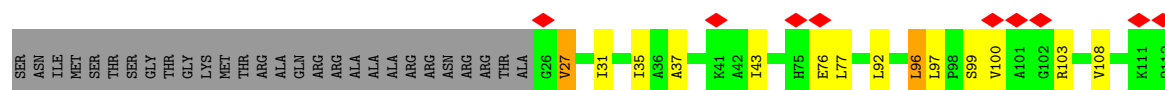
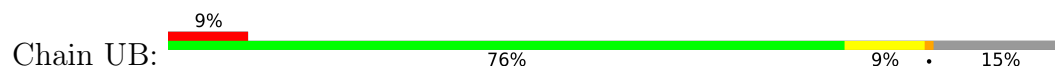


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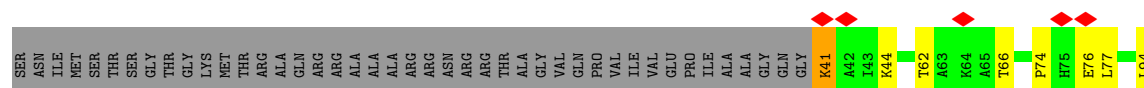




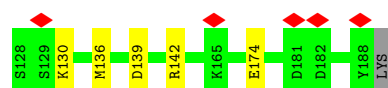
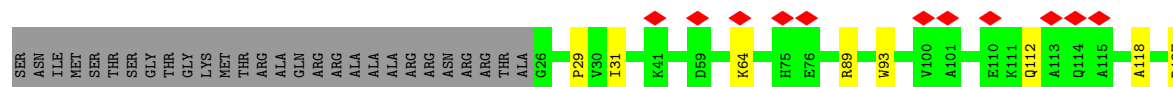
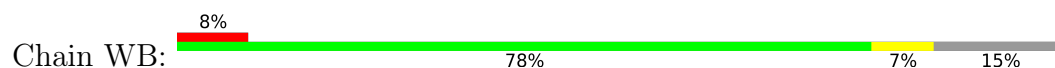
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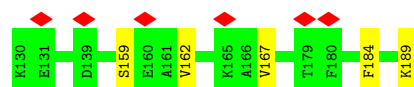
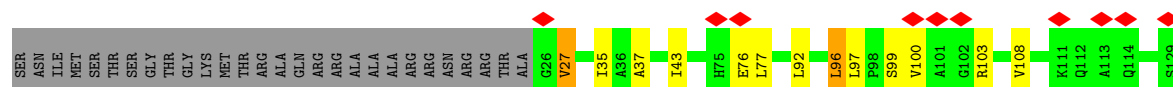
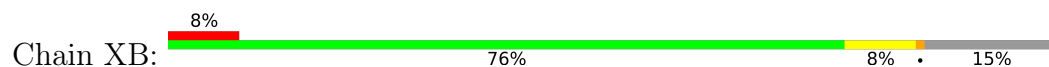
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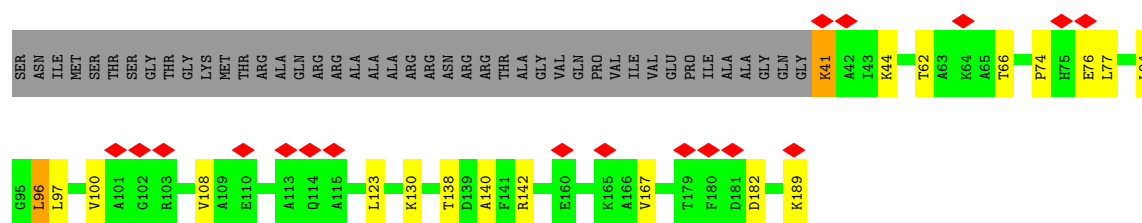
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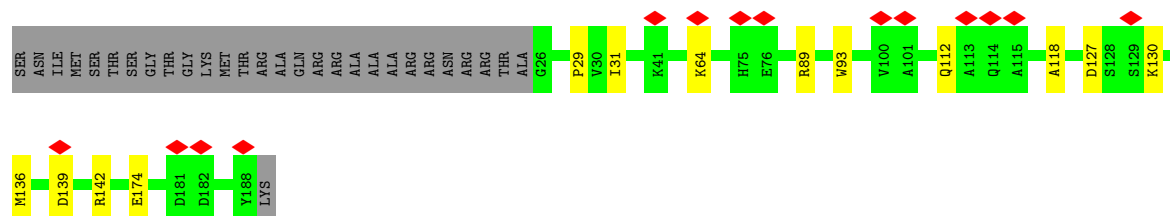
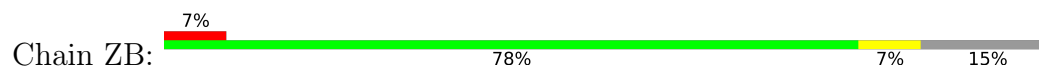
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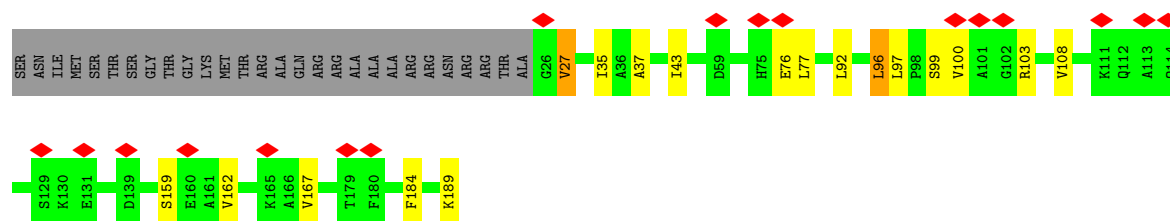
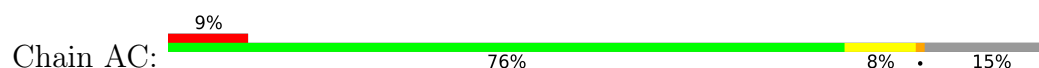
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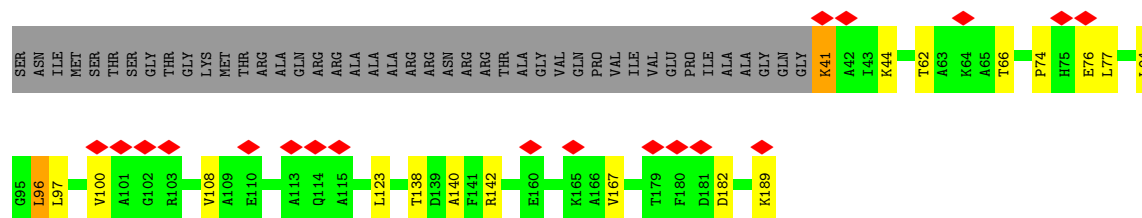
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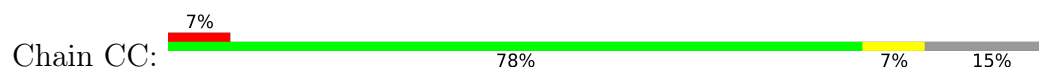
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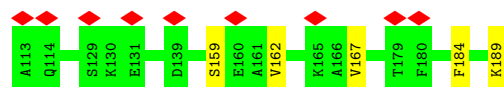
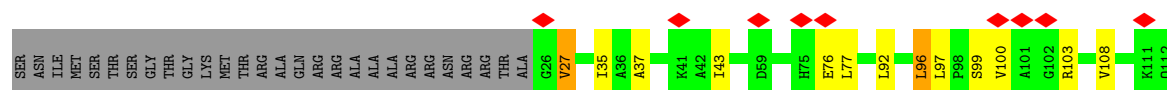
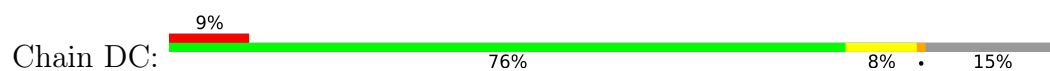


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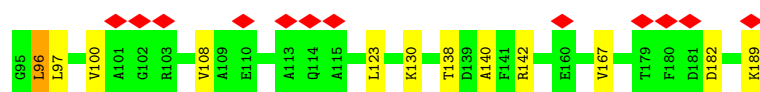
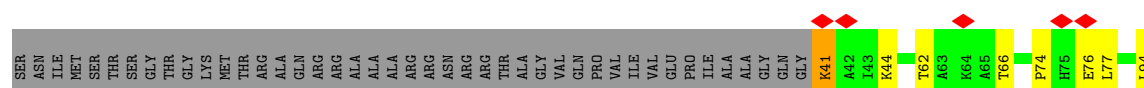




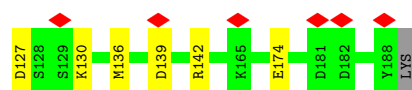
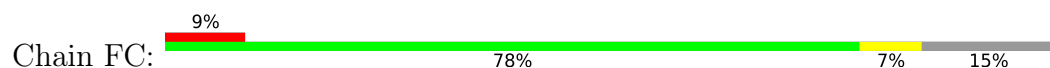
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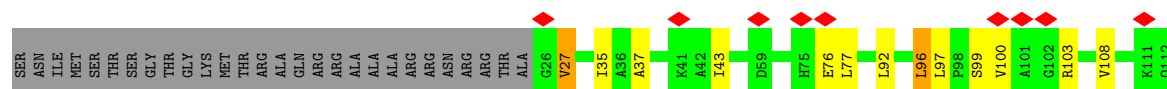
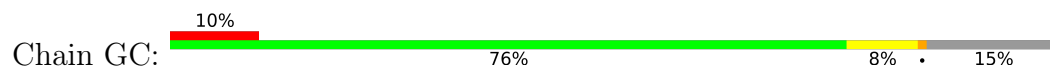
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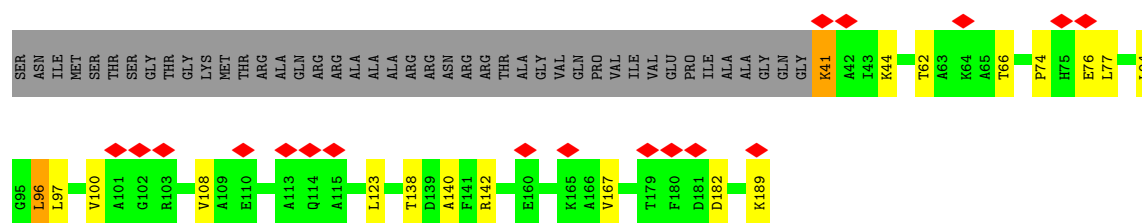
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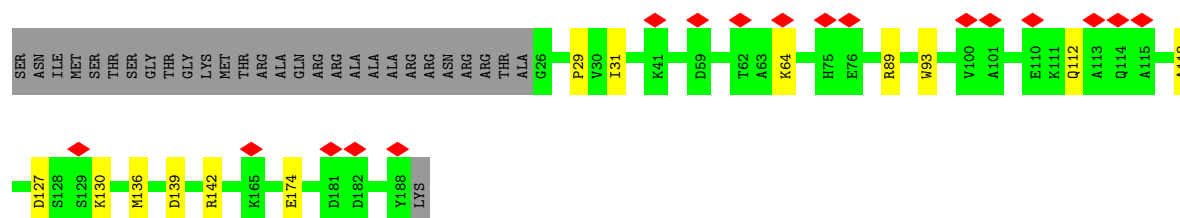
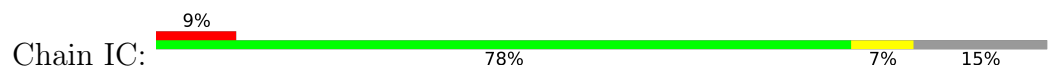
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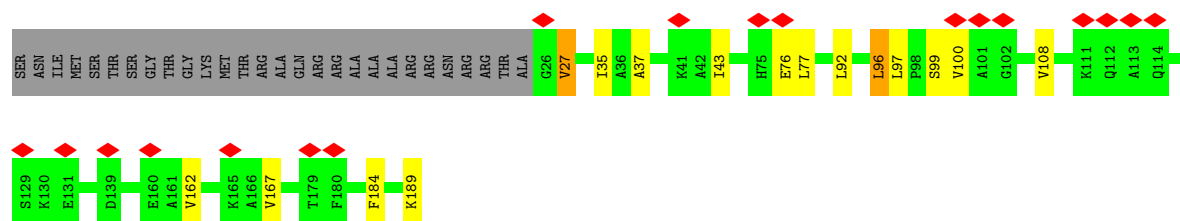
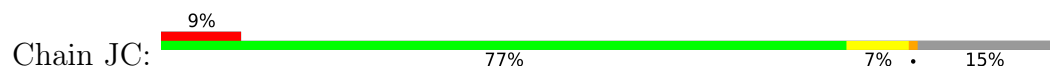
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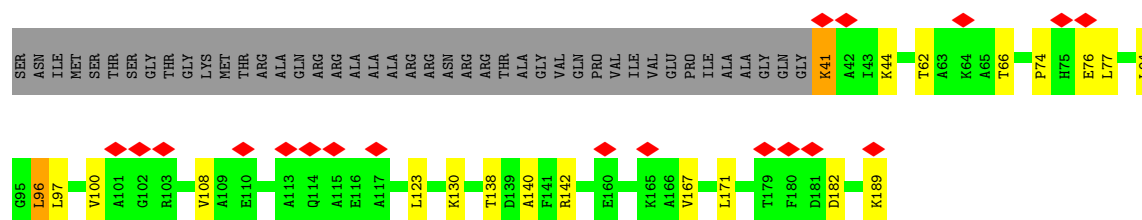
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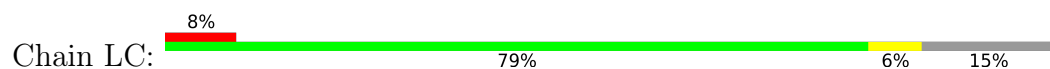
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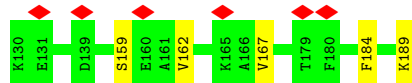
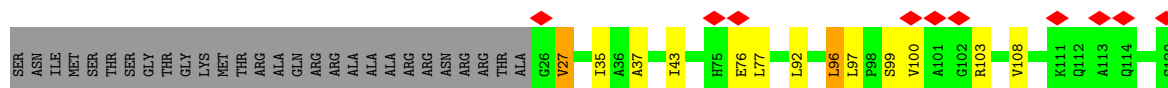
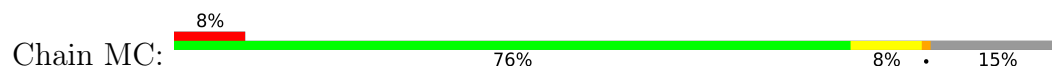


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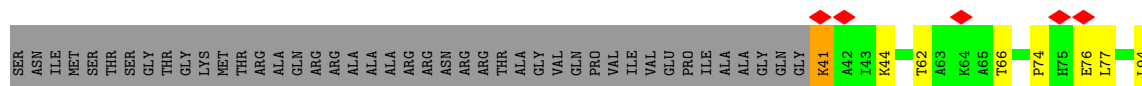




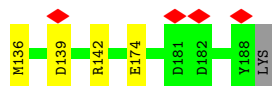
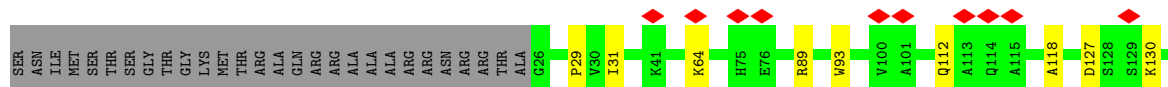
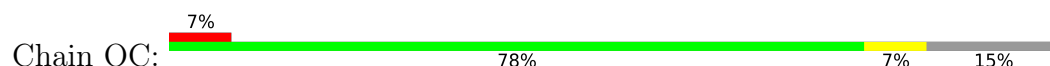
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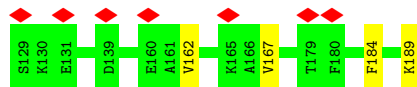
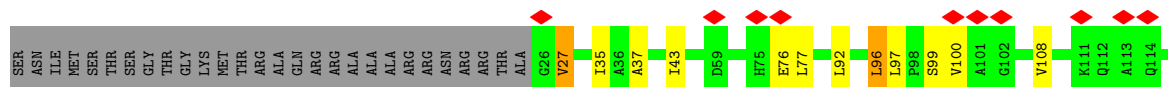
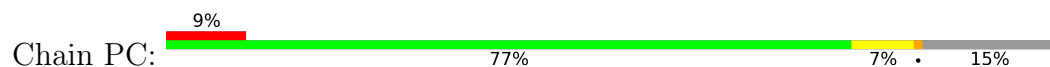
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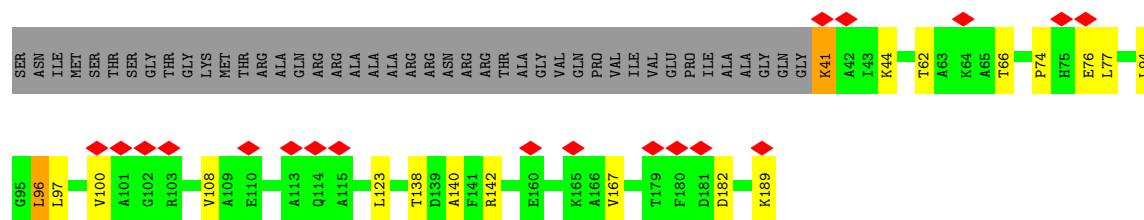
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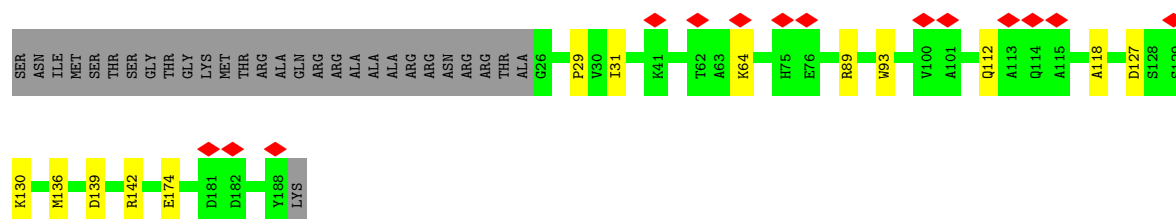
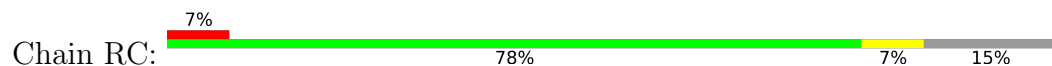
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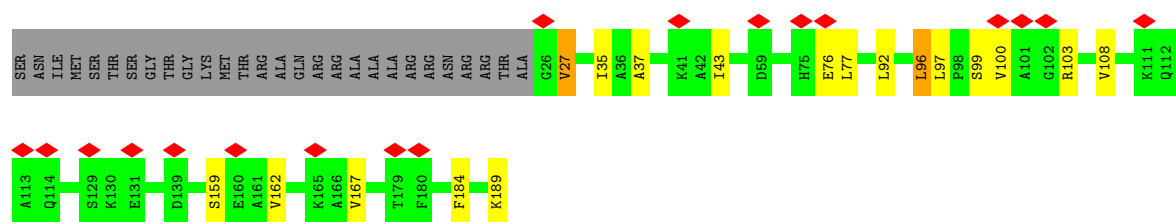
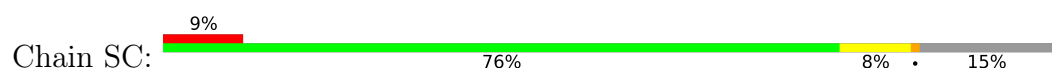
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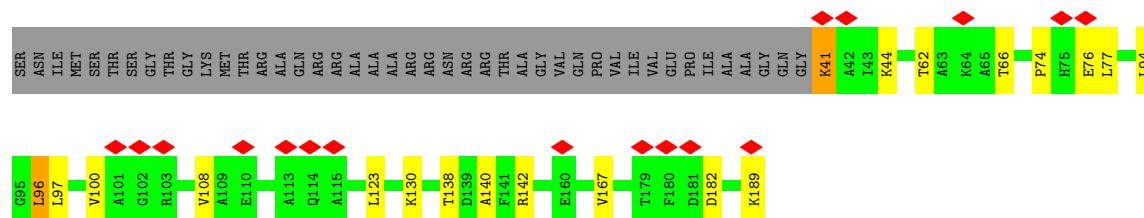
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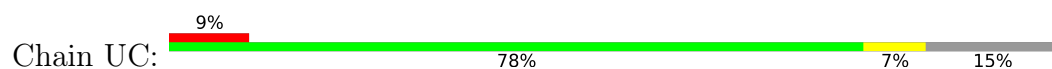
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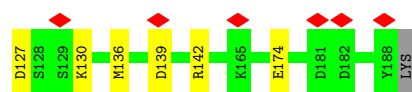


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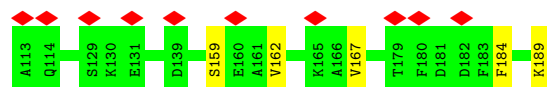
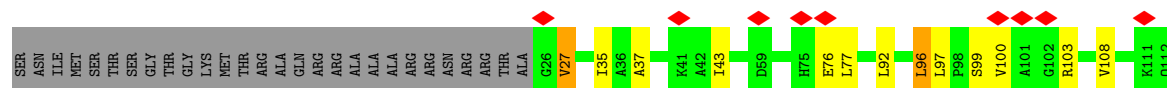
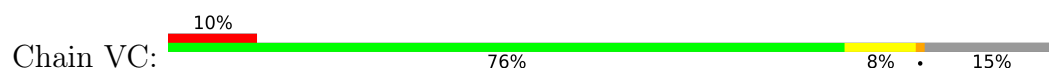


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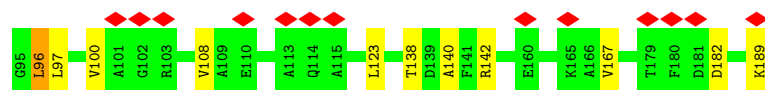
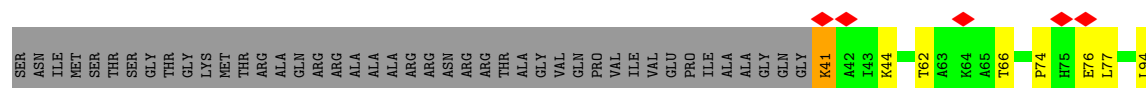




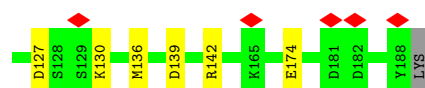
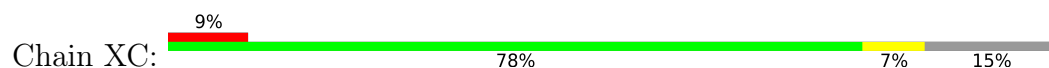
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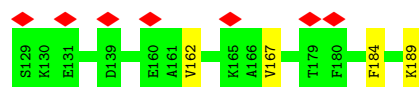
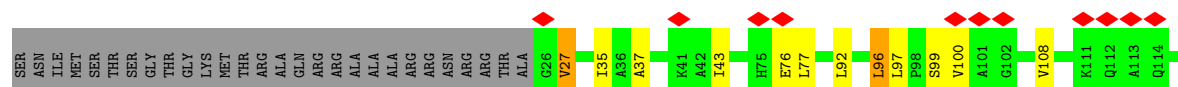
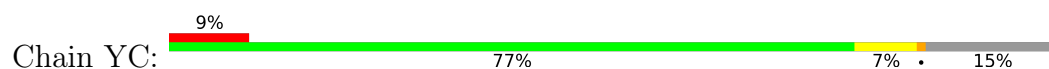
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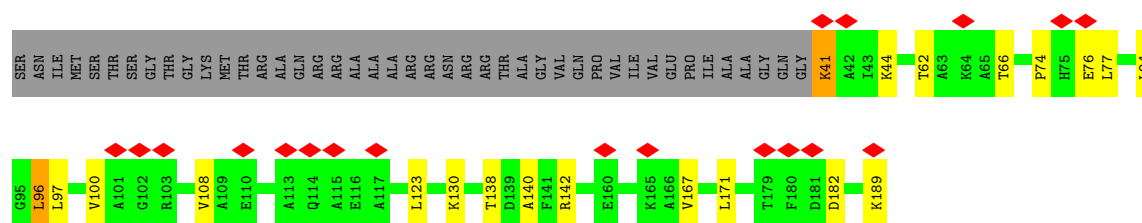
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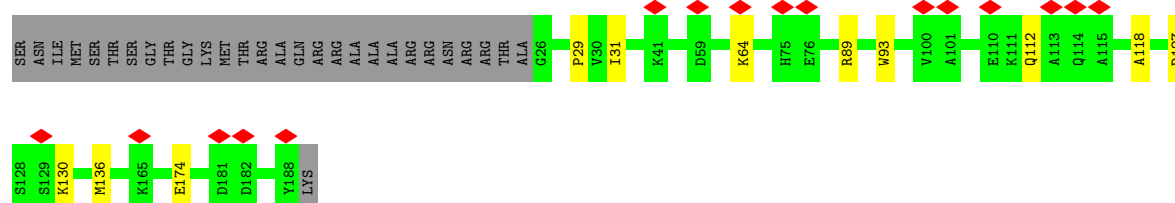
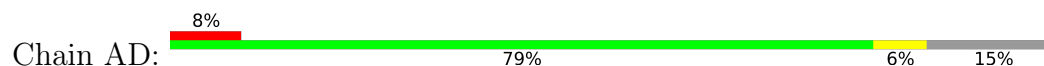
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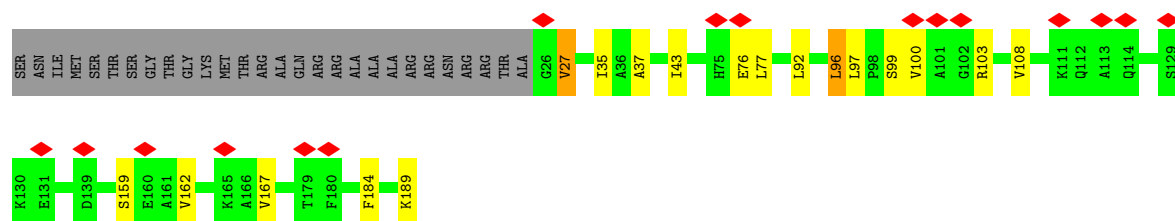
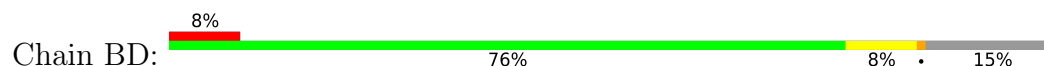
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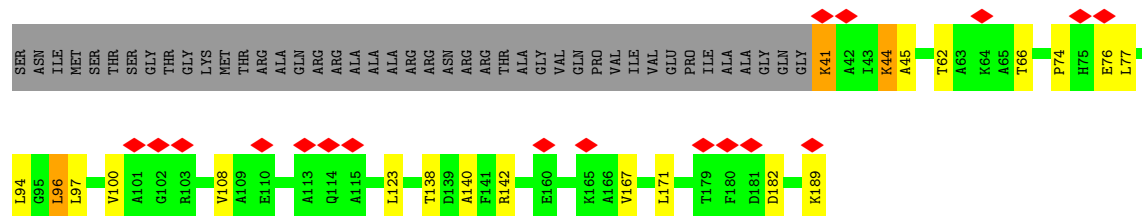
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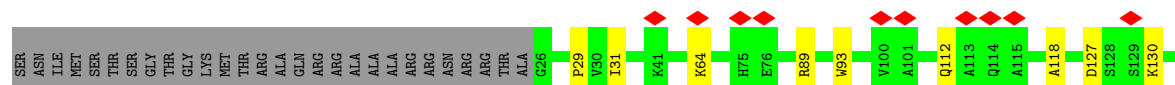
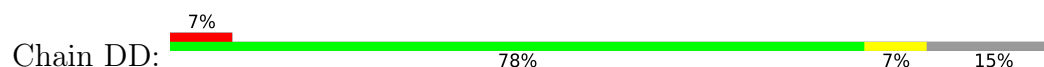
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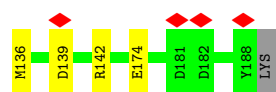


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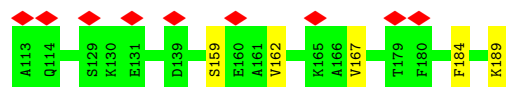
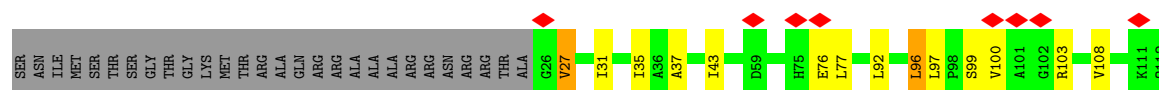
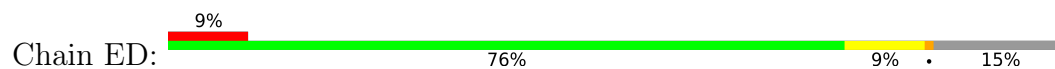


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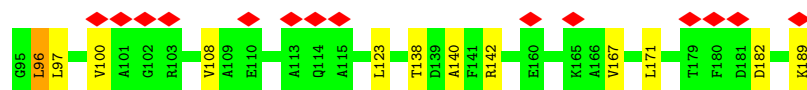
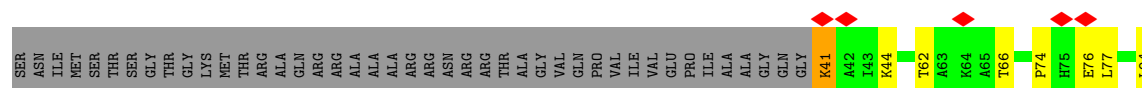




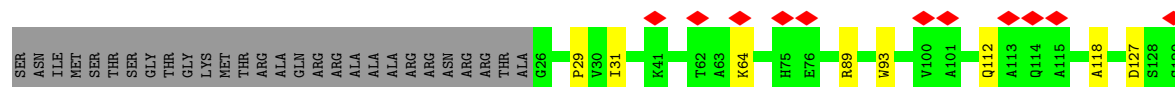
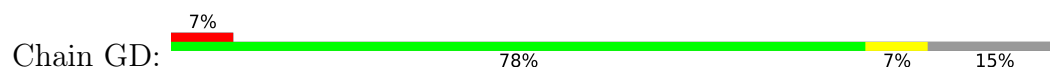
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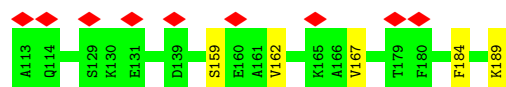
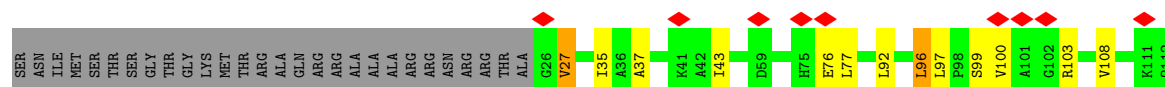
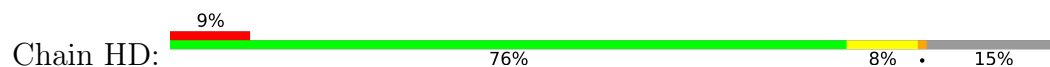
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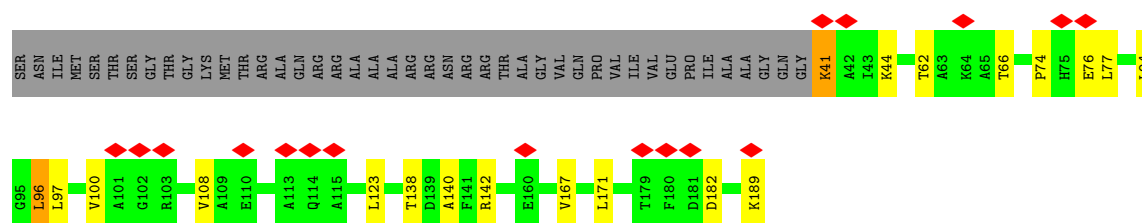
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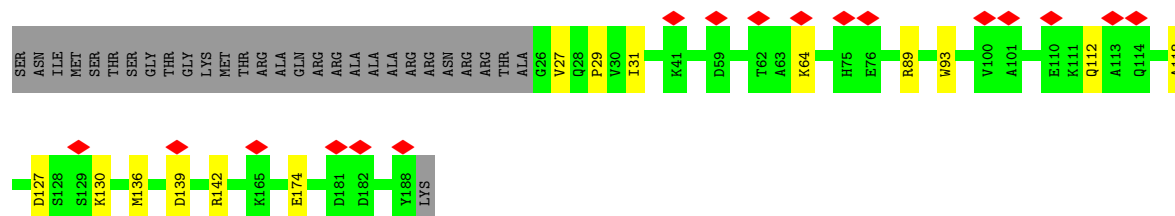
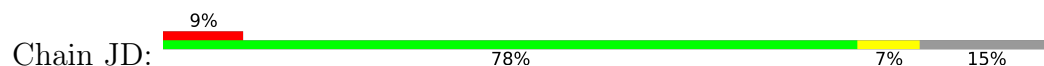
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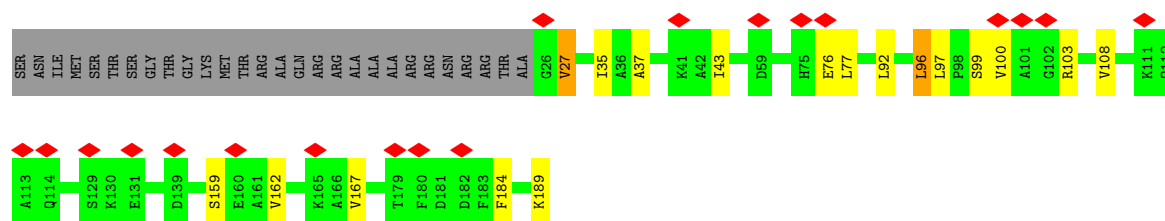
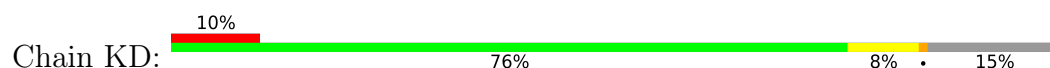
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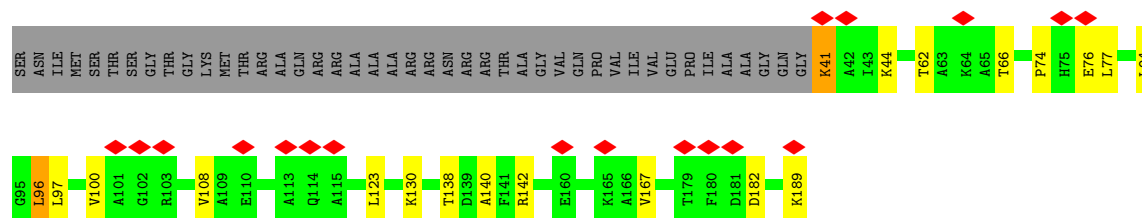
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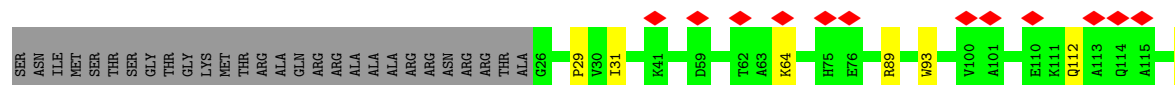
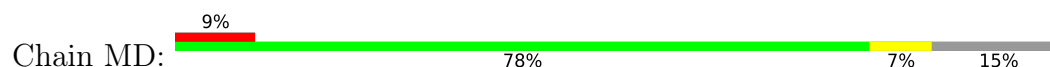
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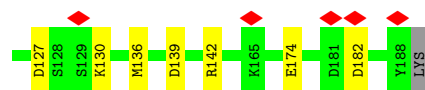


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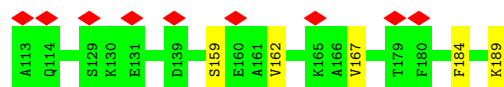
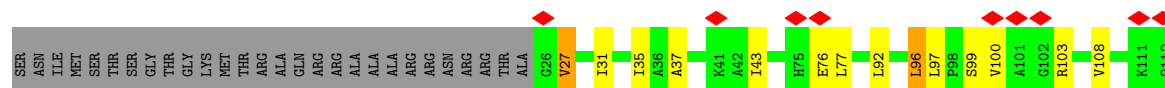
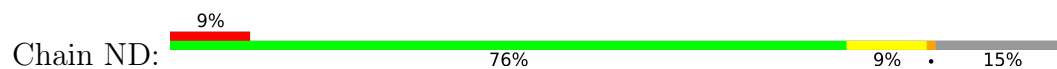


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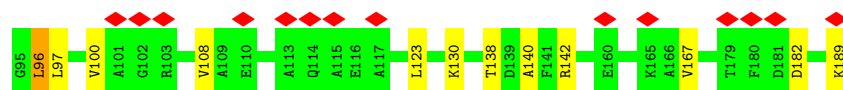
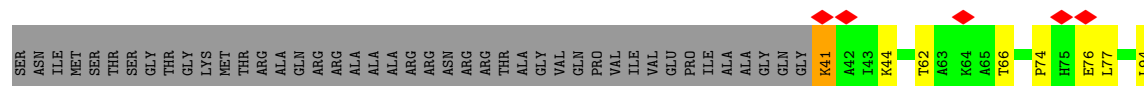




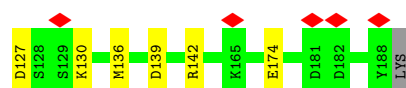
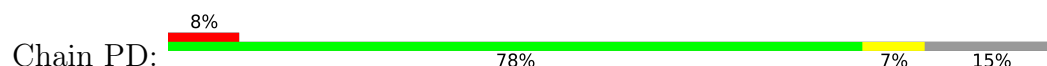
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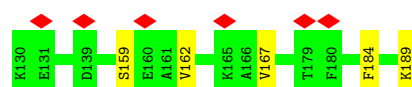
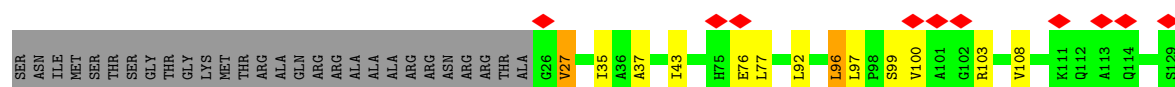
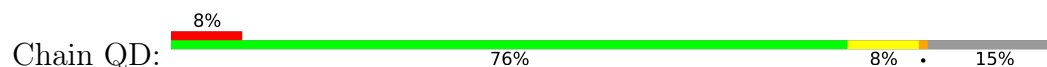
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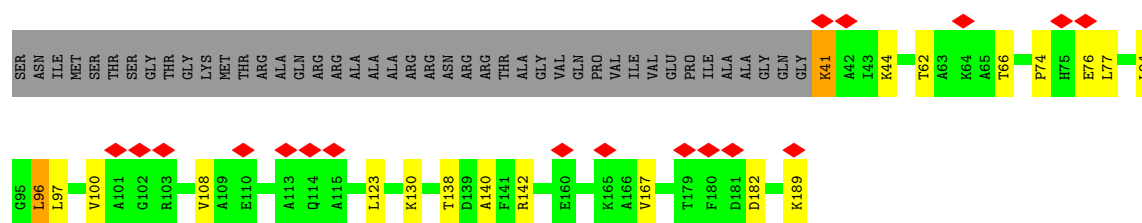
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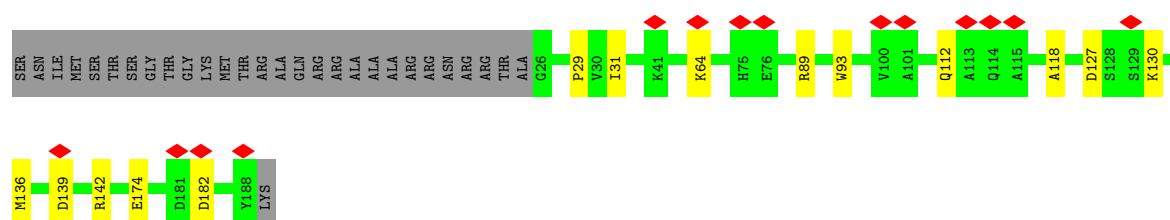
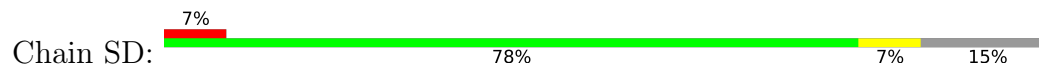
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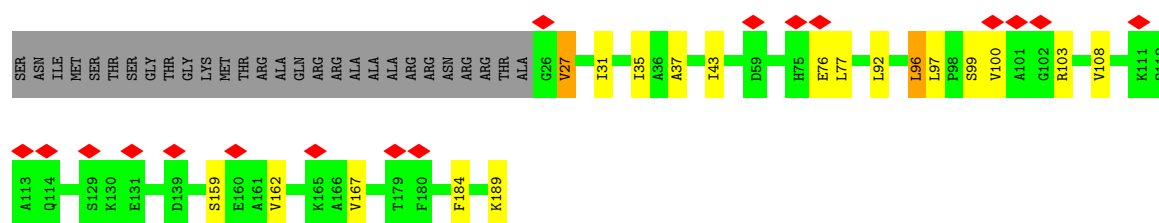
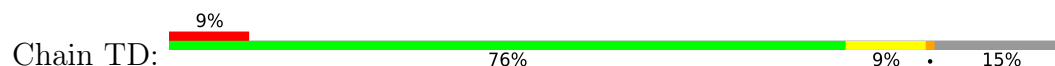
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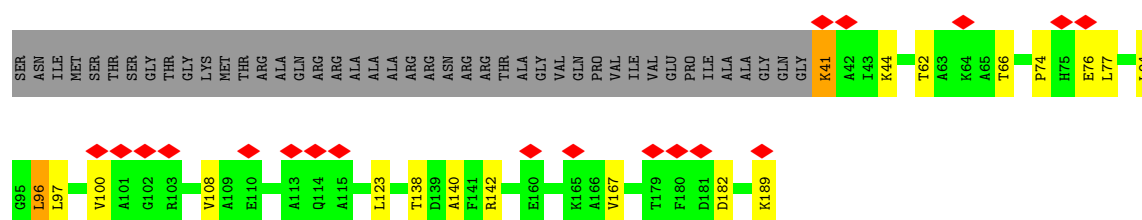
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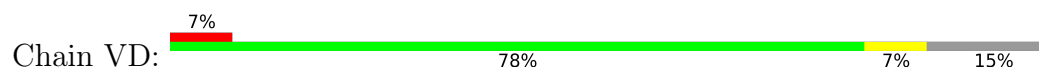
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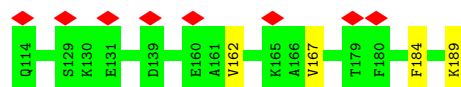
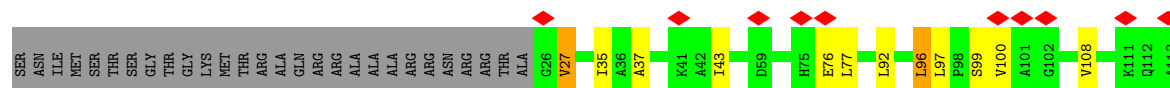
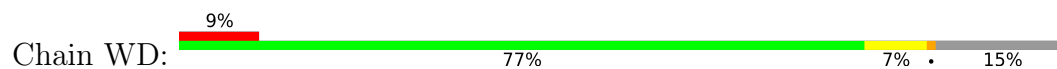


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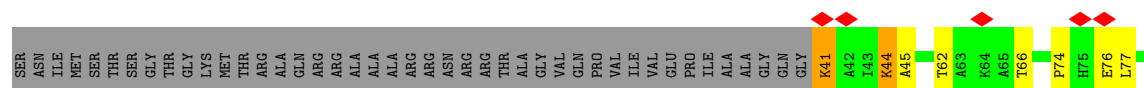




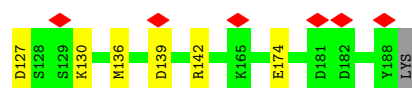
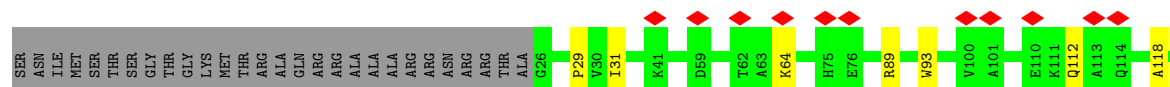
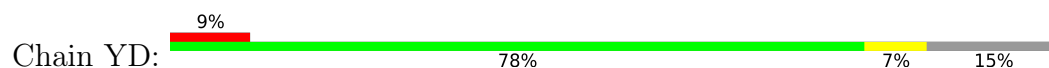
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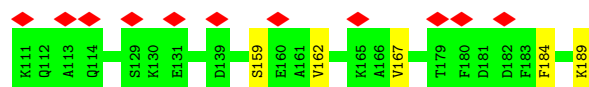
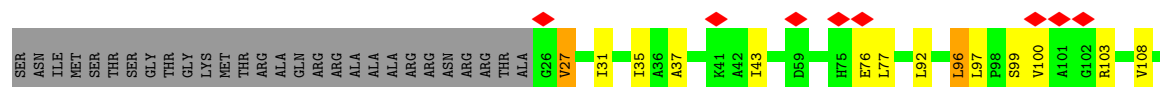
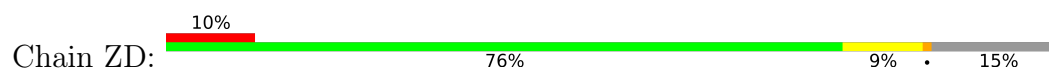
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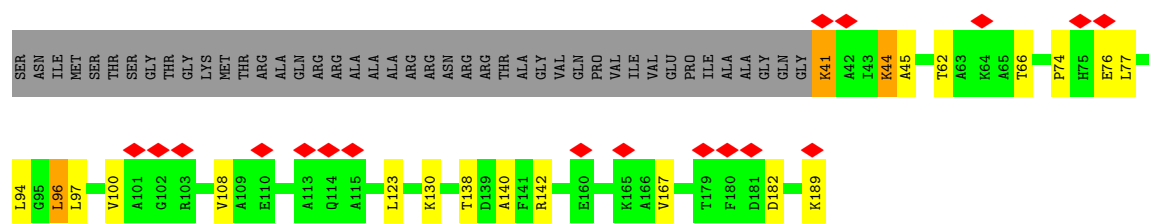
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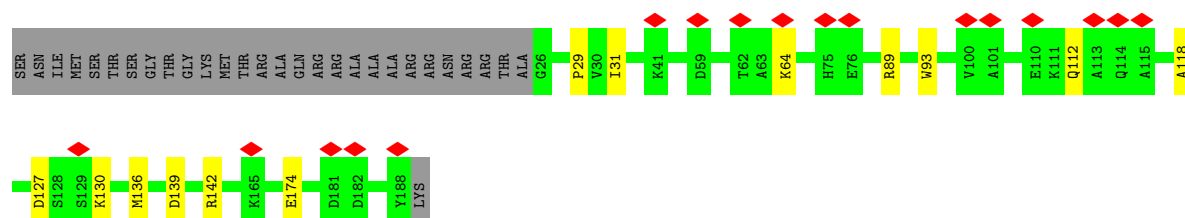
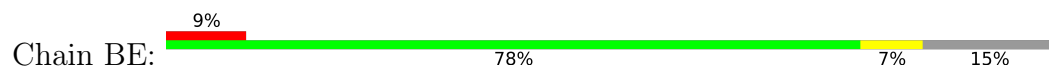
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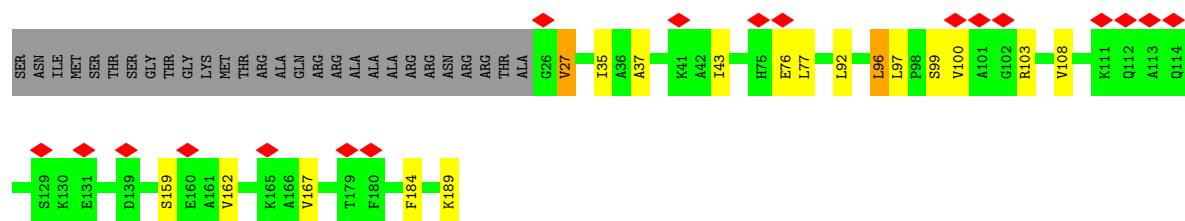
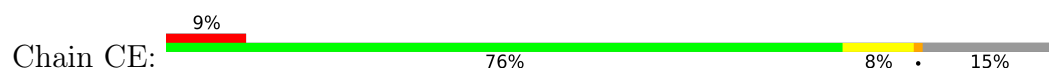
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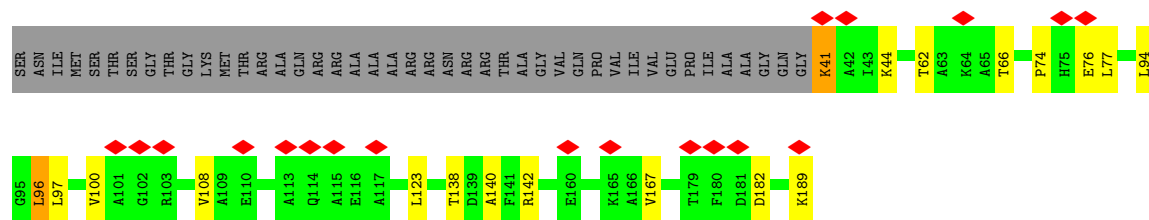
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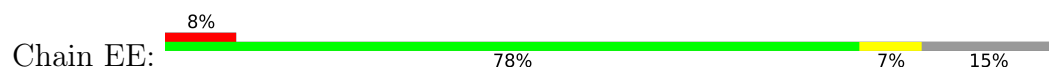
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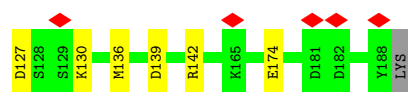


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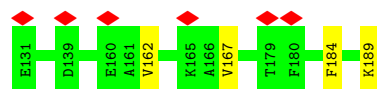
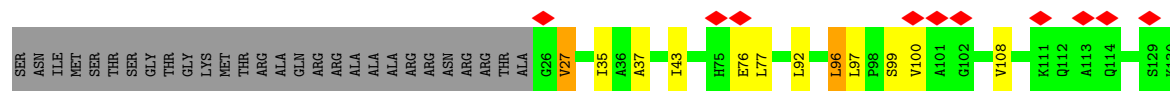
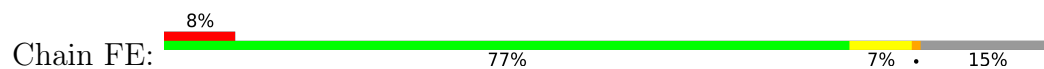


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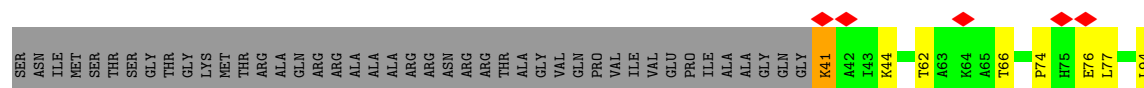




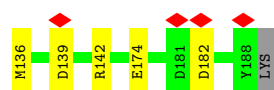
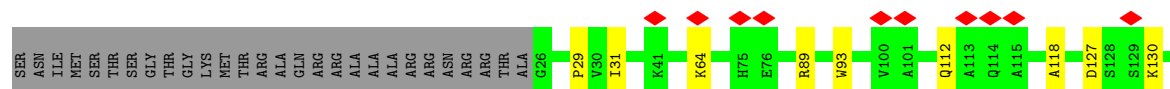
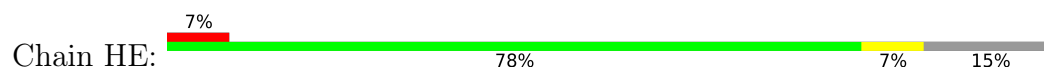
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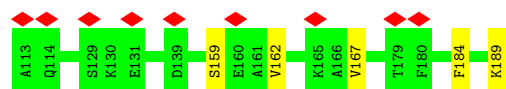
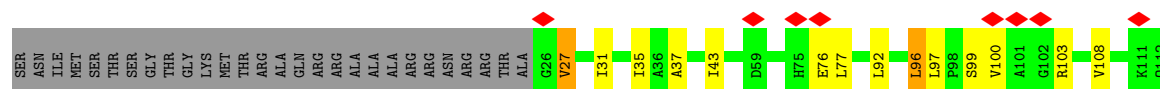
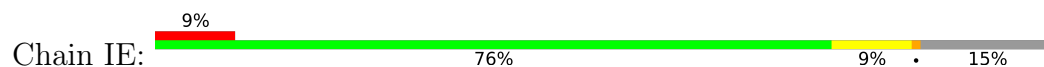
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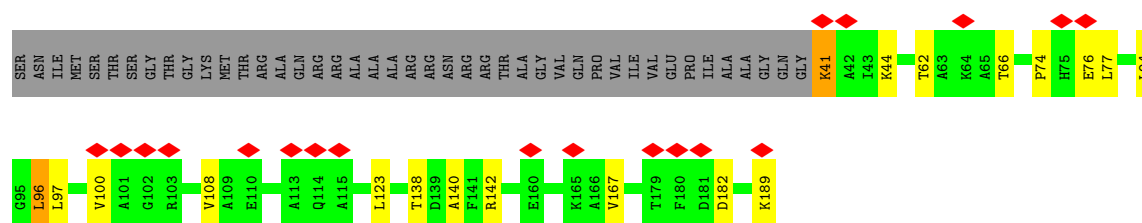
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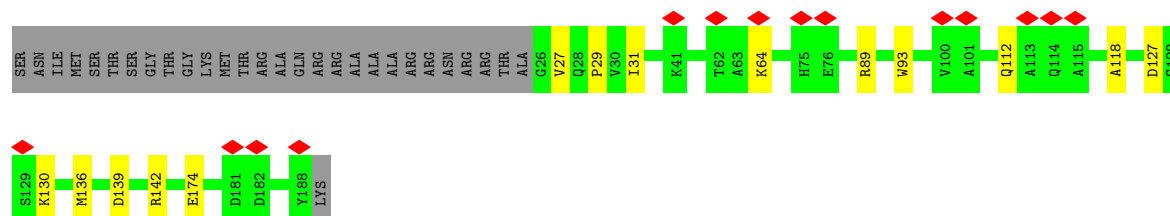
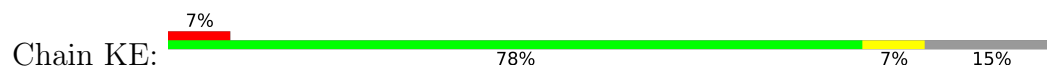
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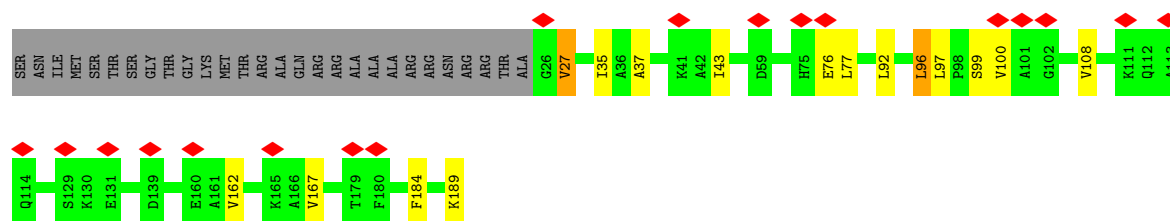
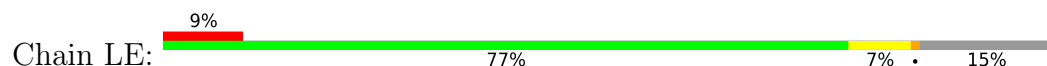
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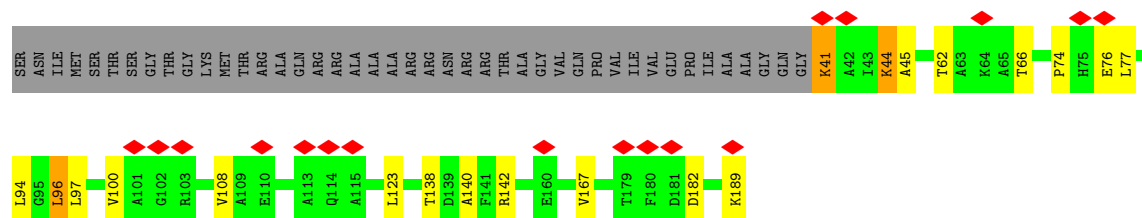
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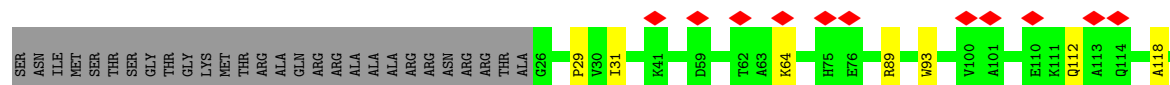
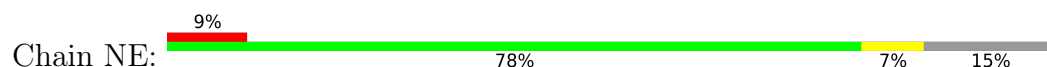
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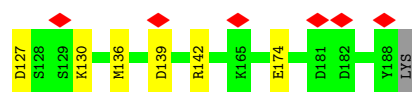


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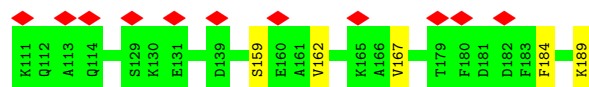
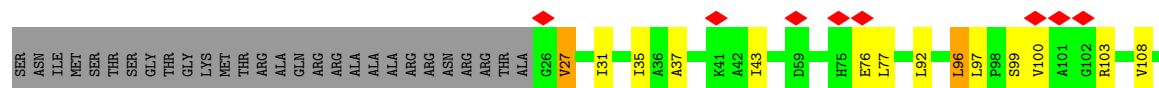
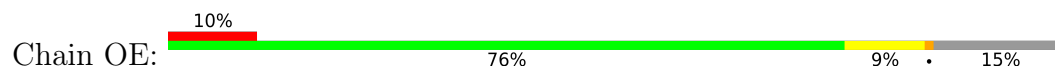


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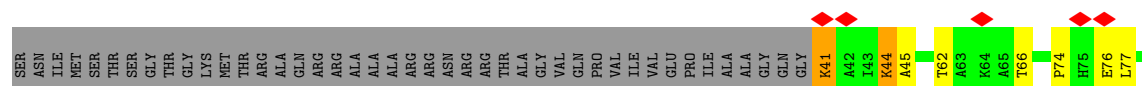




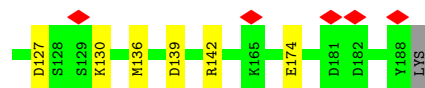
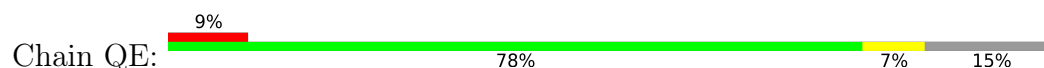
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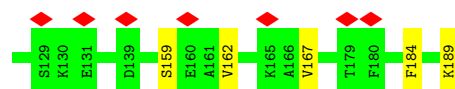
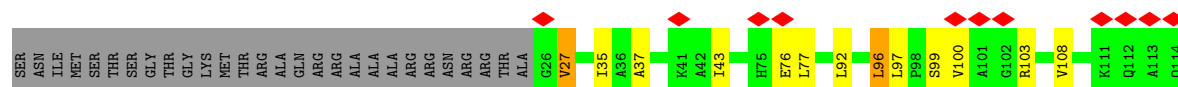
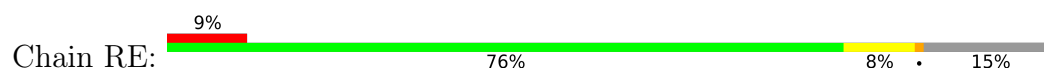
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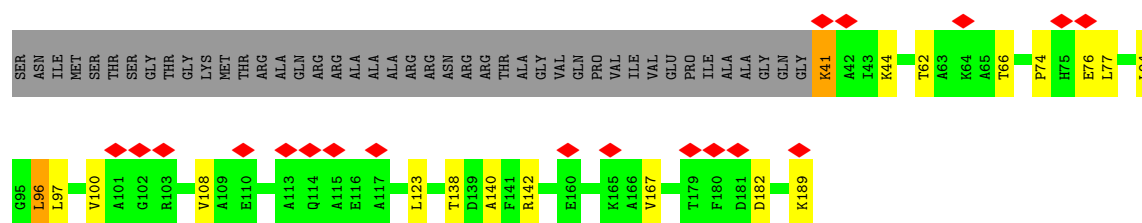
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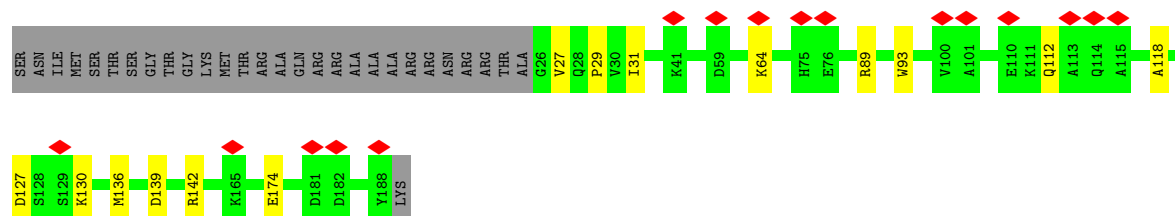
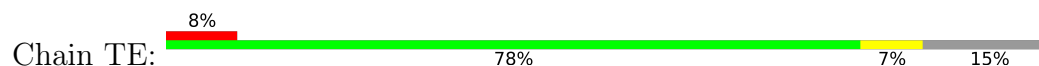
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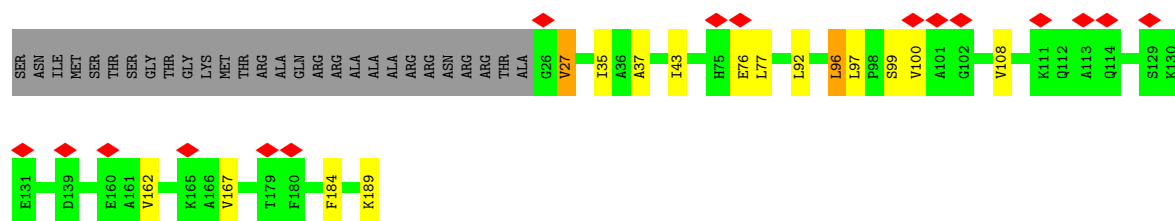
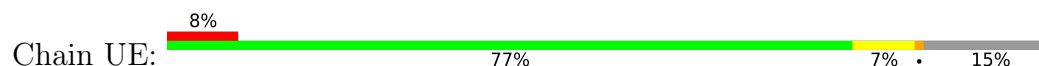
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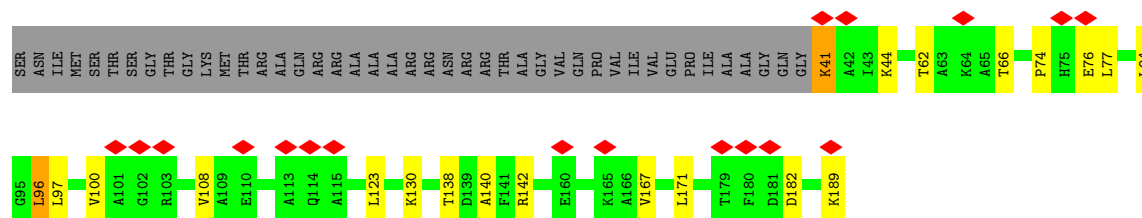
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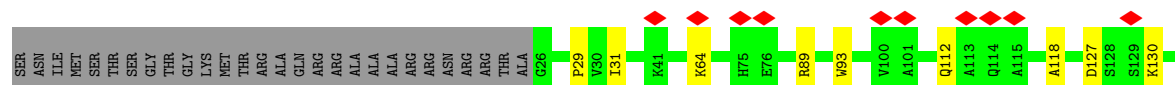
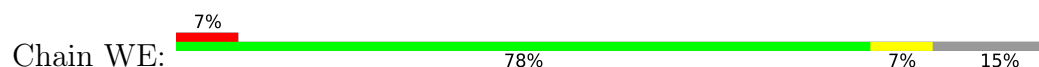
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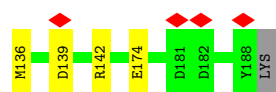


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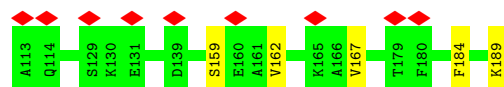
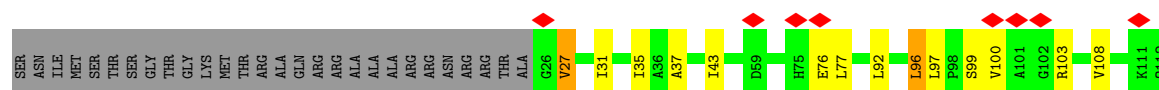
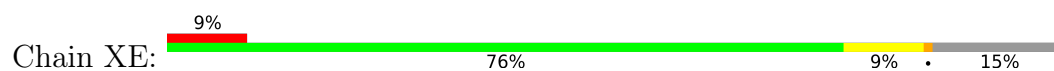


- Molecule 1: Coat protein

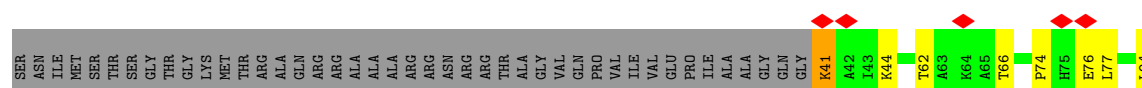




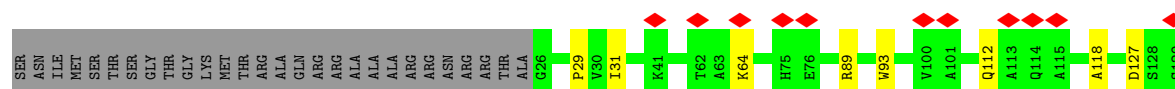
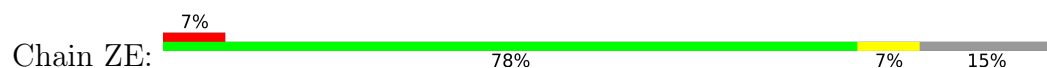
- Molecule 1: Coat protein



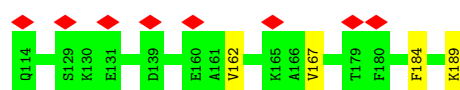
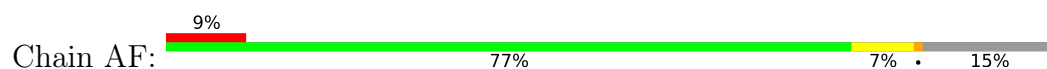
- Molecule 1: Coat protein



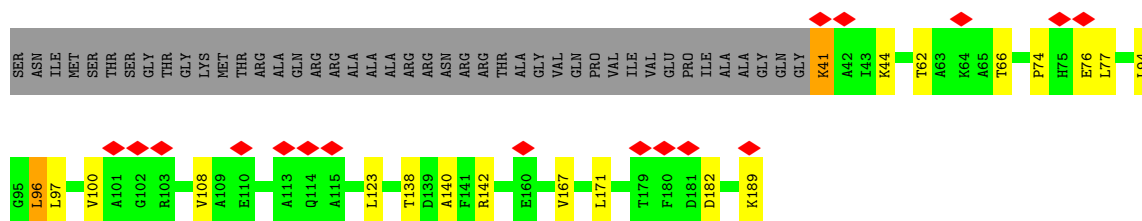
- Molecule 1: Coat protein



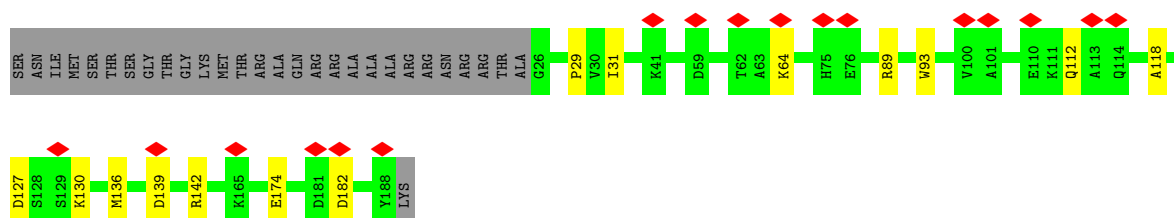
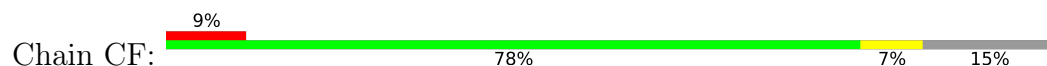
- Molecule 1: Coat protein



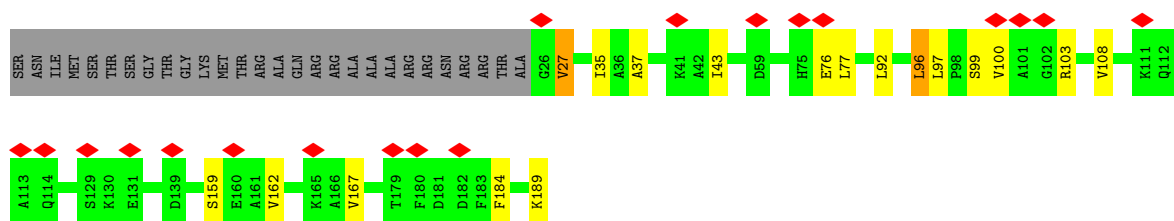
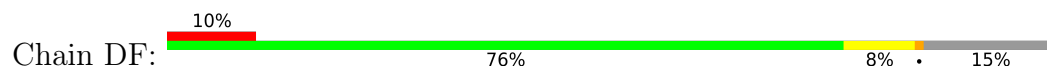
- Molecule 1: Coat protein



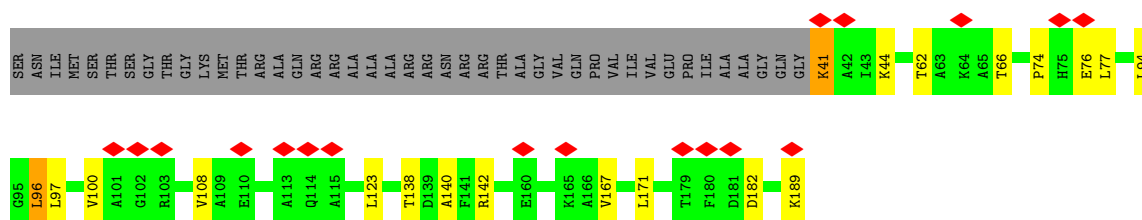
- Molecule 1: Coat protein



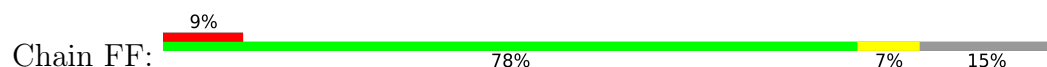
- Molecule 1: Coat protein

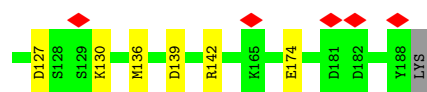


- Molecule 1: Coat protein

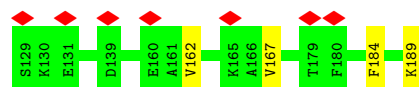
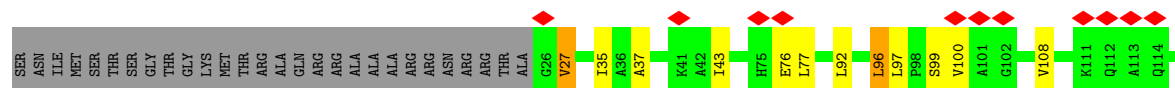
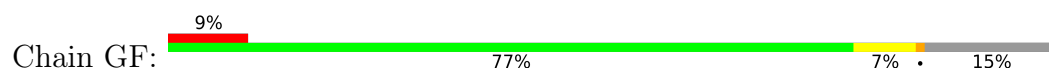


- Molecule 1: Coat protein

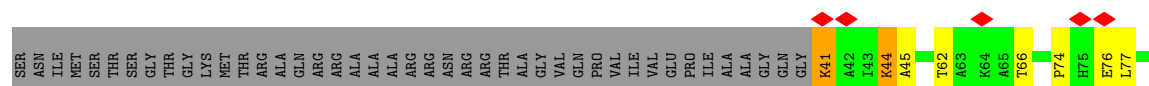




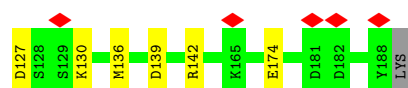
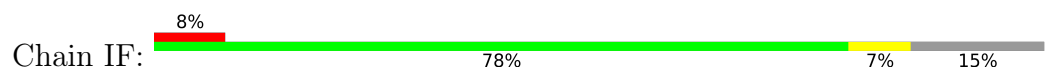
- Molecule 1: Coat protein



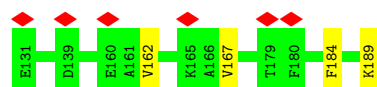
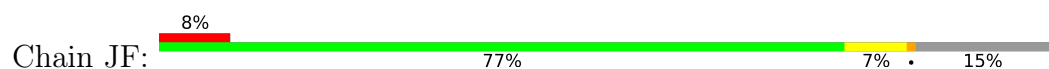
- Molecule 1: Coat protein



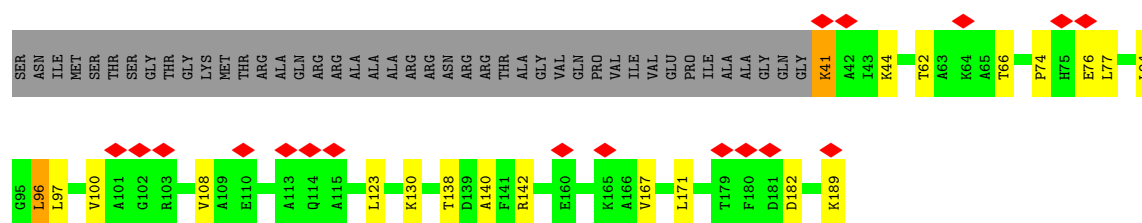
- Molecule 1: Coat protein



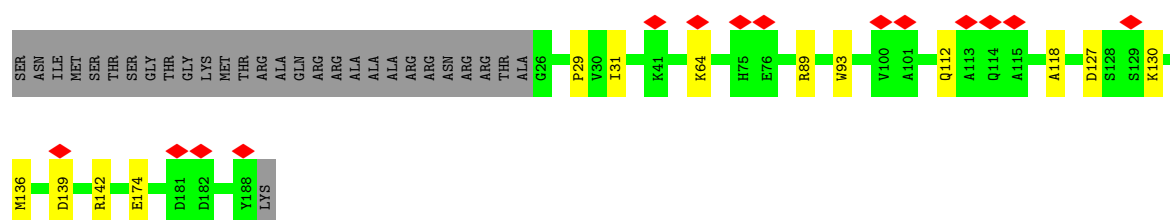
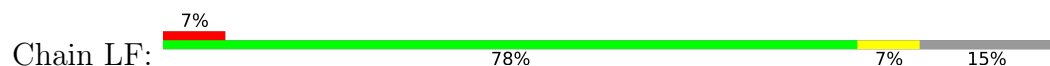
- Molecule 1: Coat protein



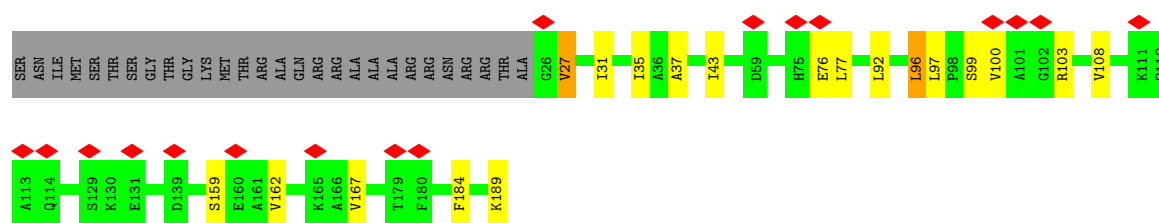
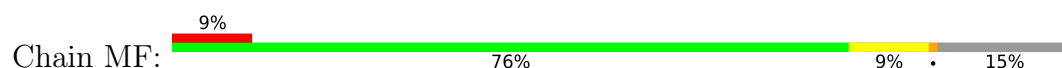
- Molecule 1: Coat protein



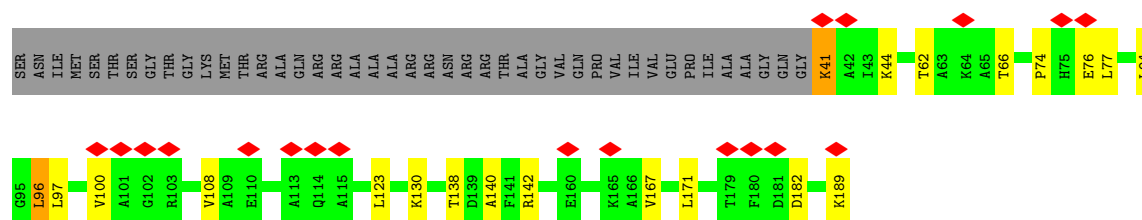
- Molecule 1: Coat protein



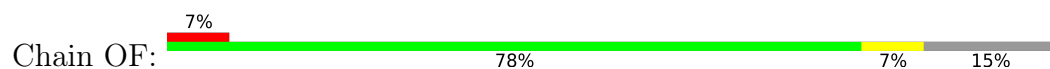
- Molecule 1: Coat protein



- Molecule 1: Coat protein

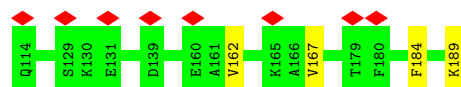
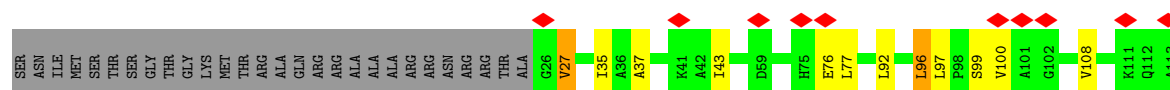
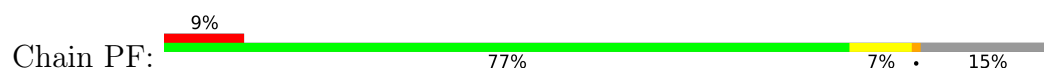


- Molecule 1: Coat protein

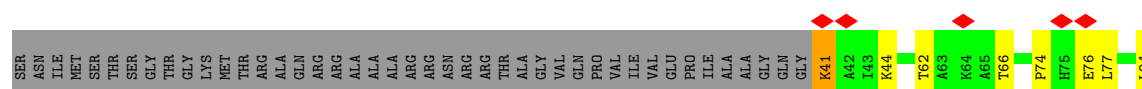




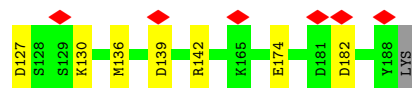
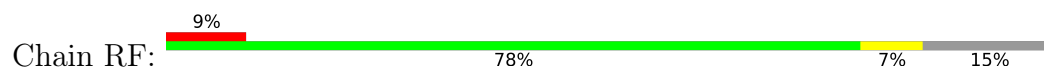
- Molecule 1: Coat protein



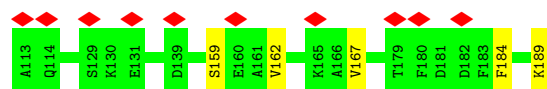
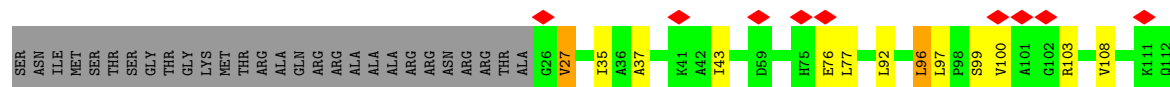
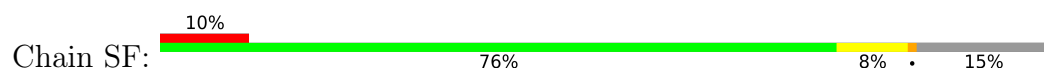
- Molecule 1: Coat protein



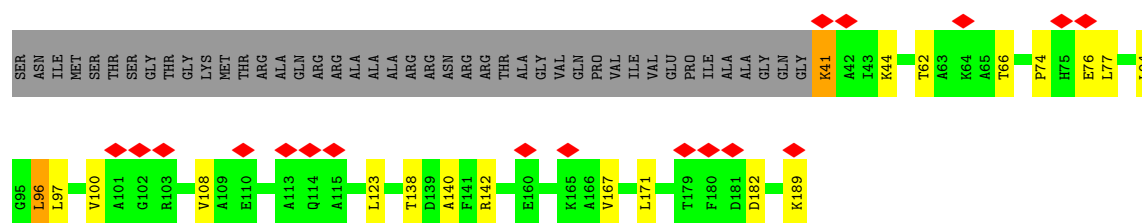
- Molecule 1: Coat protein



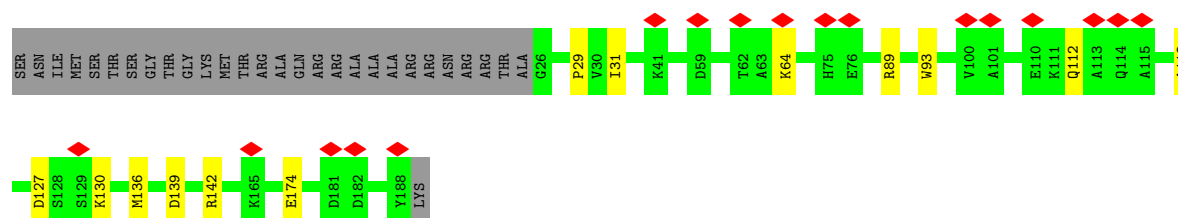
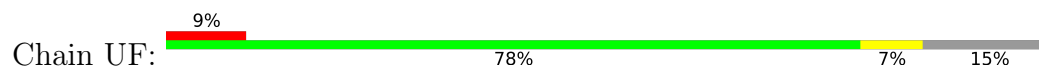
- Molecule 1: Coat protein



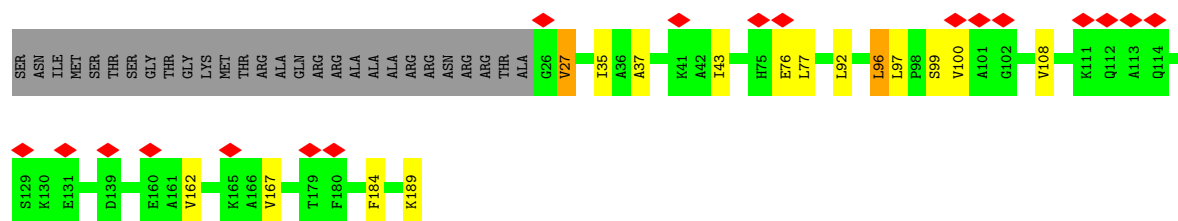
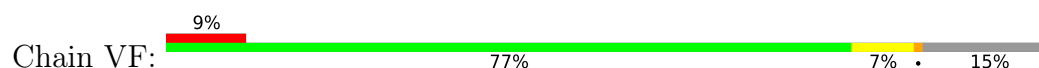
- Molecule 1: Coat protein



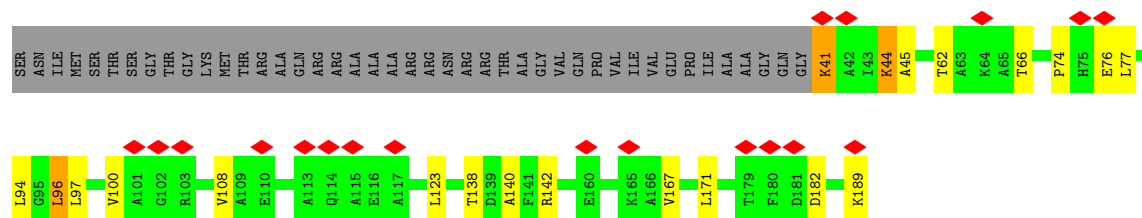
- Molecule 1: Coat protein



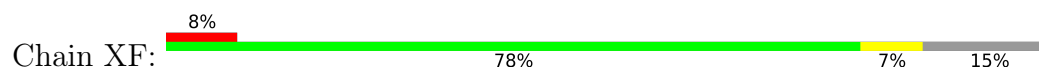
- Molecule 1: Coat protein



- Molecule 1: Coat protein

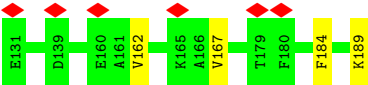
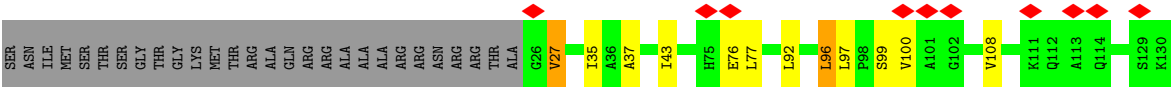
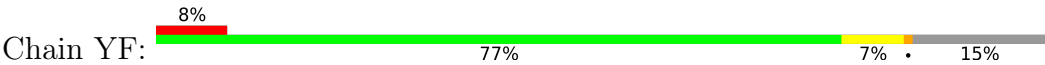


- Molecule 1: Coat protein





• Molecule 1: Coat protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	24812	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.017	Depositor
Map size ($\text{\AA}$)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	0/1152	0.26	0/1563
1	AA	0.16	0/1244	0.27	0/1693
1	AB	0.15	0/1152	0.26	0/1563
1	AC	0.16	0/1254	0.29	0/1704
1	AD	0.17	0/1244	0.28	0/1693
1	AE	0.15	0/1152	0.26	0/1563
1	AF	0.16	0/1254	0.29	0/1704
1	B	0.16	0/1244	0.28	0/1693
1	BA	0.16	0/1254	0.29	0/1704
1	BB	0.17	0/1244	0.28	0/1693
1	BC	0.15	0/1152	0.26	0/1563
1	BD	0.16	0/1254	0.29	0/1704
1	BE	0.16	0/1244	0.27	0/1693
1	BF	0.15	0/1152	0.26	0/1563
1	C	0.16	0/1254	0.29	0/1704
1	CA	0.15	0/1152	0.26	0/1563
1	CB	0.16	0/1254	0.29	0/1704
1	CC	0.17	0/1244	0.28	0/1693
1	CD	0.15	0/1152	0.26	0/1563
1	CE	0.16	0/1254	0.29	0/1704
1	CF	0.17	0/1244	0.28	0/1693
1	D	0.15	0/1152	0.26	0/1563
1	DA	0.17	0/1244	0.28	0/1693
1	DB	0.15	0/1152	0.26	0/1563
1	DC	0.16	0/1254	0.29	0/1704
1	DD	0.16	0/1244	0.28	0/1693
1	DE	0.15	0/1152	0.26	0/1563
1	DF	0.16	0/1254	0.29	0/1704
1	E	0.17	0/1244	0.28	0/1693
1	EA	0.16	0/1254	0.29	0/1704
1	EB	0.16	0/1244	0.27	0/1693
1	EC	0.15	0/1152	0.26	0/1563
1	ED	0.16	0/1254	0.29	0/1704
1	EE	0.17	0/1244	0.28	0/1693

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	EF	0.15	0/1152	0.26	0/1563
1	F	0.16	0/1254	0.29	0/1704
1	FA	0.15	0/1152	0.26	0/1563
1	FB	0.16	0/1254	0.29	0/1704
1	FC	0.17	0/1244	0.28	0/1693
1	FD	0.15	0/1152	0.26	0/1563
1	FE	0.16	0/1254	0.29	0/1704
1	FF	0.16	0/1244	0.27	0/1693
1	G	0.15	0/1152	0.26	0/1563
1	GA	0.16	0/1244	0.28	0/1693
1	GB	0.15	0/1152	0.26	0/1563
1	GC	0.16	0/1254	0.29	0/1704
1	GD	0.16	0/1244	0.28	0/1693
1	GE	0.15	0/1152	0.26	0/1563
1	GF	0.16	0/1254	0.29	0/1704
1	H	0.17	0/1244	0.28	0/1693
1	HA	0.16	0/1254	0.29	0/1704
1	HB	0.17	0/1244	0.28	0/1693
1	HC	0.15	0/1152	0.26	0/1563
1	HD	0.16	0/1254	0.29	0/1704
1	HE	0.16	0/1244	0.28	0/1693
1	HF	0.15	0/1152	0.26	0/1563
1	I	0.16	0/1254	0.29	0/1704
1	IA	0.15	0/1152	0.26	0/1563
1	IB	0.16	0/1254	0.29	0/1704
1	IC	0.17	0/1244	0.27	0/1693
1	ID	0.15	0/1152	0.26	0/1563
1	IE	0.16	0/1254	0.29	0/1704
1	IF	0.17	0/1244	0.28	0/1693
1	J	0.15	0/1152	0.26	0/1563
1	JA	0.16	0/1244	0.28	0/1693
1	JB	0.15	0/1152	0.26	0/1563
1	JC	0.16	0/1254	0.29	0/1704
1	JD	0.17	0/1244	0.28	0/1693
1	JE	0.15	0/1152	0.26	0/1563
1	JF	0.16	0/1254	0.29	0/1704
1	K	0.17	0/1244	0.27	0/1693
1	KA	0.16	0/1254	0.29	0/1704
1	KB	0.16	0/1244	0.28	0/1693
1	KC	0.15	0/1152	0.26	0/1563
1	KD	0.16	0/1254	0.29	0/1704
1	KE	0.16	0/1244	0.28	0/1693
1	KF	0.15	0/1152	0.26	0/1563

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	0.16	0/1254	0.29	0/1704
1	LA	0.15	0/1152	0.26	0/1563
1	LB	0.16	0/1254	0.29	0/1704
1	LC	0.17	0/1244	0.28	0/1693
1	LD	0.15	0/1152	0.26	0/1563
1	LE	0.16	0/1254	0.29	0/1704
1	LF	0.16	0/1244	0.28	0/1693
1	M	0.15	0/1152	0.26	0/1563
1	MA	0.17	0/1244	0.28	0/1693
1	MB	0.15	0/1152	0.26	0/1563
1	MC	0.16	0/1254	0.29	0/1704
1	MD	0.16	0/1244	0.27	0/1693
1	ME	0.15	0/1152	0.26	0/1563
1	MF	0.16	0/1254	0.29	0/1704
1	N	0.17	0/1244	0.28	0/1693
1	NA	0.16	0/1254	0.29	0/1704
1	NB	0.16	0/1244	0.28	0/1693
1	NC	0.15	0/1152	0.26	0/1563
1	ND	0.16	0/1254	0.29	0/1704
1	NE	0.17	0/1244	0.28	0/1693
1	NF	0.15	0/1152	0.26	0/1563
1	O	0.16	0/1254	0.29	0/1704
1	OA	0.15	0/1152	0.26	0/1563
1	OB	0.16	0/1254	0.29	0/1704
1	OC	0.16	0/1244	0.28	0/1693
1	OD	0.15	0/1152	0.26	0/1563
1	OE	0.16	0/1254	0.29	0/1704
1	OF	0.17	0/1244	0.28	0/1693
1	P	0.15	0/1152	0.26	0/1563
1	PA	0.16	0/1244	0.27	0/1693
1	PB	0.15	0/1152	0.26	0/1563
1	PC	0.16	0/1254	0.29	0/1704
1	PD	0.17	0/1244	0.28	0/1693
1	PE	0.15	0/1152	0.26	0/1563
1	PF	0.16	0/1254	0.29	0/1704
1	Q	0.16	0/1244	0.28	0/1693
1	QA	0.16	0/1254	0.29	0/1704
1	QB	0.17	0/1244	0.28	0/1693
1	QC	0.15	0/1152	0.26	0/1563
1	QD	0.16	0/1254	0.29	0/1704
1	QE	0.16	0/1244	0.27	0/1693
1	QF	0.15	0/1152	0.26	0/1563
1	R	0.16	0/1254	0.29	0/1704

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	RA	0.15	0/1152	0.26	0/1563
1	RB	0.16	0/1254	0.29	0/1704
1	RC	0.16	0/1244	0.28	0/1693
1	RD	0.15	0/1152	0.26	0/1563
1	RE	0.16	0/1254	0.29	0/1704
1	RF	0.17	0/1244	0.28	0/1693
1	S	0.15	0/1152	0.26	0/1563
1	SA	0.17	0/1244	0.28	0/1693
1	SB	0.15	0/1152	0.26	0/1563
1	SC	0.16	0/1254	0.29	0/1704
1	SD	0.16	0/1244	0.28	0/1693
1	SE	0.15	0/1152	0.26	0/1563
1	SF	0.16	0/1254	0.29	0/1704
1	T	0.16	0/1244	0.28	0/1693
1	TA	0.16	0/1254	0.29	0/1704
1	TB	0.16	0/1244	0.27	0/1693
1	TC	0.15	0/1152	0.26	0/1563
1	TD	0.16	0/1254	0.29	0/1704
1	TE	0.17	0/1244	0.28	0/1693
1	TF	0.15	0/1152	0.26	0/1563
1	UA	0.15	0/1152	0.26	0/1563
1	UB	0.16	0/1254	0.29	0/1704
1	UC	0.17	0/1244	0.28	0/1693
1	UD	0.15	0/1152	0.26	0/1563
1	UE	0.16	0/1254	0.29	0/1704
1	UF	0.17	0/1244	0.27	0/1693
1	V	0.16	0/1254	0.29	0/1704
1	VA	0.16	0/1244	0.28	0/1693
1	VB	0.15	0/1152	0.26	0/1563
1	VC	0.16	0/1254	0.29	0/1704
1	VD	0.16	0/1244	0.28	0/1693
1	VE	0.15	0/1152	0.26	0/1563
1	VF	0.16	0/1254	0.29	0/1704
1	W	0.15	0/1152	0.26	0/1563
1	WA	0.16	0/1254	0.29	0/1704
1	WB	0.17	0/1244	0.28	0/1693
1	WC	0.15	0/1152	0.26	0/1563
1	WD	0.16	0/1254	0.29	0/1704
1	WE	0.16	0/1244	0.28	0/1693
1	WF	0.15	0/1152	0.26	0/1563
1	X	0.17	0/1244	0.28	0/1693
1	XA	0.15	0/1152	0.26	0/1563
1	XB	0.16	0/1254	0.29	0/1704

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	XC	0.16	0/1244	0.27	0/1693
1	XD	0.15	0/1152	0.26	0/1563
1	XE	0.16	0/1254	0.29	0/1704
1	XF	0.17	0/1244	0.28	0/1693
1	Y	0.16	0/1254	0.29	0/1704
1	YA	0.16	0/1244	0.28	0/1693
1	YB	0.15	0/1152	0.26	0/1563
1	YC	0.16	0/1254	0.29	0/1704
1	YD	0.17	0/1244	0.28	0/1693
1	YE	0.15	0/1152	0.26	0/1563
1	YF	0.16	0/1254	0.29	0/1704
1	Z	0.15	0/1152	0.26	0/1563
1	ZA	0.16	0/1254	0.29	0/1704
1	ZB	0.16	0/1244	0.28	0/1693
1	ZC	0.15	0/1152	0.26	0/1563
1	ZD	0.16	0/1254	0.29	0/1704
1	ZE	0.16	0/1244	0.28	0/1693
All	All	0.16	0/219000	0.27	0/297600

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1131	0	1159	9	0
1	AA	1221	0	1250	9	0
1	AB	1131	0	1159	10	0
1	AC	1231	0	1263	12	0
1	AD	1221	0	1250	8	0
1	AE	1131	0	1159	10	0
1	AF	1231	0	1263	11	0
1	B	1221	0	1250	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	1231	0	1263	11	0
1	BB	1221	0	1250	9	0
1	BC	1131	0	1159	8	0
1	BD	1231	0	1263	12	0
1	BE	1221	0	1250	9	0
1	BF	1131	0	1159	9	0
1	C	1231	0	1263	12	0
1	CA	1131	0	1159	9	0
1	CB	1231	0	1263	11	0
1	CC	1221	0	1250	9	0
1	CD	1131	0	1159	10	0
1	CE	1231	0	1263	12	0
1	CF	1221	0	1250	10	0
1	D	1131	0	1159	9	0
1	DA	1221	0	1250	9	0
1	DB	1131	0	1159	8	0
1	DC	1231	0	1263	12	0
1	DD	1221	0	1250	9	0
1	DE	1131	0	1159	8	0
1	DF	1231	0	1263	12	0
1	E	1221	0	1250	9	0
1	EA	1231	0	1263	12	0
1	EB	1221	0	1250	9	0
1	EC	1131	0	1159	9	0
1	ED	1231	0	1263	13	0
1	EE	1221	0	1250	10	0
1	EF	1131	0	1159	9	0
1	F	1231	0	1263	11	0
1	FA	1131	0	1159	9	0
1	FB	1231	0	1263	11	0
1	FC	1221	0	1250	9	0
1	FD	1131	0	1159	9	0
1	FE	1231	0	1263	11	0
1	FF	1221	0	1250	9	0
1	G	1131	0	1159	10	0
1	GA	1221	0	1250	9	0
1	GB	1131	0	1159	9	0
1	GC	1231	0	1263	12	0
1	GD	1221	0	1250	10	0
1	GE	1131	0	1159	9	0
1	GF	1231	0	1263	11	0
1	H	1221	0	1250	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	HA	1231	0	1263	12	0
1	HB	1221	0	1250	9	0
1	HC	1131	0	1159	8	0
1	HD	1231	0	1263	12	0
1	HE	1221	0	1250	10	0
1	HF	1131	0	1159	10	0
1	I	1231	0	1263	11	0
1	IA	1131	0	1159	9	0
1	IB	1231	0	1263	12	0
1	IC	1221	0	1250	9	0
1	ID	1131	0	1159	9	0
1	IE	1231	0	1263	13	0
1	IF	1221	0	1250	10	0
1	J	1131	0	1159	9	0
1	JA	1221	0	1250	9	0
1	JB	1131	0	1159	10	0
1	JC	1231	0	1263	11	0
1	JD	1221	0	1250	10	0
1	JE	1131	0	1159	8	0
1	JF	1231	0	1263	11	0
1	K	1221	0	1250	10	0
1	KA	1231	0	1263	11	0
1	KB	1221	0	1250	9	0
1	KC	1131	0	1159	10	0
1	KD	1231	0	1263	12	0
1	KE	1221	0	1250	10	0
1	KF	1131	0	1159	10	0
1	L	1231	0	1263	12	0
1	LA	1131	0	1159	9	0
1	LB	1231	0	1263	12	0
1	LC	1221	0	1250	8	0
1	LD	1131	0	1159	9	0
1	LE	1231	0	1263	11	0
1	LF	1221	0	1250	9	0
1	M	1131	0	1159	9	0
1	MA	1221	0	1250	10	0
1	MB	1131	0	1159	9	0
1	MC	1231	0	1263	12	0
1	MD	1221	0	1250	10	0
1	ME	1131	0	1159	9	0
1	MF	1231	0	1263	13	0
1	N	1221	0	1250	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	NA	1231	0	1263	11	0
1	NB	1221	0	1250	10	0
1	NC	1131	0	1159	9	0
1	ND	1231	0	1263	13	0
1	NE	1221	0	1250	9	0
1	NF	1131	0	1159	10	0
1	O	1231	0	1263	11	0
1	OA	1131	0	1159	9	0
1	OB	1231	0	1263	12	0
1	OC	1221	0	1250	9	0
1	OD	1131	0	1159	9	0
1	OE	1231	0	1263	13	0
1	OF	1221	0	1250	9	0
1	P	1131	0	1159	8	0
1	PA	1221	0	1250	10	0
1	PB	1131	0	1159	9	0
1	PC	1231	0	1263	11	0
1	PD	1221	0	1250	10	0
1	PE	1131	0	1159	11	0
1	PF	1231	0	1263	11	0
1	Q	1221	0	1250	9	0
1	QA	1231	0	1263	11	0
1	QB	1221	0	1250	10	0
1	QC	1131	0	1159	8	0
1	QD	1231	0	1263	12	0
1	QE	1221	0	1250	9	0
1	QF	1131	0	1159	10	0
1	R	1231	0	1263	11	0
1	RA	1131	0	1159	10	0
1	RB	1231	0	1263	12	0
1	RC	1221	0	1250	9	0
1	RD	1131	0	1159	9	0
1	RE	1231	0	1263	12	0
1	RF	1221	0	1250	10	0
1	S	1131	0	1159	9	0
1	SA	1221	0	1250	10	0
1	SB	1131	0	1159	9	0
1	SC	1231	0	1263	12	0
1	SD	1221	0	1250	10	0
1	SE	1131	0	1159	8	0
1	SF	1231	0	1263	12	0
1	T	1221	0	1250	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	TA	1231	0	1263	11	0
1	TB	1221	0	1250	10	0
1	TC	1131	0	1159	10	0
1	TD	1231	0	1263	13	0
1	TE	1221	0	1250	10	0
1	TF	1131	0	1159	9	0
1	UA	1131	0	1159	8	0
1	UB	1231	0	1263	13	0
1	UC	1221	0	1250	9	0
1	UD	1131	0	1159	8	0
1	UE	1231	0	1263	11	0
1	UF	1221	0	1250	9	0
1	V	1231	0	1263	12	0
1	VA	1221	0	1250	9	0
1	VB	1131	0	1159	8	0
1	VC	1231	0	1263	12	0
1	VD	1221	0	1250	10	0
1	VE	1131	0	1159	10	0
1	VF	1231	0	1263	11	0
1	W	1131	0	1159	10	0
1	WA	1231	0	1263	11	0
1	WB	1221	0	1250	9	0
1	WC	1131	0	1159	8	0
1	WD	1231	0	1263	11	0
1	WE	1221	0	1250	9	0
1	WF	1131	0	1159	10	0
1	X	1221	0	1250	9	0
1	XA	1131	0	1159	9	0
1	XB	1231	0	1263	12	0
1	XC	1221	0	1250	9	0
1	XD	1131	0	1159	9	0
1	XE	1231	0	1263	13	0
1	XF	1221	0	1250	10	0
1	Y	1231	0	1263	11	0
1	YA	1221	0	1250	9	0
1	YB	1131	0	1159	9	0
1	YC	1231	0	1263	11	0
1	YD	1221	0	1250	9	0
1	YE	1131	0	1159	10	0
1	YF	1231	0	1263	11	0
1	Z	1131	0	1159	8	0
1	ZA	1231	0	1263	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	ZB	1221	0	1250	9	0
1	ZC	1131	0	1159	10	0
1	ZD	1231	0	1263	13	0
1	ZE	1221	0	1250	9	0
2	A	1	0	0	0	0
2	AA	1	0	0	0	0
2	AB	1	0	0	0	0
2	AC	1	0	0	0	0
2	AD	1	0	0	0	0
2	AE	1	0	0	0	0
2	AF	1	0	0	0	0
2	B	1	0	0	0	0
2	BA	1	0	0	0	0
2	BB	1	0	0	0	0
2	BC	1	0	0	0	0
2	BD	1	0	0	0	0
2	BE	1	0	0	0	0
2	BF	1	0	0	0	0
2	C	1	0	0	0	0
2	CA	1	0	0	0	0
2	CB	1	0	0	0	0
2	CC	1	0	0	0	0
2	CD	1	0	0	0	0
2	CE	1	0	0	0	0
2	CF	1	0	0	0	0
2	D	1	0	0	0	0
2	DA	1	0	0	0	0
2	DB	1	0	0	0	0
2	DC	1	0	0	0	0
2	DD	1	0	0	0	0
2	DE	1	0	0	0	0
2	DF	1	0	0	0	0
2	E	1	0	0	0	0
2	EA	1	0	0	0	0
2	EB	1	0	0	0	0
2	EC	1	0	0	0	0
2	ED	1	0	0	0	0
2	EE	1	0	0	0	0
2	EF	1	0	0	0	0
2	F	1	0	0	0	0
2	FA	1	0	0	0	0
2	FB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	FC	1	0	0	0	0
2	FD	1	0	0	0	0
2	FE	1	0	0	0	0
2	FF	1	0	0	0	0
2	G	1	0	0	0	0
2	GA	1	0	0	0	0
2	GB	1	0	0	0	0
2	GC	1	0	0	0	0
2	GD	1	0	0	0	0
2	GE	1	0	0	0	0
2	GF	1	0	0	0	0
2	H	1	0	0	0	0
2	HA	1	0	0	0	0
2	HB	1	0	0	0	0
2	HC	1	0	0	0	0
2	HD	1	0	0	0	0
2	HE	1	0	0	0	0
2	HF	1	0	0	0	0
2	I	1	0	0	0	0
2	IA	1	0	0	0	0
2	IB	1	0	0	0	0
2	IC	1	0	0	0	0
2	ID	1	0	0	0	0
2	IE	1	0	0	0	0
2	IF	1	0	0	0	0
2	J	1	0	0	0	0
2	JA	1	0	0	0	0
2	JB	1	0	0	0	0
2	JC	1	0	0	0	0
2	JD	1	0	0	0	0
2	JE	1	0	0	0	0
2	JF	1	0	0	0	0
2	K	1	0	0	0	0
2	KA	1	0	0	0	0
2	KB	1	0	0	0	0
2	KC	1	0	0	0	0
2	KD	1	0	0	0	0
2	KE	1	0	0	0	0
2	KF	1	0	0	0	0
2	L	1	0	0	0	0
2	LA	1	0	0	0	0
2	LB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	LC	1	0	0	0	0
2	LD	1	0	0	0	0
2	LE	1	0	0	0	0
2	LF	1	0	0	0	0
2	M	1	0	0	0	0
2	MA	1	0	0	0	0
2	MB	1	0	0	0	0
2	MC	1	0	0	0	0
2	MD	1	0	0	0	0
2	ME	1	0	0	0	0
2	MF	1	0	0	0	0
2	N	1	0	0	0	0
2	NA	1	0	0	0	0
2	NB	1	0	0	0	0
2	NC	1	0	0	0	0
2	ND	1	0	0	0	0
2	NE	1	0	0	0	0
2	NF	1	0	0	0	0
2	O	1	0	0	0	0
2	OA	1	0	0	0	0
2	OB	1	0	0	0	0
2	OC	1	0	0	0	0
2	OD	1	0	0	0	0
2	OE	1	0	0	0	0
2	OF	1	0	0	0	0
2	P	1	0	0	0	0
2	PA	1	0	0	0	0
2	PB	1	0	0	0	0
2	PC	1	0	0	0	0
2	PD	1	0	0	0	0
2	PE	1	0	0	0	0
2	PF	1	0	0	0	0
2	Q	1	0	0	0	0
2	QA	1	0	0	0	0
2	QB	1	0	0	0	0
2	QC	1	0	0	0	0
2	QD	1	0	0	0	0
2	QE	1	0	0	0	0
2	QF	1	0	0	0	0
2	R	1	0	0	0	0
2	RA	1	0	0	0	0
2	RB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	RC	1	0	0	0	0
2	RD	1	0	0	0	0
2	RE	1	0	0	0	0
2	RF	1	0	0	0	0
2	S	1	0	0	0	0
2	SA	1	0	0	0	0
2	SB	1	0	0	0	0
2	SC	1	0	0	0	0
2	SD	1	0	0	0	0
2	SE	1	0	0	0	0
2	SF	1	0	0	0	0
2	T	1	0	0	0	0
2	TA	1	0	0	0	0
2	TB	1	0	0	0	0
2	TC	1	0	0	0	0
2	TD	1	0	0	0	0
2	TE	1	0	0	0	0
2	TF	1	0	0	0	0
2	UA	1	0	0	0	0
2	UB	1	0	0	0	0
2	UC	1	0	0	0	0
2	UD	1	0	0	0	0
2	UE	1	0	0	0	0
2	UF	1	0	0	0	0
2	V	1	0	0	0	0
2	VA	1	0	0	0	0
2	VB	1	0	0	0	0
2	VC	1	0	0	0	0
2	VD	1	0	0	0	0
2	VE	1	0	0	0	0
2	VF	1	0	0	0	0
2	W	1	0	0	0	0
2	WA	1	0	0	0	0
2	WB	1	0	0	0	0
2	WC	1	0	0	0	0
2	WD	1	0	0	0	0
2	WE	1	0	0	0	0
2	WF	1	0	0	0	0
2	X	1	0	0	0	0
2	XA	1	0	0	0	0
2	XB	1	0	0	0	0
2	XC	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	XD	1	0	0	0	0
2	XE	1	0	0	0	0
2	XF	1	0	0	0	0
2	Y	1	0	0	0	0
2	YA	1	0	0	0	0
2	YB	1	0	0	0	0
2	YC	1	0	0	0	0
2	YD	1	0	0	0	0
2	YE	1	0	0	0	0
2	YF	1	0	0	0	0
2	Z	1	0	0	0	0
2	ZA	1	0	0	0	0
2	ZB	1	0	0	0	0
2	ZC	1	0	0	0	0
2	ZD	1	0	0	0	0
2	ZE	1	0	0	0	0
All	All	215160	0	220320	1439	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 3.

All (1439) 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:C:99:SER:HB2	1:Q:64:LYS:HE3	1.81	0.63
1:HA:99:SER:HB2	1:VA:64:LYS:HE3	1.81	0.63
1:K:64:LYS:HE3	1:UE:99:SER:HB2	1.81	0.63
1:X:64:LYS:HE3	1:PF:99:SER:HB2	1.81	0.63
1:AA:64:LYS:HE3	1:JF:99:SER:HB2	1.81	0.63
1:PA:64:LYS:HE3	1:FE:99:SER:HB2	1.81	0.63
1:EB:64:LYS:HE3	1:YF:99:SER:HB2	1.81	0.63
1:WB:64:LYS:HE3	1:GF:99:SER:HB2	1.81	0.63
1:CC:64:LYS:HE3	1:DF:99:SER:HB2	1.81	0.63
1:PD:64:LYS:HE3	1:VF:99:SER:HB2	1.81	0.63
1:H:64:LYS:HE3	1:WD:99:SER:HB2	1.81	0.63
1:BB:64:LYS:HE3	1:AF:99:SER:HB2	1.81	0.63
1:RC:64:LYS:HE3	1:SF:99:SER:HB2	1.81	0.63
1:JA:64:LYS:HE3	1:KD:99:SER:HB2	1.81	0.63
1:MA:64:LYS:HE3	1:LE:99:SER:HB2	1.81	0.63
1:MC:99:SER:HB2	1:BE:64:LYS:HE3	1.81	0.63
1:GD:64:LYS:HE3	1:OE:99:SER:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:LYS:HE3	1:RB:99:SER:HB2	1.81	0.63
1:NB:64:LYS:HE3	1:ZD:99:SER:HB2	1.81	0.63
1:BD:99:SER:HB2	1:QE:64:LYS:HE3	1.81	0.63
1:HD:99:SER:HB2	1:NE:64:LYS:HE3	1.81	0.63
1:N:64:LYS:HE3	1:YC:99:SER:HB2	1.81	0.63
1:DA:64:LYS:HE3	1:UB:99:SER:HB2	1.81	0.63
1:NA:99:SER:HB2	1:KE:64:LYS:HE3	1.81	0.63
1:HB:64:LYS:HE3	1:ND:99:SER:HB2	1.81	0.63
1:LC:64:LYS:HE3	1:CE:99:SER:HB2	1.81	0.63
1:I:99:SER:HB2	1:VD:64:LYS:HE3	1.81	0.63
1:SA:64:LYS:HE3	1:JC:99:SER:HB2	1.81	0.63
1:KB:64:LYS:HE3	1:AC:99:SER:HB2	1.81	0.63
1:OB:99:SER:HB2	1:YD:64:LYS:HE3	1.81	0.63
1:PC:99:SER:HB2	1:DD:64:LYS:HE3	1.81	0.62
1:AD:64:LYS:HE3	1:RE:99:SER:HB2	1.81	0.62
1:ZA:99:SER:HB2	1:FC:64:LYS:HE3	1.81	0.62
1:OC:64:LYS:HE3	1:ED:99:SER:HB2	1.81	0.62
1:SD:64:LYS:HE3	1:IE:99:SER:HB2	1.81	0.62
1:TD:99:SER:HB2	1:HE:64:LYS:HE3	1.81	0.62
1:T:64:LYS:HE3	1:VC:99:SER:HB2	1.81	0.62
1:V:99:SER:HB2	1:UC:64:LYS:HE3	1.81	0.62
1:QA:99:SER:HB2	1:EE:64:LYS:HE3	1.81	0.62
1:LB:99:SER:HB2	1:ZB:64:LYS:HE3	1.81	0.62
1:B:64:LYS:HE3	1:R:99:SER:HB2	1.81	0.62
1:GA:64:LYS:HE3	1:WA:99:SER:HB2	1.81	0.62
1:YA:64:LYS:HE3	1:GC:99:SER:HB2	1.81	0.62
1:IB:99:SER:HB2	1:MD:64:LYS:HE3	1.81	0.62
1:L:99:SER:HB2	1:TE:64:LYS:HE3	1.81	0.62
1:EA:99:SER:HB2	1:TB:64:LYS:HE3	1.81	0.62
1:BA:99:SER:HB2	1:IF:64:LYS:HE3	1.81	0.62
1:FB:99:SER:HB2	1:XF:64:LYS:HE3	1.81	0.62
1:WE:64:LYS:HE3	1:MF:99:SER:HB2	1.81	0.62
1:Y:99:SER:HB2	1:OF:64:LYS:HE3	1.81	0.62
1:TA:99:SER:HB2	1:IC:64:LYS:HE3	1.81	0.62
1:DC:99:SER:HB2	1:CF:64:LYS:HE3	1.81	0.62
1:SC:99:SER:HB2	1:RF:64:LYS:HE3	1.81	0.62
1:XE:99:SER:HB2	1:LF:64:LYS:HE3	1.81	0.62
1:F:99:SER:HB2	1:QB:64:LYS:HE3	1.81	0.61
1:O:99:SER:HB2	1:XC:64:LYS:HE3	1.81	0.61
1:KA:99:SER:HB2	1:JD:64:LYS:HE3	1.81	0.61
1:CB:99:SER:HB2	1:ZE:64:LYS:HE3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XB:99:SER:HB2	1:FF:64:LYS:HE3	1.81	0.61
1:QD:99:SER:HB2	1:UF:64:LYS:HE3	1.81	0.61
1:FA:138:THR:O	1:FA:142:ARG:NH2	2.35	0.60
1:RD:138:THR:O	1:RD:142:ARG:NH2	2.35	0.60
1:GE:138:THR:O	1:GE:142:ARG:NH2	2.35	0.60
1:YE:138:THR:O	1:YE:142:ARG:NH2	2.35	0.60
1:NF:138:THR:O	1:NF:142:ARG:NH2	2.35	0.60
1:A:138:THR:O	1:A:142:ARG:NH2	2.35	0.60
1:VB:138:THR:O	1:VB:142:ARG:NH2	2.35	0.60
1:OD:138:THR:O	1:OD:142:ARG:NH2	2.35	0.60
1:CA:138:THR:O	1:CA:142:ARG:NH2	2.35	0.60
1:GB:138:THR:O	1:GB:142:ARG:NH2	2.35	0.60
1:JB:138:THR:O	1:JB:142:ARG:NH2	2.35	0.60
1:CD:138:THR:O	1:CD:142:ARG:NH2	2.35	0.60
1:DE:138:THR:O	1:DE:142:ARG:NH2	2.35	0.60
1:BC:138:THR:O	1:BC:142:ARG:NH2	2.35	0.60
1:QC:138:THR:O	1:QC:142:ARG:NH2	2.35	0.60
1:SE:138:THR:O	1:SE:142:ARG:NH2	2.35	0.60
1:J:138:THR:O	1:J:142:ARG:NH2	2.35	0.60
1:OA:138:THR:O	1:OA:142:ARG:NH2	2.35	0.59
1:VE:138:THR:O	1:VE:142:ARG:NH2	2.35	0.59
1:KF:138:THR:O	1:KF:142:ARG:NH2	2.35	0.59
1:SB:138:THR:O	1:SB:142:ARG:NH2	2.35	0.59
1:LD:138:THR:O	1:LD:142:ARG:NH2	2.35	0.59
1:KC:138:THR:O	1:KC:142:ARG:NH2	2.35	0.59
1:Z:138:THR:O	1:Z:142:ARG:NH2	2.35	0.59
1:DB:138:THR:O	1:DB:142:ARG:NH2	2.35	0.59
1:ZC:138:THR:O	1:ZC:142:ARG:NH2	2.35	0.59
1:G:138:THR:O	1:G:142:ARG:NH2	2.35	0.59
1:LA:138:THR:O	1:LA:142:ARG:NH2	2.35	0.59
1:S:138:THR:O	1:S:142:ARG:NH2	2.35	0.58
1:ME:138:THR:O	1:ME:142:ARG:NH2	2.35	0.58
1:XA:138:THR:O	1:XA:142:ARG:NH2	2.35	0.58
1:MB:138:THR:O	1:MB:142:ARG:NH2	2.35	0.58
1:XD:138:THR:O	1:XD:142:ARG:NH2	2.35	0.58
1:AB:138:THR:O	1:AB:142:ARG:NH2	2.35	0.58
1:FD:138:THR:O	1:FD:142:ARG:NH2	2.35	0.58
1:W:138:THR:O	1:W:142:ARG:NH2	2.35	0.58
1:P:138:THR:O	1:P:142:ARG:NH2	2.35	0.58
1:RA:138:THR:O	1:RA:142:ARG:NH2	2.35	0.58
1:M:138:THR:O	1:M:142:ARG:NH2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UA:138:THR:O	1:UA:142:ARG:NH2	2.35	0.58
1:EC:138:THR:O	1:EC:142:ARG:NH2	2.35	0.58
1:BF:138:THR:O	1:BF:142:ARG:NH2	2.35	0.58
1:QF:138:THR:O	1:QF:142:ARG:NH2	2.35	0.58
1:WF:138:THR:O	1:WF:142:ARG:NH2	2.35	0.58
1:YB:138:THR:O	1:YB:142:ARG:NH2	2.35	0.58
1:NC:138:THR:O	1:NC:142:ARG:NH2	2.35	0.58
1:TC:138:THR:O	1:TC:142:ARG:NH2	2.35	0.58
1:ID:138:THR:O	1:ID:142:ARG:NH2	2.35	0.58
1:AE:138:THR:O	1:AE:142:ARG:NH2	2.35	0.58
1:HF:138:THR:O	1:HF:142:ARG:NH2	2.35	0.57
1:IA:138:THR:O	1:IA:142:ARG:NH2	2.35	0.57
1:PB:138:THR:O	1:PB:142:ARG:NH2	2.35	0.57
1:UD:138:THR:O	1:UD:142:ARG:NH2	2.35	0.57
1:JE:138:THR:O	1:JE:142:ARG:NH2	2.35	0.57
1:PE:138:THR:O	1:PE:142:ARG:NH2	2.35	0.57
1:D:138:THR:O	1:D:142:ARG:NH2	2.35	0.57
1:HC:138:THR:O	1:HC:142:ARG:NH2	2.35	0.57
1:WC:138:THR:O	1:WC:142:ARG:NH2	2.35	0.57
1:W:97:LEU:HB2	1:W:100:VAL:HG23	1.87	0.57
1:AB:97:LEU:HB2	1:AB:100:VAL:HG23	1.87	0.57
1:UD:97:LEU:HB2	1:UD:100:VAL:HG23	1.87	0.57
1:Z:97:LEU:HB2	1:Z:100:VAL:HG23	1.87	0.57
1:JE:97:LEU:HB2	1:JE:100:VAL:HG23	1.87	0.57
1:DB:97:LEU:HB2	1:DB:100:VAL:HG23	1.87	0.57
1:BC:97:LEU:HB2	1:BC:100:VAL:HG23	1.87	0.57
1:EF:138:THR:O	1:EF:142:ARG:NH2	2.35	0.57
1:IA:97:LEU:HB2	1:IA:100:VAL:HG23	1.87	0.56
1:XA:97:LEU:HB2	1:XA:100:VAL:HG23	1.87	0.56
1:QC:97:LEU:HB2	1:QC:100:VAL:HG23	1.87	0.56
1:TF:138:THR:O	1:TF:142:ARG:NH2	2.35	0.56
1:D:97:LEU:HB2	1:D:100:VAL:HG23	1.87	0.56
1:G:97:LEU:HB2	1:G:100:VAL:HG23	1.87	0.56
1:S:97:LEU:HB2	1:S:100:VAL:HG23	1.87	0.56
1:LA:97:LEU:HB2	1:LA:100:VAL:HG23	1.87	0.56
1:VB:97:LEU:HB2	1:VB:100:VAL:HG23	1.87	0.56
1:YB:97:LEU:HB2	1:YB:100:VAL:HG23	1.87	0.56
1:OD:97:LEU:HB2	1:OD:100:VAL:HG23	1.87	0.56
1:BF:97:LEU:HB2	1:BF:100:VAL:HG23	1.87	0.56
1:CA:97:LEU:HB2	1:CA:100:VAL:HG23	1.87	0.56
1:GB:97:LEU:HB2	1:GB:100:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NC:97:LEU:HB2	1:NC:100:VAL:HG23	1.87	0.56
1:XD:97:LEU:HB2	1:XD:100:VAL:HG23	1.87	0.56
1:ME:97:LEU:HB2	1:ME:100:VAL:HG23	1.87	0.56
1:QF:97:LEU:HB2	1:QF:100:VAL:HG23	1.87	0.56
1:ZC:97:LEU:HB2	1:ZC:100:VAL:HG23	1.87	0.56
1:CD:97:LEU:HB2	1:CD:100:VAL:HG23	1.87	0.56
1:RD:97:LEU:HB2	1:RD:100:VAL:HG23	1.87	0.56
1:J:97:LEU:HB2	1:J:100:VAL:HG23	1.87	0.56
1:HC:97:LEU:HB2	1:HC:100:VAL:HG23	1.87	0.56
1:KC:97:LEU:HB2	1:KC:100:VAL:HG23	1.87	0.56
1:GE:97:LEU:HB2	1:GE:100:VAL:HG23	1.87	0.56
1:PE:97:LEU:HB2	1:PE:100:VAL:HG23	1.87	0.56
1:OA:97:LEU:HB2	1:OA:100:VAL:HG23	1.87	0.56
1:JB:97:LEU:HB2	1:JB:100:VAL:HG23	1.87	0.56
1:WC:97:LEU:HB2	1:WC:100:VAL:HG23	1.87	0.56
1:AE:97:LEU:HB2	1:AE:100:VAL:HG23	1.87	0.56
1:UA:97:LEU:HB2	1:UA:100:VAL:HG23	1.87	0.56
1:PB:97:LEU:HB2	1:PB:100:VAL:HG23	1.87	0.56
1:DE:97:LEU:HB2	1:DE:100:VAL:HG23	1.87	0.56
1:EC:97:LEU:HB2	1:EC:100:VAL:HG23	1.87	0.56
1:TC:97:LEU:HB2	1:TC:100:VAL:HG23	1.87	0.56
1:ID:97:LEU:HB2	1:ID:100:VAL:HG23	1.87	0.56
1:SE:97:LEU:HB2	1:SE:100:VAL:HG23	1.87	0.56
1:KF:97:LEU:HB2	1:KF:100:VAL:HG23	1.87	0.56
1:M:97:LEU:HB2	1:M:100:VAL:HG23	1.87	0.56
1:P:97:LEU:HB2	1:P:100:VAL:HG23	1.87	0.56
1:RA:97:LEU:HB2	1:RA:100:VAL:HG23	1.87	0.56
1:VE:97:LEU:HB2	1:VE:100:VAL:HG23	1.87	0.55
1:YE:97:LEU:HB2	1:YE:100:VAL:HG23	1.87	0.55
1:NF:97:LEU:HB2	1:NF:100:VAL:HG23	1.87	0.55
1:FD:97:LEU:HB2	1:FD:100:VAL:HG23	1.87	0.55
1:TF:97:LEU:HB2	1:TF:100:VAL:HG23	1.87	0.55
1:MB:97:LEU:HB2	1:MB:100:VAL:HG23	1.87	0.55
1:TD:35:ILE:HD11	1:EE:31:ILE:HG23	1.89	0.55
1:EF:97:LEU:HB2	1:EF:100:VAL:HG23	1.87	0.55
1:IC:31:ILE:HG23	1:MC:35:ILE:HD11	1.89	0.55
1:LD:97:LEU:HB2	1:LD:100:VAL:HG23	1.87	0.55
1:IE:35:ILE:HD11	1:TE:31:ILE:HG23	1.89	0.55
1:ZE:31:ILE:HG23	1:DF:35:ILE:HD11	1.89	0.55
1:OF:31:ILE:HG23	1:SF:35:ILE:HD11	1.89	0.55
1:XE:35:ILE:HD11	1:IF:31:ILE:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MF:35:ILE:HD11	1:XF:31:ILE:HG23	1.89	0.55
1:SB:97:LEU:HB2	1:SB:100:VAL:HG23	1.87	0.55
1:XC:31:ILE:HG23	1:BD:35:ILE:HD11	1.89	0.55
1:LB:35:ILE:HD11	1:WB:31:ILE:HG23	1.89	0.55
1:CF:31:ILE:HG23	1:GF:35:ILE:HD11	1.89	0.55
1:RF:31:ILE:HG23	1:VF:35:ILE:HD11	1.89	0.55
1:X:31:ILE:HG23	1:BA:35:ILE:HD11	1.89	0.54
1:BB:31:ILE:HG23	1:FB:35:ILE:HD11	1.89	0.54
1:EB:31:ILE:HG23	1:IB:35:ILE:HD11	1.89	0.54
1:NB:31:ILE:HG23	1:RB:35:ILE:HD11	1.89	0.54
1:ED:35:ILE:HD11	1:PD:31:ILE:HG23	1.89	0.54
1:Q:31:ILE:HG23	1:V:35:ILE:HD11	1.89	0.54
1:AA:31:ILE:HG23	1:EA:35:ILE:HD11	1.89	0.54
1:FA:97:LEU:HB2	1:FA:100:VAL:HG23	1.87	0.54
1:KB:31:ILE:HG23	1:OB:35:ILE:HD11	1.89	0.54
1:HF:97:LEU:HB2	1:HF:100:VAL:HG23	1.87	0.54
1:K:31:ILE:HG23	1:O:35:ILE:HD11	1.89	0.54
1:PA:31:ILE:HG23	1:TA:35:ILE:HD11	1.89	0.54
1:VA:31:ILE:HG23	1:ZA:35:ILE:HD11	1.89	0.54
1:DD:31:ILE:HG23	1:HD:35:ILE:HD11	1.89	0.54
1:GD:31:ILE:HG23	1:KD:35:ILE:HD11	1.89	0.54
1:WF:97:LEU:HB2	1:WF:100:VAL:HG23	1.87	0.54
1:A:97:LEU:HB2	1:A:100:VAL:HG23	1.87	0.54
1:C:35:ILE:HD11	1:N:31:ILE:HG23	1.89	0.54
1:HA:35:ILE:HD11	1:SA:31:ILE:HG23	1.89	0.54
1:FC:31:ILE:HG23	1:JC:35:ILE:HD11	1.89	0.54
1:YA:31:ILE:HG23	1:CB:35:ILE:HD11	1.89	0.54
1:ZB:31:ILE:HG23	1:DC:35:ILE:HD11	1.89	0.54
1:UC:31:ILE:HG23	1:YC:35:ILE:HD11	1.89	0.54
1:SD:31:ILE:HG23	1:WD:35:ILE:HD11	1.89	0.54
1:VD:31:ILE:HG23	1:ZD:35:ILE:HD11	1.89	0.54
1:KE:31:ILE:HG23	1:OE:35:ILE:HD11	1.89	0.54
1:T:31:ILE:HG23	1:Y:35:ILE:HD11	1.89	0.54
1:OC:31:ILE:HG23	1:SC:35:ILE:HD11	1.89	0.54
1:PC:35:ILE:HD11	1:AD:31:ILE:HG23	1.89	0.54
1:HE:31:ILE:HG23	1:LE:35:ILE:HD11	1.89	0.54
1:AC:35:ILE:HD11	1:LC:31:ILE:HG23	1.89	0.54
1:J:182:ASP:N	1:J:182:ASP:OD1	2.42	0.53
1:OA:182:ASP:N	1:OA:182:ASP:OD1	2.42	0.53
1:JD:31:ILE:HG23	1:ND:35:ILE:HD11	1.89	0.53
1:JA:31:ILE:HG23	1:NA:35:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QB:31:ILE:HG23	1:UB:35:ILE:HD11	1.89	0.53
1:VB:182:ASP:N	1:VB:182:ASP:OD1	2.42	0.53
1:RC:31:ILE:HG23	1:VC:35:ILE:HD11	1.89	0.53
1:OD:182:ASP:OD1	1:OD:182:ASP:N	2.42	0.53
1:EF:182:ASP:N	1:EF:182:ASP:OD1	2.42	0.53
1:TF:182:ASP:OD1	1:TF:182:ASP:N	2.42	0.53
1:S:182:ASP:OD1	1:S:182:ASP:N	2.42	0.53
1:RA:182:ASP:OD1	1:RA:182:ASP:N	2.42	0.53
1:XA:182:ASP:N	1:XA:182:ASP:OD1	2.42	0.53
1:MB:182:ASP:OD1	1:MB:182:ASP:N	2.42	0.53
1:CC:31:ILE:HG23	1:GC:35:ILE:HD11	1.89	0.53
1:FD:182:ASP:OD1	1:FD:182:ASP:N	2.42	0.53
1:MD:31:ILE:HG23	1:QD:35:ILE:HD11	1.89	0.53
1:YD:31:ILE:HG23	1:CE:35:ILE:HD11	1.89	0.53
1:GE:182:ASP:OD1	1:GE:182:ASP:N	2.42	0.53
1:QE:31:ILE:HG23	1:UE:35:ILE:HD11	1.89	0.53
1:VE:182:ASP:N	1:VE:182:ASP:OD1	2.42	0.53
1:HF:182:ASP:OD1	1:HF:182:ASP:N	2.42	0.53
1:KF:182:ASP:OD1	1:KF:182:ASP:N	2.42	0.53
1:WF:182:ASP:OD1	1:WF:182:ASP:N	2.42	0.53
1:E:31:ILE:HG23	1:I:35:ILE:HD11	1.89	0.53
1:M:182:ASP:N	1:M:182:ASP:OD1	2.42	0.53
1:UA:182:ASP:OD1	1:UA:182:ASP:N	2.42	0.53
1:TB:31:ILE:HG23	1:XB:35:ILE:HD11	1.89	0.53
1:RD:182:ASP:N	1:RD:182:ASP:OD1	2.42	0.53
1:BE:31:ILE:HG23	1:FE:35:ILE:HD11	1.89	0.53
1:NE:31:ILE:HG23	1:RE:35:ILE:HD11	1.89	0.53
1:B:31:ILE:HG23	1:F:35:ILE:HD11	1.89	0.53
1:P:182:ASP:OD1	1:P:182:ASP:N	2.42	0.53
1:R:35:ILE:HD11	1:DA:31:ILE:HG23	1.89	0.53
1:GA:31:ILE:HG23	1:KA:35:ILE:HD11	1.89	0.53
1:EC:182:ASP:OD1	1:EC:182:ASP:N	2.42	0.53
1:CD:182:ASP:OD1	1:CD:182:ASP:N	2.42	0.53
1:A:182:ASP:OD1	1:A:182:ASP:N	2.42	0.53
1:JB:182:ASP:OD1	1:JB:182:ASP:N	2.42	0.53
1:BC:182:ASP:OD1	1:BC:182:ASP:N	2.42	0.53
1:QC:182:ASP:OD1	1:QC:182:ASP:N	2.42	0.53
1:TC:182:ASP:OD1	1:TC:182:ASP:N	2.42	0.53
1:FA:182:ASP:OD1	1:FA:182:ASP:N	2.42	0.53
1:WA:35:ILE:HD11	1:HB:31:ILE:HG23	1.89	0.53
1:DB:182:ASP:N	1:DB:182:ASP:OD1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FF:31:ILE:HG23	1:JF:35:ILE:HD11	1.89	0.53
1:H:31:ILE:HG23	1:L:35:ILE:HD11	1.89	0.53
1:MA:31:ILE:HG23	1:QA:35:ILE:HD11	1.89	0.53
1:SB:182:ASP:N	1:SB:182:ASP:OD1	2.42	0.53
1:UF:31:ILE:HG23	1:YF:35:ILE:HD11	1.89	0.53
1:Z:182:ASP:OD1	1:Z:182:ASP:N	2.42	0.53
1:LD:182:ASP:OD1	1:LD:182:ASP:N	2.42	0.53
1:AB:182:ASP:OD1	1:AB:182:ASP:N	2.42	0.53
1:WE:31:ILE:HG23	1:AF:35:ILE:HD11	1.89	0.53
1:QF:182:ASP:N	1:QF:182:ASP:OD1	2.42	0.53
1:BF:182:ASP:N	1:BF:182:ASP:OD1	2.42	0.52
1:NF:182:ASP:N	1:NF:182:ASP:OD1	2.42	0.52
1:B:89:ARG:H	1:B:174:GLU:HG2	1.75	0.52
1:W:182:ASP:OD1	1:W:182:ASP:N	2.42	0.52
1:GA:89:ARG:H	1:GA:174:GLU:HG2	1.75	0.52
1:VA:89:ARG:H	1:VA:174:GLU:HG2	1.75	0.52
1:WB:89:ARG:H	1:WB:174:GLU:HG2	1.75	0.52
1:YE:182:ASP:N	1:YE:182:ASP:OD1	2.42	0.52
1:LF:31:ILE:HG23	1:PF:35:ILE:HD11	1.89	0.52
1:Q:89:ARG:H	1:Q:174:GLU:HG2	1.75	0.52
1:PD:89:ARG:H	1:PD:174:GLU:HG2	1.75	0.52
1:UD:182:ASP:OD1	1:UD:182:ASP:N	2.42	0.52
1:SA:89:ARG:H	1:SA:174:GLU:HG2	1.75	0.52
1:BE:89:ARG:H	1:BE:174:GLU:HG2	1.75	0.52
1:JE:182:ASP:N	1:JE:182:ASP:OD1	2.42	0.52
1:QE:89:ARG:H	1:QE:174:GLU:HG2	1.75	0.52
1:D:182:ASP:OD1	1:D:182:ASP:N	2.42	0.52
1:G:182:ASP:OD1	1:G:182:ASP:N	2.42	0.52
1:H:89:ARG:H	1:H:174:GLU:HG2	1.74	0.52
1:N:89:ARG:H	1:N:174:GLU:HG2	1.75	0.52
1:T:89:ARG:H	1:T:174:GLU:HG2	1.75	0.52
1:IA:182:ASP:OD1	1:IA:182:ASP:N	2.42	0.52
1:LA:182:ASP:N	1:LA:182:ASP:OD1	2.42	0.52
1:YA:89:ARG:H	1:YA:174:GLU:HG2	1.75	0.52
1:GB:182:ASP:N	1:GB:182:ASP:OD1	2.42	0.52
1:YB:182:ASP:OD1	1:YB:182:ASP:N	2.42	0.52
1:HC:182:ASP:OD1	1:HC:182:ASP:N	2.42	0.52
1:NC:182:ASP:N	1:NC:182:ASP:OD1	2.42	0.52
1:SE:182:ASP:OD1	1:SE:182:ASP:N	2.42	0.52
1:OF:89:ARG:H	1:OF:174:GLU:HG2	1.75	0.52
1:CA:182:ASP:OD1	1:CA:182:ASP:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZB:89:ARG:H	1:ZB:174:GLU:HG2	1.75	0.52
1:KC:182:ASP:OD1	1:KC:182:ASP:N	2.42	0.52
1:WC:182:ASP:OD1	1:WC:182:ASP:N	2.42	0.52
1:XC:89:ARG:H	1:XC:174:GLU:HG2	1.75	0.52
1:AD:89:ARG:H	1:AD:174:GLU:HG2	1.75	0.52
1:EE:89:ARG:H	1:EE:174:GLU:HG2	1.75	0.52
1:ZE:89:ARG:H	1:ZE:174:GLU:HG2	1.75	0.52
1:MA:89:ARG:H	1:MA:174:GLU:HG2	1.74	0.52
1:EB:89:ARG:H	1:EB:174:GLU:HG2	1.75	0.52
1:QB:89:ARG:H	1:QB:174:GLU:HG2	1.74	0.52
1:LC:89:ARG:H	1:LC:174:GLU:HG2	1.75	0.52
1:OC:89:ARG:H	1:OC:174:GLU:HG2	1.75	0.52
1:ZC:182:ASP:N	1:ZC:182:ASP:OD1	2.42	0.52
1:GD:89:ARG:H	1:GD:174:GLU:HG2	1.75	0.52
1:VD:89:ARG:H	1:VD:174:GLU:HG2	1.75	0.52
1:XD:182:ASP:OD1	1:XD:182:ASP:N	2.42	0.52
1:DE:182:ASP:OD1	1:DE:182:ASP:N	2.42	0.52
1:TE:89:ARG:H	1:TE:174:GLU:HG2	1.75	0.52
1:RF:89:ARG:H	1:RF:174:GLU:HG2	1.74	0.52
1:AA:89:ARG:H	1:AA:174:GLU:HG2	1.75	0.52
1:IC:89:ARG:H	1:IC:174:GLU:HG2	1.75	0.52
1:JD:89:ARG:H	1:JD:174:GLU:HG2	1.74	0.52
1:KE:89:ARG:H	1:KE:174:GLU:HG2	1.75	0.52
1:ME:182:ASP:OD1	1:ME:182:ASP:N	2.42	0.52
1:NB:89:ARG:H	1:NB:174:GLU:HG2	1.75	0.52
1:VB:96:LEU:HD12	1:VB:167:VAL:HG22	1.92	0.52
1:YB:96:LEU:HD12	1:YB:167:VAL:HG22	1.92	0.52
1:BC:96:LEU:HD12	1:BC:167:VAL:HG22	1.92	0.52
1:QC:96:LEU:HD12	1:QC:167:VAL:HG22	1.92	0.52
1:CF:89:ARG:H	1:CF:174:GLU:HG2	1.74	0.52
1:UA:96:LEU:HD12	1:UA:167:VAL:HG22	1.92	0.52
1:NC:96:LEU:HD12	1:NC:167:VAL:HG22	1.92	0.52
1:OD:96:LEU:HD12	1:OD:167:VAL:HG22	1.92	0.52
1:UD:96:LEU:HD12	1:UD:167:VAL:HG22	1.92	0.52
1:JE:96:LEU:HD12	1:JE:167:VAL:HG22	1.92	0.52
1:P:96:LEU:HD12	1:P:167:VAL:HG22	1.92	0.51
1:SB:96:LEU:HD12	1:SB:167:VAL:HG22	1.92	0.51
1:LD:96:LEU:HD12	1:LD:167:VAL:HG22	1.92	0.51
1:SD:89:ARG:H	1:SD:174:GLU:HG2	1.75	0.51
1:HE:89:ARG:H	1:HE:174:GLU:HG2	1.75	0.51
1:W:96:LEU:HD12	1:W:167:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:89:ARG:H	1:X:174:GLU:HG2	1.74	0.51
1:PE:182:ASP:OD1	1:PE:182:ASP:N	2.42	0.51
1:FF:89:ARG:H	1:FF:174:GLU:HG2	1.75	0.51
1:M:96:LEU:HD12	1:M:167:VAL:HG22	1.92	0.51
1:RA:96:LEU:HD12	1:RA:167:VAL:HG22	1.92	0.51
1:AB:96:LEU:HD12	1:AB:167:VAL:HG22	1.92	0.51
1:BB:89:ARG:H	1:BB:174:GLU:HG2	1.74	0.51
1:TB:89:ARG:H	1:TB:174:GLU:HG2	1.75	0.51
1:KC:96:LEU:HD12	1:KC:167:VAL:HG22	1.92	0.51
1:ZC:96:LEU:HD12	1:ZC:167:VAL:HG22	1.92	0.51
1:MD:89:ARG:H	1:MD:174:GLU:HG2	1.75	0.51
1:RD:96:LEU:HD12	1:RD:167:VAL:HG22	1.92	0.51
1:AE:182:ASP:OD1	1:AE:182:ASP:N	2.42	0.51
1:GE:96:LEU:HD12	1:GE:167:VAL:HG22	1.92	0.51
1:NE:89:ARG:H	1:NE:174:GLU:HG2	1.74	0.51
1:IF:89:ARG:H	1:IF:174:GLU:HG2	1.75	0.51
1:LF:89:ARG:H	1:LF:174:GLU:HG2	1.75	0.51
1:S:96:LEU:HD12	1:S:167:VAL:HG22	1.92	0.51
1:PA:89:ARG:H	1:PA:174:GLU:HG2	1.75	0.51
1:XA:96:LEU:HD12	1:XA:167:VAL:HG22	1.92	0.51
1:DB:96:LEU:HD12	1:DB:167:VAL:HG22	1.92	0.51
1:DD:89:ARG:H	1:DD:174:GLU:HG2	1.75	0.51
1:UF:89:ARG:H	1:UF:174:GLU:HG2	1.75	0.51
1:K:89:ARG:H	1:K:174:GLU:HG2	1.75	0.51
1:Z:96:LEU:HD12	1:Z:167:VAL:HG22	1.92	0.51
1:UC:89:ARG:H	1:UC:174:GLU:HG2	1.74	0.51
1:YD:89:ARG:H	1:YD:174:GLU:HG2	1.74	0.51
1:WE:89:ARG:H	1:WE:174:GLU:HG2	1.75	0.51
1:BF:96:LEU:HD12	1:BF:167:VAL:HG22	1.92	0.51
1:EF:96:LEU:HD12	1:EF:167:VAL:HG22	1.92	0.51
1:XF:89:ARG:H	1:XF:174:GLU:HG2	1.75	0.51
1:MB:96:LEU:HD12	1:MB:167:VAL:HG22	1.92	0.51
1:FC:89:ARG:H	1:FC:174:GLU:HG2	1.74	0.51
1:FD:96:LEU:HD12	1:FD:167:VAL:HG22	1.92	0.51
1:YE:96:LEU:HD12	1:YE:167:VAL:HG22	1.92	0.51
1:QF:96:LEU:HD12	1:QF:167:VAL:HG22	1.92	0.51
1:TF:96:LEU:HD12	1:TF:167:VAL:HG22	1.92	0.51
1:J:96:LEU:HD12	1:J:167:VAL:HG22	1.92	0.51
1:FA:96:LEU:HD12	1:FA:167:VAL:HG22	1.92	0.51
1:JB:96:LEU:HD12	1:JB:167:VAL:HG22	1.92	0.51
1:KB:89:ARG:H	1:KB:174:GLU:HG2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PB:182:ASP:OD1	1:PB:182:ASP:N	2.42	0.51
1:CD:96:LEU:HD12	1:CD:167:VAL:HG22	1.92	0.51
1:NF:96:LEU:HD12	1:NF:167:VAL:HG22	1.92	0.51
1:A:96:LEU:HD12	1:A:167:VAL:HG22	1.92	0.51
1:E:89:ARG:H	1:E:174:GLU:HG2	1.75	0.51
1:JA:89:ARG:H	1:JA:174:GLU:HG2	1.75	0.51
1:OA:96:LEU:HD12	1:OA:167:VAL:HG22	1.92	0.51
1:ID:182:ASP:OD1	1:ID:182:ASP:N	2.42	0.51
1:D:96:LEU:HD12	1:D:167:VAL:HG22	1.92	0.51
1:IA:96:LEU:HD12	1:IA:167:VAL:HG22	1.92	0.51
1:WF:96:LEU:HD12	1:WF:167:VAL:HG22	1.92	0.51
1:ME:96:LEU:HD12	1:ME:167:VAL:HG22	1.92	0.51
1:CC:89:ARG:H	1:CC:174:GLU:HG2	1.75	0.50
1:RC:89:ARG:H	1:RC:174:GLU:HG2	1.75	0.50
1:XD:96:LEU:HD12	1:XD:167:VAL:HG22	1.92	0.50
1:HF:96:LEU:HD12	1:HF:167:VAL:HG22	1.92	0.50
1:EC:96:LEU:HD12	1:EC:167:VAL:HG22	1.92	0.50
1:TC:96:LEU:HD12	1:TC:167:VAL:HG22	1.92	0.50
1:AE:96:LEU:HD12	1:AE:167:VAL:HG22	1.92	0.50
1:PE:96:LEU:HD12	1:PE:167:VAL:HG22	1.92	0.50
1:SE:96:LEU:HD12	1:SE:167:VAL:HG22	1.92	0.50
1:VE:96:LEU:HD12	1:VE:167:VAL:HG22	1.92	0.50
1:KF:96:LEU:HD12	1:KF:167:VAL:HG22	1.92	0.50
1:G:96:LEU:HD12	1:G:167:VAL:HG22	1.92	0.50
1:HC:96:LEU:HD12	1:HC:167:VAL:HG22	1.92	0.50
1:LA:96:LEU:HD12	1:LA:167:VAL:HG22	1.92	0.50
1:DE:96:LEU:HD12	1:DE:167:VAL:HG22	1.92	0.50
1:WC:96:LEU:HD12	1:WC:167:VAL:HG22	1.92	0.50
1:K:89:ARG:HD2	1:K:136:MET:HE3	1.94	0.50
1:X:89:ARG:HD2	1:X:136:MET:HE3	1.94	0.50
1:CA:96:LEU:HD12	1:CA:167:VAL:HG22	1.92	0.50
1:DA:89:ARG:H	1:DA:174:GLU:HG2	1.75	0.50
1:DA:89:ARG:HD2	1:DA:136:MET:HE3	1.94	0.50
1:HB:89:ARG:HD2	1:HB:136:MET:HE3	1.94	0.50
1:KB:89:ARG:HD2	1:KB:136:MET:HE3	1.94	0.50
1:PB:96:LEU:HD12	1:PB:167:VAL:HG22	1.92	0.50
1:DD:89:ARG:HD2	1:DD:136:MET:HE3	1.94	0.50
1:YD:89:ARG:HD2	1:YD:136:MET:HE3	1.94	0.50
1:NE:89:ARG:HD2	1:NE:136:MET:HE3	1.94	0.50
1:PA:89:ARG:HD2	1:PA:136:MET:HE3	1.94	0.50
1:BB:89:ARG:HD2	1:BB:136:MET:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HB:89:ARG:H	1:HB:174:GLU:HG2	1.75	0.50
1:CC:89:ARG:HD2	1:CC:136:MET:HE3	1.94	0.50
1:LC:89:ARG:HD2	1:LC:136:MET:HE3	1.94	0.50
1:RC:89:ARG:HD2	1:RC:136:MET:HE3	1.94	0.50
1:ID:96:LEU:HD12	1:ID:167:VAL:HG22	1.92	0.50
1:EE:89:ARG:HD2	1:EE:136:MET:HE3	1.94	0.50
1:GB:96:LEU:HD12	1:GB:167:VAL:HG22	1.92	0.50
1:AD:89:ARG:HD2	1:AD:136:MET:HE3	1.94	0.50
1:TE:89:ARG:HD2	1:TE:136:MET:HE3	1.94	0.50
1:Q:89:ARG:HD2	1:Q:136:MET:HE3	1.94	0.49
1:T:89:ARG:HD2	1:T:136:MET:HE3	1.94	0.49
1:YA:89:ARG:HD2	1:YA:136:MET:HE3	1.94	0.49
1:FC:89:ARG:HD2	1:FC:136:MET:HE3	1.94	0.49
1:VA:89:ARG:HD2	1:VA:136:MET:HE3	1.94	0.49
1:UC:89:ARG:HD2	1:UC:136:MET:HE3	1.94	0.49
1:SD:89:ARG:HD2	1:SD:136:MET:HE3	1.94	0.49
1:HE:89:ARG:HD2	1:HE:136:MET:HE3	1.94	0.49
1:FF:89:ARG:HD2	1:FF:136:MET:HE3	1.94	0.49
1:UF:89:ARG:HD2	1:UF:136:MET:HE3	1.94	0.49
1:ZB:89:ARG:HD2	1:ZB:136:MET:HE3	1.94	0.49
1:OC:89:ARG:HD2	1:OC:136:MET:HE3	1.94	0.49
1:GD:89:ARG:HD2	1:GD:136:MET:HE3	1.94	0.49
1:H:89:ARG:HD2	1:H:136:MET:HE3	1.94	0.49
1:NB:89:ARG:HD2	1:NB:136:MET:HE3	1.94	0.49
1:MA:89:ARG:HD2	1:MA:136:MET:HE3	1.94	0.49
1:KE:89:ARG:HD2	1:KE:136:MET:HE3	1.94	0.49
1:GA:89:ARG:HD2	1:GA:136:MET:HE3	1.94	0.49
1:TB:89:ARG:HD2	1:TB:136:MET:HE3	1.94	0.49
1:VD:89:ARG:HD2	1:VD:136:MET:HE3	1.94	0.49
1:XF:89:ARG:HD2	1:XF:136:MET:HE3	1.94	0.49
1:B:89:ARG:HD2	1:B:136:MET:HE3	1.94	0.49
1:N:89:ARG:HD2	1:N:136:MET:HE3	1.94	0.49
1:MD:89:ARG:HD2	1:MD:136:MET:HE3	1.94	0.49
1:BE:89:ARG:HD2	1:BE:136:MET:HE3	1.94	0.49
1:IF:89:ARG:HD2	1:IF:136:MET:HE3	1.94	0.49
1:QE:89:ARG:HD2	1:QE:136:MET:HE3	1.94	0.49
1:SA:89:ARG:HD2	1:SA:136:MET:HE3	1.94	0.48
1:AA:89:ARG:HD2	1:AA:136:MET:HE3	1.94	0.48
1:P:74:PRO:HG2	1:P:77:LEU:HD12	1.96	0.48
1:W:74:PRO:HG2	1:W:77:LEU:HD12	1.96	0.48
1:Z:74:PRO:HG2	1:Z:77:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UA:74:PRO:HG2	1:UA:77:LEU:HD12	1.96	0.48
1:AB:74:PRO:HG2	1:AB:77:LEU:HD12	1.96	0.48
1:DB:74:PRO:HG2	1:DB:77:LEU:HD12	1.96	0.48
1:EB:89:ARG:HD2	1:EB:136:MET:HE3	1.94	0.48
1:QB:89:ARG:HD2	1:QB:136:MET:HE3	1.94	0.48
1:SB:74:PRO:HG2	1:SB:77:LEU:HD12	1.96	0.48
1:KC:74:PRO:HG2	1:KC:77:LEU:HD12	1.96	0.48
1:ZC:74:PRO:HG2	1:ZC:77:LEU:HD12	1.96	0.48
1:LD:74:PRO:HG2	1:LD:77:LEU:HD12	1.96	0.48
1:RD:74:PRO:HG2	1:RD:77:LEU:HD12	1.96	0.48
1:GE:74:PRO:HG2	1:GE:77:LEU:HD12	1.96	0.48
1:LF:89:ARG:HD2	1:LF:136:MET:HE3	1.94	0.48
1:RF:89:ARG:HD2	1:RF:136:MET:HE3	1.94	0.48
1:S:74:PRO:HG2	1:S:77:LEU:HD12	1.96	0.48
1:XA:74:PRO:HG2	1:XA:77:LEU:HD12	1.96	0.48
1:GB:74:PRO:HG2	1:GB:77:LEU:HD12	1.96	0.48
1:JD:89:ARG:HD2	1:JD:136:MET:HE3	1.94	0.48
1:XD:74:PRO:HG2	1:XD:77:LEU:HD12	1.96	0.48
1:WE:89:ARG:HD2	1:WE:136:MET:HE3	1.94	0.48
1:CF:89:ARG:HD2	1:CF:136:MET:HE3	1.94	0.48
1:CA:74:PRO:HG2	1:CA:77:LEU:HD12	1.96	0.48
1:XC:89:ARG:HD2	1:XC:136:MET:HE3	1.94	0.48
1:ME:74:PRO:HG2	1:ME:77:LEU:HD12	1.96	0.48
1:M:74:PRO:HG2	1:M:77:LEU:HD12	1.96	0.48
1:IC:89:ARG:HD2	1:IC:136:MET:HE3	1.94	0.48
1:JE:74:PRO:HG2	1:JE:77:LEU:HD12	1.96	0.48
1:ZE:89:ARG:HD2	1:ZE:136:MET:HE3	1.94	0.48
1:BF:74:PRO:HG2	1:BF:77:LEU:HD12	1.96	0.48
1:RA:74:PRO:HG2	1:RA:77:LEU:HD12	1.96	0.48
1:WB:89:ARG:HD2	1:WB:136:MET:HE3	1.94	0.48
1:PD:89:ARG:HD2	1:PD:136:MET:HE3	1.94	0.48
1:UD:74:PRO:HG2	1:UD:77:LEU:HD12	1.96	0.48
1:YE:74:PRO:HG2	1:YE:77:LEU:HD12	1.96	0.48
1:NF:74:PRO:HG2	1:NF:77:LEU:HD12	1.96	0.48
1:QF:74:PRO:HG2	1:QF:77:LEU:HD12	1.96	0.48
1:E:89:ARG:HD2	1:E:136:MET:HE3	1.94	0.48
1:JA:89:ARG:HD2	1:JA:136:MET:HE3	1.94	0.48
1:KF:74:PRO:HG2	1:KF:77:LEU:HD12	1.96	0.48
1:OF:89:ARG:HD2	1:OF:136:MET:HE3	1.94	0.48
1:J:74:PRO:HG2	1:J:77:LEU:HD12	1.96	0.48
1:VE:74:PRO:HG2	1:VE:77:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OA:74:PRO:HG2	1:OA:77:LEU:HD12	1.96	0.48
1:MB:74:PRO:HG2	1:MB:77:LEU:HD12	1.96	0.48
1:YB:74:PRO:HG2	1:YB:77:LEU:HD12	1.96	0.48
1:BC:74:PRO:HG2	1:BC:77:LEU:HD12	1.96	0.48
1:QC:74:PRO:HG2	1:QC:77:LEU:HD12	1.96	0.48
1:FD:74:PRO:HG2	1:FD:77:LEU:HD12	1.96	0.48
1:TF:74:PRO:HG2	1:TF:77:LEU:HD12	1.96	0.48
1:NC:74:PRO:HG2	1:NC:77:LEU:HD12	1.96	0.47
1:EF:74:PRO:HG2	1:EF:77:LEU:HD12	1.96	0.47
1:HF:74:PRO:HG2	1:HF:77:LEU:HD12	1.96	0.47
1:VA:139:ASP:OD1	1:VA:142:ARG:NE	2.45	0.47
1:ID:74:PRO:HG2	1:ID:77:LEU:HD12	1.96	0.47
1:WF:74:PRO:HG2	1:WF:77:LEU:HD12	1.96	0.47
1:EB:139:ASP:OD1	1:EB:142:ARG:NE	2.45	0.47
1:PB:74:PRO:HG2	1:PB:77:LEU:HD12	1.96	0.47
1:A:74:PRO:HG2	1:A:77:LEU:HD12	1.96	0.47
1:Q:139:ASP:OD1	1:Q:142:ARG:NE	2.45	0.47
1:AA:139:ASP:OD1	1:AA:142:ARG:NE	2.45	0.47
1:FA:74:PRO:HG2	1:FA:77:LEU:HD12	1.96	0.47
1:LA:74:PRO:HG2	1:LA:77:LEU:HD12	1.96	0.47
1:UB:92:LEU:HD22	1:UB:108:VAL:HG23	1.97	0.47
1:VB:74:PRO:HG2	1:VB:77:LEU:HD12	1.96	0.47
1:HC:74:PRO:HG2	1:HC:77:LEU:HD12	1.96	0.47
1:WC:74:PRO:HG2	1:WC:77:LEU:HD12	1.96	0.47
1:ND:92:LEU:HD22	1:ND:108:VAL:HG23	1.97	0.47
1:G:74:PRO:HG2	1:G:77:LEU:HD12	1.96	0.47
1:I:92:LEU:HD22	1:I:108:VAL:HG23	1.97	0.47
1:O:92:LEU:HD22	1:O:108:VAL:HG23	1.97	0.47
1:NA:92:LEU:HD22	1:NA:108:VAL:HG23	1.97	0.47
1:TA:92:LEU:HD22	1:TA:108:VAL:HG23	1.97	0.47
1:OD:74:PRO:HG2	1:OD:77:LEU:HD12	1.96	0.47
1:WD:92:LEU:HD22	1:WD:108:VAL:HG23	1.97	0.47
1:LE:92:LEU:HD22	1:LE:108:VAL:HG23	1.97	0.47
1:W:41:LYS:HA	1:W:41:LYS:NZ	2.30	0.47
1:AB:41:LYS:NZ	1:AB:41:LYS:HA	2.30	0.47
1:CD:74:PRO:HG2	1:CD:77:LEU:HD12	1.96	0.47
1:VE:41:LYS:HA	1:VE:41:LYS:NZ	2.30	0.47
1:XE:92:LEU:HD22	1:XE:108:VAL:HG23	1.97	0.47
1:KF:41:LYS:NZ	1:KF:41:LYS:HA	2.30	0.47
1:MF:92:LEU:HD22	1:MF:108:VAL:HG23	1.97	0.47
1:F:92:LEU:HD22	1:F:108:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:92:LEU:HD22	1:V:108:VAL:HG23	1.97	0.47
1:IA:74:PRO:HG2	1:IA:77:LEU:HD12	1.96	0.47
1:FD:41:LYS:HA	1:FD:41:LYS:NZ	2.30	0.47
1:AE:74:PRO:HG2	1:AE:77:LEU:HD12	1.96	0.47
1:CE:92:LEU:HD22	1:CE:108:VAL:HG23	1.97	0.47
1:FE:92:LEU:HD22	1:FE:108:VAL:HG23	1.97	0.47
1:QE:139:ASP:OD1	1:QE:142:ARG:NE	2.45	0.47
1:SE:74:PRO:HG2	1:SE:77:LEU:HD12	1.96	0.47
1:UE:92:LEU:HD22	1:UE:108:VAL:HG23	1.97	0.47
1:BF:41:LYS:HA	1:BF:41:LYS:NZ	2.30	0.47
1:QF:41:LYS:HA	1:QF:41:LYS:NZ	2.30	0.47
1:D:74:PRO:HG2	1:D:77:LEU:HD12	1.96	0.46
1:J:41:LYS:HA	1:J:41:LYS:NZ	2.30	0.46
1:R:92:LEU:HD22	1:R:108:VAL:HG23	1.97	0.46
1:KA:92:LEU:HD22	1:KA:108:VAL:HG23	1.97	0.46
1:ZA:92:LEU:HD22	1:ZA:108:VAL:HG23	1.97	0.46
1:JB:74:PRO:HG2	1:JB:77:LEU:HD12	1.96	0.46
1:MB:41:LYS:NZ	1:MB:41:LYS:HA	2.30	0.46
1:VB:41:LYS:HA	1:VB:41:LYS:NZ	2.30	0.46
1:EC:74:PRO:HG2	1:EC:77:LEU:HD12	1.96	0.46
1:OD:41:LYS:NZ	1:OD:41:LYS:HA	2.30	0.46
1:UD:41:LYS:HA	1:UD:41:LYS:NZ	2.30	0.46
1:JE:41:LYS:HA	1:JE:41:LYS:NZ	2.30	0.46
1:PE:74:PRO:HG2	1:PE:77:LEU:HD12	1.96	0.46
1:RE:92:LEU:HD22	1:RE:108:VAL:HG23	1.97	0.46
1:SE:41:LYS:NZ	1:SE:41:LYS:HA	2.30	0.46
1:A:41:LYS:HA	1:A:41:LYS:NZ	2.30	0.46
1:P:41:LYS:NZ	1:P:41:LYS:HA	2.30	0.46
1:CA:41:LYS:HA	1:CA:41:LYS:NZ	2.30	0.46
1:FA:41:LYS:NZ	1:FA:41:LYS:HA	2.30	0.46
1:OA:41:LYS:HA	1:OA:41:LYS:NZ	2.30	0.46
1:WA:92:LEU:HD22	1:WA:108:VAL:HG23	1.97	0.46
1:GB:41:LYS:HA	1:GB:41:LYS:NZ	2.30	0.46
1:KC:41:LYS:NZ	1:KC:41:LYS:HA	2.30	0.46
1:TC:74:PRO:HG2	1:TC:77:LEU:HD12	1.96	0.46
1:BE:139:ASP:OD1	1:BE:142:ARG:NE	2.45	0.46
1:DE:41:LYS:NZ	1:DE:41:LYS:HA	2.30	0.46
1:DE:74:PRO:HG2	1:DE:77:LEU:HD12	1.96	0.46
1:UA:41:LYS:NZ	1:UA:41:LYS:HA	2.30	0.46
1:ZC:41:LYS:HA	1:ZC:41:LYS:NZ	2.30	0.46
1:TD:92:LEU:HD22	1:TD:108:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XD:41:LYS:NZ	1:XD:41:LYS:HA	2.30	0.46
1:IE:92:LEU:HD22	1:IE:108:VAL:HG23	1.97	0.46
1:ME:41:LYS:HA	1:ME:41:LYS:NZ	2.30	0.46
1:YE:41:LYS:HA	1:YE:41:LYS:NZ	2.30	0.46
1:NF:41:LYS:NZ	1:NF:41:LYS:HA	2.30	0.46
1:YF:92:LEU:HD22	1:YF:108:VAL:HG23	1.97	0.46
1:OB:92:LEU:HD22	1:OB:108:VAL:HG23	1.97	0.46
1:GC:92:LEU:HD22	1:GC:108:VAL:HG23	1.97	0.46
1:HC:41:LYS:NZ	1:HC:41:LYS:HA	2.30	0.46
1:HF:41:LYS:NZ	1:HF:41:LYS:HA	2.30	0.46
1:JF:92:LEU:HD22	1:JF:108:VAL:HG23	1.97	0.46
1:WF:41:LYS:NZ	1:WF:41:LYS:HA	2.30	0.46
1:M:41:LYS:HA	1:M:41:LYS:NZ	2.30	0.46
1:Z:41:LYS:NZ	1:Z:41:LYS:HA	2.30	0.46
1:RA:41:LYS:HA	1:RA:41:LYS:NZ	2.30	0.46
1:DB:41:LYS:NZ	1:DB:41:LYS:HA	2.30	0.46
1:VC:92:LEU:HD22	1:VC:108:VAL:HG23	1.97	0.46
1:WC:41:LYS:NZ	1:WC:41:LYS:HA	2.30	0.46
1:HD:92:LEU:HD22	1:HD:108:VAL:HG23	1.97	0.46
1:GF:92:LEU:HD22	1:GF:108:VAL:HG23	1.97	0.46
1:VF:92:LEU:HD22	1:VF:108:VAL:HG23	1.97	0.46
1:PB:41:LYS:NZ	1:PB:41:LYS:HA	2.30	0.46
1:SB:41:LYS:HA	1:SB:41:LYS:NZ	2.30	0.46
1:YB:41:LYS:NZ	1:YB:41:LYS:HA	2.30	0.46
1:AC:92:LEU:HD22	1:AC:108:VAL:HG23	1.97	0.46
1:DC:92:LEU:HD22	1:DC:108:VAL:HG23	1.97	0.46
1:JC:92:LEU:HD22	1:JC:108:VAL:HG23	1.97	0.46
1:NC:41:LYS:HA	1:NC:41:LYS:NZ	2.30	0.46
1:PC:92:LEU:HD22	1:PC:108:VAL:HG23	1.97	0.46
1:QC:41:LYS:NZ	1:QC:41:LYS:HA	2.30	0.46
1:SC:92:LEU:HD22	1:SC:108:VAL:HG23	1.97	0.46
1:YC:92:LEU:HD22	1:YC:108:VAL:HG23	1.97	0.46
1:ID:41:LYS:NZ	1:ID:41:LYS:HA	2.30	0.46
1:LD:41:LYS:NZ	1:LD:41:LYS:HA	2.30	0.46
1:TE:112:GLN:HG3	1:TE:118:ALA:HB2	1.98	0.46
1:L:92:LEU:HD22	1:L:108:VAL:HG23	1.97	0.46
1:MA:139:ASP:OD1	1:MA:142:ARG:NE	2.45	0.46
1:QA:92:LEU:HD22	1:QA:108:VAL:HG23	1.97	0.46
1:BC:41:LYS:HA	1:BC:41:LYS:NZ	2.30	0.46
1:LC:112:GLN:HG3	1:LC:118:ALA:HB2	1.98	0.46
1:AD:112:GLN:HG3	1:AD:118:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:41:LYS:HA	1:AE:41:LYS:NZ	2.30	0.46
1:EE:112:GLN:HG3	1:EE:118:ALA:HB2	1.98	0.46
1:PE:41:LYS:NZ	1:PE:41:LYS:HA	2.30	0.46
1:VE:130:LYS:HE2	1:VE:130:LYS:HB3	1.80	0.46
1:H:139:ASP:OD1	1:H:142:ARG:NE	2.45	0.46
1:BA:92:LEU:HD22	1:BA:108:VAL:HG23	1.97	0.46
1:RB:92:LEU:HD22	1:RB:108:VAL:HG23	1.97	0.46
1:CC:112:GLN:HG3	1:CC:118:ALA:HB2	1.98	0.46
1:RC:112:GLN:HG3	1:RC:118:ALA:HB2	1.98	0.46
1:HE:139:ASP:OD1	1:HE:142:ARG:NE	2.45	0.46
1:B:112:GLN:HG3	1:B:118:ALA:HB2	1.98	0.46
1:C:92:LEU:HD22	1:C:108:VAL:HG23	1.97	0.46
1:G:41:LYS:NZ	1:G:41:LYS:HA	2.30	0.46
1:N:139:ASP:OD1	1:N:142:ARG:NE	2.45	0.46
1:Y:92:LEU:HD22	1:Y:108:VAL:HG23	1.97	0.46
1:LA:41:LYS:NZ	1:LA:41:LYS:HA	2.30	0.46
1:CB:92:LEU:HD22	1:CB:108:VAL:HG23	1.97	0.46
1:FB:92:LEU:HD22	1:FB:108:VAL:HG23	1.97	0.46
1:XB:92:LEU:HD22	1:XB:108:VAL:HG23	1.97	0.46
1:KD:92:LEU:HD22	1:KD:108:VAL:HG23	1.97	0.46
1:YD:112:GLN:HG3	1:YD:118:ALA:HB2	1.98	0.46
1:NE:112:GLN:HG3	1:NE:118:ALA:HB2	1.98	0.46
1:DA:112:GLN:HG3	1:DA:118:ALA:HB2	1.98	0.45
1:HA:92:LEU:HD22	1:HA:108:VAL:HG23	1.97	0.45
1:JB:41:LYS:HA	1:JB:41:LYS:NZ	2.30	0.45
1:TC:41:LYS:NZ	1:TC:41:LYS:HA	2.30	0.45
1:CD:41:LYS:NZ	1:CD:41:LYS:HA	2.30	0.45
1:QD:92:LEU:HD22	1:QD:108:VAL:HG23	1.97	0.45
1:KF:130:LYS:HE2	1:KF:130:LYS:HB3	1.80	0.45
1:S:41:LYS:NZ	1:S:41:LYS:HA	2.30	0.45
1:GA:112:GLN:HG3	1:GA:118:ALA:HB2	1.98	0.45
1:MA:112:GLN:HG3	1:MA:118:ALA:HB2	1.98	0.45
1:SA:139:ASP:OD1	1:SA:142:ARG:NE	2.45	0.45
1:XA:41:LYS:NZ	1:XA:41:LYS:HA	2.30	0.45
1:HB:112:GLN:HG3	1:HB:118:ALA:HB2	1.98	0.45
1:SB:130:LYS:HE2	1:SB:130:LYS:HB3	1.80	0.45
1:EC:41:LYS:NZ	1:EC:41:LYS:HA	2.30	0.45
1:VD:112:GLN:HG3	1:VD:118:ALA:HB2	1.98	0.45
1:KE:112:GLN:HG3	1:KE:118:ALA:HB2	1.98	0.45
1:AF:92:LEU:HD22	1:AF:108:VAL:HG23	1.97	0.45
1:PF:92:LEU:HD22	1:PF:108:VAL:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:112:GLN:HG3	1:H:118:ALA:HB2	1.98	0.45
1:T:112:GLN:HG3	1:T:118:ALA:HB2	1.98	0.45
1:QB:112:GLN:HG3	1:QB:118:ALA:HB2	1.98	0.45
1:XC:112:GLN:HG3	1:XC:118:ALA:HB2	1.98	0.45
1:DD:112:GLN:HG3	1:DD:118:ALA:HB2	1.98	0.45
1:RD:41:LYS:HA	1:RD:41:LYS:NZ	2.30	0.45
1:EF:41:LYS:HA	1:EF:41:LYS:NZ	2.30	0.45
1:TF:41:LYS:NZ	1:TF:41:LYS:HA	2.30	0.45
1:AA:112:GLN:HG3	1:AA:118:ALA:HB2	1.98	0.45
1:EA:92:LEU:HD22	1:EA:108:VAL:HG23	1.97	0.45
1:YA:112:GLN:HG3	1:YA:118:ALA:HB2	1.98	0.45
1:EB:112:GLN:HG3	1:EB:118:ALA:HB2	1.98	0.45
1:KB:112:GLN:HG3	1:KB:118:ALA:HB2	1.98	0.45
1:IC:112:GLN:HG3	1:IC:118:ALA:HB2	1.98	0.45
1:JD:112:GLN:HG3	1:JD:118:ALA:HB2	1.98	0.45
1:GE:41:LYS:NZ	1:GE:41:LYS:HA	2.30	0.45
1:LF:112:GLN:HG3	1:LF:118:ALA:HB2	1.98	0.45
1:NF:130:LYS:HE2	1:NF:130:LYS:HB3	1.80	0.45
1:OF:112:GLN:HG3	1:OF:118:ALA:HB2	1.98	0.45
1:IA:41:LYS:NZ	1:IA:41:LYS:HA	2.30	0.45
1:IB:92:LEU:HD22	1:IB:108:VAL:HG23	1.97	0.45
1:KB:139:ASP:OD1	1:KB:142:ARG:NE	2.45	0.45
1:DD:139:ASP:OD1	1:DD:142:ARG:NE	2.45	0.45
1:ZD:92:LEU:HD22	1:ZD:108:VAL:HG23	1.97	0.45
1:WE:112:GLN:HG3	1:WE:118:ALA:HB2	1.98	0.45
1:IF:112:GLN:HG3	1:IF:118:ALA:HB2	1.98	0.45
1:OF:139:ASP:OD1	1:OF:142:ARG:NE	2.45	0.45
1:XF:112:GLN:HG3	1:XF:118:ALA:HB2	1.98	0.45
1:I:43:ILE:HB	1:WD:184:PHE:HB2	1.99	0.45
1:O:184:PHE:HB2	1:YC:43:ILE:HB	1.99	0.45
1:NA:43:ILE:HB	1:LE:184:PHE:HB2	1.99	0.45
1:TA:184:PHE:HB2	1:JC:43:ILE:HB	1.99	0.45
1:OE:92:LEU:HD22	1:OE:108:VAL:HG23	1.97	0.45
1:XE:43:ILE:HB	1:MF:184:PHE:HB2	1.99	0.45
1:XE:184:PHE:HB2	1:MF:43:ILE:HB	1.99	0.45
1:ZE:112:GLN:HG3	1:ZE:118:ALA:HB2	1.98	0.45
1:D:41:LYS:NZ	1:D:41:LYS:HA	2.30	0.45
1:L:184:PHE:HB2	1:UE:43:ILE:HB	1.99	0.45
1:Y:43:ILE:HB	1:PF:184:PHE:HB2	1.99	0.45
1:QA:184:PHE:HB2	1:FE:43:ILE:HB	1.99	0.45
1:CB:43:ILE:HB	1:AF:184:PHE:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LB:92:LEU:HD22	1:LB:108:VAL:HG23	1.97	0.45
1:WB:112:GLN:HG3	1:WB:118:ALA:HB2	1.98	0.45
1:ZB:112:GLN:HG3	1:ZB:118:ALA:HB2	1.98	0.45
1:MD:112:GLN:HG3	1:MD:118:ALA:HB2	1.98	0.45
1:C:184:PHE:HB2	1:R:43:ILE:HB	1.99	0.45
1:V:43:ILE:HB	1:VC:184:PHE:HB2	1.99	0.45
1:X:112:GLN:HG3	1:X:118:ALA:HB2	1.98	0.45
1:EA:184:PHE:HB2	1:UB:43:ILE:HB	1.99	0.45
1:HA:184:PHE:HB2	1:WA:43:ILE:HB	1.99	0.45
1:TB:112:GLN:HG3	1:TB:118:ALA:HB2	1.98	0.45
1:XB:184:PHE:HB2	1:GF:43:ILE:HB	1.99	0.45
1:AC:96:LEU:HD12	1:AC:100:VAL:HG21	1.99	0.45
1:DC:43:ILE:HB	1:DF:184:PHE:HB2	1.99	0.45
1:FC:139:ASP:OD1	1:FC:142:ARG:NE	2.45	0.45
1:OC:112:GLN:HG3	1:OC:118:ALA:HB2	1.98	0.45
1:PC:96:LEU:HD12	1:PC:100:VAL:HG21	1.99	0.45
1:SC:43:ILE:HB	1:SF:184:PHE:HB2	1.99	0.45
1:YC:96:LEU:HD12	1:YC:100:VAL:HG21	1.99	0.45
1:BD:92:LEU:HD22	1:BD:108:VAL:HG23	1.97	0.45
1:ED:92:LEU:HD22	1:ED:108:VAL:HG23	1.97	0.45
1:PD:112:GLN:HG3	1:PD:118:ALA:HB2	1.98	0.45
1:TD:96:LEU:HD12	1:TD:100:VAL:HG21	1.99	0.45
1:IE:96:LEU:HD12	1:IE:100:VAL:HG21	1.99	0.45
1:ZE:139:ASP:OD1	1:ZE:142:ARG:NE	2.45	0.45
1:F:184:PHE:HB2	1:RB:43:ILE:HB	1.99	0.45
1:I:184:PHE:HB2	1:WD:43:ILE:HB	1.99	0.45
1:N:112:GLN:HG3	1:N:118:ALA:HB2	1.98	0.45
1:V:96:LEU:HD12	1:V:100:VAL:HG21	1.99	0.45
1:EA:96:LEU:HD12	1:EA:100:VAL:HG21	1.99	0.45
1:KA:184:PHE:HB2	1:KD:43:ILE:HB	1.99	0.45
1:YA:139:ASP:OD1	1:YA:142:ARG:NE	2.45	0.45
1:ZA:43:ILE:HB	1:GC:184:PHE:HB2	1.99	0.45
1:BB:112:GLN:HG3	1:BB:118:ALA:HB2	1.98	0.45
1:IB:184:PHE:HB2	1:ND:43:ILE:HB	1.99	0.45
1:KB:29:PRO:HB2	1:AC:27:VAL:HG13	1.99	0.45
1:JC:96:LEU:HD12	1:JC:100:VAL:HG21	1.99	0.45
1:MC:92:LEU:HD22	1:MC:108:VAL:HG23	1.97	0.45
1:PC:27:VAL:HG13	1:DD:29:PRO:HB2	1.99	0.45
1:UC:112:GLN:HG3	1:UC:118:ALA:HB2	1.98	0.45
1:LD:130:LYS:HE2	1:LD:130:LYS:HB3	1.80	0.45
1:QD:184:PHE:HB2	1:VF:43:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UE:96:LEU:HD12	1:UE:100:VAL:HG21	1.99	0.45
1:DF:96:LEU:HD12	1:DF:100:VAL:HG21	1.99	0.45
1:SF:96:LEU:HD12	1:SF:100:VAL:HG21	1.99	0.45
1:O:43:ILE:HB	1:YC:184:PHE:HB2	1.99	0.45
1:JA:112:GLN:HG3	1:JA:118:ALA:HB2	1.98	0.45
1:NA:184:PHE:HB2	1:LE:43:ILE:HB	1.99	0.45
1:TA:43:ILE:HB	1:JC:184:PHE:HB2	1.99	0.45
1:ZA:96:LEU:HD12	1:ZA:100:VAL:HG21	1.99	0.45
1:IB:96:LEU:HD12	1:IB:100:VAL:HG21	1.99	0.45
1:NB:29:PRO:HB2	1:ZD:27:VAL:HG13	1.99	0.45
1:NB:139:ASP:OD1	1:NB:142:ARG:NE	2.45	0.45
1:OB:27:VAL:HG13	1:YD:29:PRO:HB2	1.99	0.45
1:WB:29:PRO:HB2	1:GF:27:VAL:HG13	1.99	0.45
1:CC:139:ASP:OD1	1:CC:142:ARG:NE	2.45	0.45
1:DC:27:VAL:HG13	1:CF:29:PRO:HB2	1.99	0.45
1:DC:184:PHE:HB2	1:DF:43:ILE:HB	1.99	0.45
1:FC:112:GLN:HG3	1:FC:118:ALA:HB2	1.98	0.45
1:MC:27:VAL:HG13	1:BE:29:PRO:HB2	1.99	0.45
1:SC:27:VAL:HG13	1:RF:29:PRO:HB2	1.99	0.45
1:SC:96:LEU:HD12	1:SC:100:VAL:HG21	1.99	0.45
1:UC:139:ASP:OD1	1:UC:142:ARG:NE	2.45	0.45
1:BD:27:VAL:HG13	1:QE:29:PRO:HB2	1.99	0.45
1:BD:43:ILE:HB	1:RE:184:PHE:HB2	1.99	0.45
1:GD:29:PRO:HB2	1:OE:27:VAL:HG13	1.99	0.45
1:GD:139:ASP:OD1	1:GD:142:ARG:NE	2.45	0.45
1:HD:27:VAL:HG13	1:NE:29:PRO:HB2	1.99	0.45
1:PD:29:PRO:HB2	1:VF:27:VAL:HG13	1.99	0.45
1:QD:27:VAL:HG13	1:UF:29:PRO:HB2	1.99	0.45
1:FE:96:LEU:HD12	1:FE:100:VAL:HG21	1.99	0.45
1:Q:112:GLN:HG3	1:Q:118:ALA:HB2	1.98	0.44
1:T:29:PRO:HB2	1:VC:27:VAL:HG13	1.99	0.44
1:PA:29:PRO:HB2	1:FE:27:VAL:HG13	1.99	0.44
1:SA:112:GLN:HG3	1:SA:118:ALA:HB2	1.98	0.44
1:YA:29:PRO:HB2	1:GC:27:VAL:HG13	1.99	0.44
1:XB:27:VAL:HG13	1:FF:29:PRO:HB2	1.99	0.44
1:DC:96:LEU:HD12	1:DC:100:VAL:HG21	1.99	0.44
1:LC:29:PRO:HB2	1:CE:27:VAL:HG13	1.99	0.44
1:MC:43:ILE:HB	1:CE:184:PHE:HB2	1.99	0.44
1:RC:139:ASP:OD1	1:RC:142:ARG:NE	2.45	0.44
1:SC:184:PHE:HB2	1:SF:43:ILE:HB	1.99	0.44
1:ZC:130:LYS:HE2	1:ZC:130:LYS:HB3	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:29:PRO:HB2	1:RE:27:VAL:HG13	1.99	0.44
1:ND:96:LEU:HD12	1:ND:100:VAL:HG21	1.99	0.44
1:TD:184:PHE:HB2	1:IE:43:ILE:HB	1.99	0.44
1:YE:130:LYS:HE2	1:YE:130:LYS:HB3	1.80	0.44
1:CF:112:GLN:HG3	1:CF:118:ALA:HB2	1.98	0.44
1:JF:96:LEU:HD12	1:JF:100:VAL:HG21	1.99	0.44
1:RF:112:GLN:HG3	1:RF:118:ALA:HB2	1.98	0.44
1:YF:96:LEU:HD12	1:YF:100:VAL:HG21	1.99	0.44
1:A:130:LYS:HE2	1:A:130:LYS:HB3	1.80	0.44
1:E:112:GLN:HG3	1:E:118:ALA:HB2	1.98	0.44
1:K:29:PRO:HB2	1:UE:27:VAL:HG13	1.99	0.44
1:GA:139:ASP:OD1	1:GA:142:ARG:NE	2.45	0.44
1:VA:112:GLN:HG3	1:VA:118:ALA:HB2	1.98	0.44
1:TD:43:ILE:HB	1:IE:184:PHE:HB2	1.99	0.44
1:QE:112:GLN:HG3	1:QE:118:ALA:HB2	1.98	0.44
1:XE:96:LEU:HD12	1:XE:100:VAL:HG21	1.99	0.44
1:MF:96:LEU:HD12	1:MF:100:VAL:HG21	1.99	0.44
1:C:96:LEU:HD12	1:C:100:VAL:HG21	1.99	0.44
1:F:96:LEU:HD12	1:F:100:VAL:HG21	1.99	0.44
1:T:139:ASP:OD1	1:T:142:ARG:NE	2.45	0.44
1:KA:96:LEU:HD12	1:KA:100:VAL:HG21	1.99	0.44
1:PA:112:GLN:HG3	1:PA:118:ALA:HB2	1.98	0.44
1:UB:96:LEU:HD12	1:UB:100:VAL:HG21	1.99	0.44
1:XB:96:LEU:HD12	1:XB:100:VAL:HG21	1.99	0.44
1:ND:97:LEU:HB2	1:ND:100:VAL:HG13	2.00	0.44
1:BE:112:GLN:HG3	1:BE:118:ALA:HB2	1.98	0.44
1:WE:29:PRO:HB2	1:MF:27:VAL:HG13	1.99	0.44
1:CF:139:ASP:OD1	1:CF:142:ARG:NE	2.45	0.44
1:K:112:GLN:HG3	1:K:118:ALA:HB2	1.98	0.44
1:HA:96:LEU:HD12	1:HA:100:VAL:HG21	1.99	0.44
1:QA:96:LEU:HD12	1:QA:100:VAL:HG21	1.99	0.44
1:UB:97:LEU:HB2	1:UB:100:VAL:HG13	2.00	0.44
1:ZB:139:ASP:OD1	1:ZB:142:ARG:NE	2.45	0.44
1:JC:97:LEU:HB2	1:JC:100:VAL:HG13	2.00	0.44
1:YC:97:LEU:HB2	1:YC:100:VAL:HG13	2.00	0.44
1:ND:76:GLU:HG2	1:ND:77:LEU:HG	2.00	0.44
1:OD:130:LYS:HE2	1:OD:130:LYS:HB3	1.80	0.44
1:QD:96:LEU:HD12	1:QD:100:VAL:HG21	1.99	0.44
1:WD:97:LEU:HB2	1:WD:100:VAL:HG13	2.00	0.44
1:EE:139:ASP:OD1	1:EE:142:ARG:NE	2.45	0.44
1:LE:97:LEU:HB2	1:LE:100:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XE:27:VAL:HG13	1:LF:29:PRO:HB2	1.99	0.44
1:FF:112:GLN:HG3	1:FF:118:ALA:HB2	1.98	0.44
1:GF:96:LEU:HD12	1:GF:100:VAL:HG21	1.99	0.44
1:UF:112:GLN:HG3	1:UF:118:ALA:HB2	1.98	0.44
1:B:139:ASP:OD1	1:B:142:ARG:NE	2.45	0.44
1:L:96:LEU:HD12	1:L:100:VAL:HG21	1.99	0.44
1:EA:27:VAL:HG13	1:TB:29:PRO:HB2	1.99	0.44
1:JA:139:ASP:OD1	1:JA:142:ARG:NE	2.45	0.44
1:IB:97:LEU:HB2	1:IB:100:VAL:HG13	2.00	0.44
1:RB:96:LEU:HD12	1:RB:100:VAL:HG21	1.99	0.44
1:UB:76:GLU:HG2	1:UB:77:LEU:HG	2.00	0.44
1:CC:29:PRO:HB2	1:DF:27:VAL:HG13	1.99	0.44
1:OC:29:PRO:HB2	1:ED:27:VAL:HG13	1.99	0.44
1:BD:76:GLU:HG2	1:BD:77:LEU:HG	2.00	0.44
1:KD:96:LEU:HD12	1:KD:100:VAL:HG21	1.99	0.44
1:AF:76:GLU:HG2	1:AF:77:LEU:HG	2.00	0.44
1:PF:76:GLU:HG2	1:PF:77:LEU:HG	2.00	0.44
1:SF:92:LEU:HD22	1:SF:108:VAL:HG23	1.97	0.44
1:VF:96:LEU:HD12	1:VF:100:VAL:HG21	1.99	0.44
1:B:29:PRO:HB2	1:R:27:VAL:HG13	1.99	0.44
1:B:93:TRP:CE3	1:D:189:LYS:HE3	2.53	0.44
1:V:76:GLU:HG2	1:V:77:LEU:HG	2.00	0.44
1:EA:97:LEU:HB2	1:EA:100:VAL:HG13	2.00	0.44
1:GA:29:PRO:HB2	1:WA:27:VAL:HG13	1.99	0.44
1:GA:93:TRP:CE3	1:IA:189:LYS:HE3	2.53	0.44
1:FB:184:PHE:HB2	1:YF:43:ILE:HB	1.99	0.44
1:IB:27:VAL:HG13	1:MD:29:PRO:HB2	1.99	0.44
1:LB:27:VAL:HG13	1:ZB:29:PRO:HB2	1.99	0.44
1:LB:96:LEU:HD12	1:LB:100:VAL:HG21	1.99	0.44
1:OB:43:ILE:HB	1:ZD:184:PHE:HB2	1.99	0.44
1:OB:96:LEU:HD12	1:OB:100:VAL:HG21	1.99	0.44
1:RB:97:LEU:HB2	1:RB:100:VAL:HG13	2.00	0.44
1:XB:76:GLU:HG2	1:XB:77:LEU:HG	2.00	0.44
1:MC:76:GLU:HG2	1:MC:77:LEU:HG	2.00	0.44
1:RC:29:PRO:HB2	1:SF:27:VAL:HG13	1.99	0.44
1:HD:43:ILE:HB	1:OE:184:PHE:HB2	1.99	0.44
1:KD:97:LEU:HB2	1:KD:100:VAL:HG13	2.00	0.44
1:QD:76:GLU:HG2	1:QD:77:LEU:HG	2.00	0.44
1:SD:112:GLN:HG3	1:SD:118:ALA:HB2	1.98	0.44
1:ZD:76:GLU:HG2	1:ZD:77:LEU:HG	2.00	0.44
1:OE:76:GLU:HG2	1:OE:77:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AF:97:LEU:HB2	1:AF:100:VAL:HG13	2.00	0.44
1:RF:139:ASP:OD1	1:RF:142:ARG:NE	2.45	0.44
1:O:97:LEU:HB2	1:O:100:VAL:HG13	2.00	0.44
1:R:97:LEU:HB2	1:R:100:VAL:HG13	2.00	0.44
1:Y:184:PHE:HB2	1:PF:43:ILE:HB	1.99	0.44
1:BA:184:PHE:HB2	1:JF:43:ILE:HB	1.99	0.44
1:MA:93:TRP:CE3	1:OA:189:LYS:HE3	2.53	0.44
1:NA:96:LEU:HD12	1:NA:100:VAL:HG21	1.99	0.44
1:QA:43:ILE:HB	1:FE:184:PHE:HB2	1.99	0.44
1:TA:97:LEU:HB2	1:TA:100:VAL:HG13	2.00	0.44
1:ZA:76:GLU:HG2	1:ZA:77:LEU:HG	2.00	0.44
1:CB:184:PHE:HB2	1:AF:43:ILE:HB	1.99	0.44
1:FC:93:TRP:CE3	1:HC:189:LYS:HE3	2.53	0.44
1:JC:76:GLU:HG2	1:JC:77:LEU:HG	2.00	0.44
1:KC:130:LYS:HE2	1:KC:130:LYS:HB3	1.80	0.44
1:OC:139:ASP:OD1	1:OC:142:ARG:NE	2.45	0.44
1:UC:93:TRP:CE3	1:WC:189:LYS:HE3	2.53	0.44
1:YC:76:GLU:HG2	1:YC:77:LEU:HG	2.00	0.44
1:ED:96:LEU:HD12	1:ED:100:VAL:HG21	1.99	0.44
1:HD:96:LEU:HD12	1:HD:100:VAL:HG21	1.99	0.44
1:YD:93:TRP:CE3	1:AE:189:LYS:HE3	2.53	0.44
1:TE:139:ASP:OD1	1:TE:142:ARG:NE	2.45	0.44
1:DF:76:GLU:HG2	1:DF:77:LEU:HG	2.00	0.44
1:DF:92:LEU:HD22	1:DF:108:VAL:HG23	1.97	0.44
1:PF:97:LEU:HB2	1:PF:100:VAL:HG13	2.00	0.44
1:SF:76:GLU:HG2	1:SF:77:LEU:HG	2.00	0.44
1:E:139:ASP:OD1	1:E:142:ARG:NE	2.45	0.44
1:H:93:TRP:CE3	1:J:189:LYS:HE3	2.53	0.44
1:I:27:VAL:HG13	1:VD:29:PRO:HB2	1.99	0.44
1:I:96:LEU:HD12	1:I:100:VAL:HG21	1.99	0.44
1:L:43:ILE:HB	1:UE:184:PHE:HB2	1.99	0.44
1:R:96:LEU:HD12	1:R:100:VAL:HG21	1.99	0.44
1:V:97:LEU:HB2	1:V:100:VAL:HG13	2.00	0.44
1:Y:97:LEU:HB2	1:Y:100:VAL:HG13	2.00	0.44
1:BA:27:VAL:HG13	1:IF:29:PRO:HB2	1.99	0.44
1:BA:43:ILE:HB	1:JF:184:PHE:HB2	1.99	0.44
1:BA:97:LEU:HB2	1:BA:100:VAL:HG13	2.00	0.44
1:FA:130:LYS:HE2	1:FA:130:LYS:HB3	1.80	0.44
1:NA:27:VAL:HG13	1:KE:29:PRO:HB2	1.99	0.44
1:WA:96:LEU:HD12	1:WA:100:VAL:HG21	1.99	0.44
1:WA:97:LEU:HB2	1:WA:100:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CB:97:LEU:HB2	1:CB:100:VAL:HG13	2.00	0.44
1:FB:43:ILE:HB	1:YF:184:PHE:HB2	1.99	0.44
1:LB:43:ILE:HB	1:AC:184:PHE:HB2	1.99	0.44
1:LB:97:LEU:HB2	1:LB:100:VAL:HG13	2.00	0.44
1:NB:112:GLN:HG3	1:NB:118:ALA:HB2	1.98	0.44
1:OB:184:PHE:HB2	1:ZD:43:ILE:HB	1.99	0.44
1:SB:123:LEU:HD12	1:SB:140:ALA:HB2	2.00	0.44
1:ED:97:LEU:HB2	1:ED:100:VAL:HG13	2.00	0.44
1:GD:112:GLN:HG3	1:GD:118:ALA:HB2	1.98	0.44
1:HD:184:PHE:HB2	1:OE:43:ILE:HB	1.99	0.44
1:LD:123:LEU:HD12	1:LD:140:ALA:HB2	2.00	0.44
1:SD:29:PRO:HB2	1:IE:27:VAL:HG13	1.99	0.44
1:UD:123:LEU:HD12	1:UD:140:ALA:HB2	2.00	0.44
1:FE:76:GLU:HG2	1:FE:77:LEU:HG	2.00	0.44
1:HE:112:GLN:HG3	1:HE:118:ALA:HB2	1.98	0.44
1:JE:123:LEU:HD12	1:JE:140:ALA:HB2	2.00	0.44
1:NE:93:TRP:CE3	1:PE:189:LYS:HE3	2.53	0.44
1:UE:76:GLU:HG2	1:UE:77:LEU:HG	2.00	0.44
1:CF:182:ASP:OD1	1:CF:182:ASP:N	2.46	0.44
1:V:184:PHE:HB2	1:VC:43:ILE:HB	1.99	0.44
1:FA:123:LEU:HD12	1:FA:140:ALA:HB2	2.00	0.44
1:ZA:97:LEU:HB2	1:ZA:100:VAL:HG13	2.00	0.44
1:FB:27:VAL:HG13	1:XF:29:PRO:HB2	1.99	0.44
1:FB:97:LEU:HB2	1:FB:100:VAL:HG13	2.00	0.44
1:KB:93:TRP:CE3	1:MB:189:LYS:HE3	2.53	0.44
1:QB:139:ASP:OD1	1:QB:142:ARG:NE	2.45	0.44
1:CC:93:TRP:CE3	1:EC:189:LYS:HE3	2.53	0.44
1:DC:97:LEU:HB2	1:DC:100:VAL:HG13	2.00	0.44
1:PC:184:PHE:HB2	1:ED:43:ILE:HB	1.99	0.44
1:VC:96:LEU:HD12	1:VC:100:VAL:HG21	1.99	0.44
1:TD:27:VAL:HG13	1:HE:29:PRO:HB2	1.99	0.44
1:TD:76:GLU:HG2	1:TD:77:LEU:HG	2.00	0.44
1:JF:97:LEU:HB2	1:JF:100:VAL:HG13	2.00	0.44
1:VF:97:LEU:HB2	1:VF:100:VAL:HG13	2.00	0.44
1:YF:97:LEU:HB2	1:YF:100:VAL:HG13	2.00	0.44
1:A:123:LEU:HD12	1:A:140:ALA:HB2	2.00	0.43
1:L:27:VAL:HG13	1:TE:29:PRO:HB2	1.99	0.43
1:R:76:GLU:HG2	1:R:77:LEU:HG	2.00	0.43
1:Y:27:VAL:HG13	1:OF:29:PRO:HB2	1.99	0.43
1:DA:29:PRO:HB2	1:UB:27:VAL:HG13	1.99	0.43
1:PA:93:TRP:CE3	1:RA:189:LYS:HE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:27:VAL:HG13	1:EE:29:PRO:HB2	1.99	0.43
1:ZA:184:PHE:HB2	1:GC:43:ILE:HB	1.99	0.43
1:BB:139:ASP:OD1	1:BB:142:ARG:NE	2.45	0.43
1:YB:130:LYS:HE2	1:YB:130:LYS:HB3	1.80	0.43
1:MC:96:LEU:HD12	1:MC:100:VAL:HG21	1.99	0.43
1:RC:93:TRP:CE3	1:TC:189:LYS:HE3	2.53	0.43
1:SC:97:LEU:HB2	1:SC:100:VAL:HG13	2.00	0.43
1:BD:96:LEU:HD12	1:BD:100:VAL:HG21	1.99	0.43
1:DD:93:TRP:CE3	1:FD:189:LYS:HE3	2.53	0.43
1:RD:189:LYS:HE3	1:EE:93:TRP:CE3	2.53	0.43
1:XD:123:LEU:HD12	1:XD:140:ALA:HB2	2.00	0.43
1:ZD:96:LEU:HD12	1:ZD:100:VAL:HG21	1.99	0.43
1:CE:76:GLU:HG2	1:CE:77:LEU:HG	2.00	0.43
1:IE:76:GLU:HG2	1:IE:77:LEU:HG	2.00	0.43
1:OE:97:LEU:HB2	1:OE:100:VAL:HG13	2.00	0.43
1:GF:97:LEU:HB2	1:GF:100:VAL:HG13	2.00	0.43
1:JF:76:GLU:HG2	1:JF:77:LEU:HG	2.00	0.43
1:C:27:VAL:HG13	1:Q:29:PRO:HB2	1.99	0.43
1:K:93:TRP:CE3	1:M:189:LYS:HE3	2.53	0.43
1:M:123:LEU:HD12	1:M:140:ALA:HB2	2.00	0.43
1:Y:76:GLU:HG2	1:Y:77:LEU:HG	2.00	0.43
1:AA:29:PRO:HB2	1:JF:27:VAL:HG13	1.99	0.43
1:CA:123:LEU:HD12	1:CA:140:ALA:HB2	2.00	0.43
1:HA:27:VAL:HG13	1:VA:29:PRO:HB2	1.99	0.43
1:WA:76:GLU:HG2	1:WA:77:LEU:HG	2.00	0.43
1:ZA:27:VAL:HG13	1:FC:29:PRO:HB2	1.99	0.43
1:BB:93:TRP:CE3	1:DB:189:LYS:HE3	2.53	0.43
1:CB:27:VAL:HG13	1:ZE:29:PRO:HB2	1.99	0.43
1:EB:29:PRO:HB2	1:YF:27:VAL:HG13	1.99	0.43
1:GB:123:LEU:HD12	1:GB:140:ALA:HB2	2.00	0.43
1:HB:29:PRO:HB2	1:ND:27:VAL:HG13	1.99	0.43
1:LB:184:PHE:HB2	1:AC:43:ILE:HB	1.99	0.43
1:RB:76:GLU:HG2	1:RB:77:LEU:HG	2.00	0.43
1:YB:189:LYS:HE3	1:LC:93:TRP:CE3	2.53	0.43
1:GC:96:LEU:HD12	1:GC:100:VAL:HG21	1.99	0.43
1:IC:139:ASP:OD1	1:IC:142:ARG:NE	2.45	0.43
1:NC:189:LYS:HE3	1:AD:93:TRP:CE3	2.53	0.43
1:QD:97:LEU:HB2	1:QD:100:VAL:HG13	2.00	0.43
1:ZD:97:LEU:HB2	1:ZD:100:VAL:HG13	2.00	0.43
1:GE:189:LYS:HE3	1:TE:93:TRP:CE3	2.53	0.43
1:ME:123:LEU:HD12	1:ME:140:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OE:96:LEU:HD12	1:OE:100:VAL:HG21	1.99	0.43
1:QE:93:TRP:CE3	1:SE:189:LYS:HE3	2.53	0.43
1:RE:76:GLU:HG2	1:RE:77:LEU:HG	2.00	0.43
1:AF:96:LEU:HD12	1:AF:100:VAL:HG21	1.99	0.43
1:FF:93:TRP:CE3	1:HF:189:LYS:HE3	2.53	0.43
1:RF:182:ASP:OD1	1:RF:182:ASP:N	2.46	0.43
1:UF:93:TRP:CE3	1:WF:189:LYS:HE3	2.53	0.43
1:YF:76:GLU:HG2	1:YF:77:LEU:HG	2.00	0.43
1:C:43:ILE:HB	1:R:184:PHE:HB2	1.99	0.43
1:V:27:VAL:HG13	1:UC:29:PRO:HB2	1.99	0.43
1:X:93:TRP:CE3	1:Z:189:LYS:HE3	2.53	0.43
1:HA:43:ILE:HB	1:WA:184:PHE:HB2	1.99	0.43
1:RA:123:LEU:HD12	1:RA:140:ALA:HB2	2.00	0.43
1:BB:29:PRO:HB2	1:AF:27:VAL:HG13	1.99	0.43
1:CB:76:GLU:HG2	1:CB:77:LEU:HG	2.00	0.43
1:DB:123:LEU:HD12	1:DB:140:ALA:HB2	2.00	0.43
1:JB:189:LYS:HE3	1:WB:93:TRP:CE3	2.53	0.43
1:XB:43:ILE:HB	1:GF:184:PHE:HB2	1.99	0.43
1:XB:97:LEU:HB2	1:XB:100:VAL:HG13	2.00	0.43
1:MC:97:LEU:HB2	1:MC:100:VAL:HG13	2.00	0.43
1:MC:184:PHE:HB2	1:CE:43:ILE:HB	1.99	0.43
1:BD:184:PHE:HB2	1:RE:43:ILE:HB	1.99	0.43
1:JD:139:ASP:OD1	1:JD:142:ARG:NE	2.45	0.43
1:KD:76:GLU:HG2	1:KD:77:LEU:HG	2.00	0.43
1:CF:93:TRP:CE3	1:EF:189:LYS:HE3	2.53	0.43
1:PF:96:LEU:HD12	1:PF:100:VAL:HG21	1.99	0.43
1:F:43:ILE:HB	1:RB:184:PHE:HB2	1.99	0.43
1:I:97:LEU:HB2	1:I:100:VAL:HG13	2.00	0.43
1:X:139:ASP:OD1	1:X:142:ARG:NE	2.45	0.43
1:Z:123:LEU:HD12	1:Z:140:ALA:HB2	2.00	0.43
1:IA:123:LEU:HD12	1:IA:140:ALA:HB2	2.00	0.43
1:NA:97:LEU:HB2	1:NA:100:VAL:HG13	2.00	0.43
1:YA:93:TRP:CE3	1:AB:189:LYS:HE3	2.53	0.43
1:GC:76:GLU:HG2	1:GC:77:LEU:HG	2.00	0.43
1:PC:43:ILE:HB	1:ED:184:PHE:HB2	1.99	0.43
1:VC:76:GLU:HG2	1:VC:77:LEU:HG	2.00	0.43
1:BD:97:LEU:HB2	1:BD:100:VAL:HG13	2.00	0.43
1:CD:189:LYS:HE3	1:PD:93:TRP:CE3	2.53	0.43
1:QD:43:ILE:HB	1:VF:184:PHE:HB2	1.99	0.43
1:BE:93:TRP:CE3	1:DE:189:LYS:HE3	2.53	0.43
1:EF:123:LEU:HD12	1:EF:140:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OF:127:ASP:HB3	1:OF:130:LYS:HE2	2.01	0.43
1:RF:93:TRP:CE3	1:TF:189:LYS:HE3	2.53	0.43
1:TF:123:LEU:HD12	1:TF:140:ALA:HB2	2.00	0.43
1:D:123:LEU:HD12	1:D:140:ALA:HB2	2.00	0.43
1:T:93:TRP:CE3	1:W:189:LYS:HE3	2.53	0.43
1:X:29:PRO:HB2	1:PF:27:VAL:HG13	1.99	0.43
1:JA:93:TRP:CE3	1:LA:189:LYS:HE3	2.53	0.43
1:KA:43:ILE:HB	1:KD:184:PHE:HB2	1.99	0.43
1:LB:76:GLU:HG2	1:LB:77:LEU:HG	2.00	0.43
1:TB:93:TRP:CE3	1:VB:189:LYS:HE3	2.53	0.43
1:VB:123:LEU:HD12	1:VB:140:ALA:HB2	2.00	0.43
1:IC:93:TRP:CE3	1:KC:189:LYS:HE3	2.53	0.43
1:KC:123:LEU:HD12	1:KC:140:ALA:HB2	2.00	0.43
1:NC:130:LYS:HE2	1:NC:130:LYS:HB3	1.80	0.43
1:OC:93:TRP:CE3	1:QC:189:LYS:HE3	2.53	0.43
1:WC:123:LEU:HD12	1:WC:140:ALA:HB2	2.00	0.43
1:XC:139:ASP:OD1	1:XC:142:ARG:NE	2.45	0.43
1:ZC:123:LEU:HD12	1:ZC:140:ALA:HB2	2.00	0.43
1:ED:76:GLU:HG2	1:ED:77:LEU:HG	2.00	0.43
1:MD:93:TRP:CE3	1:OD:189:LYS:HE3	2.53	0.43
1:SD:93:TRP:CE3	1:UD:189:LYS:HE3	2.53	0.43
1:TD:97:LEU:HB2	1:TD:100:VAL:HG13	2.00	0.43
1:HE:93:TRP:CE3	1:JE:189:LYS:HE3	2.53	0.43
1:IE:97:LEU:HB2	1:IE:100:VAL:HG13	2.00	0.43
1:KE:93:TRP:CE3	1:ME:189:LYS:HE3	2.53	0.43
1:RE:96:LEU:HD12	1:RE:100:VAL:HG21	1.99	0.43
1:WE:93:TRP:CE3	1:YE:189:LYS:HE3	2.53	0.43
1:ZE:93:TRP:CE3	1:BF:189:LYS:HE3	2.53	0.43
1:ZE:127:ASP:HB3	1:ZE:130:LYS:HE2	2.01	0.43
1:OF:93:TRP:CE3	1:QF:189:LYS:HE3	2.53	0.43
1:E:93:TRP:CE3	1:G:189:LYS:HE3	2.53	0.43
1:J:123:LEU:HD12	1:J:140:ALA:HB2	2.00	0.43
1:S:123:LEU:HD12	1:S:140:ALA:HB2	2.00	0.43
1:FA:189:LYS:HE3	1:SA:93:TRP:CE3	2.53	0.43
1:OA:123:LEU:HD12	1:OA:140:ALA:HB2	2.00	0.43
1:TA:76:GLU:HG2	1:TA:77:LEU:HG	2.00	0.43
1:TA:96:LEU:HD12	1:TA:100:VAL:HG21	1.99	0.43
1:XA:123:LEU:HD12	1:XA:140:ALA:HB2	2.00	0.43
1:EB:93:TRP:CE3	1:GB:189:LYS:HE3	2.53	0.43
1:FB:96:LEU:HD12	1:FB:100:VAL:HG21	1.99	0.43
1:NB:127:ASP:HB3	1:NB:130:LYS:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HC:123:LEU:HD12	1:HC:140:ALA:HB2	2.00	0.43
1:XC:93:TRP:CE3	1:ZC:189:LYS:HE3	2.53	0.43
1:GD:127:ASP:HB3	1:GD:130:LYS:HE2	2.01	0.43
1:MD:127:ASP:HB3	1:MD:130:LYS:HE2	2.01	0.43
1:MD:139:ASP:OD1	1:MD:142:ARG:NE	2.45	0.43
1:OD:123:LEU:HD12	1:OD:140:ALA:HB2	2.00	0.43
1:RD:123:LEU:HD12	1:RD:140:ALA:HB2	2.00	0.43
1:SD:127:ASP:HB3	1:SD:130:LYS:HE2	2.01	0.43
1:VD:93:TRP:CE3	1:XD:189:LYS:HE3	2.53	0.43
1:WD:76:GLU:HG2	1:WD:77:LEU:HG	2.00	0.43
1:GE:123:LEU:HD12	1:GE:140:ALA:HB2	2.00	0.43
1:HE:127:ASP:HB3	1:HE:130:LYS:HE2	2.01	0.43
1:YE:123:LEU:HD12	1:YE:140:ALA:HB2	2.00	0.43
1:LF:93:TRP:CE3	1:NF:189:LYS:HE3	2.53	0.43
1:NF:123:LEU:HD12	1:NF:140:ALA:HB2	2.00	0.43
1:A:189:LYS:HE3	1:N:93:TRP:CE3	2.53	0.43
1:E:29:PRO:HB2	1:RB:27:VAL:HG13	1.99	0.43
1:G:123:LEU:HD12	1:G:140:ALA:HB2	2.00	0.43
1:N:29:PRO:HB2	1:YC:27:VAL:HG13	1.99	0.43
1:O:76:GLU:HG2	1:O:77:LEU:HG	2.00	0.43
1:P:123:LEU:HD12	1:P:140:ALA:HB2	2.00	0.43
1:AA:93:TRP:CE3	1:CA:189:LYS:HE3	2.53	0.43
1:BA:96:LEU:HD12	1:BA:100:VAL:HG21	1.99	0.43
1:JA:29:PRO:HB2	1:KD:27:VAL:HG13	1.99	0.43
1:KA:27:VAL:HG13	1:JD:29:PRO:HB2	1.99	0.43
1:NA:76:GLU:HG2	1:NA:77:LEU:HG	2.00	0.43
1:UA:123:LEU:HD12	1:UA:140:ALA:HB2	2.00	0.43
1:FB:76:GLU:HG2	1:FB:77:LEU:HG	2.00	0.43
1:JB:123:LEU:HD12	1:JB:140:ALA:HB2	2.00	0.43
1:NB:93:TRP:CE3	1:PB:189:LYS:HE3	2.53	0.43
1:TB:127:ASP:HB3	1:TB:130:LYS:HE2	2.01	0.43
1:ZB:93:TRP:CE3	1:BC:189:LYS:HE3	2.53	0.43
1:UC:127:ASP:HB3	1:UC:130:LYS:HE2	2.01	0.43
1:GD:93:TRP:CE3	1:ID:189:LYS:HE3	2.53	0.43
1:JD:93:TRP:CE3	1:LD:189:LYS:HE3	2.53	0.43
1:WD:96:LEU:HD12	1:WD:100:VAL:HG21	1.99	0.43
1:CE:96:LEU:HD12	1:CE:100:VAL:HG21	1.99	0.43
1:LE:96:LEU:HD12	1:LE:100:VAL:HG21	1.99	0.43
1:F:76:GLU:HG2	1:F:77:LEU:HG	2.00	0.43
1:O:96:LEU:HD12	1:O:100:VAL:HG21	1.99	0.43
1:LA:123:LEU:HD12	1:LA:140:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MB:123:LEU:HD12	1:MB:140:ALA:HB2	2.00	0.43
1:QB:93:TRP:CE3	1:SB:189:LYS:HE3	2.53	0.43
1:TB:139:ASP:OD1	1:TB:142:ARG:NE	2.45	0.43
1:CC:127:ASP:HB3	1:CC:130:LYS:HE2	2.01	0.43
1:FC:127:ASP:HB3	1:FC:130:LYS:HE2	2.01	0.43
1:CD:123:LEU:HD12	1:CD:140:ALA:HB2	2.00	0.43
1:FD:123:LEU:HD12	1:FD:140:ALA:HB2	2.00	0.43
1:VD:127:ASP:HB3	1:VD:130:LYS:HE2	2.01	0.43
1:KE:127:ASP:HB3	1:KE:130:LYS:HE2	2.01	0.43
1:LE:76:GLU:HG2	1:LE:77:LEU:HG	2.00	0.43
1:RE:97:LEU:HB2	1:RE:100:VAL:HG13	2.00	0.43
1:SF:97:LEU:HB2	1:SF:100:VAL:HG13	2.00	0.43
1:WF:123:LEU:HD12	1:WF:140:ALA:HB2	2.00	0.43
1:F:27:VAL:HG13	1:QB:29:PRO:HB2	1.99	0.43
1:I:76:GLU:HG2	1:I:77:LEU:HG	2.00	0.43
1:Q:93:TRP:CE3	1:S:189:LYS:HE3	2.53	0.43
1:BA:76:GLU:HG2	1:BA:77:LEU:HG	2.00	0.43
1:KA:76:GLU:HG2	1:KA:77:LEU:HG	2.00	0.43
1:SA:29:PRO:HB2	1:JC:27:VAL:HG13	1.99	0.43
1:AB:123:LEU:HD12	1:AB:140:ALA:HB2	2.00	0.43
1:CB:96:LEU:HD12	1:CB:100:VAL:HG21	1.99	0.43
1:AC:76:GLU:HG2	1:AC:77:LEU:HG	2.00	0.43
1:GC:97:LEU:HB2	1:GC:100:VAL:HG13	2.00	0.43
1:IC:127:ASP:HB3	1:IC:130:LYS:HE2	2.01	0.43
1:LC:127:ASP:HB3	1:LC:130:LYS:HE2	2.01	0.43
1:OC:127:ASP:HB3	1:OC:130:LYS:HE2	2.01	0.43
1:RC:127:ASP:HB3	1:RC:130:LYS:HE2	2.01	0.43
1:XC:127:ASP:HB3	1:XC:130:LYS:HE2	2.01	0.43
1:AD:127:ASP:HB3	1:AD:130:LYS:HE2	2.01	0.43
1:CE:97:LEU:HB2	1:CE:100:VAL:HG13	2.00	0.43
1:DF:97:LEU:HB2	1:DF:100:VAL:HG13	2.00	0.43
1:HF:123:LEU:HD12	1:HF:140:ALA:HB2	2.00	0.43
1:MF:76:GLU:HG2	1:MF:77:LEU:HG	2.00	0.43
1:H:29:PRO:HB2	1:WD:27:VAL:HG13	1.99	0.43
1:P:189:LYS:HE3	1:DA:93:TRP:CE3	2.53	0.43
1:W:123:LEU:HD12	1:W:140:ALA:HB2	2.00	0.43
1:Y:96:LEU:HD12	1:Y:100:VAL:HG21	1.99	0.43
1:EA:76:GLU:HG2	1:EA:77:LEU:HG	2.00	0.43
1:UA:189:LYS:HE3	1:HB:93:TRP:CE3	2.53	0.43
1:VA:93:TRP:CE3	1:XA:189:LYS:HE3	2.53	0.43
1:KB:127:ASP:HB3	1:KB:130:LYS:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZB:127:ASP:HB3	1:ZB:130:LYS:HE2	2.01	0.43
1:AC:97:LEU:HB2	1:AC:100:VAL:HG13	2.00	0.43
1:PC:76:GLU:HG2	1:PC:77:LEU:HG	2.00	0.43
1:VC:97:LEU:HB2	1:VC:100:VAL:HG13	2.00	0.43
1:HD:76:GLU:HG2	1:HD:77:LEU:HG	2.00	0.43
1:NE:139:ASP:OD1	1:NE:142:ARG:NE	2.45	0.43
1:XE:76:GLU:HG2	1:XE:77:LEU:HG	2.00	0.43
1:C:97:LEU:HB2	1:C:100:VAL:HG13	2.00	0.42
1:MA:29:PRO:HB2	1:LE:27:VAL:HG13	1.99	0.42
1:OB:76:GLU:HG2	1:OB:77:LEU:HG	2.00	0.42
1:PB:171:LEU:HD12	1:PB:171:LEU:HA	1.92	0.42
1:DC:76:GLU:HG2	1:DC:77:LEU:HG	2.00	0.42
1:PC:97:LEU:HB2	1:PC:100:VAL:HG13	2.00	0.42
1:DD:127:ASP:HB3	1:DD:130:LYS:HE2	2.01	0.42
1:HD:97:LEU:HB2	1:HD:100:VAL:HG13	2.00	0.42
1:KF:189:LYS:HE3	1:XF:93:TRP:CE3	2.53	0.42
1:EA:43:ILE:HB	1:UB:184:PHE:HB2	1.99	0.42
1:HA:97:LEU:HB2	1:HA:100:VAL:HG13	2.00	0.42
1:KA:97:LEU:HB2	1:KA:100:VAL:HG13	2.00	0.42
1:IB:43:ILE:HB	1:ND:184:PHE:HB2	1.99	0.42
1:IB:76:GLU:HG2	1:IB:77:LEU:HG	2.00	0.42
1:BC:123:LEU:HD12	1:BC:140:ALA:HB2	2.00	0.42
1:SC:76:GLU:HG2	1:SC:77:LEU:HG	2.00	0.42
1:VE:189:LYS:HE3	1:IF:93:TRP:CE3	2.53	0.42
1:BF:123:LEU:HD12	1:BF:140:ALA:HB2	2.00	0.42
1:QF:123:LEU:HD12	1:QF:140:ALA:HB2	2.00	0.42
1:F:97:LEU:HB2	1:F:100:VAL:HG13	2.00	0.42
1:O:27:VAL:HG13	1:XC:29:PRO:HB2	1.99	0.42
1:X:127:ASP:HB3	1:X:130:LYS:HE2	2.01	0.42
1:QA:76:GLU:HG2	1:QA:77:LEU:HG	2.00	0.42
1:TA:27:VAL:HG13	1:IC:29:PRO:HB2	1.99	0.42
1:BB:127:ASP:HB3	1:BB:130:LYS:HE2	2.01	0.42
1:OB:97:LEU:HB2	1:OB:100:VAL:HG13	2.00	0.42
1:YD:139:ASP:OD1	1:YD:142:ARG:NE	2.45	0.42
1:NE:127:ASP:HB3	1:NE:130:LYS:HE2	2.01	0.42
1:UE:97:LEU:HB2	1:UE:100:VAL:HG13	2.00	0.42
1:LF:127:ASP:HB3	1:LF:130:LYS:HE2	2.01	0.42
1:L:76:GLU:HG2	1:L:77:LEU:HG	2.00	0.42
1:QA:97:LEU:HB2	1:QA:100:VAL:HG13	2.00	0.42
1:PB:123:LEU:HD12	1:PB:140:ALA:HB2	2.00	0.42
1:QC:123:LEU:HD12	1:QC:140:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZC:171:LEU:HD12	1:ZC:171:LEU:HA	1.91	0.42
1:PD:139:ASP:OD1	1:PD:142:ARG:NE	2.45	0.42
1:YD:127:ASP:HB3	1:YD:130:LYS:HE2	2.01	0.42
1:BE:127:ASP:HB3	1:BE:130:LYS:HE2	2.01	0.42
1:FE:97:LEU:HB2	1:FE:100:VAL:HG13	2.00	0.42
1:QE:127:ASP:HB3	1:QE:130:LYS:HE2	2.01	0.42
1:VE:171:LEU:HD12	1:VE:171:LEU:HA	1.91	0.42
1:WE:127:ASP:HB3	1:WE:130:LYS:HE2	2.01	0.42
1:XE:97:LEU:HB2	1:XE:100:VAL:HG13	2.00	0.42
1:KF:171:LEU:HD12	1:KF:171:LEU:HA	1.91	0.42
1:MF:97:LEU:HB2	1:MF:100:VAL:HG13	2.00	0.42
1:C:76:GLU:HG2	1:C:77:LEU:HG	2.00	0.42
1:T:127:ASP:HB3	1:T:130:LYS:HE2	2.01	0.42
1:YA:127:ASP:HB3	1:YA:130:LYS:HE2	2.01	0.42
1:EC:123:LEU:HD12	1:EC:140:ALA:HB2	2.00	0.42
1:ID:123:LEU:HD12	1:ID:140:ALA:HB2	2.00	0.42
1:ID:171:LEU:HD12	1:ID:171:LEU:HA	1.92	0.42
1:BF:171:LEU:HD12	1:BF:171:LEU:HA	1.92	0.42
1:IF:127:ASP:HB3	1:IF:130:LYS:HE2	2.01	0.42
1:QF:171:LEU:HD12	1:QF:171:LEU:HA	1.92	0.42
1:XF:127:ASP:HB3	1:XF:130:LYS:HE2	2.01	0.42
1:B:127:ASP:HB3	1:B:130:LYS:HE2	2.01	0.42
1:L:97:LEU:HB2	1:L:100:VAL:HG13	2.00	0.42
1:GA:127:ASP:HB3	1:GA:130:LYS:HE2	2.01	0.42
1:TC:123:LEU:HD12	1:TC:140:ALA:HB2	2.00	0.42
1:DE:123:LEU:HD12	1:DE:140:ALA:HB2	2.00	0.42
1:SE:123:LEU:HD12	1:SE:140:ALA:HB2	2.00	0.42
1:HA:76:GLU:HG2	1:HA:77:LEU:HG	2.00	0.42
1:TC:130:LYS:HE2	1:TC:130:LYS:HB3	1.80	0.42
1:RD:130:LYS:HE2	1:RD:130:LYS:HB3	1.80	0.42
1:AE:123:LEU:HD12	1:AE:140:ALA:HB2	2.00	0.42
1:GE:130:LYS:HE2	1:GE:130:LYS:HB3	1.80	0.42
1:YE:171:LEU:HD12	1:YE:171:LEU:HA	1.91	0.42
1:O:37:ALA:HB1	1:YC:189:LYS:O	2.20	0.42
1:CA:130:LYS:HE2	1:CA:130:LYS:HB3	1.80	0.42
1:EA:37:ALA:HB1	1:UB:189:LYS:O	2.20	0.42
1:EA:189:LYS:O	1:UB:37:ALA:HB1	2.20	0.42
1:TA:37:ALA:HB1	1:JC:189:LYS:O	2.20	0.42
1:AB:130:LYS:HE2	1:AB:130:LYS:HB3	1.80	0.42
1:GB:130:LYS:HE2	1:GB:130:LYS:HB3	1.80	0.42
1:IB:37:ALA:HB1	1:ND:189:LYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IB:189:LYS:O	1:ND:37:ALA:HB1	2.20	0.42
1:MD:182:ASP:OD1	1:MD:182:ASP:N	2.46	0.42
1:SD:139:ASP:OD1	1:SD:142:ARG:NE	2.45	0.42
1:NF:171:LEU:HD12	1:NF:171:LEU:HA	1.91	0.42
1:XF:139:ASP:OD1	1:XF:142:ARG:NE	2.45	0.42
1:L:37:ALA:HB1	1:UE:189:LYS:O	2.20	0.42
1:N:127:ASP:HB3	1:N:130:LYS:HE2	2.01	0.42
1:W:130:LYS:HE2	1:W:130:LYS:HB3	1.80	0.42
1:DA:127:ASP:HB3	1:DA:130:LYS:HE2	2.01	0.42
1:PA:127:ASP:HB3	1:PA:130:LYS:HE2	2.01	0.42
1:QA:37:ALA:HB1	1:FE:189:LYS:O	2.20	0.42
1:SA:127:ASP:HB3	1:SA:130:LYS:HE2	2.01	0.42
1:WB:139:ASP:OD1	1:WB:142:ARG:NE	2.45	0.42
1:NC:123:LEU:HD12	1:NC:140:ALA:HB2	2.00	0.42
1:JD:127:ASP:HB3	1:JD:130:LYS:HE2	2.01	0.42
1:PE:123:LEU:HD12	1:PE:140:ALA:HB2	2.00	0.42
1:K:127:ASP:HB3	1:K:130:LYS:HE2	2.01	0.42
1:V:189:LYS:O	1:VC:37:ALA:HB1	2.20	0.42
1:ZA:189:LYS:O	1:GC:37:ALA:HB1	2.20	0.42
1:JB:171:LEU:HD12	1:JB:171:LEU:HA	1.91	0.42
1:QB:127:ASP:HB3	1:QB:130:LYS:HE2	2.01	0.42
1:KC:171:LEU:HD12	1:KC:171:LEU:HA	1.92	0.42
1:BD:37:ALA:HB1	1:RE:189:LYS:O	2.20	0.42
1:PD:127:ASP:HB3	1:PD:130:LYS:HE2	2.01	0.42
1:TE:127:ASP:HB3	1:TE:130:LYS:HE2	2.01	0.42
1:HF:171:LEU:HD12	1:HF:171:LEU:HA	1.91	0.42
1:F:189:LYS:O	1:RB:37:ALA:HB1	2.20	0.41
1:I:189:LYS:O	1:WD:37:ALA:HB1	2.20	0.41
1:O:189:LYS:O	1:YC:37:ALA:HB1	2.20	0.41
1:NA:189:LYS:O	1:LE:37:ALA:HB1	2.20	0.41
1:RA:171:LEU:HD12	1:RA:171:LEU:HA	1.92	0.41
1:TA:189:LYS:O	1:JC:37:ALA:HB1	2.20	0.41
1:CB:37:ALA:HB1	1:AF:189:LYS:O	2.20	0.41
1:HB:127:ASP:HB3	1:HB:130:LYS:HE2	2.01	0.41
1:WB:127:ASP:HB3	1:WB:130:LYS:HE2	2.01	0.41
1:YB:123:LEU:HD12	1:YB:140:ALA:HB2	2.00	0.41
1:MC:37:ALA:HB1	1:CE:189:LYS:O	2.20	0.41
1:CD:171:LEU:HD12	1:CD:171:LEU:HA	1.91	0.41
1:FF:127:ASP:HB3	1:FF:130:LYS:HE2	2.01	0.41
1:GF:76:GLU:HG2	1:GF:77:LEU:HG	2.00	0.41
1:IF:139:ASP:OD1	1:IF:142:ARG:NE	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RF:127:ASP:HB3	1:RF:130:LYS:HE2	2.01	0.41
1:UF:127:ASP:HB3	1:UF:130:LYS:HE2	2.01	0.41
1:VF:76:GLU:HG2	1:VF:77:LEU:HG	2.00	0.41
1:WF:171:LEU:HD12	1:WF:171:LEU:HA	1.92	0.41
1:H:127:ASP:HB3	1:H:130:LYS:HE2	2.01	0.41
1:W:171:LEU:HD12	1:W:171:LEU:HA	1.92	0.41
1:Y:37:ALA:HB1	1:PF:189:LYS:O	2.20	0.41
1:AA:127:ASP:HB3	1:AA:130:LYS:HE2	2.01	0.41
1:BA:189:LYS:O	1:JF:37:ALA:HB1	2.20	0.41
1:KA:37:ALA:HB1	1:KD:189:LYS:O	2.20	0.41
1:MA:127:ASP:HB3	1:MA:130:LYS:HE2	2.01	0.41
1:NB:182:ASP:OD1	1:NB:182:ASP:N	2.46	0.41
1:TB:182:ASP:OD1	1:TB:182:ASP:N	2.46	0.41
1:XB:189:LYS:O	1:GF:37:ALA:HB1	2.20	0.41
1:TC:41:LYS:HA	1:TC:41:LYS:HZ3	1.85	0.41
1:QD:37:ALA:HB1	1:VF:189:LYS:O	2.20	0.41
1:EE:127:ASP:HB3	1:EE:130:LYS:HE2	2.01	0.41
1:CF:127:ASP:HB3	1:CF:130:LYS:HE2	2.01	0.41
1:FF:139:ASP:OD1	1:FF:142:ARG:NE	2.45	0.41
1:F:37:ALA:HB1	1:RB:189:LYS:O	2.20	0.41
1:K:182:ASP:OD1	1:K:182:ASP:N	2.46	0.41
1:Q:127:ASP:HB3	1:Q:130:LYS:HE2	2.01	0.41
1:KA:189:LYS:O	1:KD:37:ALA:HB1	2.20	0.41
1:RA:130:LYS:HB3	1:RA:130:LYS:HE2	1.80	0.41
1:VA:127:ASP:HB3	1:VA:130:LYS:HE2	2.01	0.41
1:EB:127:ASP:HB3	1:EB:130:LYS:HE2	2.01	0.41
1:FB:189:LYS:O	1:YF:37:ALA:HB1	2.20	0.41
1:XB:37:ALA:HB1	1:GF:189:LYS:O	2.20	0.41
1:PC:189:LYS:O	1:ED:37:ALA:HB1	2.20	0.41
1:HD:189:LYS:O	1:OE:37:ALA:HB1	2.20	0.41
1:QD:189:LYS:O	1:VF:37:ALA:HB1	2.20	0.41
1:VD:139:ASP:OD1	1:VD:142:ARG:NE	2.45	0.41
1:KE:139:ASP:OD1	1:KE:142:ARG:NE	2.45	0.41
1:C:37:ALA:HB1	1:R:189:LYS:O	2.20	0.41
1:BA:37:ALA:HB1	1:JF:189:LYS:O	2.20	0.41
1:HA:37:ALA:HB1	1:WA:189:LYS:O	2.20	0.41
1:FB:37:ALA:HB1	1:YF:189:LYS:O	2.20	0.41
1:LB:37:ALA:HB1	1:AC:189:LYS:O	2.20	0.41
1:OB:189:LYS:O	1:ZD:37:ALA:HB1	2.20	0.41
1:DC:37:ALA:HB1	1:DF:189:LYS:O	2.20	0.41
1:EC:130:LYS:HE2	1:EC:130:LYS:HB3	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SC:37:ALA:HB1	1:SF:189:LYS:O	2.20	0.41
1:MC:189:LYS:O	1:CE:37:ALA:HB1	2.20	0.41
1:HE:182:ASP:OD1	1:HE:182:ASP:N	2.46	0.41
1:PE:171:LEU:HD12	1:PE:171:LEU:HA	1.92	0.41
1:VE:123:LEU:HD12	1:VE:140:ALA:HB2	2.00	0.41
1:EF:171:LEU:HD12	1:EF:171:LEU:HA	1.92	0.41
1:KF:123:LEU:HD12	1:KF:140:ALA:HB2	2.00	0.41
1:TF:171:LEU:HD12	1:TF:171:LEU:HA	1.92	0.41
1:MA:182:ASP:OD1	1:MA:182:ASP:N	2.46	0.41
1:PA:182:ASP:OD1	1:PA:182:ASP:N	2.46	0.41
1:HB:139:ASP:OD1	1:HB:142:ARG:NE	2.45	0.41
1:PC:37:ALA:HB1	1:ED:189:LYS:O	2.20	0.41
1:SC:189:LYS:O	1:SF:37:ALA:HB1	2.20	0.41
1:BD:189:LYS:O	1:RE:37:ALA:HB1	2.20	0.41
1:GD:182:ASP:OD1	1:GD:182:ASP:N	2.46	0.41
1:SD:182:ASP:OD1	1:SD:182:ASP:N	2.46	0.41
1:PE:130:LYS:HE2	1:PE:130:LYS:HB3	1.80	0.41
1:XE:37:ALA:HB1	1:MF:189:LYS:O	2.20	0.41
1:LF:139:ASP:OD1	1:LF:142:ARG:NE	2.45	0.41
1:UF:139:ASP:OD1	1:UF:142:ARG:NE	2.45	0.41
1:DA:139:ASP:OD1	1:DA:142:ARG:NE	2.45	0.41
1:JA:127:ASP:HB3	1:JA:130:LYS:HE2	2.01	0.41
1:QA:189:LYS:O	1:FE:37:ALA:HB1	2.20	0.41
1:AB:171:LEU:HD12	1:AB:171:LEU:HA	1.92	0.41
1:LB:189:LYS:O	1:AC:37:ALA:HB1	2.20	0.41
1:XE:189:LYS:O	1:MF:37:ALA:HB1	2.20	0.41
1:E:127:ASP:HB3	1:E:130:LYS:HE2	2.01	0.41
1:H:182:ASP:OD1	1:H:182:ASP:N	2.46	0.41
1:I:37:ALA:HB1	1:WD:189:LYS:O	2.20	0.41
1:V:37:ALA:HB1	1:VC:189:LYS:O	2.20	0.41
1:TD:37:ALA:HB1	1:IE:189:LYS:O	2.20	0.41
1:G:130:LYS:HB3	1:G:130:LYS:HE2	1.80	0.41
1:L:189:LYS:O	1:UE:37:ALA:HB1	2.20	0.41
1:M:130:LYS:HB3	1:M:130:LYS:HE2	1.80	0.41
1:Y:189:LYS:O	1:PF:37:ALA:HB1	2.20	0.41
1:NA:37:ALA:HB1	1:LE:189:LYS:O	2.20	0.41
1:PA:139:ASP:OD1	1:PA:142:ARG:NE	2.45	0.41
1:ZA:37:ALA:HB1	1:GC:189:LYS:O	2.20	0.41
1:CB:189:LYS:O	1:AF:37:ALA:HB1	2.20	0.41
1:DC:189:LYS:O	1:DF:37:ALA:HB1	2.20	0.41
1:GC:103:ARG:H	1:GC:159:SER:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:VC:103:ARG:H	1:VC:159:SER:HB3	1.86	0.41
1:ND:103:ARG:H	1:ND:159:SER:HB3	1.86	0.41
1:TD:103:ARG:H	1:TD:159:SER:HB3	1.86	0.41
1:TD:189:LYS:O	1:IE:37:ALA:HB1	2.20	0.41
1:AE:130:LYS:HE2	1:AE:130:LYS:HB3	1.80	0.41
1:IE:103:ARG:H	1:IE:159:SER:HB3	1.86	0.41
1:WE:139:ASP:OD1	1:WE:142:ARG:NE	2.45	0.41
1:K:139:ASP:OD1	1:K:142:ARG:NE	2.45	0.41
1:EA:103:ARG:H	1:EA:159:SER:HB3	1.86	0.41
1:HA:189:LYS:O	1:WA:37:ALA:HB1	2.20	0.41
1:OB:103:ARG:H	1:OB:159:SER:HB3	1.86	0.41
1:RB:103:ARG:H	1:RB:159:SER:HB3	1.86	0.41
1:UB:103:ARG:H	1:UB:159:SER:HB3	1.86	0.41
1:XB:103:ARG:H	1:XB:159:SER:HB3	1.86	0.41
1:HD:103:ARG:H	1:HD:159:SER:HB3	1.86	0.41
1:KD:103:ARG:H	1:KD:159:SER:HB3	1.86	0.41
1:QD:103:ARG:H	1:QD:159:SER:HB3	1.86	0.41
1:OA:130:LYS:HE2	1:OA:130:LYS:HB3	1.80	0.40
1:IB:103:ARG:H	1:IB:159:SER:HB3	1.86	0.40
1:LB:103:ARG:H	1:LB:159:SER:HB3	1.86	0.40
1:BD:103:ARG:H	1:BD:159:SER:HB3	1.86	0.40
1:ED:103:ARG:H	1:ED:159:SER:HB3	1.86	0.40
1:DF:103:ARG:H	1:DF:159:SER:HB3	1.86	0.40
1:SF:103:ARG:H	1:SF:159:SER:HB3	1.86	0.40
1:C:189:LYS:O	1:R:37:ALA:HB1	2.20	0.40
1:G:44:LYS:HD2	1:G:45:ALA:O	2.22	0.40
1:J:130:LYS:HE2	1:J:130:LYS:HB3	1.80	0.40
1:LA:44:LYS:HD2	1:LA:45:ALA:O	2.22	0.40
1:DC:103:ARG:H	1:DC:159:SER:HB3	1.86	0.40
1:SC:103:ARG:H	1:SC:159:SER:HB3	1.86	0.40
1:AE:44:LYS:HD2	1:AE:45:ALA:O	2.22	0.40
1:CE:103:ARG:H	1:CE:159:SER:HB3	1.86	0.40
1:ME:44:LYS:HD2	1:ME:45:ALA:O	2.22	0.40
1:XE:103:ARG:H	1:XE:159:SER:HB3	1.86	0.40
1:MF:103:ARG:H	1:MF:159:SER:HB3	1.86	0.40
1:D:44:LYS:HD2	1:D:45:ALA:O	2.22	0.40
1:S:130:LYS:HE2	1:S:130:LYS:HB3	1.80	0.40
1:IA:44:LYS:HD2	1:IA:45:ALA:O	2.22	0.40
1:JB:44:LYS:HD2	1:JB:45:ALA:O	2.22	0.40
1:MC:103:ARG:H	1:MC:159:SER:HB3	1.86	0.40
1:HD:37:ALA:HB1	1:OE:189:LYS:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XD:44:LYS:HD2	1:XD:45:ALA:O	2.22	0.40
1:ZD:103:ARG:H	1:ZD:159:SER:HB3	1.86	0.40
1:IE:31:ILE:HG13	1:TE:27:VAL:HG11	2.04	0.40
1:PE:44:LYS:HD2	1:PE:45:ALA:O	2.22	0.40
1:RE:103:ARG:H	1:RE:159:SER:HB3	1.86	0.40
1:C:31:ILE:HG13	1:N:27:VAL:HG11	2.04	0.40
1:V:103:ARG:H	1:V:159:SER:HB3	1.86	0.40
1:HA:31:ILE:HG13	1:SA:27:VAL:HG11	2.04	0.40
1:ZA:103:ARG:H	1:ZA:159:SER:HB3	1.86	0.40
1:MB:171:LEU:HD12	1:MB:171:LEU:HA	1.91	0.40
1:OB:37:ALA:HB1	1:ZD:189:LYS:O	2.20	0.40
1:CD:44:LYS:HD2	1:CD:45:ALA:O	2.22	0.40
1:FD:171:LEU:HD12	1:FD:171:LEU:HA	1.91	0.40
1:TD:31:ILE:HG13	1:EE:27:VAL:HG11	2.04	0.40
1:VD:27:VAL:HG11	1:ZD:31:ILE:HG13	2.04	0.40
1:KE:27:VAL:HG11	1:OE:31:ILE:HG13	2.04	0.40
1:OE:103:ARG:H	1:OE:159:SER:HB3	1.86	0.40
1:XE:31:ILE:HG13	1:IF:27:VAL:HG11	2.04	0.40
1:HF:44:LYS:HD2	1:HF:45:ALA:O	2.22	0.40
1:MF:31:ILE:HG13	1:XF:27:VAL:HG11	2.04	0.40
1:L:103:ARG:H	1:L:159:SER:HB3	1.86	0.40
1:XA:130:LYS:HE2	1:XA:130:LYS:HB3	1.80	0.40
1:QB:27:VAL:HG11	1:UB:31:ILE:HG13	2.04	0.40
1:AC:103:ARG:H	1:AC:159:SER:HB3	1.86	0.40
1:ED:31:ILE:HG13	1:PD:27:VAL:HG11	2.04	0.40
1:JD:27:VAL:HG11	1:ND:31:ILE:HG13	2.04	0.40
1:QF:41:LYS:HA	1:QF:41:LYS:HZ2	1.85	0.40
1:WF:44:LYS:HD2	1:WF:45:ALA:O	2.22	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	A	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	AA	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	AB	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	AC	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	AD	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	AE	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	AF	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	B	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	BA	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	BB	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	BC	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	BD	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	BE	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	BF	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	C	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	CA	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	CB	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	CC	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	CD	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	CE	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	CF	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	D	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	DA	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	DB	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	DC	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	DD	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	DE	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	DF	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	E	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	EA	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	EB	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	EC	147/192 (77%)	145 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	ED	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	EE	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	EF	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	F	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	FA	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	FB	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	FC	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	FD	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	FE	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	FF	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	G	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	GA	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	GB	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	GC	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	GD	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	GE	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	GF	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	H	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	HA	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	HB	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	HC	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	HD	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	HE	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	HF	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	I	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	IA	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	IB	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	IC	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	ID	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	IE	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	IF	161/192 (84%)	157 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	JA	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	JB	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	JC	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	JD	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	JE	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	JF	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	K	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	KA	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	KB	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	KC	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	KD	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	KE	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	KF	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	L	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	LA	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	LB	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	LC	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	LD	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	LE	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	LF	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	M	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	MA	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	MB	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	MC	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	MD	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	ME	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	MF	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	N	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	NA	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	NB	161/192 (84%)	156 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	NC	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	ND	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	NE	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	NF	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	O	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	OA	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	OB	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	OC	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	OD	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	OE	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	OF	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	P	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	PA	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	PB	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	PC	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	PD	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	PE	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	PF	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	Q	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	QA	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	QB	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	QC	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	QD	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	QE	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	QF	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	R	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	RA	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	RB	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	RC	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	RD	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	RE	162/192 (84%)	159 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	RF	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	S	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	SA	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	SB	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	SC	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	SD	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	SE	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	SF	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	T	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	TA	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	TB	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	TC	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	TD	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	TE	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	TF	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	UA	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	UB	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	UC	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	UD	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	UE	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	UF	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	V	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	VA	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	VB	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	VC	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	VD	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	VE	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	VF	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	W	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	WA	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	WB	161/192 (84%)	157 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	WC	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	WD	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	WE	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	WF	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	X	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	XA	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	XB	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	XC	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	XD	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	XE	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	XF	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	Y	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	YA	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	YB	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	YC	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	YD	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	YE	147/192 (77%)	146 (99%)	1 (1%)	0	100	100
1	YF	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	Z	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	ZA	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	ZB	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	ZC	147/192 (77%)	145 (99%)	2 (1%)	0	100	100
1	ZD	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	ZE	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
All	All	28200/34560 (82%)	27633 (98%)	567 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	AA	126/148 (85%)	126 (100%)	0	100	100
1	AB	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	AC	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	AD	126/148 (85%)	126 (100%)	0	100	100
1	AE	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	AF	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	B	126/148 (85%)	126 (100%)	0	100	100
1	BA	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	BB	126/148 (85%)	126 (100%)	0	100	100
1	BC	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	BD	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	BE	126/148 (85%)	126 (100%)	0	100	100
1	BF	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	C	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	CA	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	CB	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	CC	126/148 (85%)	126 (100%)	0	100	100
1	CD	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	CE	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	CF	126/148 (85%)	126 (100%)	0	100	100
1	D	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	DA	126/148 (85%)	126 (100%)	0	100	100
1	DB	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	DC	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	DD	126/148 (85%)	126 (100%)	0	100	100
1	DE	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	DF	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	E	126/148 (85%)	126 (100%)	0	100	100
1	EA	127/148 (86%)	123 (97%)	4 (3%)	35	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EB	126/148 (85%)	126 (100%)	0	100	100
1	EC	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	ED	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	EE	126/148 (85%)	126 (100%)	0	100	100
1	EF	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	F	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	FA	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	FB	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	FC	126/148 (85%)	126 (100%)	0	100	100
1	FD	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	FE	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	FF	126/148 (85%)	126 (100%)	0	100	100
1	G	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	GA	126/148 (85%)	126 (100%)	0	100	100
1	GB	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	GC	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	GD	126/148 (85%)	126 (100%)	0	100	100
1	GE	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	GF	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	H	126/148 (85%)	126 (100%)	0	100	100
1	HA	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	HB	126/148 (85%)	126 (100%)	0	100	100
1	HC	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	HD	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	HE	126/148 (85%)	126 (100%)	0	100	100
1	HF	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	I	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	IA	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	IB	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	IC	126/148 (85%)	126 (100%)	0	100	100
1	ID	117/148 (79%)	109 (93%)	8 (7%)	14	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	IE	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	IF	126/148 (85%)	126 (100%)	0	100	100
1	J	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	JA	126/148 (85%)	126 (100%)	0	100	100
1	JB	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	JC	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	JD	126/148 (85%)	126 (100%)	0	100	100
1	JE	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	JF	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	K	126/148 (85%)	126 (100%)	0	100	100
1	KA	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	KB	126/148 (85%)	126 (100%)	0	100	100
1	KC	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	KD	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	KE	126/148 (85%)	126 (100%)	0	100	100
1	KF	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	L	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	LA	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	LB	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	LC	126/148 (85%)	126 (100%)	0	100	100
1	LD	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	LE	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	LF	126/148 (85%)	126 (100%)	0	100	100
1	M	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	MA	126/148 (85%)	126 (100%)	0	100	100
1	MB	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	MC	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	MD	126/148 (85%)	126 (100%)	0	100	100
1	ME	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	MF	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	N	126/148 (85%)	126 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	NA	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	NB	126/148 (85%)	126 (100%)	0	100	100
1	NC	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	ND	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	NE	126/148 (85%)	126 (100%)	0	100	100
1	NF	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	O	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	OA	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	OB	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	OC	126/148 (85%)	126 (100%)	0	100	100
1	OD	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	OE	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	OF	126/148 (85%)	126 (100%)	0	100	100
1	P	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	PA	126/148 (85%)	126 (100%)	0	100	100
1	PB	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	PC	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	PD	126/148 (85%)	126 (100%)	0	100	100
1	PE	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	PF	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	Q	126/148 (85%)	126 (100%)	0	100	100
1	QA	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	QB	126/148 (85%)	126 (100%)	0	100	100
1	QC	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	QD	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	QE	126/148 (85%)	126 (100%)	0	100	100
1	QF	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	R	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	RA	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	RB	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	RC	126/148 (85%)	126 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	RD	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	RE	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	RF	126/148 (85%)	126 (100%)	0	100	100
1	S	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	SA	126/148 (85%)	126 (100%)	0	100	100
1	SB	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	SC	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	SD	126/148 (85%)	126 (100%)	0	100	100
1	SE	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	SF	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	T	126/148 (85%)	126 (100%)	0	100	100
1	TA	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	TB	126/148 (85%)	126 (100%)	0	100	100
1	TC	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	TD	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	TE	126/148 (85%)	126 (100%)	0	100	100
1	TF	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	UA	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	UB	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	UC	126/148 (85%)	126 (100%)	0	100	100
1	UD	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	UE	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	UF	126/148 (85%)	126 (100%)	0	100	100
1	V	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	VA	126/148 (85%)	126 (100%)	0	100	100
1	VB	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	VC	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	VD	126/148 (85%)	126 (100%)	0	100	100
1	VE	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	VF	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	W	117/148 (79%)	109 (93%)	8 (7%)	14	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	WA	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	WB	126/148 (85%)	126 (100%)	0	100	100
1	WC	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	WD	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	WE	126/148 (85%)	126 (100%)	0	100	100
1	WF	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	X	126/148 (85%)	126 (100%)	0	100	100
1	XA	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	XB	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	XC	126/148 (85%)	126 (100%)	0	100	100
1	XD	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	XE	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	XF	126/148 (85%)	126 (100%)	0	100	100
1	Y	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	YA	126/148 (85%)	126 (100%)	0	100	100
1	YB	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	YC	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	YD	126/148 (85%)	126 (100%)	0	100	100
1	YE	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	YF	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	Z	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	ZA	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	ZB	126/148 (85%)	126 (100%)	0	100	100
1	ZC	117/148 (79%)	109 (93%)	8 (7%)	14	45
1	ZD	127/148 (86%)	123 (97%)	4 (3%)	35	68
1	ZE	126/148 (85%)	126 (100%)	0	100	100
All	All	22200/26640 (83%)	21480 (97%)	720 (3%)	35	67

All (720) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	44	LYS

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Mol	Chain	Res	Type
1	A	62	THR
1	A	66	THR
1	A	76	GLU
1	A	94	LEU
1	A	96	LEU
1	A	108	VAL
1	C	27	VAL
1	C	96	LEU
1	C	162	VAL
1	C	167	VAL
1	D	41	LYS
1	D	44	LYS
1	D	62	THR
1	D	66	THR
1	D	76	GLU
1	D	94	LEU
1	D	96	LEU
1	D	108	VAL
1	F	27	VAL
1	F	96	LEU
1	F	162	VAL
1	F	167	VAL
1	G	41	LYS
1	G	44	LYS
1	G	62	THR
1	G	66	THR
1	G	76	GLU
1	G	94	LEU
1	G	96	LEU
1	G	108	VAL
1	I	27	VAL
1	I	96	LEU
1	I	162	VAL
1	I	167	VAL
1	J	41	LYS
1	J	44	LYS
1	J	62	THR
1	J	66	THR
1	J	76	GLU
1	J	94	LEU
1	J	96	LEU
1	J	108	VAL

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Mol	Chain	Res	Type
1	L	27	VAL
1	L	96	LEU
1	L	162	VAL
1	L	167	VAL
1	M	41	LYS
1	M	44	LYS
1	M	62	THR
1	M	66	THR
1	M	76	GLU
1	M	94	LEU
1	M	96	LEU
1	M	108	VAL
1	O	27	VAL
1	O	96	LEU
1	O	162	VAL
1	O	167	VAL
1	P	41	LYS
1	P	44	LYS
1	P	62	THR
1	P	66	THR
1	P	76	GLU
1	P	94	LEU
1	P	96	LEU
1	P	108	VAL
1	R	27	VAL
1	R	96	LEU
1	R	162	VAL
1	R	167	VAL
1	S	41	LYS
1	S	44	LYS
1	S	62	THR
1	S	66	THR
1	S	76	GLU
1	S	94	LEU
1	S	96	LEU
1	S	108	VAL
1	V	27	VAL
1	V	96	LEU
1	V	162	VAL
1	V	167	VAL
1	W	41	LYS
1	W	44	LYS

Continued on next page...

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Mol	Chain	Res	Type
1	W	62	THR
1	W	66	THR
1	W	76	GLU
1	W	94	LEU
1	W	96	LEU
1	W	108	VAL
1	Y	27	VAL
1	Y	96	LEU
1	Y	162	VAL
1	Y	167	VAL
1	Z	41	LYS
1	Z	44	LYS
1	Z	62	THR
1	Z	66	THR
1	Z	76	GLU
1	Z	94	LEU
1	Z	96	LEU
1	Z	108	VAL
1	BA	27	VAL
1	BA	96	LEU
1	BA	162	VAL
1	BA	167	VAL
1	CA	41	LYS
1	CA	44	LYS
1	CA	62	THR
1	CA	66	THR
1	CA	76	GLU
1	CA	94	LEU
1	CA	96	LEU
1	CA	108	VAL
1	EA	27	VAL
1	EA	96	LEU
1	EA	162	VAL
1	EA	167	VAL
1	FA	41	LYS
1	FA	44	LYS
1	FA	62	THR
1	FA	66	THR
1	FA	76	GLU
1	FA	94	LEU
1	FA	96	LEU
1	FA	108	VAL

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Mol	Chain	Res	Type
1	HA	27	VAL
1	HA	96	LEU
1	HA	162	VAL
1	HA	167	VAL
1	IA	41	LYS
1	IA	44	LYS
1	IA	62	THR
1	IA	66	THR
1	IA	76	GLU
1	IA	94	LEU
1	IA	96	LEU
1	IA	108	VAL
1	KA	27	VAL
1	KA	96	LEU
1	KA	162	VAL
1	KA	167	VAL
1	LA	41	LYS
1	LA	44	LYS
1	LA	62	THR
1	LA	66	THR
1	LA	76	GLU
1	LA	94	LEU
1	LA	96	LEU
1	LA	108	VAL
1	NA	27	VAL
1	NA	96	LEU
1	NA	162	VAL
1	NA	167	VAL
1	OA	41	LYS
1	OA	44	LYS
1	OA	62	THR
1	OA	66	THR
1	OA	76	GLU
1	OA	94	LEU
1	OA	96	LEU
1	OA	108	VAL
1	QA	27	VAL
1	QA	96	LEU
1	QA	162	VAL
1	QA	167	VAL
1	RA	41	LYS
1	RA	44	LYS

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Mol	Chain	Res	Type
1	RA	62	THR
1	RA	66	THR
1	RA	76	GLU
1	RA	94	LEU
1	RA	96	LEU
1	RA	108	VAL
1	TA	27	VAL
1	TA	96	LEU
1	TA	162	VAL
1	TA	167	VAL
1	UA	41	LYS
1	UA	44	LYS
1	UA	62	THR
1	UA	66	THR
1	UA	76	GLU
1	UA	94	LEU
1	UA	96	LEU
1	UA	108	VAL
1	WA	27	VAL
1	WA	96	LEU
1	WA	162	VAL
1	WA	167	VAL
1	XA	41	LYS
1	XA	44	LYS
1	XA	62	THR
1	XA	66	THR
1	XA	76	GLU
1	XA	94	LEU
1	XA	96	LEU
1	XA	108	VAL
1	ZA	27	VAL
1	ZA	96	LEU
1	ZA	162	VAL
1	ZA	167	VAL
1	AB	41	LYS
1	AB	44	LYS
1	AB	62	THR
1	AB	66	THR
1	AB	76	GLU
1	AB	94	LEU
1	AB	96	LEU
1	AB	108	VAL

Continued on next page...

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Mol	Chain	Res	Type
1	CB	27	VAL
1	CB	96	LEU
1	CB	162	VAL
1	CB	167	VAL
1	DB	41	LYS
1	DB	44	LYS
1	DB	62	THR
1	DB	66	THR
1	DB	76	GLU
1	DB	94	LEU
1	DB	96	LEU
1	DB	108	VAL
1	FB	27	VAL
1	FB	96	LEU
1	FB	162	VAL
1	FB	167	VAL
1	GB	41	LYS
1	GB	44	LYS
1	GB	62	THR
1	GB	66	THR
1	GB	76	GLU
1	GB	94	LEU
1	GB	96	LEU
1	GB	108	VAL
1	IB	27	VAL
1	IB	96	LEU
1	IB	162	VAL
1	IB	167	VAL
1	JB	41	LYS
1	JB	44	LYS
1	JB	62	THR
1	JB	66	THR
1	JB	76	GLU
1	JB	94	LEU
1	JB	96	LEU
1	JB	108	VAL
1	LB	27	VAL
1	LB	96	LEU
1	LB	162	VAL
1	LB	167	VAL
1	MB	41	LYS
1	MB	44	LYS

Continued on next page...

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Mol	Chain	Res	Type
1	MB	62	THR
1	MB	66	THR
1	MB	76	GLU
1	MB	94	LEU
1	MB	96	LEU
1	MB	108	VAL
1	OB	27	VAL
1	OB	96	LEU
1	OB	162	VAL
1	OB	167	VAL
1	PB	41	LYS
1	PB	44	LYS
1	PB	62	THR
1	PB	66	THR
1	PB	76	GLU
1	PB	94	LEU
1	PB	96	LEU
1	PB	108	VAL
1	RB	27	VAL
1	RB	96	LEU
1	RB	162	VAL
1	RB	167	VAL
1	SB	41	LYS
1	SB	44	LYS
1	SB	62	THR
1	SB	66	THR
1	SB	76	GLU
1	SB	94	LEU
1	SB	96	LEU
1	SB	108	VAL
1	UB	27	VAL
1	UB	96	LEU
1	UB	162	VAL
1	UB	167	VAL
1	VB	41	LYS
1	VB	44	LYS
1	VB	62	THR
1	VB	66	THR
1	VB	76	GLU
1	VB	94	LEU
1	VB	96	LEU
1	VB	108	VAL

Continued on next page...

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Mol	Chain	Res	Type
1	XB	27	VAL
1	XB	96	LEU
1	XB	162	VAL
1	XB	167	VAL
1	YB	41	LYS
1	YB	44	LYS
1	YB	62	THR
1	YB	66	THR
1	YB	76	GLU
1	YB	94	LEU
1	YB	96	LEU
1	YB	108	VAL
1	AC	27	VAL
1	AC	96	LEU
1	AC	162	VAL
1	AC	167	VAL
1	BC	41	LYS
1	BC	44	LYS
1	BC	62	THR
1	BC	66	THR
1	BC	76	GLU
1	BC	94	LEU
1	BC	96	LEU
1	BC	108	VAL
1	DC	27	VAL
1	DC	96	LEU
1	DC	162	VAL
1	DC	167	VAL
1	EC	41	LYS
1	EC	44	LYS
1	EC	62	THR
1	EC	66	THR
1	EC	76	GLU
1	EC	94	LEU
1	EC	96	LEU
1	EC	108	VAL
1	GC	27	VAL
1	GC	96	LEU
1	GC	162	VAL
1	GC	167	VAL
1	HC	41	LYS
1	HC	44	LYS

Continued on next page...

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Mol	Chain	Res	Type
1	HC	62	THR
1	HC	66	THR
1	HC	76	GLU
1	HC	94	LEU
1	HC	96	LEU
1	HC	108	VAL
1	JC	27	VAL
1	JC	96	LEU
1	JC	162	VAL
1	JC	167	VAL
1	KC	41	LYS
1	KC	44	LYS
1	KC	62	THR
1	KC	66	THR
1	KC	76	GLU
1	KC	94	LEU
1	KC	96	LEU
1	KC	108	VAL
1	MC	27	VAL
1	MC	96	LEU
1	MC	162	VAL
1	MC	167	VAL
1	NC	41	LYS
1	NC	44	LYS
1	NC	62	THR
1	NC	66	THR
1	NC	76	GLU
1	NC	94	LEU
1	NC	96	LEU
1	NC	108	VAL
1	PC	27	VAL
1	PC	96	LEU
1	PC	162	VAL
1	PC	167	VAL
1	QC	41	LYS
1	QC	44	LYS
1	QC	62	THR
1	QC	66	THR
1	QC	76	GLU
1	QC	94	LEU
1	QC	96	LEU
1	QC	108	VAL

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Mol	Chain	Res	Type
1	SC	27	VAL
1	SC	96	LEU
1	SC	162	VAL
1	SC	167	VAL
1	TC	41	LYS
1	TC	44	LYS
1	TC	62	THR
1	TC	66	THR
1	TC	76	GLU
1	TC	94	LEU
1	TC	96	LEU
1	TC	108	VAL
1	VC	27	VAL
1	VC	96	LEU
1	VC	162	VAL
1	VC	167	VAL
1	WC	41	LYS
1	WC	44	LYS
1	WC	62	THR
1	WC	66	THR
1	WC	76	GLU
1	WC	94	LEU
1	WC	96	LEU
1	WC	108	VAL
1	YC	27	VAL
1	YC	96	LEU
1	YC	162	VAL
1	YC	167	VAL
1	ZC	41	LYS
1	ZC	44	LYS
1	ZC	62	THR
1	ZC	66	THR
1	ZC	76	GLU
1	ZC	94	LEU
1	ZC	96	LEU
1	ZC	108	VAL
1	BD	27	VAL
1	BD	96	LEU
1	BD	162	VAL
1	BD	167	VAL
1	CD	41	LYS
1	CD	44	LYS

Continued on next page...

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Mol	Chain	Res	Type
1	CD	62	THR
1	CD	66	THR
1	CD	76	GLU
1	CD	94	LEU
1	CD	96	LEU
1	CD	108	VAL
1	ED	27	VAL
1	ED	96	LEU
1	ED	162	VAL
1	ED	167	VAL
1	FD	41	LYS
1	FD	44	LYS
1	FD	62	THR
1	FD	66	THR
1	FD	76	GLU
1	FD	94	LEU
1	FD	96	LEU
1	FD	108	VAL
1	HD	27	VAL
1	HD	96	LEU
1	HD	162	VAL
1	HD	167	VAL
1	ID	41	LYS
1	ID	44	LYS
1	ID	62	THR
1	ID	66	THR
1	ID	76	GLU
1	ID	94	LEU
1	ID	96	LEU
1	ID	108	VAL
1	KD	27	VAL
1	KD	96	LEU
1	KD	162	VAL
1	KD	167	VAL
1	LD	41	LYS
1	LD	44	LYS
1	LD	62	THR
1	LD	66	THR
1	LD	76	GLU
1	LD	94	LEU
1	LD	96	LEU
1	LD	108	VAL

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Mol	Chain	Res	Type
1	ND	27	VAL
1	ND	96	LEU
1	ND	162	VAL
1	ND	167	VAL
1	OD	41	LYS
1	OD	44	LYS
1	OD	62	THR
1	OD	66	THR
1	OD	76	GLU
1	OD	94	LEU
1	OD	96	LEU
1	OD	108	VAL
1	QD	27	VAL
1	QD	96	LEU
1	QD	162	VAL
1	QD	167	VAL
1	RD	41	LYS
1	RD	44	LYS
1	RD	62	THR
1	RD	66	THR
1	RD	76	GLU
1	RD	94	LEU
1	RD	96	LEU
1	RD	108	VAL
1	TD	27	VAL
1	TD	96	LEU
1	TD	162	VAL
1	TD	167	VAL
1	UD	41	LYS
1	UD	44	LYS
1	UD	62	THR
1	UD	66	THR
1	UD	76	GLU
1	UD	94	LEU
1	UD	96	LEU
1	UD	108	VAL
1	WD	27	VAL
1	WD	96	LEU
1	WD	162	VAL
1	WD	167	VAL
1	XD	41	LYS
1	XD	44	LYS

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Mol	Chain	Res	Type
1	XD	62	THR
1	XD	66	THR
1	XD	76	GLU
1	XD	94	LEU
1	XD	96	LEU
1	XD	108	VAL
1	ZD	27	VAL
1	ZD	96	LEU
1	ZD	162	VAL
1	ZD	167	VAL
1	AE	41	LYS
1	AE	44	LYS
1	AE	62	THR
1	AE	66	THR
1	AE	76	GLU
1	AE	94	LEU
1	AE	96	LEU
1	AE	108	VAL
1	CE	27	VAL
1	CE	96	LEU
1	CE	162	VAL
1	CE	167	VAL
1	DE	41	LYS
1	DE	44	LYS
1	DE	62	THR
1	DE	66	THR
1	DE	76	GLU
1	DE	94	LEU
1	DE	96	LEU
1	DE	108	VAL
1	FE	27	VAL
1	FE	96	LEU
1	FE	162	VAL
1	FE	167	VAL
1	GE	41	LYS
1	GE	44	LYS
1	GE	62	THR
1	GE	66	THR
1	GE	76	GLU
1	GE	94	LEU
1	GE	96	LEU
1	GE	108	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	IE	27	VAL
1	IE	96	LEU
1	IE	162	VAL
1	IE	167	VAL
1	JE	41	LYS
1	JE	44	LYS
1	JE	62	THR
1	JE	66	THR
1	JE	76	GLU
1	JE	94	LEU
1	JE	96	LEU
1	JE	108	VAL
1	LE	27	VAL
1	LE	96	LEU
1	LE	162	VAL
1	LE	167	VAL
1	ME	41	LYS
1	ME	44	LYS
1	ME	62	THR
1	ME	66	THR
1	ME	76	GLU
1	ME	94	LEU
1	ME	96	LEU
1	ME	108	VAL
1	OE	27	VAL
1	OE	96	LEU
1	OE	162	VAL
1	OE	167	VAL
1	PE	41	LYS
1	PE	44	LYS
1	PE	62	THR
1	PE	66	THR
1	PE	76	GLU
1	PE	94	LEU
1	PE	96	LEU
1	PE	108	VAL
1	RE	27	VAL
1	RE	96	LEU
1	RE	162	VAL
1	RE	167	VAL
1	SE	41	LYS
1	SE	44	LYS

Continued on next page...

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Mol	Chain	Res	Type
1	SE	62	THR
1	SE	66	THR
1	SE	76	GLU
1	SE	94	LEU
1	SE	96	LEU
1	SE	108	VAL
1	UE	27	VAL
1	UE	96	LEU
1	UE	162	VAL
1	UE	167	VAL
1	VE	41	LYS
1	VE	44	LYS
1	VE	62	THR
1	VE	66	THR
1	VE	76	GLU
1	VE	94	LEU
1	VE	96	LEU
1	VE	108	VAL
1	XE	27	VAL
1	XE	96	LEU
1	XE	162	VAL
1	XE	167	VAL
1	YE	41	LYS
1	YE	44	LYS
1	YE	62	THR
1	YE	66	THR
1	YE	76	GLU
1	YE	94	LEU
1	YE	96	LEU
1	YE	108	VAL
1	AF	27	VAL
1	AF	96	LEU
1	AF	162	VAL
1	AF	167	VAL
1	BF	41	LYS
1	BF	44	LYS
1	BF	62	THR
1	BF	66	THR
1	BF	76	GLU
1	BF	94	LEU
1	BF	96	LEU
1	BF	108	VAL

Continued on next page...

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Mol	Chain	Res	Type
1	DF	27	VAL
1	DF	96	LEU
1	DF	162	VAL
1	DF	167	VAL
1	EF	41	LYS
1	EF	44	LYS
1	EF	62	THR
1	EF	66	THR
1	EF	76	GLU
1	EF	94	LEU
1	EF	96	LEU
1	EF	108	VAL
1	GF	27	VAL
1	GF	96	LEU
1	GF	162	VAL
1	GF	167	VAL
1	HF	41	LYS
1	HF	44	LYS
1	HF	62	THR
1	HF	66	THR
1	HF	76	GLU
1	HF	94	LEU
1	HF	96	LEU
1	HF	108	VAL
1	JF	27	VAL
1	JF	96	LEU
1	JF	162	VAL
1	JF	167	VAL
1	KF	41	LYS
1	KF	44	LYS
1	KF	62	THR
1	KF	66	THR
1	KF	76	GLU
1	KF	94	LEU
1	KF	96	LEU
1	KF	108	VAL
1	MF	27	VAL
1	MF	96	LEU
1	MF	162	VAL
1	MF	167	VAL
1	NF	41	LYS
1	NF	44	LYS

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Mol	Chain	Res	Type
1	NF	62	THR
1	NF	66	THR
1	NF	76	GLU
1	NF	94	LEU
1	NF	96	LEU
1	NF	108	VAL
1	PF	27	VAL
1	PF	96	LEU
1	PF	162	VAL
1	PF	167	VAL
1	QF	41	LYS
1	QF	44	LYS
1	QF	62	THR
1	QF	66	THR
1	QF	76	GLU
1	QF	94	LEU
1	QF	96	LEU
1	QF	108	VAL
1	SF	27	VAL
1	SF	96	LEU
1	SF	162	VAL
1	SF	167	VAL
1	TF	41	LYS
1	TF	44	LYS
1	TF	62	THR
1	TF	66	THR
1	TF	76	GLU
1	TF	94	LEU
1	TF	96	LEU
1	TF	108	VAL
1	VF	27	VAL
1	VF	96	LEU
1	VF	162	VAL
1	VF	167	VAL
1	WF	41	LYS
1	WF	44	LYS
1	WF	62	THR
1	WF	66	THR
1	WF	76	GLU
1	WF	94	LEU
1	WF	96	LEU
1	WF	108	VAL

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Mol	Chain	Res	Type
1	YF	27	VAL
1	YF	96	LEU
1	YF	162	VAL
1	YF	167	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (166) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	82	ASN
1	B	153	GLN
1	C	28	GLN
1	E	82	ASN
1	E	153	GLN
1	F	28	GLN
1	H	82	ASN
1	I	28	GLN
1	K	82	ASN
1	K	153	GLN
1	L	28	GLN
1	N	82	ASN
1	O	28	GLN
1	Q	82	ASN
1	R	28	GLN
1	T	82	ASN
1	V	28	GLN
1	X	82	ASN
1	X	153	GLN
1	Y	28	GLN
1	AA	82	ASN
1	AA	153	GLN
1	BA	28	GLN
1	DA	82	ASN
1	EA	28	GLN
1	GA	82	ASN
1	GA	153	GLN
1	HA	28	GLN
1	JA	82	ASN
1	JA	153	GLN
1	KA	28	GLN
1	MA	82	ASN
1	NA	28	GLN
1	PA	82	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	PA	153	GLN
1	QA	28	GLN
1	SA	82	ASN
1	SA	153	GLN
1	TA	28	GLN
1	VA	82	ASN
1	WA	28	GLN
1	YA	82	ASN
1	YA	153	GLN
1	ZA	28	GLN
1	BB	82	ASN
1	BB	153	GLN
1	CB	28	GLN
1	EB	82	ASN
1	EB	153	GLN
1	FB	28	GLN
1	HB	82	ASN
1	IB	28	GLN
1	KB	82	ASN
1	LB	28	GLN
1	NB	82	ASN
1	NB	153	GLN
1	OB	28	GLN
1	QB	82	ASN
1	QB	153	GLN
1	RB	28	GLN
1	TB	82	ASN
1	TB	153	GLN
1	UB	28	GLN
1	WB	82	ASN
1	XB	28	GLN
1	ZB	82	ASN
1	ZB	153	GLN
1	AC	28	GLN
1	CC	82	ASN
1	CC	153	GLN
1	DC	28	GLN
1	FC	82	ASN
1	FC	153	GLN
1	GC	28	GLN
1	IC	82	ASN
1	IC	153	GLN

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Mol	Chain	Res	Type
1	JC	28	GLN
1	LC	82	ASN
1	MC	28	GLN
1	OC	82	ASN
1	OC	153	GLN
1	PC	28	GLN
1	RC	82	ASN
1	RC	153	GLN
1	SC	28	GLN
1	UC	82	ASN
1	UC	153	GLN
1	VC	28	GLN
1	XC	82	ASN
1	XC	153	GLN
1	YC	28	GLN
1	AD	82	ASN
1	AD	153	GLN
1	BD	28	GLN
1	DD	82	ASN
1	ED	28	GLN
1	GD	82	ASN
1	GD	153	GLN
1	HD	28	GLN
1	JD	82	ASN
1	JD	153	GLN
1	KD	28	GLN
1	MD	82	ASN
1	MD	153	GLN
1	ND	28	GLN
1	PD	82	ASN
1	PD	153	GLN
1	QD	28	GLN
1	SD	82	ASN
1	SD	153	GLN
1	TD	28	GLN
1	VD	82	ASN
1	VD	153	GLN
1	WD	28	GLN
1	YD	82	ASN
1	YD	153	GLN
1	ZD	28	GLN
1	BE	82	ASN

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Mol	Chain	Res	Type
1	BE	153	GLN
1	CE	28	GLN
1	EE	82	ASN
1	EE	153	GLN
1	FE	28	GLN
1	HE	82	ASN
1	HE	153	GLN
1	IE	28	GLN
1	KE	82	ASN
1	KE	153	GLN
1	LE	28	GLN
1	NE	82	ASN
1	NE	153	GLN
1	OE	28	GLN
1	QE	82	ASN
1	QE	153	GLN
1	RE	28	GLN
1	TE	82	ASN
1	TE	153	GLN
1	UE	28	GLN
1	WE	82	ASN
1	WE	153	GLN
1	XE	28	GLN
1	ZE	82	ASN
1	ZE	153	GLN
1	AF	28	GLN
1	CF	82	ASN
1	CF	153	GLN
1	DF	28	GLN
1	FF	82	ASN
1	GF	28	GLN
1	IF	82	ASN
1	IF	153	GLN
1	JF	28	GLN
1	LF	82	ASN
1	LF	153	GLN
1	MF	28	GLN
1	OF	82	ASN
1	OF	153	GLN
1	PF	28	GLN
1	RF	82	ASN
1	RF	153	GLN

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Mol	Chain	Res	Type
1	SF	28	GLN
1	UF	82	ASN
1	VF	28	GLN
1	XF	82	ASN
1	XF	153	GLN
1	YF	28	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

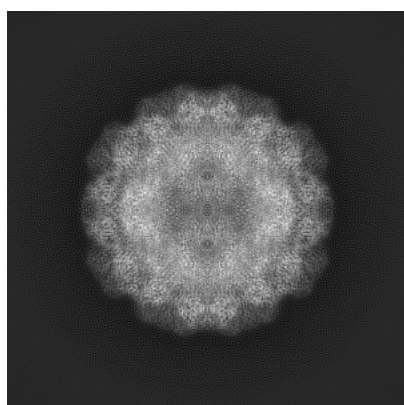
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13344. These allow visual inspection of the internal detail of the map and identification of artifacts.

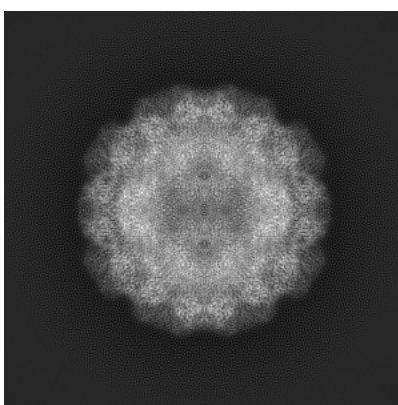
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

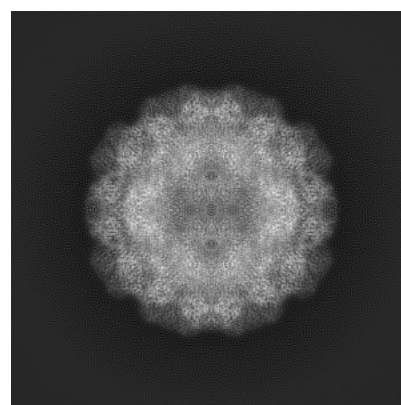
6.1.1 Primary map



X



Y

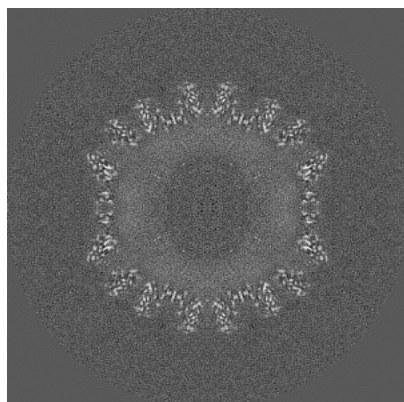


Z

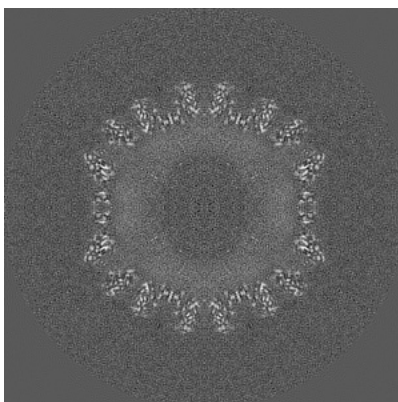
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

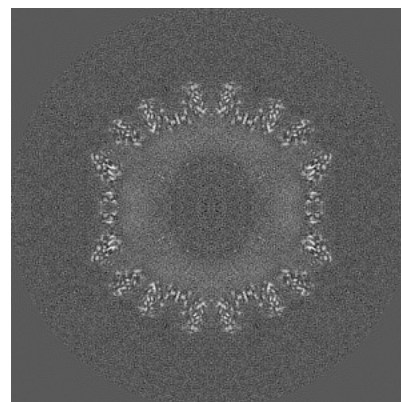
6.2.1 Primary map



X Index: 256



Y Index: 256

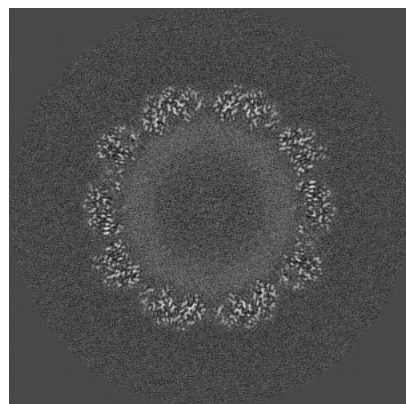


Z Index: 256

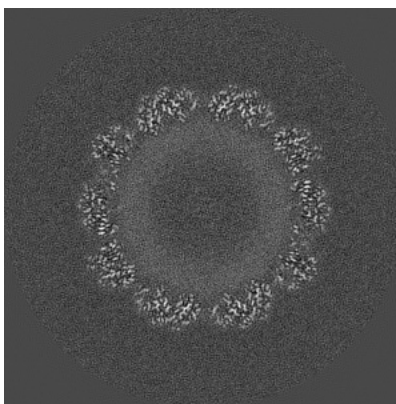
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

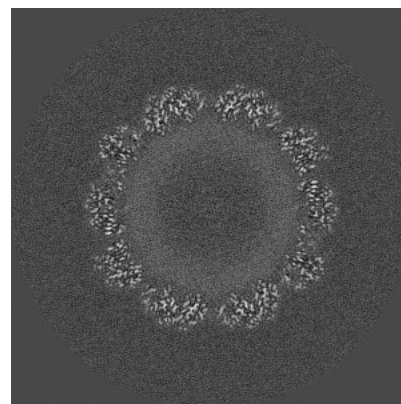
6.3.1 Primary map



X Index: 230



Y Index: 230

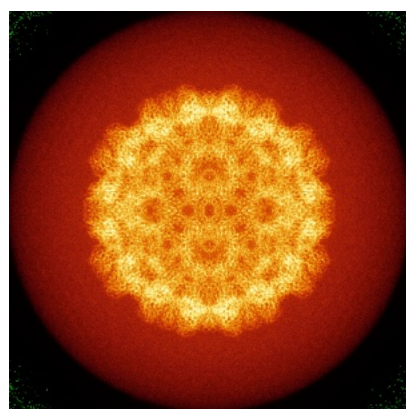


Z Index: 230

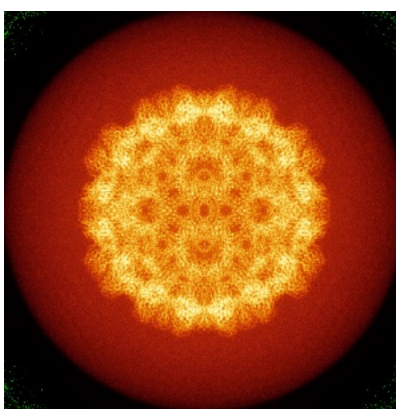
The images above show the largest variance slices of the map in three orthogonal directions.

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

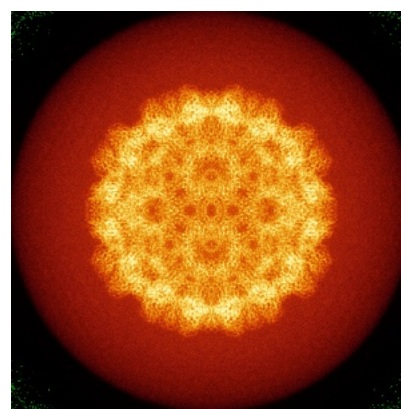
6.4.1 Primary map



X



Y

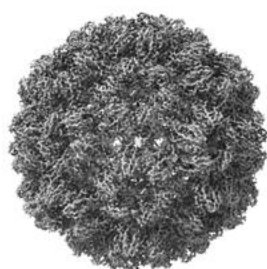


Z

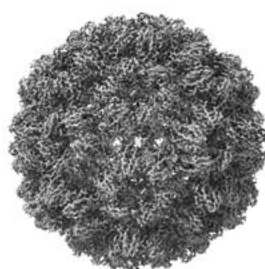
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

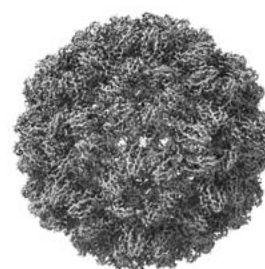
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

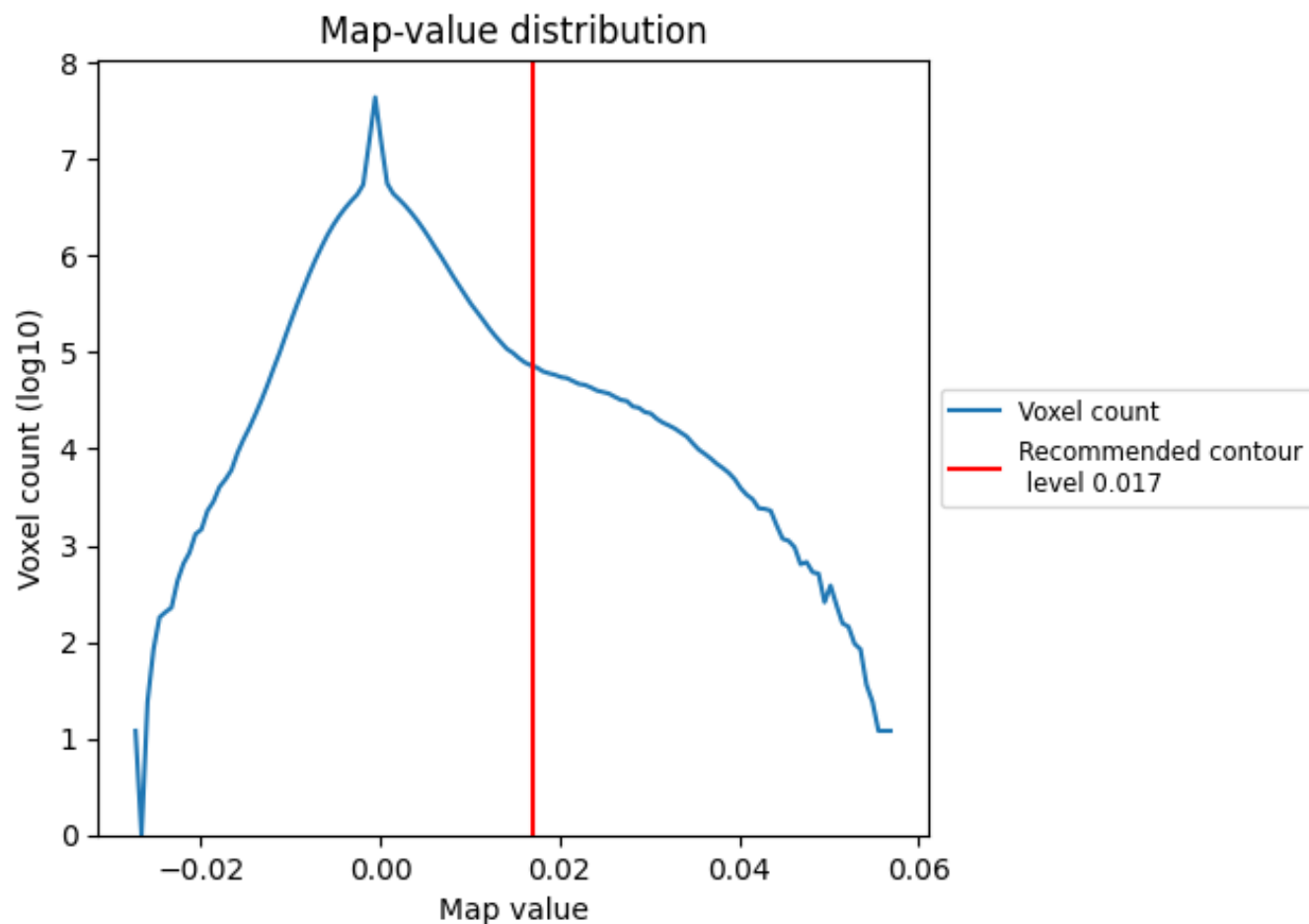
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

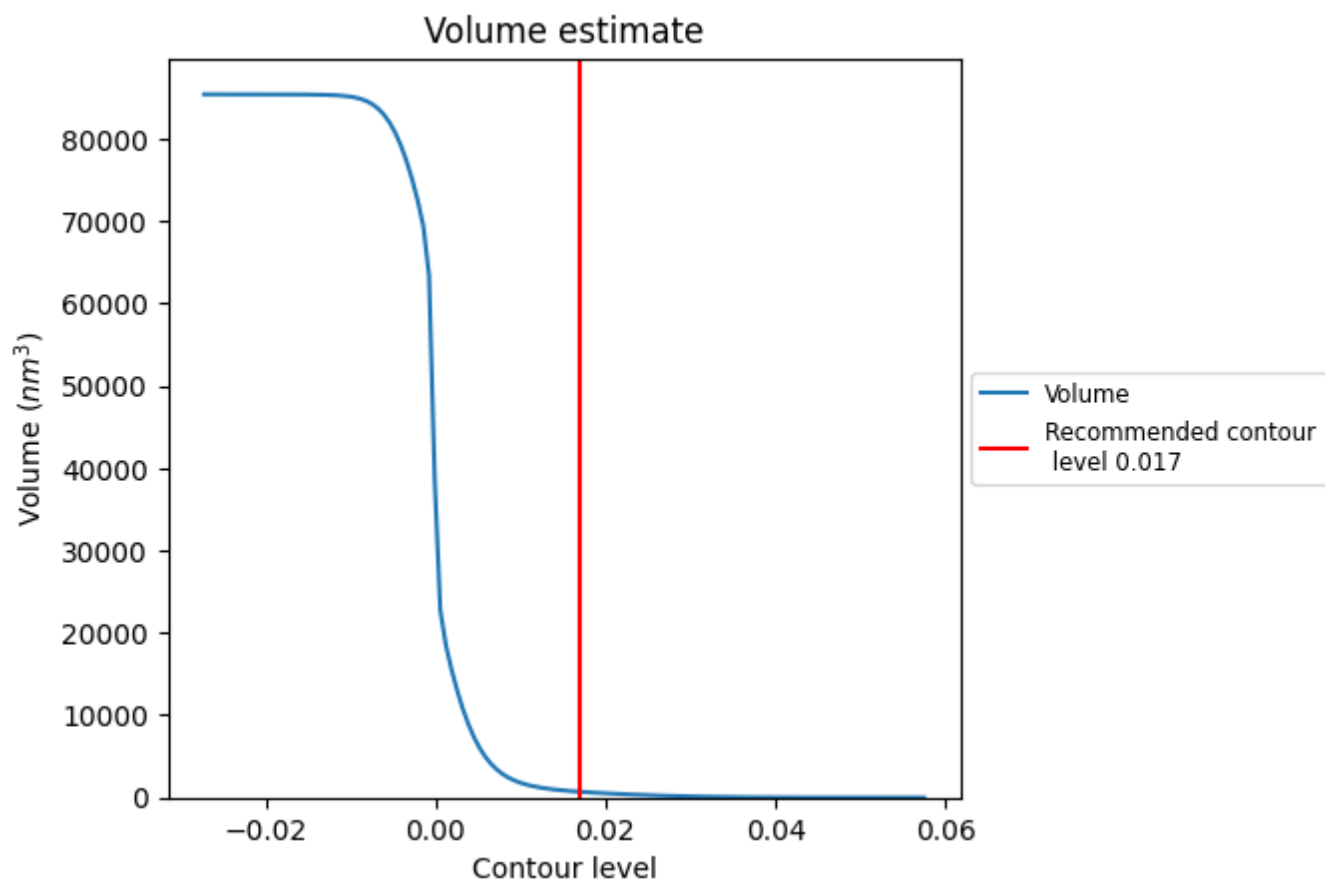
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

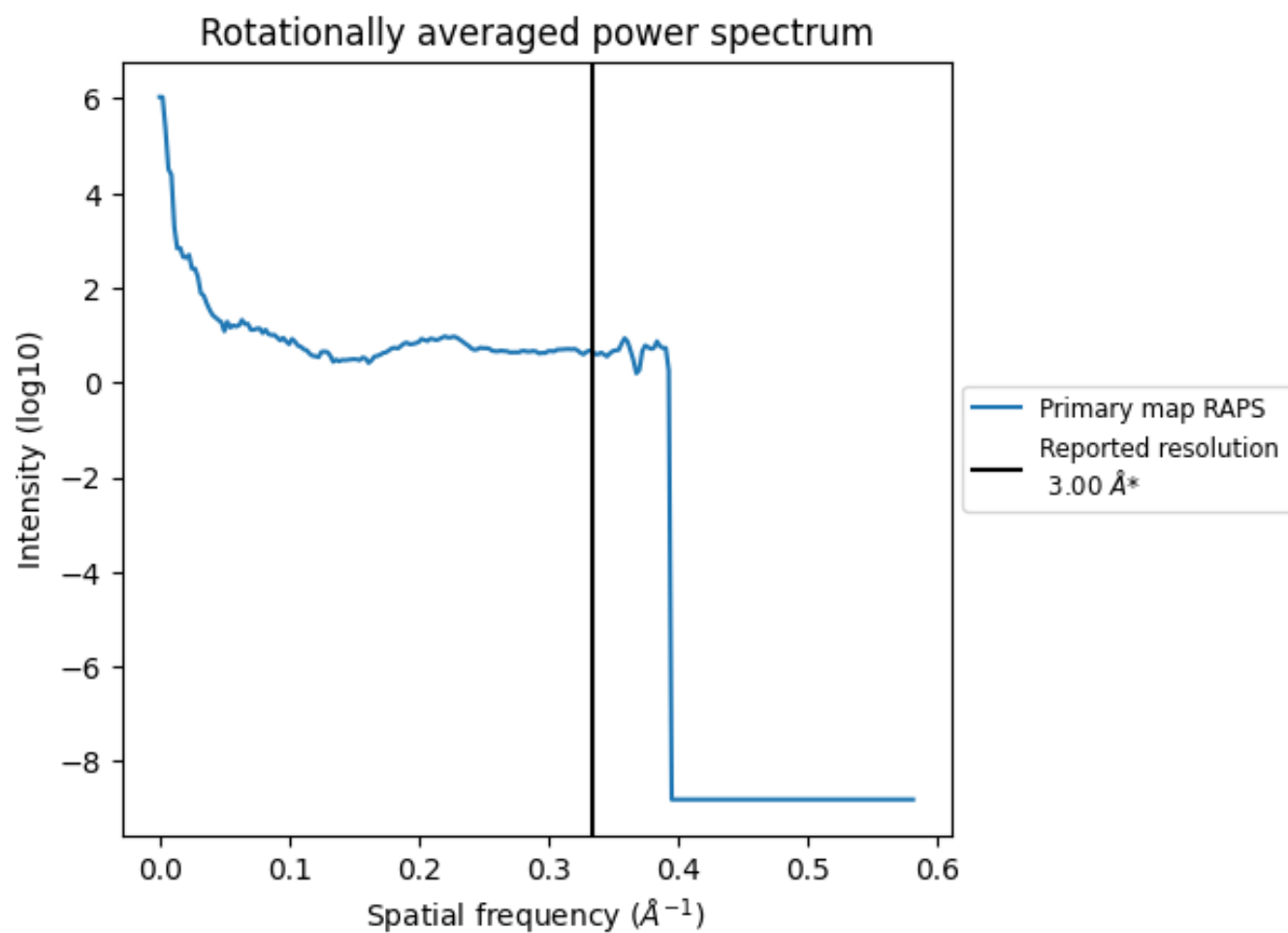
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 702 nm³; this corresponds to an approximate mass of 634 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

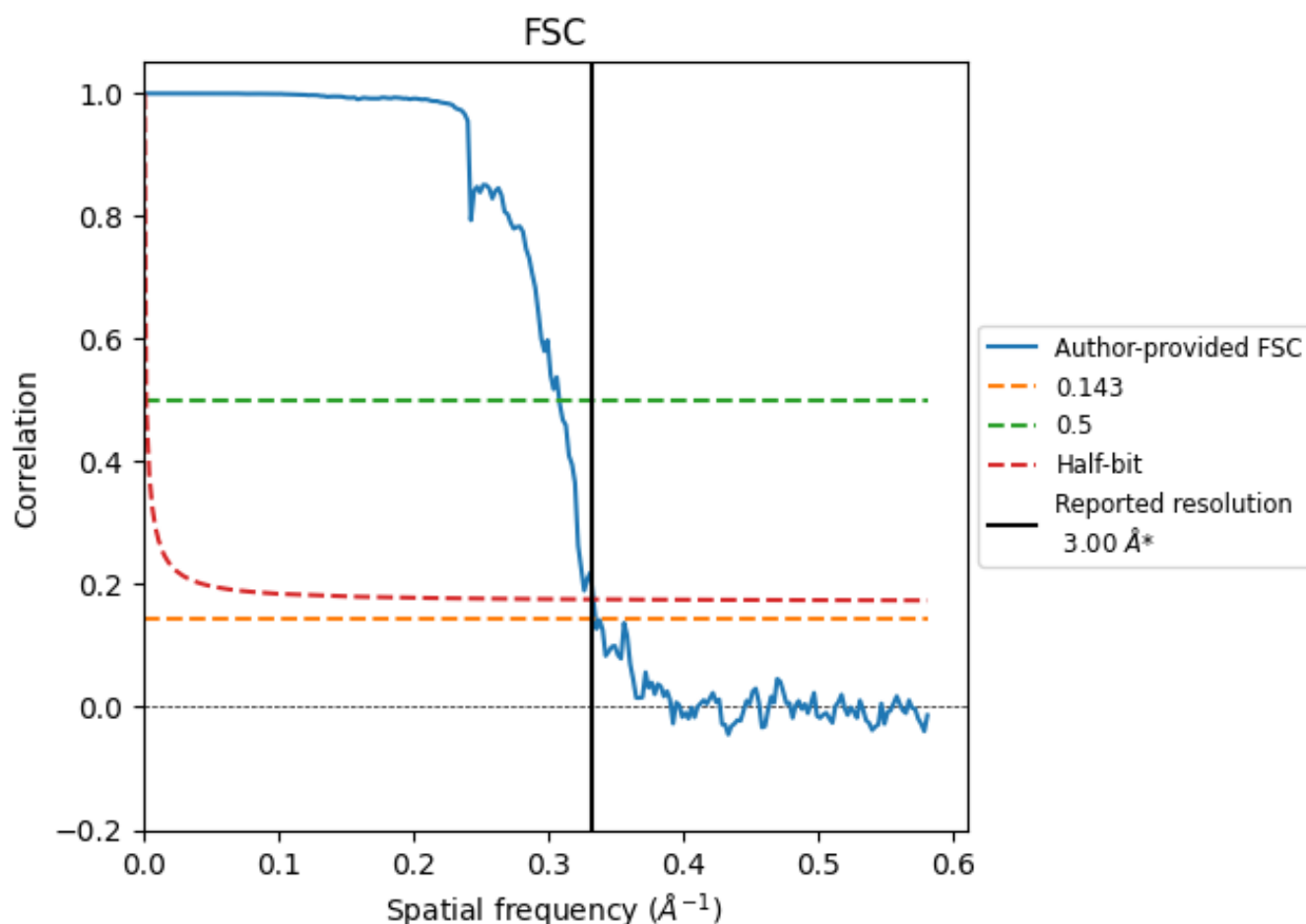


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

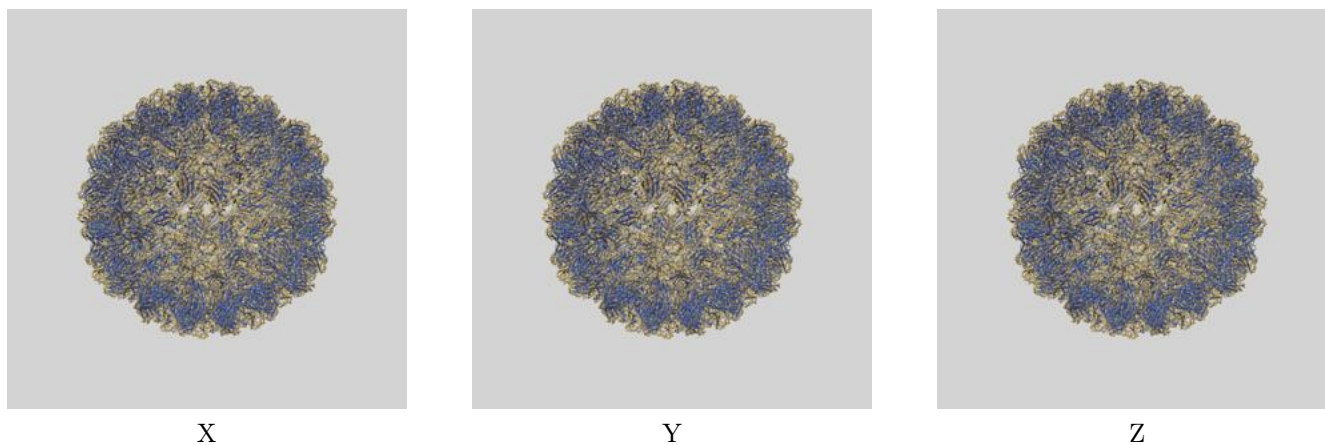
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.24	2.99
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

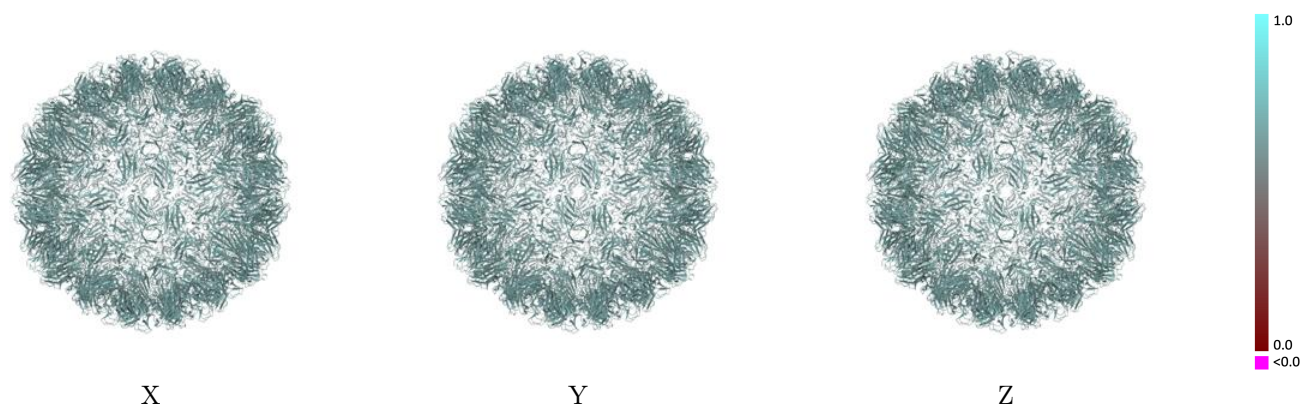
This section contains information regarding the fit between EMDB map EMD-13344 and PDB model 7PE1. Per-residue inclusion information can be found in [section 3](#) on [page 46](#).

9.1 Map-model overlay [i](#)



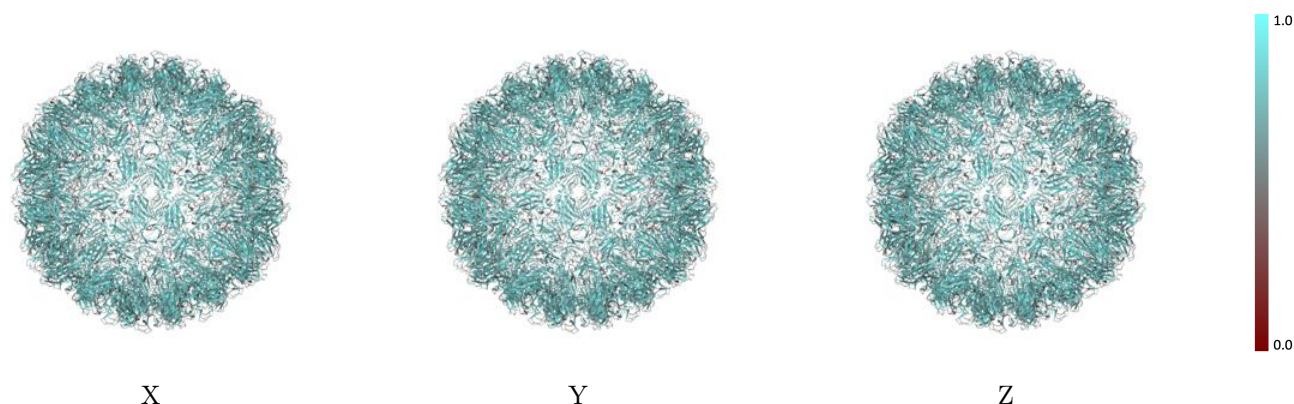
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



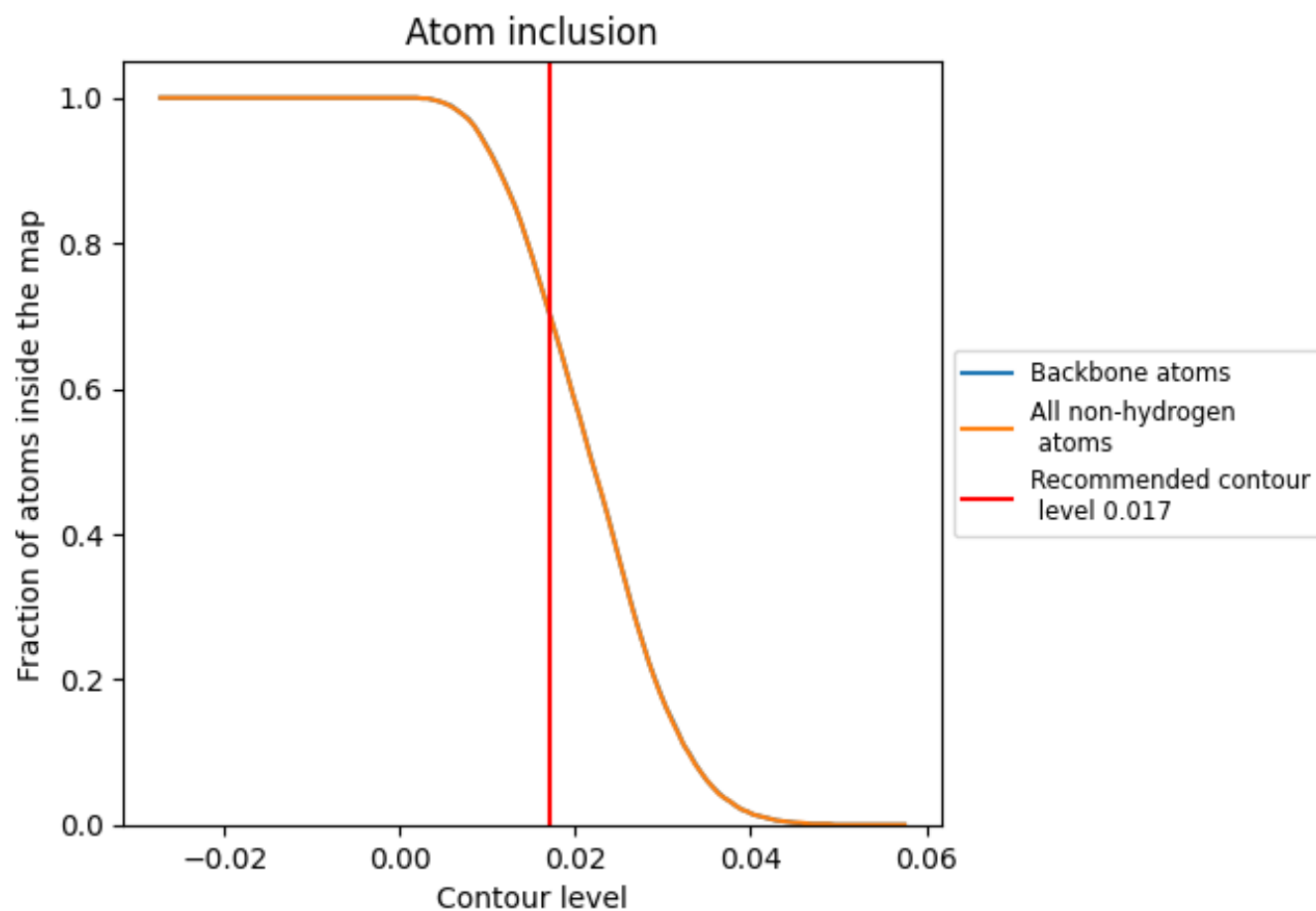
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 71% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7060	 0.6260
A	 0.7070	 0.6270
AA	 0.7130	 0.6270
AB	 0.7010	 0.6250
AC	 0.7200	 0.6260
AD	 0.7160	 0.6290
AE	 0.7030	 0.6270
AF	 0.7090	 0.6250
B	 0.7250	 0.6300
BA	 0.7090	 0.6230
BB	 0.7170	 0.6300
BC	 0.6910	 0.6230
BD	 0.7080	 0.6250
BE	 0.7130	 0.6260
BF	 0.7010	 0.6260
C	 0.7200	 0.6250
CA	 0.6970	 0.6220
CB	 0.7150	 0.6230
CC	 0.7210	 0.6290
CD	 0.7070	 0.6280
CE	 0.7090	 0.6230
CF	 0.7170	 0.6300
D	 0.6910	 0.6240
DA	 0.7160	 0.6270
DB	 0.7030	 0.6250
DC	 0.7090	 0.6230
DD	 0.7250	 0.6310
DE	 0.6970	 0.6230
DF	 0.7150	 0.6230
E	 0.7210	 0.6290
EA	 0.7080	 0.6210
EB	 0.7130	 0.6270
EC	 0.7010	 0.6250
ED	 0.7200	 0.6260
EE	 0.7160	 0.6270



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Chain	Atom inclusion	Q-score
EF	 0.7030	 0.6260
F	 0.7090	 0.6240
FA	 0.7070	 0.6270
FB	 0.7090	 0.6230
FC	 0.7170	 0.6250
FD	 0.6910	 0.6260
FE	 0.7080	 0.6230
FF	 0.7130	 0.6270
G	 0.7010	 0.6250
GA	 0.7250	 0.6300
GB	 0.6970	 0.6240
GC	 0.7150	 0.6230
GD	 0.7220	 0.6270
GE	 0.7070	 0.6270
GF	 0.7090	 0.6240
H	 0.7170	 0.6290
HA	 0.7200	 0.6250
HB	 0.7160	 0.6260
HC	 0.7030	 0.6250
HD	 0.7090	 0.6230
HE	 0.7250	 0.6310
HF	 0.6970	 0.6240
I	 0.7150	 0.6230
IA	 0.6910	 0.6240
IB	 0.7080	 0.6220
IC	 0.7130	 0.6270
ID	 0.7010	 0.6250
IE	 0.7200	 0.6260
IF	 0.7160	 0.6290
J	 0.7030	 0.6250
JA	 0.7220	 0.6270
JB	 0.7070	 0.6270
JC	 0.7090	 0.6220
JD	 0.7170	 0.6250
JE	 0.6910	 0.6250
JF	 0.7080	 0.6230
K	 0.7130	 0.6280
KA	 0.7090	 0.6220
KB	 0.7250	 0.6300
KC	 0.6970	 0.6240
KD	 0.7150	 0.6240
KE	 0.7220	 0.6270

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Chain	Atom inclusion	Q-score
KF	 0.7070	 0.6280
L	 0.7090	 0.6220
LA	 0.7010	 0.6250
LB	 0.7200	 0.6270
LC	 0.7160	 0.6290
LD	 0.7030	 0.6260
LE	 0.7090	 0.6240
LF	 0.7250	 0.6300
M	 0.6970	 0.6240
MA	 0.7170	 0.6280
MB	 0.6910	 0.6250
MC	 0.7080	 0.6230
MD	 0.7140	 0.6290
ME	 0.7010	 0.6260
MF	 0.7200	 0.6270
N	 0.7160	 0.6260
NA	 0.7150	 0.6210
NB	 0.7210	 0.6300
NC	 0.7070	 0.6270
ND	 0.7090	 0.6200
NE	 0.7170	 0.6280
NF	 0.6910	 0.6240
O	 0.7080	 0.6230
OA	 0.7030	 0.6230
OB	 0.7090	 0.6230
OC	 0.7250	 0.6310
OD	 0.6970	 0.6240
OE	 0.7150	 0.6210
OF	 0.7210	 0.6270
P	 0.7070	 0.6260
PA	 0.7140	 0.6260
PB	 0.7010	 0.6230
PC	 0.7200	 0.6270
PD	 0.7160	 0.6290
PE	 0.7030	 0.6270
PF	 0.7090	 0.6230
Q	 0.7250	 0.6290
QA	 0.7090	 0.6220
QB	 0.7170	 0.6250
QC	 0.6910	 0.6230
QD	 0.7080	 0.6250
QE	 0.7140	 0.6280

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Chain	Atom inclusion	Q-score
QF	 0.7010	 0.6250
R	 0.7200	 0.6240
RA	 0.6970	 0.6230
RB	 0.7150	 0.6230
RC	 0.7220	 0.6250
RD	 0.7070	 0.6270
RE	 0.7090	 0.6230
RF	 0.7170	 0.6300
S	 0.6910	 0.6220
SA	 0.7160	 0.6280
SB	 0.7030	 0.6240
SC	 0.7090	 0.6230
SD	 0.7250	 0.6320
SE	 0.6970	 0.6250
SF	 0.7150	 0.6220
T	 0.7210	 0.6280
TA	 0.7080	 0.6210
TB	 0.7130	 0.6270
TC	 0.7010	 0.6260
TD	 0.7200	 0.6260
TE	 0.7160	 0.6290
TF	 0.7030	 0.6260
UA	 0.7070	 0.6270
UB	 0.7090	 0.6210
UC	 0.7170	 0.6250
UD	 0.6910	 0.6240
UE	 0.7080	 0.6230
UF	 0.7130	 0.6280
V	 0.7090	 0.6220
VA	 0.7250	 0.6280
VB	 0.6970	 0.6260
VC	 0.7150	 0.6230
VD	 0.7220	 0.6280
VE	 0.7070	 0.6290
VF	 0.7090	 0.6250
W	 0.7010	 0.6230
WA	 0.7200	 0.6260
WB	 0.7160	 0.6290
WC	 0.7030	 0.6250
WD	 0.7090	 0.6230
WE	 0.7250	 0.6320
WF	 0.6970	 0.6240

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Chain	Atom inclusion	Q-score
X	 0.7170	 0.6290
XA	 0.6910	 0.6240
XB	 0.7080	 0.6230
XC	 0.7130	 0.6270
XD	 0.7010	 0.6250
XE	 0.7200	 0.6250
XF	 0.7160	 0.6300
Y	 0.7150	 0.6200
YA	 0.7220	 0.6280
YB	 0.7070	 0.6280
YC	 0.7090	 0.6210
YD	 0.7170	 0.6280
YE	 0.6910	 0.6260
YF	 0.7080	 0.6250
Z	 0.7030	 0.6240
ZA	 0.7090	 0.6220
ZB	 0.7250	 0.6310
ZC	 0.6970	 0.6240
ZD	 0.7150	 0.6220
ZE	 0.7210	 0.6300