



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 11:04 PM UTC

PDB ID : 6ZW7 / pdb_00006zw7
EMDB ID : EMD-11483
Title : C17 symmetry: Bacterial Vipp1 and PspA are members of the ancient ESCRT-III membrane-remodeling superfamily.
Authors : Liu, J.; Tassinari, M.; Souza, D.P.; Naskar, S.; Noel, J.K.; Bohuszewicz, O.; Buck, M.; Williams, T.A.; Baum, B.; Low, H.H.
Deposited on : 2020-07-27
Resolution : 9.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

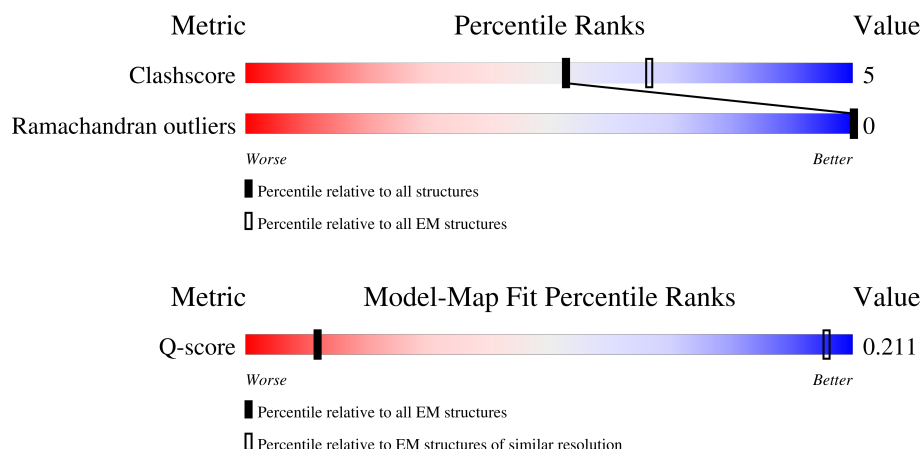
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 9.40 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	-
Q-score	-	25397	224 (8.90 - 9.90)

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	258	
1	AA	258	
1	AB	258	
1	AC	258	
1	AD	258	

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Mol	Chain	Length	Quality of chain
1	B	258	
1	BA	258	
1	BB	258	
1	BC	258	
1	BD	258	
1	C	258	
1	CA	258	
1	CB	258	
1	CC	258	
1	CD	258	
1	D	258	
1	DA	258	
1	DB	258	
1	DC	258	
1	DD	258	
1	E	258	
1	EA	258	
1	EB	258	
1	EC	258	
1	ED	258	
1	F	258	
1	FA	258	
1	FB	258	
1	FC	258	
1	FD	258	

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Mol	Chain	Length	Quality of chain
1	G	258	
1	GA	258	
1	GB	258	
1	GC	258	
1	GD	258	
1	H	258	
1	HA	258	
1	HB	258	
1	HC	258	
1	HD	258	
1	I	258	
1	IA	258	
1	IB	258	
1	IC	258	
1	ID	258	
1	J	258	
1	JA	258	
1	JB	258	
1	JC	258	
1	JD	258	
1	K	258	
1	KA	258	
1	KB	258	
1	KC	258	
1	KD	258	

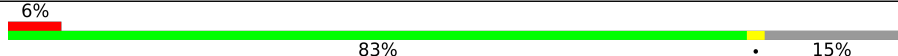
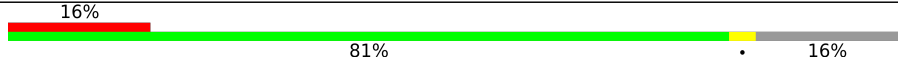
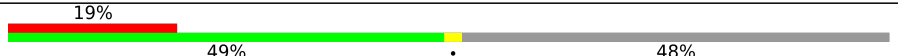
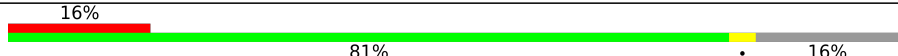
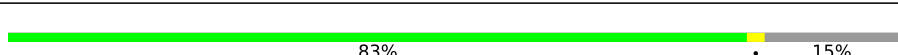
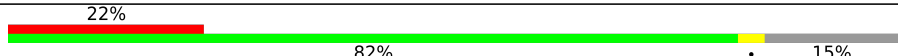
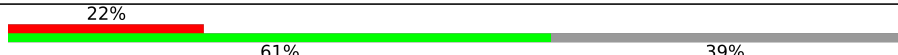
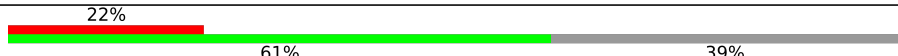
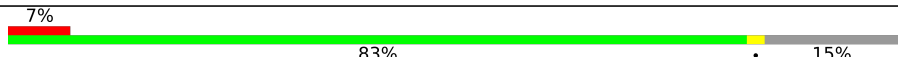
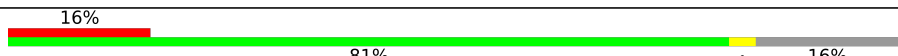
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Mol	Chain	Length	Quality of chain
1	L	258	
1	LA	258	
1	LB	258	
1	LC	258	
1	LD	258	
1	M	258	
1	MA	258	
1	MB	258	
1	MC	258	
1	MD	258	
1	N	258	
1	NA	258	
1	NB	258	
1	NC	258	
1	ND	258	
1	O	258	
1	OA	258	
1	OB	258	
1	OC	258	
1	OD	258	
1	P	258	
1	PA	258	
1	PB	258	
1	PC	258	
1	PD	258	

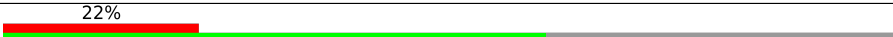
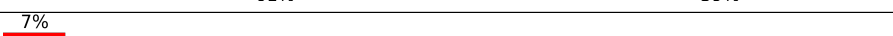
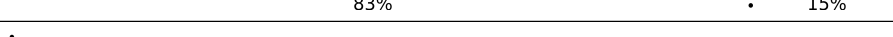
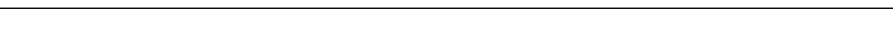
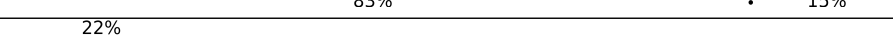
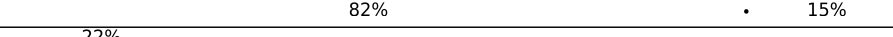
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Mol	Chain	Length	Quality of chain
1	Q	258	
1	QA	258	
1	QB	258	
1	QC	258	
1	R	258	
1	RA	258	
1	RB	258	
1	RC	258	
1	S	258	
1	SA	258	
1	SB	258	
1	SC	258	
1	T	258	
1	TA	258	
1	TB	258	
1	TC	258	
1	UA	258	
1	UB	258	
1	UC	258	
1	V	258	
1	VA	258	
1	VB	258	
1	VC	258	
1	W	258	
1	WA	258	

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Mol	Chain	Length	Quality of chain
1	WB	258	
1	WC	258	
1	X	258	
1	XA	258	
1	XB	258	
1	XC	258	
1	Y	258	
1	YA	258	
1	YB	258	
1	YC	258	
1	Z	258	
1	ZA	258	
1	ZB	258	
1	ZC	258	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 116807 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 vipp1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	133	Total 661	C 395	N 133	O 133	0	0
1	B	219	Total 1086	C 648	N 219	O 219	0	0
1	C	219	Total 1086	C 648	N 219	O 219	0	0
1	D	219	Total 1086	C 648	N 219	O 219	0	0
1	E	219	Total 1086	C 648	N 219	O 219	0	0
1	F	218	Total 1081	C 645	N 218	O 218	0	0
1	G	158	Total 785	C 469	N 158	O 158	0	0
1	H	133	Total 661	C 395	N 133	O 133	0	0
1	I	219	Total 1086	C 648	N 219	O 219	0	0
1	J	219	Total 1086	C 648	N 219	O 219	0	0
1	K	219	Total 1086	C 648	N 219	O 219	0	0
1	L	219	Total 1086	C 648	N 219	O 219	0	0
1	M	218	Total 1081	C 645	N 218	O 218	0	0
1	N	158	Total 785	C 469	N 158	O 158	0	0
1	O	133	Total 661	C 395	N 133	O 133	0	0
1	P	219	Total 1086	C 648	N 219	O 219	0	0
1	Q	219	Total 1086	C 648	N 219	O 219	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	R	219	Total 1086	C 648	N 219	O 219	0	0
1	S	219	Total 1086	C 648	N 219	O 219	0	0
1	T	218	Total 1081	C 645	N 218	O 218	0	0
1	V	158	Total 785	C 469	N 158	O 158	0	0
1	W	133	Total 661	C 395	N 133	O 133	0	0
1	X	219	Total 1086	C 648	N 219	O 219	0	0
1	Y	219	Total 1086	C 648	N 219	O 219	0	0
1	Z	219	Total 1086	C 648	N 219	O 219	0	0
1	AA	219	Total 1086	C 648	N 219	O 219	0	0
1	BA	218	Total 1081	C 645	N 218	O 218	0	0
1	CA	158	Total 785	C 469	N 158	O 158	0	0
1	DA	133	Total 661	C 395	N 133	O 133	0	0
1	EA	219	Total 1086	C 648	N 219	O 219	0	0
1	FA	219	Total 1086	C 648	N 219	O 219	0	0
1	GA	219	Total 1086	C 648	N 219	O 219	0	0
1	HA	219	Total 1086	C 648	N 219	O 219	0	0
1	IA	218	Total 1081	C 645	N 218	O 218	0	0
1	JA	158	Total 785	C 469	N 158	O 158	0	0
1	KA	133	Total 661	C 395	N 133	O 133	0	0
1	LA	219	Total 1086	C 648	N 219	O 219	0	0
1	MA	219	Total 1086	C 648	N 219	O 219	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	NA	219	Total 1086	C 648	N 219	O 219	0	0
1	OA	219	Total 1086	C 648	N 219	O 219	0	0
1	PA	218	Total 1081	C 645	N 218	O 218	0	0
1	QA	158	Total 785	C 469	N 158	O 158	0	0
1	RA	133	Total 661	C 395	N 133	O 133	0	0
1	SA	219	Total 1086	C 648	N 219	O 219	0	0
1	TA	219	Total 1086	C 648	N 219	O 219	0	0
1	UA	219	Total 1086	C 648	N 219	O 219	0	0
1	VA	219	Total 1086	C 648	N 219	O 219	0	0
1	WA	218	Total 1081	C 645	N 218	O 218	0	0
1	XA	158	Total 785	C 469	N 158	O 158	0	0
1	YA	133	Total 661	C 395	N 133	O 133	0	0
1	ZA	219	Total 1086	C 648	N 219	O 219	0	0
1	AB	219	Total 1086	C 648	N 219	O 219	0	0
1	BB	219	Total 1086	C 648	N 219	O 219	0	0
1	CB	219	Total 1086	C 648	N 219	O 219	0	0
1	DB	218	Total 1081	C 645	N 218	O 218	0	0
1	EB	158	Total 785	C 469	N 158	O 158	0	0
1	FB	133	Total 661	C 395	N 133	O 133	0	0
1	GB	219	Total 1086	C 648	N 219	O 219	0	0
1	HB	219	Total 1086	C 648	N 219	O 219	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	IB	219	Total 1086	C 648	N 219	O 219	0	0
1	JB	219	Total 1086	C 648	N 219	O 219	0	0
1	KB	218	Total 1081	C 645	N 218	O 218	0	0
1	LB	158	Total 785	C 469	N 158	O 158	0	0
1	MB	133	Total 661	C 395	N 133	O 133	0	0
1	NB	219	Total 1086	C 648	N 219	O 219	0	0
1	OB	219	Total 1086	C 648	N 219	O 219	0	0
1	PB	219	Total 1086	C 648	N 219	O 219	0	0
1	QB	219	Total 1086	C 648	N 219	O 219	0	0
1	RB	218	Total 1081	C 645	N 218	O 218	0	0
1	SB	158	Total 785	C 469	N 158	O 158	0	0
1	TB	133	Total 661	C 395	N 133	O 133	0	0
1	UB	219	Total 1086	C 648	N 219	O 219	0	0
1	VB	219	Total 1086	C 648	N 219	O 219	0	0
1	WB	219	Total 1086	C 648	N 219	O 219	0	0
1	XB	219	Total 1086	C 648	N 219	O 219	0	0
1	YB	218	Total 1081	C 645	N 218	O 218	0	0
1	ZB	158	Total 785	C 469	N 158	O 158	0	0
1	AC	133	Total 661	C 395	N 133	O 133	0	0
1	BC	219	Total 1086	C 648	N 219	O 219	0	0
1	CC	219	Total 1086	C 648	N 219	O 219	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	DC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	EC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	FC	218	Total	C	N	O	0	0
			1081	645	218	218		
1	GC	158	Total	C	N	O	0	0
			785	469	158	158		
1	HC	133	Total	C	N	O	0	0
			661	395	133	133		
1	IC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	JC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	KC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	LC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	MC	218	Total	C	N	O	0	0
			1081	645	218	218		
1	NC	158	Total	C	N	O	0	0
			785	469	158	158		
1	OC	133	Total	C	N	O	0	0
			661	395	133	133		
1	PC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	QC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	RC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	SC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	TC	218	Total	C	N	O	0	0
			1081	645	218	218		
1	UC	158	Total	C	N	O	0	0
			785	469	158	158		
1	VC	133	Total	C	N	O	0	0
			661	395	133	133		
1	WC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	XC	219	Total	C	N	O	0	0
			1086	648	219	219		

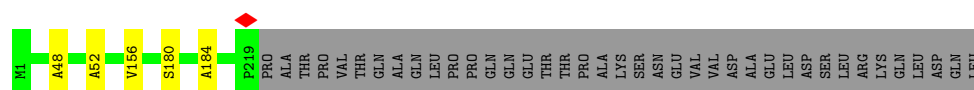
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Mol	Chain	Residues	Atoms				AltConf	Trace
1	YC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	ZC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	AD	218	Total	C	N	O	0	0
			1081	645	218	218		
1	BD	158	Total	C	N	O	0	0
			785	469	158	158		
1	CD	133	Total	C	N	O	0	0
			661	395	133	133		
1	DD	219	Total	C	N	O	0	0
			1086	648	219	219		
1	ED	219	Total	C	N	O	0	0
			1086	648	219	219		
1	FD	219	Total	C	N	O	0	0
			1086	648	219	219		
1	GD	219	Total	C	N	O	0	0
			1086	648	219	219		
1	HD	218	Total	C	N	O	0	0
			1081	645	218	218		
1	ID	158	Total	C	N	O	0	0
			785	469	158	158		
1	JD	133	Total	C	N	O	0	0
			661	395	133	133		
1	KD	219	Total	C	N	O	0	0
			1086	648	219	219		
1	LD	219	Total	C	N	O	0	0
			1086	648	219	219		
1	MD	219	Total	C	N	O	0	0
			1086	648	219	219		
1	ND	219	Total	C	N	O	0	0
			1086	648	219	219		
1	OD	218	Total	C	N	O	0	0
			1081	645	218	218		
1	PD	158	Total	C	N	O	0	0
			785	469	158	158		

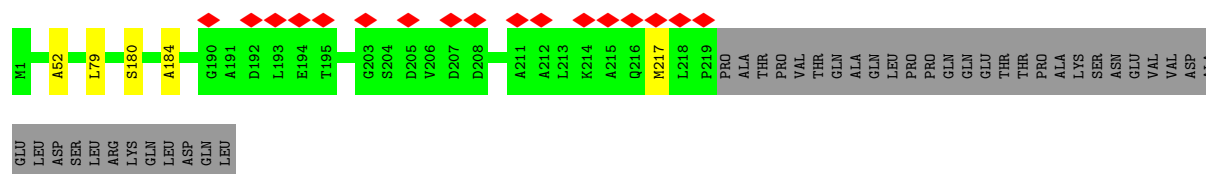
- Molecule 1: vippl

Chain D:  83% 15%



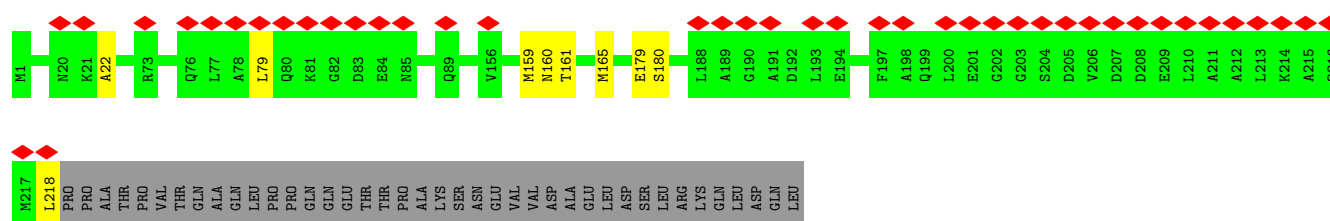
- Molecule 1: vippl

Chain E:  7% 83% 15%



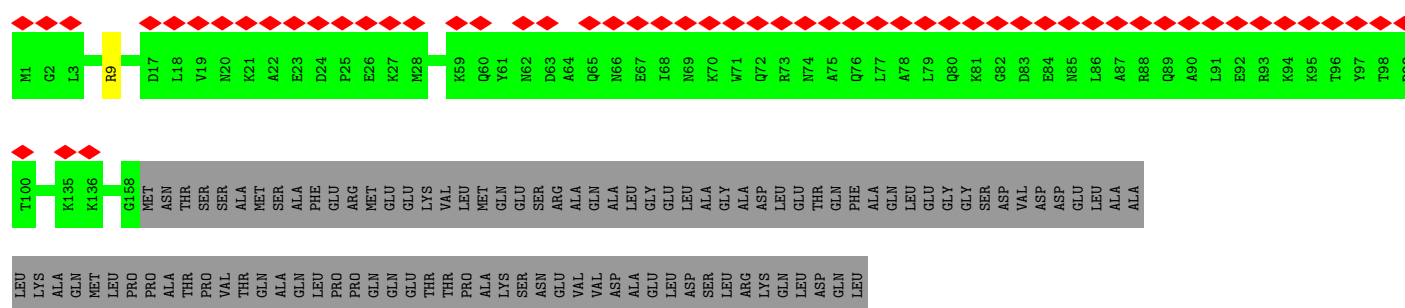
- Molecule 1: vippl

Chain F:  16% 81% 16%



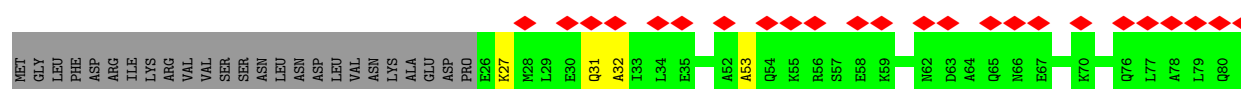
- Molecule 1: vippl

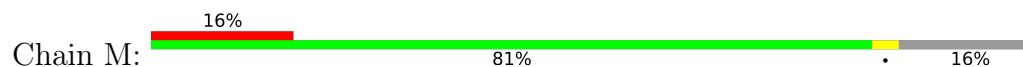
Chain G:  22% 61% 39%

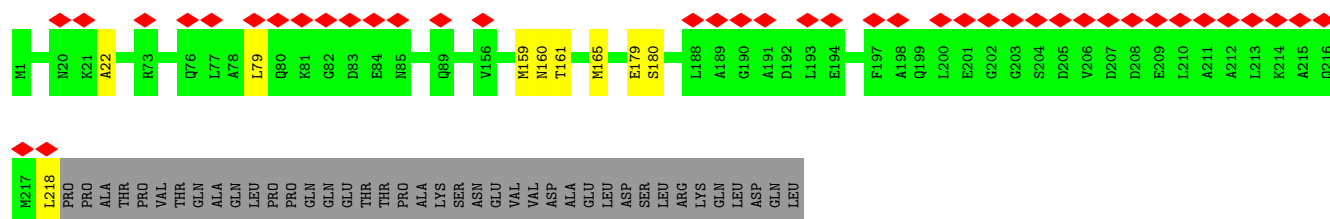


- Molecule 1: vippl

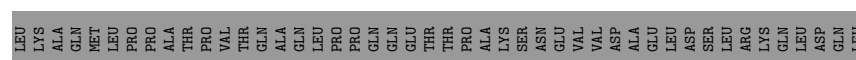
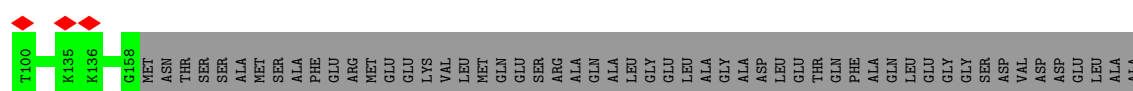
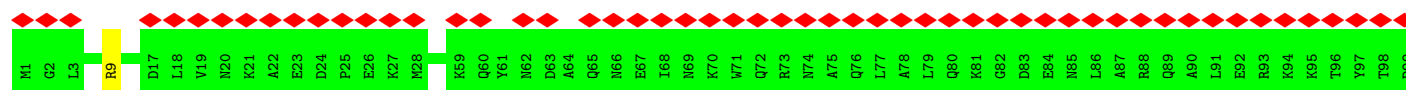
Chain H:  19% 49% 48%



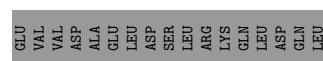
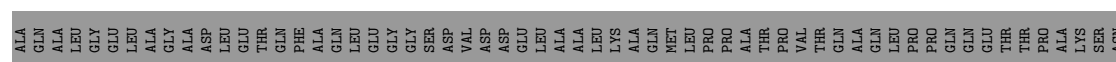
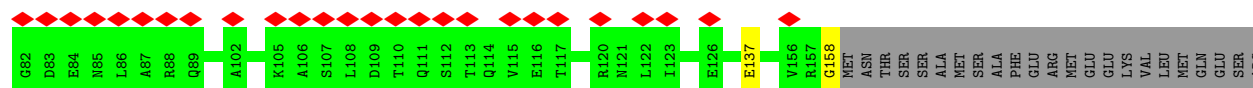
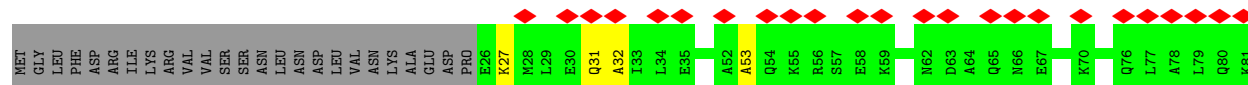




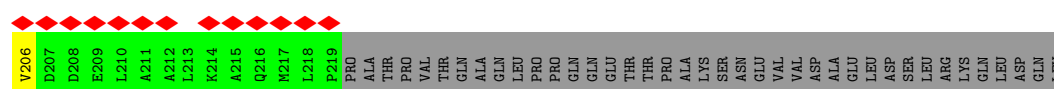
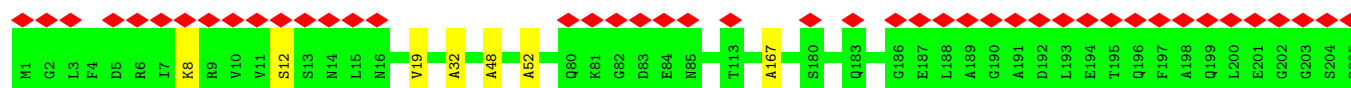
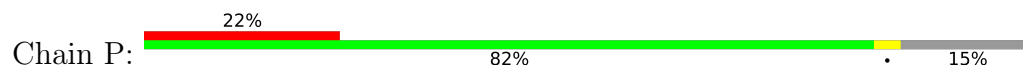
- Molecule 1: vipp1



- Molecule 1: vipp1

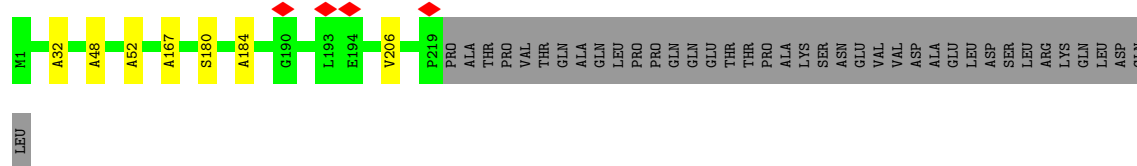


- Molecule 1: vipp1



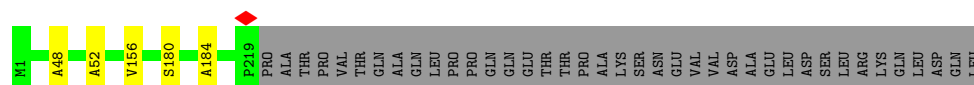
- Molecule 1: vipp1

Chain Q:  82% 15%



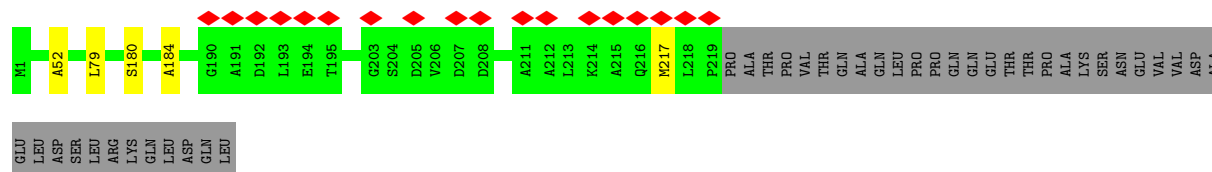
• Molecule 1: vipp1

Chain R:  83% 15%



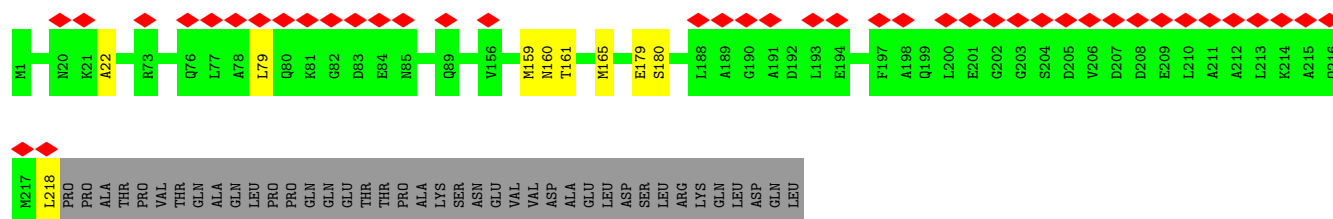
• Molecule 1: vipp1

Chain S:  7% 83% 15%



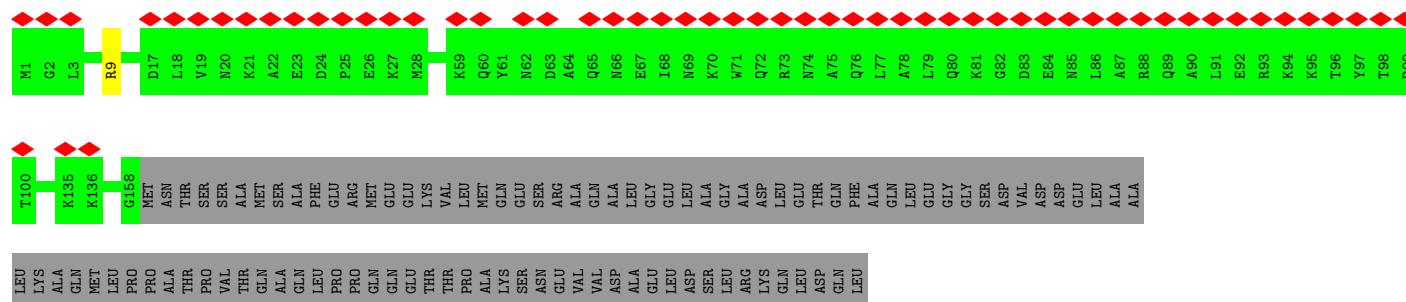
• Molecule 1: vipp1

Chain T:  16% 81% 16%

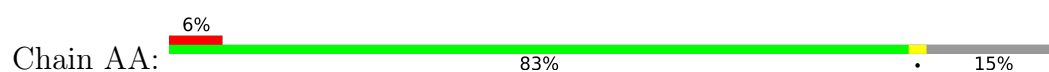
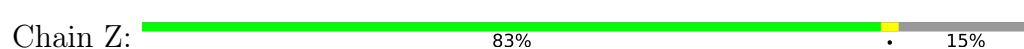
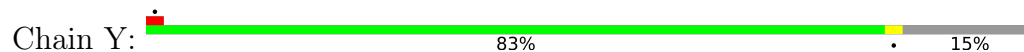
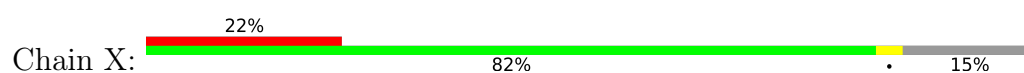


• Molecule 1: vipp1

Chain V:  22% 61% 39%



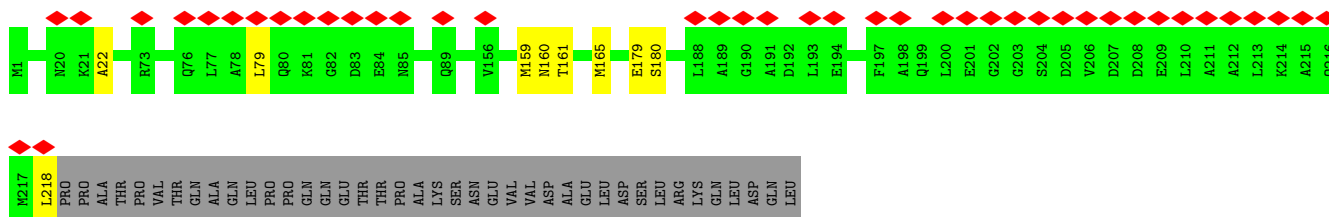
Chain W:



ASP
SER
LEU
LEU
ARG
LYS
GLN
LEU
ASP
GLN
LEU

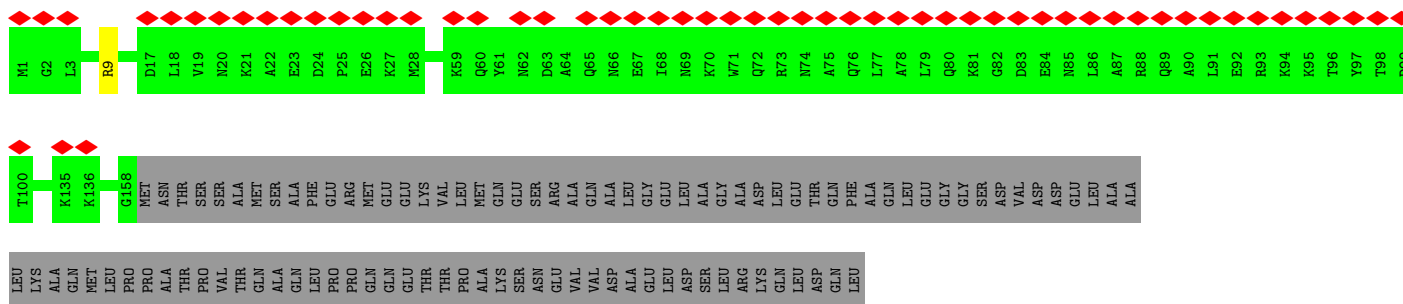
• Molecule 1: vipp1

Chain BA: 16% 81% 16%



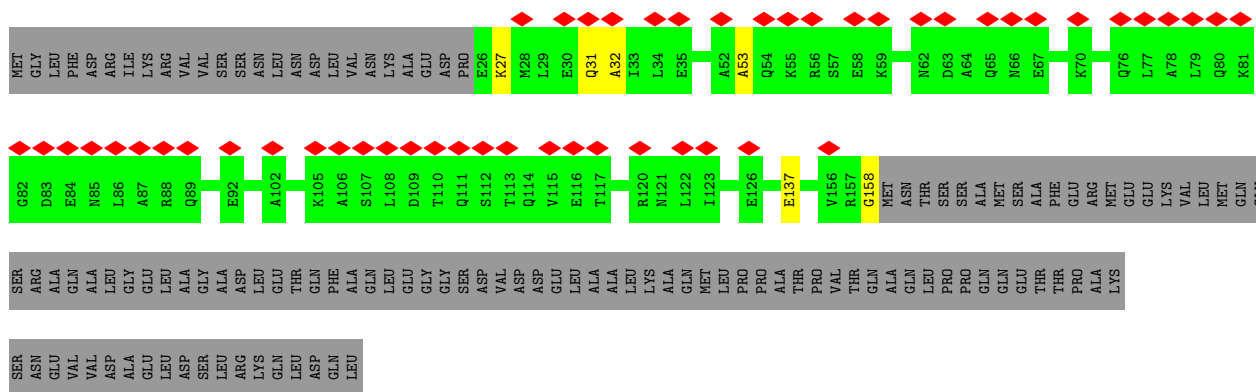
• Molecule 1: vipp1

Chain CA: 22% 61% 39%



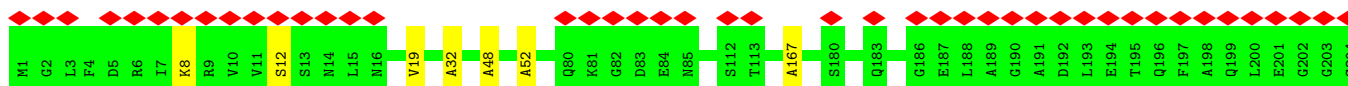
• Molecule 1: vipp1

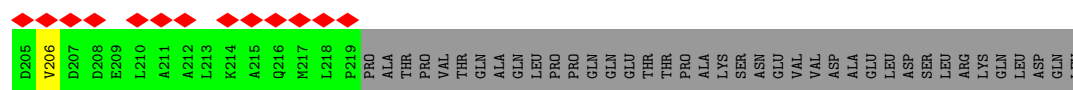
Chain DA: 20% 49% 48%



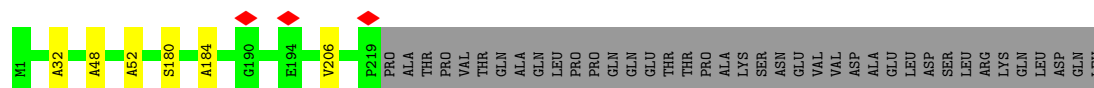
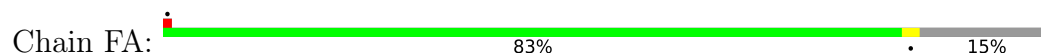
• Molecule 1: vipp1

Chain EA: 22% 82% 15%

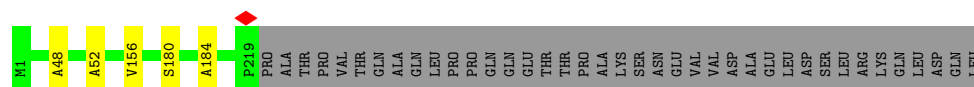
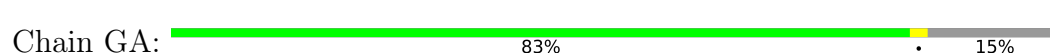




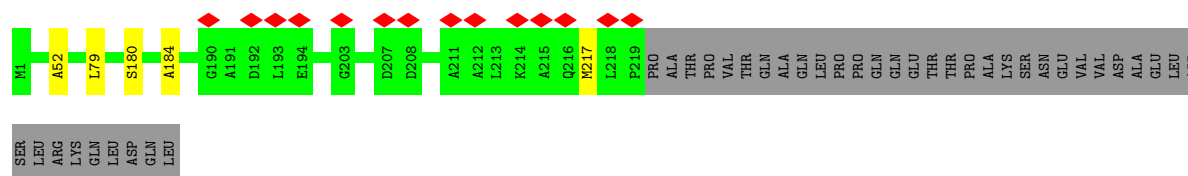
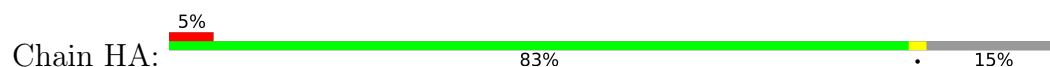
- Molecule 1: vipp1



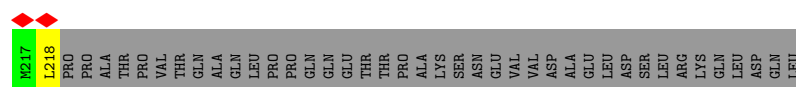
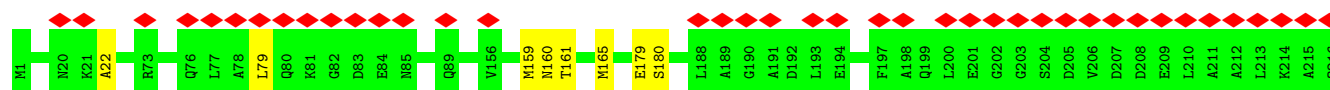
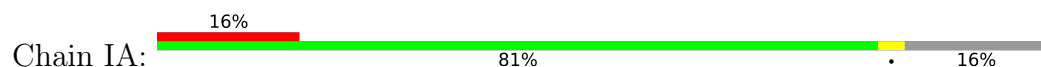
- Molecule 1: vipp1



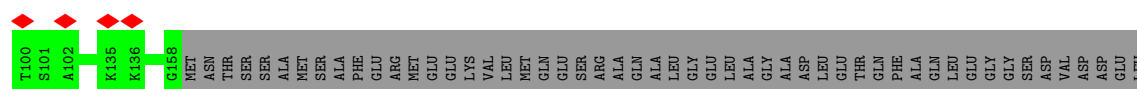
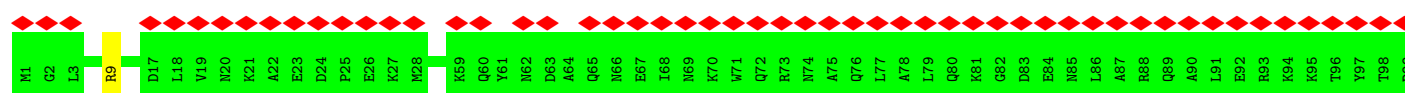
- Molecule 1: vipp1



- Molecule 1: vipp1



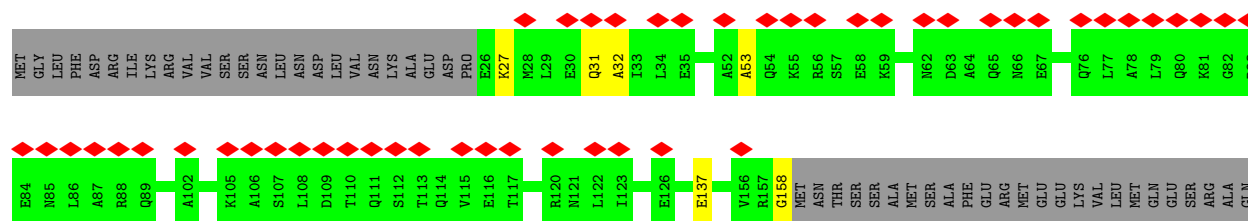
- Molecule 1: vipp1



ALA
ALA
LEU
LEU
LYS
PHE
LEU
ASP
ARG
GLN
MET
LEU
PRO
PRO
PRO
ALA
THR
PRO
VAL
THR
GLN
ALA
GLN
LEU
LEU
PRO
PRO
GLN
GLN
GLU
GLU
THR
THR
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PRO
ALA
LYS
SER
SER
ASN
GLU
VAL
VAL
ASP
ALA
GLU
LEU
ASP
SER
LEU
LEU
ARG
LYS
GLN
LEU
ASP
GLN
LEU

• Molecule 1: vipp1

Chain KA: 19% 49% 48%

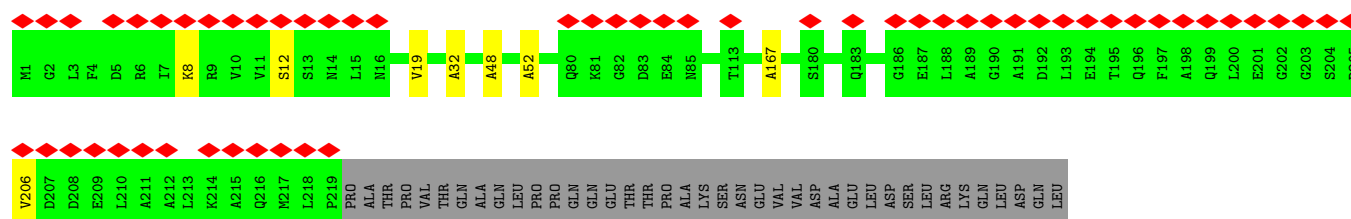


ALA
LEU
GLY
GLU
LEU
LEU
ALA
GLY
ALA
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LEU
LEU
THR
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PHE
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GLY
GLY
SER
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LEU
PRO
PRO
GLN
GLN
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GLN
LEU

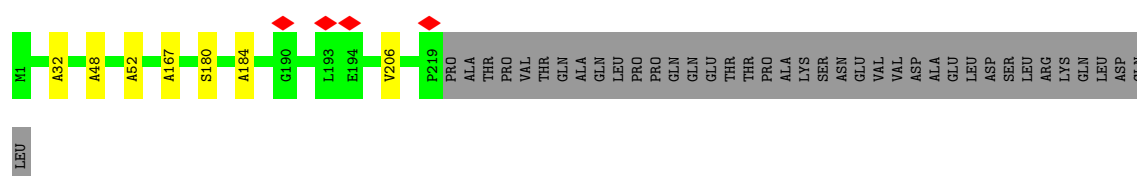
• Molecule 1: vipp1

Chain LA: 22% 82% 15%



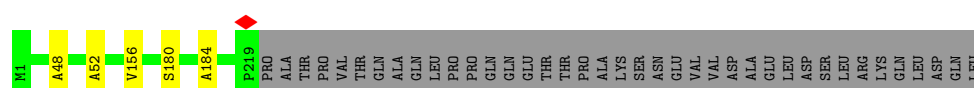
• Molecule 1: vipp1

Chain MA: 82% 15%



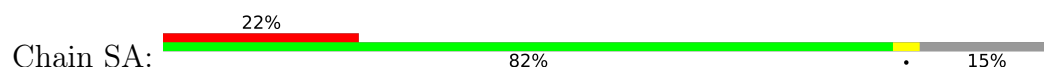
• Molecule 1: vipp1

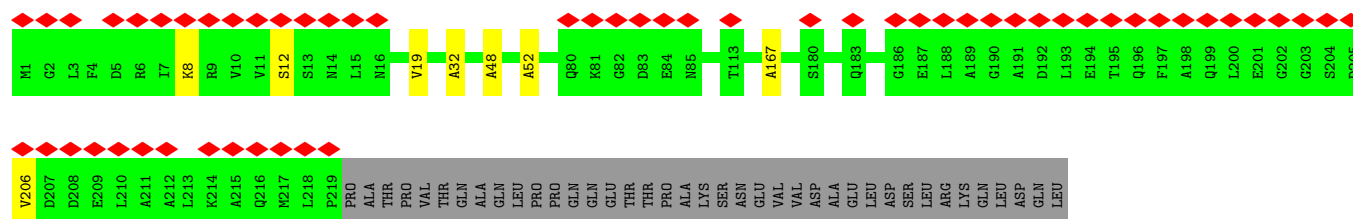
Chain NA: 83% 15%



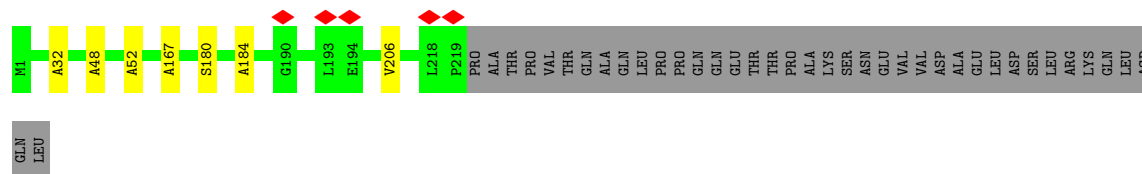
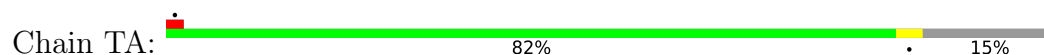
• Molecule 1: vipp1

Chain OA: 7% 83% 15%

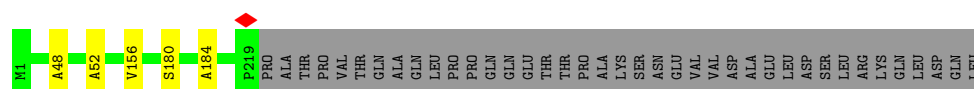
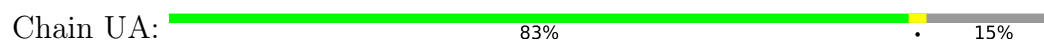




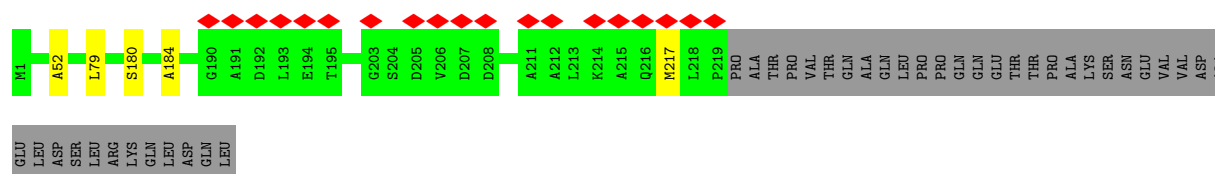
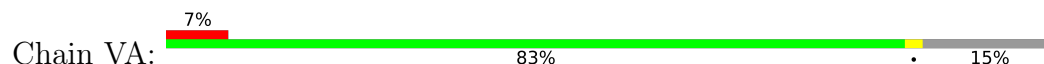
- Molecule 1: vipp1



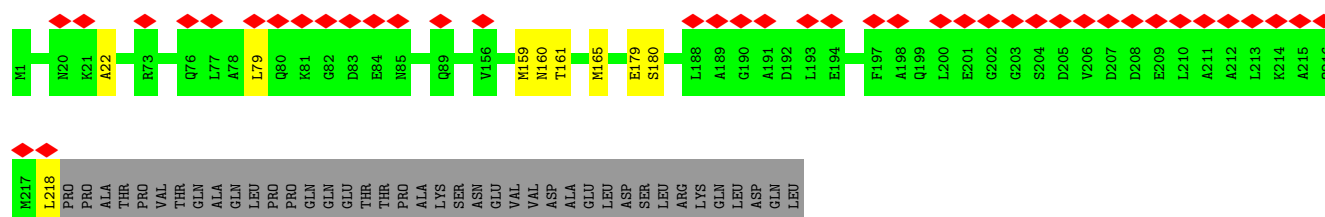
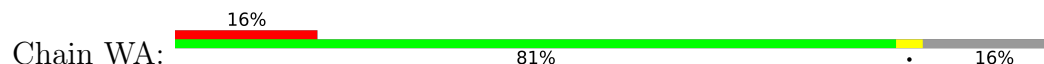
- Molecule 1: vipp1



- Molecule 1: vipp1

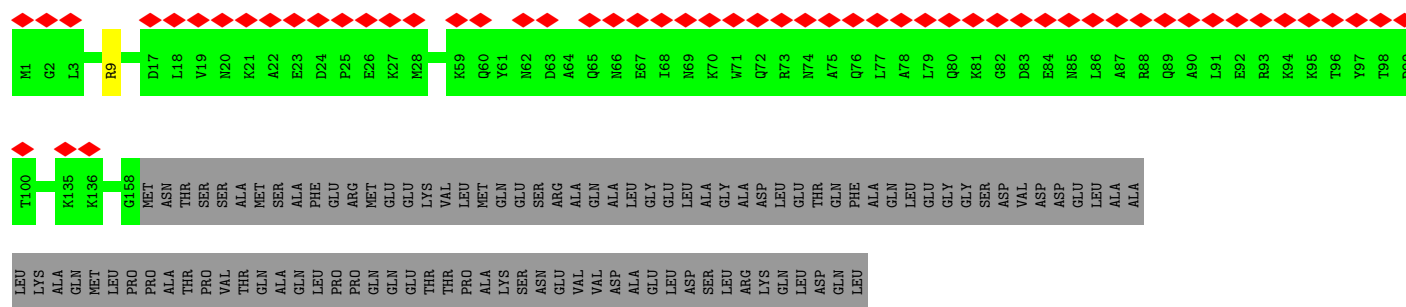


- Molecule 1: vipp1

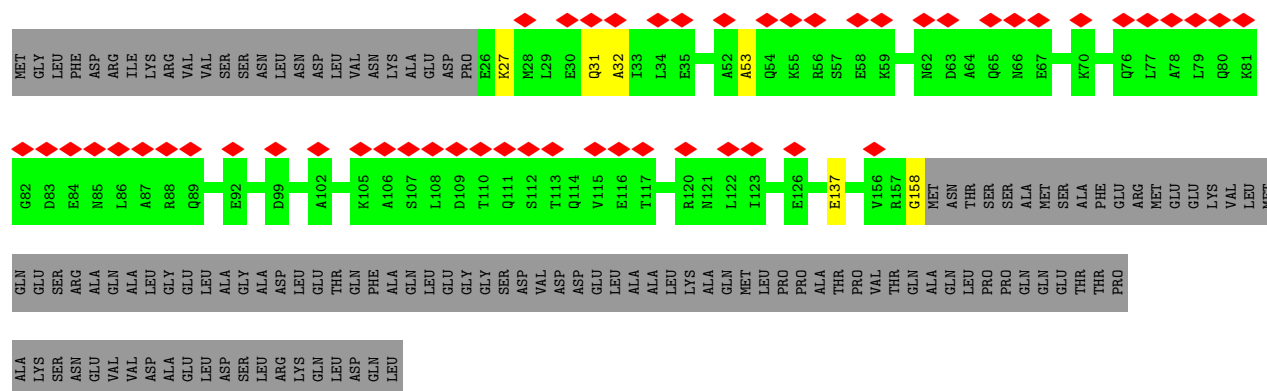


- Molecule 1: vipp1

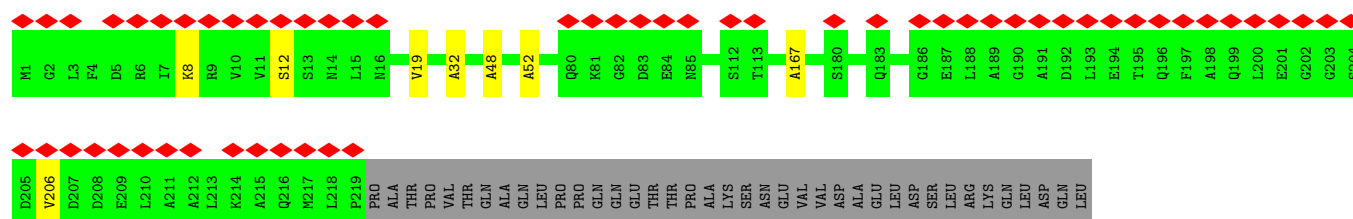
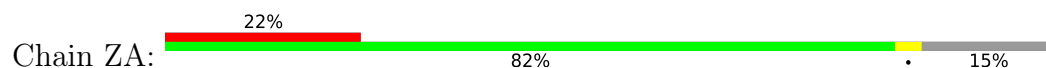




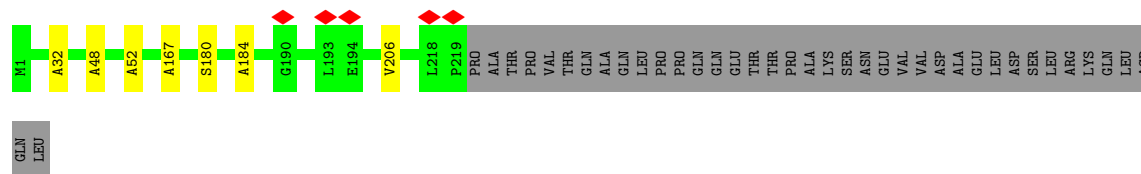
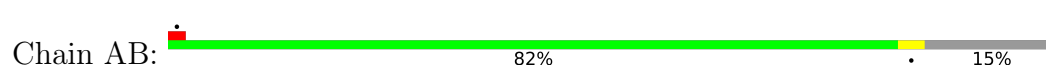
- Molecule 1: vippp1



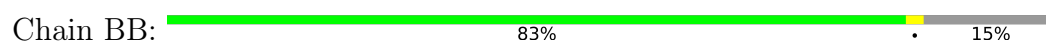
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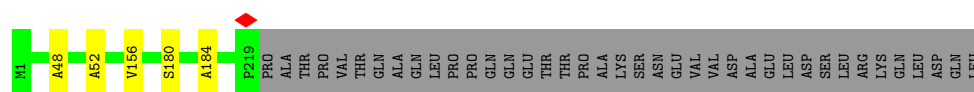


- Molecule 1: vippp1

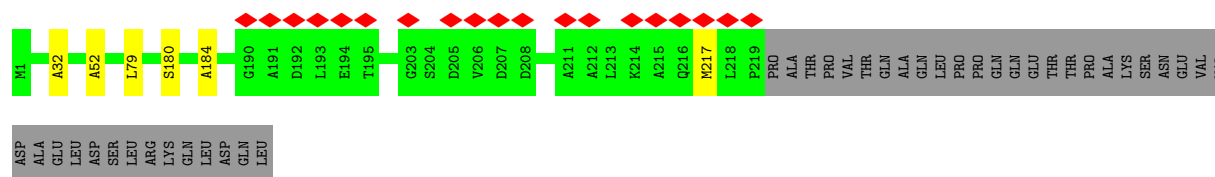
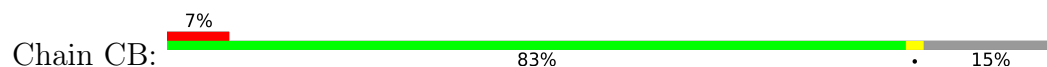


- Molecule 1: vippp1

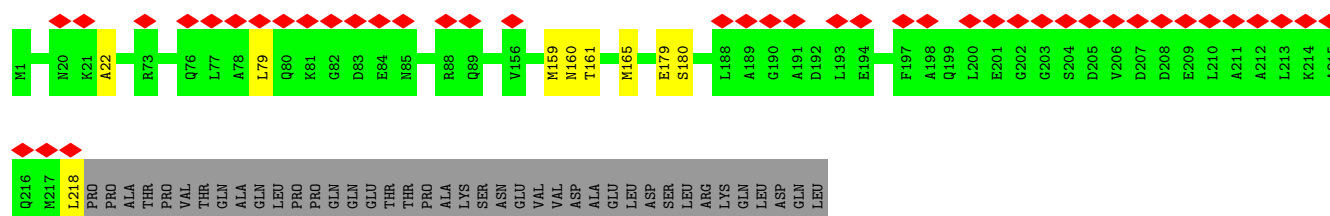
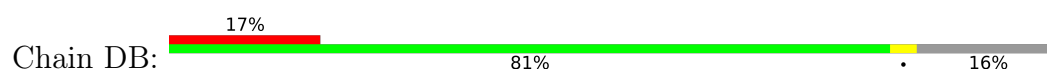




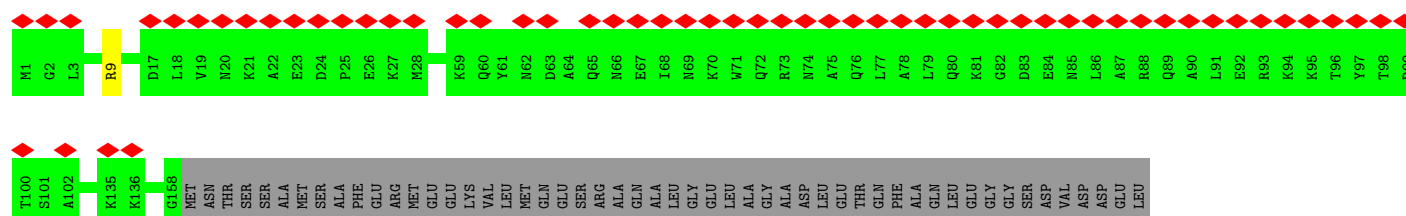
• Molecule 1: vipp1



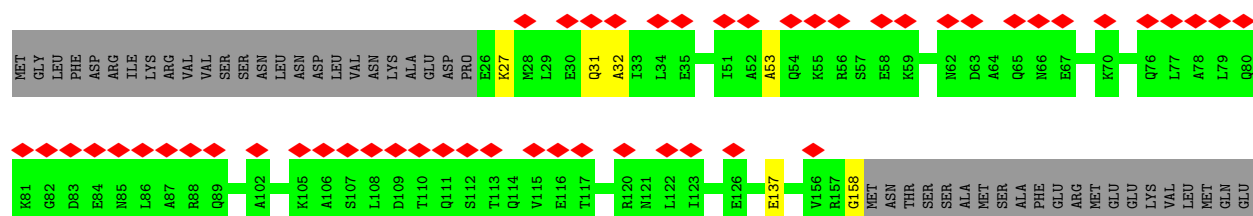
• Molecule 1: vipp1

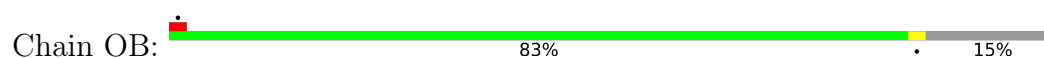


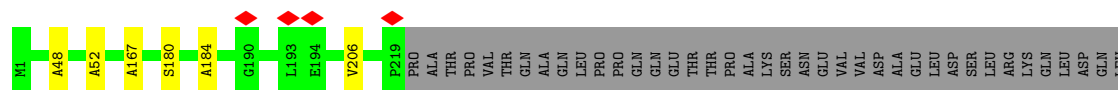
• Molecule 1: vipp1



• Molecule 1: vipp1

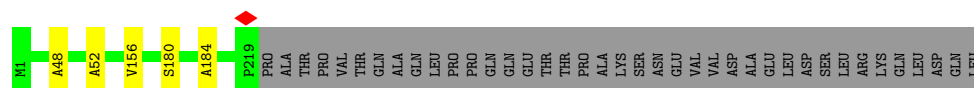






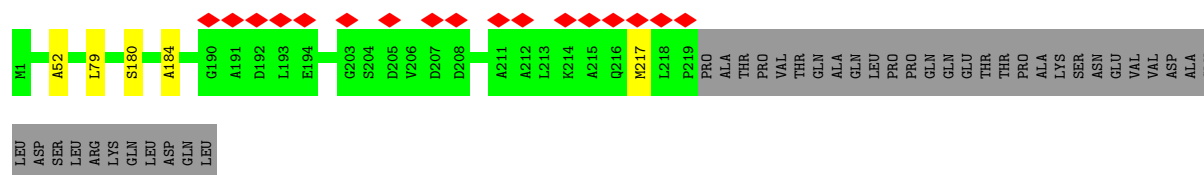
- Molecule 1: vipp1

Chain PB:
83% 15%



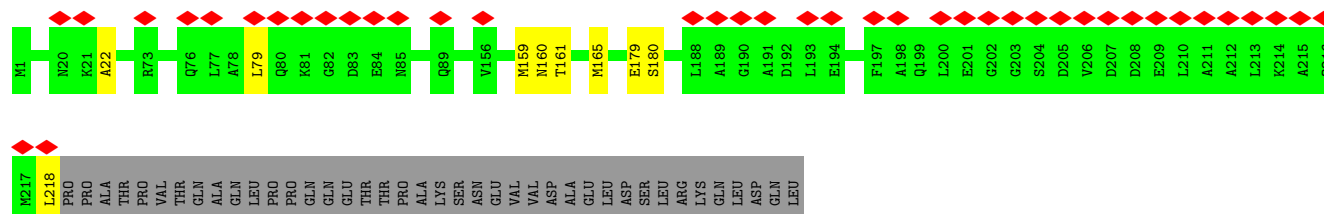
- Molecule 1: vipp1

Chain QB:
7% 83% 15%



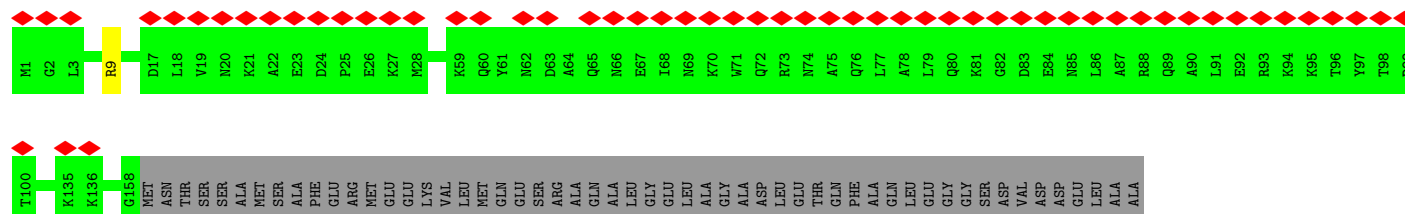
- Molecule 1: vipp1

Chain RB:
16% 81% 16%



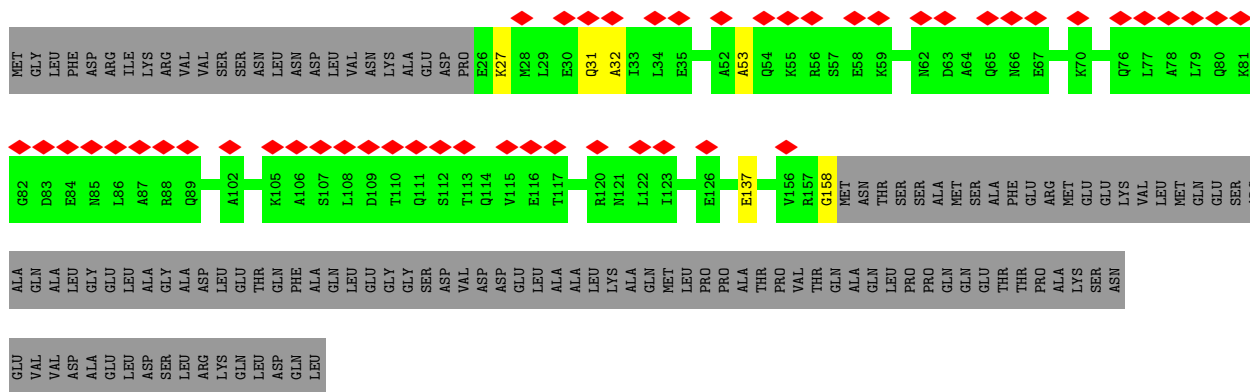
- Molecule 1: vipp1

Chain SB:
22% 61% 39%

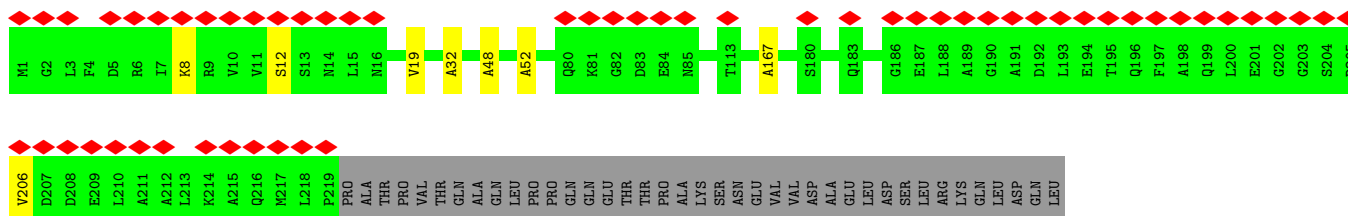
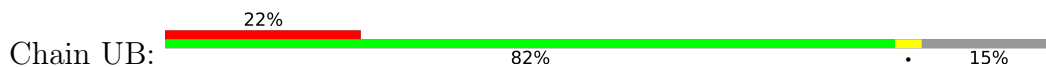


- Molecule 1: vipp1

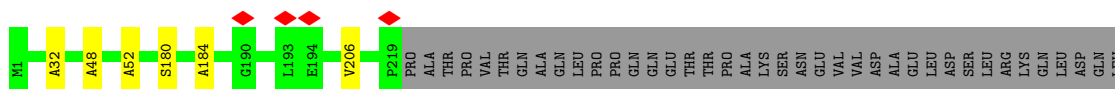
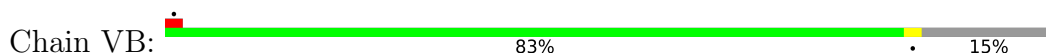
Chain TB:
19% 49% 48%



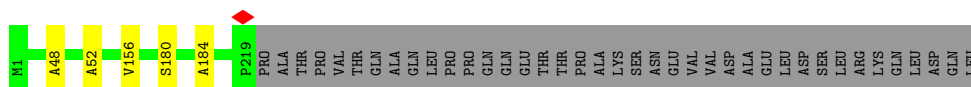
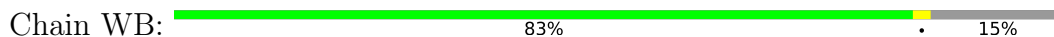
- Molecule 1: vippp1



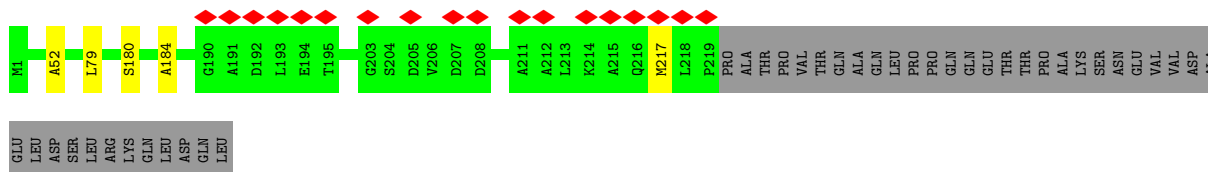
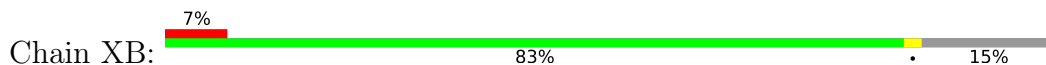
- Molecule 1: vippp1



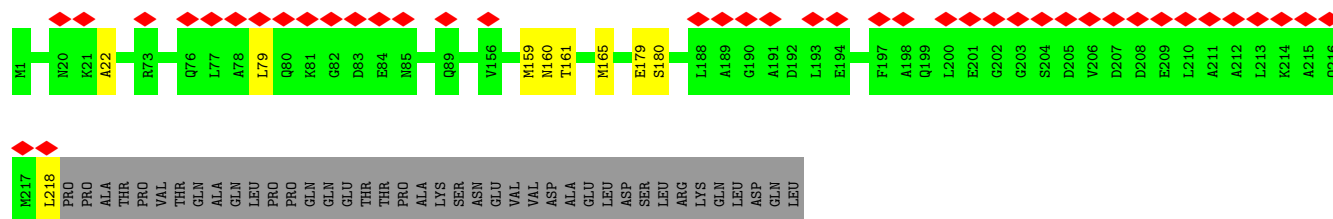
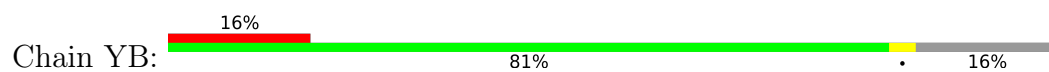
- Molecule 1: vippp1



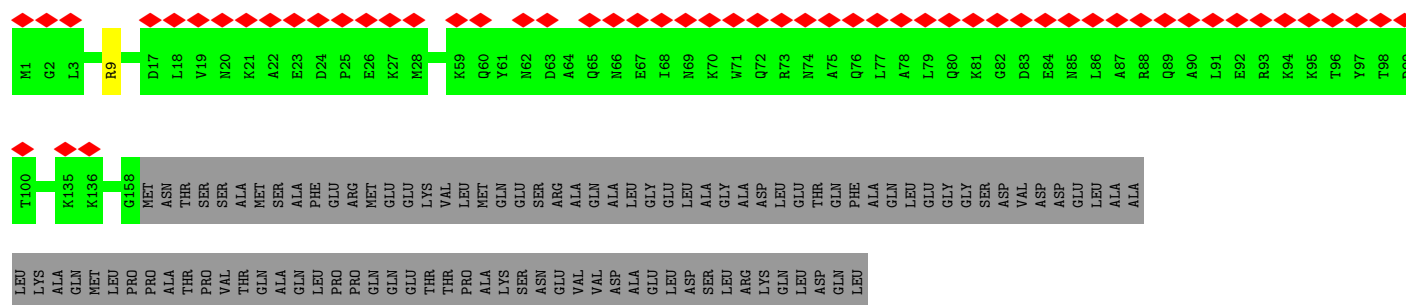
- Molecule 1: vippp1



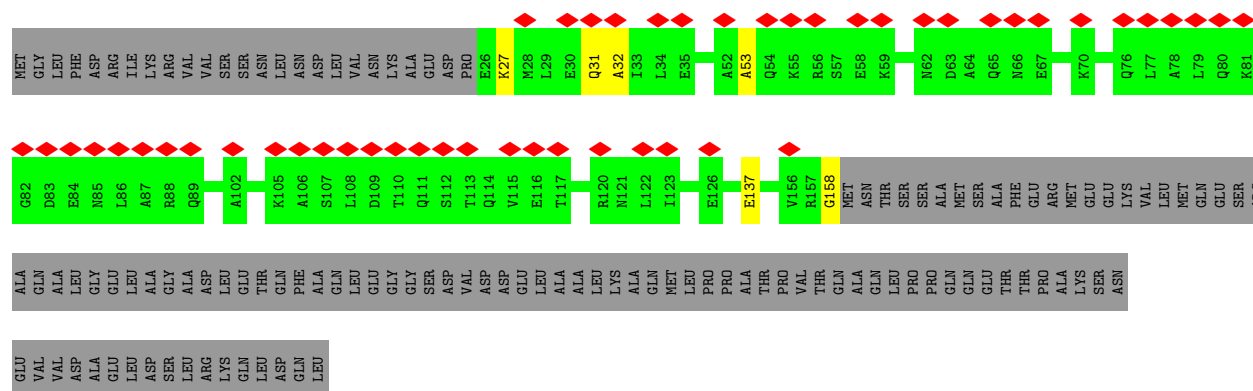
- Molecule 1: vippp1



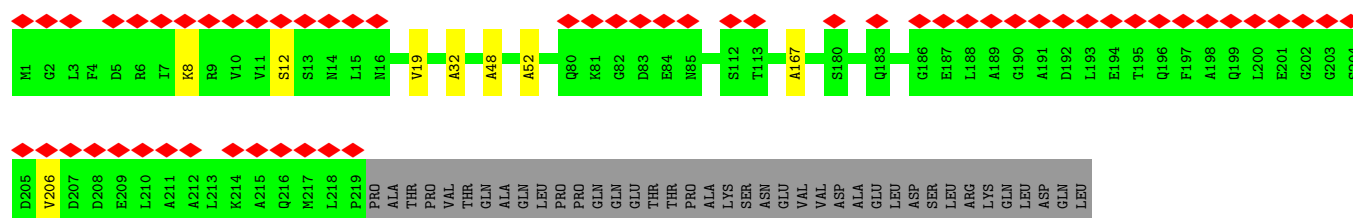
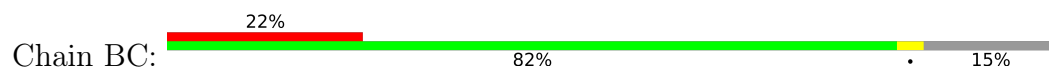
• Molecule 1: vipp1

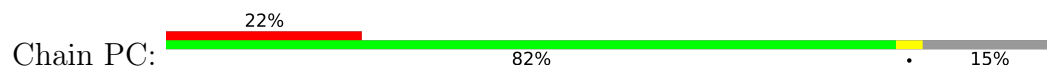


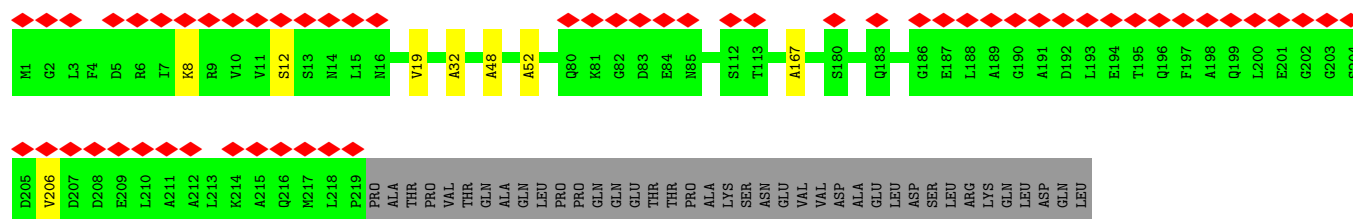
• Molecule 1: vipp1



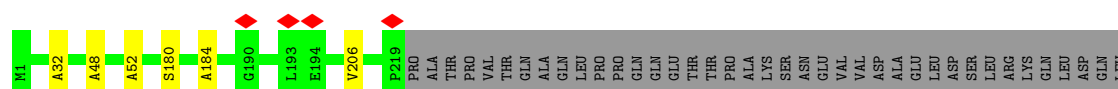
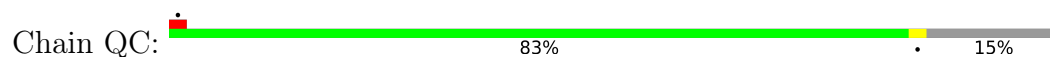
• Molecule 1: vipp1



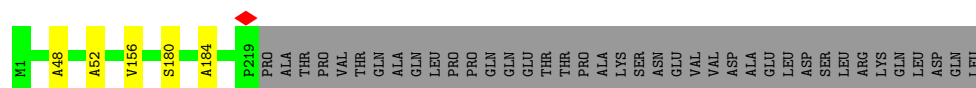
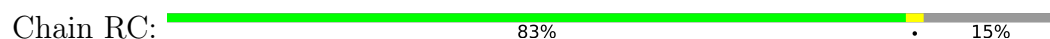




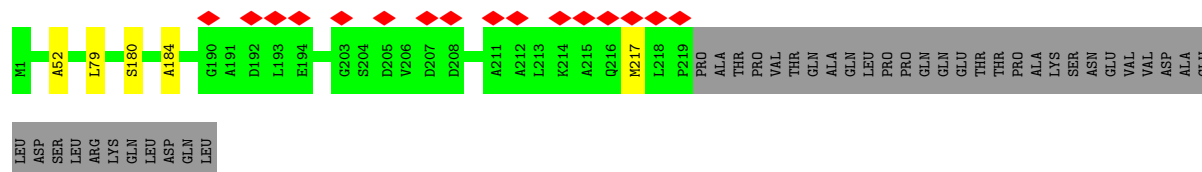
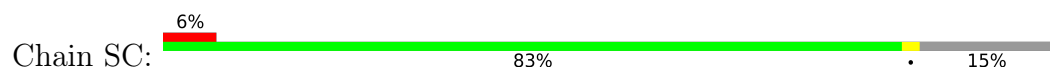
- Molecule 1: vipp1



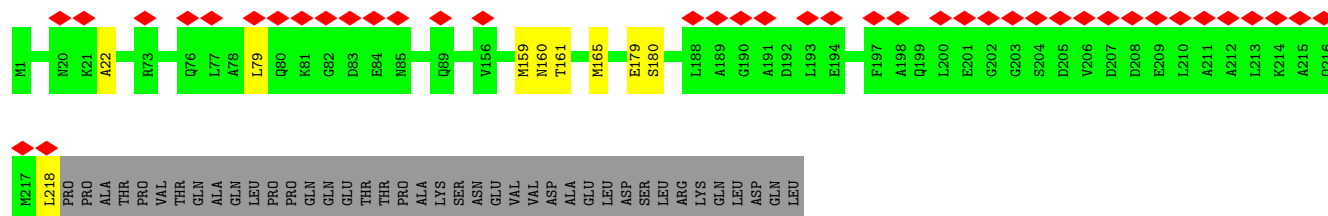
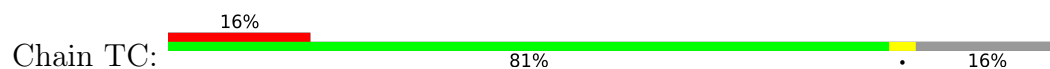
- Molecule 1: vipp1



- Molecule 1: vipp1

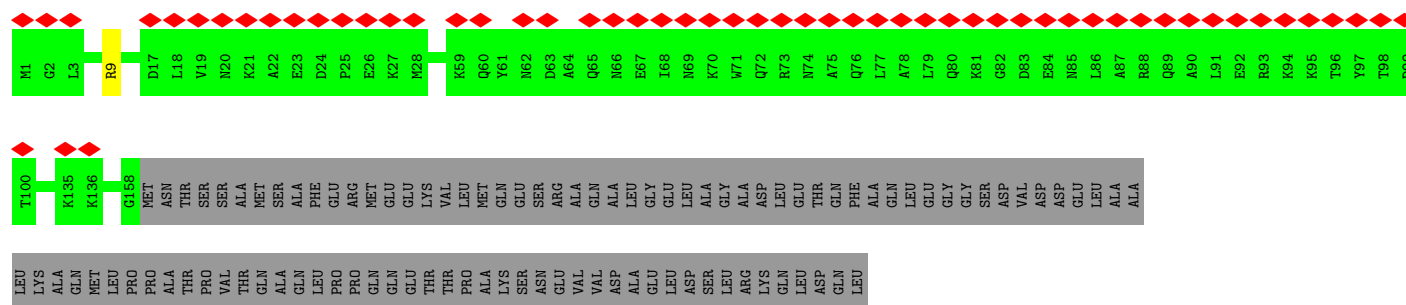


- Molecule 1: vipp1

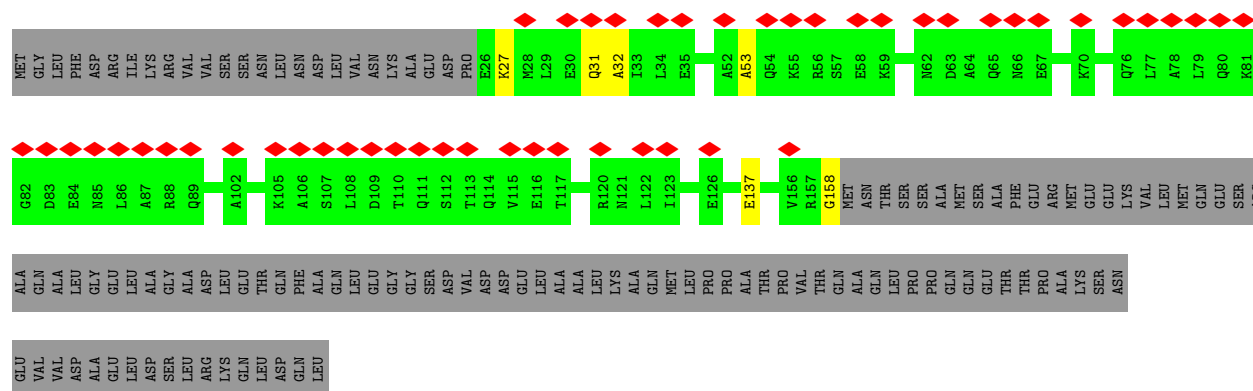


- Molecule 1: vipp1

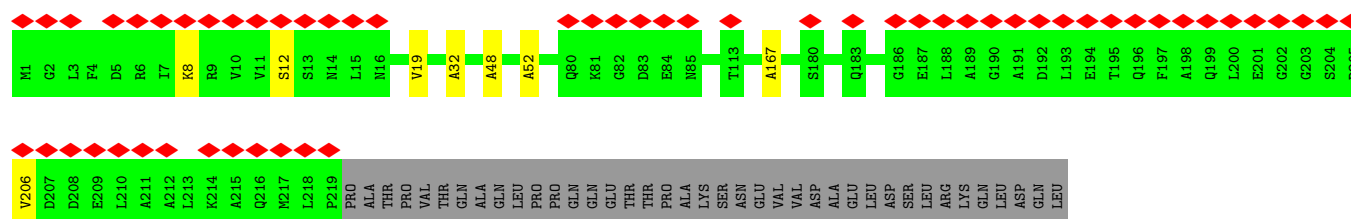
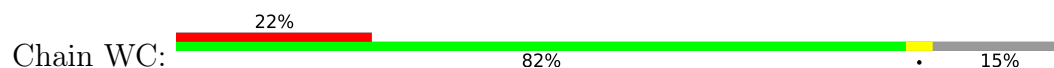




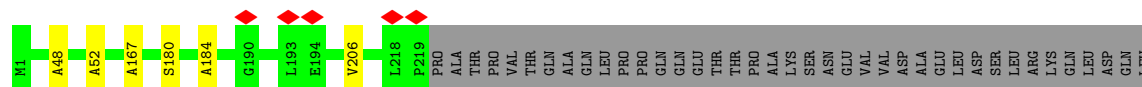
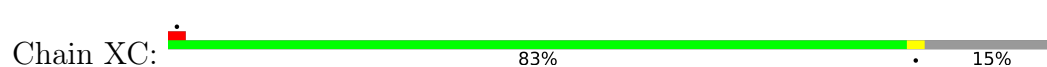
• Molecule 1: vipp1



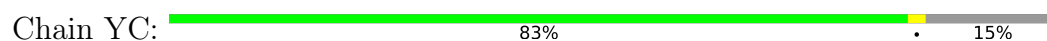
• Molecule 1: vipp1

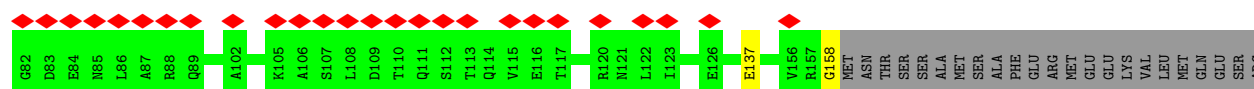


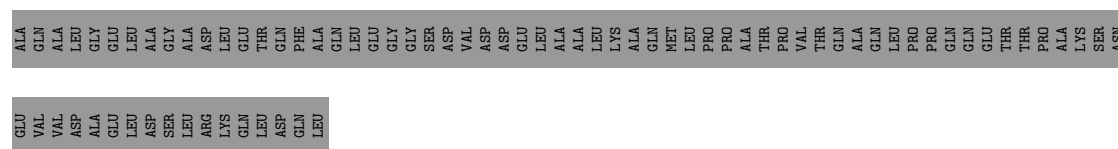
• Molecule 1: vipp1



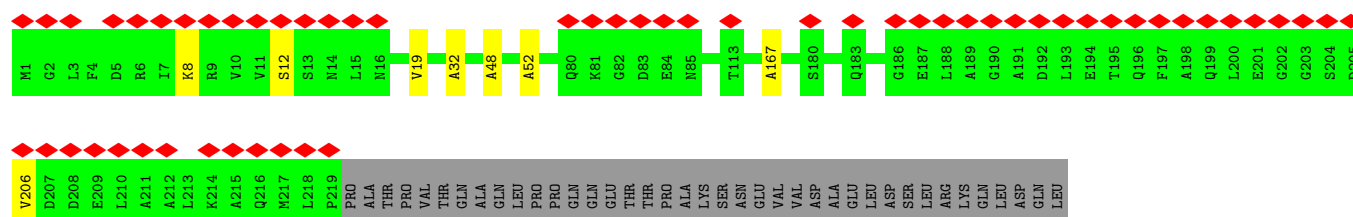
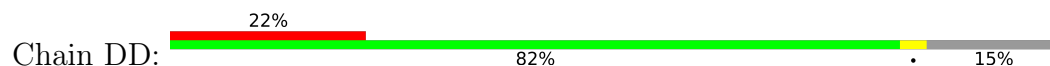
• Molecule 1: vipp1



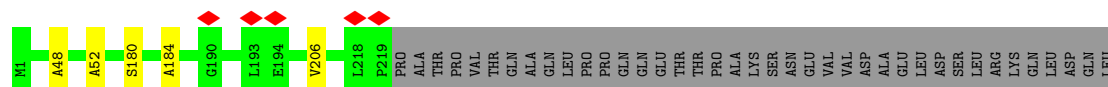
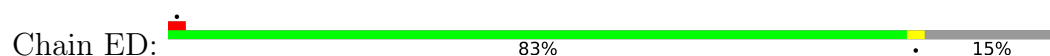




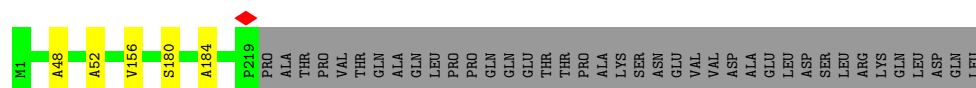
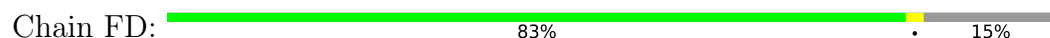
• Molecule 1: vipp1



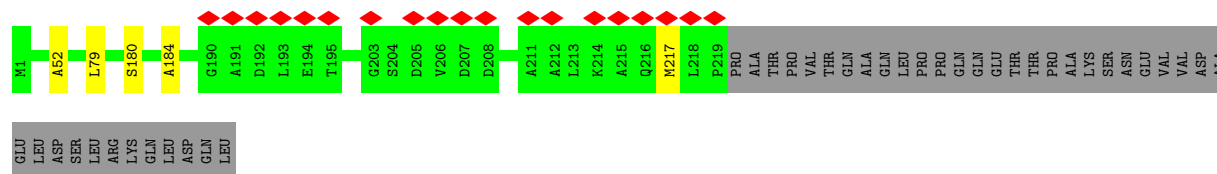
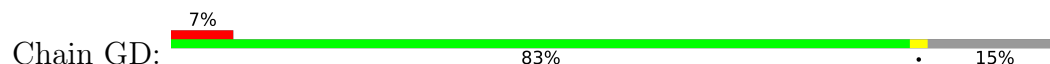
• Molecule 1: vipp1



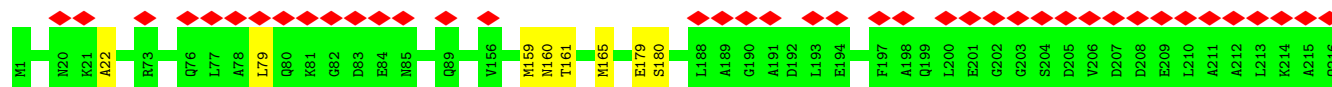
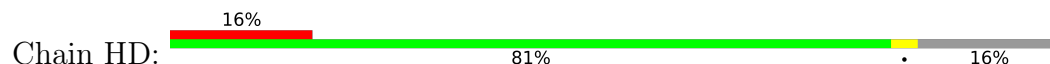
• Molecule 1: vipp1

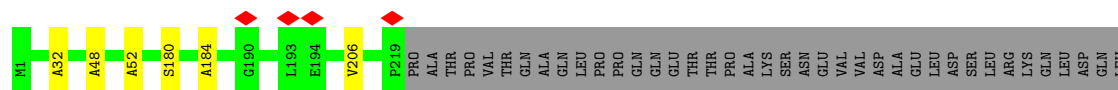


• Molecule 1: vipp1

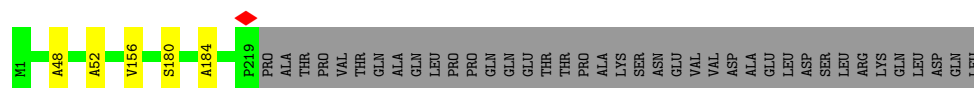
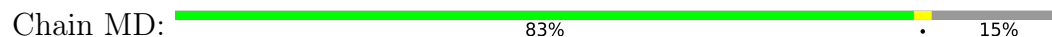


• Molecule 1: vipp1

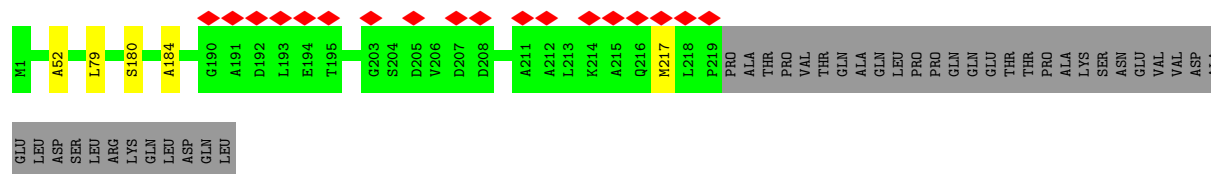
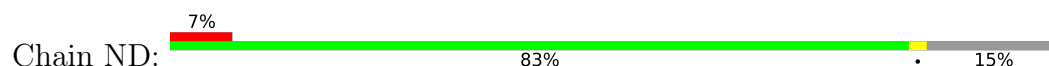




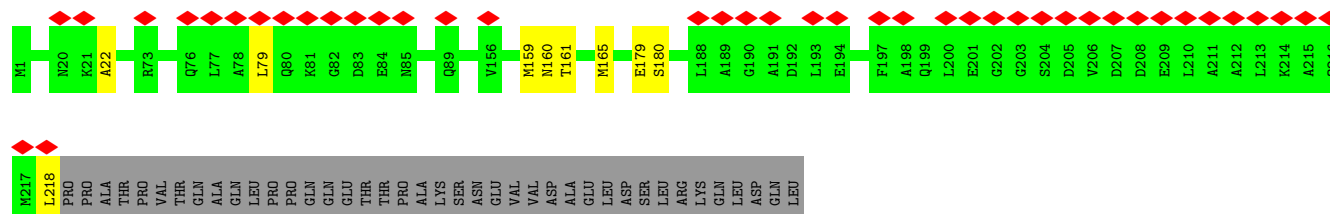
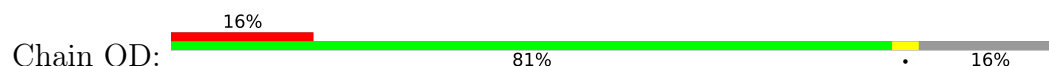
- Molecule 1: vipp1



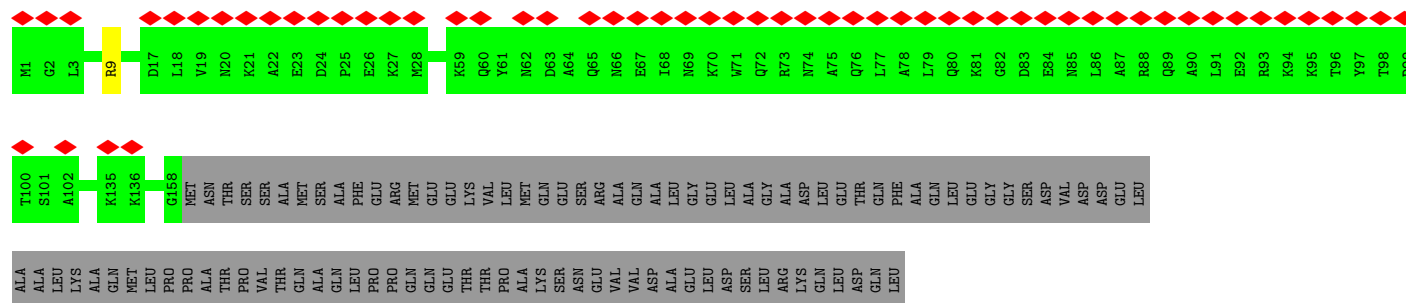
- Molecule 1: vipp1



- Molecule 1: vipp1



- Molecule 1: vipp1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4055	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size ($\text{\AA}$)	467.04, 467.04, 467.04	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.39, 1.39, 1.39	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/660	0.89	0/920
1	AA	0.36	0/1085	0.89	0/1512
1	AB	0.35	0/1085	0.91	1/1512 (0.1%)
1	AC	0.34	0/660	0.89	0/920
1	AD	0.38	0/1080	0.94	0/1505
1	B	0.35	0/1085	0.93	2/1512 (0.1%)
1	BA	0.38	0/1080	0.94	0/1505
1	BB	0.37	0/1085	0.97	1/1512 (0.1%)
1	BC	0.35	0/1085	0.93	2/1512 (0.1%)
1	BD	0.35	0/784	0.95	0/1093
1	C	0.35	0/1085	0.91	1/1512 (0.1%)
1	CA	0.35	0/784	0.95	0/1093
1	CB	0.35	0/1085	0.89	0/1512
1	CC	0.35	0/1085	0.92	1/1512 (0.1%)
1	CD	0.34	0/660	0.89	0/920
1	D	0.37	0/1085	0.97	1/1512 (0.1%)
1	DA	0.34	0/660	0.89	0/920
1	DB	0.38	0/1080	0.94	0/1505
1	DC	0.37	0/1085	0.97	1/1512 (0.1%)
1	DD	0.35	0/1085	0.93	2/1512 (0.1%)
1	E	0.35	0/1085	0.89	0/1512
1	EA	0.35	0/1085	0.93	2/1512 (0.1%)
1	EB	0.35	0/784	0.95	0/1093
1	EC	0.35	0/1085	0.89	0/1512
1	ED	0.35	0/1085	0.91	1/1512 (0.1%)
1	F	0.38	0/1080	0.94	0/1505
1	FA	0.35	0/1085	0.91	1/1512 (0.1%)
1	FB	0.34	0/660	0.89	0/920
1	FC	0.38	0/1080	0.94	0/1505
1	FD	0.37	0/1085	0.97	1/1512 (0.1%)
1	G	0.35	0/784	0.95	0/1093
1	GA	0.37	0/1085	0.97	1/1512 (0.1%)
1	GB	0.35	0/1085	0.93	2/1512 (0.1%)
1	GC	0.35	0/784	0.95	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	GD	0.36	0/1085	0.89	0/1512
1	H	0.34	0/660	0.89	0/920
1	HA	0.36	0/1085	0.89	0/1512
1	HB	0.36	0/1085	0.91	1/1512 (0.1%)
1	HC	0.34	0/660	0.89	0/920
1	HD	0.38	0/1080	0.94	0/1505
1	I	0.35	0/1085	0.93	2/1512 (0.1%)
1	IA	0.38	0/1080	0.94	0/1505
1	IB	0.37	0/1085	0.97	1/1512 (0.1%)
1	IC	0.35	0/1085	0.93	2/1512 (0.1%)
1	ID	0.35	0/784	0.95	0/1093
1	J	0.35	0/1085	0.91	1/1512 (0.1%)
1	JA	0.35	0/784	0.95	0/1093
1	JB	0.36	0/1085	0.89	0/1512
1	JC	0.36	0/1085	0.91	1/1512 (0.1%)
1	JD	0.34	0/660	0.89	0/920
1	K	0.37	0/1085	0.97	1/1512 (0.1%)
1	KA	0.34	0/660	0.89	0/920
1	KB	0.38	0/1080	0.94	0/1505
1	KC	0.37	0/1085	0.97	1/1512 (0.1%)
1	KD	0.35	0/1085	0.93	2/1512 (0.1%)
1	L	0.36	0/1085	0.89	0/1512
1	LA	0.35	0/1085	0.93	2/1512 (0.1%)
1	LB	0.35	0/784	0.95	0/1093
1	LC	0.36	0/1085	0.89	0/1512
1	LD	0.36	0/1085	0.91	1/1512 (0.1%)
1	M	0.38	0/1080	0.94	0/1505
1	MA	0.36	0/1085	0.91	1/1512 (0.1%)
1	MB	0.34	0/660	0.89	0/920
1	MC	0.38	0/1080	0.94	0/1505
1	MD	0.37	0/1085	0.97	1/1512 (0.1%)
1	N	0.35	0/784	0.95	0/1093
1	NA	0.37	0/1085	0.97	1/1512 (0.1%)
1	NB	0.35	0/1085	0.93	2/1512 (0.1%)
1	NC	0.35	0/784	0.95	0/1093
1	ND	0.36	0/1085	0.89	0/1512
1	O	0.34	0/660	0.89	0/920
1	OA	0.36	0/1085	0.89	0/1512
1	OB	0.36	0/1085	0.91	1/1512 (0.1%)
1	OC	0.34	0/660	0.89	0/920
1	OD	0.38	0/1080	0.94	0/1505
1	P	0.35	0/1085	0.93	2/1512 (0.1%)
1	PA	0.38	0/1080	0.94	0/1505

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	PB	0.37	0/1085	0.97	1/1512 (0.1%)
1	PC	0.35	0/1085	0.93	2/1512 (0.1%)
1	PD	0.35	0/784	0.95	0/1093
1	Q	0.35	0/1085	0.91	1/1512 (0.1%)
1	QA	0.35	0/784	0.95	0/1093
1	QB	0.36	0/1085	0.89	0/1512
1	QC	0.35	0/1085	0.91	1/1512 (0.1%)
1	R	0.37	0/1085	0.97	1/1512 (0.1%)
1	RA	0.34	0/660	0.89	0/920
1	RB	0.38	0/1080	0.94	0/1505
1	RC	0.37	0/1085	0.96	1/1512 (0.1%)
1	S	0.35	0/1085	0.89	0/1512
1	SA	0.35	0/1085	0.93	2/1512 (0.1%)
1	SB	0.35	0/784	0.95	0/1093
1	SC	0.35	0/1085	0.89	0/1512
1	T	0.38	0/1080	0.94	0/1505
1	TA	0.35	0/1085	0.91	1/1512 (0.1%)
1	TB	0.34	0/660	0.89	0/920
1	TC	0.38	0/1080	0.94	0/1505
1	UA	0.37	0/1085	0.97	1/1512 (0.1%)
1	UB	0.35	0/1085	0.93	2/1512 (0.1%)
1	UC	0.35	0/784	0.95	0/1093
1	V	0.35	0/784	0.95	0/1093
1	VA	0.36	0/1085	0.89	0/1512
1	VB	0.35	0/1085	0.91	1/1512 (0.1%)
1	VC	0.34	0/660	0.89	0/920
1	W	0.34	0/660	0.89	0/920
1	WA	0.38	0/1080	0.94	0/1505
1	WB	0.37	0/1085	0.97	1/1512 (0.1%)
1	WC	0.35	0/1085	0.93	2/1512 (0.1%)
1	X	0.35	0/1085	0.93	2/1512 (0.1%)
1	XA	0.35	0/784	0.95	0/1093
1	XB	0.35	0/1085	0.89	0/1512
1	XC	0.35	0/1085	0.92	1/1512 (0.1%)
1	Y	0.35	0/1085	0.91	1/1512 (0.1%)
1	YA	0.34	0/660	0.89	0/920
1	YB	0.38	0/1080	0.94	0/1505
1	YC	0.37	0/1085	0.97	1/1512 (0.1%)
1	Z	0.37	0/1085	0.97	1/1512 (0.1%)
1	ZA	0.35	0/1085	0.93	2/1512 (0.1%)
1	ZB	0.35	0/784	0.95	0/1093
1	ZC	0.36	0/1085	0.89	0/1512
All	All	0.36	0/116688	0.93	68/162622 (0.0%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YC	156	VAL	N-CA-C	6.24	116.39	110.53
1	WB	156	VAL	N-CA-C	6.23	116.38	110.53
1	PB	156	VAL	N-CA-C	6.22	116.38	110.53
1	DC	156	VAL	N-CA-C	6.22	116.37	110.53
1	GA	156	VAL	N-CA-C	6.21	116.36	110.53
1	UA	156	VAL	N-CA-C	6.21	116.36	110.53
1	D	156	VAL	N-CA-C	6.20	116.36	110.53
1	Z	156	VAL	N-CA-C	6.20	116.36	110.53
1	IB	156	VAL	N-CA-C	6.20	116.35	110.53
1	FD	156	VAL	N-CA-C	6.19	116.35	110.53
1	BB	156	VAL	N-CA-C	6.19	116.35	110.53
1	MD	156	VAL	N-CA-C	6.19	116.35	110.53
1	NA	156	VAL	N-CA-C	6.19	116.35	110.53
1	R	156	VAL	N-CA-C	6.19	116.35	110.53
1	KC	156	VAL	N-CA-C	6.19	116.35	110.53
1	K	156	VAL	N-CA-C	6.18	116.34	110.53
1	RC	156	VAL	N-CA-C	6.17	116.33	110.53
1	EA	206	VAL	N-CA-C	5.48	116.21	110.62
1	LA	206	VAL	N-CA-C	5.48	116.21	110.62
1	ZA	206	VAL	N-CA-C	5.47	116.20	110.62
1	GB	206	VAL	N-CA-C	5.47	116.20	110.62
1	NB	206	VAL	N-CA-C	5.46	116.19	110.62
1	BC	206	VAL	N-CA-C	5.46	116.19	110.62
1	IC	206	VAL	N-CA-C	5.46	116.19	110.62
1	P	206	VAL	N-CA-C	5.45	116.18	110.62
1	WC	206	VAL	N-CA-C	5.45	116.18	110.62
1	B	206	VAL	N-CA-C	5.45	116.18	110.62
1	UB	206	VAL	N-CA-C	5.45	116.17	110.62
1	PC	206	VAL	N-CA-C	5.44	116.17	110.62
1	I	206	VAL	N-CA-C	5.43	116.16	110.62
1	DD	206	VAL	N-CA-C	5.43	116.16	110.62
1	KD	206	VAL	N-CA-C	5.43	116.16	110.62
1	SA	206	VAL	N-CA-C	5.42	116.15	110.62
1	X	206	VAL	N-CA-C	5.41	116.14	110.62
1	QC	206	VAL	N-CA-C	5.32	116.05	110.62
1	CC	206	VAL	N-CA-C	5.30	116.03	110.62
1	Y	206	VAL	N-CA-C	5.29	116.02	110.62
1	MA	206	VAL	N-CA-C	5.29	116.02	110.62
1	J	206	VAL	N-CA-C	5.29	116.02	110.62
1	XC	206	VAL	N-CA-C	5.29	116.01	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	VB	206	VAL	N-CA-C	5.28	116.01	110.62
1	LD	206	VAL	N-CA-C	5.28	116.01	110.62
1	C	206	VAL	N-CA-C	5.28	116.01	110.62
1	TA	206	VAL	N-CA-C	5.28	116.00	110.62
1	OB	206	VAL	N-CA-C	5.28	116.00	110.62
1	Q	206	VAL	N-CA-C	5.27	116.00	110.62
1	AB	206	VAL	N-CA-C	5.27	115.99	110.62
1	FA	206	VAL	N-CA-C	5.26	115.99	110.62
1	HB	206	VAL	N-CA-C	5.26	115.98	110.62
1	JC	206	VAL	N-CA-C	5.25	115.98	110.62
1	ED	206	VAL	N-CA-C	5.24	115.96	110.62
1	I	19	VAL	N-CA-C	5.21	115.94	110.62
1	ZA	19	VAL	N-CA-C	5.20	115.93	110.62
1	BC	19	VAL	N-CA-C	5.17	115.90	110.62
1	WC	19	VAL	N-CA-C	5.17	115.89	110.62
1	P	19	VAL	N-CA-C	5.17	115.89	110.62
1	SA	19	VAL	N-CA-C	5.17	115.89	110.62
1	IC	19	VAL	N-CA-C	5.17	115.89	110.62
1	UB	19	VAL	N-CA-C	5.16	115.89	110.62
1	B	19	VAL	N-CA-C	5.15	115.88	110.62
1	DD	19	VAL	N-CA-C	5.15	115.88	110.62
1	X	19	VAL	N-CA-C	5.15	115.87	110.62
1	LA	19	VAL	N-CA-C	5.15	115.87	110.62
1	EA	19	VAL	N-CA-C	5.15	115.87	110.62
1	GB	19	VAL	N-CA-C	5.15	115.87	110.62
1	KD	19	VAL	N-CA-C	5.14	115.87	110.62
1	PC	19	VAL	N-CA-C	5.14	115.86	110.62
1	NB	19	VAL	N-CA-C	5.11	115.83	110.62

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	661	0	320	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1086	0	531	12	0
1	AB	1086	0	531	27	0
1	AC	661	0	320	12	0
1	AD	1081	0	530	14	0
1	B	1086	0	531	15	0
1	BA	1081	0	530	14	0
1	BB	1086	0	531	22	0
1	BC	1086	0	531	15	0
1	BD	785	0	376	3	0
1	C	1086	0	531	27	0
1	CA	785	0	376	3	0
1	CB	1086	0	531	13	0
1	CC	1086	0	531	26	0
1	CD	661	0	320	12	0
1	D	1086	0	531	23	0
1	DA	661	0	320	12	0
1	DB	1081	0	530	13	0
1	DC	1086	0	531	21	0
1	DD	1086	0	531	15	0
1	E	1086	0	531	12	0
1	EA	1086	0	531	15	0
1	EB	785	0	376	3	0
1	EC	1086	0	531	13	0
1	ED	1086	0	531	24	0
1	F	1081	0	530	14	0
1	FA	1086	0	531	25	0
1	FB	661	0	320	12	0
1	FC	1081	0	530	15	0
1	FD	1086	0	531	23	0
1	G	785	0	376	3	0
1	GA	1086	0	531	22	0
1	GB	1086	0	531	15	0
1	GC	785	0	376	3	0
1	GD	1086	0	531	12	0
1	H	661	0	320	12	0
1	HA	1086	0	531	13	0
1	HB	1086	0	531	26	0
1	HC	661	0	320	12	0
1	HD	1081	0	530	14	0
1	I	1086	0	531	15	0
1	IA	1081	0	530	14	0
1	IB	1086	0	531	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	IC	1086	0	531	15	0
1	ID	785	0	376	3	0
1	J	1086	0	531	27	0
1	JA	785	0	376	3	0
1	JB	1086	0	531	14	0
1	JC	1086	0	531	26	0
1	JD	661	0	320	12	0
1	K	1086	0	531	23	0
1	KA	661	0	320	12	0
1	KB	1081	0	530	13	0
1	KC	1086	0	531	22	0
1	KD	1086	0	531	15	0
1	L	1086	0	531	12	0
1	LA	1086	0	531	15	0
1	LB	785	0	376	3	0
1	LC	1086	0	531	13	0
1	LD	1086	0	531	26	0
1	M	1081	0	530	14	0
1	MA	1086	0	531	26	0
1	MB	661	0	320	12	0
1	MC	1081	0	530	14	0
1	MD	1086	0	531	22	0
1	N	785	0	376	3	0
1	NA	1086	0	531	22	0
1	NB	1086	0	531	15	0
1	NC	785	0	376	3	0
1	ND	1086	0	531	13	0
1	O	661	0	320	12	0
1	OA	1086	0	531	12	0
1	OB	1086	0	531	24	0
1	OC	661	0	320	12	0
1	OD	1081	0	530	15	0
1	P	1086	0	531	15	0
1	PA	1081	0	530	13	0
1	PB	1086	0	531	23	0
1	PC	1086	0	531	15	0
1	PD	785	0	376	3	0
1	Q	1086	0	531	26	0
1	QA	785	0	376	3	0
1	QB	1086	0	531	13	0
1	QC	1086	0	531	26	0
1	R	1086	0	531	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	RA	661	0	320	12	0
1	RB	1081	0	530	14	0
1	RC	1086	0	531	22	0
1	S	1086	0	531	13	0
1	SA	1086	0	531	15	0
1	SB	785	0	376	3	0
1	SC	1086	0	531	12	0
1	T	1081	0	530	14	0
1	TA	1086	0	531	27	0
1	TB	661	0	320	12	0
1	TC	1081	0	530	14	0
1	UA	1086	0	531	22	0
1	UB	1086	0	531	15	0
1	UC	785	0	376	3	0
1	V	785	0	376	3	0
1	VA	1086	0	531	12	0
1	VB	1086	0	531	25	0
1	VC	661	0	320	12	0
1	W	661	0	320	12	0
1	WA	1081	0	530	13	0
1	WB	1086	0	531	22	0
1	WC	1086	0	531	15	0
1	X	1086	0	531	15	0
1	XA	785	0	376	3	0
1	XB	1086	0	531	12	0
1	XC	1086	0	531	25	0
1	Y	1086	0	531	25	0
1	YA	661	0	320	12	0
1	YB	1081	0	530	15	0
1	YC	1086	0	531	24	0
1	Z	1086	0	531	23	0
1	ZA	1086	0	531	15	0
1	ZB	785	0	376	3	0
1	ZC	1086	0	531	13	0
All	All	116807	0	56950	923	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (923) 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:SA:48:ALA:CB	1:HB:184:ALA:HB1	1.57	1.33
1:C:184:ALA:HB1	1:DD:48:ALA:CB	1.59	1.32
1:I:48:ALA:CB	1:Y:184:ALA:HB1	1.58	1.32
1:IC:48:ALA:CB	1:XC:184:ALA:HB1	1.60	1.32
1:X:48:ALA:CB	1:MA:184:ALA:HB1	1.60	1.32
1:P:48:ALA:CB	1:FA:184:ALA:HB1	1.60	1.32
1:ZA:48:ALA:CB	1:OB:184:ALA:HB1	1.57	1.32
1:LA:48:ALA:CB	1:AB:184:ALA:HB1	1.59	1.31
1:B:48:ALA:CB	1:Q:184:ALA:HB1	1.59	1.31
1:J:184:ALA:HB1	1:KD:48:ALA:CB	1.60	1.31
1:BC:48:ALA:CB	1:QC:184:ALA:HB1	1.60	1.31
1:PC:48:ALA:CB	1:ED:184:ALA:HB1	1.59	1.31
1:EA:48:ALA:CB	1:TA:184:ALA:HB1	1.59	1.30
1:UB:48:ALA:CB	1:JC:184:ALA:HB1	1.58	1.30
1:AC:31:GLN:CB	1:BC:8:LYS:O	1.80	1.30
1:VC:31:GLN:CB	1:WC:8:LYS:O	1.80	1.30
1:JD:31:GLN:CB	1:KD:8:LYS:O	1.80	1.30
1:OC:31:GLN:CB	1:PC:8:LYS:O	1.80	1.30
1:GB:48:ALA:CB	1:VB:184:ALA:HB1	1.61	1.29
1:NB:48:ALA:CB	1:CC:184:ALA:HB1	1.62	1.29
1:UA:52:ALA:HB2	1:JB:180:SER:CB	1.63	1.29
1:WC:48:ALA:CB	1:LD:184:ALA:HB1	1.60	1.29
1:A:31:GLN:CB	1:B:8:LYS:O	1.80	1.29
1:MB:31:GLN:CB	1:NB:8:LYS:O	1.80	1.29
1:BB:52:ALA:HB2	1:QB:180:SER:CB	1.62	1.29
1:O:31:GLN:CB	1:P:8:LYS:O	1.80	1.28
1:FB:31:GLN:CB	1:GB:8:LYS:O	1.80	1.28
1:TB:31:GLN:CB	1:UB:8:LYS:O	1.80	1.28
1:H:31:GLN:CB	1:I:8:LYS:O	1.80	1.28
1:HC:31:GLN:CB	1:IC:8:LYS:O	1.80	1.28
1:DA:31:GLN:CB	1:EA:8:LYS:O	1.80	1.28
1:RA:31:GLN:CB	1:SA:8:LYS:O	1.80	1.28
1:YC:52:ALA:HB2	1:ND:180:SER:CB	1.62	1.28
1:K:52:ALA:HB2	1:AA:180:SER:CB	1.63	1.28
1:Z:52:ALA:HB2	1:OA:180:SER:CB	1.64	1.28
1:IB:52:ALA:CB	1:XB:180:SER:CB	2.12	1.28
1:YC:52:ALA:CB	1:ND:180:SER:CB	2.11	1.27
1:CD:31:GLN:CB	1:DD:8:LYS:O	1.80	1.27
1:D:52:ALA:HB2	1:S:180:SER:CB	1.64	1.27
1:GA:52:ALA:HB2	1:VA:180:SER:CB	1.64	1.27
1:K:52:ALA:CB	1:AA:180:SER:CB	2.13	1.27
1:W:31:GLN:CB	1:X:8:LYS:O	1.80	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NA:52:ALA:HB2	1:CB:180:SER:CB	1.63	1.27
1:NA:52:ALA:CB	1:CB:180:SER:CB	2.13	1.27
1:YA:31:GLN:CB	1:ZA:8:LYS:O	1.80	1.27
1:PB:52:ALA:HB2	1:EC:180:SER:CB	1.64	1.27
1:E:180:SER:CB	1:FD:52:ALA:CB	2.13	1.26
1:WB:52:ALA:HB2	1:LC:180:SER:CB	1.64	1.26
1:PB:52:ALA:CB	1:EC:180:SER:CB	2.12	1.26
1:D:52:ALA:CB	1:S:180:SER:CB	2.13	1.26
1:KA:31:GLN:CB	1:LA:8:LYS:O	1.80	1.26
1:BB:52:ALA:CB	1:QB:180:SER:CB	2.13	1.26
1:GA:52:ALA:CB	1:VA:180:SER:CB	2.14	1.26
1:ZA:48:ALA:HB1	1:OB:184:ALA:CB	1.65	1.26
1:IB:52:ALA:HB2	1:XB:180:SER:CB	1.63	1.26
1:R:52:ALA:HB2	1:HA:180:SER:CB	1.64	1.25
1:E:180:SER:CB	1:FD:52:ALA:HB2	1.64	1.25
1:R:52:ALA:CB	1:HA:180:SER:CB	2.13	1.25
1:Z:52:ALA:CB	1:OA:180:SER:CB	2.14	1.25
1:SA:48:ALA:HB1	1:HB:184:ALA:CB	1.65	1.25
1:UA:52:ALA:CB	1:JB:180:SER:CB	2.14	1.25
1:WB:52:ALA:CB	1:LC:180:SER:CB	2.14	1.25
1:RC:52:ALA:HB2	1:GD:180:SER:CB	1.65	1.25
1:DC:52:ALA:CB	1:SC:180:SER:CB	2.13	1.24
1:DC:52:ALA:HB2	1:SC:180:SER:CB	1.64	1.24
1:KC:52:ALA:HB2	1:ZC:180:SER:CB	1.65	1.24
1:KC:52:ALA:CB	1:ZC:180:SER:CB	2.14	1.24
1:UB:48:ALA:HB1	1:JC:184:ALA:CB	1.67	1.24
1:L:180:SER:CB	1:MD:52:ALA:HB2	1.66	1.24
1:LA:48:ALA:HB1	1:AB:184:ALA:CB	1.68	1.24
1:RC:52:ALA:CB	1:GD:180:SER:CB	2.15	1.24
1:I:48:ALA:HB1	1:Y:184:ALA:CB	1.66	1.23
1:L:180:SER:CB	1:MD:52:ALA:CB	2.15	1.23
1:B:48:ALA:HB1	1:Q:184:ALA:CB	1.67	1.23
1:C:184:ALA:CB	1:DD:48:ALA:HB1	1.68	1.23
1:EA:48:ALA:HB1	1:TA:184:ALA:CB	1.68	1.23
1:BC:48:ALA:HB1	1:QC:184:ALA:CB	1.68	1.23
1:GB:48:ALA:HB1	1:VB:184:ALA:CB	1.69	1.22
1:P:48:ALA:HB1	1:FA:184:ALA:CB	1.68	1.21
1:IC:48:ALA:HB1	1:XC:184:ALA:CB	1.68	1.21
1:PC:48:ALA:HB1	1:ED:184:ALA:CB	1.67	1.21
1:J:184:ALA:CB	1:KD:48:ALA:HB1	1.68	1.21
1:X:48:ALA:HB1	1:MA:184:ALA:CB	1.68	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WC:48:ALA:HB1	1:LD:184:ALA:CB	1.68	1.20
1:NB:48:ALA:HB1	1:CC:184:ALA:CB	1.70	1.20
1:FC:79:LEU:CB	1:AD:218:LEU:O	1.93	1.17
1:M:218:LEU:O	1:HD:79:LEU:CB	1.94	1.16
1:IA:79:LEU:CB	1:DB:218:LEU:O	1.94	1.15
1:YB:79:LEU:CB	1:TC:218:LEU:O	1.95	1.15
1:TC:79:LEU:CB	1:OD:218:LEU:O	1.95	1.15
1:M:79:LEU:CB	1:IA:218:LEU:O	1.94	1.15
1:T:218:LEU:O	1:OD:79:LEU:CB	1.94	1.15
1:MC:79:LEU:CB	1:HD:218:LEU:O	1.95	1.15
1:F:218:LEU:O	1:AD:79:LEU:CB	1.96	1.14
1:DB:79:LEU:CB	1:YB:218:LEU:O	1.96	1.14
1:KB:79:LEU:CB	1:FC:218:LEU:O	1.96	1.14
1:T:79:LEU:CB	1:PA:218:LEU:O	1.94	1.14
1:F:79:LEU:CB	1:BA:218:LEU:O	1.95	1.13
1:RB:79:LEU:CB	1:MC:218:LEU:O	1.96	1.13
1:WA:79:LEU:CB	1:RB:218:LEU:O	1.95	1.13
1:AB:52:ALA:HB1	1:PB:180:SER:CB	1.77	1.13
1:TA:52:ALA:HB1	1:IB:180:SER:CB	1.78	1.12
1:J:52:ALA:HB1	1:Z:180:SER:CB	1.78	1.12
1:BA:79:LEU:CB	1:WA:218:LEU:O	1.96	1.12
1:PA:79:LEU:CB	1:KB:218:LEU:O	1.97	1.12
1:C:52:ALA:HB1	1:R:180:SER:CB	1.80	1.11
1:MA:52:ALA:HB1	1:BB:180:SER:CB	1.81	1.11
1:XC:52:ALA:HB1	1:MD:180:SER:CB	1.81	1.11
1:CC:52:ALA:HB1	1:RC:180:SER:CB	1.81	1.11
1:VB:52:ALA:HB1	1:KC:180:SER:CB	1.80	1.11
1:Q:52:ALA:HB1	1:GA:180:SER:CB	1.81	1.10
1:Y:52:ALA:HB1	1:NA:180:SER:CB	1.81	1.10
1:HB:52:ALA:HB1	1:WB:180:SER:CB	1.82	1.10
1:JC:52:ALA:HB1	1:YC:180:SER:CB	1.81	1.10
1:QC:52:ALA:HB1	1:FD:180:SER:CB	1.81	1.10
1:FA:52:ALA:HB1	1:UA:180:SER:CB	1.81	1.10
1:D:180:SER:CB	1:ED:52:ALA:HB1	1.81	1.10
1:K:180:SER:CB	1:LD:52:ALA:HB1	1.82	1.09
1:AB:48:ALA:CA	1:PB:184:ALA:HB1	1.84	1.08
1:OB:52:ALA:HB1	1:DC:180:SER:CB	1.83	1.07
1:TA:48:ALA:CA	1:IB:184:ALA:HB1	1.84	1.07
1:JC:48:ALA:CA	1:YC:184:ALA:HB1	1.85	1.07
1:J:48:ALA:CA	1:Z:184:ALA:HB1	1.85	1.07
1:FA:48:ALA:CA	1:UA:184:ALA:HB1	1.85	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ALA:HB1	1:ED:48:ALA:CA	1.85	1.06
1:QC:48:ALA:CA	1:FD:184:ALA:HB1	1.85	1.06
1:K:184:ALA:HB1	1:LD:48:ALA:CA	1.85	1.06
1:VB:48:ALA:CA	1:KC:184:ALA:HB1	1.85	1.06
1:CC:48:ALA:CA	1:RC:184:ALA:HB1	1.85	1.06
1:Y:48:ALA:CA	1:NA:184:ALA:HB1	1.85	1.06
1:TA:48:ALA:CB	1:IB:184:ALA:HB1	1.86	1.06
1:VB:48:ALA:HB1	1:KC:184:ALA:HB1	1.38	1.06
1:QC:48:ALA:HB1	1:FD:184:ALA:HB1	1.37	1.06
1:C:48:ALA:CA	1:R:184:ALA:HB1	1.85	1.05
1:HB:48:ALA:CA	1:WB:184:ALA:HB1	1.87	1.05
1:MA:48:ALA:CA	1:BB:184:ALA:HB1	1.86	1.05
1:JC:48:ALA:HB1	1:YC:184:ALA:HB1	1.38	1.05
1:Q:48:ALA:CA	1:GA:184:ALA:HB1	1.85	1.05
1:XC:48:ALA:CA	1:MD:184:ALA:HB1	1.87	1.05
1:QC:48:ALA:CB	1:FD:184:ALA:HB1	1.86	1.04
1:K:184:ALA:HB1	1:LD:48:ALA:CB	1.87	1.04
1:JC:48:ALA:CB	1:YC:184:ALA:HB1	1.88	1.04
1:AB:48:ALA:CB	1:PB:184:ALA:HB1	1.87	1.04
1:OB:48:ALA:CA	1:DC:184:ALA:HB1	1.87	1.04
1:J:48:ALA:CB	1:Z:184:ALA:HB1	1.88	1.04
1:VB:48:ALA:CB	1:KC:184:ALA:HB1	1.87	1.04
1:D:184:ALA:HB1	1:ED:48:ALA:CB	1.89	1.03
1:FA:48:ALA:CB	1:UA:184:ALA:HB1	1.88	1.03
1:TA:48:ALA:HB1	1:IB:184:ALA:HB1	1.38	1.03
1:AB:48:ALA:HB1	1:PB:184:ALA:HB1	1.38	1.03
1:C:48:ALA:CB	1:R:184:ALA:HB1	1.88	1.03
1:Y:48:ALA:CB	1:NA:184:ALA:HB1	1.88	1.03
1:CC:48:ALA:HB1	1:RC:184:ALA:HB1	1.40	1.03
1:YC:52:ALA:HB1	1:ND:180:SER:CB	1.88	1.03
1:D:184:ALA:HB1	1:ED:48:ALA:HB1	1.40	1.03
1:K:184:ALA:HB1	1:LD:48:ALA:HB1	1.37	1.02
1:MA:48:ALA:CB	1:BB:184:ALA:HB1	1.89	1.02
1:CC:48:ALA:CB	1:RC:184:ALA:HB1	1.89	1.02
1:Q:48:ALA:CB	1:GA:184:ALA:HB1	1.89	1.01
1:C:48:ALA:HB1	1:R:184:ALA:HB1	1.39	1.01
1:MA:48:ALA:HB1	1:BB:184:ALA:HB1	1.40	1.01
1:HB:48:ALA:HB1	1:WB:184:ALA:HB1	1.42	1.01
1:OB:48:ALA:HB1	1:DC:184:ALA:HB1	1.43	1.01
1:AB:48:ALA:HB1	1:PB:184:ALA:CB	1.91	1.01
1:IB:52:ALA:HB1	1:XB:180:SER:CB	1.89	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:48:ALA:HB1	1:Z:184:ALA:HB1	1.39	1.00
1:VB:48:ALA:HB1	1:KC:184:ALA:CB	1.91	1.00
1:QC:48:ALA:HB1	1:FD:184:ALA:CB	1.91	1.00
1:FA:48:ALA:HB1	1:UA:184:ALA:HB1	1.39	1.00
1:NA:52:ALA:HB1	1:CB:180:SER:CB	1.90	1.00
1:OB:48:ALA:CB	1:DC:184:ALA:HB1	1.92	1.00
1:Y:48:ALA:HB1	1:NA:184:ALA:HB1	1.40	1.00
1:HB:48:ALA:CB	1:WB:184:ALA:HB1	1.91	1.00
1:XC:48:ALA:CB	1:MD:184:ALA:HB1	1.92	1.00
1:E:180:SER:CB	1:FD:52:ALA:HB1	1.91	1.00
1:Q:48:ALA:HB1	1:GA:184:ALA:HB1	1.40	0.99
1:XC:48:ALA:HB1	1:MD:184:ALA:HB1	1.43	0.99
1:TA:48:ALA:HB1	1:IB:184:ALA:CB	1.91	0.99
1:K:184:ALA:CB	1:LD:48:ALA:HB1	1.91	0.99
1:J:48:ALA:HB1	1:Z:184:ALA:CB	1.92	0.98
1:GA:52:ALA:HB1	1:VA:180:SER:CB	1.91	0.98
1:PB:52:ALA:HB1	1:EC:180:SER:CB	1.88	0.98
1:D:52:ALA:HB1	1:S:180:SER:CB	1.91	0.98
1:Z:52:ALA:HB1	1:OA:180:SER:CB	1.91	0.98
1:JC:48:ALA:HB1	1:YC:184:ALA:CB	1.92	0.98
1:R:52:ALA:HB1	1:HA:180:SER:CB	1.91	0.98
1:CC:48:ALA:HB1	1:RC:184:ALA:CB	1.93	0.98
1:K:52:ALA:HB1	1:AA:180:SER:CB	1.92	0.98
1:FA:48:ALA:HB1	1:UA:184:ALA:CB	1.93	0.98
1:MA:52:ALA:HB2	1:BB:180:SER:O	1.65	0.97
1:UA:52:ALA:HB1	1:JB:180:SER:CB	1.93	0.97
1:FA:52:ALA:HB2	1:UA:180:SER:O	1.65	0.97
1:BB:52:ALA:HB1	1:QB:180:SER:CB	1.92	0.97
1:C:48:ALA:HB1	1:R:184:ALA:CB	1.93	0.97
1:TA:52:ALA:HB2	1:IB:180:SER:O	1.65	0.97
1:L:180:SER:CB	1:MD:52:ALA:HB1	1.92	0.97
1:Y:52:ALA:HB2	1:NA:180:SER:O	1.65	0.97
1:MA:48:ALA:HB1	1:BB:184:ALA:CB	1.94	0.97
1:HB:52:ALA:HB2	1:WB:180:SER:O	1.65	0.97
1:AB:52:ALA:HB2	1:PB:180:SER:O	1.65	0.97
1:J:52:ALA:HB2	1:Z:180:SER:O	1.65	0.97
1:RC:52:ALA:HB1	1:GD:180:SER:CB	1.92	0.97
1:Q:48:ALA:HB1	1:GA:184:ALA:CB	1.93	0.97
1:D:184:ALA:CB	1:ED:48:ALA:HB1	1.93	0.96
1:Q:52:ALA:HB2	1:GA:180:SER:O	1.65	0.96
1:OB:52:ALA:HB2	1:DC:180:SER:O	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KC:52:ALA:HB1	1:ZC:180:SER:CB	1.92	0.96
1:Y:48:ALA:HB1	1:NA:184:ALA:CB	1.93	0.96
1:C:52:ALA:HB2	1:R:180:SER:O	1.65	0.96
1:Y:48:ALA:O	1:NA:184:ALA:HB2	1.66	0.96
1:FA:48:ALA:O	1:UA:184:ALA:HB2	1.66	0.96
1:XC:52:ALA:HB2	1:MD:180:SER:O	1.65	0.96
1:VB:52:ALA:HB2	1:KC:180:SER:O	1.65	0.96
1:CC:52:ALA:HB2	1:RC:180:SER:O	1.65	0.96
1:DC:52:ALA:HB1	1:SC:180:SER:CB	1.91	0.96
1:D:180:SER:O	1:ED:52:ALA:HB2	1.65	0.95
1:AB:48:ALA:O	1:PB:184:ALA:HB2	1.67	0.95
1:HB:48:ALA:HB1	1:WB:184:ALA:CB	1.96	0.95
1:VB:48:ALA:O	1:KC:184:ALA:HB2	1.66	0.95
1:C:48:ALA:O	1:R:184:ALA:HB2	1.66	0.95
1:J:48:ALA:O	1:Z:184:ALA:HB2	1.66	0.95
1:K:180:SER:O	1:LD:52:ALA:HB2	1.65	0.95
1:JC:52:ALA:HB2	1:YC:180:SER:O	1.65	0.95
1:J:184:ALA:HB1	1:KD:48:ALA:HB1	0.95	0.95
1:OB:48:ALA:O	1:DC:184:ALA:HB2	1.66	0.95
1:QC:52:ALA:HB2	1:FD:180:SER:O	1.65	0.95
1:HB:48:ALA:O	1:WB:184:ALA:HB2	1.66	0.94
1:D:184:ALA:HB2	1:ED:48:ALA:O	1.66	0.94
1:Q:48:ALA:O	1:GA:184:ALA:HB2	1.66	0.94
1:TA:48:ALA:O	1:IB:184:ALA:HB2	1.66	0.94
1:XC:48:ALA:HB1	1:MD:184:ALA:CB	1.96	0.94
1:CC:48:ALA:O	1:RC:184:ALA:HB2	1.66	0.94
1:QC:48:ALA:O	1:FD:184:ALA:HB2	1.66	0.94
1:MA:48:ALA:O	1:BB:184:ALA:HB2	1.66	0.94
1:WB:52:ALA:HB1	1:LC:180:SER:CB	1.92	0.94
1:JC:48:ALA:O	1:YC:184:ALA:HB2	1.66	0.94
1:XC:48:ALA:O	1:MD:184:ALA:HB2	1.66	0.94
1:NB:48:ALA:HB1	1:CC:184:ALA:HB1	0.95	0.94
1:OB:48:ALA:HB1	1:DC:184:ALA:CB	1.97	0.94
1:PC:48:ALA:HB1	1:ED:184:ALA:HB1	0.94	0.94
1:K:184:ALA:HB2	1:LD:48:ALA:O	1.66	0.93
1:P:48:ALA:HB1	1:FA:184:ALA:HB1	0.94	0.93
1:BC:48:ALA:HB1	1:QC:184:ALA:HB1	0.94	0.93
1:C:184:ALA:HB1	1:DD:48:ALA:HB1	0.93	0.93
1:IC:48:ALA:HB1	1:XC:184:ALA:HB1	0.94	0.92
1:DA:31:GLN:CB	1:EA:12:SER:N	2.33	0.92
1:W:31:GLN:CB	1:X:12:SER:N	2.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:48:ALA:HB1	1:TA:184:ALA:HB1	0.93	0.92
1:KA:31:GLN:CB	1:LA:12:SER:N	2.33	0.92
1:O:31:GLN:CB	1:P:12:SER:N	2.33	0.92
1:UB:48:ALA:HB1	1:JC:184:ALA:HB1	0.92	0.92
1:GB:48:ALA:HB1	1:VB:184:ALA:HB1	0.94	0.91
1:X:48:ALA:HB1	1:MA:184:ALA:HB1	0.93	0.91
1:RA:31:GLN:CB	1:SA:12:SER:N	2.33	0.91
1:H:31:GLN:CB	1:I:12:SER:N	2.33	0.91
1:YA:31:GLN:CB	1:ZA:12:SER:N	2.33	0.91
1:A:31:GLN:CB	1:B:12:SER:N	2.33	0.91
1:WC:48:ALA:HB1	1:LD:184:ALA:HB1	0.92	0.91
1:LA:48:ALA:HB1	1:AB:184:ALA:HB1	0.93	0.91
1:FB:31:GLN:CB	1:GB:12:SER:N	2.33	0.91
1:AC:31:GLN:CB	1:BC:12:SER:N	2.33	0.91
1:CD:31:GLN:CB	1:DD:12:SER:N	2.33	0.91
1:B:48:ALA:HB1	1:Q:184:ALA:HB1	0.92	0.91
1:I:48:ALA:HB1	1:Y:184:ALA:HB1	0.91	0.91
1:MB:31:GLN:CB	1:NB:12:SER:N	2.33	0.91
1:VC:31:GLN:CB	1:WC:12:SER:N	2.33	0.91
1:JD:31:GLN:CB	1:KD:12:SER:N	2.33	0.91
1:TB:31:GLN:CB	1:UB:12:SER:N	2.33	0.90
1:HC:31:GLN:CB	1:IC:12:SER:N	2.33	0.90
1:OC:31:GLN:CB	1:PC:12:SER:N	2.33	0.90
1:TA:52:ALA:HB1	1:IB:180:SER:CA	2.02	0.90
1:AB:52:ALA:HB1	1:PB:180:SER:CA	2.01	0.90
1:VB:52:ALA:HB1	1:KC:180:SER:CA	2.03	0.89
1:Y:52:ALA:HB1	1:NA:180:SER:CA	2.03	0.89
1:MA:52:ALA:HB1	1:BB:180:SER:CA	2.03	0.89
1:CC:52:ALA:HB1	1:RC:180:SER:CA	2.03	0.89
1:C:52:ALA:HB1	1:R:180:SER:CA	2.03	0.89
1:Q:52:ALA:HB1	1:GA:180:SER:CA	2.03	0.88
1:QC:52:ALA:HB1	1:FD:180:SER:CA	2.03	0.88
1:J:52:ALA:HB1	1:Z:180:SER:CA	2.02	0.88
1:XC:52:ALA:HB1	1:MD:180:SER:CA	2.03	0.88
1:ZA:48:ALA:HB1	1:OB:184:ALA:HB1	0.90	0.88
1:FA:52:ALA:HB1	1:UA:180:SER:CA	2.03	0.88
1:K:180:SER:CA	1:LD:52:ALA:HB1	2.03	0.88
1:KA:31:GLN:CB	1:LA:12:SER:H	1.87	0.88
1:SA:48:ALA:HB1	1:HB:184:ALA:HB1	0.91	0.88
1:DA:31:GLN:CB	1:EA:12:SER:H	1.87	0.87
1:W:31:GLN:CB	1:X:12:SER:H	1.87	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:31:GLN:CB	1:SA:12:SER:H	1.87	0.87
1:JC:52:ALA:HB1	1:YC:180:SER:CA	2.03	0.87
1:O:31:GLN:CB	1:P:12:SER:H	1.87	0.87
1:VC:31:GLN:CB	1:WC:12:SER:H	1.87	0.87
1:YA:31:GLN:CB	1:ZA:12:SER:H	1.87	0.87
1:OB:52:ALA:HB1	1:DC:180:SER:CA	2.04	0.87
1:H:31:GLN:CB	1:I:12:SER:H	1.87	0.87
1:D:180:SER:CA	1:ED:52:ALA:HB1	2.03	0.87
1:HB:52:ALA:HB1	1:WB:180:SER:CA	2.04	0.87
1:OC:31:GLN:CB	1:PC:12:SER:H	1.87	0.87
1:A:31:GLN:CB	1:B:12:SER:H	1.87	0.86
1:FB:31:GLN:CB	1:GB:12:SER:H	1.87	0.86
1:MB:31:GLN:CB	1:NB:12:SER:H	1.87	0.86
1:CD:31:GLN:CB	1:DD:12:SER:H	1.87	0.86
1:JD:31:GLN:CB	1:KD:12:SER:H	1.87	0.86
1:TB:31:GLN:CB	1:UB:12:SER:H	1.87	0.86
1:AC:31:GLN:CB	1:BC:12:SER:H	1.87	0.86
1:HC:31:GLN:CB	1:IC:12:SER:H	1.87	0.85
1:OB:52:ALA:CB	1:DC:180:SER:O	2.25	0.85
1:Y:52:ALA:CB	1:NA:180:SER:O	2.26	0.84
1:K:180:SER:O	1:LD:52:ALA:CB	2.26	0.83
1:FA:52:ALA:CB	1:UA:180:SER:O	2.26	0.83
1:JC:52:ALA:CB	1:YC:180:SER:O	2.26	0.83
1:XC:52:ALA:CB	1:MD:180:SER:O	2.26	0.83
1:D:180:SER:O	1:ED:52:ALA:CB	2.26	0.83
1:C:52:ALA:CB	1:R:180:SER:O	2.26	0.83
1:YA:27:LYS:O	1:ZA:12:SER:CB	2.27	0.83
1:FB:27:LYS:O	1:GB:12:SER:CB	2.27	0.83
1:Q:52:ALA:CB	1:GA:180:SER:O	2.26	0.83
1:HB:52:ALA:CB	1:WB:180:SER:O	2.25	0.83
1:KA:27:LYS:O	1:LA:12:SER:CB	2.27	0.83
1:QC:52:ALA:CB	1:FD:180:SER:O	2.27	0.83
1:MA:52:ALA:CB	1:BB:180:SER:O	2.26	0.83
1:MB:27:LYS:O	1:NB:12:SER:CB	2.27	0.83
1:DA:27:LYS:O	1:EA:12:SER:CB	2.27	0.82
1:TB:27:LYS:O	1:UB:12:SER:CB	2.27	0.82
1:VB:52:ALA:CB	1:KC:180:SER:O	2.27	0.82
1:O:27:LYS:O	1:P:12:SER:CB	2.27	0.82
1:AC:27:LYS:O	1:BC:12:SER:CB	2.27	0.82
1:CC:52:ALA:CB	1:RC:180:SER:O	2.26	0.82
1:J:52:ALA:CB	1:Z:180:SER:O	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:27:LYS:O	1:SA:12:SER:CB	2.27	0.82
1:TB:31:GLN:CB	1:UB:12:SER:CB	2.58	0.82
1:HC:27:LYS:O	1:IC:12:SER:CB	2.27	0.82
1:HC:31:GLN:CB	1:IC:12:SER:CB	2.58	0.82
1:J:184:ALA:CA	1:KD:48:ALA:HB1	2.09	0.82
1:RA:31:GLN:CB	1:SA:12:SER:CB	2.58	0.82
1:FB:31:GLN:CB	1:GB:12:SER:CB	2.58	0.82
1:TA:52:ALA:CB	1:IB:180:SER:O	2.27	0.82
1:AB:52:ALA:CB	1:PB:180:SER:O	2.28	0.82
1:MB:31:GLN:CB	1:NB:12:SER:CB	2.58	0.82
1:A:27:LYS:O	1:B:12:SER:CB	2.27	0.82
1:KA:31:GLN:CB	1:LA:12:SER:CB	2.58	0.82
1:YA:31:GLN:CB	1:ZA:12:SER:CB	2.58	0.82
1:AC:31:GLN:CB	1:BC:12:SER:CB	2.58	0.82
1:JD:27:LYS:O	1:KD:12:SER:CB	2.27	0.82
1:W:27:LYS:O	1:X:12:SER:CB	2.27	0.81
1:DA:31:GLN:CB	1:EA:12:SER:CB	2.58	0.81
1:OC:31:GLN:CB	1:PC:12:SER:CB	2.58	0.81
1:VC:27:LYS:O	1:WC:12:SER:CB	2.27	0.81
1:VC:31:GLN:CB	1:WC:12:SER:CB	2.58	0.81
1:H:27:LYS:O	1:I:12:SER:CB	2.27	0.81
1:I:48:ALA:HB1	1:Y:184:ALA:CA	2.10	0.81
1:EA:48:ALA:HB1	1:TA:184:ALA:CA	2.10	0.81
1:OB:48:ALA:O	1:DC:184:ALA:CB	2.27	0.81
1:OC:27:LYS:O	1:PC:12:SER:CB	2.27	0.81
1:CD:27:LYS:O	1:DD:12:SER:CB	2.27	0.81
1:B:48:ALA:HB1	1:Q:184:ALA:CA	2.11	0.81
1:W:31:GLN:CB	1:X:12:SER:CB	2.58	0.81
1:HB:48:ALA:O	1:WB:184:ALA:CB	2.28	0.81
1:PC:48:ALA:HB1	1:ED:184:ALA:CA	2.09	0.81
1:D:184:ALA:CB	1:ED:48:ALA:O	2.29	0.81
1:Q:48:ALA:O	1:GA:184:ALA:CB	2.28	0.81
1:CD:31:GLN:CB	1:DD:12:SER:CB	2.58	0.81
1:X:48:ALA:HB1	1:MA:184:ALA:CA	2.11	0.81
1:SA:48:ALA:HB1	1:HB:184:ALA:CA	2.09	0.81
1:K:184:ALA:CB	1:LD:48:ALA:O	2.28	0.81
1:O:31:GLN:CB	1:P:12:SER:CB	2.58	0.81
1:A:31:GLN:CB	1:B:12:SER:CB	2.58	0.81
1:H:31:GLN:CB	1:I:12:SER:CB	2.58	0.81
1:ZA:48:ALA:HB1	1:OB:184:ALA:CA	2.10	0.81
1:IC:48:ALA:HB1	1:XC:184:ALA:CA	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XC:48:ALA:O	1:MD:184:ALA:CB	2.28	0.81
1:JD:31:GLN:CB	1:KD:12:SER:CB	2.58	0.81
1:UB:48:ALA:HB1	1:JC:184:ALA:CA	2.10	0.80
1:M:22:ALA:HB2	1:N:9:ARG:CB	2.12	0.80
1:MC:22:ALA:HB2	1:NC:9:ARG:CB	2.12	0.80
1:HD:22:ALA:HB2	1:ID:9:ARG:CB	2.12	0.80
1:T:22:ALA:HB2	1:V:9:ARG:CB	2.12	0.80
1:LA:48:ALA:HB1	1:AB:184:ALA:CA	2.11	0.80
1:PA:22:ALA:HB2	1:QA:9:ARG:CB	2.12	0.80
1:Y:48:ALA:O	1:NA:184:ALA:CB	2.29	0.80
1:MA:48:ALA:O	1:BB:184:ALA:CB	2.29	0.80
1:IA:22:ALA:HB2	1:JA:9:ARG:CB	2.12	0.80
1:OD:22:ALA:HB2	1:PD:9:ARG:CB	2.12	0.80
1:FC:22:ALA:HB2	1:GC:9:ARG:CB	2.12	0.80
1:TC:22:ALA:HB2	1:UC:9:ARG:CB	2.12	0.80
1:XC:52:ALA:HB1	1:MD:180:SER:C	2.07	0.80
1:P:48:ALA:HB1	1:FA:184:ALA:CA	2.11	0.80
1:KB:22:ALA:HB2	1:LB:9:ARG:CB	2.12	0.80
1:CC:48:ALA:O	1:RC:184:ALA:CB	2.28	0.80
1:JC:48:ALA:O	1:YC:184:ALA:CB	2.29	0.80
1:AD:22:ALA:HB2	1:BD:9:ARG:CB	2.12	0.80
1:RB:22:ALA:HB2	1:SB:9:ARG:CB	2.12	0.80
1:BC:48:ALA:HB1	1:QC:184:ALA:CA	2.11	0.79
1:C:48:ALA:O	1:R:184:ALA:CB	2.29	0.79
1:C:184:ALA:CA	1:DD:48:ALA:HB1	2.11	0.79
1:FA:48:ALA:O	1:UA:184:ALA:CB	2.29	0.79
1:OB:52:ALA:HB1	1:DC:180:SER:C	2.07	0.79
1:HB:52:ALA:HB1	1:WB:180:SER:C	2.07	0.79
1:VB:48:ALA:O	1:KC:184:ALA:CB	2.29	0.79
1:F:22:ALA:HB2	1:G:9:ARG:CB	2.12	0.79
1:BA:22:ALA:HB2	1:CA:9:ARG:CB	2.12	0.79
1:DB:22:ALA:HB2	1:EB:9:ARG:CB	2.11	0.79
1:TA:48:ALA:O	1:IB:184:ALA:CB	2.30	0.79
1:WA:22:ALA:HB2	1:XA:9:ARG:CB	2.12	0.79
1:J:48:ALA:O	1:Z:184:ALA:CB	2.30	0.79
1:AB:48:ALA:O	1:PB:184:ALA:CB	2.30	0.79
1:MA:52:ALA:HB1	1:BB:180:SER:C	2.08	0.79
1:YB:22:ALA:HB2	1:ZB:9:ARG:CB	2.12	0.79
1:Q:52:ALA:HB1	1:GA:180:SER:C	2.09	0.78
1:QC:48:ALA:O	1:FD:184:ALA:CB	2.29	0.78
1:Y:52:ALA:HB1	1:NA:180:SER:C	2.09	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:SER:C	1:ED:52:ALA:HB1	2.09	0.78
1:GB:48:ALA:HB1	1:VB:184:ALA:CA	2.13	0.78
1:PA:22:ALA:CB	1:QA:9:ARG:CB	2.62	0.78
1:YB:22:ALA:CB	1:ZB:9:ARG:CB	2.62	0.78
1:WC:48:ALA:HB1	1:LD:184:ALA:CA	2.13	0.78
1:FA:52:ALA:HB1	1:UA:180:SER:C	2.09	0.78
1:IA:22:ALA:CB	1:JA:9:ARG:CB	2.62	0.78
1:FC:22:ALA:CB	1:GC:9:ARG:CB	2.62	0.78
1:BA:22:ALA:CB	1:CA:9:ARG:CB	2.62	0.78
1:WA:22:ALA:CB	1:XA:9:ARG:CB	2.62	0.78
1:DB:22:ALA:CB	1:EB:9:ARG:CB	2.62	0.78
1:RB:22:ALA:CB	1:SB:9:ARG:CB	2.62	0.78
1:KB:22:ALA:CB	1:LB:9:ARG:CB	2.62	0.78
1:T:22:ALA:CB	1:V:9:ARG:CB	2.62	0.78
1:CC:52:ALA:HB1	1:RC:180:SER:C	2.08	0.78
1:MC:22:ALA:CB	1:NC:9:ARG:CB	2.62	0.78
1:M:22:ALA:CB	1:N:9:ARG:CB	2.62	0.77
1:F:22:ALA:CB	1:G:9:ARG:CB	2.62	0.77
1:K:180:SER:C	1:LD:52:ALA:HB1	2.10	0.77
1:TC:22:ALA:CB	1:UC:9:ARG:CB	2.62	0.77
1:C:52:ALA:HB1	1:R:180:SER:C	2.09	0.77
1:TA:52:ALA:HB1	1:IB:180:SER:C	2.10	0.77
1:OD:22:ALA:CB	1:PD:9:ARG:CB	2.62	0.77
1:J:52:ALA:HB1	1:Z:180:SER:C	2.09	0.77
1:JC:52:ALA:HB1	1:YC:180:SER:C	2.09	0.77
1:AD:22:ALA:CB	1:BD:9:ARG:CB	2.62	0.77
1:HD:22:ALA:CB	1:ID:9:ARG:CB	2.62	0.77
1:NB:48:ALA:HB1	1:CC:184:ALA:CA	2.13	0.77
1:J:48:ALA:HA	1:Z:184:ALA:HB1	1.66	0.77
1:AB:52:ALA:HB1	1:PB:180:SER:C	2.09	0.77
1:QC:52:ALA:HB1	1:FD:180:SER:C	2.10	0.77
1:VB:52:ALA:HB1	1:KC:180:SER:C	2.09	0.76
1:C:48:ALA:HA	1:R:184:ALA:HB1	1.67	0.76
1:XC:48:ALA:HA	1:MD:184:ALA:HB1	1.67	0.76
1:D:184:ALA:HB1	1:ED:48:ALA:HA	1.67	0.75
1:Q:48:ALA:HA	1:GA:184:ALA:HB1	1.68	0.75
1:Y:48:ALA:HA	1:NA:184:ALA:HB1	1.68	0.75
1:TA:48:ALA:HA	1:IB:184:ALA:HB1	1.66	0.75
1:VB:48:ALA:HA	1:KC:184:ALA:HB1	1.67	0.75
1:FA:48:ALA:HA	1:UA:184:ALA:HB1	1.67	0.74
1:QC:48:ALA:HA	1:FD:184:ALA:HB1	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JC:48:ALA:HA	1:YC:184:ALA:HB1	1.68	0.74
1:K:184:ALA:HB1	1:LD:48:ALA:HA	1.68	0.74
1:MA:48:ALA:HA	1:BB:184:ALA:HB1	1.67	0.74
1:CC:48:ALA:HA	1:RC:184:ALA:HB1	1.68	0.74
1:AB:48:ALA:HA	1:PB:184:ALA:HB1	1.66	0.73
1:HB:48:ALA:HA	1:WB:184:ALA:HB1	1.68	0.73
1:OB:48:ALA:HA	1:DC:184:ALA:HB1	1.69	0.72
1:XC:52:ALA:CB	1:MD:180:SER:C	2.62	0.72
1:HB:52:ALA:CB	1:WB:180:SER:C	2.63	0.72
1:Y:52:ALA:CB	1:NA:180:SER:C	2.63	0.71
1:FA:52:ALA:CB	1:UA:180:SER:C	2.63	0.71
1:MA:52:ALA:CB	1:BB:180:SER:C	2.63	0.71
1:AB:52:ALA:CB	1:PB:180:SER:C	2.63	0.71
1:CC:52:ALA:CB	1:RC:180:SER:C	2.63	0.71
1:CB:52:ALA:HA	1:RB:179:GLU:CB	2.20	0.71
1:C:52:ALA:CB	1:R:180:SER:C	2.63	0.71
1:D:180:SER:C	1:ED:52:ALA:CB	2.63	0.71
1:JC:52:ALA:CB	1:YC:180:SER:C	2.64	0.71
1:J:52:ALA:CB	1:Z:180:SER:C	2.63	0.71
1:VB:52:ALA:CB	1:KC:180:SER:C	2.63	0.71
1:OB:52:ALA:CB	1:DC:180:SER:C	2.63	0.71
1:Q:52:ALA:CB	1:GA:180:SER:C	2.63	0.71
1:QC:52:ALA:CB	1:FD:180:SER:C	2.64	0.71
1:VA:52:ALA:HA	1:KB:179:GLU:CB	2.21	0.71
1:TA:52:ALA:CB	1:IB:180:SER:C	2.63	0.70
1:L:52:ALA:HA	1:BA:179:GLU:CB	2.21	0.70
1:ZC:52:ALA:HA	1:OD:179:GLU:CB	2.22	0.70
1:K:180:SER:C	1:LD:52:ALA:CB	2.64	0.70
1:XB:52:ALA:HA	1:MC:179:GLU:CB	2.22	0.70
1:K:184:ALA:HB1	1:LD:48:ALA:C	2.17	0.69
1:F:179:GLU:CB	1:GD:52:ALA:HA	2.22	0.69
1:E:52:ALA:HA	1:T:179:GLU:CB	2.22	0.69
1:AA:52:ALA:HA	1:PA:179:GLU:CB	2.23	0.69
1:OA:52:ALA:HA	1:DB:179:GLU:CB	2.22	0.69
1:EC:52:ALA:HA	1:TC:179:GLU:CB	2.23	0.69
1:JC:48:ALA:C	1:YC:184:ALA:HB1	2.18	0.69
1:OB:48:ALA:C	1:DC:184:ALA:HB1	2.17	0.69
1:S:52:ALA:HA	1:IA:179:GLU:CB	2.23	0.68
1:ZA:52:ALA:HB1	1:OB:180:SER:CB	2.23	0.68
1:SC:52:ALA:HA	1:HD:179:GLU:CB	2.23	0.68
1:HA:52:ALA:HA	1:WA:179:GLU:CB	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HB:48:ALA:C	1:WB:184:ALA:HB1	2.18	0.68
1:QB:52:ALA:HA	1:FC:179:GLU:CB	2.24	0.68
1:QC:48:ALA:C	1:FD:184:ALA:HB1	2.18	0.68
1:JB:52:ALA:HA	1:YB:179:GLU:CB	2.23	0.68
1:LC:52:ALA:HA	1:AD:179:GLU:CB	2.23	0.68
1:D:184:ALA:HB1	1:ED:48:ALA:C	2.18	0.68
1:MA:48:ALA:C	1:BB:184:ALA:HB1	2.18	0.68
1:C:48:ALA:C	1:R:184:ALA:HB1	2.18	0.68
1:FA:48:ALA:C	1:UA:184:ALA:HB1	2.18	0.68
1:Q:48:ALA:C	1:GA:184:ALA:HB1	2.18	0.67
1:I:52:ALA:HB1	1:Y:180:SER:CB	2.24	0.67
1:SA:52:ALA:HB1	1:HB:180:SER:CB	2.24	0.67
1:VB:48:ALA:C	1:KC:184:ALA:HB1	2.18	0.67
1:Y:48:ALA:C	1:NA:184:ALA:HB1	2.18	0.67
1:TA:48:ALA:C	1:IB:184:ALA:HB1	2.19	0.67
1:CC:48:ALA:C	1:RC:184:ALA:HB1	2.18	0.67
1:WC:52:ALA:HB1	1:LD:180:SER:CB	2.24	0.67
1:J:48:ALA:HB1	1:Z:184:ALA:HB3	1.77	0.67
1:M:179:GLU:CB	1:ND:52:ALA:HA	2.24	0.67
1:LA:52:ALA:HB1	1:AB:180:SER:CB	2.25	0.67
1:ZA:48:ALA:HB3	1:OB:184:ALA:HB1	1.72	0.67
1:AB:48:ALA:C	1:PB:184:ALA:HB1	2.20	0.67
1:XC:48:ALA:C	1:MD:184:ALA:HB1	2.19	0.67
1:YA:53:ALA:HB1	1:FB:137:GLU:CB	2.25	0.67
1:C:184:ALA:HB1	1:DD:48:ALA:HB3	1.74	0.66
1:EA:52:ALA:HB1	1:TA:180:SER:CB	2.26	0.66
1:X:52:ALA:HB1	1:MA:180:SER:CB	2.26	0.66
1:K:184:ALA:HB3	1:LD:48:ALA:HB1	1.78	0.66
1:P:52:ALA:HB1	1:FA:180:SER:CB	2.26	0.66
1:GB:52:ALA:HB1	1:VB:180:SER:CB	2.25	0.66
1:B:52:ALA:HB1	1:Q:180:SER:CB	2.25	0.66
1:AB:48:ALA:HB1	1:PB:184:ALA:HB3	1.76	0.66
1:PA:161:THR:O	1:PA:165:MET:N	2.24	0.66
1:AC:53:ALA:HB1	1:HC:137:GLU:CB	2.26	0.66
1:LA:48:ALA:HB3	1:AB:184:ALA:HB1	1.74	0.66
1:WA:161:THR:O	1:WA:165:MET:N	2.24	0.66
1:UB:52:ALA:HB1	1:JC:180:SER:CB	2.25	0.66
1:J:48:ALA:C	1:Z:184:ALA:HB1	2.19	0.65
1:IA:161:THR:O	1:IA:165:MET:N	2.24	0.65
1:DB:161:THR:O	1:DB:165:MET:N	2.24	0.65
1:KB:161:THR:O	1:KB:165:MET:N	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:SER:CB	1:DD:52:ALA:HB1	2.25	0.65
1:I:48:ALA:HB3	1:Y:184:ALA:HB1	1.73	0.65
1:PC:48:ALA:HB3	1:ED:184:ALA:HB1	1.72	0.65
1:BA:161:THR:O	1:BA:165:MET:N	2.24	0.65
1:RB:161:THR:O	1:RB:165:MET:N	2.24	0.65
1:QC:48:ALA:HB1	1:FD:184:ALA:HB3	1.77	0.65
1:X:48:ALA:HB3	1:MA:184:ALA:HB1	1.74	0.65
1:YB:161:THR:O	1:YB:165:MET:N	2.24	0.65
1:Y:48:ALA:C	1:NA:184:ALA:CB	2.70	0.65
1:FA:48:ALA:C	1:UA:184:ALA:CB	2.70	0.65
1:TA:48:ALA:C	1:IB:184:ALA:CB	2.70	0.65
1:VB:48:ALA:C	1:KC:184:ALA:CB	2.70	0.65
1:FC:161:THR:O	1:FC:165:MET:N	2.24	0.65
1:QC:48:ALA:C	1:FD:184:ALA:CB	2.69	0.65
1:K:184:ALA:CB	1:LD:48:ALA:C	2.69	0.65
1:TA:48:ALA:HB1	1:IB:184:ALA:HB3	1.76	0.65
1:NB:52:ALA:HB1	1:CC:180:SER:CB	2.26	0.65
1:BC:52:ALA:HB1	1:QC:180:SER:CB	2.26	0.65
1:C:48:ALA:C	1:R:184:ALA:CB	2.70	0.65
1:D:184:ALA:CB	1:ED:48:ALA:C	2.70	0.65
1:J:48:ALA:C	1:Z:184:ALA:CB	2.70	0.65
1:T:161:THR:O	1:T:165:MET:N	2.24	0.65
1:OB:48:ALA:C	1:DC:184:ALA:CB	2.70	0.65
1:MC:161:THR:O	1:MC:165:MET:N	2.24	0.65
1:Y:48:ALA:HB1	1:NA:184:ALA:HB3	1.78	0.65
1:DA:53:ALA:HB1	1:KA:137:GLU:CB	2.27	0.65
1:TC:161:THR:O	1:TC:165:MET:N	2.24	0.65
1:M:161:THR:O	1:M:165:MET:N	2.24	0.65
1:JC:48:ALA:C	1:YC:184:ALA:CB	2.69	0.65
1:PC:52:ALA:HB1	1:ED:180:SER:CB	2.27	0.65
1:AD:161:THR:O	1:AD:165:MET:N	2.24	0.64
1:IC:52:ALA:HB1	1:XC:180:SER:CB	2.26	0.64
1:F:161:THR:O	1:F:165:MET:N	2.24	0.64
1:VB:48:ALA:HB1	1:KC:184:ALA:HB3	1.77	0.64
1:HD:161:THR:O	1:HD:165:MET:N	2.24	0.64
1:O:53:ALA:HB1	1:W:137:GLU:CB	2.27	0.64
1:CC:48:ALA:C	1:RC:184:ALA:CB	2.70	0.64
1:XC:48:ALA:C	1:MD:184:ALA:CB	2.71	0.64
1:OD:161:THR:O	1:OD:165:MET:N	2.24	0.64
1:FB:53:ALA:HB1	1:MB:137:GLU:CB	2.28	0.64
1:AB:48:ALA:C	1:PB:184:ALA:CB	2.70	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OC:53:ALA:HB1	1:VC:137:GLU:CB	2.27	0.64
1:XC:48:ALA:HB1	1:MD:184:ALA:HB3	1.80	0.64
1:RA:53:ALA:HB1	1:YA:137:GLU:CB	2.28	0.64
1:HB:48:ALA:C	1:WB:184:ALA:CB	2.70	0.64
1:H:53:ALA:HB1	1:O:137:GLU:CB	2.27	0.64
1:MA:48:ALA:C	1:BB:184:ALA:CB	2.70	0.64
1:MA:48:ALA:HB1	1:BB:184:ALA:HB3	1.79	0.63
1:D:184:ALA:HB3	1:ED:48:ALA:HB1	1.78	0.63
1:Q:48:ALA:C	1:GA:184:ALA:CB	2.70	0.63
1:M:179:GLU:CB	1:ND:52:ALA:HB1	2.29	0.63
1:NB:32:ALA:HB2	1:UB:167:ALA:CB	2.29	0.63
1:WC:32:ALA:HB2	1:DD:167:ALA:CB	2.29	0.63
1:BC:48:ALA:HB3	1:QC:184:ALA:HB1	1.74	0.63
1:CC:48:ALA:HB1	1:RC:184:ALA:HB3	1.79	0.63
1:VC:53:ALA:HB1	1:CD:137:GLU:CB	2.28	0.63
1:A:137:GLU:CB	1:JD:53:ALA:HB1	2.28	0.63
1:J:180:SER:CB	1:KD:52:ALA:HB1	2.27	0.63
1:SC:52:ALA:HB1	1:HD:179:GLU:CB	2.29	0.63
1:VA:52:ALA:HB1	1:KB:179:GLU:CB	2.29	0.63
1:CD:53:ALA:HB1	1:JD:137:GLU:CB	2.28	0.63
1:TB:53:ALA:HB1	1:AC:137:GLU:CB	2.29	0.63
1:DD:32:ALA:HB2	1:KD:167:ALA:CB	2.29	0.63
1:C:48:ALA:HB1	1:R:184:ALA:HB3	1.78	0.62
1:X:32:ALA:HB2	1:EA:167:ALA:CB	2.29	0.62
1:KA:53:ALA:HB1	1:RA:137:GLU:CB	2.28	0.62
1:IC:32:ALA:HB2	1:PC:167:ALA:CB	2.28	0.62
1:LA:32:ALA:HB2	1:SA:167:ALA:CB	2.29	0.62
1:GB:32:ALA:HB2	1:NB:167:ALA:CB	2.29	0.62
1:HA:52:ALA:HB1	1:WA:179:GLU:CB	2.30	0.62
1:MB:53:ALA:HB1	1:TB:137:GLU:CB	2.29	0.62
1:UB:32:ALA:HB2	1:BC:167:ALA:CB	2.29	0.62
1:A:53:ALA:HB1	1:H:137:GLU:CB	2.29	0.62
1:CB:52:ALA:HB1	1:RB:179:GLU:CB	2.30	0.62
1:XB:52:ALA:HB1	1:MC:179:GLU:CB	2.29	0.62
1:AA:52:ALA:HB1	1:PA:179:GLU:CB	2.30	0.62
1:LC:52:ALA:HB1	1:AD:179:GLU:CB	2.29	0.62
1:L:52:ALA:HB1	1:BA:179:GLU:CB	2.30	0.62
1:JC:48:ALA:HB1	1:YC:184:ALA:HB3	1.78	0.62
1:B:32:ALA:HB2	1:I:167:ALA:CB	2.29	0.62
1:I:32:ALA:HB2	1:P:167:ALA:CB	2.29	0.62
1:S:52:ALA:HB1	1:IA:179:GLU:CB	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:ALA:HB1	1:T:179:GLU:CB	2.30	0.62
1:P:32:ALA:HB2	1:X:167:ALA:CB	2.29	0.62
1:CB:52:ALA:CA	1:RB:179:GLU:CB	2.78	0.62
1:SA:32:ALA:HB2	1:ZA:167:ALA:CB	2.30	0.62
1:SA:48:ALA:HB3	1:HB:184:ALA:HB1	1.72	0.62
1:OA:52:ALA:HB1	1:DB:179:GLU:CB	2.31	0.61
1:VA:52:ALA:CA	1:KB:179:GLU:CB	2.78	0.61
1:EC:52:ALA:HB1	1:TC:179:GLU:CB	2.30	0.61
1:F:179:GLU:CB	1:GD:52:ALA:HB1	2.30	0.61
1:J:184:ALA:HB1	1:KD:48:ALA:HB3	1.72	0.61
1:HC:53:ALA:HB1	1:OC:137:GLU:CB	2.30	0.61
1:NB:48:ALA:HB3	1:CC:184:ALA:HB1	1.77	0.61
1:PC:32:ALA:HB2	1:WC:167:ALA:CB	2.31	0.61
1:W:53:ALA:HB1	1:DA:137:GLU:CB	2.29	0.61
1:ZA:32:ALA:HB2	1:GB:167:ALA:CB	2.30	0.61
1:EA:32:ALA:HB2	1:LA:167:ALA:CB	2.30	0.61
1:BC:32:ALA:HB2	1:IC:167:ALA:CB	2.30	0.61
1:B:167:ALA:CB	1:KD:32:ALA:HB2	2.30	0.61
1:L:52:ALA:CA	1:BA:179:GLU:CB	2.78	0.61
1:OA:52:ALA:CA	1:DB:179:GLU:CB	2.79	0.61
1:JB:52:ALA:HB1	1:YB:179:GLU:CB	2.31	0.60
1:Q:48:ALA:HB1	1:GA:184:ALA:HB3	1.79	0.60
1:HA:52:ALA:CA	1:WA:179:GLU:CB	2.79	0.60
1:QB:52:ALA:HB1	1:FC:179:GLU:CB	2.31	0.60
1:FA:48:ALA:HB1	1:UA:184:ALA:HB3	1.78	0.60
1:XB:52:ALA:CA	1:MC:179:GLU:CB	2.79	0.60
1:OB:48:ALA:HB1	1:DC:184:ALA:HB3	1.81	0.60
1:AA:52:ALA:CA	1:PA:179:GLU:CB	2.80	0.60
1:JB:52:ALA:CA	1:YB:179:GLU:CB	2.80	0.60
1:EC:52:ALA:CA	1:TC:179:GLU:CB	2.80	0.60
1:E:52:ALA:CA	1:T:179:GLU:CB	2.79	0.59
1:ZC:52:ALA:HB1	1:OD:179:GLU:CB	2.32	0.59
1:S:52:ALA:CA	1:IA:179:GLU:CB	2.80	0.59
1:LC:52:ALA:CA	1:AD:179:GLU:CB	2.80	0.59
1:SC:52:ALA:CA	1:HD:179:GLU:CB	2.80	0.59
1:ZC:52:ALA:CA	1:OD:179:GLU:CB	2.79	0.59
1:EA:48:ALA:HB3	1:TA:184:ALA:HB1	1.73	0.59
1:F:179:GLU:CB	1:GD:52:ALA:CA	2.79	0.59
1:KA:31:GLN:CB	1:LA:12:SER:CA	2.81	0.59
1:QB:52:ALA:CA	1:FC:179:GLU:CB	2.80	0.59
1:CD:31:GLN:CB	1:DD:12:SER:CA	2.81	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HC:31:GLN:CB	1:IC:12:SER:CA	2.81	0.59
1:W:31:GLN:CB	1:X:12:SER:CA	2.81	0.59
1:A:31:GLN:CB	1:B:12:SER:CA	2.81	0.59
1:RA:31:GLN:CB	1:SA:12:SER:CA	2.81	0.59
1:UB:48:ALA:HB3	1:JC:184:ALA:HB1	1.72	0.59
1:OC:31:GLN:CB	1:PC:12:SER:CA	2.81	0.59
1:O:31:GLN:CB	1:P:12:SER:CA	2.81	0.59
1:MB:31:GLN:CB	1:NB:12:SER:CA	2.81	0.59
1:FB:31:GLN:CB	1:GB:12:SER:CA	2.81	0.58
1:H:31:GLN:CB	1:I:12:SER:CA	2.81	0.58
1:VC:31:GLN:CB	1:WC:12:SER:CA	2.81	0.58
1:M:179:GLU:CB	1:ND:52:ALA:CA	2.80	0.58
1:HB:48:ALA:HB1	1:WB:184:ALA:HB3	1.81	0.58
1:WC:48:ALA:HB3	1:LD:184:ALA:HB1	1.76	0.58
1:AC:31:GLN:CB	1:BC:12:SER:CA	2.81	0.58
1:JD:31:GLN:CB	1:KD:12:SER:CA	2.81	0.58
1:DA:31:GLN:CB	1:EA:12:SER:CA	2.81	0.58
1:TB:31:GLN:CB	1:UB:12:SER:CA	2.81	0.58
1:RC:52:ALA:HB2	1:GD:180:SER:CA	2.33	0.58
1:IC:48:ALA:HB3	1:XC:184:ALA:HB1	1.73	0.58
1:D:52:ALA:HB2	1:S:180:SER:CA	2.33	0.58
1:YA:31:GLN:CB	1:ZA:12:SER:CA	2.81	0.58
1:YC:52:ALA:HB2	1:ND:180:SER:CA	2.33	0.58
1:WB:52:ALA:HB2	1:LC:180:SER:CA	2.33	0.57
1:GB:48:ALA:HB3	1:VB:184:ALA:HB1	1.76	0.57
1:NA:52:ALA:HB2	1:CB:180:SER:CA	2.33	0.57
1:UA:52:ALA:HB2	1:JB:180:SER:CA	2.33	0.57
1:BB:52:ALA:HB2	1:QB:180:SER:CA	2.33	0.57
1:P:48:ALA:HB3	1:FA:184:ALA:HB1	1.74	0.56
1:GA:52:ALA:HB2	1:VA:180:SER:CA	2.33	0.56
1:K:52:ALA:HB2	1:AA:180:SER:CA	2.33	0.56
1:Z:52:ALA:HB2	1:OA:180:SER:CA	2.33	0.56
1:IB:52:ALA:HB2	1:XB:180:SER:CA	2.33	0.56
1:R:52:ALA:HB2	1:HA:180:SER:CA	2.33	0.55
1:B:48:ALA:HB3	1:Q:184:ALA:HB1	1.73	0.55
1:L:52:ALA:CB	1:BA:179:GLU:CB	2.85	0.55
1:L:180:SER:CA	1:MD:52:ALA:HB2	2.34	0.55
1:PB:52:ALA:HB2	1:EC:180:SER:CA	2.33	0.55
1:XB:52:ALA:CB	1:MC:179:GLU:CB	2.85	0.55
1:E:180:SER:CA	1:FD:52:ALA:HB2	2.33	0.54
1:M:179:GLU:CB	1:ND:52:ALA:CB	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZC:52:ALA:HB2	1:OD:180:SER:N	2.22	0.54
1:E:52:ALA:CB	1:T:179:GLU:CB	2.86	0.54
1:VA:52:ALA:CB	1:KB:179:GLU:CB	2.85	0.54
1:HA:52:ALA:CB	1:WA:179:GLU:CB	2.86	0.54
1:TA:52:ALA:CB	1:IB:180:SER:CB	2.71	0.54
1:S:52:ALA:CB	1:IA:179:GLU:CB	2.86	0.54
1:AA:52:ALA:CB	1:PA:179:GLU:CB	2.86	0.54
1:QB:52:ALA:HB2	1:FC:180:SER:N	2.23	0.54
1:JB:52:ALA:HB2	1:YB:180:SER:N	2.23	0.54
1:SC:52:ALA:CB	1:HD:179:GLU:CB	2.85	0.54
1:F:179:GLU:CB	1:GD:52:ALA:CB	2.86	0.54
1:CB:52:ALA:CB	1:RB:179:GLU:CB	2.85	0.54
1:LC:52:ALA:CB	1:AD:179:GLU:CB	2.86	0.53
1:DC:52:ALA:HB2	1:SC:180:SER:CA	2.33	0.53
1:EC:52:ALA:CB	1:TC:179:GLU:CB	2.86	0.53
1:KC:52:ALA:HB2	1:ZC:180:SER:CA	2.33	0.53
1:E:52:ALA:HB2	1:T:180:SER:N	2.24	0.53
1:OA:52:ALA:HB2	1:DB:180:SER:N	2.24	0.53
1:EC:79:LEU:CB	1:ZC:217:MET:HA	2.39	0.53
1:J:52:ALA:CB	1:Z:180:SER:CB	2.71	0.53
1:OA:52:ALA:CB	1:DB:179:GLU:CB	2.86	0.53
1:AA:52:ALA:HB2	1:PA:180:SER:N	2.24	0.53
1:HA:52:ALA:HB2	1:WA:180:SER:N	2.24	0.53
1:KA:32:ALA:HB1	1:RA:158:GLY:HA3	1.91	0.53
1:EC:52:ALA:HB2	1:TC:180:SER:N	2.24	0.53
1:F:180:SER:N	1:GD:52:ALA:HB2	2.24	0.53
1:H:32:ALA:HB1	1:O:158:GLY:HA3	1.91	0.53
1:L:52:ALA:HB2	1:BA:180:SER:N	2.24	0.53
1:O:32:ALA:HB1	1:W:158:GLY:HA3	1.91	0.52
1:TC:22:ALA:HB1	1:UC:9:ARG:CB	2.39	0.52
1:AD:22:ALA:HB1	1:BD:9:ARG:CB	2.39	0.52
1:DB:22:ALA:HB1	1:EB:9:ARG:CB	2.39	0.52
1:S:52:ALA:HB2	1:IA:180:SER:N	2.24	0.52
1:CB:52:ALA:HB2	1:RB:180:SER:N	2.24	0.52
1:FB:32:ALA:HB1	1:MB:158:GLY:HA3	1.91	0.52
1:LC:52:ALA:HB2	1:AD:180:SER:N	2.24	0.52
1:ZC:52:ALA:CB	1:OD:179:GLU:CB	2.87	0.52
1:CD:32:ALA:HB1	1:JD:158:GLY:HA3	1.91	0.52
1:DA:32:ALA:HB1	1:KA:158:GLY:HA3	1.92	0.52
1:RA:32:ALA:HB1	1:YA:158:GLY:HA3	1.91	0.52
1:HD:22:ALA:HB1	1:ID:9:ARG:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLY:HA3	1:JD:32:ALA:HB1	1.91	0.52
1:VA:52:ALA:HB2	1:KB:180:SER:N	2.24	0.52
1:YA:32:ALA:HB1	1:FB:158:GLY:HA3	1.91	0.52
1:XB:52:ALA:HB2	1:MC:180:SER:N	2.24	0.52
1:HC:32:ALA:HB1	1:OC:158:GLY:HA3	1.91	0.52
1:MC:22:ALA:HB1	1:NC:9:ARG:CB	2.39	0.52
1:SC:52:ALA:HB2	1:HD:180:SER:N	2.25	0.52
1:W:32:ALA:HB1	1:DA:158:GLY:HA3	1.91	0.52
1:M:180:SER:N	1:ND:52:ALA:HB2	2.25	0.52
1:MB:32:ALA:HB1	1:TB:158:GLY:HA3	1.91	0.52
1:QB:52:ALA:CB	1:FC:179:GLU:CB	2.88	0.52
1:A:32:ALA:HB1	1:H:158:GLY:HA3	1.91	0.51
1:M:22:ALA:HB1	1:N:9:ARG:CB	2.39	0.51
1:JB:52:ALA:CB	1:YB:179:GLU:CB	2.87	0.51
1:F:22:ALA:HB1	1:G:9:ARG:CB	2.39	0.51
1:HA:79:LEU:CB	1:CB:217:MET:HA	2.40	0.51
1:T:22:ALA:HB1	1:V:9:ARG:CB	2.39	0.51
1:OC:32:ALA:HB1	1:VC:158:GLY:HA3	1.92	0.51
1:L:217:MET:HA	1:GD:79:LEU:CB	2.40	0.51
1:VC:32:ALA:HB1	1:CD:158:GLY:HA3	1.91	0.51
1:OD:22:ALA:HB1	1:PD:9:ARG:CB	2.39	0.51
1:WA:22:ALA:HB1	1:XA:9:ARG:CB	2.39	0.51
1:TB:32:ALA:HB1	1:AC:158:GLY:HA3	1.91	0.51
1:FC:22:ALA:HB1	1:GC:9:ARG:CB	2.39	0.51
1:AC:32:ALA:HB1	1:HC:158:GLY:HA3	1.91	0.51
1:BA:22:ALA:HB1	1:CA:9:ARG:CB	2.39	0.50
1:S:217:MET:HA	1:ND:79:LEU:CB	2.41	0.50
1:SC:79:LEU:CB	1:ND:217:MET:HA	2.41	0.50
1:S:79:LEU:CB	1:OA:217:MET:HA	2.41	0.50
1:L:79:LEU:CB	1:HA:217:MET:HA	2.41	0.50
1:YB:22:ALA:HB1	1:ZB:9:ARG:CB	2.39	0.50
1:IA:22:ALA:HB1	1:JA:9:ARG:CB	2.39	0.49
1:LC:79:LEU:CB	1:GD:217:MET:HA	2.42	0.49
1:T:159:MET:C	1:T:161:THR:H	2.21	0.49
1:BA:159:MET:C	1:BA:161:THR:H	2.21	0.49
1:XB:79:LEU:CB	1:SC:217:MET:HA	2.42	0.49
1:YB:159:MET:C	1:YB:161:THR:H	2.21	0.49
1:J:184:ALA:C	1:KD:48:ALA:HB1	2.37	0.49
1:PA:22:ALA:HB1	1:QA:9:ARG:CB	2.39	0.49
1:FC:159:MET:C	1:FC:161:THR:H	2.21	0.49
1:C:52:ALA:CB	1:R:180:SER:CB	2.73	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RB:22:ALA:HB1	1:SB:9:ARG:CB	2.39	0.49
1:WA:159:MET:C	1:WA:161:THR:H	2.21	0.49
1:DB:159:MET:C	1:DB:161:THR:H	2.21	0.48
1:QB:79:LEU:CB	1:LC:217:MET:HA	2.43	0.48
1:E:217:MET:HA	1:ZC:79:LEU:CB	2.43	0.48
1:AB:52:ALA:CB	1:PB:180:SER:CB	2.70	0.48
1:HD:159:MET:C	1:HD:161:THR:H	2.21	0.48
1:RB:159:MET:C	1:RB:161:THR:H	2.21	0.48
1:IC:48:ALA:HB1	1:XC:184:ALA:C	2.38	0.48
1:P:48:ALA:HB1	1:FA:184:ALA:C	2.38	0.48
1:X:48:ALA:HB1	1:MA:184:ALA:C	2.38	0.48
1:JB:79:LEU:CB	1:EC:217:MET:HA	2.43	0.48
1:KB:22:ALA:HB1	1:LB:9:ARG:CB	2.39	0.48
1:AD:159:MET:C	1:AD:161:THR:H	2.21	0.48
1:OD:159:MET:C	1:OD:161:THR:H	2.21	0.48
1:M:159:MET:C	1:M:161:THR:H	2.21	0.48
1:AA:79:LEU:CB	1:VA:217:MET:HA	2.42	0.48
1:EA:48:ALA:HB1	1:TA:184:ALA:C	2.38	0.48
1:VA:79:LEU:CB	1:QB:217:MET:HA	2.42	0.48
1:IA:159:MET:C	1:IA:161:THR:H	2.21	0.48
1:E:79:LEU:CB	1:AA:217:MET:HA	2.43	0.48
1:C:184:ALA:C	1:DD:48:ALA:HB1	2.38	0.48
1:PA:159:MET:C	1:PA:161:THR:H	2.21	0.48
1:CB:79:LEU:CB	1:XB:217:MET:HA	2.43	0.48
1:MC:159:MET:C	1:MC:161:THR:H	2.21	0.48
1:FA:52:ALA:CB	1:UA:180:SER:CB	2.73	0.48
1:BC:48:ALA:HB1	1:QC:184:ALA:C	2.38	0.48
1:KB:159:MET:C	1:KB:161:THR:H	2.21	0.47
1:LA:48:ALA:HB1	1:AB:184:ALA:C	2.39	0.47
1:PC:48:ALA:HB1	1:ED:184:ALA:C	2.38	0.47
1:TC:159:MET:C	1:TC:161:THR:H	2.21	0.47
1:F:159:MET:C	1:F:161:THR:H	2.21	0.47
1:F:160:ASN:O	1:F:161:THR:C	2.58	0.47
1:BA:160:ASN:O	1:BA:161:THR:C	2.58	0.47
1:YB:160:ASN:O	1:YB:161:THR:C	2.58	0.47
1:TC:160:ASN:O	1:TC:161:THR:C	2.58	0.47
1:B:48:ALA:HB1	1:Q:184:ALA:C	2.39	0.47
1:L:184:ALA:HB2	1:MD:48:ALA:HB1	1.97	0.47
1:NB:48:ALA:HB1	1:CC:184:ALA:C	2.38	0.47
1:OD:160:ASN:O	1:OD:161:THR:C	2.58	0.47
1:I:48:ALA:HB1	1:Y:184:ALA:C	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:160:ASN:O	1:T:161:THR:C	2.58	0.47
1:PA:160:ASN:O	1:PA:161:THR:C	2.58	0.47
1:GB:48:ALA:HB1	1:VB:184:ALA:C	2.39	0.47
1:AD:160:ASN:O	1:AD:161:THR:C	2.58	0.47
1:SA:48:ALA:HB1	1:HB:184:ALA:C	2.39	0.47
1:DB:160:ASN:O	1:DB:161:THR:C	2.58	0.47
1:KB:160:ASN:O	1:KB:161:THR:C	2.58	0.47
1:MC:160:ASN:O	1:MC:161:THR:C	2.58	0.47
1:OA:79:LEU:CB	1:JB:217:MET:HA	2.44	0.46
1:RB:160:ASN:O	1:RB:161:THR:C	2.58	0.46
1:UB:48:ALA:HB1	1:JC:184:ALA:C	2.38	0.46
1:WA:160:ASN:O	1:WA:161:THR:C	2.58	0.46
1:AB:48:ALA:CB	1:PB:184:ALA:CB	2.65	0.46
1:RC:48:ALA:HB1	1:GD:184:ALA:HB2	1.98	0.46
1:JC:48:ALA:CB	1:YC:184:ALA:CB	2.67	0.46
1:ZA:48:ALA:HB1	1:OB:184:ALA:C	2.40	0.46
1:KC:48:ALA:HB1	1:ZC:184:ALA:HB2	1.98	0.46
1:IA:160:ASN:O	1:IA:161:THR:C	2.58	0.46
1:HD:160:ASN:O	1:HD:161:THR:C	2.58	0.46
1:WC:48:ALA:HB1	1:LD:184:ALA:C	2.40	0.46
1:M:160:ASN:O	1:M:161:THR:C	2.58	0.45
1:FC:160:ASN:O	1:FC:161:THR:C	2.58	0.45
1:E:184:ALA:HB2	1:FD:48:ALA:HB1	1.99	0.45
1:DC:48:ALA:HB1	1:SC:184:ALA:HB2	1.98	0.45
1:D:180:SER:CB	1:ED:52:ALA:CB	2.73	0.45
1:D:48:ALA:HB1	1:S:184:ALA:HB2	1.99	0.44
1:Y:52:ALA:CB	1:NA:180:SER:CB	2.74	0.44
1:PB:48:ALA:HB1	1:EC:184:ALA:HB2	1.99	0.44
1:WB:48:ALA:HB1	1:LC:184:ALA:HB2	1.99	0.44
1:K:180:SER:CB	1:LD:52:ALA:CB	2.75	0.44
1:R:48:ALA:HB1	1:HA:184:ALA:HB2	1.98	0.44
1:XC:52:ALA:CB	1:MD:180:SER:CB	2.73	0.44
1:Z:48:ALA:HB1	1:OA:184:ALA:HB2	1.98	0.44
1:GA:48:ALA:HB1	1:VA:184:ALA:HB2	1.98	0.43
1:TA:48:ALA:CB	1:IB:184:ALA:CB	2.65	0.43
1:UA:48:ALA:HB1	1:JB:184:ALA:HB2	1.99	0.43
1:NA:48:ALA:HB1	1:CB:184:ALA:HB2	1.99	0.43
1:IB:48:ALA:HB1	1:XB:184:ALA:HB2	1.99	0.43
1:O:32:ALA:CB	1:W:158:GLY:HA3	2.49	0.43
1:MA:52:ALA:CB	1:BB:180:SER:CB	2.73	0.43
1:AC:32:ALA:CB	1:HC:158:GLY:HA3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YC:48:ALA:HB1	1:ND:184:ALA:HB2	2.00	0.43
1:DA:32:ALA:CB	1:KA:158:GLY:HA3	2.49	0.43
1:K:48:ALA:HB1	1:AA:184:ALA:HB2	2.00	0.43
1:YA:32:ALA:CB	1:FB:158:GLY:HA3	2.48	0.43
1:A:158:GLY:HA3	1:JD:32:ALA:CB	2.49	0.43
1:OC:32:ALA:CB	1:VC:158:GLY:HA3	2.48	0.43
1:A:32:ALA:CB	1:H:158:GLY:HA3	2.49	0.43
1:K:184:ALA:CB	1:LD:48:ALA:CB	2.66	0.43
1:HB:52:ALA:CB	1:WB:180:SER:CB	2.75	0.43
1:BB:48:ALA:HB1	1:QB:184:ALA:HB2	2.00	0.42
1:VC:32:ALA:CB	1:CD:158:GLY:HA3	2.49	0.42
1:KA:32:ALA:CB	1:RA:158:GLY:HA3	2.49	0.42
1:VB:52:ALA:CB	1:KC:180:SER:CB	2.73	0.42
1:H:32:ALA:CB	1:O:158:GLY:HA3	2.49	0.42
1:FB:32:ALA:CB	1:MB:158:GLY:HA3	2.49	0.42
1:CB:32:ALA:HB1	1:JB:163:SER:CB	2.50	0.42
1:CD:32:ALA:CB	1:JD:158:GLY:HA3	2.49	0.42
1:FA:32:ALA:HB2	1:MA:167:ALA:CB	2.50	0.42
1:QC:32:ALA:HB2	1:XC:167:ALA:CB	2.50	0.42
1:D:52:ALA:CB	1:S:180:SER:CA	2.95	0.41
1:W:32:ALA:CB	1:DA:158:GLY:HA3	2.50	0.41
1:CC:32:ALA:HB2	1:JC:167:ALA:CB	2.50	0.41
1:QB:52:ALA:HB2	1:FC:180:SER:CA	2.50	0.41
1:C:32:ALA:HB2	1:J:167:ALA:CB	2.51	0.41
1:C:48:ALA:CB	1:R:184:ALA:CB	2.67	0.41
1:C:167:ALA:CB	1:LD:32:ALA:HB2	2.50	0.41
1:J:48:ALA:CB	1:Z:184:ALA:CB	2.66	0.41
1:MC:159:MET:C	1:MC:161:THR:N	2.79	0.41
1:M:159:MET:C	1:M:161:THR:N	2.79	0.41
1:R:52:ALA:CB	1:HA:180:SER:CA	2.95	0.41
1:RA:32:ALA:CB	1:YA:158:GLY:HA3	2.49	0.41
1:QC:52:ALA:CB	1:FD:180:SER:CB	2.73	0.41
1:HD:159:MET:C	1:HD:161:THR:N	2.79	0.41
1:EC:32:ALA:HB1	1:LC:163:SER:CB	2.51	0.41
1:Q:52:ALA:CB	1:GA:180:SER:CB	2.74	0.41
1:AB:32:ALA:HB2	1:HB:167:ALA:CB	2.51	0.41
1:JB:52:ALA:HB2	1:YB:180:SER:CA	2.51	0.41
1:F:159:MET:C	1:F:161:THR:N	2.79	0.41
1:MB:32:ALA:CB	1:TB:158:GLY:HA3	2.50	0.41
1:RB:159:MET:C	1:RB:161:THR:N	2.79	0.41
1:TB:32:ALA:CB	1:AC:158:GLY:HA3	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FC:159:MET:C	1:FC:161:THR:N	2.79	0.41
1:HC:32:ALA:CB	1:OC:158:GLY:HA3	2.50	0.41
1:AD:159:MET:C	1:AD:161:THR:N	2.79	0.41
1:J:32:ALA:HB2	1:Q:167:ALA:CB	2.51	0.41
1:TA:32:ALA:HB2	1:AB:167:ALA:CB	2.51	0.41
1:TC:159:MET:C	1:TC:161:THR:N	2.79	0.41
1:OD:159:MET:C	1:OD:161:THR:N	2.79	0.41
1:BA:159:MET:C	1:BA:161:THR:N	2.79	0.40
1:YB:159:MET:C	1:YB:161:THR:N	2.79	0.40
1:HB:32:ALA:HB2	1:OB:167:ALA:CB	2.51	0.40
1:QC:48:ALA:CB	1:FD:184:ALA:CB	2.66	0.40
1:MA:32:ALA:HB2	1:TA:167:ALA:CB	2.52	0.40
1:YC:52:ALA:CB	1:ND:180:SER:CA	2.94	0.40
1:IA:159:MET:C	1:IA:161:THR:N	2.79	0.40
1:VB:32:ALA:HB2	1:CC:167:ALA:CB	2.51	0.40
1:JC:52:ALA:CB	1:YC:180:SER:CB	2.74	0.40
1:Q:32:ALA:HB2	1:Y:167:ALA:CB	2.51	0.40
1:T:159:MET:C	1:T:161:THR:N	2.79	0.40
1:CC:52:ALA:CB	1:RC:180:SER:CB	2.74	0.40
1:ZC:52:ALA:HB2	1:OD:180:SER:CA	2.51	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	131/258 (51%)	131 (100%)	0	0	100	100
1	AA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	AB	217/258 (84%)	217 (100%)	0	0	100	100
1	AC	131/258 (51%)	131 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AD	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	B	217/258 (84%)	217 (100%)	0	0	100	100
1	BA	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	BB	217/258 (84%)	217 (100%)	0	0	100	100
1	BC	217/258 (84%)	217 (100%)	0	0	100	100
1	BD	156/258 (60%)	156 (100%)	0	0	100	100
1	C	217/258 (84%)	217 (100%)	0	0	100	100
1	CA	156/258 (60%)	156 (100%)	0	0	100	100
1	CB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	CC	217/258 (84%)	217 (100%)	0	0	100	100
1	CD	131/258 (51%)	131 (100%)	0	0	100	100
1	D	217/258 (84%)	217 (100%)	0	0	100	100
1	DA	131/258 (51%)	131 (100%)	0	0	100	100
1	DB	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	DC	217/258 (84%)	217 (100%)	0	0	100	100
1	DD	217/258 (84%)	217 (100%)	0	0	100	100
1	E	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	EA	217/258 (84%)	217 (100%)	0	0	100	100
1	EB	156/258 (60%)	156 (100%)	0	0	100	100
1	EC	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	ED	217/258 (84%)	217 (100%)	0	0	100	100
1	F	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	FA	217/258 (84%)	217 (100%)	0	0	100	100
1	FB	131/258 (51%)	131 (100%)	0	0	100	100
1	FC	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	FD	217/258 (84%)	217 (100%)	0	0	100	100
1	G	156/258 (60%)	156 (100%)	0	0	100	100
1	GA	217/258 (84%)	217 (100%)	0	0	100	100
1	GB	217/258 (84%)	217 (100%)	0	0	100	100
1	GC	156/258 (60%)	156 (100%)	0	0	100	100
1	GD	217/258 (84%)	216 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	131/258 (51%)	131 (100%)	0	0	100	100
1	HA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	HB	217/258 (84%)	217 (100%)	0	0	100	100
1	HC	131/258 (51%)	131 (100%)	0	0	100	100
1	HD	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	I	217/258 (84%)	217 (100%)	0	0	100	100
1	IA	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	IB	217/258 (84%)	217 (100%)	0	0	100	100
1	IC	217/258 (84%)	217 (100%)	0	0	100	100
1	ID	156/258 (60%)	156 (100%)	0	0	100	100
1	J	217/258 (84%)	217 (100%)	0	0	100	100
1	JA	156/258 (60%)	156 (100%)	0	0	100	100
1	JB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	JC	217/258 (84%)	217 (100%)	0	0	100	100
1	JD	131/258 (51%)	131 (100%)	0	0	100	100
1	K	217/258 (84%)	217 (100%)	0	0	100	100
1	KA	131/258 (51%)	131 (100%)	0	0	100	100
1	KB	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	KC	217/258 (84%)	217 (100%)	0	0	100	100
1	KD	217/258 (84%)	217 (100%)	0	0	100	100
1	L	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	LA	217/258 (84%)	217 (100%)	0	0	100	100
1	LB	156/258 (60%)	156 (100%)	0	0	100	100
1	LC	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	LD	217/258 (84%)	217 (100%)	0	0	100	100
1	M	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	MA	217/258 (84%)	217 (100%)	0	0	100	100
1	MB	131/258 (51%)	131 (100%)	0	0	100	100
1	MC	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	MD	217/258 (84%)	217 (100%)	0	0	100	100
1	N	156/258 (60%)	156 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	NA	217/258 (84%)	217 (100%)	0	0	100	100
1	NB	217/258 (84%)	217 (100%)	0	0	100	100
1	NC	156/258 (60%)	156 (100%)	0	0	100	100
1	ND	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	O	131/258 (51%)	131 (100%)	0	0	100	100
1	OA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	OB	217/258 (84%)	217 (100%)	0	0	100	100
1	OC	131/258 (51%)	131 (100%)	0	0	100	100
1	OD	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	P	217/258 (84%)	217 (100%)	0	0	100	100
1	PA	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	PB	217/258 (84%)	217 (100%)	0	0	100	100
1	PC	217/258 (84%)	217 (100%)	0	0	100	100
1	PD	156/258 (60%)	156 (100%)	0	0	100	100
1	Q	217/258 (84%)	217 (100%)	0	0	100	100
1	QA	156/258 (60%)	156 (100%)	0	0	100	100
1	QB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	QC	217/258 (84%)	217 (100%)	0	0	100	100
1	R	217/258 (84%)	217 (100%)	0	0	100	100
1	RA	131/258 (51%)	131 (100%)	0	0	100	100
1	RB	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	RC	217/258 (84%)	217 (100%)	0	0	100	100
1	S	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	SA	217/258 (84%)	217 (100%)	0	0	100	100
1	SB	156/258 (60%)	156 (100%)	0	0	100	100
1	SC	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	T	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	TA	217/258 (84%)	217 (100%)	0	0	100	100
1	TB	131/258 (51%)	131 (100%)	0	0	100	100
1	TC	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	UA	217/258 (84%)	217 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UB	217/258 (84%)	217 (100%)	0	0	100	100
1	UC	156/258 (60%)	156 (100%)	0	0	100	100
1	V	156/258 (60%)	156 (100%)	0	0	100	100
1	VA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	VB	217/258 (84%)	217 (100%)	0	0	100	100
1	VC	131/258 (51%)	131 (100%)	0	0	100	100
1	W	131/258 (51%)	131 (100%)	0	0	100	100
1	WA	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	WB	217/258 (84%)	217 (100%)	0	0	100	100
1	WC	217/258 (84%)	217 (100%)	0	0	100	100
1	X	217/258 (84%)	217 (100%)	0	0	100	100
1	XA	156/258 (60%)	156 (100%)	0	0	100	100
1	XB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	XC	217/258 (84%)	217 (100%)	0	0	100	100
1	Y	217/258 (84%)	217 (100%)	0	0	100	100
1	YA	131/258 (51%)	131 (100%)	0	0	100	100
1	YB	216/258 (84%)	214 (99%)	2 (1%)	0	100	100
1	YC	217/258 (84%)	217 (100%)	0	0	100	100
1	Z	217/258 (84%)	217 (100%)	0	0	100	100
1	ZA	217/258 (84%)	217 (100%)	0	0	100	100
1	ZB	156/258 (60%)	156 (100%)	0	0	100	100
1	ZC	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
All	All	23307/30702 (76%)	23256 (100%)	51 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

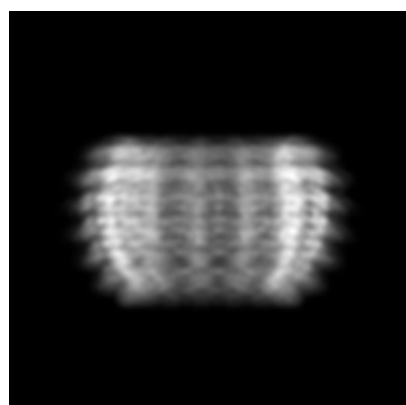
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11483. These allow visual inspection of the internal detail of the map and identification of artifacts.

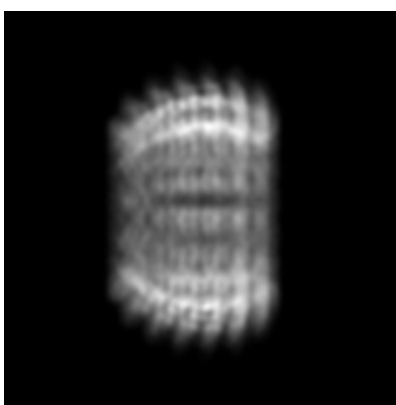
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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: 168



Y Index: 168



Z Index: 168

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: 238



Y Index: 234

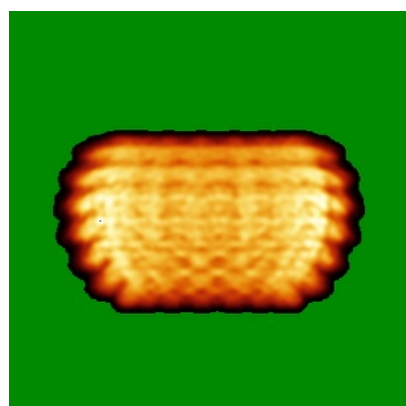


Z Index: 178

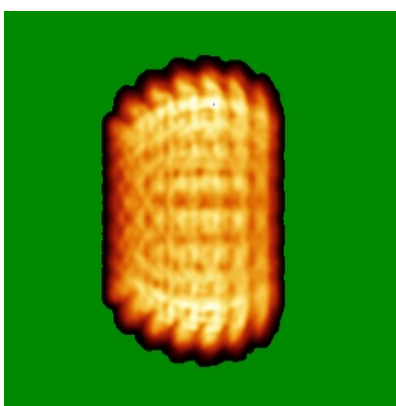
The images above show the largest variance slices of the map in three orthogonal directions.

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

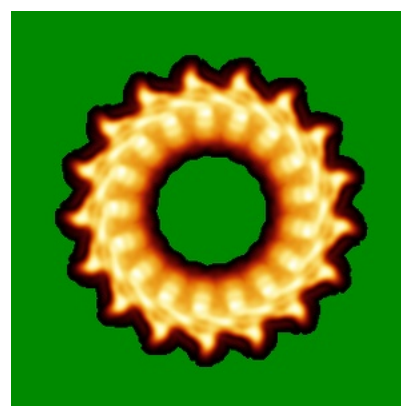
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

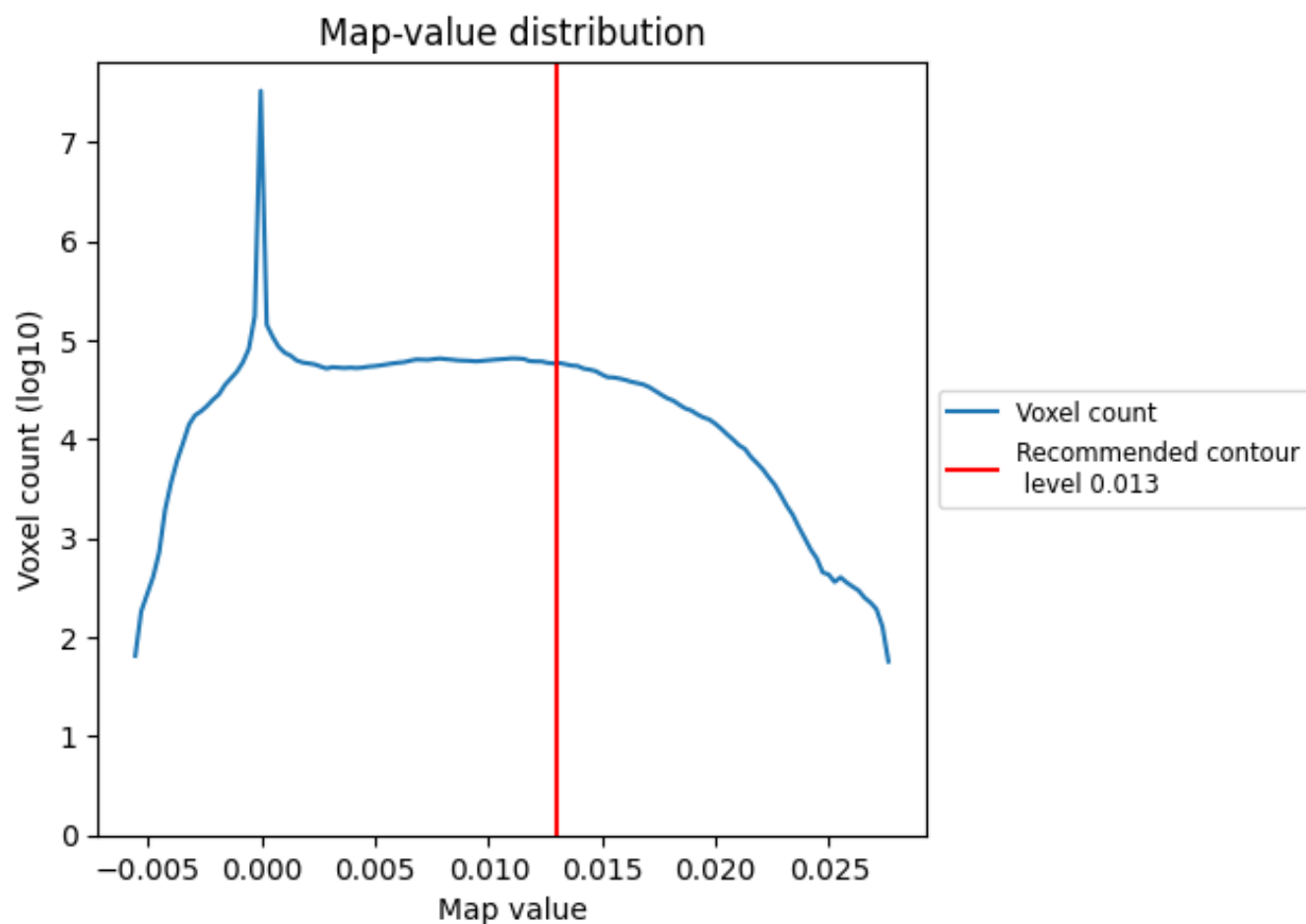
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

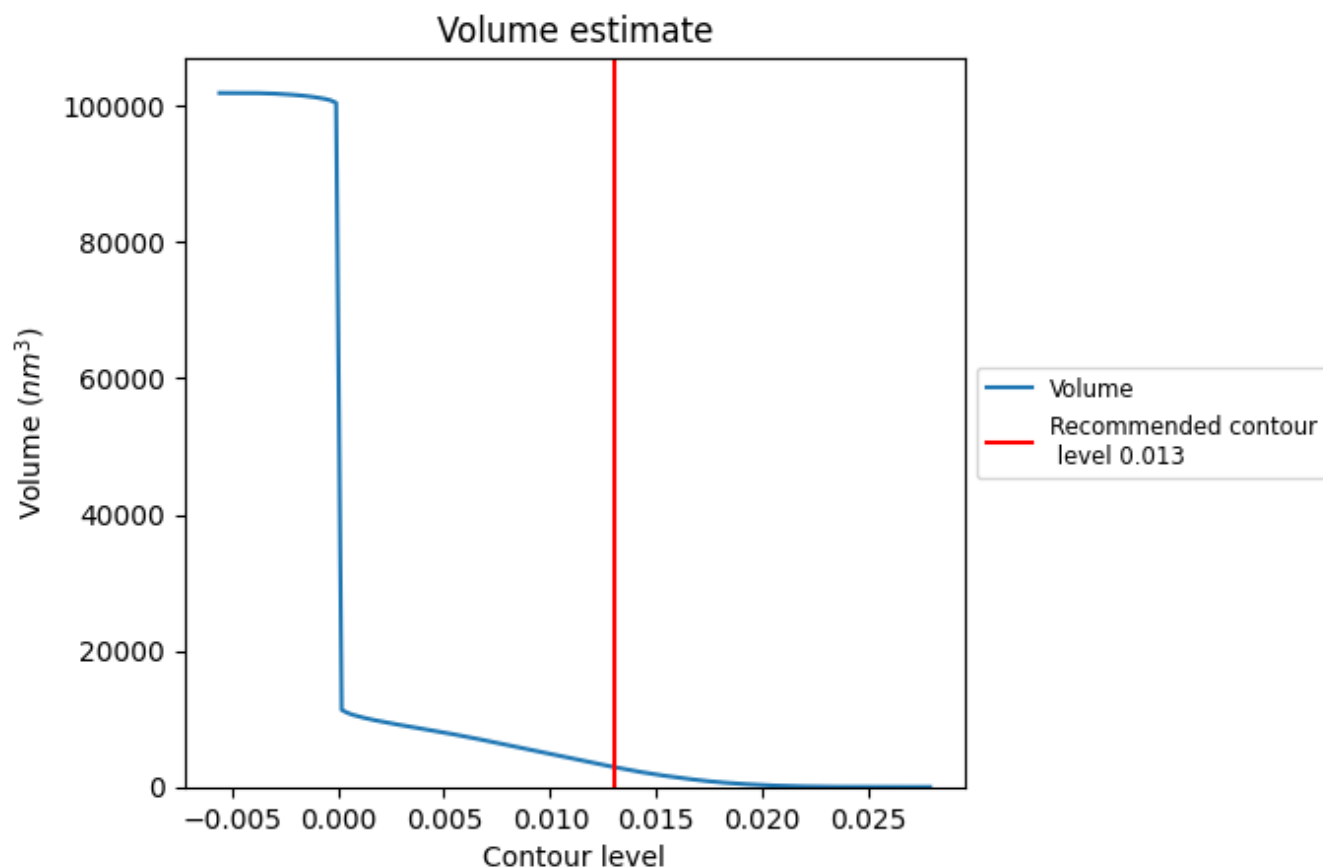
This section contains the results of statistical analysis of the map.

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.

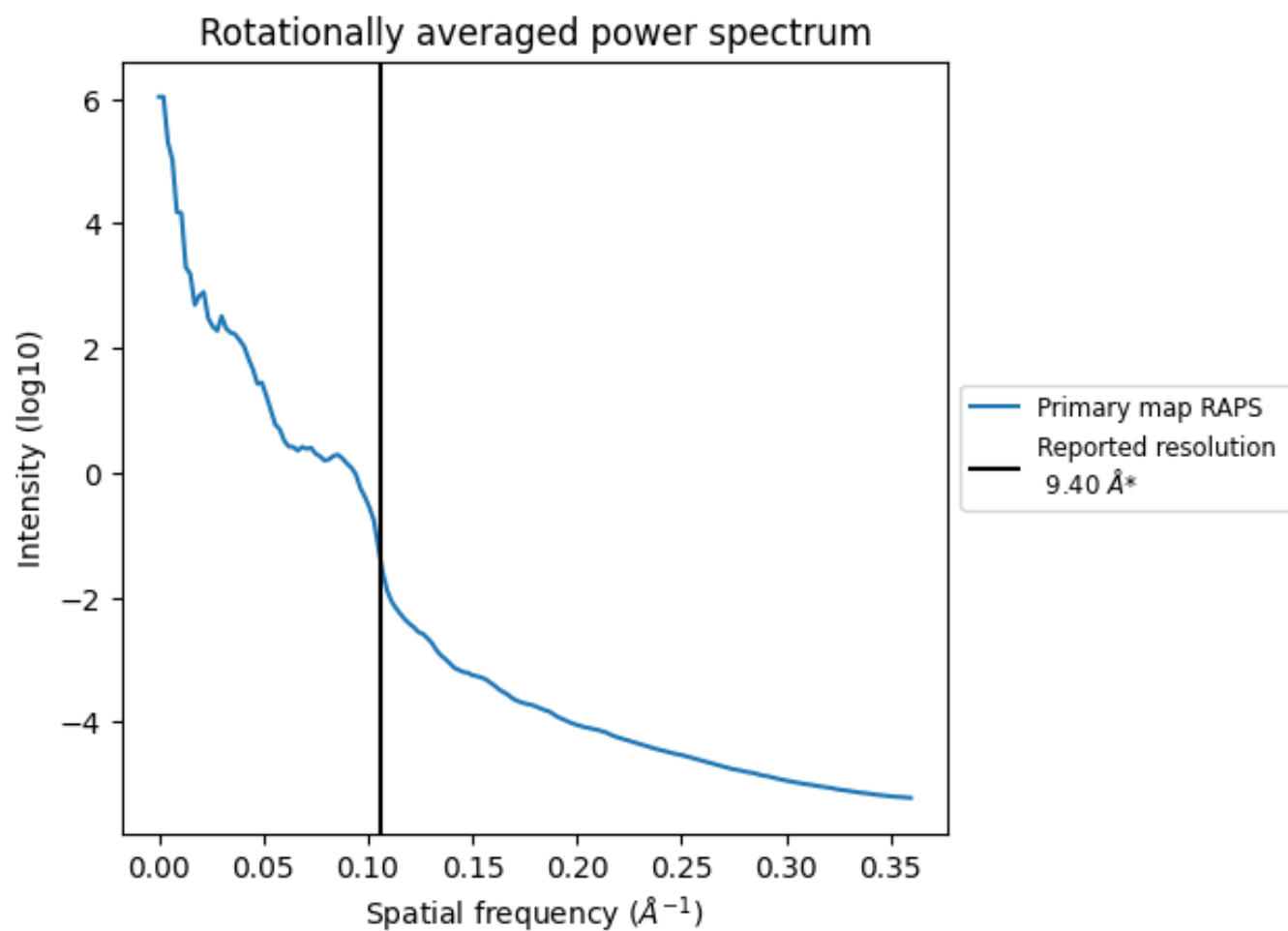
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2925 nm³; this corresponds to an approximate mass of 2643 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 0.106 Å⁻¹

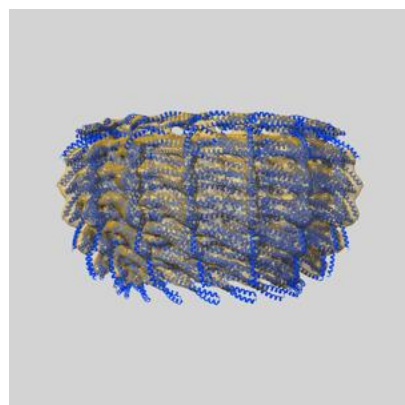
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

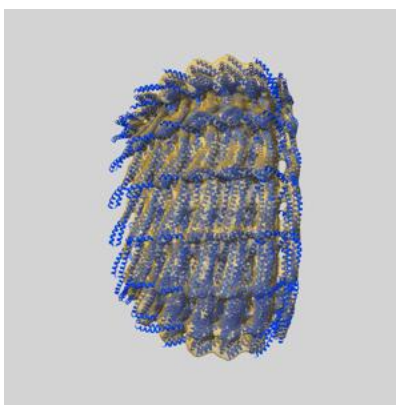
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11483 and PDB model 6ZW7. Per-residue inclusion information can be found in section 3 on page 14.

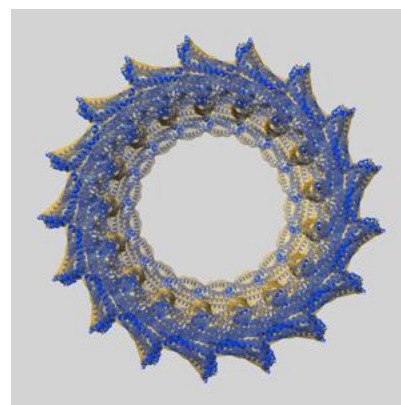
9.1 Map-model overlay [i](#)



X



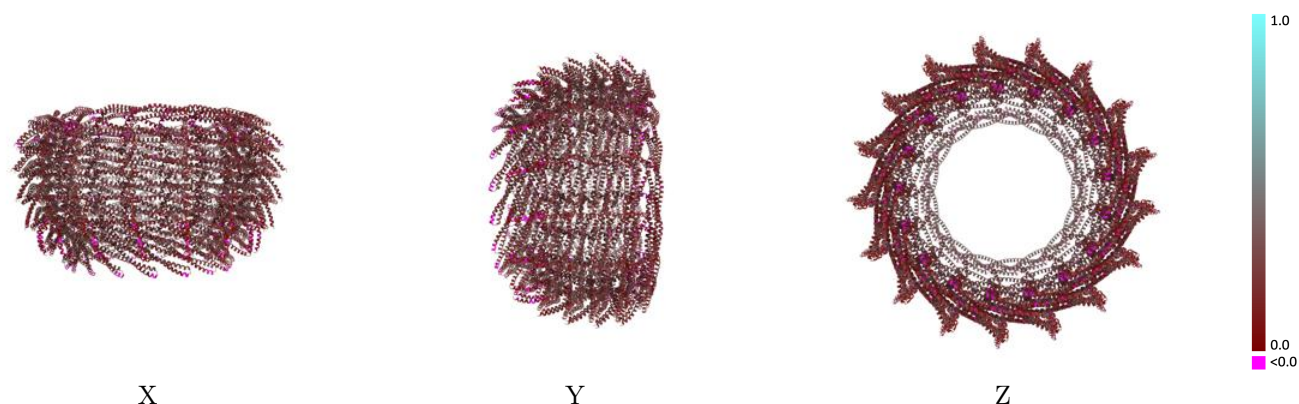
Y



Z

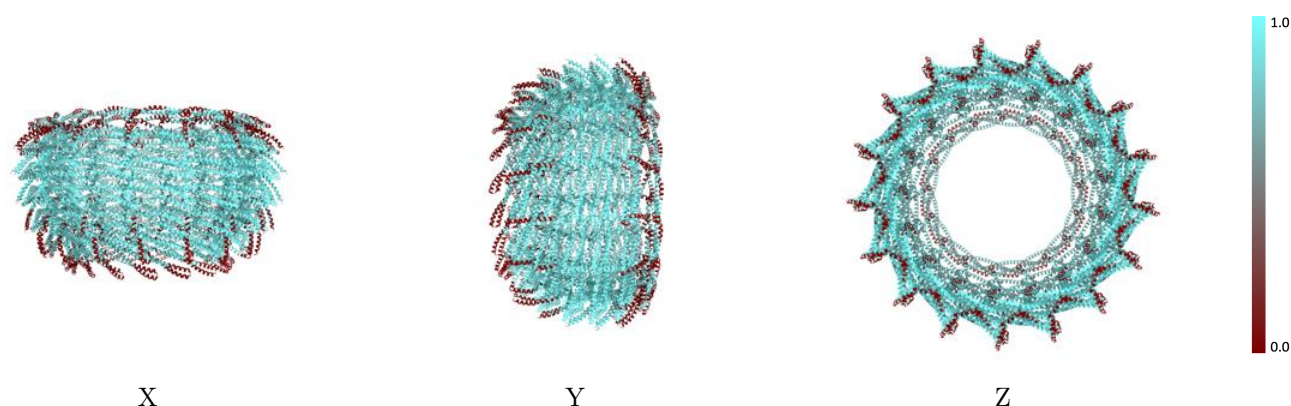
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



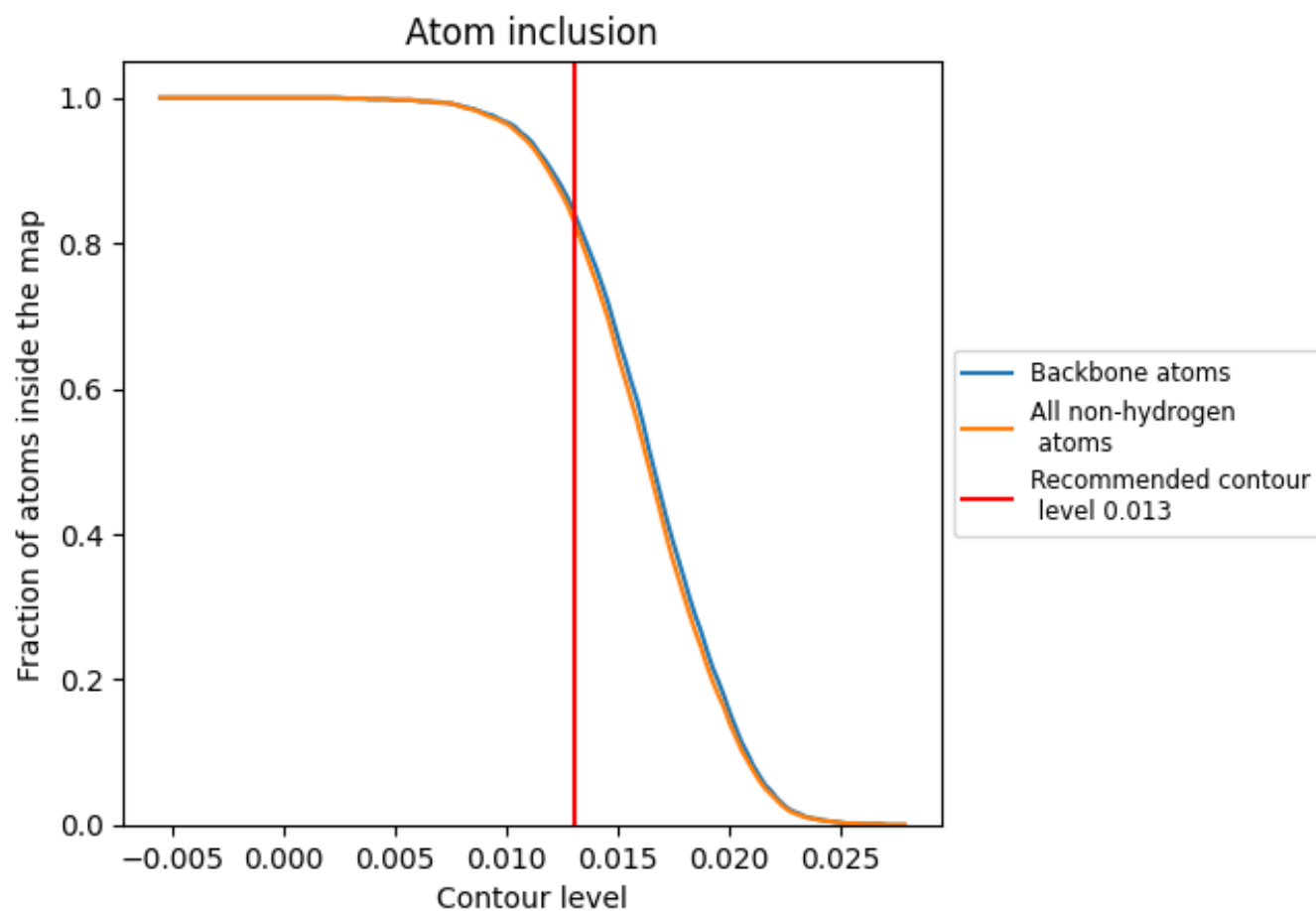
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 83% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8320	 0.2110
A	 0.6280	 0.1800
AA	 0.9190	 0.2230
AB	 0.9740	 0.2260
AC	 0.6260	 0.1800
AD	 0.8060	 0.1870
B	 0.7470	 0.1920
BA	 0.8050	 0.1910
BB	 0.9870	 0.2450
BC	 0.7470	 0.1930
BD	 0.6250	 0.2200
C	 0.9760	 0.2220
CA	 0.6270	 0.2210
CB	 0.9120	 0.2200
CC	 0.9770	 0.2250
CD	 0.6310	 0.1780
D	 0.9920	 0.2420
DA	 0.6260	 0.1790
DB	 0.8030	 0.1900
DC	 0.9910	 0.2420
DD	 0.7470	 0.1890
E	 0.9190	 0.2200
EA	 0.7480	 0.1930
EB	 0.6230	 0.2210
EC	 0.9150	 0.2190
ED	 0.9740	 0.2220
F	 0.8050	 0.1900
FA	 0.9800	 0.2250
FB	 0.6260	 0.1790
FC	 0.8030	 0.1890
FD	 0.9880	 0.2410
G	 0.6250	 0.2210
GA	 0.9920	 0.2450
GB	 0.7480	 0.1920
GC	 0.6250	 0.2220



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Chain	Atom inclusion	Q-score
GD	 0.9130	 0.2200
H	 0.6320	 0.1770
HA	 0.9220	 0.2230
HB	 0.9760	 0.2250
HC	 0.6260	 0.1800
HD	 0.8030	 0.1870
I	 0.7480	 0.1900
IA	 0.8050	 0.1900
IB	 0.9920	 0.2430
IC	 0.7490	 0.1920
ID	 0.6250	 0.2190
J	 0.9780	 0.2210
JA	 0.6240	 0.2230
JB	 0.9160	 0.2190
JC	 0.9790	 0.2240
JD	 0.6230	 0.1790
K	 0.9920	 0.2420
KA	 0.6370	 0.1790
KB	 0.8050	 0.1890
KC	 0.9920	 0.2430
KD	 0.7460	 0.1910
L	 0.9140	 0.2220
LA	 0.7500	 0.1930
LB	 0.6250	 0.2210
LC	 0.9220	 0.2200
LD	 0.9770	 0.2230
M	 0.8050	 0.1900
MA	 0.9770	 0.2260
MB	 0.6310	 0.1770
MC	 0.8070	 0.1880
MD	 0.9910	 0.2430
N	 0.6270	 0.2220
NA	 0.9910	 0.2450
NB	 0.7500	 0.1920
NC	 0.6250	 0.2190
ND	 0.9150	 0.2220
O	 0.6310	 0.1780
OA	 0.9150	 0.2220
OB	 0.9780	 0.2230
OC	 0.6260	 0.1780
OD	 0.8050	 0.1890
P	 0.7480	 0.1920

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Chain	Atom inclusion	Q-score
PA	 0.8060	 0.1900
PB	 0.9920	 0.2430
PC	 0.7490	 0.1930
PD	 0.6240	 0.2200
Q	 0.9760	 0.2240
QA	 0.6250	 0.2230
QB	 0.9170	 0.2180
QC	 0.9770	 0.2240
R	 0.9900	 0.2450
RA	 0.6370	 0.1790
RB	 0.8060	 0.1870
RC	 0.9920	 0.2440
S	 0.9130	 0.2230
SA	 0.7480	 0.1940
SB	 0.6270	 0.2220
SC	 0.9180	 0.2210
T	 0.8030	 0.1920
TA	 0.9740	 0.2250
TB	 0.6340	 0.1780
TC	 0.8070	 0.1880
UA	 0.9890	 0.2460
UB	 0.7480	 0.1930
UC	 0.6270	 0.2190
V	 0.6250	 0.2220
VA	 0.9130	 0.2220
VB	 0.9750	 0.2240
VC	 0.6350	 0.1790
W	 0.6220	 0.1770
WA	 0.8040	 0.1900
WB	 0.9900	 0.2440
WC	 0.7500	 0.1910
X	 0.7470	 0.1940
XA	 0.6250	 0.2230
XB	 0.9140	 0.2200
XC	 0.9750	 0.2230
Y	 0.9790	 0.2260
YA	 0.6250	 0.1760
YB	 0.8030	 0.1890
YC	 0.9900	 0.2410
Z	 0.9910	 0.2460
ZA	 0.7460	 0.1950
ZB	 0.6240	 0.2220

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Chain	Atom inclusion	Q-score
ZC	 0.9150	 0.2210