



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:00 PM UTC

PDB ID : 7PE2 / pdb_00007pe2
EMDB ID : EMD-13345
Title : Cryo-EM structure of BMV-derived VLP expressed in E. coli (eVLP)
Authors : Ruszkowski, M.; Strugala, A.; Indyka, P.; Urbanowicz, A.
Deposited on : 2021-08-09
Resolution : 3.20 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:

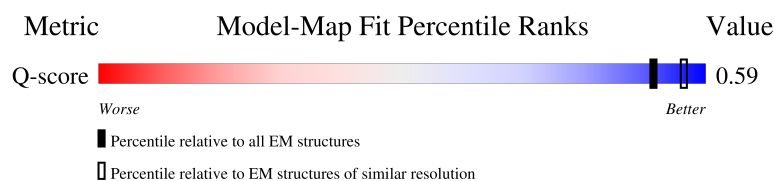
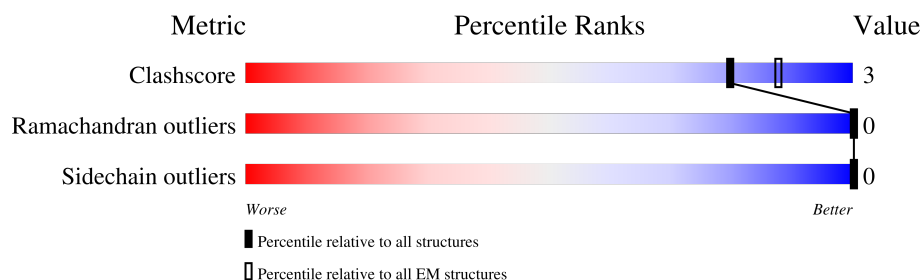
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.20 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	15020 (2.70 - 3.70)

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	
1	AA	192	
1	AB	192	
1	AC	192	

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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	

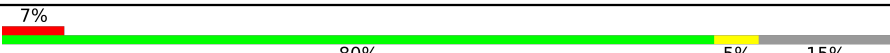
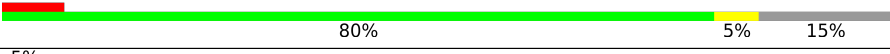
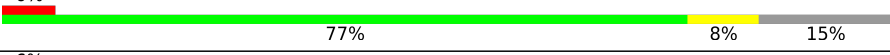
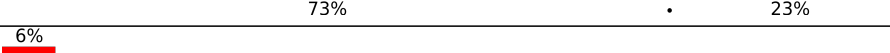
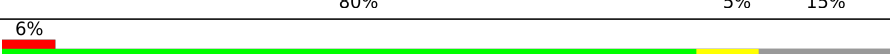
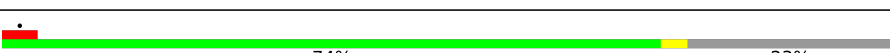
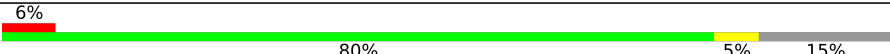
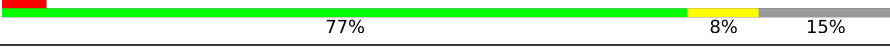
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Mol	Chain	Length	Quality of chain
1	SC	192	
1	SD	192	
1	SE	192	
1	SF	192	
1	T	192	
1	TA	192	
1	TB	192	
1	TC	192	
1	TD	192	
1	TE	192	
1	TF	192	
1	UA	192	
1	UB	192	
1	UC	192	
1	UD	192	
1	UE	192	
1	UF	192	
1	V	192	
1	VA	192	
1	VB	192	
1	VC	192	
1	VD	192	
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	6% 77% 8% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 214200 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	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	B	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	C	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	D	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	E	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	F	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	G	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	H	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	I	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	J	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	K	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	L	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	M	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	N	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	O	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	P	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	Q	163	Total	C	N	O	S	0	0
			1214	780	203	228	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	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	T	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	V	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	W	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	X	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	Y	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	Z	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	AA	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	BA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	CA	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	DA	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	EA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	FA	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	GA	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	HA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	IA	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	JA	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	KA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	LA	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	MA	163	Total	C	N	O	S	0	0
			1214	780	203	228	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	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	PA	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	QA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	RA	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	SA	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	TA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	UA	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	VA	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	WA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	XA	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	YA	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	ZA	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	AB	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	BB	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	CB	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	DB	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	EB	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	FB	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	GB	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	HB	163	Total	C	N	O	S	0	0
			1214	780	203	228	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	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	KB	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	LB	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	MB	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	NB	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	OB	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	PB	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	QB	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	RB	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	SB	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	TB	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	UB	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	VB	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	WB	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	XB	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	YB	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	ZB	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	AC	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	BC	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	CC	163	Total	C	N	O	S	0	0
			1214	780	203	228	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	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	FC	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	GC	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	HC	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	IC	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	JC	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	KC	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	LC	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	MC	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	NC	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	OC	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	PC	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	QC	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	RC	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	SC	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	TC	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	UC	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	VC	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	WC	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	XC	163	Total	C	N	O	S	0	0
			1214	780	203	228	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	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	AD	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	BD	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	CD	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	DD	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	ED	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	FD	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	GD	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	HD	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	ID	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	JD	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	KD	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	LD	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	MD	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	ND	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	OD	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	PD	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	QD	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	RD	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	SD	163	Total	C	N	O	S	0	0
			1214	780	203	228	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	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	VD	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	WD	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	XD	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	YD	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	ZD	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	AE	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	BE	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	CE	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	DE	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	EE	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	FE	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	GE	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	HE	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	IE	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	JE	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	KE	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	LE	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	ME	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	NE	163	Total	C	N	O	S	0	0
			1214	780	203	228	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	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	QE	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	RE	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	SE	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	TE	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	UE	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	VE	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	WE	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	XE	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	YE	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	ZE	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	AF	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	BF	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	CF	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	DF	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	EF	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	FF	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	GF	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	HF	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	IF	163	Total	C	N	O	S	0	0
			1214	780	203	228	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	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	LF	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	MF	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	NF	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	OF	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	PF	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	QF	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	RF	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	SF	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	TF	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	UF	163	Total	C	N	O	S	0	0
			1214	780	203	228	3		
1	VF	164	Total	C	N	O	S	0	0
			1231	792	205	231	3		
1	WF	148	Total	C	N	O	S	0	0
			1122	722	186	211	3		
1	XF	163	Total	C	N	O	S	0	0
			1214	780	203	228	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 Q9QJC1
IA	0	ILE	-	expression tag	UNP Q9QJC1
IA	189	LYS	-	expression tag	UNP Q9QJC1
JA	-2	SER	-	expression tag	UNP Q9QJC1
JA	-1	ASN	-	expression tag	UNP Q9QJC1
JA	0	ILE	-	expression tag	UNP Q9QJC1
JA	189	LYS	-	expression tag	UNP Q9QJC1
KA	-2	SER	-	expression tag	UNP Q9QJC1
KA	-1	ASN	-	expression tag	UNP Q9QJC1
KA	0	ILE	-	expression tag	UNP Q9QJC1
KA	189	LYS	-	expression tag	UNP Q9QJC1
LA	-2	SER	-	expression tag	UNP Q9QJC1
LA	-1	ASN	-	expression tag	UNP Q9QJC1
LA	0	ILE	-	expression tag	UNP Q9QJC1
LA	189	LYS	-	expression tag	UNP Q9QJC1
MA	-2	SER	-	expression tag	UNP Q9QJC1
MA	-1	ASN	-	expression tag	UNP Q9QJC1
MA	0	ILE	-	expression tag	UNP Q9QJC1
MA	189	LYS	-	expression tag	UNP Q9QJC1
NA	-2	SER	-	expression tag	UNP Q9QJC1
NA	-1	ASN	-	expression tag	UNP Q9QJC1
NA	0	ILE	-	expression tag	UNP Q9QJC1
NA	189	LYS	-	expression tag	UNP Q9QJC1
OA	-2	SER	-	expression tag	UNP Q9QJC1
OA	-1	ASN	-	expression tag	UNP Q9QJC1
OA	0	ILE	-	expression tag	UNP Q9QJC1
OA	189	LYS	-	expression tag	UNP Q9QJC1
PA	-2	SER	-	expression tag	UNP Q9QJC1
PA	-1	ASN	-	expression tag	UNP Q9QJC1
PA	0	ILE	-	expression tag	UNP Q9QJC1
PA	189	LYS	-	expression tag	UNP Q9QJC1
QA	-2	SER	-	expression tag	UNP Q9QJC1
QA	-1	ASN	-	expression tag	UNP Q9QJC1
QA	0	ILE	-	expression tag	UNP Q9QJC1
QA	189	LYS	-	expression tag	UNP Q9QJC1
RA	-2	SER	-	expression tag	UNP Q9QJC1
RA	-1	ASN	-	expression tag	UNP Q9QJC1
RA	0	ILE	-	expression tag	UNP Q9QJC1
RA	189	LYS	-	expression tag	UNP Q9QJC1
SA	-2	SER	-	expression tag	UNP Q9QJC1
SA	-1	ASN	-	expression tag	UNP Q9QJC1
SA	0	ILE	-	expression tag	UNP Q9QJC1

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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 Q9QJC1
DB	0	ILE	-	expression tag	UNP Q9QJC1
DB	189	LYS	-	expression tag	UNP Q9QJC1
EB	-2	SER	-	expression tag	UNP Q9QJC1
EB	-1	ASN	-	expression tag	UNP Q9QJC1
EB	0	ILE	-	expression tag	UNP Q9QJC1
EB	189	LYS	-	expression tag	UNP Q9QJC1
FB	-2	SER	-	expression tag	UNP Q9QJC1
FB	-1	ASN	-	expression tag	UNP Q9QJC1
FB	0	ILE	-	expression tag	UNP Q9QJC1
FB	189	LYS	-	expression tag	UNP Q9QJC1
GB	-2	SER	-	expression tag	UNP Q9QJC1
GB	-1	ASN	-	expression tag	UNP Q9QJC1
GB	0	ILE	-	expression tag	UNP Q9QJC1
GB	189	LYS	-	expression tag	UNP Q9QJC1
HB	-2	SER	-	expression tag	UNP Q9QJC1
HB	-1	ASN	-	expression tag	UNP Q9QJC1
HB	0	ILE	-	expression tag	UNP Q9QJC1
HB	189	LYS	-	expression tag	UNP Q9QJC1
IB	-2	SER	-	expression tag	UNP Q9QJC1
IB	-1	ASN	-	expression tag	UNP Q9QJC1
IB	0	ILE	-	expression tag	UNP Q9QJC1
IB	189	LYS	-	expression tag	UNP Q9QJC1
JB	-2	SER	-	expression tag	UNP Q9QJC1
JB	-1	ASN	-	expression tag	UNP Q9QJC1
JB	0	ILE	-	expression tag	UNP Q9QJC1
JB	189	LYS	-	expression tag	UNP Q9QJC1
KB	-2	SER	-	expression tag	UNP Q9QJC1
KB	-1	ASN	-	expression tag	UNP Q9QJC1
KB	0	ILE	-	expression tag	UNP Q9QJC1
KB	189	LYS	-	expression tag	UNP Q9QJC1
LB	-2	SER	-	expression tag	UNP Q9QJC1
LB	-1	ASN	-	expression tag	UNP Q9QJC1
LB	0	ILE	-	expression tag	UNP Q9QJC1
LB	189	LYS	-	expression tag	UNP Q9QJC1
MB	-2	SER	-	expression tag	UNP Q9QJC1
MB	-1	ASN	-	expression tag	UNP Q9QJC1
MB	0	ILE	-	expression tag	UNP Q9QJC1
MB	189	LYS	-	expression tag	UNP Q9QJC1
NB	-2	SER	-	expression tag	UNP Q9QJC1
NB	-1	ASN	-	expression tag	UNP Q9QJC1
NB	0	ILE	-	expression tag	UNP Q9QJC1

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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 Q9QJC1
TC	0	ILE	-	expression tag	UNP Q9QJC1
TC	189	LYS	-	expression tag	UNP Q9QJC1
UC	-2	SER	-	expression tag	UNP Q9QJC1
UC	-1	ASN	-	expression tag	UNP Q9QJC1
UC	0	ILE	-	expression tag	UNP Q9QJC1
UC	189	LYS	-	expression tag	UNP Q9QJC1
VC	-2	SER	-	expression tag	UNP Q9QJC1
VC	-1	ASN	-	expression tag	UNP Q9QJC1
VC	0	ILE	-	expression tag	UNP Q9QJC1
VC	189	LYS	-	expression tag	UNP Q9QJC1
WC	-2	SER	-	expression tag	UNP Q9QJC1
WC	-1	ASN	-	expression tag	UNP Q9QJC1
WC	0	ILE	-	expression tag	UNP Q9QJC1
WC	189	LYS	-	expression tag	UNP Q9QJC1
XC	-2	SER	-	expression tag	UNP Q9QJC1
XC	-1	ASN	-	expression tag	UNP Q9QJC1
XC	0	ILE	-	expression tag	UNP Q9QJC1
XC	189	LYS	-	expression tag	UNP Q9QJC1
YC	-2	SER	-	expression tag	UNP Q9QJC1
YC	-1	ASN	-	expression tag	UNP Q9QJC1
YC	0	ILE	-	expression tag	UNP Q9QJC1
YC	189	LYS	-	expression tag	UNP Q9QJC1
ZC	-2	SER	-	expression tag	UNP Q9QJC1
ZC	-1	ASN	-	expression tag	UNP Q9QJC1
ZC	0	ILE	-	expression tag	UNP Q9QJC1
ZC	189	LYS	-	expression tag	UNP Q9QJC1
AD	-2	SER	-	expression tag	UNP Q9QJC1
AD	-1	ASN	-	expression tag	UNP Q9QJC1
AD	0	ILE	-	expression tag	UNP Q9QJC1
AD	189	LYS	-	expression tag	UNP Q9QJC1
BD	-2	SER	-	expression tag	UNP Q9QJC1
BD	-1	ASN	-	expression tag	UNP Q9QJC1
BD	0	ILE	-	expression tag	UNP Q9QJC1
BD	189	LYS	-	expression tag	UNP Q9QJC1
CD	-2	SER	-	expression tag	UNP Q9QJC1
CD	-1	ASN	-	expression tag	UNP Q9QJC1
CD	0	ILE	-	expression tag	UNP Q9QJC1
CD	189	LYS	-	expression tag	UNP Q9QJC1
DD	-2	SER	-	expression tag	UNP Q9QJC1
DD	-1	ASN	-	expression tag	UNP Q9QJC1
DD	0	ILE	-	expression tag	UNP Q9QJC1

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Chain	Residue	Modelled	Actual	Comment	Reference
DD	189	LYS	-	expression tag	UNP Q9Q CJ1
ED	-2	SER	-	expression tag	UNP Q9Q CJ1
ED	-1	ASN	-	expression tag	UNP Q9Q CJ1
ED	0	ILE	-	expression tag	UNP Q9Q CJ1
ED	189	LYS	-	expression tag	UNP Q9Q CJ1
FD	-2	SER	-	expression tag	UNP Q9Q CJ1
FD	-1	ASN	-	expression tag	UNP Q9Q CJ1
FD	0	ILE	-	expression tag	UNP Q9Q CJ1
FD	189	LYS	-	expression tag	UNP Q9Q CJ1
GD	-2	SER	-	expression tag	UNP Q9Q CJ1
GD	-1	ASN	-	expression tag	UNP Q9Q CJ1
GD	0	ILE	-	expression tag	UNP Q9Q CJ1
GD	189	LYS	-	expression tag	UNP Q9Q CJ1
HD	-2	SER	-	expression tag	UNP Q9Q CJ1
HD	-1	ASN	-	expression tag	UNP Q9Q CJ1
HD	0	ILE	-	expression tag	UNP Q9Q CJ1
HD	189	LYS	-	expression tag	UNP Q9Q CJ1
ID	-2	SER	-	expression tag	UNP Q9Q CJ1
ID	-1	ASN	-	expression tag	UNP Q9Q CJ1
ID	0	ILE	-	expression tag	UNP Q9Q CJ1
ID	189	LYS	-	expression tag	UNP Q9Q CJ1
JD	-2	SER	-	expression tag	UNP Q9Q CJ1
JD	-1	ASN	-	expression tag	UNP Q9Q CJ1
JD	0	ILE	-	expression tag	UNP Q9Q CJ1
JD	189	LYS	-	expression tag	UNP Q9Q CJ1
KD	-2	SER	-	expression tag	UNP Q9Q CJ1
KD	-1	ASN	-	expression tag	UNP Q9Q CJ1
KD	0	ILE	-	expression tag	UNP Q9Q CJ1
KD	189	LYS	-	expression tag	UNP Q9Q CJ1
LD	-2	SER	-	expression tag	UNP Q9Q CJ1
LD	-1	ASN	-	expression tag	UNP Q9Q CJ1
LD	0	ILE	-	expression tag	UNP Q9Q CJ1
LD	189	LYS	-	expression tag	UNP Q9Q CJ1
MD	-2	SER	-	expression tag	UNP Q9Q CJ1
MD	-1	ASN	-	expression tag	UNP Q9Q CJ1
MD	0	ILE	-	expression tag	UNP Q9Q CJ1
MD	189	LYS	-	expression tag	UNP Q9Q CJ1
ND	-2	SER	-	expression tag	UNP Q9Q CJ1
ND	-1	ASN	-	expression tag	UNP Q9Q CJ1
ND	0	ILE	-	expression tag	UNP Q9Q CJ1
ND	189	LYS	-	expression tag	UNP Q9Q CJ1
OD	-2	SER	-	expression tag	UNP Q9Q CJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
OD	-1	ASN	-	expression tag	UNP Q9QJC1
OD	0	ILE	-	expression tag	UNP Q9QJC1
OD	189	LYS	-	expression tag	UNP Q9QJC1
PD	-2	SER	-	expression tag	UNP Q9QJC1
PD	-1	ASN	-	expression tag	UNP Q9QJC1
PD	0	ILE	-	expression tag	UNP Q9QJC1
PD	189	LYS	-	expression tag	UNP Q9QJC1
QD	-2	SER	-	expression tag	UNP Q9QJC1
QD	-1	ASN	-	expression tag	UNP Q9QJC1
QD	0	ILE	-	expression tag	UNP Q9QJC1
QD	189	LYS	-	expression tag	UNP Q9QJC1
RD	-2	SER	-	expression tag	UNP Q9QJC1
RD	-1	ASN	-	expression tag	UNP Q9QJC1
RD	0	ILE	-	expression tag	UNP Q9QJC1
RD	189	LYS	-	expression tag	UNP Q9QJC1
SD	-2	SER	-	expression tag	UNP Q9QJC1
SD	-1	ASN	-	expression tag	UNP Q9QJC1
SD	0	ILE	-	expression tag	UNP Q9QJC1
SD	189	LYS	-	expression tag	UNP Q9QJC1
TD	-2	SER	-	expression tag	UNP Q9QJC1
TD	-1	ASN	-	expression tag	UNP Q9QJC1
TD	0	ILE	-	expression tag	UNP Q9QJC1
TD	189	LYS	-	expression tag	UNP Q9QJC1
UD	-2	SER	-	expression tag	UNP Q9QJC1
UD	-1	ASN	-	expression tag	UNP Q9QJC1
UD	0	ILE	-	expression tag	UNP Q9QJC1
UD	189	LYS	-	expression tag	UNP Q9QJC1
VD	-2	SER	-	expression tag	UNP Q9QJC1
VD	-1	ASN	-	expression tag	UNP Q9QJC1
VD	0	ILE	-	expression tag	UNP Q9QJC1
VD	189	LYS	-	expression tag	UNP Q9QJC1
WD	-2	SER	-	expression tag	UNP Q9QJC1
WD	-1	ASN	-	expression tag	UNP Q9QJC1
WD	0	ILE	-	expression tag	UNP Q9QJC1
WD	189	LYS	-	expression tag	UNP Q9QJC1
XD	-2	SER	-	expression tag	UNP Q9QJC1
XD	-1	ASN	-	expression tag	UNP Q9QJC1
XD	0	ILE	-	expression tag	UNP Q9QJC1
XD	189	LYS	-	expression tag	UNP Q9QJC1
YD	-2	SER	-	expression tag	UNP Q9QJC1
YD	-1	ASN	-	expression tag	UNP Q9QJC1
YD	0	ILE	-	expression tag	UNP Q9QJC1

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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 Q9QJC1
UE	-2	SER	-	expression tag	UNP Q9QJC1
UE	-1	ASN	-	expression tag	UNP Q9QJC1
UE	0	ILE	-	expression tag	UNP Q9QJC1
UE	189	LYS	-	expression tag	UNP Q9QJC1
VE	-2	SER	-	expression tag	UNP Q9QJC1
VE	-1	ASN	-	expression tag	UNP Q9QJC1
VE	0	ILE	-	expression tag	UNP Q9QJC1
VE	189	LYS	-	expression tag	UNP Q9QJC1
WE	-2	SER	-	expression tag	UNP Q9QJC1
WE	-1	ASN	-	expression tag	UNP Q9QJC1
WE	0	ILE	-	expression tag	UNP Q9QJC1
WE	189	LYS	-	expression tag	UNP Q9QJC1
XE	-2	SER	-	expression tag	UNP Q9QJC1
XE	-1	ASN	-	expression tag	UNP Q9QJC1
XE	0	ILE	-	expression tag	UNP Q9QJC1
XE	189	LYS	-	expression tag	UNP Q9QJC1
YE	-2	SER	-	expression tag	UNP Q9QJC1
YE	-1	ASN	-	expression tag	UNP Q9QJC1
YE	0	ILE	-	expression tag	UNP Q9QJC1
YE	189	LYS	-	expression tag	UNP Q9QJC1
ZE	-2	SER	-	expression tag	UNP Q9QJC1
ZE	-1	ASN	-	expression tag	UNP Q9QJC1
ZE	0	ILE	-	expression tag	UNP Q9QJC1
ZE	189	LYS	-	expression tag	UNP Q9QJC1
AF	-2	SER	-	expression tag	UNP Q9QJC1
AF	-1	ASN	-	expression tag	UNP Q9QJC1
AF	0	ILE	-	expression tag	UNP Q9QJC1
AF	189	LYS	-	expression tag	UNP Q9QJC1
BF	-2	SER	-	expression tag	UNP Q9QJC1
BF	-1	ASN	-	expression tag	UNP Q9QJC1
BF	0	ILE	-	expression tag	UNP Q9QJC1
BF	189	LYS	-	expression tag	UNP Q9QJC1
CF	-2	SER	-	expression tag	UNP Q9QJC1
CF	-1	ASN	-	expression tag	UNP Q9QJC1
CF	0	ILE	-	expression tag	UNP Q9QJC1
CF	189	LYS	-	expression tag	UNP Q9QJC1
DF	-2	SER	-	expression tag	UNP Q9QJC1
DF	-1	ASN	-	expression tag	UNP Q9QJC1
DF	0	ILE	-	expression tag	UNP Q9QJC1
DF	189	LYS	-	expression tag	UNP Q9QJC1
EF	-2	SER	-	expression tag	UNP Q9QJC1

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Chain	Residue	Modelled	Actual	Comment	Reference
EF	-1	ASN	-	expression tag	UNP Q9QJC1
EF	0	ILE	-	expression tag	UNP Q9QJC1
EF	189	LYS	-	expression tag	UNP Q9QJC1
FF	-2	SER	-	expression tag	UNP Q9QJC1
FF	-1	ASN	-	expression tag	UNP Q9QJC1
FF	0	ILE	-	expression tag	UNP Q9QJC1
FF	189	LYS	-	expression tag	UNP Q9QJC1
GF	-2	SER	-	expression tag	UNP Q9QJC1
GF	-1	ASN	-	expression tag	UNP Q9QJC1
GF	0	ILE	-	expression tag	UNP Q9QJC1
GF	189	LYS	-	expression tag	UNP Q9QJC1
HF	-2	SER	-	expression tag	UNP Q9QJC1
HF	-1	ASN	-	expression tag	UNP Q9QJC1
HF	0	ILE	-	expression tag	UNP Q9QJC1
HF	189	LYS	-	expression tag	UNP Q9QJC1
IF	-2	SER	-	expression tag	UNP Q9QJC1
IF	-1	ASN	-	expression tag	UNP Q9QJC1
IF	0	ILE	-	expression tag	UNP Q9QJC1
IF	189	LYS	-	expression tag	UNP Q9QJC1
JF	-2	SER	-	expression tag	UNP Q9QJC1
JF	-1	ASN	-	expression tag	UNP Q9QJC1
JF	0	ILE	-	expression tag	UNP Q9QJC1
JF	189	LYS	-	expression tag	UNP Q9QJC1
KF	-2	SER	-	expression tag	UNP Q9QJC1
KF	-1	ASN	-	expression tag	UNP Q9QJC1
KF	0	ILE	-	expression tag	UNP Q9QJC1
KF	189	LYS	-	expression tag	UNP Q9QJC1
LF	-2	SER	-	expression tag	UNP Q9QJC1
LF	-1	ASN	-	expression tag	UNP Q9QJC1
LF	0	ILE	-	expression tag	UNP Q9QJC1
LF	189	LYS	-	expression tag	UNP Q9QJC1
MF	-2	SER	-	expression tag	UNP Q9QJC1
MF	-1	ASN	-	expression tag	UNP Q9QJC1
MF	0	ILE	-	expression tag	UNP Q9QJC1
MF	189	LYS	-	expression tag	UNP Q9QJC1
NF	-2	SER	-	expression tag	UNP Q9QJC1
NF	-1	ASN	-	expression tag	UNP Q9QJC1
NF	0	ILE	-	expression tag	UNP Q9QJC1
NF	189	LYS	-	expression tag	UNP Q9QJC1
OF	-2	SER	-	expression tag	UNP Q9QJC1
OF	-1	ASN	-	expression tag	UNP Q9QJC1
OF	0	ILE	-	expression tag	UNP Q9QJC1

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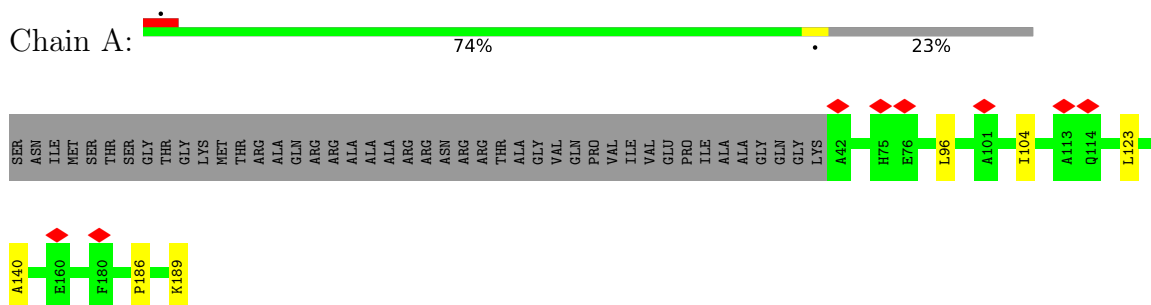
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Mol	Chain	Residues	Atoms		AltConf
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2	PF	1	Total 1	O 1	0
2	QF	1	Total 1	O 1	0
2	RF	1	Total 1	O 1	0
2	SF	1	Total 1	O 1	0
2	TF	1	Total 1	O 1	0
2	UF	1	Total 1	O 1	0
2	VF	1	Total 1	O 1	0
2	WF	1	Total 1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

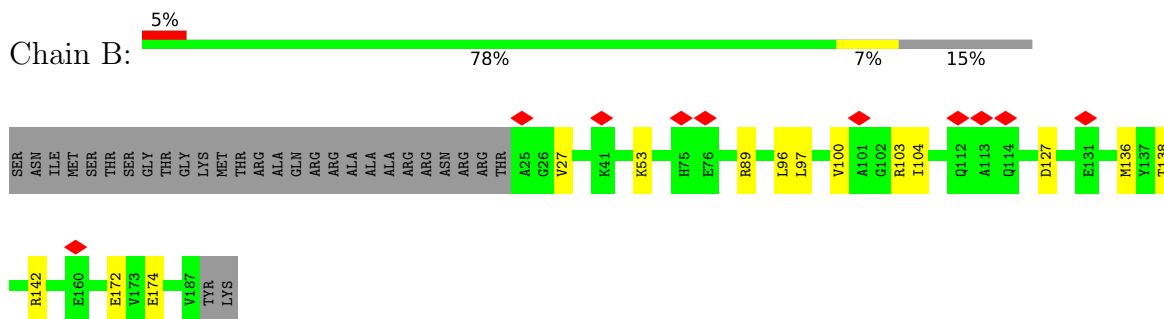
3 Residue-property plots [i](#)

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.

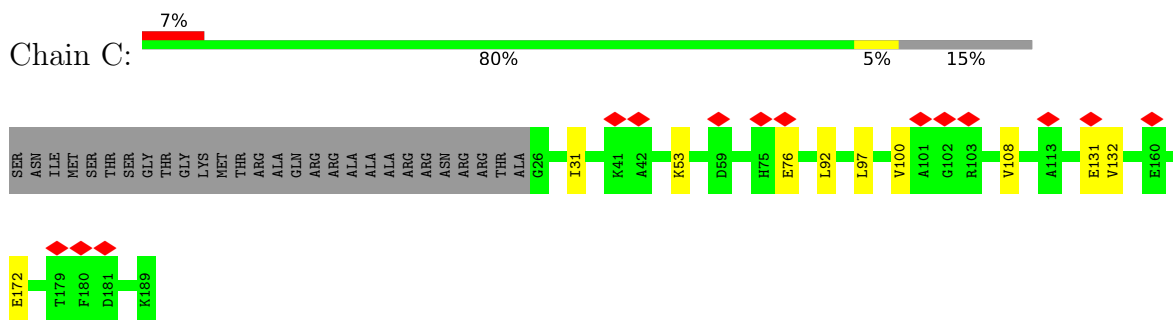
- Molecule 1: Coat protein



- Molecule 1: Coat protein

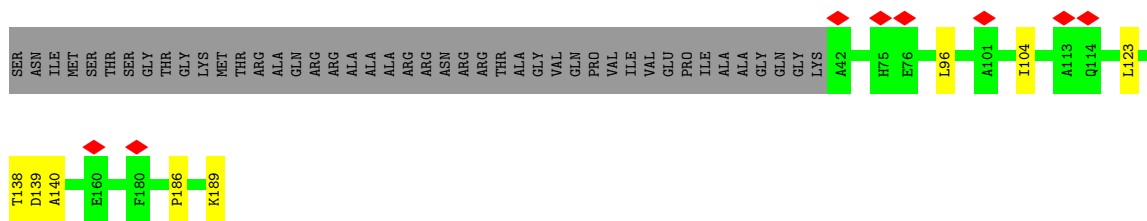


- Molecule 1: Coat protein

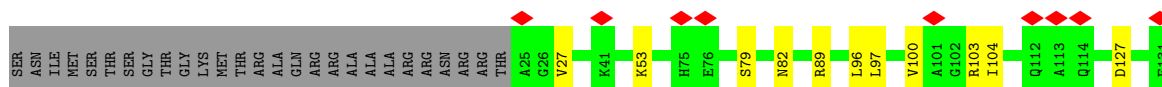
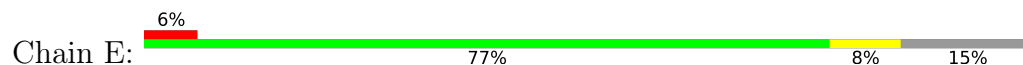


- Molecule 1: Coat protein

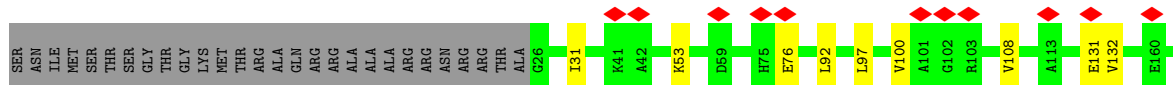
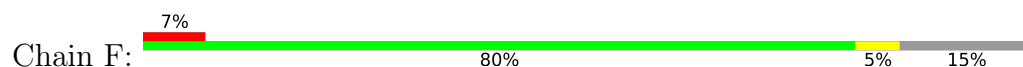




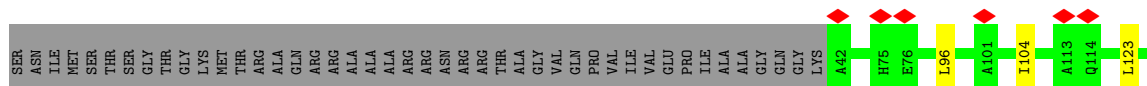
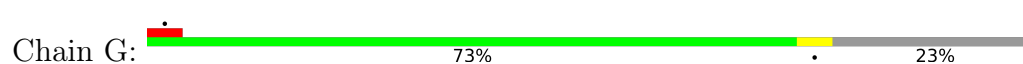
• Molecule 1: Coat protein



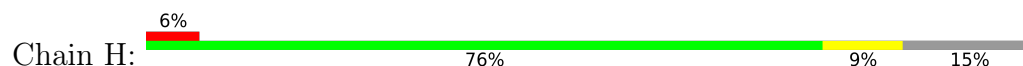
• Molecule 1: Coat protein



• Molecule 1: Coat protein

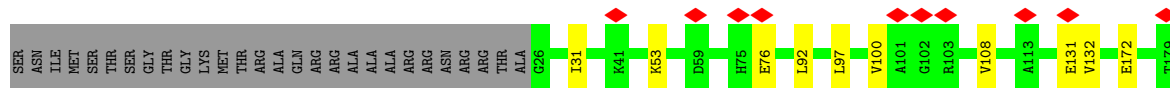
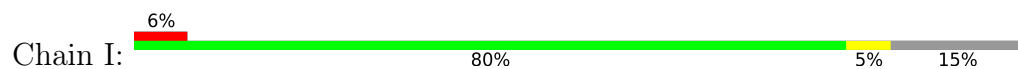


• Molecule 1: Coat protein

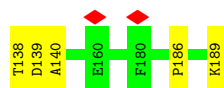
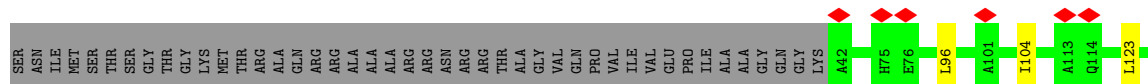




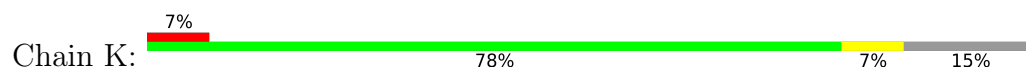
- Molecule 1: Coat protein



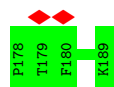
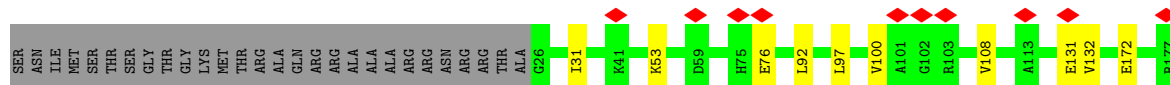
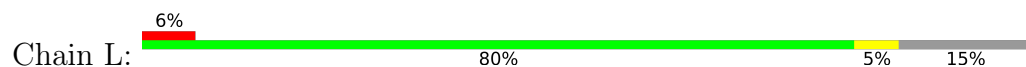
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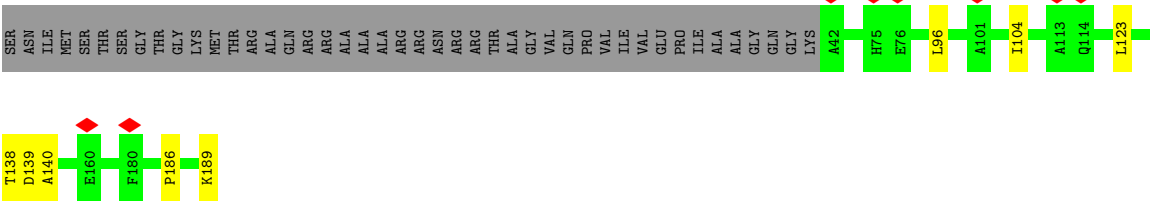
- Molecule 1: Coat protein



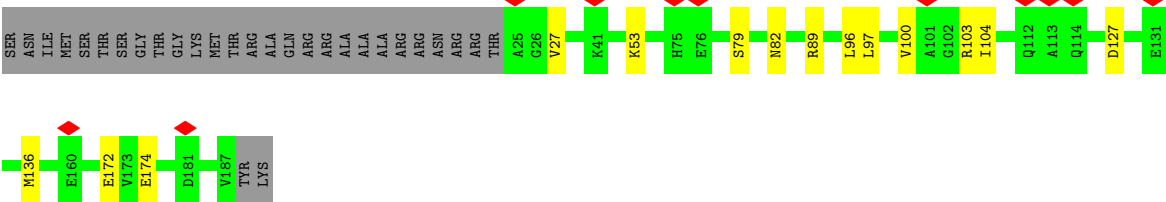
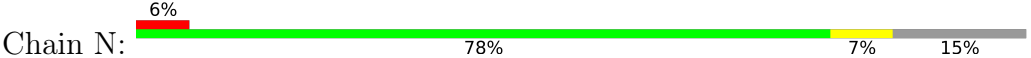
- Molecule 1: Coat protein



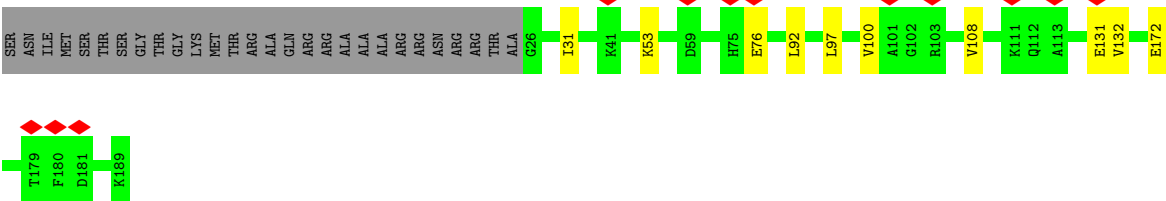
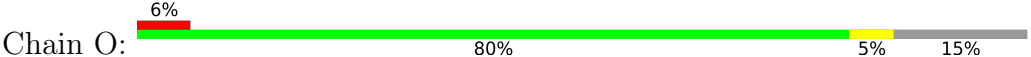
- Molecule 1: Coat protein



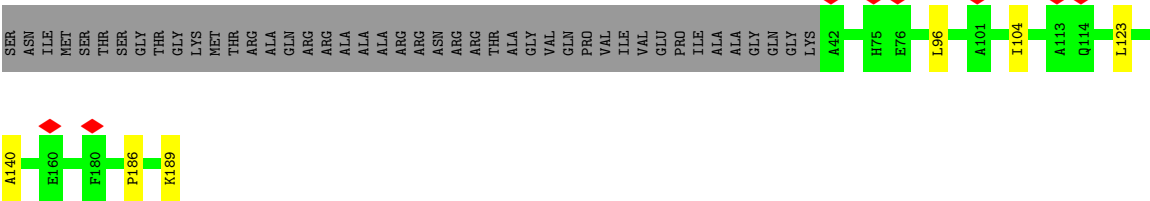
• Molecule 1: Coat protein



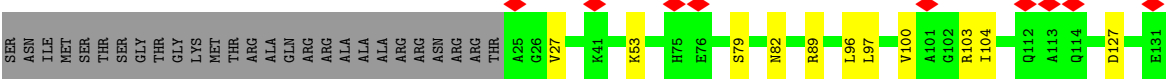
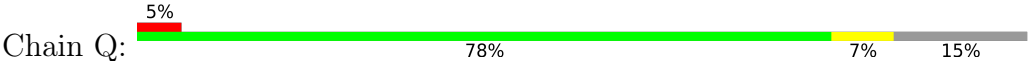
• Molecule 1: Coat protein



• Molecule 1: Coat protein

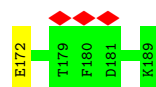
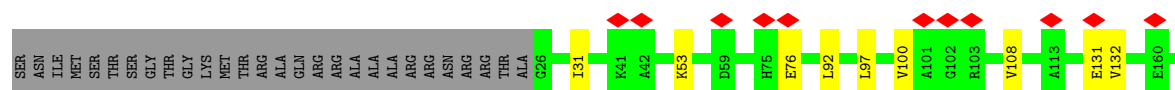
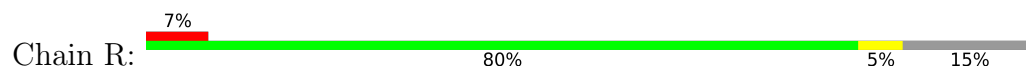


• Molecule 1: Coat protein

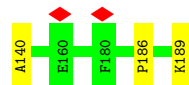
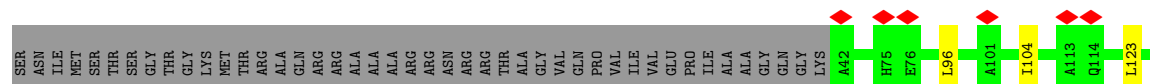




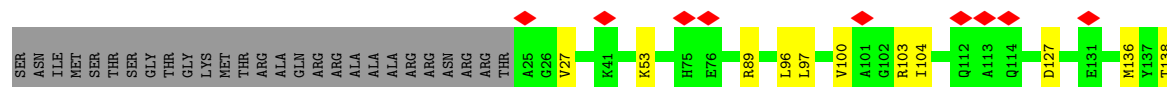
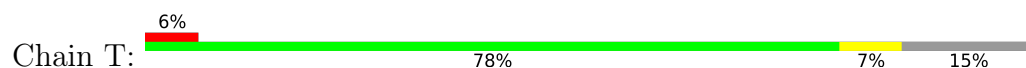
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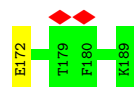
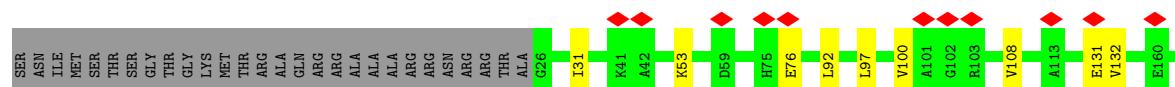
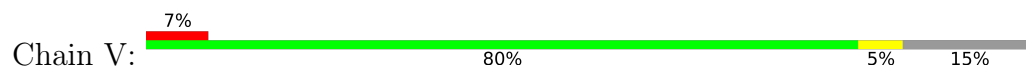
- Molecule 1: Coat protein



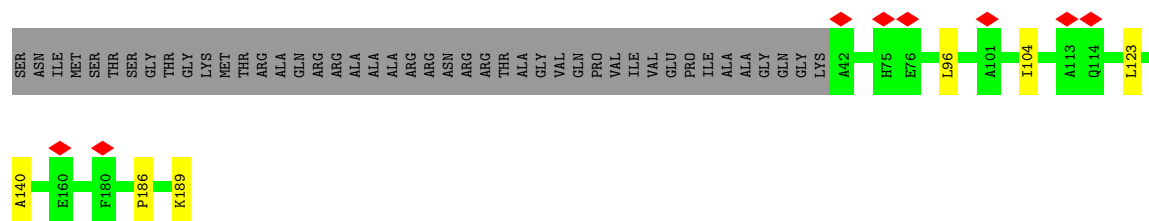
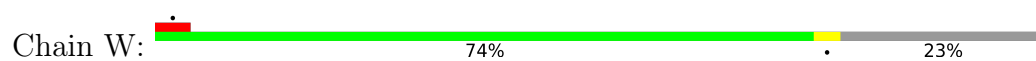
- Molecule 1: Coat protein



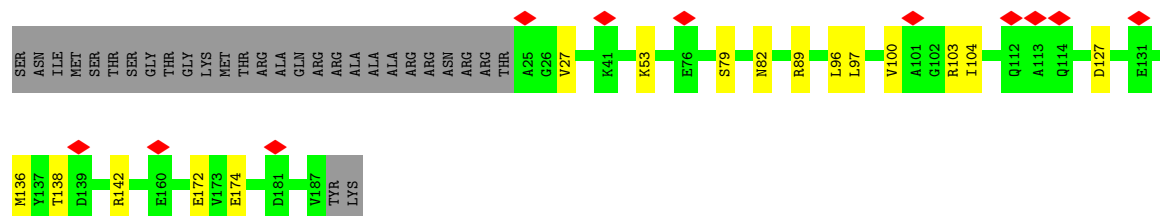
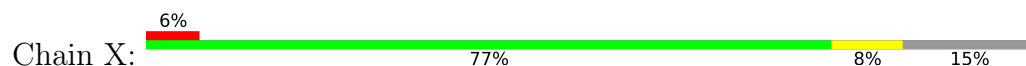
- Molecule 1: Coat protein



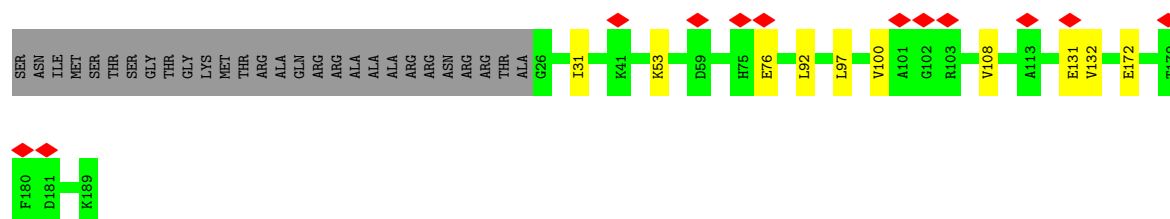
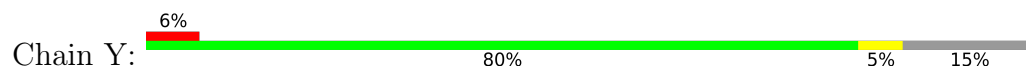
- Molecule 1: Coat protein



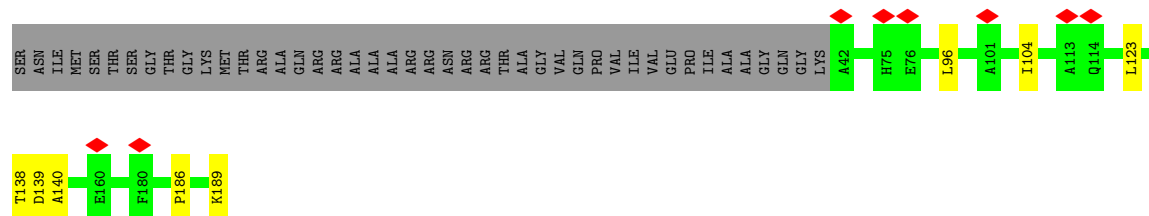
- Molecule 1: Coat protein



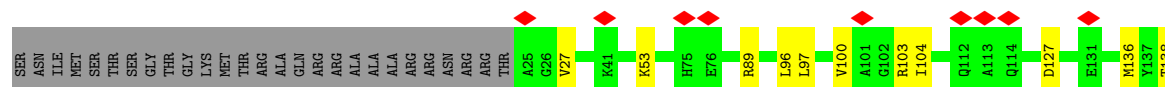
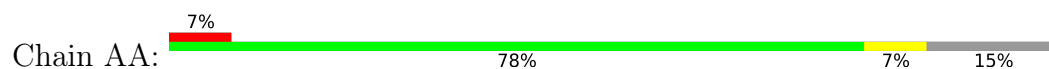
- Molecule 1: Coat protein

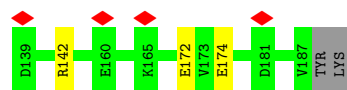


- Molecule 1: Coat protein

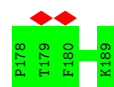
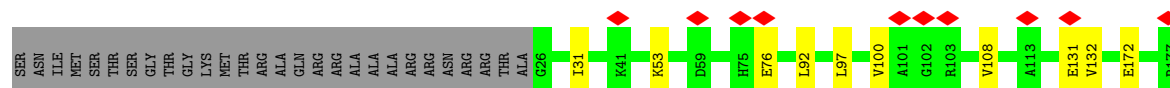
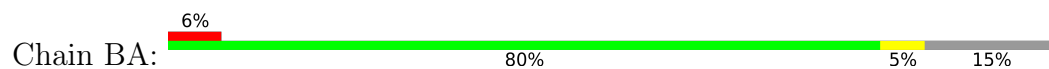


- Molecule 1: Coat protein

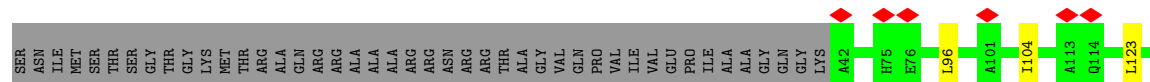
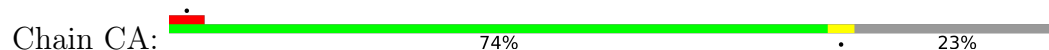




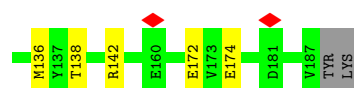
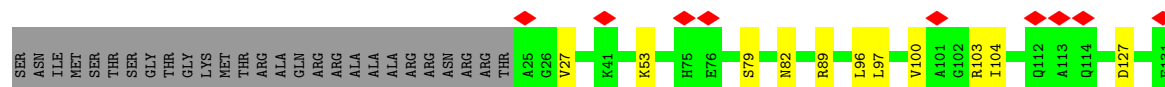
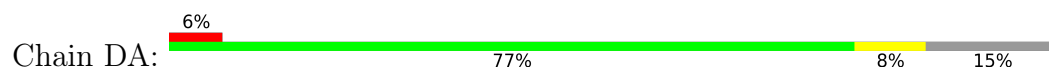
- Molecule 1: Coat protein



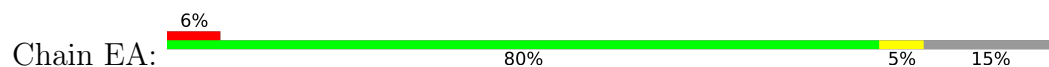
- Molecule 1: Coat protein



- Molecule 1: Coat protein

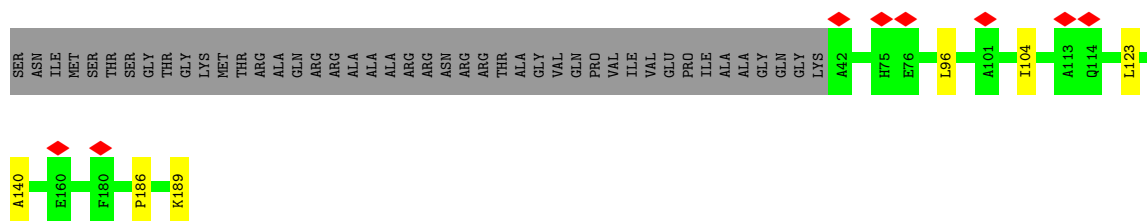


- Molecule 1: Coat protein



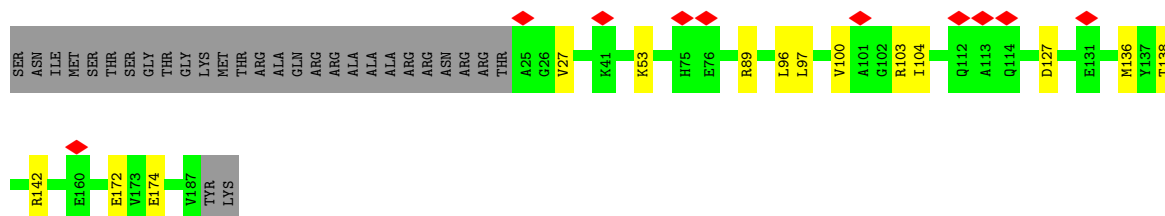
- Molecule 1: Coat protein

Chain FA:  74% 23%



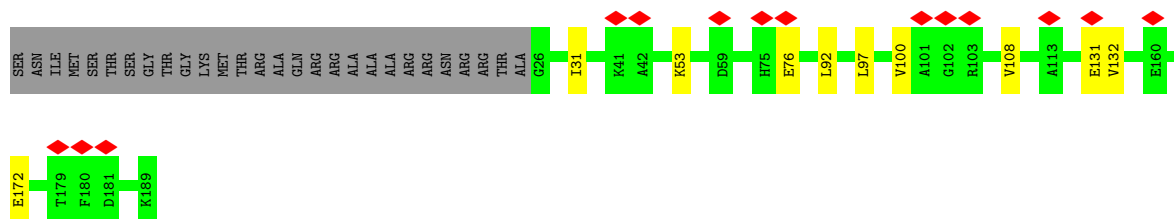
- Molecule 1: Coat protein

Chain GA:  78% 7% 15%



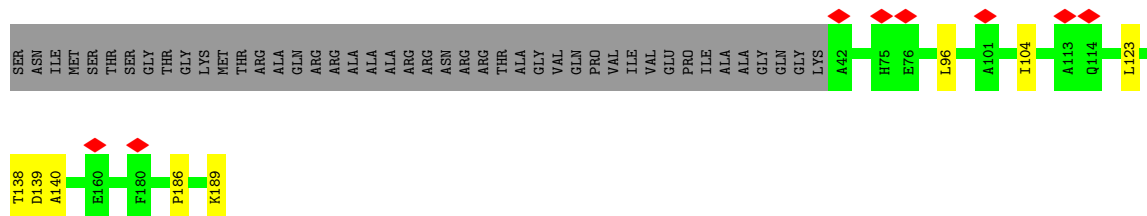
- Molecule 1: Coat protein

Chain HA:  80% 5% 15%



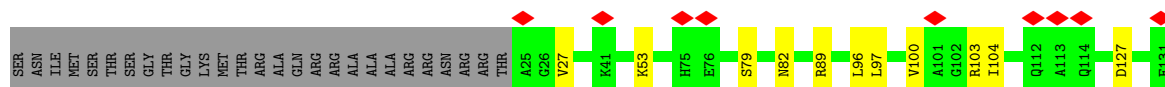
- Molecule 1: Coat protein

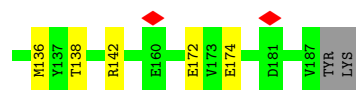
Chain IA:  73% 23%



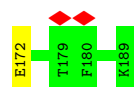
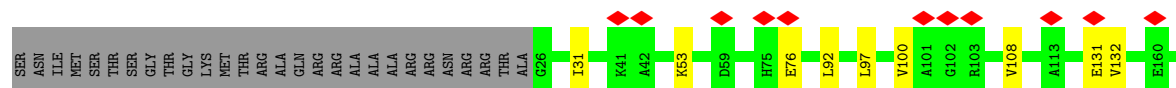
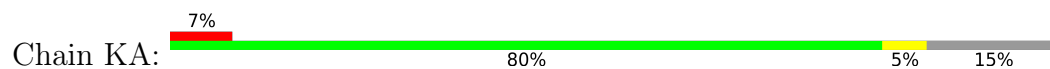
- Molecule 1: Coat protein

Chain JA:  77% 8% 15%

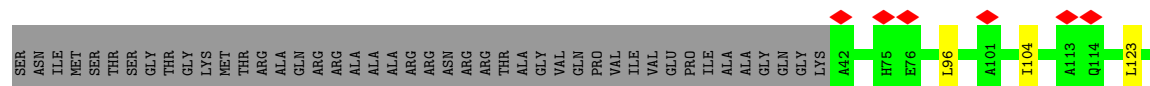
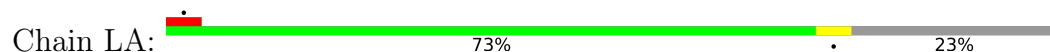




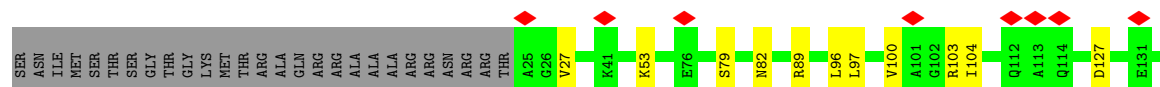
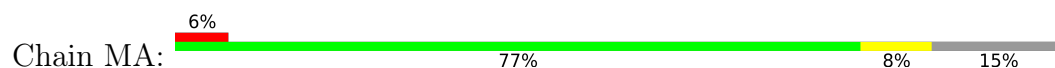
- Molecule 1: Coat protein



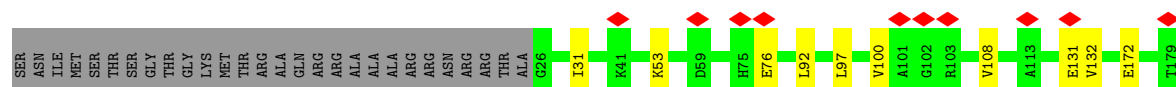
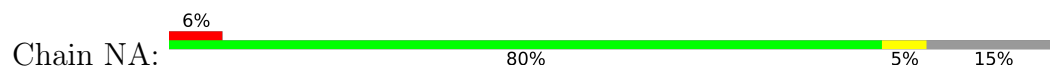
- Molecule 1: Coat protein



- Molecule 1: Coat protein

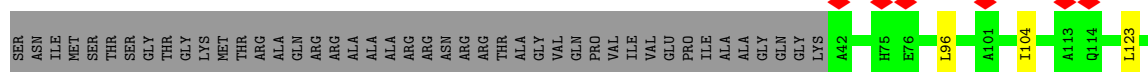


- Molecule 1: Coat protein



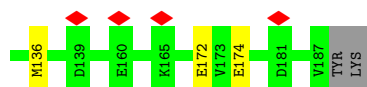
- Molecule 1: Coat protein

Chain OA:  73% 23%



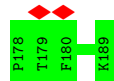
- Molecule 1: Coat protein

Chain PA:  78% 7% 15%



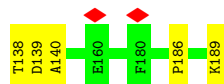
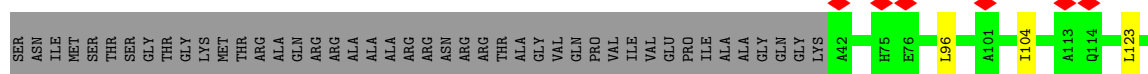
- Molecule 1: Coat protein

Chain QA:  80% 5% 15%



- Molecule 1: Coat protein

Chain RA:  73% 23%



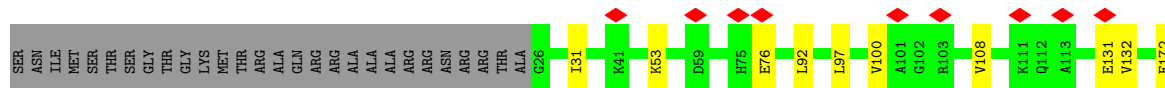
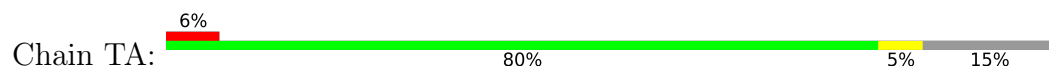
- Molecule 1: Coat protein

Chain SA:  78% 7% 15%

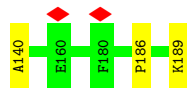
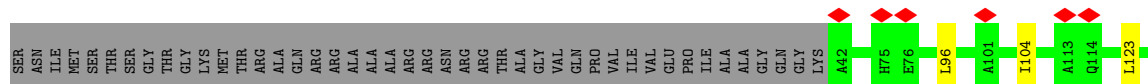
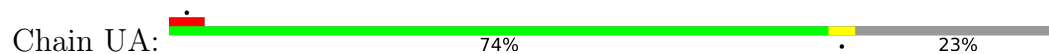




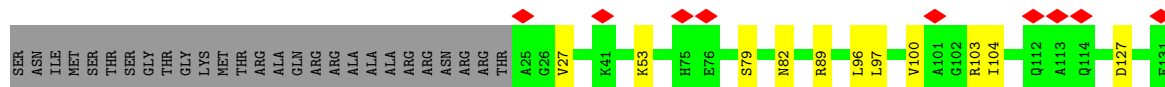
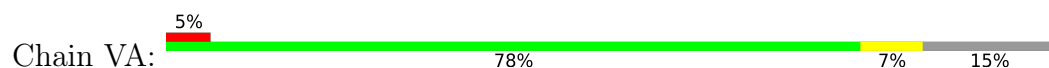
- Molecule 1: Coat protein



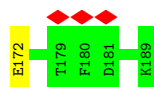
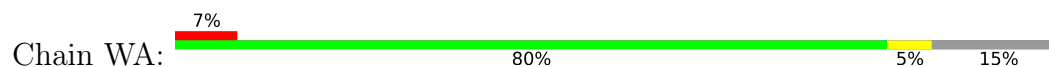
- Molecule 1: Coat protein



- Molecule 1: Coat protein

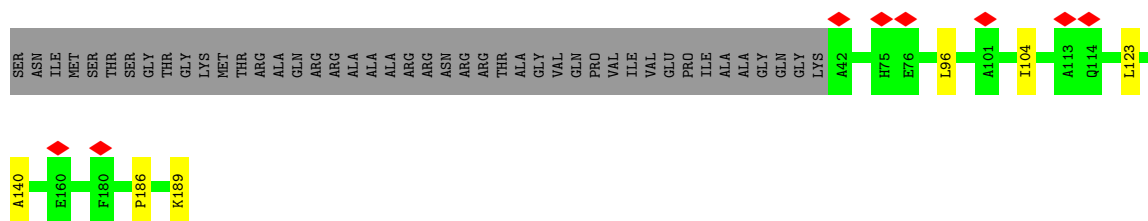


- Molecule 1: Coat protein



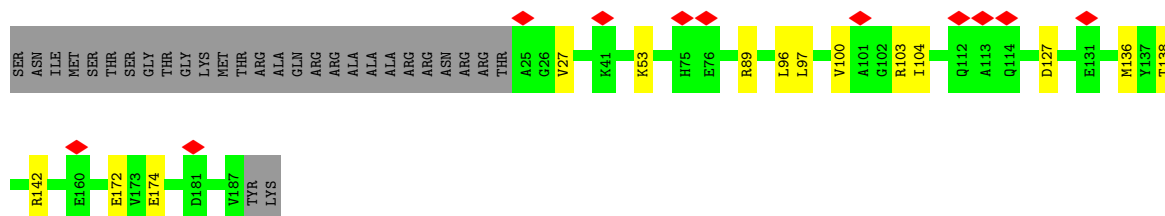
- Molecule 1: Coat protein

Chain XA:  74% 23%



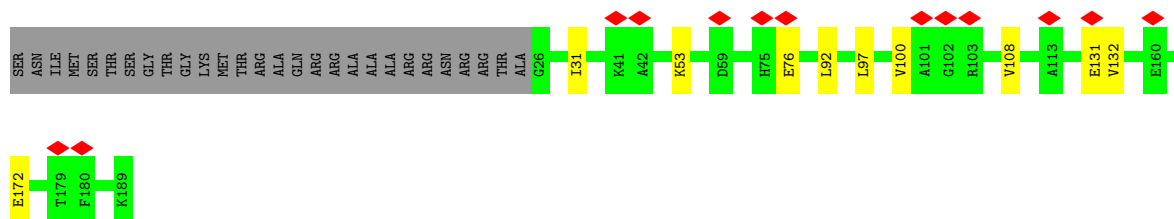
- Molecule 1: Coat protein

Chain YA:  6% 78% 7% 15%



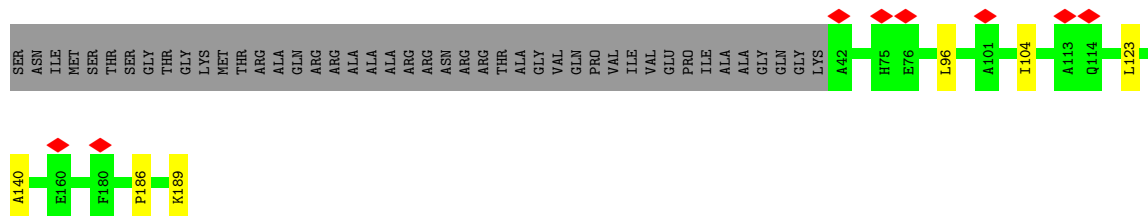
- Molecule 1: Coat protein

Chain ZA:  7% 80% 5% 15%



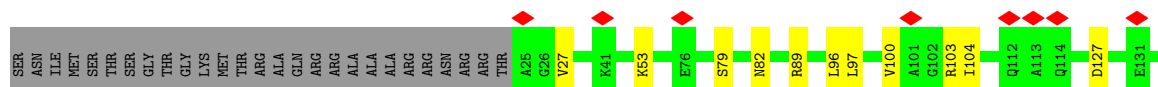
- Molecule 1: Coat protein

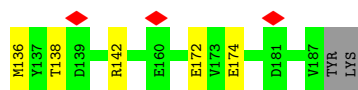
Chain AB:  74% 23%



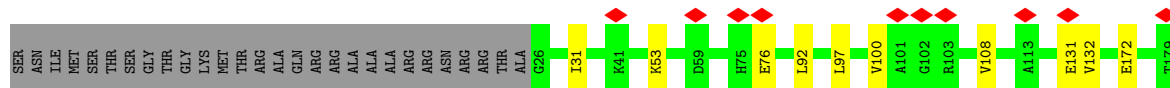
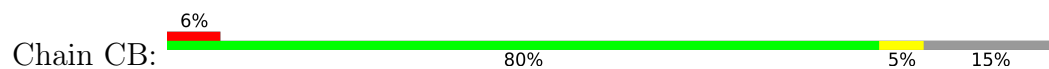
- Molecule 1: Coat protein

Chain BB:  6% 77% 8% 15%

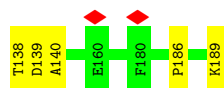
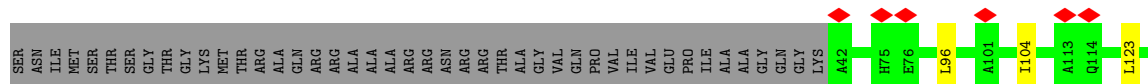
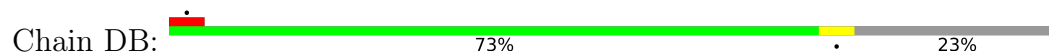




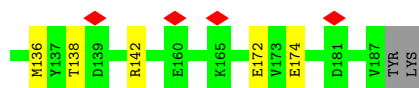
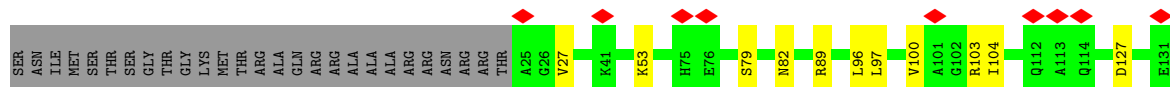
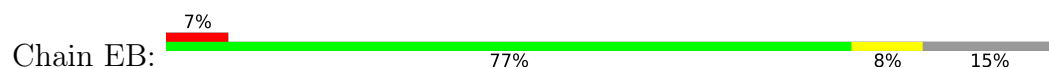
- Molecule 1: Coat protein



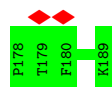
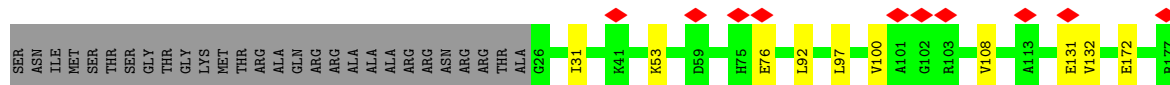
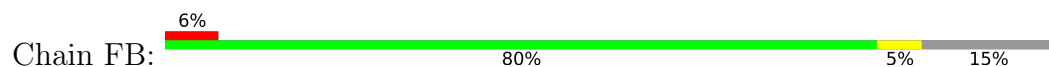
- Molecule 1: Coat protein



- Molecule 1: Coat protein

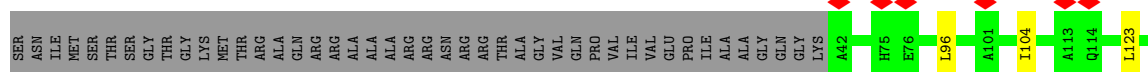


- Molecule 1: Coat protein



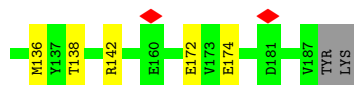
- Molecule 1: Coat protein

Chain GB:  73% 23%



- Molecule 1: Coat protein

Chain HB:  77% 8% 15%



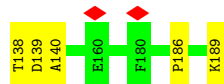
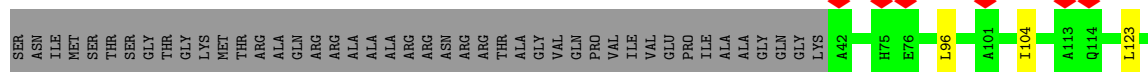
- Molecule 1: Coat protein

Chain IB:  80% 5% 15%



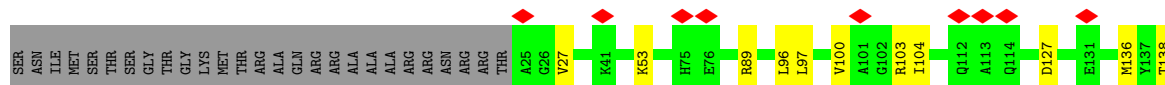
- Molecule 1: Coat protein

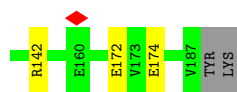
Chain JB:  73% 23%



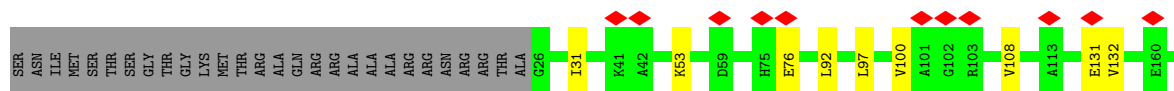
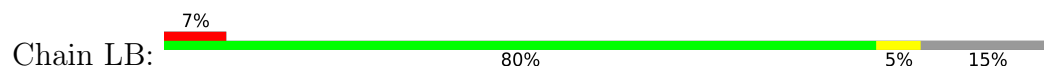
- Molecule 1: Coat protein

Chain KB:  78% 7% 15%

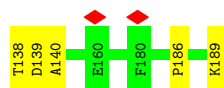
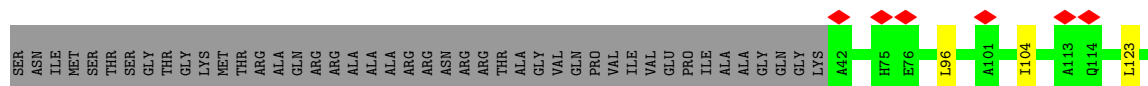
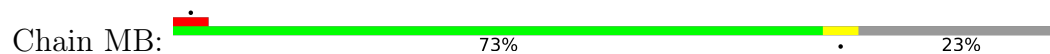




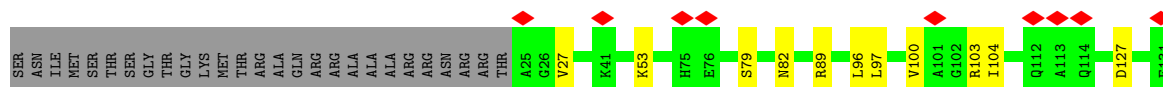
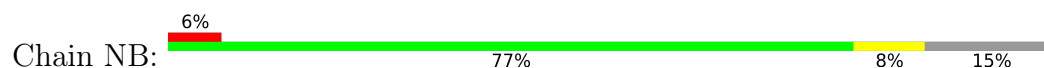
- Molecule 1: Coat protein



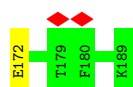
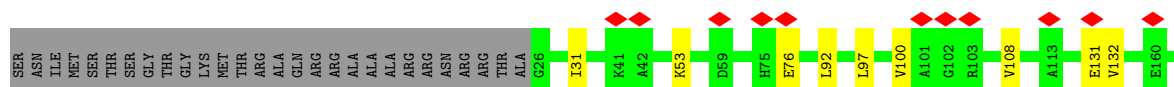
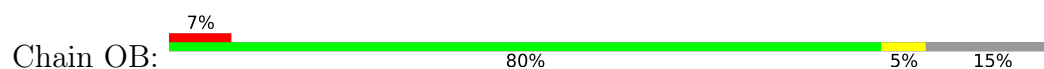
- Molecule 1: Coat protein



- Molecule 1: Coat protein

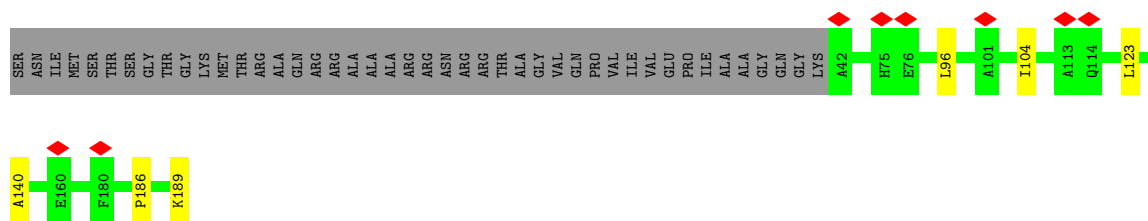


- Molecule 1: Coat protein



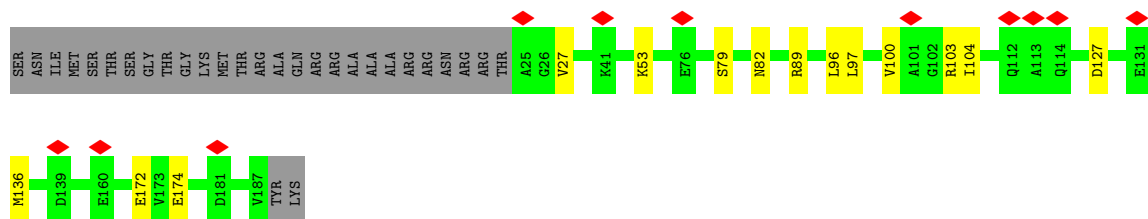
- Molecule 1: Coat protein

Chain PB:  74% 23%



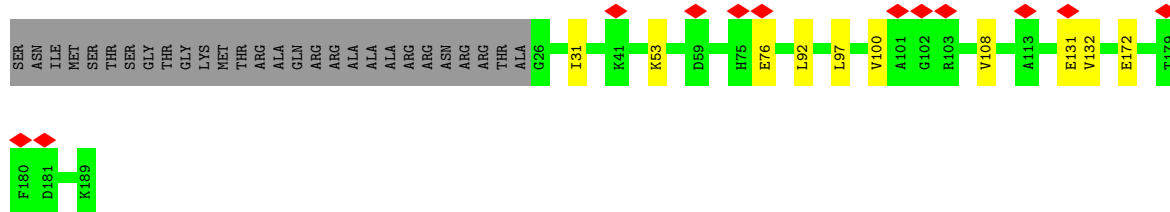
- Molecule 1: Coat protein

Chain QB:  78% 7% 15% 6%



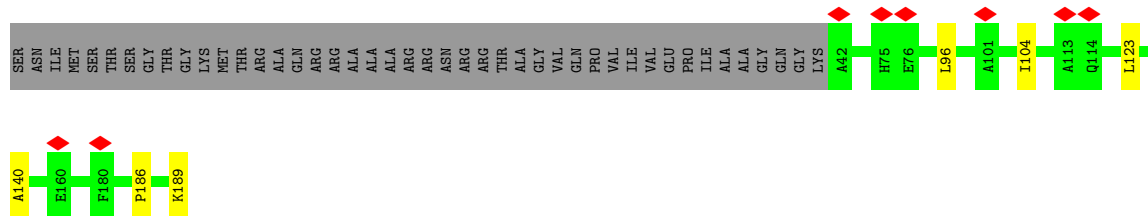
- Molecule 1: Coat protein

Chain RB:  80% 5% 15% 6%



- Molecule 1: Coat protein

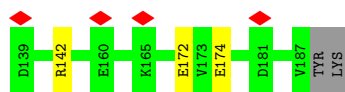
Chain SB:  74% 23%



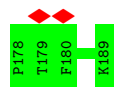
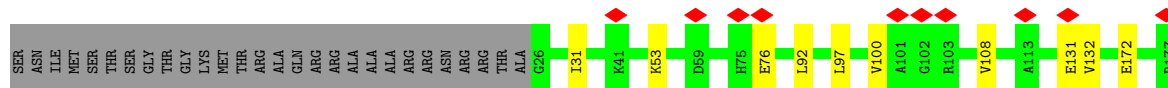
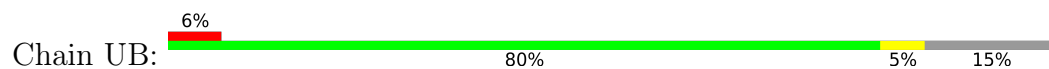
- Molecule 1: Coat protein

Chain TB:  78% 7% 15% 7%

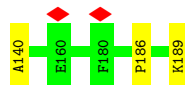
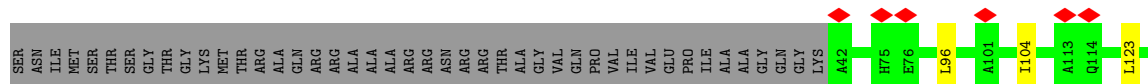
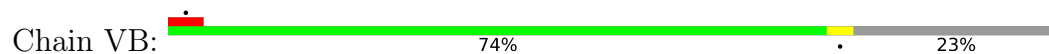




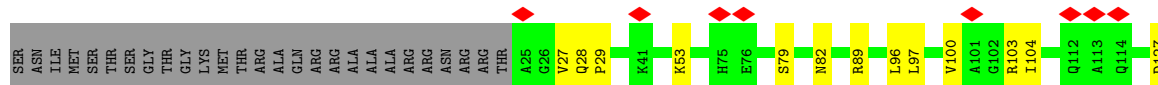
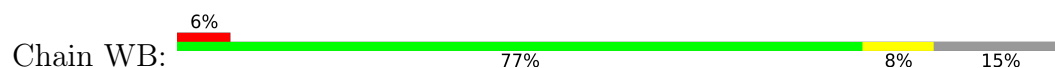
- Molecule 1: Coat protein



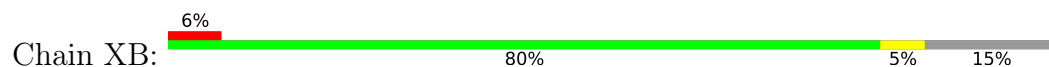
- Molecule 1: Coat protein



- Molecule 1: Coat protein

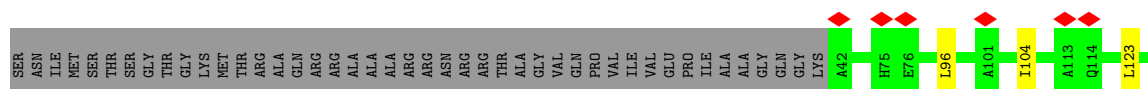


- Molecule 1: Coat protein



- Molecule 1: Coat protein

Chain YB:  73% 23%



- Molecule 1: Coat protein

Chain ZB:  5% 77% 8% 15%



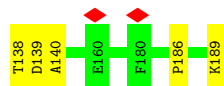
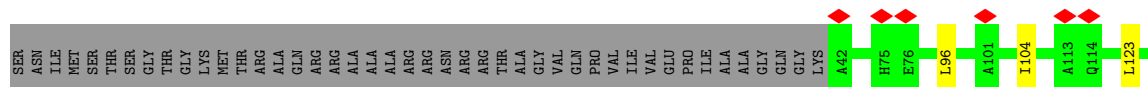
- Molecule 1: Coat protein

Chain AC:  7% 80% 5% 15%



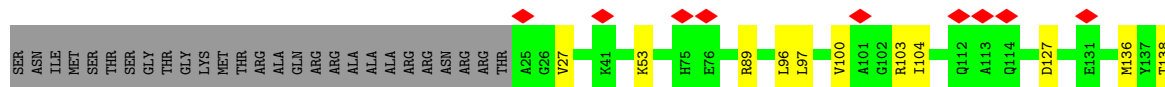
- Molecule 1: Coat protein

Chain BC:  73% 23%



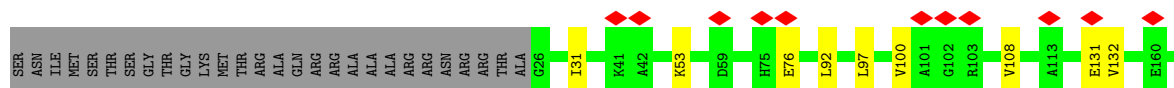
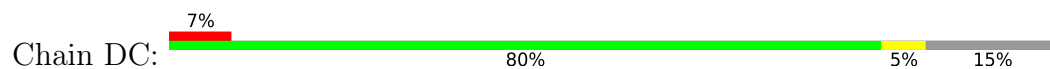
- Molecule 1: Coat protein

Chain CC:  6% 78% 7% 15%

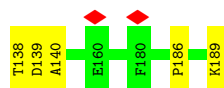
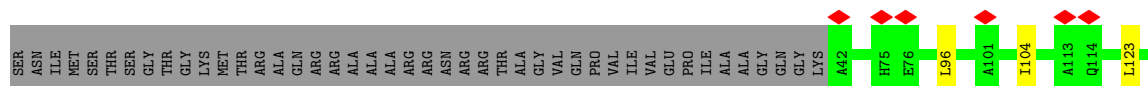
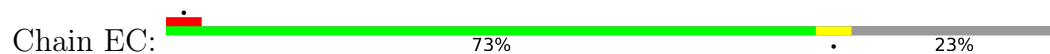




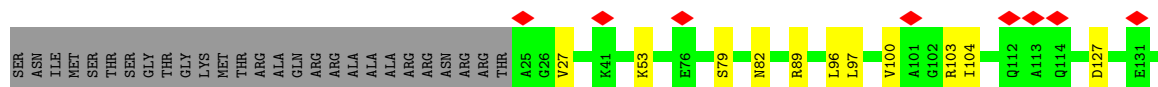
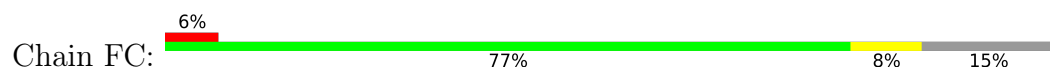
- Molecule 1: Coat protein



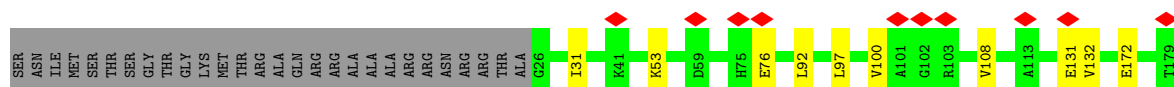
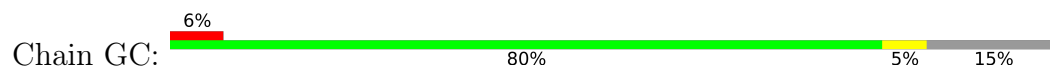
- Molecule 1: Coat protein



- Molecule 1: Coat protein

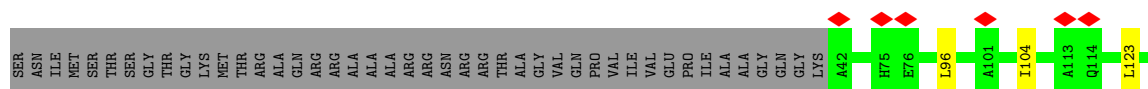


- Molecule 1: Coat protein



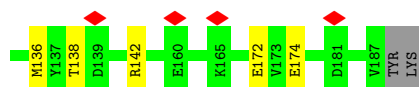
- Molecule 1: Coat protein

Chain HC:  74% 23%



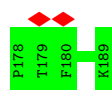
- Molecule 1: Coat protein

Chain IC:  77% 8% 15%



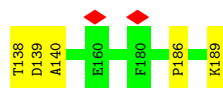
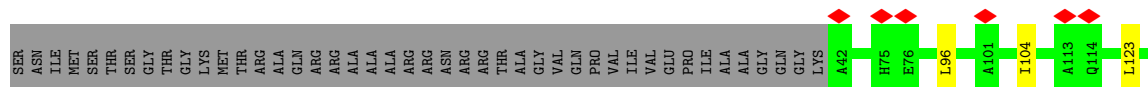
- Molecule 1: Coat protein

Chain JC:  80% 5% 15%



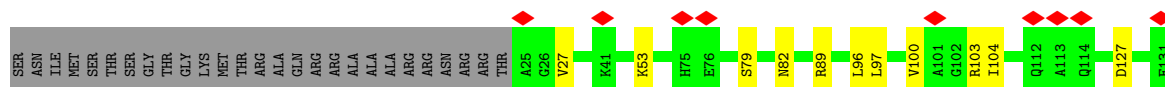
- Molecule 1: Coat protein

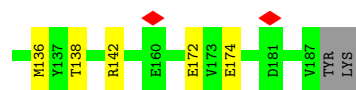
Chain KC:  73% 23%



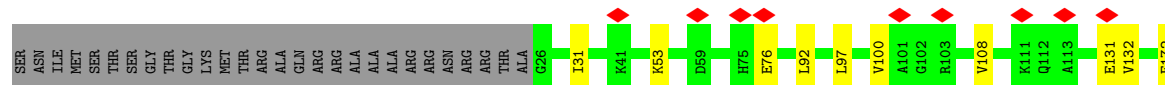
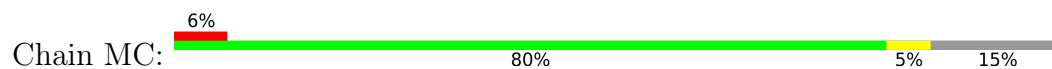
- Molecule 1: Coat protein

Chain LC:  77% 8% 15%

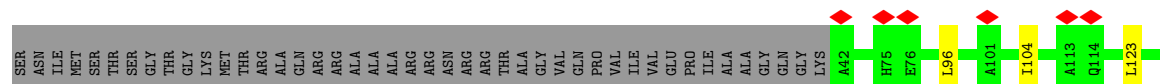
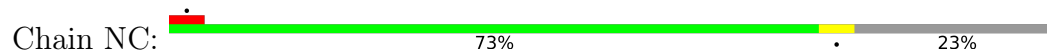




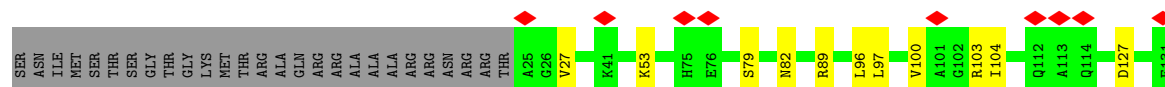
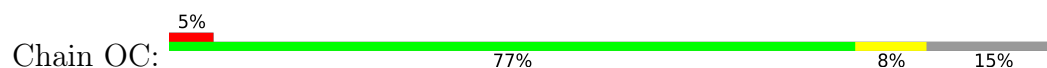
- Molecule 1: Coat protein



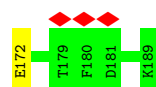
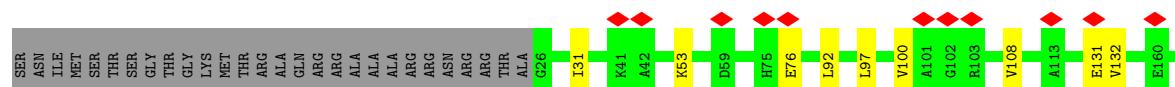
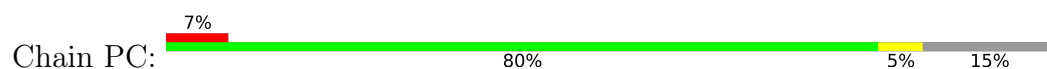
- Molecule 1: Coat protein



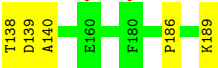
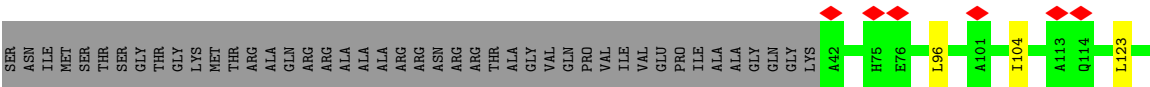
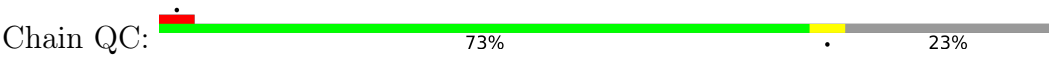
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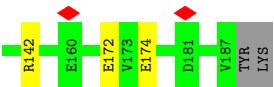
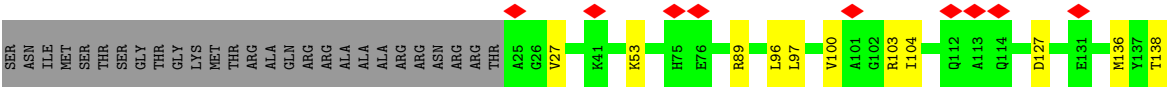
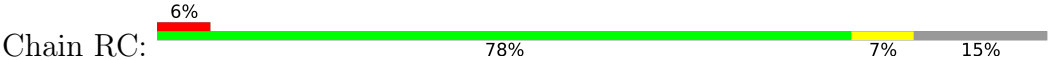
- Molecule 1: Coat protein



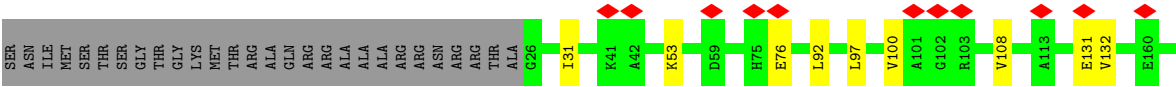
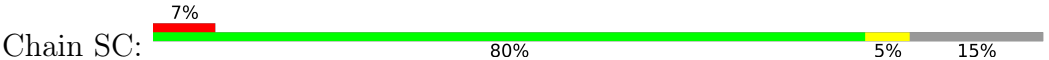
- Molecule 1: Coat protein



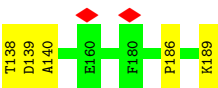
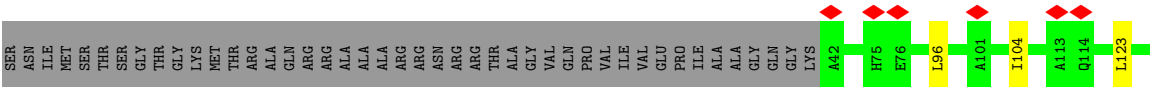
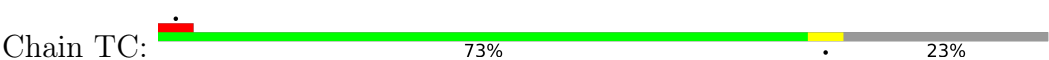
• Molecule 1: Coat protein



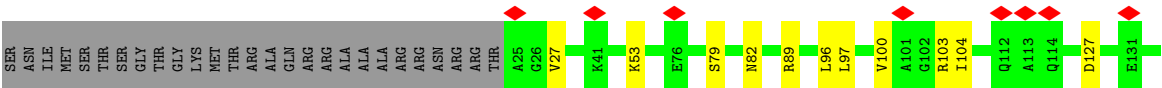
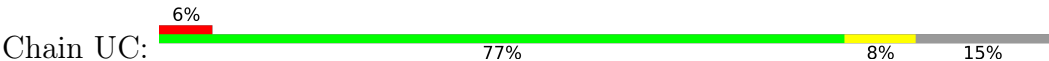
• Molecule 1: Coat protein

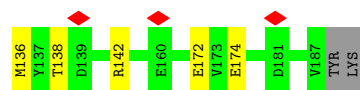


• Molecule 1: Coat protein

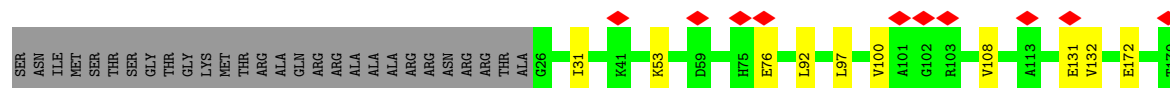
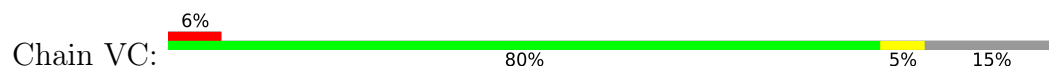


• Molecule 1: Coat protein

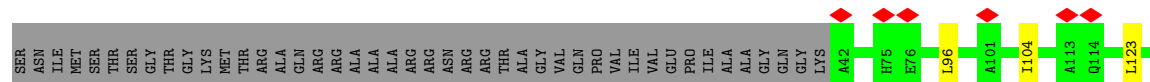
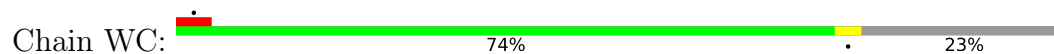




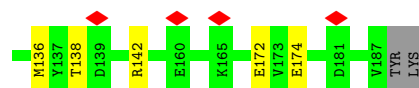
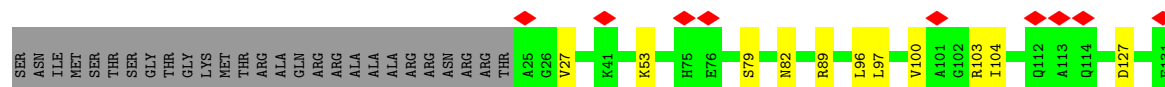
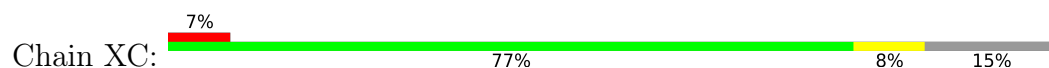
- Molecule 1: Coat protein



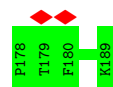
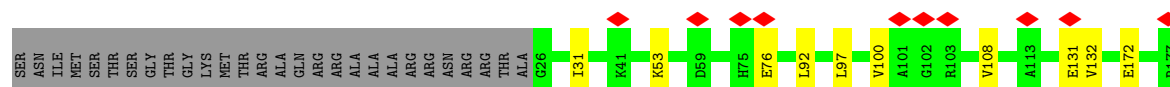
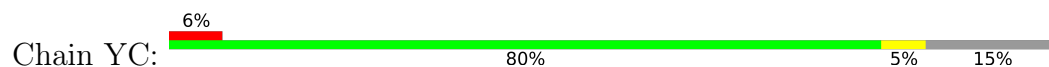
- Molecule 1: Coat protein



- Molecule 1: Coat protein

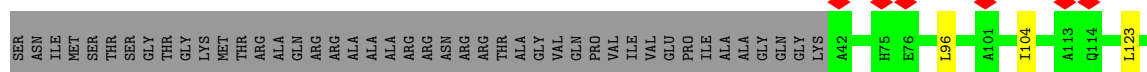


- Molecule 1: Coat protein



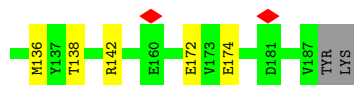
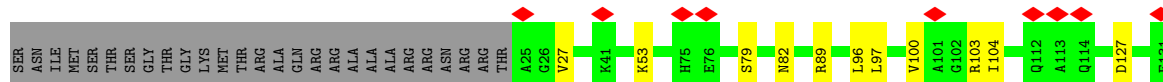
- Molecule 1: Coat protein

Chain ZC:  73% 23%



- Molecule 1: Coat protein

Chain AD:  6% 77% 8% 15%



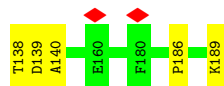
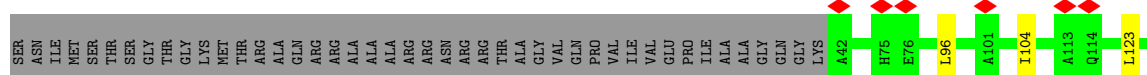
- Molecule 1: Coat protein

Chain BD:  7% 80% 5% 15%



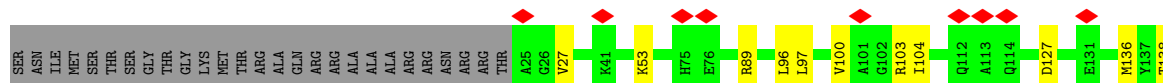
- Molecule 1: Coat protein

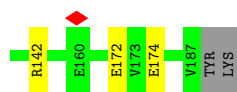
Chain CD:  73% 23%



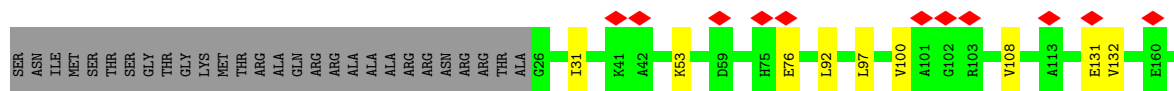
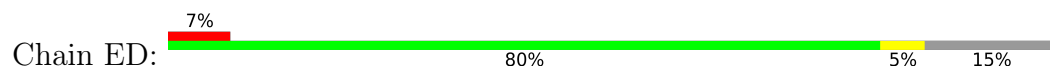
- Molecule 1: Coat protein

Chain DD:  5% 78% 7% 15%

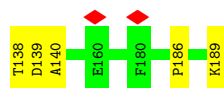
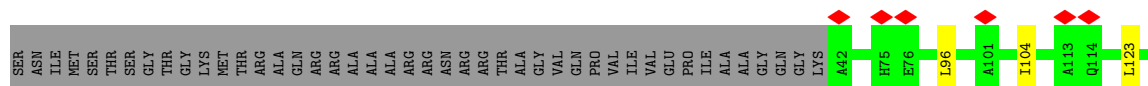
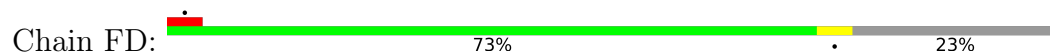




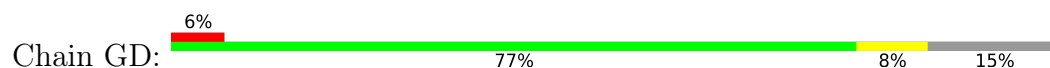
- Molecule 1: Coat protein



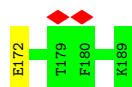
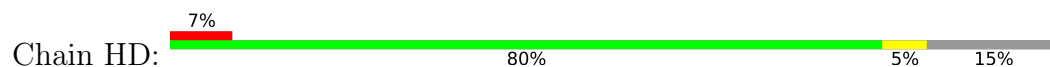
- Molecule 1: Coat protein



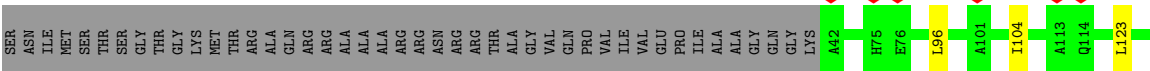
- Molecule 1: Coat protein



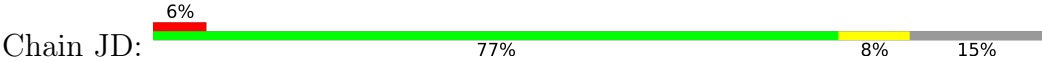
- Molecule 1: Coat protein



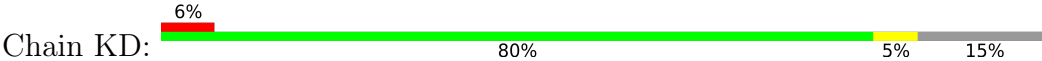
- Molecule 1: Coat protein



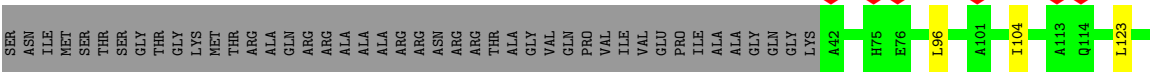
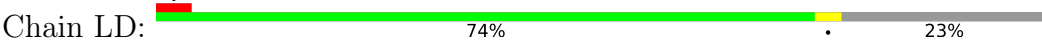
• Molecule 1: Coat protein



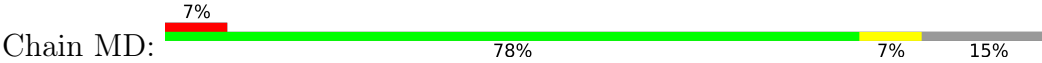
• Molecule 1: Coat protein

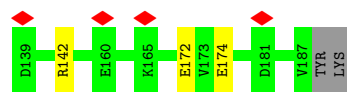


• Molecule 1: Coat protein

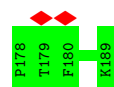
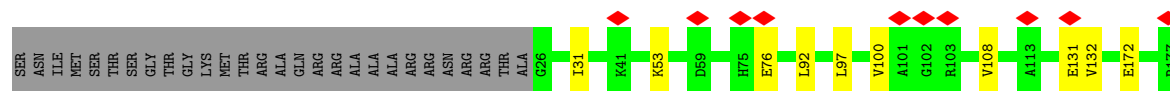
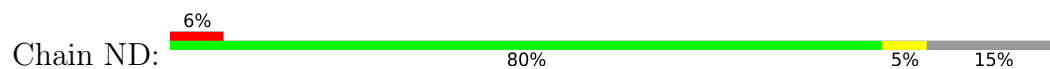


• Molecule 1: Coat protein

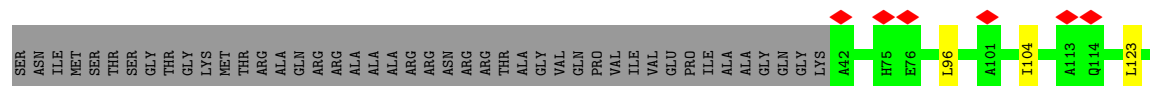
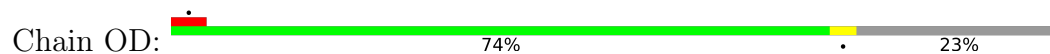




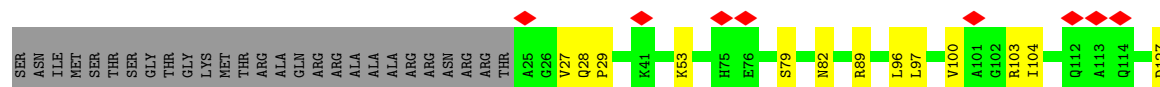
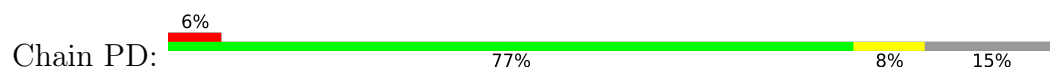
- Molecule 1: Coat protein



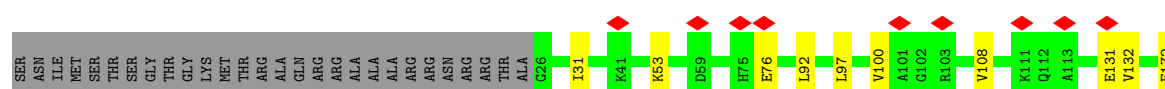
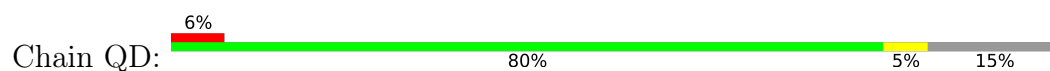
- Molecule 1: Coat protein



- Molecule 1: Coat protein

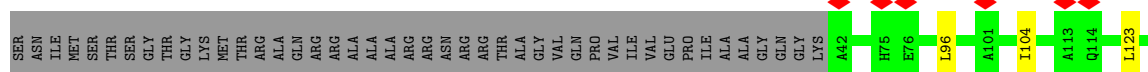


- Molecule 1: Coat protein



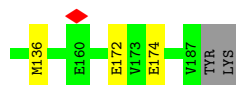
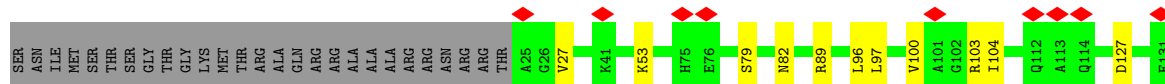
- Molecule 1: Coat protein

Chain RD:  73% 23%



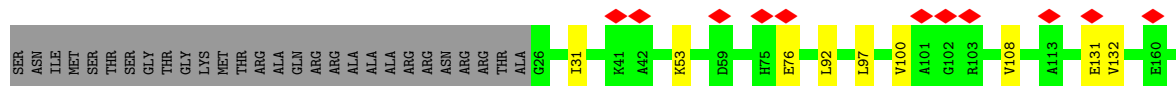
- Molecule 1: Coat protein

Chain SD:  78% 7% 15%



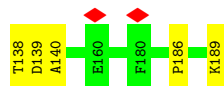
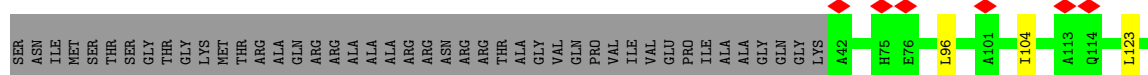
- Molecule 1: Coat protein

Chain TD:  80% 5% 15%



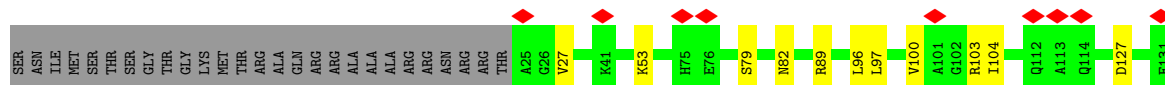
- Molecule 1: Coat protein

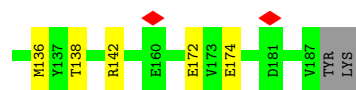
Chain UD:  73% 23%



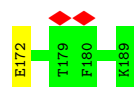
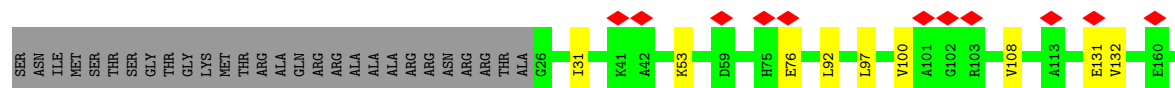
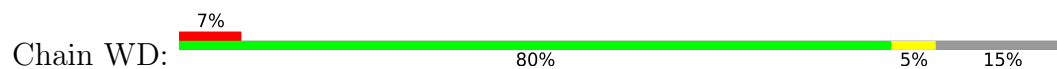
- Molecule 1: Coat protein

Chain VD:  77% 8% 15%

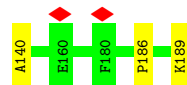
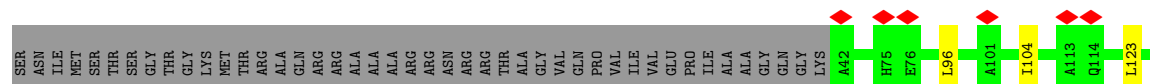
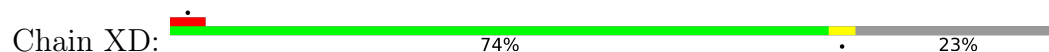




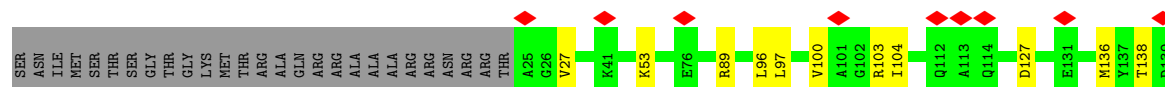
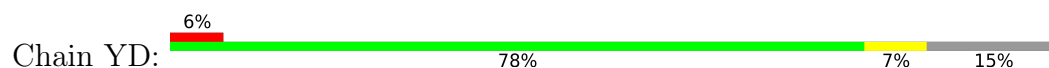
- Molecule 1: Coat protein



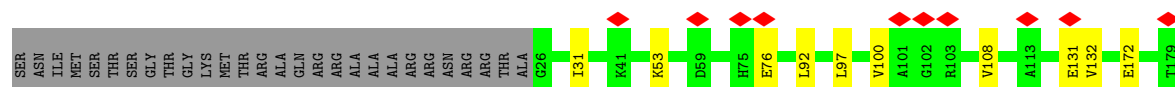
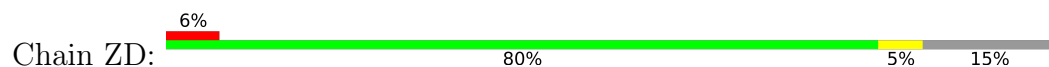
- Molecule 1: Coat protein



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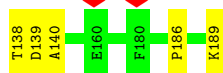
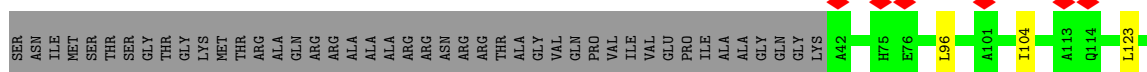


- Molecule 1: Coat protein



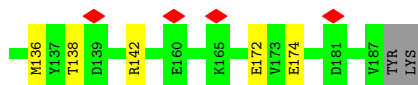
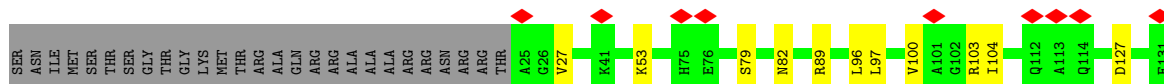
- Molecule 1: Coat protein

Chain AE:  73% 23%



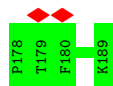
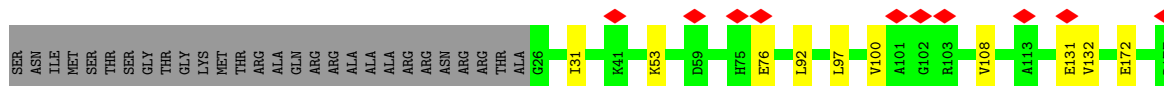
- Molecule 1: Coat protein

Chain BE:  77% 8% 15%



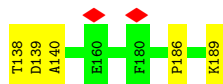
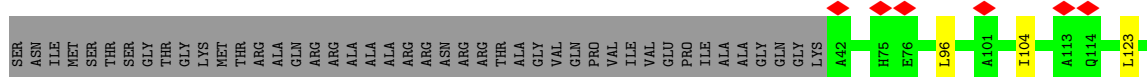
- Molecule 1: Coat protein

Chain CE:  80% 5% 15%



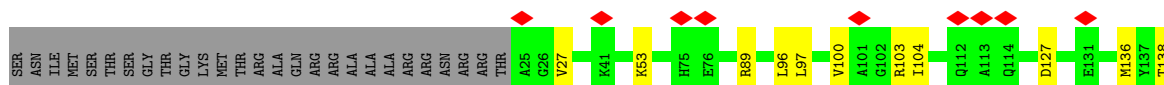
- Molecule 1: Coat protein

Chain DE:  73% 23%



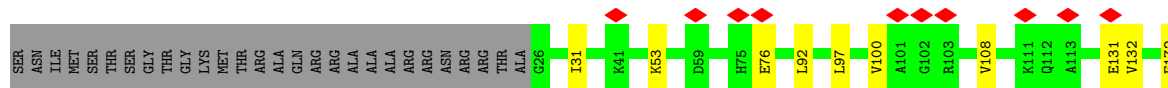
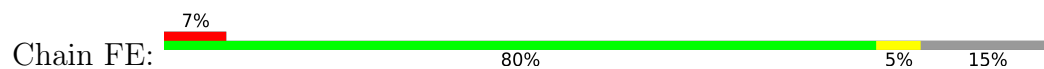
- Molecule 1: Coat protein

Chain EE:  78% 7% 15%

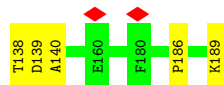
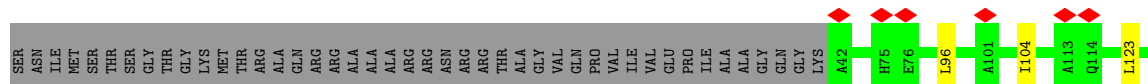
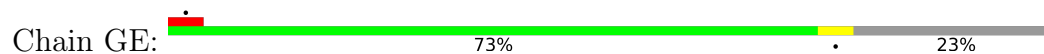




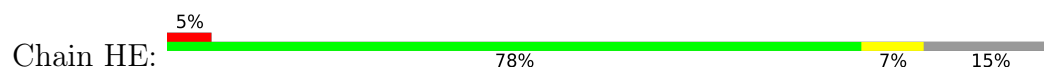
- Molecule 1: Coat protein



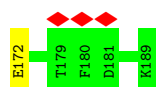
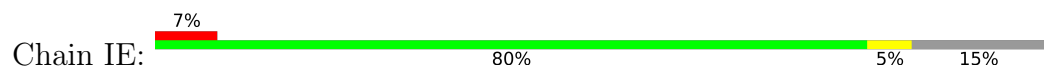
- Molecule 1: Coat protein



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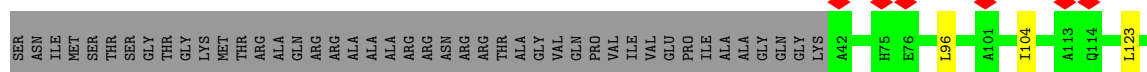


- Molecule 1: Coat protein



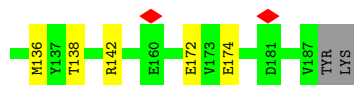
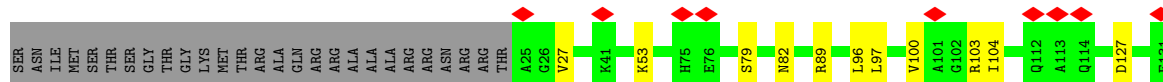
- Molecule 1: Coat protein

Chain JE:  73% 23%



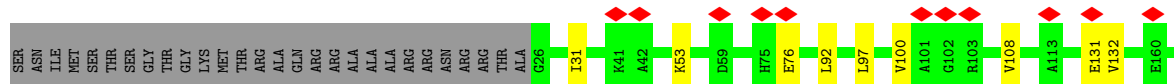
- Molecule 1: Coat protein

Chain KE:  77% 8% 15%



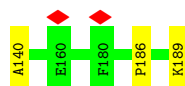
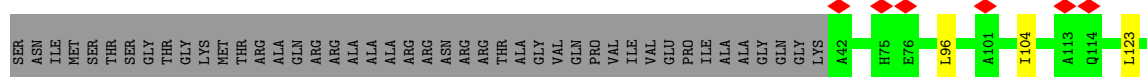
- Molecule 1: Coat protein

Chain LE:  80% 5% 15%



- Molecule 1: Coat protein

Chain ME:  74% 23%



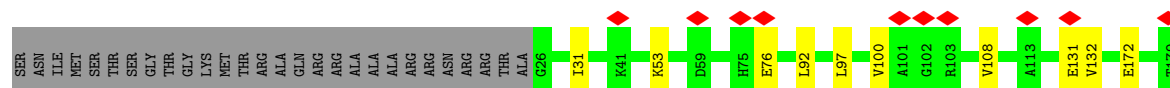
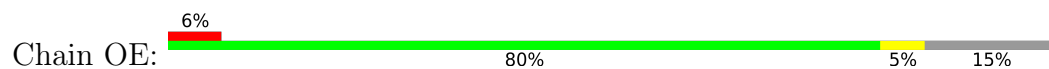
- Molecule 1: Coat protein

Chain NE:  78% 7% 15%

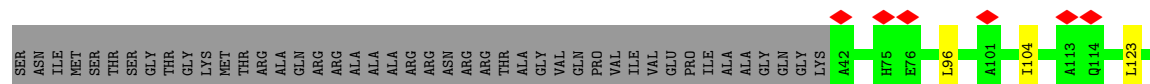
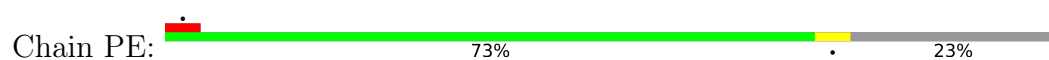




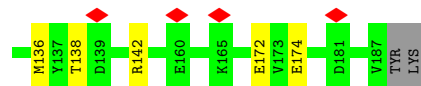
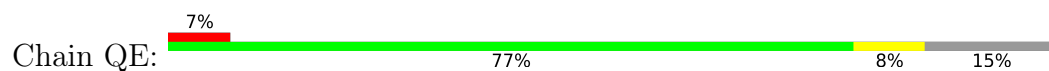
- Molecule 1: Coat protein



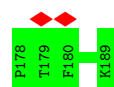
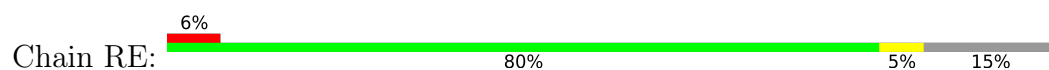
- Molecule 1: Coat protein



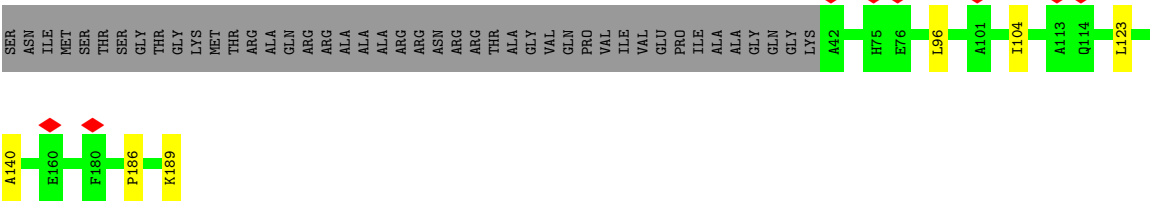
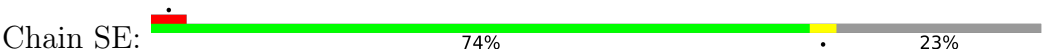
- Molecule 1: Coat protein



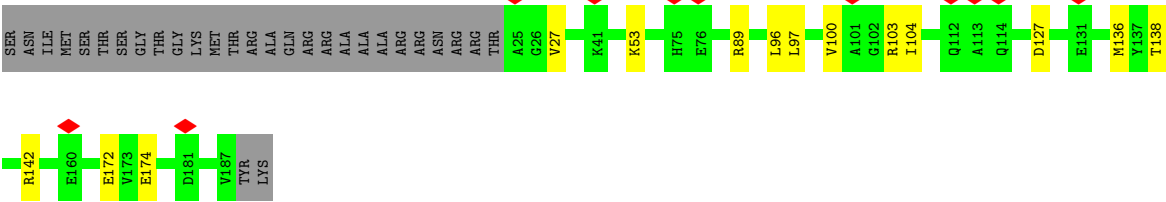
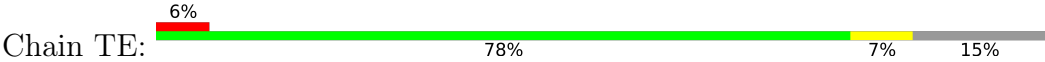
- Molecule 1: Coat protein



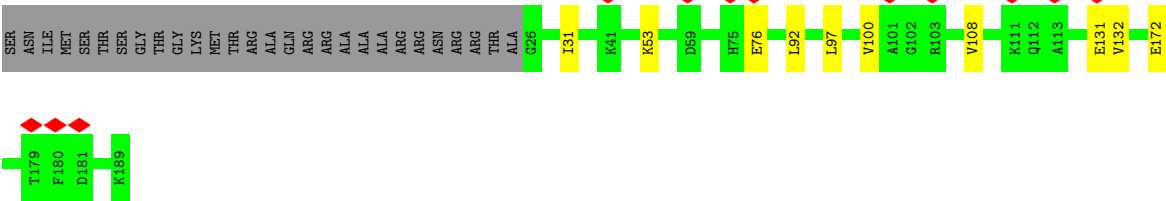
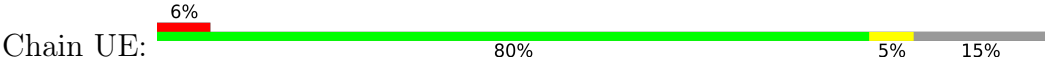
- Molecule 1: Coat protein



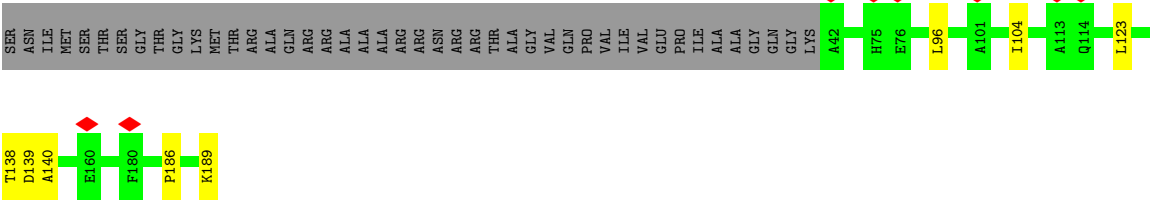
• Molecule 1: Coat protein



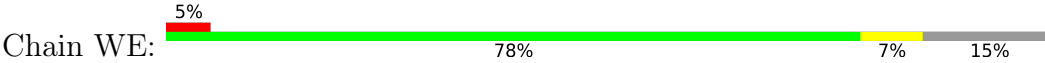
• Molecule 1: Coat protein

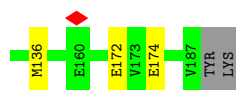


• Molecule 1: Coat protein

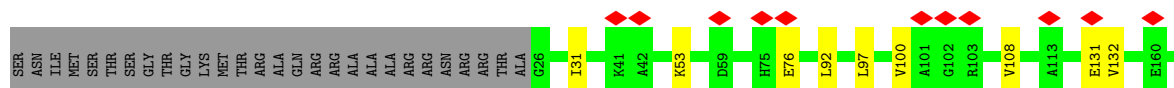
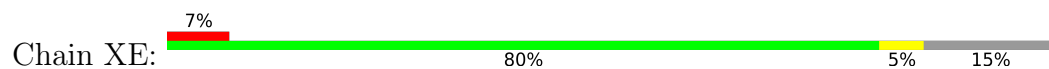


• Molecule 1: Coat protein

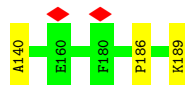
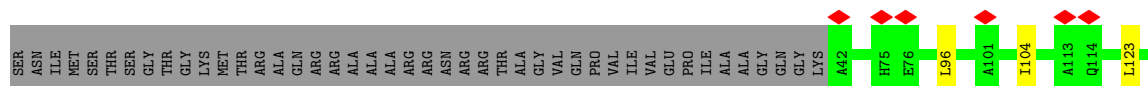
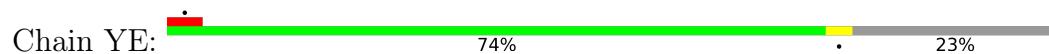




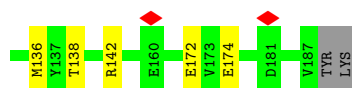
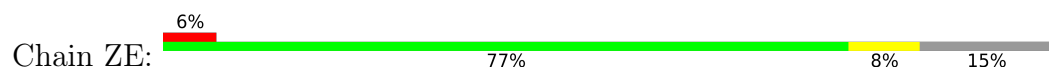
- Molecule 1: Coat protein



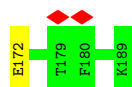
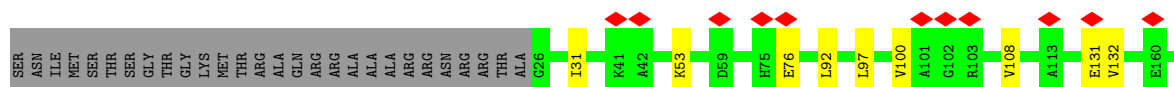
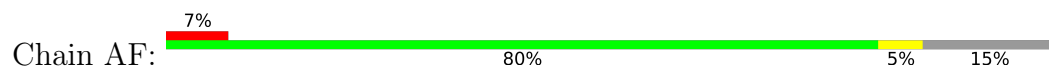
- Molecule 1: Coat protein



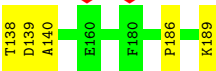
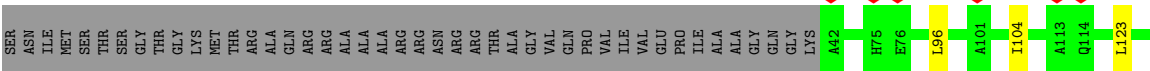
- Molecule 1: Coat protein



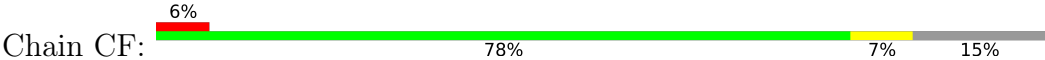
- Molecule 1: Coat protein



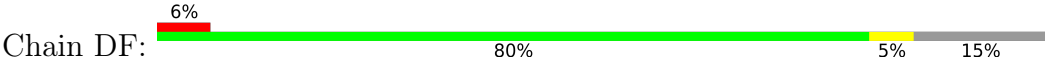
- Molecule 1: Coat protein



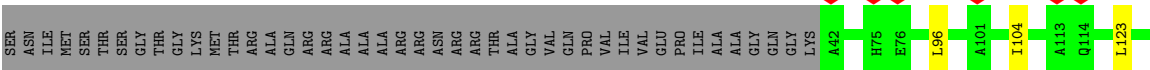
• Molecule 1: Coat protein



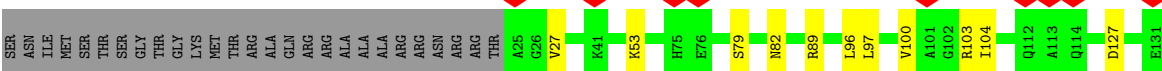
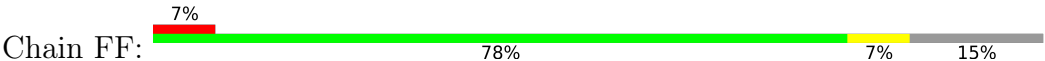
• Molecule 1: Coat protein



• Molecule 1: Coat protein

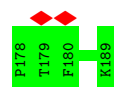
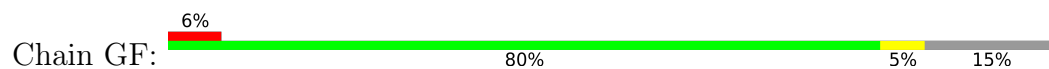


• Molecule 1: Coat protein

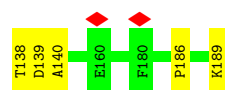
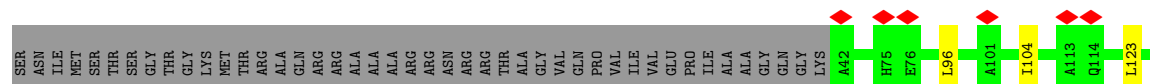
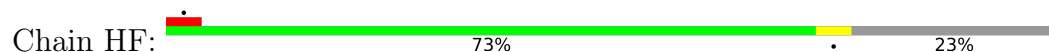




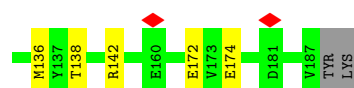
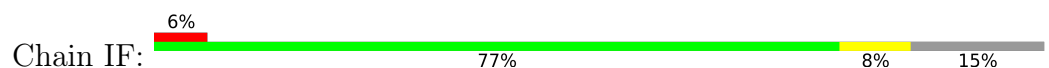
- Molecule 1: Coat protein



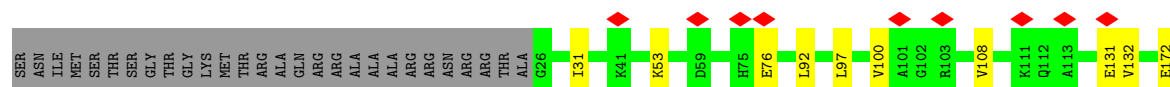
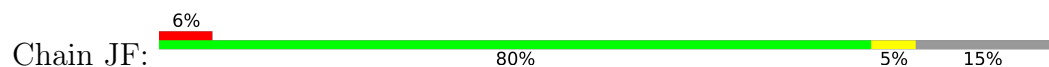
- Molecule 1: Coat protein



- Molecule 1: Coat protein

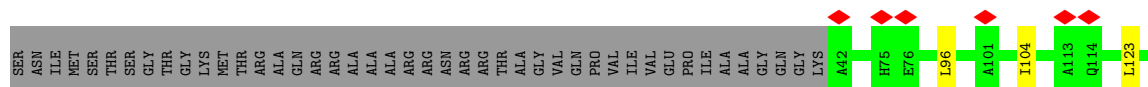


- Molecule 1: Coat protein



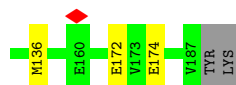
- Molecule 1: Coat protein

Chain KF:  74% 23%



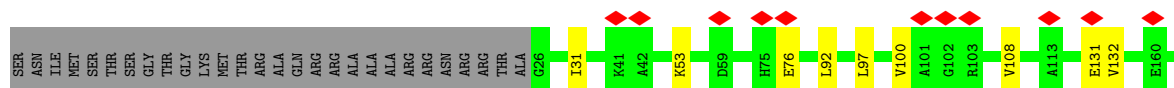
- Molecule 1: Coat protein

Chain LF:  5% 78% 7% 15%



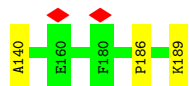
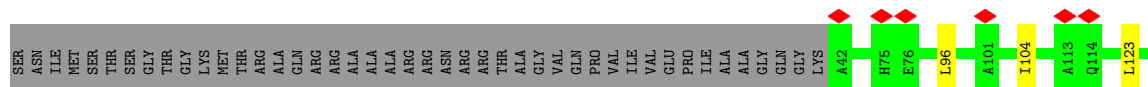
- Molecule 1: Coat protein

Chain MF:  7% 80% 5% 15%



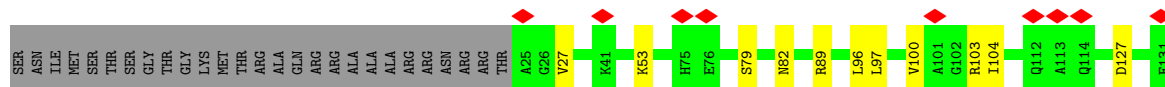
- Molecule 1: Coat protein

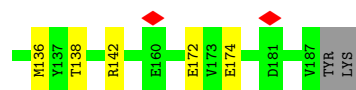
Chain NF:  74% 23%



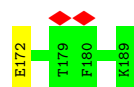
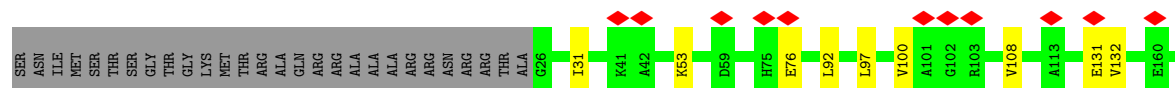
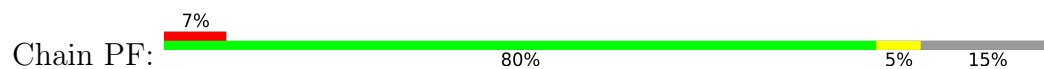
- Molecule 1: Coat protein

Chain OF:  6% 77% 8% 15%

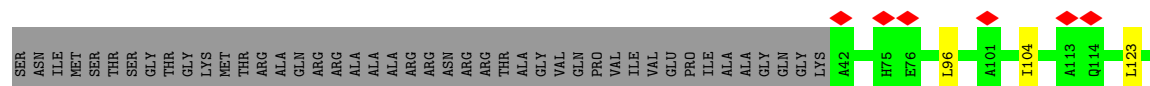
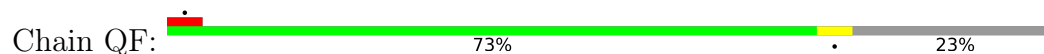




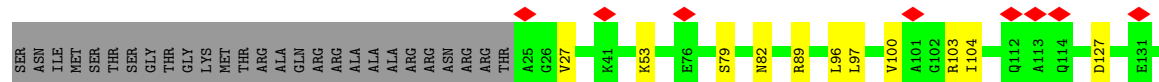
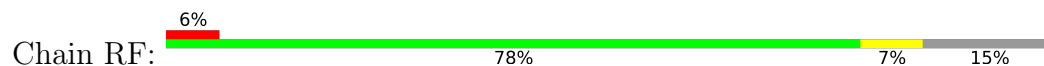
- Molecule 1: Coat protein



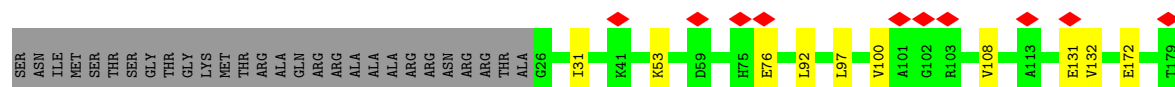
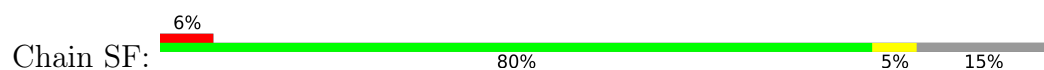
- Molecule 1: Coat protein



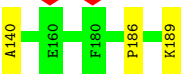
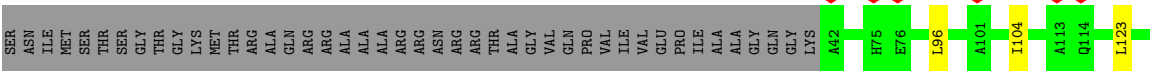
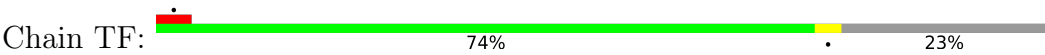
- Molecule 1: Coat protein



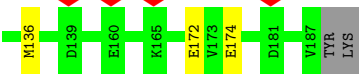
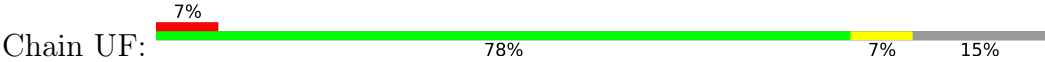
- Molecule 1: Coat protein



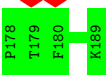
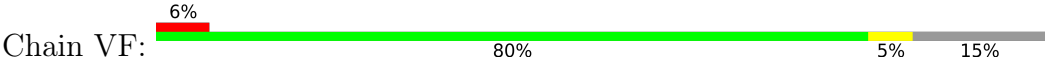
- Molecule 1: Coat protein



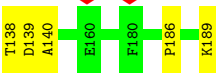
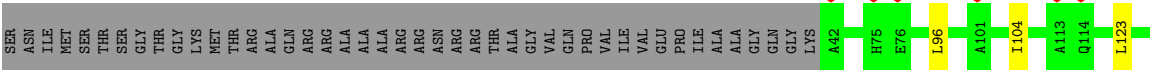
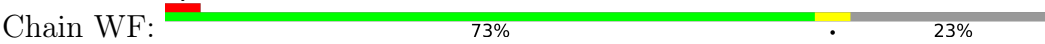
• Molecule 1: Coat protein



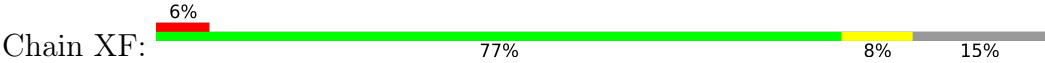
• Molecule 1: Coat protein

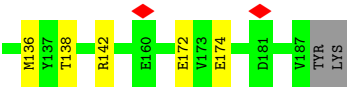


• Molecule 1: Coat protein

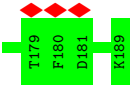
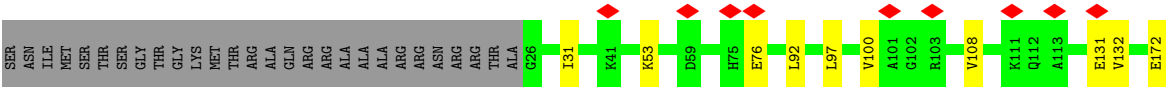
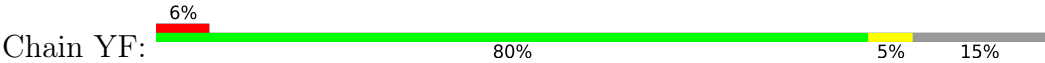


• Molecule 1: Coat protein





• 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	11521	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	0.062	Depositor
Minimum map value	-0.029	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	0/1143	0.30	0/1552
1	AA	0.16	0/1236	0.30	0/1682
1	AB	0.15	0/1143	0.30	0/1552
1	AC	0.15	0/1254	0.33	0/1704
1	AD	0.16	0/1236	0.30	0/1682
1	AE	0.15	0/1143	0.30	0/1552
1	AF	0.15	0/1254	0.33	0/1704
1	B	0.16	0/1236	0.30	0/1682
1	BA	0.15	0/1254	0.33	0/1704
1	BB	0.16	0/1236	0.30	0/1682
1	BC	0.15	0/1143	0.30	0/1552
1	BD	0.15	0/1254	0.33	0/1704
1	BE	0.16	0/1236	0.30	0/1682
1	BF	0.15	0/1143	0.30	0/1552
1	C	0.15	0/1254	0.33	0/1704
1	CA	0.15	0/1143	0.30	0/1552
1	CB	0.15	0/1254	0.33	0/1704
1	CC	0.16	0/1236	0.30	0/1682
1	CD	0.15	0/1143	0.30	0/1552
1	CE	0.15	0/1254	0.33	0/1704
1	CF	0.16	0/1236	0.30	0/1682
1	D	0.15	0/1143	0.30	0/1552
1	DA	0.16	0/1236	0.30	0/1682
1	DB	0.15	0/1143	0.30	0/1552
1	DC	0.15	0/1254	0.33	0/1704
1	DD	0.16	0/1236	0.30	0/1682
1	DE	0.15	0/1143	0.30	0/1552
1	DF	0.15	0/1254	0.33	0/1704
1	E	0.16	0/1236	0.30	0/1682
1	EA	0.15	0/1254	0.33	0/1704
1	EB	0.16	0/1236	0.30	0/1682
1	EC	0.15	0/1143	0.30	0/1552
1	ED	0.15	0/1254	0.33	0/1704
1	EE	0.16	0/1236	0.30	0/1682

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	EF	0.15	0/1143	0.30	0/1552
1	F	0.15	0/1254	0.33	0/1704
1	FA	0.15	0/1143	0.30	0/1552
1	FB	0.15	0/1254	0.33	0/1704
1	FC	0.16	0/1236	0.30	0/1682
1	FD	0.15	0/1143	0.30	0/1552
1	FE	0.15	0/1254	0.33	0/1704
1	FF	0.16	0/1236	0.30	0/1682
1	G	0.15	0/1143	0.30	0/1552
1	GA	0.16	0/1236	0.30	0/1682
1	GB	0.15	0/1143	0.30	0/1552
1	GC	0.15	0/1254	0.33	0/1704
1	GD	0.16	0/1236	0.30	0/1682
1	GE	0.15	0/1143	0.30	0/1552
1	GF	0.15	0/1254	0.33	0/1704
1	H	0.16	0/1236	0.30	0/1682
1	HA	0.15	0/1254	0.33	0/1704
1	HB	0.16	0/1236	0.30	0/1682
1	HC	0.15	0/1143	0.30	0/1552
1	HD	0.15	0/1254	0.33	0/1704
1	HE	0.16	0/1236	0.30	0/1682
1	HF	0.15	0/1143	0.30	0/1552
1	I	0.15	0/1254	0.33	0/1704
1	IA	0.15	0/1143	0.30	0/1552
1	IB	0.15	0/1254	0.33	0/1704
1	IC	0.16	0/1236	0.30	0/1682
1	ID	0.15	0/1143	0.30	0/1552
1	IE	0.15	0/1254	0.33	0/1704
1	IF	0.16	0/1236	0.30	0/1682
1	J	0.15	0/1143	0.30	0/1552
1	JA	0.16	0/1236	0.30	0/1682
1	JB	0.15	0/1143	0.30	0/1552
1	JC	0.15	0/1254	0.33	0/1704
1	JD	0.16	0/1236	0.30	0/1682
1	JE	0.15	0/1143	0.30	0/1552
1	JF	0.15	0/1254	0.33	0/1704
1	K	0.16	0/1236	0.30	0/1682
1	KA	0.15	0/1254	0.33	0/1704
1	KB	0.16	0/1236	0.30	0/1682
1	KC	0.15	0/1143	0.30	0/1552
1	KD	0.15	0/1254	0.33	0/1704
1	KE	0.16	0/1236	0.30	0/1682
1	KF	0.15	0/1143	0.30	0/1552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	0.15	0/1254	0.33	0/1704
1	LA	0.15	0/1143	0.30	0/1552
1	LB	0.15	0/1254	0.33	0/1704
1	LC	0.16	0/1236	0.30	0/1682
1	LD	0.15	0/1143	0.30	0/1552
1	LE	0.15	0/1254	0.33	0/1704
1	LF	0.16	0/1236	0.30	0/1682
1	M	0.15	0/1143	0.30	0/1552
1	MA	0.16	0/1236	0.30	0/1682
1	MB	0.15	0/1143	0.30	0/1552
1	MC	0.15	0/1254	0.33	0/1704
1	MD	0.16	0/1236	0.30	0/1682
1	ME	0.15	0/1143	0.30	0/1552
1	MF	0.15	0/1254	0.33	0/1704
1	N	0.16	0/1236	0.30	0/1682
1	NA	0.15	0/1254	0.33	0/1704
1	NB	0.16	0/1236	0.30	0/1682
1	NC	0.15	0/1143	0.30	0/1552
1	ND	0.15	0/1254	0.33	0/1704
1	NE	0.16	0/1236	0.30	0/1682
1	NF	0.15	0/1143	0.30	0/1552
1	O	0.15	0/1254	0.33	0/1704
1	OA	0.15	0/1143	0.30	0/1552
1	OB	0.15	0/1254	0.33	0/1704
1	OC	0.16	0/1236	0.30	0/1682
1	OD	0.15	0/1143	0.30	0/1552
1	OE	0.15	0/1254	0.33	0/1704
1	OF	0.16	0/1236	0.30	0/1682
1	P	0.15	0/1143	0.30	0/1552
1	PA	0.16	0/1236	0.30	0/1682
1	PB	0.15	0/1143	0.30	0/1552
1	PC	0.15	0/1254	0.33	0/1704
1	PD	0.16	0/1236	0.30	0/1682
1	PE	0.15	0/1143	0.30	0/1552
1	PF	0.15	0/1254	0.33	0/1704
1	Q	0.16	0/1236	0.30	0/1682
1	QA	0.15	0/1254	0.33	0/1704
1	QB	0.16	0/1236	0.30	0/1682
1	QC	0.15	0/1143	0.30	0/1552
1	QD	0.15	0/1254	0.33	0/1704
1	QE	0.16	0/1236	0.30	0/1682
1	QF	0.15	0/1143	0.30	0/1552
1	R	0.15	0/1254	0.33	0/1704

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	RA	0.15	0/1143	0.30	0/1552
1	RB	0.15	0/1254	0.33	0/1704
1	RC	0.16	0/1236	0.30	0/1682
1	RD	0.15	0/1143	0.30	0/1552
1	RE	0.15	0/1254	0.33	0/1704
1	RF	0.16	0/1236	0.30	0/1682
1	S	0.15	0/1143	0.30	0/1552
1	SA	0.16	0/1236	0.30	0/1682
1	SB	0.15	0/1143	0.30	0/1552
1	SC	0.15	0/1254	0.33	0/1704
1	SD	0.16	0/1236	0.30	0/1682
1	SE	0.15	0/1143	0.30	0/1552
1	SF	0.15	0/1254	0.33	0/1704
1	T	0.16	0/1236	0.30	0/1682
1	TA	0.15	0/1254	0.33	0/1704
1	TB	0.16	0/1236	0.30	0/1682
1	TC	0.15	0/1143	0.30	0/1552
1	TD	0.15	0/1254	0.33	0/1704
1	TE	0.16	0/1236	0.30	0/1682
1	TF	0.15	0/1143	0.30	0/1552
1	UA	0.15	0/1143	0.30	0/1552
1	UB	0.15	0/1254	0.33	0/1704
1	UC	0.16	0/1236	0.30	0/1682
1	UD	0.15	0/1143	0.30	0/1552
1	UE	0.15	0/1254	0.33	0/1704
1	UF	0.16	0/1236	0.30	0/1682
1	V	0.15	0/1254	0.33	0/1704
1	VA	0.16	0/1236	0.30	0/1682
1	VB	0.15	0/1143	0.30	0/1552
1	VC	0.15	0/1254	0.33	0/1704
1	VD	0.16	0/1236	0.30	0/1682
1	VE	0.15	0/1143	0.30	0/1552
1	VF	0.15	0/1254	0.33	0/1704
1	W	0.15	0/1143	0.30	0/1552
1	WA	0.15	0/1254	0.33	0/1704
1	WB	0.16	0/1236	0.30	0/1682
1	WC	0.15	0/1143	0.30	0/1552
1	WD	0.15	0/1254	0.33	0/1704
1	WE	0.16	0/1236	0.30	0/1682
1	WF	0.15	0/1143	0.30	0/1552
1	X	0.16	0/1236	0.30	0/1682
1	XA	0.15	0/1143	0.30	0/1552
1	XB	0.15	0/1254	0.33	0/1704

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	XC	0.16	0/1236	0.30	0/1682
1	XD	0.15	0/1143	0.30	0/1552
1	XE	0.15	0/1254	0.33	0/1704
1	XF	0.16	0/1236	0.30	0/1682
1	Y	0.15	0/1254	0.33	0/1704
1	YA	0.16	0/1236	0.30	0/1682
1	YB	0.15	0/1143	0.30	0/1552
1	YC	0.15	0/1254	0.33	0/1704
1	YD	0.16	0/1236	0.30	0/1682
1	YE	0.15	0/1143	0.30	0/1552
1	YF	0.15	0/1254	0.33	0/1704
1	Z	0.15	0/1143	0.30	0/1552
1	ZA	0.15	0/1254	0.33	0/1704
1	ZB	0.16	0/1236	0.30	0/1682
1	ZC	0.15	0/1143	0.30	0/1552
1	ZD	0.15	0/1254	0.33	0/1704
1	ZE	0.16	0/1236	0.30	0/1682
All	All	0.15	0/217980	0.31	0/296280

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	1122	0	1146	3	0
1	AA	1214	0	1246	10	0
1	AB	1122	0	1146	3	0
1	AC	1231	0	1263	9	0
1	AD	1214	0	1246	11	0
1	AE	1122	0	1146	4	0
1	AF	1231	0	1263	8	0
1	B	1214	0	1246	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	1231	0	1263	9	0
1	BB	1214	0	1246	11	0
1	BC	1122	0	1146	4	0
1	BD	1231	0	1263	9	0
1	BE	1214	0	1246	11	0
1	BF	1122	0	1146	4	0
1	C	1231	0	1263	9	0
1	CA	1122	0	1146	3	0
1	CB	1231	0	1263	8	0
1	CC	1214	0	1246	9	0
1	CD	1122	0	1146	4	0
1	CE	1231	0	1263	8	0
1	CF	1214	0	1246	10	0
1	D	1122	0	1146	4	0
1	DA	1214	0	1246	10	0
1	DB	1122	0	1146	4	0
1	DC	1231	0	1263	9	0
1	DD	1214	0	1246	10	0
1	DE	1122	0	1146	4	0
1	DF	1231	0	1263	9	0
1	E	1214	0	1246	11	0
1	EA	1231	0	1263	9	0
1	EB	1214	0	1246	11	0
1	EC	1122	0	1146	4	0
1	ED	1231	0	1263	9	0
1	EE	1214	0	1246	10	0
1	EF	1122	0	1146	3	0
1	F	1231	0	1263	9	0
1	FA	1122	0	1146	3	0
1	FB	1231	0	1263	9	0
1	FC	1214	0	1246	10	0
1	FD	1122	0	1146	4	0
1	FE	1231	0	1263	9	0
1	FF	1214	0	1246	10	0
1	G	1122	0	1146	4	0
1	GA	1214	0	1246	10	0
1	GB	1122	0	1146	4	0
1	GC	1231	0	1263	8	0
1	GD	1214	0	1246	11	0
1	GE	1122	0	1146	4	0
1	GF	1231	0	1263	9	0
1	H	1214	0	1246	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	HA	1231	0	1263	9	0
1	HB	1214	0	1246	10	0
1	HC	1122	0	1146	3	0
1	HD	1231	0	1263	9	0
1	HE	1214	0	1246	10	0
1	HF	1122	0	1146	4	0
1	I	1231	0	1263	9	0
1	IA	1122	0	1146	4	0
1	IB	1231	0	1263	8	0
1	IC	1214	0	1246	11	0
1	ID	1122	0	1146	3	0
1	IE	1231	0	1263	9	0
1	IF	1214	0	1246	11	0
1	J	1122	0	1146	4	0
1	JA	1214	0	1246	11	0
1	JB	1122	0	1146	4	0
1	JC	1231	0	1263	8	0
1	JD	1214	0	1246	11	0
1	JE	1122	0	1146	4	0
1	JF	1231	0	1263	9	0
1	K	1214	0	1246	10	0
1	KA	1231	0	1263	9	0
1	KB	1214	0	1246	10	0
1	KC	1122	0	1146	4	0
1	KD	1231	0	1263	9	0
1	KE	1214	0	1246	11	0
1	KF	1122	0	1146	3	0
1	L	1231	0	1263	9	0
1	LA	1122	0	1146	4	0
1	LB	1231	0	1263	9	0
1	LC	1214	0	1246	11	0
1	LD	1122	0	1146	3	0
1	LE	1231	0	1263	9	0
1	LF	1214	0	1246	9	0
1	M	1122	0	1146	4	0
1	MA	1214	0	1246	11	0
1	MB	1122	0	1146	4	0
1	MC	1231	0	1263	9	0
1	MD	1214	0	1246	10	0
1	ME	1122	0	1146	3	0
1	MF	1231	0	1263	8	0
1	N	1214	0	1246	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	NA	1231	0	1263	9	0
1	NB	1214	0	1246	11	0
1	NC	1122	0	1146	4	0
1	ND	1231	0	1263	9	0
1	NE	1214	0	1246	10	0
1	NF	1122	0	1146	3	0
1	O	1231	0	1263	9	0
1	OA	1122	0	1146	4	0
1	OB	1231	0	1263	9	0
1	OC	1214	0	1246	11	0
1	OD	1122	0	1146	3	0
1	OE	1231	0	1263	8	0
1	OF	1214	0	1246	11	0
1	P	1122	0	1146	3	0
1	PA	1214	0	1246	10	0
1	PB	1122	0	1146	3	0
1	PC	1231	0	1263	9	0
1	PD	1214	0	1246	11	0
1	PE	1122	0	1146	4	0
1	PF	1231	0	1263	8	0
1	Q	1214	0	1246	10	0
1	QA	1231	0	1263	9	0
1	QB	1214	0	1246	10	0
1	QC	1122	0	1146	4	0
1	QD	1231	0	1263	8	0
1	QE	1214	0	1246	11	0
1	QF	1122	0	1146	4	0
1	R	1231	0	1263	8	0
1	RA	1122	0	1146	4	0
1	RB	1231	0	1263	9	0
1	RC	1214	0	1246	9	0
1	RD	1122	0	1146	4	0
1	RE	1231	0	1263	9	0
1	RF	1214	0	1246	10	0
1	S	1122	0	1146	3	0
1	SA	1214	0	1246	10	0
1	SB	1122	0	1146	3	0
1	SC	1231	0	1263	9	0
1	SD	1214	0	1246	10	0
1	SE	1122	0	1146	3	0
1	SF	1231	0	1263	9	0
1	T	1214	0	1246	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	TA	1231	0	1263	9	0
1	TB	1214	0	1246	8	0
1	TC	1122	0	1146	4	0
1	TD	1231	0	1263	9	0
1	TE	1214	0	1246	10	0
1	TF	1122	0	1146	3	0
1	UA	1122	0	1146	3	0
1	UB	1231	0	1263	9	0
1	UC	1214	0	1246	11	0
1	UD	1122	0	1146	4	0
1	UE	1231	0	1263	9	0
1	UF	1214	0	1246	10	0
1	V	1231	0	1263	9	0
1	VA	1214	0	1246	10	0
1	VB	1122	0	1146	3	0
1	VC	1231	0	1263	8	0
1	VD	1214	0	1246	11	0
1	VE	1122	0	1146	4	0
1	VF	1231	0	1263	9	0
1	W	1122	0	1146	3	0
1	WA	1231	0	1263	8	0
1	WB	1214	0	1246	11	0
1	WC	1122	0	1146	3	0
1	WD	1231	0	1263	9	0
1	WE	1214	0	1246	9	0
1	WF	1122	0	1146	4	0
1	X	1214	0	1246	11	0
1	XA	1122	0	1146	3	0
1	XB	1231	0	1263	6	0
1	XC	1214	0	1246	11	0
1	XD	1122	0	1146	3	0
1	XE	1231	0	1263	9	0
1	XF	1214	0	1246	11	0
1	Y	1231	0	1263	8	0
1	YA	1214	0	1246	9	0
1	YB	1122	0	1146	4	0
1	YC	1231	0	1263	9	0
1	YD	1214	0	1246	9	0
1	YE	1122	0	1146	3	0
1	YF	1231	0	1263	9	0
1	Z	1122	0	1146	4	0
1	ZA	1231	0	1263	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	ZB	1214	0	1246	11	0
1	ZC	1122	0	1146	4	0
1	ZD	1231	0	1263	8	0
1	ZE	1214	0	1246	11	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	214200	0	219300	1188	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 (1188) 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:CF:97:LEU:HB2	1:CF:100:VAL:HG23	1.82	0.62
1:RF:97:LEU:HB2	1:RF:100:VAL:HG23	1.82	0.62
1:JA:97:LEU:HB2	1:JA:100:VAL:HG23	1.82	0.62
1:SA:97:LEU:HB2	1:SA:100:VAL:HG23	1.82	0.62
1:LF:97:LEU:HB2	1:LF:100:VAL:HG23	1.82	0.62
1:E:97:LEU:HB2	1:E:100:VAL:HG23	1.82	0.62
1:K:97:LEU:HB2	1:K:100:VAL:HG23	1.82	0.62
1:N:97:LEU:HB2	1:N:100:VAL:HG23	1.82	0.62
1:IC:97:LEU:HB2	1:IC:100:VAL:HG23	1.82	0.62
1:XC:97:LEU:HB2	1:XC:100:VAL:HG23	1.82	0.62
1:WE:97:LEU:HB2	1:WE:100:VAL:HG23	1.82	0.62
1:UF:97:LEU:HB2	1:UF:100:VAL:HG23	1.82	0.62
1:X:53:LYS:HG2	1:X:172:GLU:HG3	1.82	0.62
1:PA:97:LEU:HB2	1:PA:100:VAL:HG23	1.82	0.62
1:FF:97:LEU:HB2	1:FF:100:VAL:HG23	1.82	0.62
1:H:97:LEU:HB2	1:H:100:VAL:HG23	1.82	0.62
1:Q:53:LYS:HG2	1:Q:172:GLU:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MA:97:LEU:HB2	1:MA:100:VAL:HG23	1.82	0.62
1:VA:53:LYS:HG2	1:VA:172:GLU:HG3	1.82	0.62
1:BB:53:LYS:HG2	1:BB:172:GLU:HG3	1.82	0.62
1:EE:53:LYS:HG2	1:EE:172:GLU:HG3	1.82	0.62
1:TE:53:LYS:HG2	1:TE:172:GLU:HG3	1.82	0.62
1:SA:53:LYS:HG2	1:SA:172:GLU:HG3	1.82	0.62
1:ZB:53:LYS:HG2	1:ZB:172:GLU:HG3	1.82	0.62
1:OC:53:LYS:HG2	1:OC:172:GLU:HG3	1.82	0.62
1:BE:97:LEU:HB2	1:BE:100:VAL:HG23	1.82	0.62
1:QE:97:LEU:HB2	1:QE:100:VAL:HG23	1.82	0.62
1:B:53:LYS:HG2	1:B:172:GLU:HG3	1.82	0.61
1:N:53:LYS:HG2	1:N:172:GLU:HG3	1.82	0.61
1:GA:53:LYS:HG2	1:GA:172:GLU:HG3	1.82	0.61
1:T:97:LEU:HB2	1:T:100:VAL:HG23	1.82	0.61
1:AA:97:LEU:HB2	1:AA:100:VAL:HG23	1.82	0.61
1:YA:97:LEU:HB2	1:YA:100:VAL:HG23	1.82	0.61
1:EB:97:LEU:HB2	1:EB:100:VAL:HG23	1.82	0.61
1:XF:97:LEU:HB2	1:XF:100:VAL:HG23	1.82	0.61
1:F:97:LEU:HB2	1:F:100:VAL:HG23	1.83	0.61
1:H:53:LYS:HG2	1:H:172:GLU:HG3	1.82	0.61
1:T:53:LYS:HG2	1:T:172:GLU:HG3	1.82	0.61
1:X:97:LEU:HB2	1:X:100:VAL:HG23	1.82	0.61
1:KA:97:LEU:HB2	1:KA:100:VAL:HG23	1.83	0.61
1:BB:97:LEU:HB2	1:BB:100:VAL:HG23	1.82	0.61
1:SD:97:LEU:HB2	1:SD:100:VAL:HG23	1.82	0.61
1:YD:97:LEU:HB2	1:YD:100:VAL:HG23	1.82	0.61
1:Y:97:LEU:HB2	1:Y:100:VAL:HG23	1.83	0.61
1:EA:97:LEU:HB2	1:EA:100:VAL:HG23	1.83	0.61
1:MA:53:LYS:HG2	1:MA:172:GLU:HG3	1.82	0.61
1:YA:53:LYS:HG2	1:YA:172:GLU:HG3	1.82	0.61
1:IB:97:LEU:HB2	1:IB:100:VAL:HG23	1.83	0.61
1:TB:97:LEU:HB2	1:TB:100:VAL:HG23	1.82	0.61
1:WB:97:LEU:HB2	1:WB:100:VAL:HG23	1.82	0.61
1:GC:97:LEU:HB2	1:GC:100:VAL:HG23	1.83	0.61
1:PD:97:LEU:HB2	1:PD:100:VAL:HG23	1.82	0.61
1:HE:97:LEU:HB2	1:HE:100:VAL:HG23	1.82	0.61
1:WE:53:LYS:HG2	1:WE:172:GLU:HG3	1.82	0.61
1:IF:97:LEU:HB2	1:IF:100:VAL:HG23	1.82	0.61
1:LF:53:LYS:HG2	1:LF:172:GLU:HG3	1.82	0.61
1:B:97:LEU:HB2	1:B:100:VAL:HG23	1.82	0.61
1:K:53:LYS:HG2	1:K:172:GLU:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:97:LEU:HB2	1:Q:100:VAL:HG23	1.82	0.61
1:PA:53:LYS:HG2	1:PA:172:GLU:HG3	1.82	0.61
1:VA:97:LEU:HB2	1:VA:100:VAL:HG23	1.82	0.61
1:CB:97:LEU:HB2	1:CB:100:VAL:HG23	1.83	0.61
1:WB:53:LYS:HG2	1:WB:172:GLU:HG3	1.82	0.61
1:VC:97:LEU:HB2	1:VC:100:VAL:HG23	1.83	0.61
1:MD:97:LEU:HB2	1:MD:100:VAL:HG23	1.82	0.61
1:VD:53:LYS:HG2	1:VD:172:GLU:HG3	1.82	0.61
1:NE:97:LEU:HB2	1:NE:100:VAL:HG23	1.82	0.61
1:O:97:LEU:HB2	1:O:100:VAL:HG23	1.83	0.61
1:QB:97:LEU:HB2	1:QB:100:VAL:HG23	1.82	0.61
1:DD:97:LEU:HB2	1:DD:100:VAL:HG23	1.82	0.61
1:JD:97:LEU:HB2	1:JD:100:VAL:HG23	1.82	0.61
1:PD:53:LYS:HG2	1:PD:172:GLU:HG3	1.82	0.61
1:TD:97:LEU:HB2	1:TD:100:VAL:HG23	1.83	0.61
1:KE:53:LYS:HG2	1:KE:172:GLU:HG3	1.82	0.61
1:C:97:LEU:HB2	1:C:100:VAL:HG23	1.83	0.61
1:GA:97:LEU:HB2	1:GA:100:VAL:HG23	1.82	0.61
1:TA:97:LEU:HB2	1:TA:100:VAL:HG23	1.83	0.61
1:RB:97:LEU:HB2	1:RB:100:VAL:HG23	1.83	0.61
1:UC:97:LEU:HB2	1:UC:100:VAL:HG23	1.82	0.61
1:AD:97:LEU:HB2	1:AD:100:VAL:HG23	1.82	0.61
1:KD:97:LEU:HB2	1:KD:100:VAL:HG23	1.83	0.61
1:VD:97:LEU:HB2	1:VD:100:VAL:HG23	1.82	0.61
1:IE:97:LEU:HB2	1:IE:100:VAL:HG23	1.83	0.61
1:HA:97:LEU:HB2	1:HA:100:VAL:HG23	1.83	0.61
1:ZA:97:LEU:HB2	1:ZA:100:VAL:HG23	1.83	0.61
1:KB:97:LEU:HB2	1:KB:100:VAL:HG23	1.82	0.61
1:FC:97:LEU:HB2	1:FC:100:VAL:HG23	1.82	0.61
1:LC:97:LEU:HB2	1:LC:100:VAL:HG23	1.82	0.61
1:MD:53:LYS:HG2	1:MD:172:GLU:HG3	1.82	0.61
1:KE:97:LEU:HB2	1:KE:100:VAL:HG23	1.82	0.61
1:V:97:LEU:HB2	1:V:100:VAL:HG23	1.83	0.61
1:TB:53:LYS:HG2	1:TB:172:GLU:HG3	1.82	0.61
1:JC:97:LEU:HB2	1:JC:100:VAL:HG23	1.83	0.61
1:LC:53:LYS:HG2	1:LC:172:GLU:HG3	1.82	0.61
1:XC:53:LYS:HG2	1:XC:172:GLU:HG3	1.82	0.61
1:JD:53:LYS:HG2	1:JD:172:GLU:HG3	1.82	0.61
1:FE:97:LEU:HB2	1:FE:100:VAL:HG23	1.83	0.61
1:UE:97:LEU:HB2	1:UE:100:VAL:HG23	1.83	0.61
1:UF:53:LYS:HG2	1:UF:172:GLU:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IC:53:LYS:HG2	1:IC:172:GLU:HG3	1.82	0.61
1:AD:53:LYS:HG2	1:AD:172:GLU:HG3	1.82	0.61
1:YD:53:LYS:HG2	1:YD:172:GLU:HG3	1.82	0.61
1:HE:53:LYS:HG2	1:HE:172:GLU:HG3	1.82	0.61
1:LE:97:LEU:HB2	1:LE:100:VAL:HG23	1.83	0.61
1:FF:53:LYS:HG2	1:FF:172:GLU:HG3	1.82	0.61
1:QB:53:LYS:HG2	1:QB:172:GLU:HG3	1.82	0.60
1:RC:97:LEU:HB2	1:RC:100:VAL:HG23	1.82	0.60
1:YC:97:LEU:HB2	1:YC:100:VAL:HG23	1.83	0.60
1:SD:53:LYS:HG2	1:SD:172:GLU:HG3	1.82	0.60
1:WD:97:LEU:HB2	1:WD:100:VAL:HG23	1.83	0.60
1:NE:53:LYS:HG2	1:NE:172:GLU:HG3	1.82	0.60
1:GF:97:LEU:HB2	1:GF:100:VAL:HG23	1.83	0.60
1:BA:97:LEU:HB2	1:BA:100:VAL:HG23	1.83	0.60
1:OB:97:LEU:HB2	1:OB:100:VAL:HG23	1.83	0.60
1:IF:53:LYS:HG2	1:IF:172:GLU:HG3	1.82	0.60
1:VF:97:LEU:HB2	1:VF:100:VAL:HG23	1.83	0.60
1:XF:53:LYS:HG2	1:XF:172:GLU:HG3	1.82	0.60
1:R:97:LEU:HB2	1:R:100:VAL:HG23	1.83	0.60
1:WA:97:LEU:HB2	1:WA:100:VAL:HG23	1.83	0.60
1:FB:97:LEU:HB2	1:FB:100:VAL:HG23	1.83	0.60
1:CC:97:LEU:HB2	1:CC:100:VAL:HG23	1.82	0.60
1:HD:97:LEU:HB2	1:HD:100:VAL:HG23	1.83	0.60
1:OF:97:LEU:HB2	1:OF:100:VAL:HG23	1.82	0.60
1:HB:97:LEU:HB2	1:HB:100:VAL:HG23	1.82	0.60
1:DF:97:LEU:HB2	1:DF:100:VAL:HG23	1.83	0.60
1:MF:97:LEU:HB2	1:MF:100:VAL:HG23	1.83	0.60
1:E:53:LYS:HG2	1:E:172:GLU:HG3	1.82	0.60
1:DA:97:LEU:HB2	1:DA:100:VAL:HG23	1.82	0.60
1:JA:53:LYS:HG2	1:JA:172:GLU:HG3	1.82	0.60
1:BE:53:LYS:HG2	1:BE:172:GLU:HG3	1.82	0.60
1:QE:53:LYS:HG2	1:QE:172:GLU:HG3	1.82	0.60
1:XE:97:LEU:HB2	1:XE:100:VAL:HG23	1.83	0.60
1:SF:97:LEU:HB2	1:SF:100:VAL:HG23	1.83	0.60
1:I:97:LEU:HB2	1:I:100:VAL:HG23	1.83	0.60
1:L:97:LEU:HB2	1:L:100:VAL:HG23	1.83	0.60
1:NA:97:LEU:HB2	1:NA:100:VAL:HG23	1.83	0.60
1:XB:97:LEU:HB2	1:XB:100:VAL:HG23	1.83	0.60
1:CC:53:LYS:HG2	1:CC:172:GLU:HG3	1.82	0.60
1:CE:97:LEU:HB2	1:CE:100:VAL:HG23	1.83	0.60
1:ZE:97:LEU:HB2	1:ZE:100:VAL:HG23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RC:53:LYS:HG2	1:RC:172:GLU:HG3	1.82	0.60
1:SC:97:LEU:HB2	1:SC:100:VAL:HG23	1.83	0.60
1:CF:53:LYS:HG2	1:CF:172:GLU:HG3	1.82	0.60
1:OF:53:LYS:HG2	1:OF:172:GLU:HG3	1.82	0.60
1:PF:97:LEU:HB2	1:PF:100:VAL:HG23	1.83	0.60
1:DA:53:LYS:HG2	1:DA:172:GLU:HG3	1.82	0.60
1:QA:97:LEU:HB2	1:QA:100:VAL:HG23	1.83	0.60
1:HB:53:LYS:HG2	1:HB:172:GLU:HG3	1.82	0.60
1:ZB:97:LEU:HB2	1:ZB:100:VAL:HG23	1.82	0.60
1:MC:97:LEU:HB2	1:MC:100:VAL:HG23	1.83	0.60
1:GD:53:LYS:HG2	1:GD:172:GLU:HG3	1.82	0.60
1:ND:97:LEU:HB2	1:ND:100:VAL:HG23	1.83	0.60
1:QD:97:LEU:HB2	1:QD:100:VAL:HG23	1.83	0.60
1:RE:97:LEU:HB2	1:RE:100:VAL:HG23	1.83	0.60
1:ZE:53:LYS:HG2	1:ZE:172:GLU:HG3	1.82	0.60
1:AF:97:LEU:HB2	1:AF:100:VAL:HG23	1.83	0.60
1:RF:53:LYS:HG2	1:RF:172:GLU:HG3	1.82	0.60
1:AA:53:LYS:HG2	1:AA:172:GLU:HG3	1.82	0.60
1:NB:53:LYS:HG2	1:NB:172:GLU:HG3	1.82	0.60
1:EB:53:LYS:HG2	1:EB:172:GLU:HG3	1.82	0.60
1:UB:97:LEU:HB2	1:UB:100:VAL:HG23	1.83	0.60
1:DC:97:LEU:HB2	1:DC:100:VAL:HG23	1.83	0.60
1:FC:53:LYS:HG2	1:FC:172:GLU:HG3	1.82	0.60
1:OC:97:LEU:HB2	1:OC:100:VAL:HG23	1.82	0.60
1:PC:97:LEU:HB2	1:PC:100:VAL:HG23	1.83	0.60
1:BD:97:LEU:HB2	1:BD:100:VAL:HG23	1.83	0.60
1:KB:53:LYS:HG2	1:KB:172:GLU:HG3	1.82	0.59
1:AC:97:LEU:HB2	1:AC:100:VAL:HG23	1.83	0.59
1:EE:97:LEU:HB2	1:EE:100:VAL:HG23	1.82	0.59
1:UC:53:LYS:HG2	1:UC:172:GLU:HG3	1.82	0.59
1:DD:53:LYS:HG2	1:DD:172:GLU:HG3	1.82	0.59
1:YF:97:LEU:HB2	1:YF:100:VAL:HG23	1.83	0.59
1:TE:97:LEU:HB2	1:TE:100:VAL:HG23	1.82	0.59
1:NB:97:LEU:HB2	1:NB:100:VAL:HG23	1.82	0.59
1:JF:97:LEU:HB2	1:JF:100:VAL:HG23	1.83	0.59
1:GD:97:LEU:HB2	1:GD:100:VAL:HG23	1.82	0.59
1:LB:97:LEU:HB2	1:LB:100:VAL:HG23	1.83	0.59
1:ED:97:LEU:HB2	1:ED:100:VAL:HG23	1.83	0.59
1:ZD:92:LEU:HD22	1:ZD:108:VAL:HG23	1.85	0.59
1:CE:92:LEU:HD22	1:CE:108:VAL:HG23	1.85	0.59
1:OE:92:LEU:HD22	1:OE:108:VAL:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DC:92:LEU:HD22	1:DC:108:VAL:HG23	1.85	0.58
1:RE:92:LEU:HD22	1:RE:108:VAL:HG23	1.85	0.58
1:XE:92:LEU:HD22	1:XE:108:VAL:HG23	1.85	0.58
1:MF:92:LEU:HD22	1:MF:108:VAL:HG23	1.85	0.58
1:EA:92:LEU:HD22	1:EA:108:VAL:HG23	1.85	0.58
1:IB:92:LEU:HD22	1:IB:108:VAL:HG23	1.85	0.58
1:SC:92:LEU:HD22	1:SC:108:VAL:HG23	1.85	0.58
1:YC:92:LEU:HD22	1:YC:108:VAL:HG23	1.85	0.58
1:OE:97:LEU:HB2	1:OE:100:VAL:HG23	1.83	0.58
1:GF:92:LEU:HD22	1:GF:108:VAL:HG23	1.85	0.58
1:VF:92:LEU:HD22	1:VF:108:VAL:HG23	1.85	0.58
1:Y:92:LEU:HD22	1:Y:108:VAL:HG23	1.85	0.58
1:LB:92:LEU:HD22	1:LB:108:VAL:HG23	1.85	0.58
1:JC:92:LEU:HD22	1:JC:108:VAL:HG23	1.85	0.58
1:ED:92:LEU:HD22	1:ED:108:VAL:HG23	1.85	0.58
1:ZD:97:LEU:HB2	1:ZD:100:VAL:HG23	1.83	0.58
1:SF:92:LEU:HD22	1:SF:108:VAL:HG23	1.85	0.58
1:CB:92:LEU:HD22	1:CB:108:VAL:HG23	1.85	0.58
1:BD:92:LEU:HD22	1:BD:108:VAL:HG23	1.85	0.58
1:KD:92:LEU:HD22	1:KD:108:VAL:HG23	1.85	0.58
1:XE:131:GLU:HG2	1:XE:132:VAL:HG23	1.86	0.58
1:DF:92:LEU:HD22	1:DF:108:VAL:HG23	1.85	0.58
1:MF:131:GLU:HG2	1:MF:132:VAL:HG23	1.86	0.58
1:F:131:GLU:HG2	1:F:132:VAL:HG23	1.86	0.58
1:O:131:GLU:HG2	1:O:132:VAL:HG23	1.86	0.58
1:KA:92:LEU:HD22	1:KA:108:VAL:HG23	1.85	0.58
1:RB:92:LEU:HD22	1:RB:108:VAL:HG23	1.85	0.58
1:MC:92:LEU:HD22	1:MC:108:VAL:HG23	1.85	0.58
1:C:92:LEU:HD22	1:C:108:VAL:HG23	1.85	0.58
1:F:92:LEU:HD22	1:F:108:VAL:HG23	1.85	0.58
1:EA:131:GLU:HG2	1:EA:132:VAL:HG23	1.86	0.58
1:HA:92:LEU:HD22	1:HA:108:VAL:HG23	1.85	0.58
1:KA:131:GLU:HG2	1:KA:132:VAL:HG23	1.86	0.58
1:TA:131:GLU:HG2	1:TA:132:VAL:HG23	1.86	0.58
1:ZA:131:GLU:HG2	1:ZA:132:VAL:HG23	1.86	0.58
1:BD:131:GLU:HG2	1:BD:132:VAL:HG23	1.86	0.58
1:ED:131:GLU:HG2	1:ED:132:VAL:HG23	1.86	0.58
1:HD:92:LEU:HD22	1:HD:108:VAL:HG23	1.85	0.58
1:L:92:LEU:HD22	1:L:108:VAL:HG23	1.85	0.58
1:V:131:GLU:HG2	1:V:132:VAL:HG23	1.86	0.58
1:IB:131:GLU:HG2	1:IB:132:VAL:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LB:131:GLU:HG2	1:LB:132:VAL:HG23	1.86	0.58
1:OB:92:LEU:HD22	1:OB:108:VAL:HG23	1.85	0.58
1:GC:92:LEU:HD22	1:GC:108:VAL:HG23	1.85	0.58
1:MC:131:GLU:HG2	1:MC:132:VAL:HG23	1.86	0.58
1:VC:92:LEU:HD22	1:VC:108:VAL:HG23	1.85	0.58
1:QA:92:LEU:HD22	1:QA:108:VAL:HG23	1.85	0.58
1:XB:92:LEU:HD22	1:XB:108:VAL:HG23	1.85	0.58
1:DC:131:GLU:HG2	1:DC:132:VAL:HG23	1.86	0.58
1:SC:131:GLU:HG2	1:SC:132:VAL:HG23	1.86	0.58
1:QD:92:LEU:HD22	1:QD:108:VAL:HG23	1.85	0.58
1:O:92:LEU:HD22	1:O:108:VAL:HG23	1.85	0.58
1:BA:131:GLU:HG2	1:BA:132:VAL:HG23	1.86	0.58
1:TA:92:LEU:HD22	1:TA:108:VAL:HG23	1.85	0.58
1:FB:131:GLU:HG2	1:FB:132:VAL:HG23	1.86	0.58
1:PC:92:LEU:HD22	1:PC:108:VAL:HG23	1.85	0.58
1:DF:131:GLU:HG2	1:DF:132:VAL:HG23	1.86	0.58
1:SF:131:GLU:HG2	1:SF:132:VAL:HG23	1.86	0.58
1:R:131:GLU:HG2	1:R:132:VAL:HG23	1.86	0.57
1:FB:92:LEU:HD22	1:FB:108:VAL:HG23	1.85	0.57
1:JC:131:GLU:HG2	1:JC:132:VAL:HG23	1.86	0.57
1:YC:131:GLU:HG2	1:YC:132:VAL:HG23	1.86	0.57
1:QD:53:LYS:HG2	1:QD:172:GLU:HG3	1.86	0.57
1:WD:53:LYS:HG2	1:WD:172:GLU:HG3	1.86	0.57
1:ZD:131:GLU:HG2	1:ZD:132:VAL:HG23	1.86	0.57
1:OE:131:GLU:HG2	1:OE:132:VAL:HG23	1.86	0.57
1:R:53:LYS:HG2	1:R:172:GLU:HG3	1.86	0.57
1:BA:92:LEU:HD22	1:BA:108:VAL:HG23	1.85	0.57
1:WA:53:LYS:HG2	1:WA:172:GLU:HG3	1.86	0.57
1:LB:53:LYS:HG2	1:LB:172:GLU:HG3	1.86	0.57
1:XB:53:LYS:HG2	1:XB:172:GLU:HG3	1.86	0.57
1:AC:92:LEU:HD22	1:AC:108:VAL:HG23	1.85	0.57
1:JC:53:LYS:HG2	1:JC:172:GLU:HG3	1.86	0.57
1:PC:131:GLU:HG2	1:PC:132:VAL:HG23	1.86	0.57
1:YC:53:LYS:HG2	1:YC:172:GLU:HG3	1.86	0.57
1:ED:53:LYS:HG2	1:ED:172:GLU:HG3	1.86	0.57
1:LE:53:LYS:HG2	1:LE:172:GLU:HG3	1.86	0.57
1:AF:53:LYS:HG2	1:AF:172:GLU:HG3	1.86	0.57
1:AF:92:LEU:HD22	1:AF:108:VAL:HG23	1.85	0.57
1:JF:92:LEU:HD22	1:JF:108:VAL:HG23	1.85	0.57
1:WA:131:GLU:HG2	1:WA:132:VAL:HG23	1.86	0.57
1:UB:53:LYS:HG2	1:UB:172:GLU:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UB:92:LEU:HD22	1:UB:108:VAL:HG23	1.85	0.57
1:AC:131:GLU:HG2	1:AC:132:VAL:HG23	1.86	0.57
1:ND:53:LYS:HG2	1:ND:172:GLU:HG3	1.86	0.57
1:ND:131:GLU:HG2	1:ND:132:VAL:HG23	1.86	0.57
1:ZD:53:LYS:HG2	1:ZD:172:GLU:HG3	1.87	0.57
1:OE:53:LYS:HG2	1:OE:172:GLU:HG3	1.87	0.57
1:PF:53:LYS:HG2	1:PF:172:GLU:HG3	1.86	0.57
1:PF:92:LEU:HD22	1:PF:108:VAL:HG23	1.85	0.57
1:YF:92:LEU:HD22	1:YF:108:VAL:HG23	1.85	0.57
1:I:92:LEU:HD22	1:I:108:VAL:HG23	1.85	0.57
1:P:186:PRO:O	1:P:189:LYS:NZ	2.38	0.57
1:NA:92:LEU:HD22	1:NA:108:VAL:HG23	1.85	0.57
1:NA:131:GLU:HG2	1:NA:132:VAL:HG23	1.86	0.57
1:UA:186:PRO:O	1:UA:189:LYS:NZ	2.38	0.57
1:UB:131:GLU:HG2	1:UB:132:VAL:HG23	1.86	0.57
1:GC:131:GLU:HG2	1:GC:132:VAL:HG23	1.86	0.57
1:VC:131:GLU:HG2	1:VC:132:VAL:HG23	1.86	0.57
1:ND:92:LEU:HD22	1:ND:108:VAL:HG23	1.85	0.57
1:LE:92:LEU:HD22	1:LE:108:VAL:HG23	1.85	0.57
1:JF:53:LYS:HG2	1:JF:172:GLU:HG3	1.86	0.57
1:YF:53:LYS:HG2	1:YF:172:GLU:HG3	1.86	0.57
1:I:131:GLU:HG2	1:I:132:VAL:HG23	1.86	0.57
1:S:186:PRO:O	1:S:189:LYS:NZ	2.38	0.57
1:XA:186:PRO:O	1:XA:189:LYS:NZ	2.38	0.57
1:RB:53:LYS:HG2	1:RB:172:GLU:HG3	1.87	0.57
1:CD:186:PRO:O	1:CD:189:LYS:NZ	2.38	0.57
1:VE:186:PRO:O	1:VE:189:LYS:NZ	2.38	0.57
1:KF:186:PRO:O	1:KF:189:LYS:NZ	2.38	0.57
1:NA:53:LYS:HG2	1:NA:172:GLU:HG3	1.87	0.57
1:KD:53:LYS:HG2	1:KD:172:GLU:HG3	1.87	0.57
1:QD:131:GLU:HG2	1:QD:132:VAL:HG23	1.86	0.57
1:WD:92:LEU:HD22	1:WD:108:VAL:HG23	1.85	0.57
1:RE:131:GLU:HG2	1:RE:132:VAL:HG23	1.86	0.57
1:GF:53:LYS:HG2	1:GF:172:GLU:HG3	1.86	0.57
1:SF:53:LYS:HG2	1:SF:172:GLU:HG3	1.87	0.57
1:VF:53:LYS:HG2	1:VF:172:GLU:HG3	1.86	0.57
1:I:53:LYS:HG2	1:I:172:GLU:HG3	1.87	0.57
1:J:186:PRO:O	1:J:189:LYS:NZ	2.38	0.57
1:O:53:LYS:HG2	1:O:172:GLU:HG3	1.86	0.57
1:TA:53:LYS:HG2	1:TA:172:GLU:HG3	1.86	0.57
1:WA:92:LEU:HD22	1:WA:108:VAL:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EC:186:PRO:O	1:EC:189:LYS:NZ	2.38	0.57
1:LE:131:GLU:HG2	1:LE:132:VAL:HG23	1.86	0.57
1:DF:53:LYS:HG2	1:DF:172:GLU:HG3	1.87	0.57
1:YF:131:GLU:HG2	1:YF:132:VAL:HG23	1.86	0.57
1:A:186:PRO:O	1:A:189:LYS:NZ	2.38	0.57
1:L:131:GLU:HG2	1:L:132:VAL:HG23	1.86	0.57
1:R:92:LEU:HD22	1:R:108:VAL:HG23	1.85	0.57
1:Z:186:PRO:O	1:Z:189:LYS:NZ	2.38	0.57
1:QA:131:GLU:HG2	1:QA:132:VAL:HG23	1.86	0.57
1:DB:186:PRO:O	1:DB:189:LYS:NZ	2.38	0.57
1:XB:131:GLU:HG2	1:XB:132:VAL:HG23	1.86	0.57
1:TC:186:PRO:O	1:TC:189:LYS:NZ	2.38	0.57
1:WD:131:GLU:HG2	1:WD:132:VAL:HG23	1.86	0.57
1:CE:131:GLU:HG2	1:CE:132:VAL:HG23	1.86	0.57
1:MF:53:LYS:HG2	1:MF:172:GLU:HG3	1.86	0.57
1:V:92:LEU:HD22	1:V:108:VAL:HG23	1.85	0.57
1:OA:186:PRO:O	1:OA:189:LYS:NZ	2.38	0.57
1:ZA:92:LEU:HD22	1:ZA:108:VAL:HG23	1.85	0.57
1:RB:131:GLU:HG2	1:RB:132:VAL:HG23	1.86	0.57
1:XE:53:LYS:HG2	1:XE:172:GLU:HG3	1.86	0.57
1:EF:186:PRO:O	1:EF:189:LYS:NZ	2.38	0.57
1:JF:131:GLU:HG2	1:JF:132:VAL:HG23	1.86	0.57
1:TF:186:PRO:O	1:TF:189:LYS:NZ	2.38	0.57
1:BD:53:LYS:HG2	1:BD:172:GLU:HG3	1.86	0.57
1:KD:131:GLU:HG2	1:KD:132:VAL:HG23	1.86	0.57
1:TD:92:LEU:HD22	1:TD:108:VAL:HG23	1.85	0.57
1:TD:131:GLU:HG2	1:TD:132:VAL:HG23	1.86	0.57
1:IE:92:LEU:HD22	1:IE:108:VAL:HG23	1.85	0.57
1:AF:131:GLU:HG2	1:AF:132:VAL:HG23	1.86	0.57
1:BA:53:LYS:HG2	1:BA:172:GLU:HG3	1.86	0.56
1:FB:53:LYS:HG2	1:FB:172:GLU:HG3	1.86	0.56
1:AC:53:LYS:HG2	1:AC:172:GLU:HG3	1.86	0.56
1:IE:131:GLU:HG2	1:IE:132:VAL:HG23	1.86	0.56
1:C:131:GLU:HG2	1:C:132:VAL:HG23	1.86	0.56
1:L:53:LYS:HG2	1:L:172:GLU:HG3	1.86	0.56
1:IB:53:LYS:HG2	1:IB:172:GLU:HG3	1.86	0.56
1:DC:53:LYS:HG2	1:DC:172:GLU:HG3	1.86	0.56
1:MC:53:LYS:HG2	1:MC:172:GLU:HG3	1.86	0.56
1:SC:53:LYS:HG2	1:SC:172:GLU:HG3	1.86	0.56
1:PF:131:GLU:HG2	1:PF:132:VAL:HG23	1.86	0.56
1:G:186:PRO:O	1:G:189:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:53:LYS:HG2	1:Y:172:GLU:HG3	1.87	0.56
1:EA:53:LYS:HG2	1:EA:172:GLU:HG3	1.86	0.56
1:HA:131:GLU:HG2	1:HA:132:VAL:HG23	1.86	0.56
1:LA:186:PRO:O	1:LA:189:LYS:NZ	2.38	0.56
1:QA:53:LYS:HG2	1:QA:172:GLU:HG3	1.86	0.56
1:CB:53:LYS:HG2	1:CB:172:GLU:HG3	1.87	0.56
1:PC:53:LYS:HG2	1:PC:172:GLU:HG3	1.86	0.56
1:OD:186:PRO:O	1:OD:189:LYS:NZ	2.38	0.56
1:TD:53:LYS:HG2	1:TD:172:GLU:HG3	1.86	0.56
1:FE:53:LYS:HG2	1:FE:172:GLU:HG3	1.86	0.56
1:IE:53:LYS:HG2	1:IE:172:GLU:HG3	1.86	0.56
1:HA:53:LYS:HG2	1:HA:172:GLU:HG3	1.86	0.56
1:CB:131:GLU:HG2	1:CB:132:VAL:HG23	1.86	0.56
1:VB:186:PRO:O	1:VB:189:LYS:NZ	2.38	0.56
1:UE:53:LYS:HG2	1:UE:172:GLU:HG3	1.86	0.56
1:C:53:LYS:HG2	1:C:172:GLU:HG3	1.86	0.56
1:OB:131:GLU:HG2	1:OB:132:VAL:HG23	1.86	0.56
1:BC:186:PRO:O	1:BC:189:LYS:NZ	2.38	0.56
1:FE:92:LEU:HD22	1:FE:108:VAL:HG23	1.85	0.56
1:UE:92:LEU:HD22	1:UE:108:VAL:HG23	1.85	0.56
1:V:53:LYS:HG2	1:V:172:GLU:HG3	1.86	0.56
1:Y:131:GLU:HG2	1:Y:132:VAL:HG23	1.86	0.56
1:ZA:53:LYS:HG2	1:ZA:172:GLU:HG3	1.86	0.56
1:QC:186:PRO:O	1:QC:189:LYS:NZ	2.38	0.56
1:HD:131:GLU:HG2	1:HD:132:VAL:HG23	1.86	0.56
1:CE:53:LYS:HG2	1:CE:172:GLU:HG3	1.86	0.56
1:RE:53:LYS:HG2	1:RE:172:GLU:HG3	1.86	0.56
1:GF:131:GLU:HG2	1:GF:132:VAL:HG23	1.86	0.56
1:VF:131:GLU:HG2	1:VF:132:VAL:HG23	1.86	0.56
1:KA:53:LYS:HG2	1:KA:172:GLU:HG3	1.86	0.56
1:FE:131:GLU:HG2	1:FE:132:VAL:HG23	1.86	0.56
1:GC:53:LYS:HG2	1:GC:172:GLU:HG3	1.87	0.56
1:VC:53:LYS:HG2	1:VC:172:GLU:HG3	1.87	0.56
1:BF:186:PRO:O	1:BF:189:LYS:NZ	2.38	0.56
1:QF:186:PRO:O	1:QF:189:LYS:NZ	2.38	0.56
1:F:53:LYS:HG2	1:F:172:GLU:HG3	1.86	0.55
1:GB:186:PRO:O	1:GB:189:LYS:NZ	2.38	0.55
1:UE:131:GLU:HG2	1:UE:132:VAL:HG23	1.86	0.55
1:CA:186:PRO:O	1:CA:189:LYS:NZ	2.38	0.55
1:WF:186:PRO:O	1:WF:189:LYS:NZ	2.38	0.55
1:OB:53:LYS:HG2	1:OB:172:GLU:HG3	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HD:53:LYS:HG2	1:HD:172:GLU:HG3	1.86	0.55
1:XD:186:PRO:O	1:XD:189:LYS:NZ	2.38	0.55
1:ME:186:PRO:O	1:ME:189:LYS:NZ	2.38	0.55
1:M:186:PRO:O	1:M:189:LYS:NZ	2.38	0.55
1:RA:186:PRO:O	1:RA:189:LYS:NZ	2.38	0.55
1:HF:186:PRO:O	1:HF:189:LYS:NZ	2.38	0.55
1:JE:186:PRO:O	1:JE:189:LYS:NZ	2.38	0.55
1:NC:186:PRO:O	1:NC:189:LYS:NZ	2.38	0.55
1:DE:186:PRO:O	1:DE:189:LYS:NZ	2.38	0.55
1:HB:103:ARG:NH2	1:HB:127:ASP:OD2	2.38	0.55
1:UD:186:PRO:O	1:UD:189:LYS:NZ	2.38	0.55
1:YB:186:PRO:O	1:YB:189:LYS:NZ	2.38	0.55
1:SE:186:PRO:O	1:SE:189:LYS:NZ	2.38	0.55
1:YE:186:PRO:O	1:YE:189:LYS:NZ	2.38	0.55
1:NF:186:PRO:O	1:NF:189:LYS:NZ	2.38	0.54
1:TB:103:ARG:NH2	1:TB:127:ASP:OD2	2.38	0.54
1:AE:186:PRO:O	1:AE:189:LYS:NZ	2.38	0.54
1:MD:103:ARG:NH2	1:MD:127:ASP:OD2	2.38	0.54
1:K:103:ARG:NH2	1:K:127:ASP:OD2	2.38	0.54
1:NB:103:ARG:NH2	1:NB:127:ASP:OD2	2.38	0.54
1:LD:186:PRO:O	1:LD:189:LYS:NZ	2.38	0.54
1:PE:186:PRO:O	1:PE:189:LYS:NZ	2.38	0.54
1:SB:186:PRO:O	1:SB:189:LYS:NZ	2.38	0.54
1:GD:103:ARG:NH2	1:GD:127:ASP:OD2	2.38	0.54
1:PA:103:ARG:NH2	1:PA:127:ASP:OD2	2.38	0.54
1:ZC:186:PRO:O	1:ZC:189:LYS:NZ	2.38	0.54
1:HC:186:PRO:O	1:HC:189:LYS:NZ	2.38	0.54
1:RC:103:ARG:NH2	1:RC:127:ASP:OD2	2.38	0.54
1:ID:186:PRO:O	1:ID:189:LYS:NZ	2.38	0.54
1:EE:103:ARG:NH2	1:EE:127:ASP:OD2	2.38	0.54
1:FF:103:ARG:NH2	1:FF:127:ASP:OD2	2.38	0.54
1:UF:103:ARG:NH2	1:UF:127:ASP:OD2	2.38	0.54
1:PB:186:PRO:O	1:PB:189:LYS:NZ	2.38	0.53
1:KC:186:PRO:O	1:KC:189:LYS:NZ	2.38	0.53
1:WC:186:PRO:O	1:WC:189:LYS:NZ	2.38	0.53
1:TE:103:ARG:NH2	1:TE:127:ASP:OD2	2.38	0.53
1:XF:103:ARG:NH2	1:XF:127:ASP:OD2	2.38	0.53
1:CC:103:ARG:NH2	1:CC:127:ASP:OD2	2.38	0.53
1:D:186:PRO:O	1:D:189:LYS:NZ	2.38	0.53
1:IA:186:PRO:O	1:IA:189:LYS:NZ	2.38	0.53
1:IF:103:ARG:NH2	1:IF:127:ASP:OD2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SD:103:ARG:NH2	1:SD:127:ASP:OD2	2.38	0.53
1:HE:103:ARG:NH2	1:HE:127:ASP:OD2	2.38	0.53
1:ZE:103:ARG:NH2	1:ZE:127:ASP:OD2	2.38	0.53
1:OF:103:ARG:NH2	1:OF:127:ASP:OD2	2.38	0.53
1:RD:186:PRO:O	1:RD:189:LYS:NZ	2.38	0.53
1:GE:186:PRO:O	1:GE:189:LYS:NZ	2.38	0.53
1:IC:103:ARG:NH2	1:IC:127:ASP:OD2	2.38	0.52
1:LF:103:ARG:NH2	1:LF:127:ASP:OD2	2.38	0.52
1:FA:186:PRO:O	1:FA:189:LYS:NZ	2.38	0.52
1:XC:103:ARG:NH2	1:XC:127:ASP:OD2	2.38	0.52
1:FD:186:PRO:O	1:FD:189:LYS:NZ	2.38	0.52
1:AA:103:ARG:NH2	1:AA:127:ASP:OD2	2.38	0.52
1:MB:186:PRO:O	1:MB:189:LYS:NZ	2.38	0.52
1:WE:103:ARG:NH2	1:WE:127:ASP:OD2	2.38	0.52
1:H:103:ARG:NH2	1:H:127:ASP:OD2	2.38	0.52
1:X:103:ARG:NH2	1:X:127:ASP:OD2	2.38	0.52
1:MA:103:ARG:NH2	1:MA:127:ASP:OD2	2.38	0.52
1:OC:103:ARG:NH2	1:OC:127:ASP:OD2	2.38	0.52
1:EB:103:ARG:NH2	1:EB:127:ASP:OD2	2.38	0.52
1:GC:76:GLU:H	1:GC:76:GLU:CD	2.18	0.52
1:BB:103:ARG:NH2	1:BB:127:ASP:OD2	2.38	0.52
1:ZB:103:ARG:NH2	1:ZB:127:ASP:OD2	2.38	0.52
1:MC:76:GLU:CD	1:MC:76:GLU:H	2.18	0.52
1:VC:76:GLU:CD	1:VC:76:GLU:H	2.18	0.52
1:DA:89:ARG:HD2	1:DA:136:MET:HE3	1.92	0.52
1:MA:89:ARG:HD2	1:MA:136:MET:HE3	1.92	0.52
1:HB:89:ARG:HD2	1:HB:136:MET:HE3	1.92	0.52
1:LB:76:GLU:CD	1:LB:76:GLU:H	2.18	0.52
1:ED:76:GLU:CD	1:ED:76:GLU:H	2.18	0.52
1:HD:76:GLU:CD	1:HD:76:GLU:H	2.18	0.52
1:MD:89:ARG:HD2	1:MD:136:MET:HE3	1.92	0.52
1:OE:76:GLU:H	1:OE:76:GLU:CD	2.18	0.52
1:WE:89:ARG:HD2	1:WE:136:MET:HE3	1.92	0.52
1:LF:89:ARG:HD2	1:LF:136:MET:HE3	1.92	0.52
1:H:89:ARG:HD2	1:H:136:MET:HE3	1.92	0.52
1:TB:89:ARG:HD2	1:TB:136:MET:HE3	1.92	0.52
1:YC:76:GLU:CD	1:YC:76:GLU:H	2.18	0.52
1:BD:76:GLU:CD	1:BD:76:GLU:H	2.18	0.52
1:ZD:76:GLU:H	1:ZD:76:GLU:CD	2.18	0.52
1:XE:76:GLU:CD	1:XE:76:GLU:H	2.18	0.52
1:MF:76:GLU:CD	1:MF:76:GLU:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SF:76:GLU:CD	1:SF:76:GLU:H	2.18	0.52
1:GA:89:ARG:HD2	1:GA:136:MET:HE3	1.92	0.52
1:SA:89:ARG:HD2	1:SA:136:MET:HE3	1.92	0.52
1:OB:76:GLU:H	1:OB:76:GLU:CD	2.18	0.52
1:JC:76:GLU:CD	1:JC:76:GLU:H	2.18	0.52
1:DF:76:GLU:CD	1:DF:76:GLU:H	2.18	0.52
1:B:89:ARG:HD2	1:B:136:MET:HE3	1.92	0.51
1:N:89:ARG:HD2	1:N:136:MET:HE3	1.92	0.51
1:R:31:ILE:HG13	1:DA:27:VAL:HG11	1.92	0.51
1:HA:76:GLU:H	1:HA:76:GLU:CD	2.18	0.51
1:WA:31:ILE:HG13	1:HB:27:VAL:HG11	1.92	0.51
1:BB:89:ARG:HD2	1:BB:136:MET:HE3	1.92	0.51
1:LB:31:ILE:HG13	1:WB:27:VAL:HG11	1.92	0.51
1:IC:89:ARG:HD2	1:IC:136:MET:HE3	1.92	0.51
1:LC:89:ARG:HD2	1:LC:136:MET:HE3	1.92	0.51
1:UC:89:ARG:HD2	1:UC:136:MET:HE3	1.92	0.51
1:XC:27:VAL:HG11	1:BD:31:ILE:HG13	1.93	0.51
1:AD:89:ARG:HD2	1:AD:136:MET:HE3	1.92	0.51
1:SD:89:ARG:HD2	1:SD:136:MET:HE3	1.92	0.51
1:TD:76:GLU:CD	1:TD:76:GLU:H	2.18	0.51
1:IE:76:GLU:CD	1:IE:76:GLU:H	2.18	0.51
1:JF:76:GLU:H	1:JF:76:GLU:CD	2.18	0.51
1:UF:89:ARG:HD2	1:UF:136:MET:HE3	1.92	0.51
1:C:76:GLU:CD	1:C:76:GLU:H	2.18	0.51
1:X:89:ARG:HD2	1:X:136:MET:HE3	1.92	0.51
1:KB:103:ARG:NH2	1:KB:127:ASP:OD2	2.38	0.51
1:FC:27:VAL:HG11	1:JC:31:ILE:HG13	1.93	0.51
1:FC:89:ARG:HD2	1:FC:136:MET:HE3	1.92	0.51
1:IC:27:VAL:HG11	1:MC:31:ILE:HG13	1.93	0.51
1:XC:89:ARG:HD2	1:XC:136:MET:HE3	1.92	0.51
1:ED:31:ILE:HG13	1:PD:27:VAL:HG11	1.92	0.51
1:HE:89:ARG:HD2	1:HE:136:MET:HE3	1.92	0.51
1:FF:89:ARG:HD2	1:FF:136:MET:HE3	1.92	0.51
1:RF:27:VAL:HG11	1:VF:31:ILE:HG13	1.93	0.51
1:YF:76:GLU:CD	1:YF:76:GLU:H	2.18	0.51
1:F:76:GLU:H	1:F:76:GLU:CD	2.18	0.51
1:L:76:GLU:CD	1:L:76:GLU:H	2.18	0.51
1:KA:76:GLU:H	1:KA:76:GLU:CD	2.18	0.51
1:QB:103:ARG:NH2	1:QB:127:ASP:OD2	2.38	0.51
1:CC:27:VAL:HG11	1:GC:31:ILE:HG13	1.93	0.51
1:CE:76:GLU:H	1:CE:76:GLU:CD	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EE:89:ARG:HD2	1:EE:136:MET:HE3	1.92	0.51
1:RE:76:GLU:H	1:RE:76:GLU:CD	2.18	0.51
1:TE:89:ARG:HD2	1:TE:136:MET:HE3	1.92	0.51
1:R:76:GLU:H	1:R:76:GLU:CD	2.18	0.51
1:Y:76:GLU:CD	1:Y:76:GLU:H	2.18	0.51
1:OC:89:ARG:HD2	1:OC:136:MET:HE3	1.92	0.51
1:RC:27:VAL:HG11	1:VC:31:ILE:HG13	1.93	0.51
1:UC:27:VAL:HG11	1:YC:31:ILE:HG13	1.93	0.51
1:CF:27:VAL:HG11	1:GF:31:ILE:HG13	1.93	0.51
1:GF:76:GLU:CD	1:GF:76:GLU:H	2.18	0.51
1:VF:76:GLU:H	1:VF:76:GLU:CD	2.18	0.51
1:E:89:ARG:HD2	1:E:136:MET:HE3	1.92	0.51
1:H:27:VAL:HG11	1:L:31:ILE:HG13	1.93	0.51
1:JA:89:ARG:HD2	1:JA:136:MET:HE3	1.92	0.51
1:QA:76:GLU:CD	1:QA:76:GLU:H	2.18	0.51
1:CB:76:GLU:H	1:CB:76:GLU:CD	2.18	0.51
1:XB:76:GLU:CD	1:XB:76:GLU:H	2.18	0.51
1:ZB:89:ARG:HD2	1:ZB:136:MET:HE3	1.92	0.51
1:QE:89:ARG:HD2	1:QE:136:MET:HE3	1.92	0.51
1:ZE:27:VAL:HG11	1:DF:31:ILE:HG13	1.93	0.51
1:FF:27:VAL:HG11	1:JF:31:ILE:HG13	1.93	0.51
1:OF:27:VAL:HG11	1:SF:31:ILE:HG13	1.93	0.51
1:O:76:GLU:CD	1:O:76:GLU:H	2.18	0.51
1:V:76:GLU:CD	1:V:76:GLU:H	2.18	0.51
1:MA:27:VAL:HG11	1:QA:31:ILE:HG13	1.93	0.51
1:WA:76:GLU:H	1:WA:76:GLU:CD	2.18	0.51
1:KB:27:VAL:HG11	1:OB:31:ILE:HG13	1.93	0.51
1:ZB:27:VAL:HG11	1:DC:31:ILE:HG13	1.93	0.51
1:OC:27:VAL:HG11	1:SC:31:ILE:HG13	1.93	0.51
1:DD:27:VAL:HG11	1:HD:31:ILE:HG13	1.93	0.51
1:DD:103:ARG:NH2	1:DD:127:ASP:OD2	2.38	0.51
1:JD:89:ARG:HD2	1:JD:136:MET:HE3	1.92	0.51
1:JD:103:ARG:NH2	1:JD:127:ASP:OD2	2.38	0.51
1:SD:27:VAL:HG11	1:WD:31:ILE:HG13	1.93	0.51
1:BE:89:ARG:HD2	1:BE:136:MET:HE3	1.92	0.51
1:HE:27:VAL:HG11	1:LE:31:ILE:HG13	1.93	0.51
1:NE:27:VAL:HG11	1:RE:31:ILE:HG13	1.93	0.51
1:AF:76:GLU:CD	1:AF:76:GLU:H	2.18	0.51
1:PF:76:GLU:CD	1:PF:76:GLU:H	2.18	0.51
1:UF:27:VAL:HG11	1:YF:31:ILE:HG13	1.93	0.51
1:T:89:ARG:HD2	1:T:136:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZA:76:GLU:CD	1:ZA:76:GLU:H	2.18	0.51
1:RB:76:GLU:CD	1:RB:76:GLU:H	2.18	0.51
1:KD:76:GLU:H	1:KD:76:GLU:CD	2.18	0.51
1:QD:76:GLU:CD	1:QD:76:GLU:H	2.18	0.51
1:YD:27:VAL:HG11	1:CE:31:ILE:HG13	1.93	0.51
1:UE:76:GLU:CD	1:UE:76:GLU:H	2.18	0.51
1:CF:103:ARG:NH2	1:CF:127:ASP:OD2	2.38	0.51
1:RF:103:ARG:NH2	1:RF:127:ASP:OD2	2.38	0.51
1:I:76:GLU:CD	1:I:76:GLU:H	2.18	0.51
1:HA:31:ILE:HG13	1:SA:27:VAL:HG11	1.92	0.51
1:NA:76:GLU:CD	1:NA:76:GLU:H	2.18	0.51
1:TA:76:GLU:H	1:TA:76:GLU:CD	2.18	0.51
1:YA:89:ARG:HD2	1:YA:136:MET:HE3	1.92	0.51
1:QB:89:ARG:HD2	1:QB:136:MET:HE3	1.92	0.51
1:DC:76:GLU:CD	1:DC:76:GLU:H	2.18	0.51
1:B:27:VAL:HG11	1:F:31:ILE:HG13	1.93	0.51
1:GA:27:VAL:HG11	1:KA:31:ILE:HG13	1.93	0.51
1:SC:76:GLU:H	1:SC:76:GLU:CD	2.18	0.51
1:WD:76:GLU:H	1:WD:76:GLU:CD	2.18	0.51
1:BE:27:VAL:HG11	1:FE:31:ILE:HG13	1.93	0.51
1:FE:76:GLU:H	1:FE:76:GLU:CD	2.18	0.51
1:QE:27:VAL:HG11	1:UE:31:ILE:HG13	1.93	0.51
1:MF:31:ILE:HG13	1:XF:27:VAL:HG11	1.92	0.51
1:C:31:ILE:HG13	1:N:27:VAL:HG11	1.92	0.51
1:GD:89:ARG:HD2	1:GD:136:MET:HE3	1.92	0.51
1:LE:76:GLU:CD	1:LE:76:GLU:H	2.18	0.51
1:XE:31:ILE:HG13	1:IF:27:VAL:HG11	1.92	0.51
1:X:27:VAL:HG11	1:BA:31:ILE:HG13	1.93	0.50
1:NB:89:ARG:HD2	1:NB:136:MET:HE3	1.92	0.50
1:RC:89:ARG:HD2	1:RC:136:MET:HE3	1.92	0.50
1:GD:27:VAL:HG11	1:KD:31:ILE:HG13	1.93	0.50
1:VD:27:VAL:HG11	1:ZD:31:ILE:HG13	1.93	0.50
1:RF:89:ARG:HD2	1:RF:136:MET:HE3	1.92	0.50
1:BB:27:VAL:HG11	1:FB:31:ILE:HG13	1.93	0.50
1:NB:27:VAL:HG11	1:RB:31:ILE:HG13	1.93	0.50
1:AC:76:GLU:CD	1:AC:76:GLU:H	2.18	0.50
1:CC:89:ARG:HD2	1:CC:136:MET:HE3	1.92	0.50
1:KE:27:VAL:HG11	1:OE:31:ILE:HG13	1.93	0.50
1:T:103:ARG:NH2	1:T:127:ASP:OD2	2.38	0.50
1:AA:89:ARG:HD2	1:AA:136:MET:HE3	1.92	0.50
1:IB:76:GLU:CD	1:IB:76:GLU:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PC:76:GLU:CD	1:PC:76:GLU:H	2.18	0.50
1:VD:89:ARG:HD2	1:VD:136:MET:HE3	1.92	0.50
1:CF:89:ARG:HD2	1:CF:136:MET:HE3	1.92	0.50
1:Q:103:ARG:NH2	1:Q:127:ASP:OD2	2.38	0.50
1:T:27:VAL:HG11	1:Y:31:ILE:HG13	1.93	0.50
1:BA:76:GLU:CD	1:BA:76:GLU:H	2.18	0.50
1:YA:27:VAL:HG11	1:CB:31:ILE:HG13	1.93	0.50
1:YA:103:ARG:NH2	1:YA:127:ASP:OD2	2.38	0.50
1:JB:186:PRO:O	1:JB:189:LYS:NZ	2.38	0.50
1:YD:89:ARG:HD2	1:YD:136:MET:HE3	1.92	0.50
1:E:27:VAL:HG11	1:I:31:ILE:HG13	1.93	0.50
1:EA:76:GLU:CD	1:EA:76:GLU:H	2.18	0.50
1:JA:27:VAL:HG11	1:NA:31:ILE:HG13	1.93	0.50
1:PA:89:ARG:HD2	1:PA:136:MET:HE3	1.92	0.50
1:VA:103:ARG:NH2	1:VA:127:ASP:OD2	2.38	0.50
1:EB:89:ARG:HD2	1:EB:136:MET:HE3	1.92	0.50
1:AC:31:ILE:HG13	1:LC:27:VAL:HG11	1.92	0.50
1:PC:31:ILE:HG13	1:AD:27:VAL:HG11	1.92	0.50
1:ND:76:GLU:H	1:ND:76:GLU:CD	2.18	0.50
1:PD:89:ARG:HD2	1:PD:136:MET:HE3	1.92	0.50
1:TD:31:ILE:HG13	1:EE:27:VAL:HG11	1.92	0.50
1:KE:89:ARG:HD2	1:KE:136:MET:HE3	1.92	0.50
1:NE:89:ARG:HD2	1:NE:136:MET:HE3	1.92	0.50
1:K:89:ARG:HD2	1:K:136:MET:HE3	1.92	0.50
1:N:103:ARG:NH2	1:N:127:ASP:OD2	2.38	0.50
1:FB:76:GLU:CD	1:FB:76:GLU:H	2.18	0.50
1:UB:76:GLU:CD	1:UB:76:GLU:H	2.18	0.50
1:WB:89:ARG:HD2	1:WB:136:MET:HE3	1.92	0.50
1:IE:31:ILE:HG13	1:TE:27:VAL:HG11	1.92	0.50
1:WE:27:VAL:HG11	1:AF:31:ILE:HG13	1.93	0.50
1:LF:27:VAL:HG11	1:PF:31:ILE:HG13	1.93	0.50
1:OF:89:ARG:HD2	1:OF:136:MET:HE3	1.92	0.50
1:EB:27:VAL:HG11	1:IB:31:ILE:HG13	1.93	0.50
1:VA:27:VAL:HG11	1:ZA:31:ILE:HG13	1.93	0.50
1:VA:89:ARG:HD2	1:VA:136:MET:HE3	1.92	0.50
1:TB:27:VAL:HG11	1:XB:31:ILE:HG13	1.93	0.50
1:MD:27:VAL:HG11	1:QD:31:ILE:HG13	1.93	0.50
1:NE:103:ARG:NH2	1:NE:127:ASP:OD2	2.38	0.50
1:ZE:89:ARG:HD2	1:ZE:136:MET:HE3	1.92	0.50
1:IF:89:ARG:HD2	1:IF:136:MET:HE3	1.92	0.50
1:XF:89:ARG:HD2	1:XF:136:MET:HE3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:27:VAL:HG11	1:V:31:ILE:HG13	1.93	0.50
1:AA:27:VAL:HG11	1:EA:31:ILE:HG13	1.93	0.50
1:QB:27:VAL:HG11	1:UB:31:ILE:HG13	1.93	0.50
1:UC:103:ARG:NH2	1:UC:127:ASP:OD2	2.38	0.50
1:Q:89:ARG:HD2	1:Q:136:MET:HE3	1.92	0.49
1:SA:103:ARG:NH2	1:SA:127:ASP:OD2	2.38	0.49
1:KB:89:ARG:HD2	1:KB:136:MET:HE3	1.92	0.49
1:JD:27:VAL:HG11	1:ND:31:ILE:HG13	1.93	0.49
1:KE:103:ARG:NH2	1:KE:127:ASP:OD2	2.38	0.49
1:DD:89:ARG:HD2	1:DD:136:MET:HE3	1.92	0.49
1:YD:103:ARG:NH2	1:YD:127:ASP:OD2	2.38	0.49
1:VD:103:ARG:NH2	1:VD:127:ASP:OD2	2.38	0.49
1:K:27:VAL:HG11	1:O:31:ILE:HG13	1.93	0.49
1:FC:103:ARG:NH2	1:FC:127:ASP:OD2	2.38	0.49
1:PA:27:VAL:HG11	1:TA:31:ILE:HG13	1.93	0.49
1:P:123:LEU:HD12	1:P:140:ALA:HB2	1.95	0.49
1:W:123:LEU:HD12	1:W:140:ALA:HB2	1.95	0.49
1:AD:103:ARG:NH2	1:AD:127:ASP:OD2	2.38	0.49
1:UA:123:LEU:HD12	1:UA:140:ALA:HB2	1.95	0.49
1:AB:123:LEU:HD12	1:AB:140:ALA:HB2	1.95	0.49
1:LC:103:ARG:NH2	1:LC:127:ASP:OD2	2.38	0.49
1:CA:123:LEU:HD12	1:CA:140:ALA:HB2	1.95	0.48
1:UD:123:LEU:HD12	1:UD:140:ALA:HB2	1.95	0.48
1:EF:123:LEU:HD12	1:EF:140:ALA:HB2	1.95	0.48
1:TF:123:LEU:HD12	1:TF:140:ALA:HB2	1.95	0.48
1:Z:123:LEU:HD12	1:Z:140:ALA:HB2	1.95	0.48
1:GB:123:LEU:HD12	1:GB:140:ALA:HB2	1.95	0.48
1:JB:123:LEU:HD12	1:JB:140:ALA:HB2	1.95	0.48
1:HC:123:LEU:HD12	1:HC:140:ALA:HB2	1.95	0.48
1:CD:123:LEU:HD12	1:CD:140:ALA:HB2	1.95	0.48
1:FD:123:LEU:HD12	1:FD:140:ALA:HB2	1.95	0.48
1:OD:123:LEU:HD12	1:OD:140:ALA:HB2	1.95	0.48
1:AE:123:LEU:HD12	1:AE:140:ALA:HB2	1.95	0.48
1:PE:123:LEU:HD12	1:PE:140:ALA:HB2	1.95	0.48
1:E:103:ARG:NH2	1:E:127:ASP:OD2	2.38	0.48
1:DB:123:LEU:HD12	1:DB:140:ALA:HB2	1.95	0.48
1:MB:123:LEU:HD12	1:MB:140:ALA:HB2	1.95	0.48
1:VB:123:LEU:HD12	1:VB:140:ALA:HB2	1.95	0.48
1:WC:123:LEU:HD12	1:WC:140:ALA:HB2	1.95	0.48
1:JE:123:LEU:HD12	1:JE:140:ALA:HB2	1.95	0.48
1:NC:123:LEU:HD12	1:NC:140:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BE:103:ARG:NH2	1:BE:127:ASP:OD2	2.38	0.48
1:DE:123:LEU:HD12	1:DE:140:ALA:HB2	1.95	0.48
1:SE:123:LEU:HD12	1:SE:140:ALA:HB2	1.95	0.48
1:YB:123:LEU:HD12	1:YB:140:ALA:HB2	1.95	0.48
1:QE:103:ARG:NH2	1:QE:127:ASP:OD2	2.38	0.48
1:A:123:LEU:HD12	1:A:140:ALA:HB2	1.95	0.48
1:FA:123:LEU:HD12	1:FA:140:ALA:HB2	1.95	0.48
1:ID:123:LEU:HD12	1:ID:140:ALA:HB2	1.95	0.48
1:B:103:ARG:NH2	1:B:127:ASP:OD2	2.38	0.48
1:JA:103:ARG:NH2	1:JA:127:ASP:OD2	2.38	0.48
1:PB:123:LEU:HD12	1:PB:140:ALA:HB2	1.95	0.48
1:XD:123:LEU:HD12	1:XD:140:ALA:HB2	1.95	0.48
1:ME:123:LEU:HD12	1:ME:140:ALA:HB2	1.95	0.48
1:BF:123:LEU:HD12	1:BF:140:ALA:HB2	1.95	0.48
1:SB:123:LEU:HD12	1:SB:140:ALA:HB2	1.95	0.48
1:QF:123:LEU:HD12	1:QF:140:ALA:HB2	1.95	0.48
1:LD:123:LEU:HD12	1:LD:140:ALA:HB2	1.95	0.48
1:KF:123:LEU:HD12	1:KF:140:ALA:HB2	1.95	0.48
1:W:186:PRO:O	1:W:189:LYS:NZ	2.38	0.48
1:VE:123:LEU:HD12	1:VE:140:ALA:HB2	1.95	0.48
1:G:123:LEU:HD12	1:G:140:ALA:HB2	1.95	0.47
1:GA:103:ARG:NH2	1:GA:127:ASP:OD2	2.38	0.47
1:LA:123:LEU:HD12	1:LA:140:ALA:HB2	1.95	0.47
1:NF:123:LEU:HD12	1:NF:140:ALA:HB2	1.95	0.47
1:M:123:LEU:HD12	1:M:140:ALA:HB2	1.95	0.47
1:S:123:LEU:HD12	1:S:140:ALA:HB2	1.95	0.47
1:RA:123:LEU:HD12	1:RA:140:ALA:HB2	1.95	0.47
1:XA:123:LEU:HD12	1:XA:140:ALA:HB2	1.95	0.47
1:EC:123:LEU:HD12	1:EC:140:ALA:HB2	1.95	0.47
1:ZC:123:LEU:HD12	1:ZC:140:ALA:HB2	1.95	0.47
1:RD:123:LEU:HD12	1:RD:140:ALA:HB2	1.95	0.47
1:GE:123:LEU:HD12	1:GE:140:ALA:HB2	1.95	0.47
1:YE:123:LEU:HD12	1:YE:140:ALA:HB2	1.95	0.47
1:AB:186:PRO:O	1:AB:189:LYS:NZ	2.38	0.47
1:BC:123:LEU:HD12	1:BC:140:ALA:HB2	1.95	0.47
1:KC:123:LEU:HD12	1:KC:140:ALA:HB2	1.95	0.47
1:TC:123:LEU:HD12	1:TC:140:ALA:HB2	1.95	0.47
1:J:123:LEU:HD12	1:J:140:ALA:HB2	1.95	0.47
1:QC:123:LEU:HD12	1:QC:140:ALA:HB2	1.95	0.47
1:D:123:LEU:HD12	1:D:140:ALA:HB2	1.95	0.47
1:OA:123:LEU:HD12	1:OA:140:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HF:123:LEU:HD12	1:HF:140:ALA:HB2	1.95	0.47
1:WF:123:LEU:HD12	1:WF:140:ALA:HB2	1.95	0.47
1:IA:123:LEU:HD12	1:IA:140:ALA:HB2	1.95	0.47
1:DA:103:ARG:NH2	1:DA:127:ASP:OD2	2.38	0.46
1:YE:96:LEU:HD21	1:YE:104:ILE:HG13	1.98	0.46
1:NF:96:LEU:HD21	1:NF:104:ILE:HG13	1.98	0.46
1:A:96:LEU:HD21	1:A:104:ILE:HG13	1.98	0.46
1:JB:96:LEU:HD21	1:JB:104:ILE:HG13	1.98	0.46
1:OD:96:LEU:HD21	1:OD:104:ILE:HG13	1.98	0.46
1:RD:96:LEU:HD21	1:RD:104:ILE:HG13	1.98	0.46
1:S:96:LEU:HD21	1:S:104:ILE:HG13	1.98	0.45
1:FA:96:LEU:HD21	1:FA:104:ILE:HG13	1.98	0.45
1:LA:96:LEU:HD21	1:LA:104:ILE:HG13	1.98	0.45
1:XA:96:LEU:HD21	1:XA:104:ILE:HG13	1.98	0.45
1:MB:96:LEU:HD21	1:MB:104:ILE:HG13	1.98	0.45
1:VB:96:LEU:HD21	1:VB:104:ILE:HG13	1.98	0.45
1:CD:96:LEU:HD21	1:CD:104:ILE:HG13	1.98	0.45
1:GE:96:LEU:HD21	1:GE:104:ILE:HG13	1.98	0.45
1:EF:96:LEU:HD21	1:EF:104:ILE:HG13	1.98	0.45
1:G:96:LEU:HD21	1:G:104:ILE:HG13	1.98	0.45
1:EC:96:LEU:HD21	1:EC:104:ILE:HG13	1.98	0.45
1:TC:96:LEU:HD21	1:TC:104:ILE:HG13	1.98	0.45
1:FD:96:LEU:HD21	1:FD:104:ILE:HG13	1.98	0.45
1:TF:96:LEU:HD21	1:TF:104:ILE:HG13	1.98	0.45
1:M:96:LEU:HD21	1:M:104:ILE:HG13	1.98	0.45
1:RA:96:LEU:HD21	1:RA:104:ILE:HG13	1.98	0.45
1:WB:103:ARG:NH2	1:WB:127:ASP:OD2	2.38	0.45
1:PD:103:ARG:NH2	1:PD:127:ASP:OD2	2.38	0.45
1:QB:96:LEU:HD21	1:QB:104:ILE:HG13	1.99	0.45
1:JD:96:LEU:HD21	1:JD:104:ILE:HG13	1.99	0.45
1:SB:96:LEU:HD21	1:SB:104:ILE:HG13	1.98	0.45
1:AE:96:LEU:HD21	1:AE:104:ILE:HG13	1.98	0.45
1:HF:96:LEU:HD21	1:HF:104:ILE:HG13	1.98	0.45
1:QF:96:LEU:HD21	1:QF:104:ILE:HG13	1.98	0.45
1:WF:96:LEU:HD21	1:WF:104:ILE:HG13	1.98	0.45
1:N:96:LEU:HD21	1:N:104:ILE:HG13	1.99	0.45
1:W:96:LEU:HD21	1:W:104:ILE:HG13	1.98	0.45
1:AA:96:LEU:HD21	1:AA:104:ILE:HG13	1.99	0.45
1:SA:96:LEU:HD21	1:SA:104:ILE:HG13	1.99	0.45
1:AB:96:LEU:HD21	1:AB:104:ILE:HG13	1.98	0.45
1:UC:96:LEU:HD21	1:UC:104:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LD:96:LEU:HD21	1:LD:104:ILE:HG13	1.98	0.45
1:PE:96:LEU:HD21	1:PE:104:ILE:HG13	1.98	0.45
1:BF:96:LEU:HD21	1:BF:104:ILE:HG13	1.98	0.45
1:EB:96:LEU:HD21	1:EB:104:ILE:HG13	1.99	0.45
1:CC:96:LEU:HD21	1:CC:104:ILE:HG13	1.99	0.45
1:FC:96:LEU:HD21	1:FC:104:ILE:HG13	1.99	0.45
1:SD:96:LEU:HD21	1:SD:104:ILE:HG13	1.99	0.45
1:HE:96:LEU:HD21	1:HE:104:ILE:HG13	1.99	0.45
1:ME:96:LEU:HD21	1:ME:104:ILE:HG13	1.98	0.45
1:WE:96:LEU:HD21	1:WE:104:ILE:HG13	1.99	0.45
1:LF:96:LEU:HD21	1:LF:104:ILE:HG13	1.99	0.45
1:D:96:LEU:HD21	1:D:104:ILE:HG13	1.98	0.45
1:K:96:LEU:HD21	1:K:104:ILE:HG13	1.99	0.45
1:IA:96:LEU:HD21	1:IA:104:ILE:HG13	1.98	0.45
1:YB:96:LEU:HD21	1:YB:104:ILE:HG13	1.98	0.45
1:RC:96:LEU:HD21	1:RC:104:ILE:HG13	1.99	0.45
1:XD:96:LEU:HD21	1:XD:104:ILE:HG13	1.98	0.45
1:YD:96:LEU:HD21	1:YD:104:ILE:HG13	1.99	0.45
1:PA:96:LEU:HD21	1:PA:104:ILE:HG13	1.99	0.45
1:BC:96:LEU:HD21	1:BC:104:ILE:HG13	1.98	0.45
1:NC:96:LEU:HD21	1:NC:104:ILE:HG13	1.98	0.45
1:NE:96:LEU:HD21	1:NE:104:ILE:HG13	1.99	0.45
1:QE:96:LEU:HD21	1:QE:104:ILE:HG13	1.99	0.45
1:ZE:96:LEU:HD21	1:ZE:104:ILE:HG13	1.99	0.45
1:B:96:LEU:HD21	1:B:104:ILE:HG13	1.99	0.45
1:QC:96:LEU:HD21	1:QC:104:ILE:HG13	1.98	0.45
1:BE:96:LEU:HD21	1:BE:104:ILE:HG13	1.99	0.45
1:DE:96:LEU:HD21	1:DE:104:ILE:HG13	1.98	0.45
1:OF:96:LEU:HD21	1:OF:104:ILE:HG13	1.99	0.45
1:GA:96:LEU:HD21	1:GA:104:ILE:HG13	1.99	0.44
1:IC:96:LEU:HD21	1:IC:104:ILE:HG13	1.99	0.44
1:UD:96:LEU:HD21	1:UD:104:ILE:HG13	1.98	0.44
1:EE:96:LEU:HD21	1:EE:104:ILE:HG13	1.99	0.44
1:JE:96:LEU:HD21	1:JE:104:ILE:HG13	1.98	0.44
1:SE:96:LEU:HD21	1:SE:104:ILE:HG13	1.98	0.44
1:H:96:LEU:HD21	1:H:104:ILE:HG13	1.99	0.44
1:DB:96:LEU:HD21	1:DB:104:ILE:HG13	1.98	0.44
1:GB:96:LEU:HD21	1:GB:104:ILE:HG13	1.98	0.44
1:KB:96:LEU:HD21	1:KB:104:ILE:HG13	1.99	0.44
1:LC:96:LEU:HD21	1:LC:104:ILE:HG13	1.99	0.44
1:XC:96:LEU:HD21	1:XC:104:ILE:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:96:LEU:HD21	1:AD:104:ILE:HG13	1.99	0.44
1:DD:96:LEU:HD21	1:DD:104:ILE:HG13	1.99	0.44
1:TE:96:LEU:HD21	1:TE:104:ILE:HG13	1.99	0.44
1:Z:96:LEU:HD21	1:Z:104:ILE:HG13	1.98	0.44
1:MA:96:LEU:HD21	1:MA:104:ILE:HG13	1.99	0.44
1:TB:96:LEU:HD21	1:TB:104:ILE:HG13	1.99	0.44
1:MD:96:LEU:HD21	1:MD:104:ILE:HG13	1.99	0.44
1:KF:96:LEU:HD21	1:KF:104:ILE:HG13	1.98	0.44
1:XF:96:LEU:HD21	1:XF:104:ILE:HG13	1.99	0.44
1:T:96:LEU:HD21	1:T:104:ILE:HG13	1.99	0.44
1:CA:96:LEU:HD21	1:CA:104:ILE:HG13	1.98	0.44
1:KC:96:LEU:HD21	1:KC:104:ILE:HG13	1.98	0.44
1:VE:96:LEU:HD21	1:VE:104:ILE:HG13	1.98	0.44
1:IF:96:LEU:HD21	1:IF:104:ILE:HG13	1.99	0.44
1:UA:96:LEU:HD21	1:UA:104:ILE:HG13	1.98	0.44
1:YA:96:LEU:HD21	1:YA:104:ILE:HG13	1.99	0.44
1:ZC:96:LEU:HD21	1:ZC:104:ILE:HG13	1.98	0.44
1:P:96:LEU:HD21	1:P:104:ILE:HG13	1.98	0.44
1:PB:96:LEU:HD21	1:PB:104:ILE:HG13	1.98	0.44
1:J:96:LEU:HD21	1:J:104:ILE:HG13	1.98	0.44
1:KB:89:ARG:H	1:KB:174:GLU:HG2	1.83	0.44
1:DD:89:ARG:H	1:DD:174:GLU:HG2	1.83	0.44
1:ID:96:LEU:HD21	1:ID:104:ILE:HG13	1.98	0.44
1:IF:89:ARG:H	1:IF:174:GLU:HG2	1.83	0.44
1:XF:89:ARG:H	1:XF:174:GLU:HG2	1.83	0.44
1:K:89:ARG:H	1:K:174:GLU:HG2	1.83	0.44
1:QB:89:ARG:H	1:QB:174:GLU:HG2	1.83	0.44
1:TB:89:ARG:H	1:TB:174:GLU:HG2	1.83	0.44
1:WC:96:LEU:HD21	1:WC:104:ILE:HG13	1.98	0.44
1:JD:89:ARG:H	1:JD:174:GLU:HG2	1.83	0.44
1:MD:89:ARG:H	1:MD:174:GLU:HG2	1.83	0.44
1:HE:89:ARG:H	1:HE:174:GLU:HG2	1.83	0.44
1:B:89:ARG:H	1:B:174:GLU:HG2	1.83	0.44
1:OA:96:LEU:HD21	1:OA:104:ILE:HG13	1.98	0.44
1:PA:89:ARG:H	1:PA:174:GLU:HG2	1.83	0.44
1:NB:96:LEU:HD21	1:NB:104:ILE:HG13	1.99	0.44
1:SD:89:ARG:H	1:SD:174:GLU:HG2	1.83	0.44
1:DA:89:ARG:H	1:DA:174:GLU:HG2	1.83	0.43
1:GA:89:ARG:H	1:GA:174:GLU:HG2	1.83	0.43
1:JA:89:ARG:H	1:JA:174:GLU:HG2	1.83	0.43
1:HC:96:LEU:HD21	1:HC:104:ILE:HG13	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RC:89:ARG:H	1:RC:174:GLU:HG2	1.83	0.43
1:GD:96:LEU:HD21	1:GD:104:ILE:HG13	1.99	0.43
1:CF:96:LEU:HD21	1:CF:104:ILE:HG13	1.99	0.43
1:RF:96:LEU:HD21	1:RF:104:ILE:HG13	1.99	0.43
1:E:89:ARG:H	1:E:174:GLU:HG2	1.83	0.43
1:AA:89:ARG:H	1:AA:174:GLU:HG2	1.83	0.43
1:EB:89:ARG:H	1:EB:174:GLU:HG2	1.83	0.43
1:HB:89:ARG:H	1:HB:174:GLU:HG2	1.83	0.43
1:WB:96:LEU:HD21	1:WB:104:ILE:HG13	1.99	0.43
1:CC:89:ARG:H	1:CC:174:GLU:HG2	1.83	0.43
1:FF:89:ARG:H	1:FF:174:GLU:HG2	1.83	0.43
1:UF:89:ARG:H	1:UF:174:GLU:HG2	1.83	0.43
1:Q:96:LEU:HD21	1:Q:104:ILE:HG13	1.99	0.43
1:JA:96:LEU:HD21	1:JA:104:ILE:HG13	1.99	0.43
1:VA:96:LEU:HD21	1:VA:104:ILE:HG13	1.99	0.43
1:HB:96:LEU:HD21	1:HB:104:ILE:HG13	1.99	0.43
1:UC:89:ARG:H	1:UC:174:GLU:HG2	1.83	0.43
1:PD:96:LEU:HD21	1:PD:104:ILE:HG13	1.99	0.43
1:VD:96:LEU:HD21	1:VD:104:ILE:HG13	1.99	0.43
1:CF:89:ARG:H	1:CF:174:GLU:HG2	1.83	0.43
1:RF:89:ARG:H	1:RF:174:GLU:HG2	1.83	0.43
1:Q:89:ARG:H	1:Q:174:GLU:HG2	1.83	0.43
1:X:96:LEU:HD21	1:X:104:ILE:HG13	1.99	0.43
1:DA:96:LEU:HD21	1:DA:104:ILE:HG13	1.99	0.43
1:VA:89:ARG:H	1:VA:174:GLU:HG2	1.83	0.43
1:KE:96:LEU:HD21	1:KE:104:ILE:HG13	1.99	0.43
1:TE:89:ARG:H	1:TE:174:GLU:HG2	1.83	0.43
1:E:96:LEU:HD21	1:E:104:ILE:HG13	1.99	0.43
1:FC:89:ARG:H	1:FC:174:GLU:HG2	1.83	0.43
1:LC:89:ARG:H	1:LC:174:GLU:HG2	1.83	0.43
1:AD:89:ARG:H	1:AD:174:GLU:HG2	1.83	0.43
1:EE:89:ARG:H	1:EE:174:GLU:HG2	1.83	0.43
1:NE:89:ARG:H	1:NE:174:GLU:HG2	1.83	0.43
1:ZE:89:ARG:H	1:ZE:174:GLU:HG2	1.83	0.43
1:FF:96:LEU:HD21	1:FF:104:ILE:HG13	1.99	0.43
1:BB:96:LEU:HD21	1:BB:104:ILE:HG13	1.99	0.43
1:OC:89:ARG:H	1:OC:174:GLU:HG2	1.83	0.43
1:YD:89:ARG:H	1:YD:174:GLU:HG2	1.83	0.43
1:UF:96:LEU:HD21	1:UF:104:ILE:HG13	1.99	0.43
1:ZB:89:ARG:H	1:ZB:174:GLU:HG2	1.83	0.43
1:OF:89:ARG:H	1:OF:174:GLU:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:89:ARG:H	1:T:174:GLU:HG2	1.83	0.43
1:X:89:ARG:H	1:X:174:GLU:HG2	1.83	0.43
1:BB:89:ARG:H	1:BB:174:GLU:HG2	1.83	0.43
1:OC:96:LEU:HD21	1:OC:104:ILE:HG13	1.99	0.43
1:KE:89:ARG:H	1:KE:174:GLU:HG2	1.83	0.43
1:WE:89:ARG:H	1:WE:174:GLU:HG2	1.83	0.43
1:LF:89:ARG:H	1:LF:174:GLU:HG2	1.83	0.43
1:MA:89:ARG:H	1:MA:174:GLU:HG2	1.83	0.43
1:YA:89:ARG:H	1:YA:174:GLU:HG2	1.83	0.43
1:ZB:96:LEU:HD21	1:ZB:104:ILE:HG13	1.99	0.43
1:H:89:ARG:H	1:H:174:GLU:HG2	1.83	0.42
1:VD:89:ARG:H	1:VD:174:GLU:HG2	1.83	0.42
1:PD:89:ARG:H	1:PD:174:GLU:HG2	1.83	0.42
1:WB:89:ARG:H	1:WB:174:GLU:HG2	1.83	0.42
1:XC:89:ARG:H	1:XC:174:GLU:HG2	1.83	0.42
1:NB:89:ARG:H	1:NB:174:GLU:HG2	1.83	0.42
1:IC:89:ARG:H	1:IC:174:GLU:HG2	1.83	0.42
1:N:89:ARG:H	1:N:174:GLU:HG2	1.83	0.42
1:SA:89:ARG:H	1:SA:174:GLU:HG2	1.83	0.42
1:GD:89:ARG:H	1:GD:174:GLU:HG2	1.83	0.42
1:BE:89:ARG:H	1:BE:174:GLU:HG2	1.83	0.42
1:QE:89:ARG:H	1:QE:174:GLU:HG2	1.83	0.42
1:BE:27:VAL:CG1	1:FE:31:ILE:HG13	2.50	0.42
1:QE:27:VAL:CG1	1:UE:31:ILE:HG13	2.50	0.42
1:R:31:ILE:HG13	1:DA:27:VAL:CG1	2.50	0.42
1:IC:27:VAL:CG1	1:MC:31:ILE:HG13	2.50	0.42
1:XC:27:VAL:CG1	1:BD:31:ILE:HG13	2.50	0.42
1:VD:27:VAL:CG1	1:ZD:31:ILE:HG13	2.50	0.42
1:IE:31:ILE:HG13	1:TE:27:VAL:CG1	2.50	0.42
1:KE:27:VAL:CG1	1:OE:31:ILE:HG13	2.50	0.42
1:MF:31:ILE:HG13	1:XF:27:VAL:CG1	2.50	0.42
1:K:27:VAL:CG1	1:O:31:ILE:HG13	2.50	0.42
1:WA:31:ILE:HG13	1:HB:27:VAL:CG1	2.50	0.42
1:ZB:27:VAL:CG1	1:DC:31:ILE:HG13	2.50	0.42
1:OC:27:VAL:CG1	1:SC:31:ILE:HG13	2.50	0.42
1:PD:79:SER:OG	1:PD:82:ASN:ND2	2.53	0.42
1:TD:31:ILE:HG13	1:EE:27:VAL:CG1	2.50	0.42
1:XE:31:ILE:HG13	1:IF:27:VAL:CG1	2.50	0.42
1:UF:79:SER:OG	1:UF:82:ASN:ND2	2.53	0.42
1:PA:27:VAL:CG1	1:TA:31:ILE:HG13	2.50	0.41
1:NB:79:SER:OG	1:NB:82:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WB:79:SER:OG	1:WB:82:ASN:ND2	2.53	0.41
1:AC:31:ILE:HG13	1:LC:27:VAL:CG1	2.50	0.41
1:GD:79:SER:OG	1:GD:82:ASN:ND2	2.53	0.41
1:JD:27:VAL:CG1	1:ND:31:ILE:HG13	2.50	0.41
1:FE:131:GLU:HG2	1:FE:132:VAL:N	2.35	0.41
1:UE:131:GLU:HG2	1:UE:132:VAL:N	2.35	0.41
1:WE:79:SER:OG	1:WE:82:ASN:ND2	2.53	0.41
1:FF:79:SER:OG	1:FF:82:ASN:ND2	2.53	0.41
1:H:27:VAL:CG1	1:L:31:ILE:HG13	2.50	0.41
1:Q:27:VAL:CG1	1:V:31:ILE:HG13	2.50	0.41
1:PA:79:SER:OG	1:PA:82:ASN:ND2	2.53	0.41
1:QB:27:VAL:CG1	1:UB:31:ILE:HG13	2.50	0.41
1:PC:31:ILE:HG13	1:AD:27:VAL:CG1	2.50	0.41
1:RE:131:GLU:HG2	1:RE:132:VAL:N	2.35	0.41
1:DF:131:GLU:HG2	1:DF:132:VAL:N	2.35	0.41
1:LF:79:SER:OG	1:LF:82:ASN:ND2	2.53	0.41
1:SF:131:GLU:HG2	1:SF:132:VAL:N	2.35	0.41
1:K:79:SER:OG	1:K:82:ASN:ND2	2.53	0.41
1:MA:27:VAL:CG1	1:QA:31:ILE:HG13	2.50	0.41
1:SA:79:SER:OG	1:SA:82:ASN:ND2	2.53	0.41
1:VA:27:VAL:CG1	1:ZA:31:ILE:HG13	2.50	0.41
1:CE:131:GLU:HG2	1:CE:132:VAL:N	2.35	0.41
1:LE:131:GLU:HG2	1:LE:132:VAL:N	2.35	0.41
1:E:27:VAL:HG11	1:I:31:ILE:CD1	2.51	0.41
1:E:27:VAL:CG1	1:I:31:ILE:HG13	2.50	0.41
1:V:131:GLU:HG2	1:V:132:VAL:N	2.35	0.41
1:JA:27:VAL:HG11	1:NA:31:ILE:CD1	2.51	0.41
1:JA:27:VAL:CG1	1:NA:31:ILE:HG13	2.50	0.41
1:NB:27:VAL:HG11	1:RB:31:ILE:CD1	2.51	0.41
1:IC:79:SER:OG	1:IC:82:ASN:ND2	2.53	0.41
1:GD:27:VAL:HG11	1:KD:31:ILE:CD1	2.51	0.41
1:ND:131:GLU:HG2	1:ND:132:VAL:N	2.35	0.41
1:WD:131:GLU:HG2	1:WD:132:VAL:N	2.35	0.41
1:RF:27:VAL:CG1	1:VF:31:ILE:HG13	2.50	0.41
1:F:131:GLU:HG2	1:F:132:VAL:N	2.35	0.41
1:N:79:SER:OG	1:N:82:ASN:ND2	2.53	0.41
1:O:131:GLU:HG2	1:O:132:VAL:N	2.35	0.41
1:TA:131:GLU:HG2	1:TA:132:VAL:N	2.35	0.41
1:VA:79:SER:OG	1:VA:82:ASN:ND2	2.53	0.41
1:ZA:131:GLU:HG2	1:ZA:132:VAL:N	2.35	0.41
1:UB:131:GLU:HG2	1:UB:132:VAL:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XC:79:SER:OG	1:XC:82:ASN:ND2	2.53	0.41
1:CF:27:VAL:CG1	1:GF:31:ILE:HG13	2.50	0.41
1:IF:79:SER:OG	1:IF:82:ASN:ND2	2.53	0.41
1:UF:27:VAL:HG11	1:YF:31:ILE:CD1	2.51	0.41
1:C:31:ILE:HG13	1:N:27:VAL:CG1	2.50	0.41
1:C:131:GLU:HG2	1:C:132:VAL:N	2.35	0.41
1:Q:79:SER:OG	1:Q:82:ASN:ND2	2.53	0.41
1:DA:79:SER:OG	1:DA:82:ASN:ND2	2.53	0.41
1:HA:31:ILE:HG13	1:SA:27:VAL:CG1	2.50	0.41
1:KA:131:GLU:HG2	1:KA:132:VAL:N	2.35	0.41
1:YA:27:VAL:CG1	1:CB:31:ILE:HG13	2.50	0.41
1:BB:79:SER:OG	1:BB:82:ASN:ND2	2.53	0.41
1:OB:131:GLU:HG2	1:OB:132:VAL:N	2.35	0.41
1:ZB:79:SER:OG	1:ZB:82:ASN:ND2	2.53	0.41
1:UC:79:SER:OG	1:UC:82:ASN:ND2	2.53	0.41
1:BE:138:THR:O	1:BE:142:ARG:NH2	2.54	0.41
1:QE:138:THR:O	1:QE:142:ARG:NH2	2.54	0.41
1:ZE:138:THR:O	1:ZE:142:ARG:NH2	2.54	0.41
1:FF:27:VAL:HG11	1:JF:31:ILE:CD1	2.51	0.41
1:OF:138:THR:O	1:OF:142:ARG:NH2	2.54	0.41
1:T:27:VAL:CG1	1:Y:31:ILE:HG13	2.50	0.41
1:X:79:SER:OG	1:X:82:ASN:ND2	2.53	0.41
1:AA:27:VAL:HG11	1:EA:31:ILE:CD1	2.51	0.41
1:DA:138:THR:O	1:DA:142:ARG:NH2	2.54	0.41
1:HA:131:GLU:HG2	1:HA:132:VAL:N	2.35	0.41
1:HB:79:SER:OG	1:HB:82:ASN:ND2	2.53	0.41
1:HB:138:THR:O	1:HB:142:ARG:NH2	2.54	0.41
1:FC:79:SER:OG	1:FC:82:ASN:ND2	2.53	0.41
1:FC:138:THR:O	1:FC:142:ARG:NH2	2.54	0.41
1:GC:131:GLU:HG2	1:GC:132:VAL:N	2.35	0.41
1:OC:79:SER:OG	1:OC:82:ASN:ND2	2.53	0.41
1:SC:131:GLU:HG2	1:SC:132:VAL:N	2.35	0.41
1:UC:138:THR:O	1:UC:142:ARG:NH2	2.54	0.41
1:VC:131:GLU:HG2	1:VC:132:VAL:N	2.35	0.41
1:YD:138:THR:O	1:YD:142:ARG:NH2	2.54	0.41
1:NE:138:THR:O	1:NE:142:ARG:NH2	2.54	0.41
1:WE:27:VAL:HG11	1:AF:31:ILE:CD1	2.51	0.41
1:CF:27:VAL:HG11	1:GF:31:ILE:CD1	2.51	0.41
1:RF:27:VAL:HG11	1:VF:31:ILE:CD1	2.51	0.41
1:UF:27:VAL:CG1	1:YF:31:ILE:HG13	2.50	0.41
1:XF:79:SER:OG	1:XF:82:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:THR:O	1:E:142:ARG:NH2	2.54	0.41
1:H:27:VAL:HG11	1:L:31:ILE:CD1	2.51	0.41
1:X:138:THR:O	1:X:142:ARG:NH2	2.54	0.41
1:JA:138:THR:O	1:JA:142:ARG:NH2	2.54	0.41
1:MA:27:VAL:HG11	1:QA:31:ILE:CD1	2.51	0.41
1:WA:131:GLU:HG2	1:WA:132:VAL:N	2.35	0.41
1:BB:138:THR:O	1:BB:142:ARG:NH2	2.54	0.41
1:EB:27:VAL:HG11	1:IB:31:ILE:CD1	2.51	0.41
1:EB:138:THR:O	1:EB:142:ARG:NH2	2.54	0.41
1:LB:31:ILE:HG13	1:WB:27:VAL:CG1	2.50	0.41
1:DC:131:GLU:HG2	1:DC:132:VAL:N	2.35	0.41
1:IC:27:VAL:HG11	1:MC:31:ILE:CD1	2.51	0.41
1:LC:138:THR:O	1:LC:142:ARG:NH2	2.54	0.41
1:AD:138:THR:O	1:AD:142:ARG:NH2	2.54	0.41
1:HD:131:GLU:HG2	1:HD:132:VAL:N	2.35	0.41
1:TD:131:GLU:HG2	1:TD:132:VAL:N	2.35	0.41
1:EE:138:THR:O	1:EE:142:ARG:NH2	2.54	0.41
1:IE:131:GLU:HG2	1:IE:132:VAL:N	2.35	0.41
1:TE:138:THR:O	1:TE:142:ARG:NH2	2.54	0.41
1:FF:27:VAL:CG1	1:JF:31:ILE:HG13	2.50	0.41
1:LF:27:VAL:HG11	1:PF:31:ILE:CD1	2.51	0.41
1:XF:138:THR:O	1:XF:142:ARG:NH2	2.54	0.41
1:B:27:VAL:HG11	1:F:31:ILE:CD1	2.51	0.41
1:B:27:VAL:CG1	1:F:31:ILE:HG13	2.50	0.41
1:E:79:SER:OG	1:E:82:ASN:ND2	2.53	0.41
1:H:79:SER:OG	1:H:82:ASN:ND2	2.53	0.41
1:M:138:THR:HG22	1:M:139:ASP:OD1	2.21	0.41
1:R:131:GLU:HG2	1:R:132:VAL:N	2.35	0.41
1:T:138:THR:O	1:T:142:ARG:NH2	2.54	0.41
1:X:27:VAL:CG1	1:BA:31:ILE:HG13	2.50	0.41
1:Z:138:THR:HG22	1:Z:139:ASP:OD1	2.21	0.41
1:AA:27:VAL:CG1	1:EA:31:ILE:HG13	2.50	0.41
1:AA:138:THR:O	1:AA:142:ARG:NH2	2.54	0.41
1:GA:27:VAL:HG11	1:KA:31:ILE:CD1	2.51	0.41
1:GA:27:VAL:CG1	1:KA:31:ILE:HG13	2.50	0.41
1:JA:79:SER:OG	1:JA:82:ASN:ND2	2.53	0.41
1:MA:79:SER:OG	1:MA:82:ASN:ND2	2.53	0.41
1:RA:138:THR:HG22	1:RA:139:ASP:OD1	2.21	0.41
1:YA:138:THR:O	1:YA:142:ARG:NH2	2.54	0.41
1:CB:131:GLU:HG2	1:CB:132:VAL:N	2.35	0.41
1:DB:138:THR:HG22	1:DB:139:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:27:VAL:CG1	1:IB:31:ILE:HG13	2.50	0.41
1:KB:27:VAL:HG11	1:OB:31:ILE:CD1	2.51	0.41
1:KB:138:THR:O	1:KB:142:ARG:NH2	2.54	0.41
1:NB:27:VAL:CG1	1:RB:31:ILE:HG13	2.50	0.41
1:NB:138:THR:O	1:NB:142:ARG:NH2	2.54	0.41
1:QB:79:SER:OG	1:QB:82:ASN:ND2	2.53	0.41
1:AC:31:ILE:CD1	1:LC:27:VAL:HG11	2.51	0.41
1:CC:27:VAL:CG1	1:GC:31:ILE:HG13	2.50	0.41
1:JC:131:GLU:HG2	1:JC:132:VAL:N	2.35	0.41
1:MC:131:GLU:HG2	1:MC:132:VAL:N	2.35	0.41
1:OC:27:VAL:HG11	1:SC:31:ILE:CD1	2.51	0.41
1:PC:31:ILE:CD1	1:AD:27:VAL:HG11	2.51	0.41
1:RC:27:VAL:CG1	1:VC:31:ILE:HG13	2.50	0.41
1:XC:27:VAL:HG11	1:BD:31:ILE:CD1	2.51	0.41
1:YC:131:GLU:HG2	1:YC:132:VAL:N	2.35	0.41
1:AD:79:SER:OG	1:AD:82:ASN:ND2	2.53	0.41
1:BD:131:GLU:HG2	1:BD:132:VAL:N	2.35	0.41
1:DD:27:VAL:HG11	1:HD:31:ILE:CD1	2.51	0.41
1:DD:138:THR:O	1:DD:142:ARG:NH2	2.54	0.41
1:ED:31:ILE:HG13	1:PD:27:VAL:CG1	2.50	0.41
1:GD:138:THR:O	1:GD:142:ARG:NH2	2.54	0.41
1:JD:79:SER:OG	1:JD:82:ASN:ND2	2.53	0.41
1:SD:79:SER:OG	1:SD:82:ASN:ND2	2.53	0.41
1:VD:27:VAL:HG11	1:ZD:31:ILE:CD1	2.51	0.41
1:VD:138:THR:O	1:VD:142:ARG:NH2	2.54	0.41
1:HE:79:SER:OG	1:HE:82:ASN:ND2	2.53	0.41
1:KE:27:VAL:HG11	1:OE:31:ILE:CD1	2.51	0.41
1:KE:138:THR:O	1:KE:142:ARG:NH2	2.54	0.41
1:ZE:27:VAL:HG11	1:DF:31:ILE:CD1	2.51	0.41
1:ZE:27:VAL:CG1	1:DF:31:ILE:HG13	2.50	0.41
1:ZE:79:SER:OG	1:ZE:82:ASN:ND2	2.53	0.41
1:AF:131:GLU:HG2	1:AF:132:VAL:N	2.35	0.41
1:HF:138:THR:HG22	1:HF:139:ASP:OD1	2.21	0.41
1:IF:138:THR:O	1:IF:142:ARG:NH2	2.54	0.41
1:OF:27:VAL:HG11	1:SF:31:ILE:CD1	2.51	0.41
1:OF:27:VAL:CG1	1:SF:31:ILE:HG13	2.50	0.41
1:OF:79:SER:OG	1:OF:82:ASN:ND2	2.53	0.41
1:PF:131:GLU:HG2	1:PF:132:VAL:N	2.35	0.41
1:RF:79:SER:OG	1:RF:82:ASN:ND2	2.53	0.41
1:WF:138:THR:HG22	1:WF:139:ASP:OD1	2.21	0.41
1:H:138:THR:O	1:H:142:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:27:VAL:HG11	1:O:31:ILE:CD1	2.51	0.41
1:Y:131:GLU:HG2	1:Y:132:VAL:N	2.35	0.41
1:LA:138:THR:HG22	1:LA:139:ASP:OD1	2.21	0.41
1:QA:131:GLU:HG2	1:QA:132:VAL:N	2.35	0.41
1:BB:27:VAL:CG1	1:FB:31:ILE:HG13	2.50	0.41
1:MB:138:THR:HG22	1:MB:139:ASP:OD1	2.21	0.41
1:RB:131:GLU:HG2	1:RB:132:VAL:N	2.35	0.41
1:YB:138:THR:HG22	1:YB:139:ASP:OD1	2.21	0.41
1:ZB:27:VAL:HG11	1:DC:31:ILE:CD1	2.51	0.41
1:FC:27:VAL:CG1	1:JC:31:ILE:HG13	2.50	0.41
1:NC:138:THR:HG22	1:NC:139:ASP:OD1	2.21	0.41
1:FD:138:THR:HG22	1:FD:139:ASP:OD1	2.21	0.41
1:TD:31:ILE:CD1	1:EE:27:VAL:HG11	2.51	0.41
1:VD:79:SER:OG	1:VD:82:ASN:ND2	2.53	0.41
1:CF:79:SER:OG	1:CF:82:ASN:ND2	2.53	0.41
1:GF:131:GLU:HG2	1:GF:132:VAL:N	2.35	0.41
1:G:138:THR:HG22	1:G:139:ASP:OD1	2.21	0.40
1:L:131:GLU:HG2	1:L:132:VAL:N	2.35	0.40
1:MA:138:THR:O	1:MA:142:ARG:NH2	2.54	0.40
1:AC:131:GLU:HG2	1:AC:132:VAL:N	2.35	0.40
1:BC:138:THR:HG22	1:BC:139:ASP:OD1	2.21	0.40
1:CC:138:THR:O	1:CC:142:ARG:NH2	2.54	0.40
1:LC:79:SER:OG	1:LC:82:ASN:ND2	2.53	0.40
1:QC:138:THR:HG22	1:QC:139:ASP:OD1	2.21	0.40
1:RC:138:THR:O	1:RC:142:ARG:NH2	2.54	0.40
1:TC:138:THR:HG22	1:TC:139:ASP:OD1	2.21	0.40
1:UC:27:VAL:CG1	1:YC:31:ILE:HG13	2.50	0.40
1:ED:31:ILE:CD1	1:PD:27:VAL:HG11	2.51	0.40
1:MD:138:THR:O	1:MD:142:ARG:NH2	2.54	0.40
1:IE:31:ILE:CD1	1:TE:27:VAL:HG11	2.51	0.40
1:NE:27:VAL:HG11	1:RE:31:ILE:CD1	2.51	0.40
1:QF:138:THR:HG22	1:QF:139:ASP:OD1	2.21	0.40
1:VF:131:GLU:HG2	1:VF:132:VAL:N	2.35	0.40
1:NA:131:GLU:HG2	1:NA:132:VAL:N	2.35	0.40
1:PA:27:VAL:HG11	1:TA:31:ILE:CD1	2.51	0.40
1:VA:27:VAL:HG11	1:ZA:31:ILE:CD1	2.51	0.40
1:KB:27:VAL:CG1	1:OB:31:ILE:HG13	2.50	0.40
1:LB:31:ILE:CD1	1:WB:27:VAL:HG11	2.51	0.40
1:WB:28:GLN:HA	1:WB:29:PRO:HD3	1.97	0.40
1:EC:138:THR:HG22	1:EC:139:ASP:OD1	2.21	0.40
1:IC:138:THR:O	1:IC:142:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PC:131:GLU:HG2	1:PC:132:VAL:N	2.35	0.40
1:XC:138:THR:O	1:XC:142:ARG:NH2	2.54	0.40
1:DD:27:VAL:CG1	1:HD:31:ILE:HG13	2.50	0.40
1:KD:131:GLU:HG2	1:KD:132:VAL:N	2.35	0.40
1:RD:138:THR:HG22	1:RD:139:ASP:OD1	2.21	0.40
1:SD:27:VAL:HG11	1:WD:31:ILE:CD1	2.51	0.40
1:YD:27:VAL:HG11	1:CE:31:ILE:CD1	2.51	0.40
1:BE:27:VAL:HG11	1:FE:31:ILE:CD1	2.51	0.40
1:BE:79:SER:OG	1:BE:82:ASN:ND2	2.53	0.40
1:GE:138:THR:HG22	1:GE:139:ASP:OD1	2.21	0.40
1:HE:27:VAL:HG11	1:LE:31:ILE:CD1	2.51	0.40
1:JE:138:THR:HG22	1:JE:139:ASP:OD1	2.21	0.40
1:KE:79:SER:OG	1:KE:82:ASN:ND2	2.53	0.40
1:BF:138:THR:HG22	1:BF:139:ASP:OD1	2.21	0.40
1:MF:31:ILE:CD1	1:XF:27:VAL:HG11	2.51	0.40
1:B:138:THR:O	1:B:142:ARG:NH2	2.54	0.40
1:I:131:GLU:HG2	1:I:132:VAL:N	2.35	0.40
1:Q:27:VAL:HG11	1:V:31:ILE:CD1	2.51	0.40
1:IA:138:THR:HG22	1:IA:139:ASP:OD1	2.21	0.40
1:BB:27:VAL:HG11	1:FB:31:ILE:CD1	2.51	0.40
1:FB:131:GLU:HG2	1:FB:132:VAL:N	2.35	0.40
1:TB:138:THR:O	1:TB:142:ARG:NH2	2.54	0.40
1:KC:138:THR:HG22	1:KC:139:ASP:OD1	2.21	0.40
1:ED:131:GLU:HG2	1:ED:132:VAL:N	2.35	0.40
1:JD:27:VAL:HG11	1:ND:31:ILE:CD1	2.51	0.40
1:PD:28:GLN:HA	1:PD:29:PRO:HD3	1.97	0.40
1:UD:138:THR:HG22	1:UD:139:ASP:OD1	2.21	0.40
1:HE:27:VAL:CG1	1:LE:31:ILE:HG13	2.50	0.40
1:QE:27:VAL:HG11	1:UE:31:ILE:CD1	2.51	0.40
1:QE:79:SER:OG	1:QE:82:ASN:ND2	2.53	0.40
1:XE:31:ILE:CD1	1:IF:27:VAL:HG11	2.51	0.40
1:C:31:ILE:CD1	1:N:27:VAL:HG11	2.51	0.40
1:D:138:THR:HG22	1:D:139:ASP:OD1	2.21	0.40
1:H:28:GLN:HA	1:H:29:PRO:HD3	1.97	0.40
1:GA:138:THR:O	1:GA:142:ARG:NH2	2.54	0.40
1:EB:79:SER:OG	1:EB:82:ASN:ND2	2.53	0.40
1:JB:138:THR:HG22	1:JB:139:ASP:OD1	2.21	0.40
1:QB:27:VAL:HG11	1:UB:31:ILE:CD1	2.51	0.40
1:ZB:138:THR:O	1:ZB:142:ARG:NH2	2.54	0.40
1:OC:138:THR:O	1:OC:142:ARG:NH2	2.54	0.40
1:ZC:138:THR:HG22	1:ZC:139:ASP:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MD:27:VAL:HG11	1:QD:31:ILE:CD1	2.51	0.40
1:SD:27:VAL:CG1	1:WD:31:ILE:HG13	2.50	0.40
1:AE:138:THR:HG22	1:AE:139:ASP:OD1	2.21	0.40
1:PE:138:THR:HG22	1:PE:139:ASP:OD1	2.21	0.40
1:J:138:THR:HG22	1:J:139:ASP:OD1	2.21	0.40
1:X:27:VAL:HG11	1:BA:31:ILE:CD1	2.51	0.40
1:BA:131:GLU:HG2	1:BA:132:VAL:N	2.35	0.40
1:EA:131:GLU:HG2	1:EA:132:VAL:N	2.35	0.40
1:HA:31:ILE:CD1	1:SA:27:VAL:HG11	2.51	0.40
1:OA:138:THR:HG22	1:OA:139:ASP:OD1	2.21	0.40
1:GB:138:THR:HG22	1:GB:139:ASP:OD1	2.21	0.40
1:LB:131:GLU:HG2	1:LB:132:VAL:N	2.35	0.40
1:UC:27:VAL:HG11	1:YC:31:ILE:CD1	2.51	0.40
1:CD:138:THR:HG22	1:CD:139:ASP:OD1	2.21	0.40
1:GD:27:VAL:CG1	1:KD:31:ILE:HG13	2.50	0.40
1:JD:138:THR:O	1:JD:142:ARG:NH2	2.54	0.40
1:MD:27:VAL:CG1	1:QD:31:ILE:HG13	2.50	0.40
1:DE:138:THR:HG22	1:DE:139:ASP:OD1	2.21	0.40
1:NE:27:VAL:CG1	1:RE:31:ILE:HG13	2.50	0.40
1:VE:138:THR:HG22	1:VE:139:ASP:OD1	2.21	0.40
1:XE:131:GLU:HG2	1:XE:132:VAL:N	2.35	0.40
1:JF:131:GLU:HG2	1:JF:132:VAL:N	2.35	0.40
1:YF:131:GLU:HG2	1:YF:132:VAL:N	2.35	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	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	AA	161/192 (84%)	156 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	AC	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	AD	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	AE	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	AF	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	B	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	BA	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	BB	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	BC	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	BD	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	BE	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	BF	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	C	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	CA	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	CB	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	CC	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	CD	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	CE	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	CF	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	D	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	DA	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	DB	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	DC	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	DD	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	DE	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	DF	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	E	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	EA	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	EB	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	EC	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	ED	162/192 (84%)	160 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EE	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	EF	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	F	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	FA	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	FB	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	FC	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	FD	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	FE	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	FF	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	G	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	GA	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	GB	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	GC	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	GD	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	GE	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	GF	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	H	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	HA	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	HB	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	HC	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	HD	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	HE	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	HF	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	I	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	IA	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	IB	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	IC	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	ID	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	IE	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	IF	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	J	146/192 (76%)	144 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	JA	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	JB	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	JC	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	JD	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	JE	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	JF	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	K	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	KA	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	KB	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	KC	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	KD	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	KE	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	KF	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	L	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	LA	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	LB	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	LC	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	LD	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	LE	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	LF	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	M	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	MA	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	MB	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	MC	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	MD	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	ME	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	MF	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	N	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	NA	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	NB	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	NC	146/192 (76%)	144 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	ND	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	NE	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	NF	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	O	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	OA	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	OB	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	OC	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	OD	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	OE	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	OF	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	P	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	PA	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	PB	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	PC	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	PD	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	PE	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	PF	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	Q	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	QA	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	QB	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	QC	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	QD	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	QE	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	QF	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	R	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	RA	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	RB	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	RC	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	RD	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	RE	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	RF	161/192 (84%)	156 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	SA	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	SB	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	SC	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	SD	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	SE	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	SF	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	T	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	TA	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	TB	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	TC	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	TD	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	TE	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	TF	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	UA	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	UB	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	UC	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	UD	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	UE	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	UF	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	V	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	VA	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	VB	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	VC	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	VD	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	VE	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	VF	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	W	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	WA	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	WB	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	WC	146/192 (76%)	144 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	WD	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	WE	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	WF	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	X	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	XA	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	XB	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	XC	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	XD	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	XE	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	XF	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	Y	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	YA	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	YB	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	YC	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	YD	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	YE	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	YF	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	Z	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	ZA	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	ZB	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	ZC	146/192 (76%)	144 (99%)	2 (1%)	0	100	100
1	ZD	162/192 (84%)	160 (99%)	2 (1%)	0	100	100
1	ZE	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
All	All	28140/34560 (81%)	27600 (98%)	540 (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	116/148 (78%)	116 (100%)	0	100	100
1	AA	125/148 (84%)	125 (100%)	0	100	100
1	AB	116/148 (78%)	116 (100%)	0	100	100
1	AC	127/148 (86%)	127 (100%)	0	100	100
1	AD	125/148 (84%)	125 (100%)	0	100	100
1	AE	116/148 (78%)	116 (100%)	0	100	100
1	AF	127/148 (86%)	127 (100%)	0	100	100
1	B	125/148 (84%)	125 (100%)	0	100	100
1	BA	127/148 (86%)	127 (100%)	0	100	100
1	BB	125/148 (84%)	125 (100%)	0	100	100
1	BC	116/148 (78%)	116 (100%)	0	100	100
1	BD	127/148 (86%)	127 (100%)	0	100	100
1	BE	125/148 (84%)	125 (100%)	0	100	100
1	BF	116/148 (78%)	116 (100%)	0	100	100
1	C	127/148 (86%)	127 (100%)	0	100	100
1	CA	116/148 (78%)	116 (100%)	0	100	100
1	CB	127/148 (86%)	127 (100%)	0	100	100
1	CC	125/148 (84%)	125 (100%)	0	100	100
1	CD	116/148 (78%)	116 (100%)	0	100	100
1	CE	127/148 (86%)	127 (100%)	0	100	100
1	CF	125/148 (84%)	125 (100%)	0	100	100
1	D	116/148 (78%)	116 (100%)	0	100	100
1	DA	125/148 (84%)	125 (100%)	0	100	100
1	DB	116/148 (78%)	116 (100%)	0	100	100
1	DC	127/148 (86%)	127 (100%)	0	100	100
1	DD	125/148 (84%)	125 (100%)	0	100	100
1	DE	116/148 (78%)	116 (100%)	0	100	100
1	DF	127/148 (86%)	127 (100%)	0	100	100
1	E	125/148 (84%)	125 (100%)	0	100	100
1	EA	127/148 (86%)	127 (100%)	0	100	100
1	EB	125/148 (84%)	125 (100%)	0	100	100
1	EC	116/148 (78%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	ED	127/148 (86%)	127 (100%)	0	100	100
1	EE	125/148 (84%)	125 (100%)	0	100	100
1	EF	116/148 (78%)	116 (100%)	0	100	100
1	F	127/148 (86%)	127 (100%)	0	100	100
1	FA	116/148 (78%)	116 (100%)	0	100	100
1	FB	127/148 (86%)	127 (100%)	0	100	100
1	FC	125/148 (84%)	125 (100%)	0	100	100
1	FD	116/148 (78%)	116 (100%)	0	100	100
1	FE	127/148 (86%)	127 (100%)	0	100	100
1	FF	125/148 (84%)	125 (100%)	0	100	100
1	G	116/148 (78%)	116 (100%)	0	100	100
1	GA	125/148 (84%)	125 (100%)	0	100	100
1	GB	116/148 (78%)	116 (100%)	0	100	100
1	GC	127/148 (86%)	127 (100%)	0	100	100
1	GD	125/148 (84%)	125 (100%)	0	100	100
1	GE	116/148 (78%)	116 (100%)	0	100	100
1	GF	127/148 (86%)	127 (100%)	0	100	100
1	H	125/148 (84%)	125 (100%)	0	100	100
1	HA	127/148 (86%)	127 (100%)	0	100	100
1	HB	125/148 (84%)	125 (100%)	0	100	100
1	HC	116/148 (78%)	116 (100%)	0	100	100
1	HD	127/148 (86%)	127 (100%)	0	100	100
1	HE	125/148 (84%)	125 (100%)	0	100	100
1	HF	116/148 (78%)	116 (100%)	0	100	100
1	I	127/148 (86%)	127 (100%)	0	100	100
1	IA	116/148 (78%)	116 (100%)	0	100	100
1	IB	127/148 (86%)	127 (100%)	0	100	100
1	IC	125/148 (84%)	125 (100%)	0	100	100
1	ID	116/148 (78%)	116 (100%)	0	100	100
1	IE	127/148 (86%)	127 (100%)	0	100	100
1	IF	125/148 (84%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	116/148 (78%)	116 (100%)	0	100	100
1	JA	125/148 (84%)	125 (100%)	0	100	100
1	JB	116/148 (78%)	116 (100%)	0	100	100
1	JC	127/148 (86%)	127 (100%)	0	100	100
1	JD	125/148 (84%)	125 (100%)	0	100	100
1	JE	116/148 (78%)	116 (100%)	0	100	100
1	JF	127/148 (86%)	127 (100%)	0	100	100
1	K	125/148 (84%)	125 (100%)	0	100	100
1	KA	127/148 (86%)	127 (100%)	0	100	100
1	KB	125/148 (84%)	125 (100%)	0	100	100
1	KC	116/148 (78%)	116 (100%)	0	100	100
1	KD	127/148 (86%)	127 (100%)	0	100	100
1	KE	125/148 (84%)	125 (100%)	0	100	100
1	KF	116/148 (78%)	116 (100%)	0	100	100
1	L	127/148 (86%)	127 (100%)	0	100	100
1	LA	116/148 (78%)	116 (100%)	0	100	100
1	LB	127/148 (86%)	127 (100%)	0	100	100
1	LC	125/148 (84%)	125 (100%)	0	100	100
1	LD	116/148 (78%)	116 (100%)	0	100	100
1	LE	127/148 (86%)	127 (100%)	0	100	100
1	LF	125/148 (84%)	125 (100%)	0	100	100
1	M	116/148 (78%)	116 (100%)	0	100	100
1	MA	125/148 (84%)	125 (100%)	0	100	100
1	MB	116/148 (78%)	116 (100%)	0	100	100
1	MC	127/148 (86%)	127 (100%)	0	100	100
1	MD	125/148 (84%)	125 (100%)	0	100	100
1	ME	116/148 (78%)	116 (100%)	0	100	100
1	MF	127/148 (86%)	127 (100%)	0	100	100
1	N	125/148 (84%)	125 (100%)	0	100	100
1	NA	127/148 (86%)	127 (100%)	0	100	100
1	NB	125/148 (84%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	NC	116/148 (78%)	116 (100%)	0	100	100
1	ND	127/148 (86%)	127 (100%)	0	100	100
1	NE	125/148 (84%)	125 (100%)	0	100	100
1	NF	116/148 (78%)	116 (100%)	0	100	100
1	O	127/148 (86%)	127 (100%)	0	100	100
1	OA	116/148 (78%)	116 (100%)	0	100	100
1	OB	127/148 (86%)	127 (100%)	0	100	100
1	OC	125/148 (84%)	125 (100%)	0	100	100
1	OD	116/148 (78%)	116 (100%)	0	100	100
1	OE	127/148 (86%)	127 (100%)	0	100	100
1	OF	125/148 (84%)	125 (100%)	0	100	100
1	P	116/148 (78%)	116 (100%)	0	100	100
1	PA	125/148 (84%)	125 (100%)	0	100	100
1	PB	116/148 (78%)	116 (100%)	0	100	100
1	PC	127/148 (86%)	127 (100%)	0	100	100
1	PD	125/148 (84%)	125 (100%)	0	100	100
1	PE	116/148 (78%)	116 (100%)	0	100	100
1	PF	127/148 (86%)	127 (100%)	0	100	100
1	Q	125/148 (84%)	125 (100%)	0	100	100
1	QA	127/148 (86%)	127 (100%)	0	100	100
1	QB	125/148 (84%)	125 (100%)	0	100	100
1	QC	116/148 (78%)	116 (100%)	0	100	100
1	QD	127/148 (86%)	127 (100%)	0	100	100
1	QE	125/148 (84%)	125 (100%)	0	100	100
1	QF	116/148 (78%)	116 (100%)	0	100	100
1	R	127/148 (86%)	127 (100%)	0	100	100
1	RA	116/148 (78%)	116 (100%)	0	100	100
1	RB	127/148 (86%)	127 (100%)	0	100	100
1	RC	125/148 (84%)	125 (100%)	0	100	100
1	RD	116/148 (78%)	116 (100%)	0	100	100
1	RE	127/148 (86%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	RF	125/148 (84%)	125 (100%)	0	100	100
1	S	116/148 (78%)	116 (100%)	0	100	100
1	SA	125/148 (84%)	125 (100%)	0	100	100
1	SB	116/148 (78%)	116 (100%)	0	100	100
1	SC	127/148 (86%)	127 (100%)	0	100	100
1	SD	125/148 (84%)	125 (100%)	0	100	100
1	SE	116/148 (78%)	116 (100%)	0	100	100
1	SF	127/148 (86%)	127 (100%)	0	100	100
1	T	125/148 (84%)	125 (100%)	0	100	100
1	TA	127/148 (86%)	127 (100%)	0	100	100
1	TB	125/148 (84%)	125 (100%)	0	100	100
1	TC	116/148 (78%)	116 (100%)	0	100	100
1	TD	127/148 (86%)	127 (100%)	0	100	100
1	TE	125/148 (84%)	125 (100%)	0	100	100
1	TF	116/148 (78%)	116 (100%)	0	100	100
1	UA	116/148 (78%)	116 (100%)	0	100	100
1	UB	127/148 (86%)	127 (100%)	0	100	100
1	UC	125/148 (84%)	125 (100%)	0	100	100
1	UD	116/148 (78%)	116 (100%)	0	100	100
1	UE	127/148 (86%)	127 (100%)	0	100	100
1	UF	125/148 (84%)	125 (100%)	0	100	100
1	V	127/148 (86%)	127 (100%)	0	100	100
1	VA	125/148 (84%)	125 (100%)	0	100	100
1	VB	116/148 (78%)	116 (100%)	0	100	100
1	VC	127/148 (86%)	127 (100%)	0	100	100
1	VD	125/148 (84%)	125 (100%)	0	100	100
1	VE	116/148 (78%)	116 (100%)	0	100	100
1	VF	127/148 (86%)	127 (100%)	0	100	100
1	W	116/148 (78%)	116 (100%)	0	100	100
1	WA	127/148 (86%)	127 (100%)	0	100	100
1	WB	125/148 (84%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	WC	116/148 (78%)	116 (100%)	0	100	100
1	WD	127/148 (86%)	127 (100%)	0	100	100
1	WE	125/148 (84%)	125 (100%)	0	100	100
1	WF	116/148 (78%)	116 (100%)	0	100	100
1	X	125/148 (84%)	125 (100%)	0	100	100
1	XA	116/148 (78%)	116 (100%)	0	100	100
1	XB	127/148 (86%)	127 (100%)	0	100	100
1	XC	125/148 (84%)	125 (100%)	0	100	100
1	XD	116/148 (78%)	116 (100%)	0	100	100
1	XE	127/148 (86%)	127 (100%)	0	100	100
1	XF	125/148 (84%)	125 (100%)	0	100	100
1	Y	127/148 (86%)	127 (100%)	0	100	100
1	YA	125/148 (84%)	125 (100%)	0	100	100
1	YB	116/148 (78%)	116 (100%)	0	100	100
1	YC	127/148 (86%)	127 (100%)	0	100	100
1	YD	125/148 (84%)	125 (100%)	0	100	100
1	YE	116/148 (78%)	116 (100%)	0	100	100
1	YF	127/148 (86%)	127 (100%)	0	100	100
1	Z	116/148 (78%)	116 (100%)	0	100	100
1	ZA	127/148 (86%)	127 (100%)	0	100	100
1	ZB	125/148 (84%)	125 (100%)	0	100	100
1	ZC	116/148 (78%)	116 (100%)	0	100	100
1	ZD	127/148 (86%)	127 (100%)	0	100	100
1	ZE	125/148 (84%)	125 (100%)	0	100	100
All	All	22080/26640 (83%)	22080 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	B	153	GLN

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Mol	Chain	Res	Type
1	D	114	GLN
1	E	153	GLN
1	G	114	GLN
1	H	153	GLN
1	J	114	GLN
1	K	153	GLN
1	M	114	GLN
1	N	153	GLN
1	O	28	GLN
1	P	114	GLN
1	Q	153	GLN
1	S	114	GLN
1	T	153	GLN
1	V	28	GLN
1	W	114	GLN
1	X	153	GLN
1	Y	28	GLN
1	Z	114	GLN
1	AA	153	GLN
1	CA	114	GLN
1	DA	153	GLN
1	FA	114	GLN
1	GA	153	GLN
1	IA	114	GLN
1	JA	153	GLN
1	KA	75	HIS
1	LA	114	GLN
1	MA	153	GLN
1	NA	28	GLN
1	OA	114	GLN
1	PA	153	GLN
1	RA	114	GLN
1	SA	153	GLN
1	TA	28	GLN
1	UA	114	GLN
1	VA	153	GLN
1	XA	114	GLN
1	YA	153	GLN
1	ZA	28	GLN
1	AB	114	GLN
1	BB	82	ASN
1	BB	153	GLN

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Mol	Chain	Res	Type
1	CB	28	GLN
1	DB	114	GLN
1	EB	153	GLN
1	GB	114	GLN
1	HB	153	GLN
1	JB	114	GLN
1	KB	153	GLN
1	MB	114	GLN
1	NB	82	ASN
1	NB	153	GLN
1	OB	75	HIS
1	PB	114	GLN
1	QB	153	GLN
1	RB	75	HIS
1	SB	114	GLN
1	TB	153	GLN
1	VB	114	GLN
1	WB	153	GLN
1	YB	114	GLN
1	ZB	153	GLN
1	AC	75	HIS
1	BC	114	GLN
1	CC	153	GLN
1	DC	28	GLN
1	EC	114	GLN
1	FC	153	GLN
1	HC	114	GLN
1	IC	153	GLN
1	KC	114	GLN
1	LC	153	GLN
1	MC	28	GLN
1	NC	114	GLN
1	OC	153	GLN
1	PC	75	HIS
1	QC	67	ASN
1	QC	114	GLN
1	RC	153	GLN
1	SC	28	GLN
1	TC	114	GLN
1	UC	153	GLN
1	WC	114	GLN
1	XC	153	GLN

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Mol	Chain	Res	Type
1	ZC	114	GLN
1	AD	153	GLN
1	BD	28	GLN
1	CD	114	GLN
1	DD	153	GLN
1	FD	114	GLN
1	GD	82	ASN
1	GD	153	GLN
1	HD	75	HIS
1	ID	114	GLN
1	JD	153	GLN
1	LD	114	GLN
1	MD	82	ASN
1	MD	153	GLN
1	OD	114	GLN
1	PD	153	GLN
1	RD	114	GLN
1	SD	153	GLN
1	TD	28	GLN
1	UD	114	GLN
1	VD	153	GLN
1	WD	28	GLN
1	XD	114	GLN
1	YD	153	GLN
1	AE	114	GLN
1	BE	153	GLN
1	DE	67	ASN
1	DE	114	GLN
1	EE	153	GLN
1	FE	28	GLN
1	GE	114	GLN
1	HE	153	GLN
1	IE	28	GLN
1	JE	114	GLN
1	KE	153	GLN
1	LE	28	GLN
1	ME	114	GLN
1	NE	153	GLN
1	PE	114	GLN
1	QE	153	GLN
1	SE	67	ASN
1	SE	114	GLN

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Mol	Chain	Res	Type
1	TE	153	GLN
1	UE	28	GLN
1	VE	114	GLN
1	WE	153	GLN
1	YE	114	GLN
1	ZE	153	GLN
1	AF	75	HIS
1	BF	114	GLN
1	CF	153	GLN
1	EF	114	GLN
1	FF	153	GLN
1	GF	28	GLN
1	HF	114	GLN
1	IF	153	GLN
1	JF	28	GLN
1	KF	114	GLN
1	LF	153	GLN
1	MF	28	GLN
1	NF	114	GLN
1	OF	153	GLN
1	PF	75	HIS
1	QF	114	GLN
1	RF	153	GLN
1	TF	114	GLN
1	UF	153	GLN
1	VF	28	GLN
1	WF	114	GLN
1	XF	153	GLN
1	YF	28	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

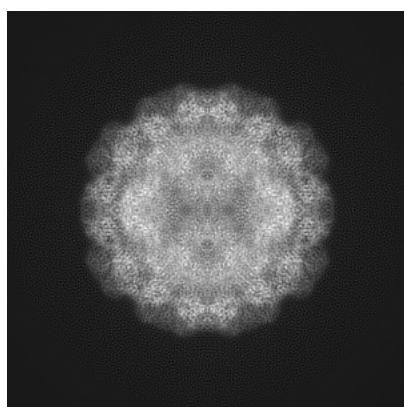
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13345. These allow visual inspection of the internal detail of the map and identification of artifacts.

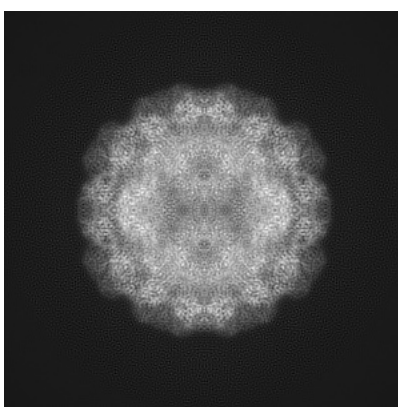
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

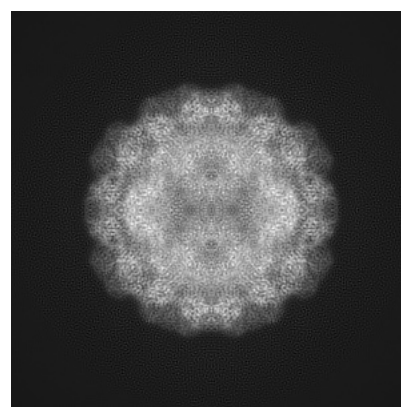
6.1.1 Primary map



X



Y

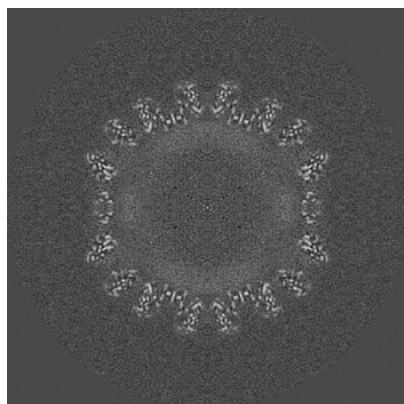


Z

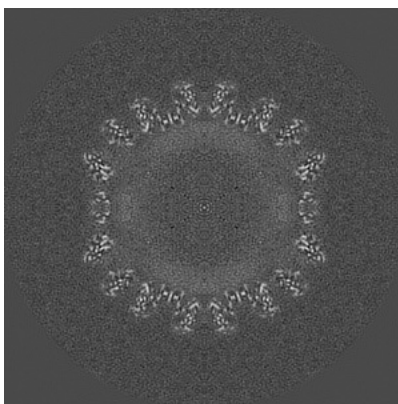
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

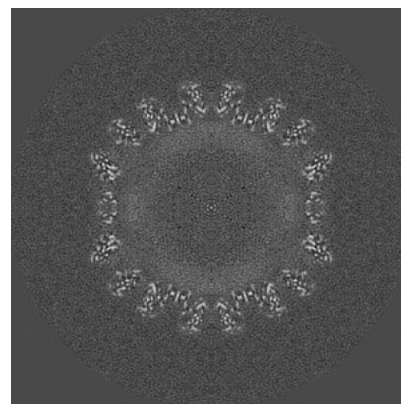
6.2.1 Primary map



X Index: 256



Y Index: 256

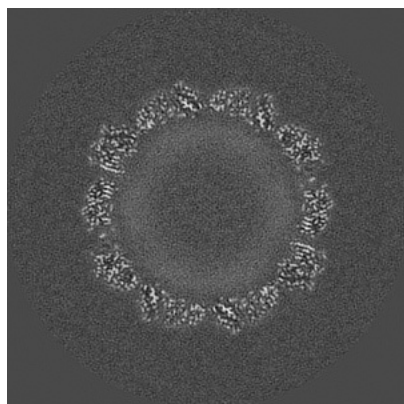


Z Index: 256

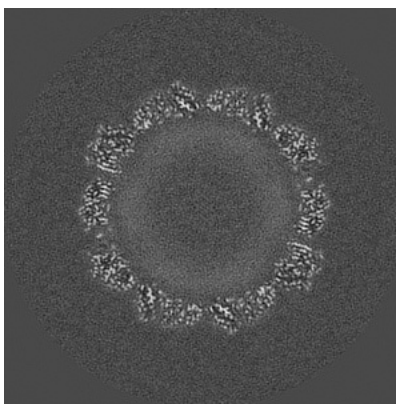
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

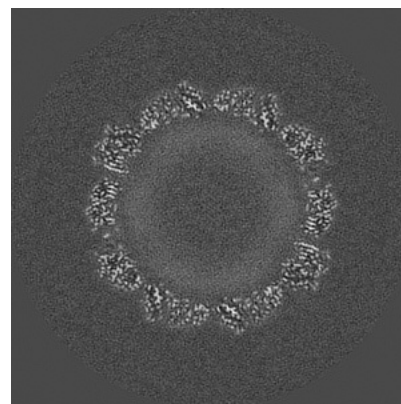
6.3.1 Primary map



X Index: 277



Y Index: 277

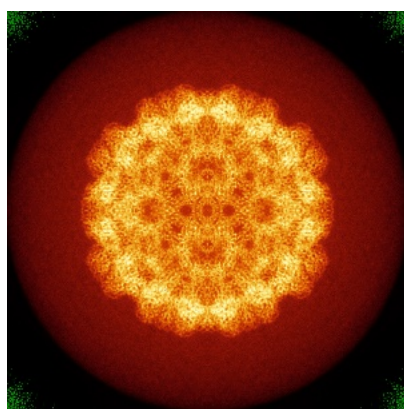


Z Index: 277

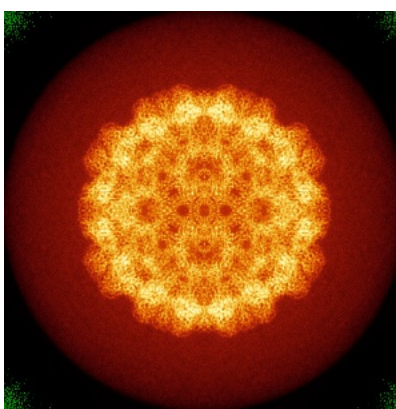
The images above show the largest variance slices of the map in three orthogonal directions.

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

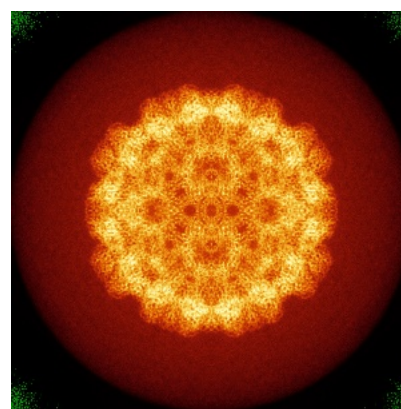
6.4.1 Primary map



X



Y



Z

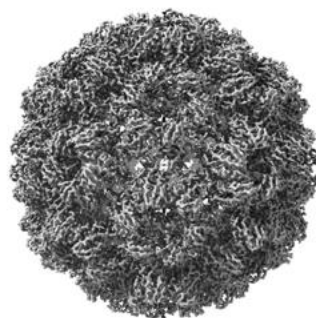
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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.

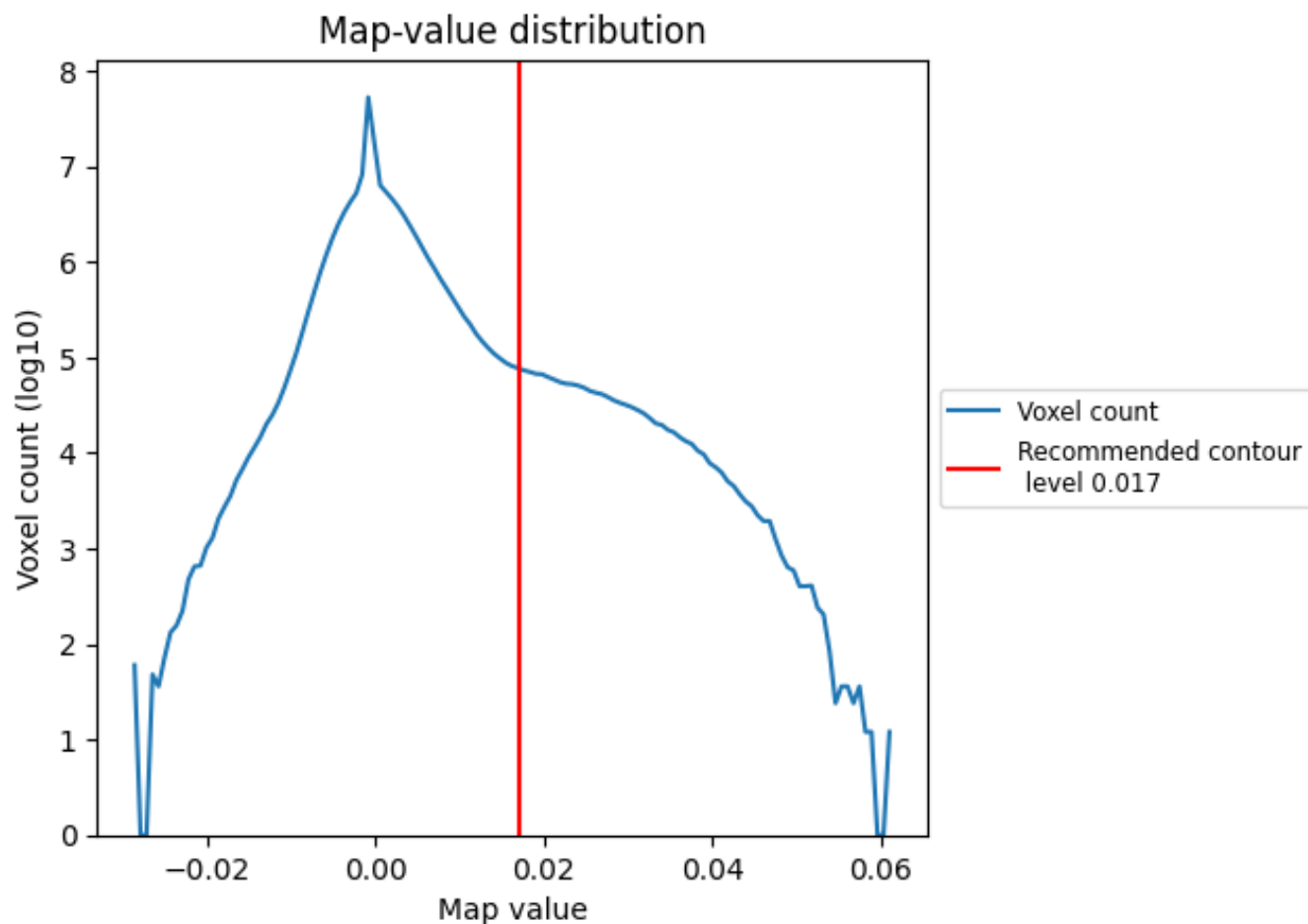
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

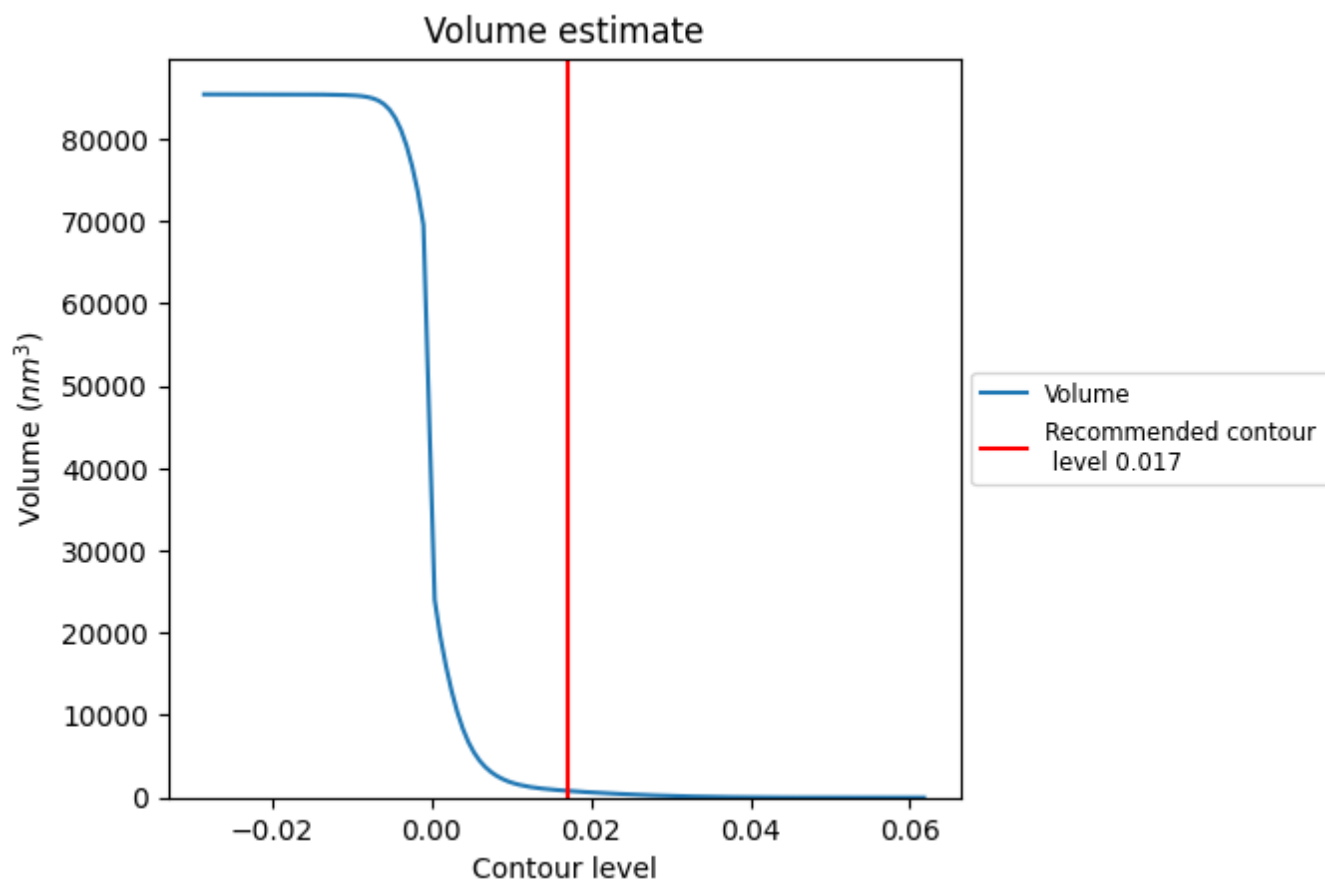
This section contains the results of statistical analysis of the map.

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.

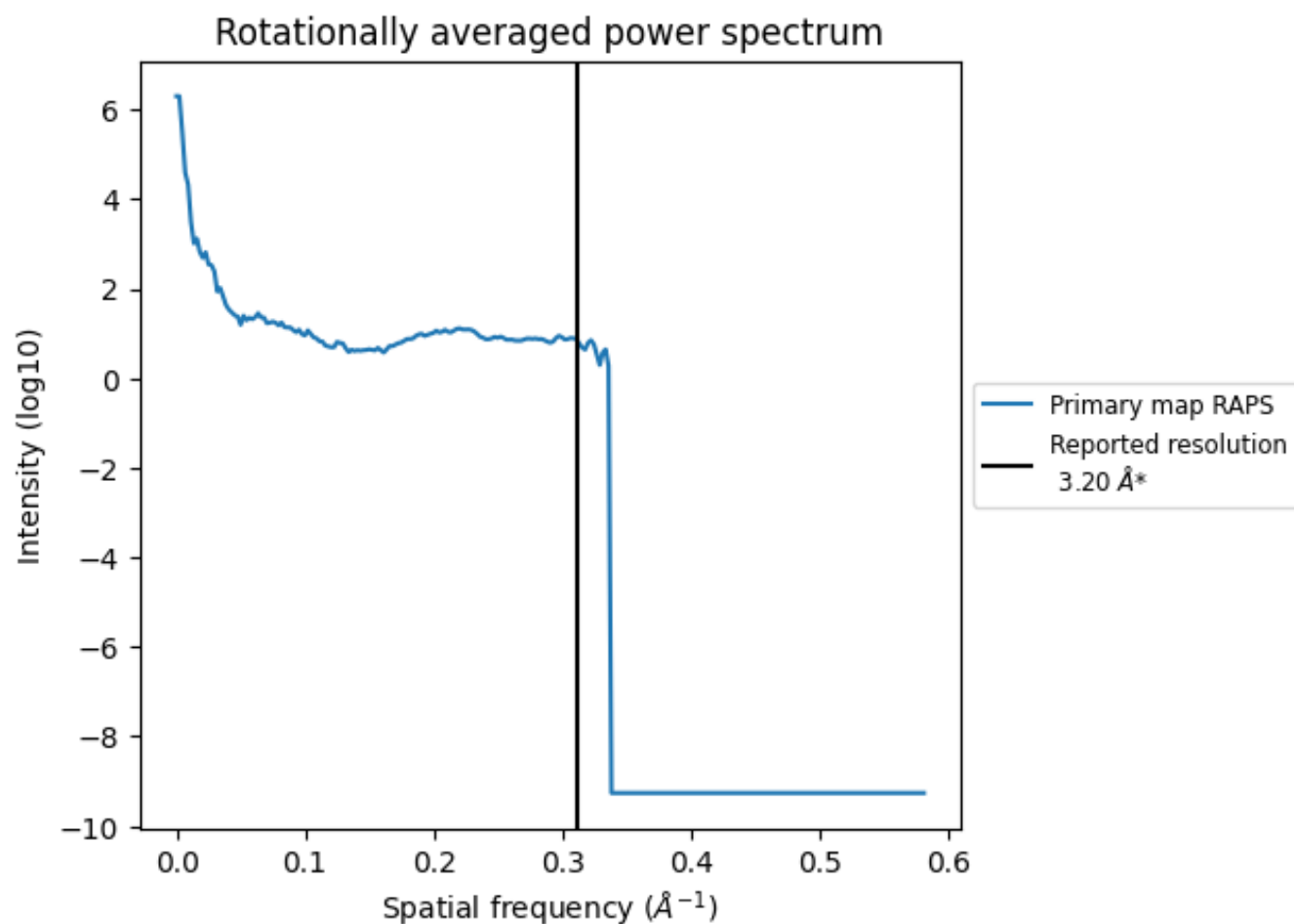
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 821 nm³; this corresponds to an approximate mass of 742 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 ⓘ

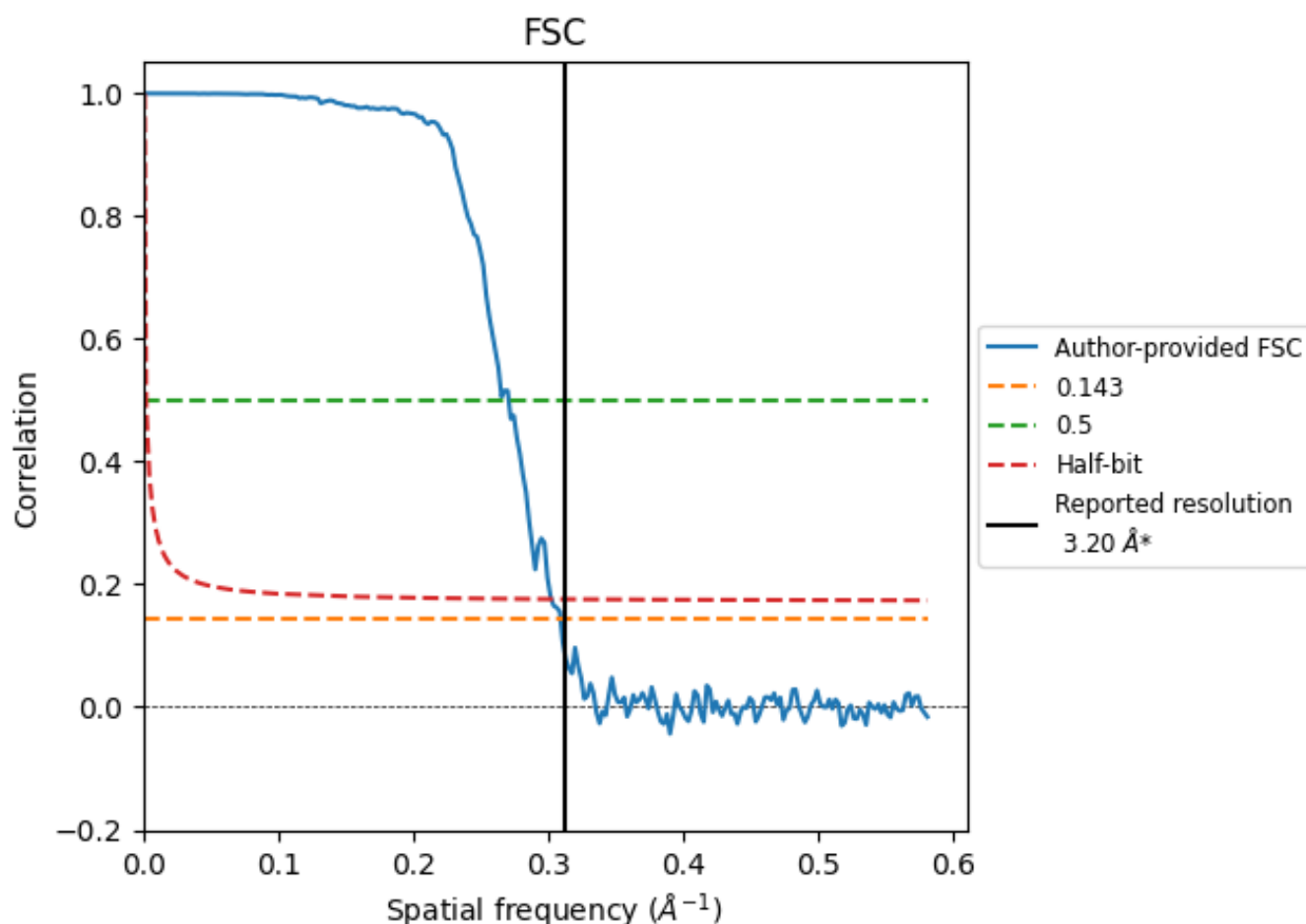


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

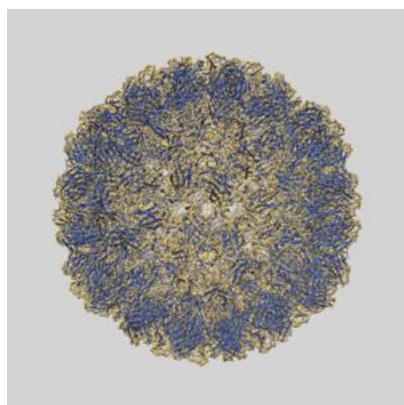
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.69	3.30
Unmasked-calculated*	-	-	-

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

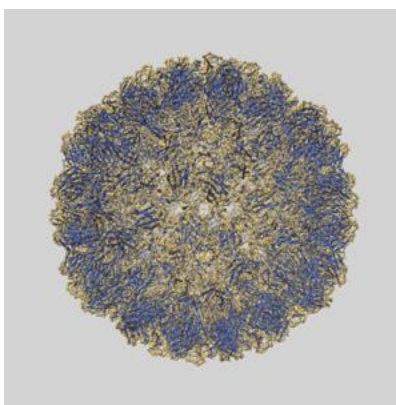
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13345 and PDB model 7PE2. Per-residue inclusion information can be found in section [3](#) on page [46](#).

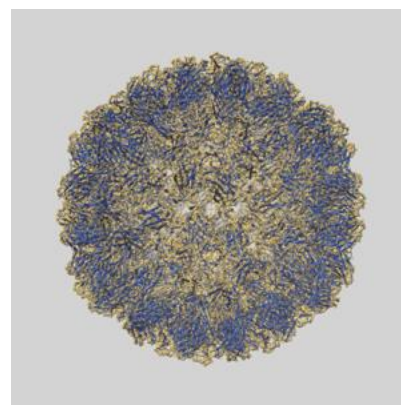
9.1 Map-model overlay [i](#)



X



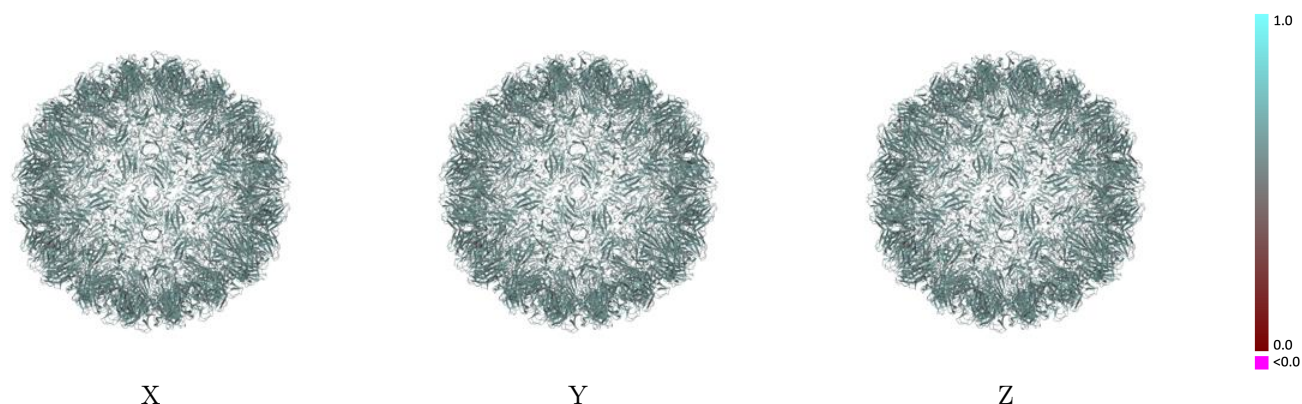
Y



Z

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](#)

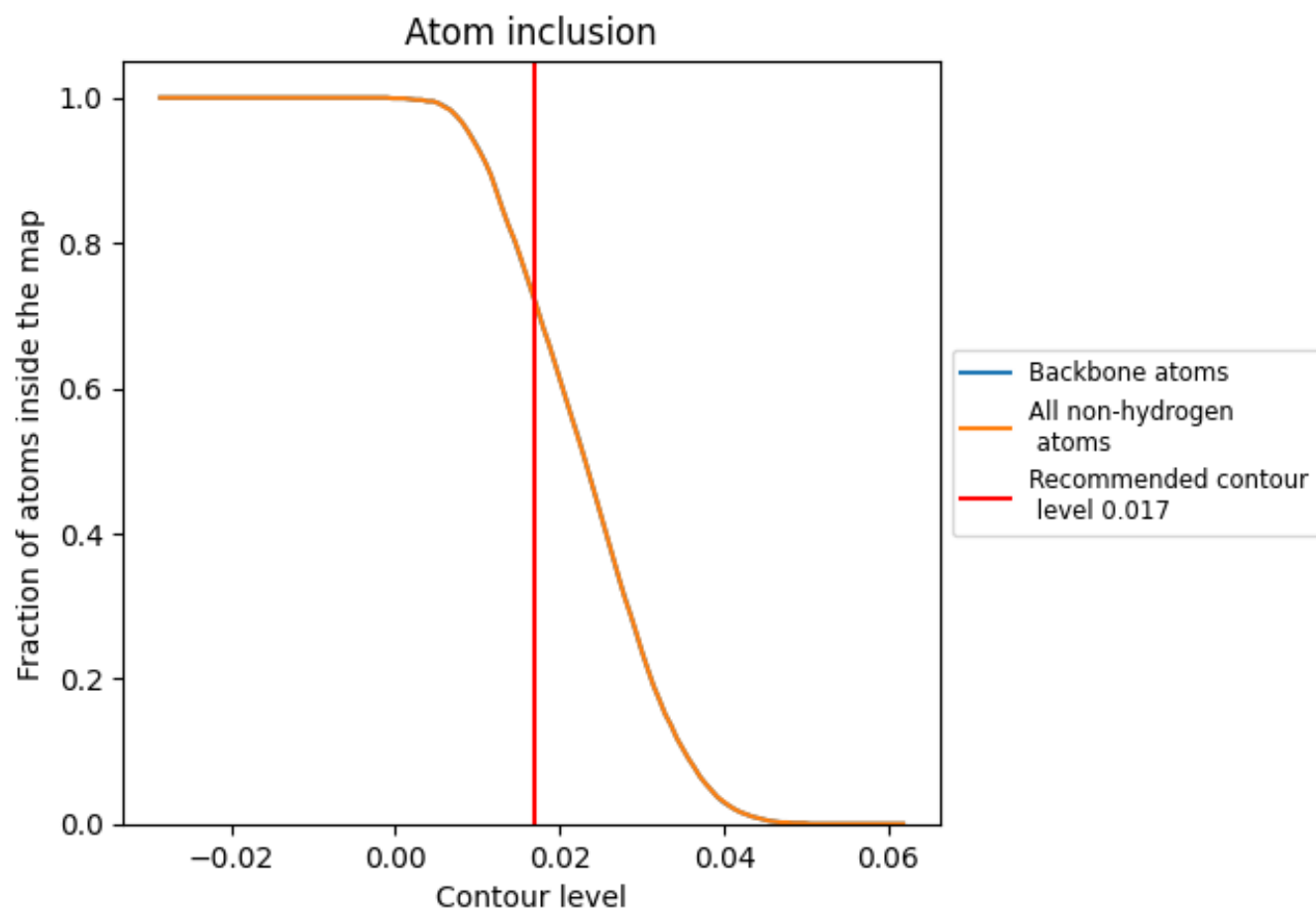


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 72% 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	 0.7200	 0.5900
A	 0.7220	 0.5920
AA	 0.7300	 0.5910
AB	 0.7180	 0.5900
AC	 0.7200	 0.5860
AD	 0.7410	 0.5930
AE	 0.7230	 0.5930
AF	 0.7170	 0.5880
B	 0.7420	 0.5920
BA	 0.7230	 0.5850
BB	 0.7330	 0.5930
BC	 0.7140	 0.5880
BD	 0.7220	 0.5870
BE	 0.7300	 0.5920
BF	 0.7180	 0.5920
C	 0.7200	 0.5860
CA	 0.7170	 0.5890
CB	 0.7190	 0.5840
CC	 0.7360	 0.5930
CD	 0.7220	 0.5900
CE	 0.7230	 0.5850
CF	 0.7330	 0.5930
D	 0.7140	 0.5900
DA	 0.7410	 0.5910
DB	 0.7230	 0.5900
DC	 0.7170	 0.5850
DD	 0.7420	 0.5940
DE	 0.7170	 0.5920
DF	 0.7190	 0.5870
E	 0.7360	 0.5930
EA	 0.7230	 0.5830
EB	 0.7300	 0.5930
EC	 0.7180	 0.5900
ED	 0.7200	 0.5870
EE	 0.7410	 0.5920



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Chain	Atom inclusion	Q-score
EF	 0.7230	 0.5900
F	 0.7170	 0.5860
FA	 0.7220	 0.5910
FB	 0.7230	 0.5850
FC	 0.7330	 0.5890
FD	 0.7140	 0.5910
FE	 0.7220	 0.5840
FF	 0.7300	 0.5920
G	 0.7180	 0.5910
GA	 0.7420	 0.5930
GB	 0.7170	 0.5920
GC	 0.7190	 0.5850
GD	 0.7360	 0.5910
GE	 0.7220	 0.5920
GF	 0.7230	 0.5860
H	 0.7330	 0.5920
HA	 0.7200	 0.5860
HB	 0.7410	 0.5910
HC	 0.7220	 0.5920
HD	 0.7170	 0.5880
HE	 0.7420	 0.5930
HF	 0.7170	 0.5930
I	 0.7190	 0.5850
IA	 0.7140	 0.5890
IB	 0.7220	 0.5850
IC	 0.7300	 0.5930
ID	 0.7180	 0.5900
IE	 0.7200	 0.5890
IF	 0.7410	 0.5930
J	 0.7220	 0.5920
JA	 0.7360	 0.5920
JB	 0.7220	 0.5920
JC	 0.7230	 0.5860
JD	 0.7330	 0.5900
JE	 0.7140	 0.5900
JF	 0.7230	 0.5840
K	 0.7300	 0.5940
KA	 0.7170	 0.5860
KB	 0.7420	 0.5910
KC	 0.7170	 0.5910
KD	 0.7190	 0.5850
KE	 0.7360	 0.5930

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Chain	Atom inclusion	Q-score
KF	 0.7220	 0.5930
L	 0.7230	 0.5860
LA	 0.7180	 0.5890
LB	 0.7200	 0.5880
LC	 0.7410	 0.5930
LD	 0.7220	 0.5910
LE	 0.7170	 0.5850
LF	 0.7420	 0.5920
M	 0.7170	 0.5920
MA	 0.7330	 0.5920
MB	 0.7140	 0.5910
MC	 0.7230	 0.5840
MD	 0.7300	 0.5940
ME	 0.7180	 0.5900
MF	 0.7200	 0.5880
N	 0.7410	 0.5910
NA	 0.7190	 0.5850
NB	 0.7360	 0.5930
NC	 0.7220	 0.5910
ND	 0.7230	 0.5820
NE	 0.7330	 0.5930
NF	 0.7140	 0.5900
O	 0.7230	 0.5860
OA	 0.7220	 0.5890
OB	 0.7170	 0.5860
OC	 0.7420	 0.5940
OD	 0.7170	 0.5910
OE	 0.7190	 0.5830
OF	 0.7360	 0.5920
P	 0.7220	 0.5910
PA	 0.7300	 0.5900
PB	 0.7180	 0.5900
PC	 0.7200	 0.5880
PD	 0.7410	 0.5940
PE	 0.7220	 0.5920
PF	 0.7170	 0.5850
Q	 0.7420	 0.5930
QA	 0.7230	 0.5850
QB	 0.7330	 0.5910
QC	 0.7140	 0.5890
QD	 0.7220	 0.5870
QE	 0.7300	 0.5940

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Chain	Atom inclusion	Q-score
QF	 0.7180	 0.5920
R	 0.7200	 0.5850
RA	 0.7170	 0.5910
RB	 0.7190	 0.5860
RC	 0.7360	 0.5890
RD	 0.7220	 0.5920
RE	 0.7230	 0.5850
RF	 0.7330	 0.5940
S	 0.7140	 0.5890
SA	 0.7410	 0.5930
SB	 0.7230	 0.5890
SC	 0.7180	 0.5860
SD	 0.7420	 0.5940
SE	 0.7170	 0.5930
SF	 0.7190	 0.5850
T	 0.7360	 0.5920
TA	 0.7220	 0.5850
TB	 0.7300	 0.5920
TC	 0.7180	 0.5890
TD	 0.7200	 0.5850
TE	 0.7410	 0.5930
TF	 0.7220	 0.5920
UA	 0.7220	 0.5910
UB	 0.7230	 0.5840
UC	 0.7330	 0.5900
UD	 0.7140	 0.5910
UE	 0.7220	 0.5850
UF	 0.7300	 0.5930
V	 0.7170	 0.5850
VA	 0.7420	 0.5930
VB	 0.7170	 0.5930
VC	 0.7190	 0.5830
VD	 0.7360	 0.5920
VE	 0.7220	 0.5940
VF	 0.7230	 0.5880
W	 0.7180	 0.5880
WA	 0.7200	 0.5870
WB	 0.7410	 0.5940
WC	 0.7230	 0.5920
WD	 0.7180	 0.5850
WE	 0.7420	 0.5950
WF	 0.7170	 0.5920

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Chain	Atom inclusion	Q-score
X	 0.7330	 0.5920
XA	 0.7140	 0.5900
XB	 0.7230	 0.5850
XC	 0.7300	 0.5930
XD	 0.7180	 0.5900
XE	 0.7200	 0.5860
XF	 0.7410	 0.5940
Y	 0.7190	 0.5840
YA	 0.7360	 0.5920
YB	 0.7220	 0.5930
YC	 0.7230	 0.5830
YD	 0.7330	 0.5910
YE	 0.7140	 0.5920
YF	 0.7230	 0.5860
Z	 0.7230	 0.5880
ZA	 0.7180	 0.5850
ZB	 0.7420	 0.5930
ZC	 0.7170	 0.5920
ZD	 0.7190	 0.5850
ZE	 0.7360	 0.5920