



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 12:07 AM EDT

PDB ID : 6N4V
EMDB ID : EMD-0344
Title : CryoEM structure of Leviviridae PP7 WT coat protein dimer capsid (PP7PP7-WT)
Authors : Liangjun, Z.; Kopylov, M.; Potter, C.S.; Carragher, B.; Finn, M.G.
Deposited on : 2018-11-20
Resolution : 3.00 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

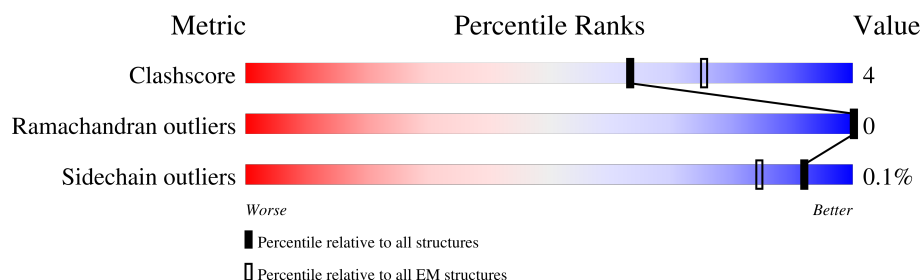
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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









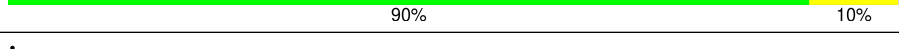
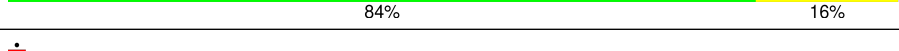
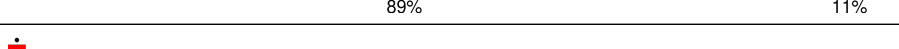
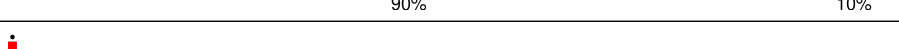
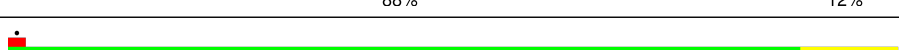

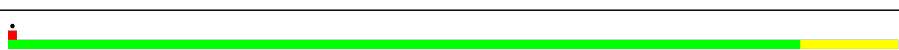

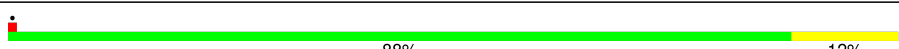





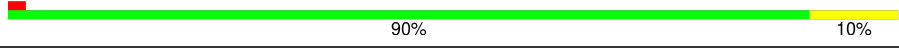
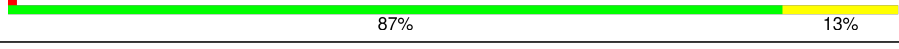



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	
1	Af	258	
1	B	258	
1	BA	258	





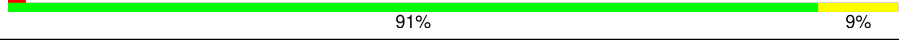

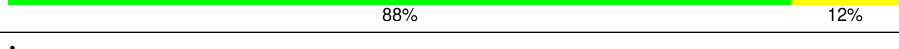
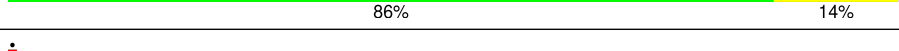
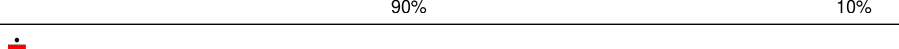
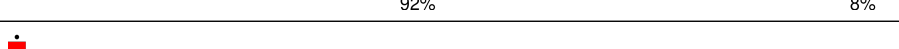
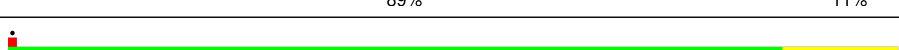

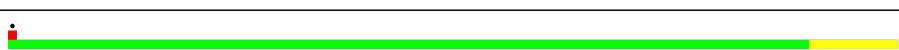

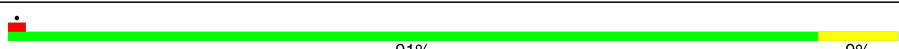




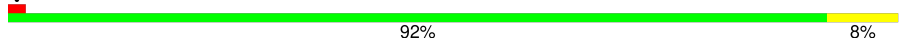
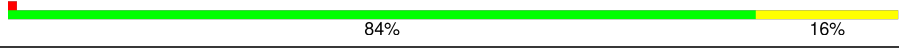
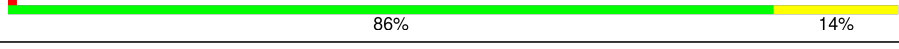



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Mol	Chain	Length	Quality of chain
1	BB	258	
1	BC	258	
1	BD	258	
1	C	258	
1	CA	258	
1	CB	258	
1	CC	258	
1	CD	258	
1	D	258	
1	DA	258	
1	DB	258	
1	DC	258	
1	DD	258	
1	E	258	
1	EA	258	
1	EB	258	
1	EC	258	
1	ED	258	
1	F	258	
1	FA	258	
1	FB	258	
1	FC	258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






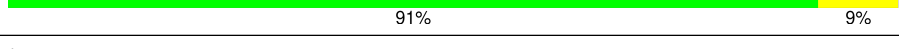
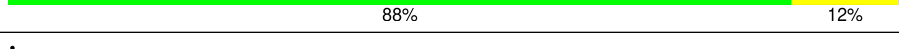
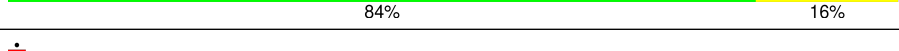
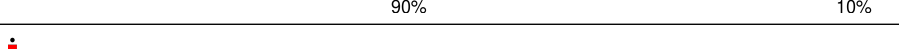
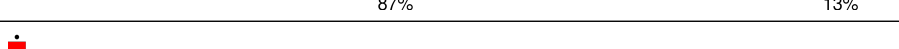
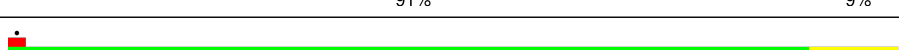

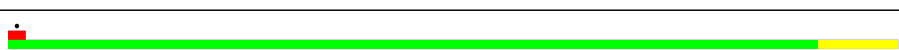

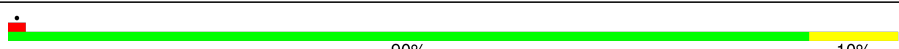





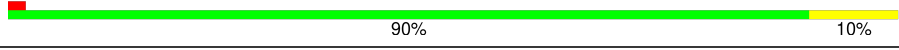
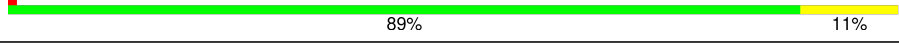
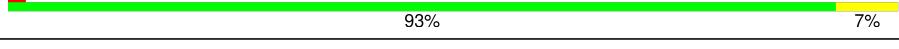


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Mol	Chain	Length	Quality of chain
1	GB	258	
1	GC	258	
1	GD	258	
1	H	258	
1	HA	258	
1	HB	258	
1	HC	258	
1	HD	258	
1	I	258	
1	IA	258	
1	IB	258	
1	IC	258	
1	ID	258	
1	J	258	
1	JA	258	
1	JB	258	
1	JC	258	
1	JD	258	
1	K	258	
1	KA	258	
1	KB	258	
1	KC	258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



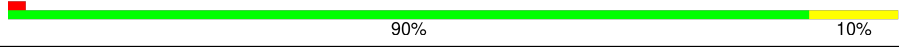



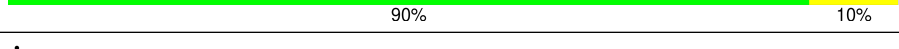
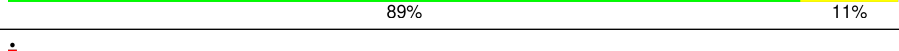
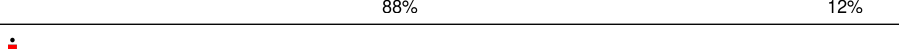
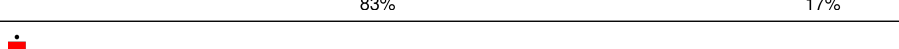


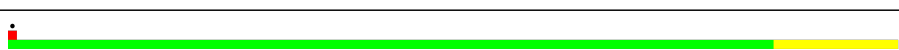

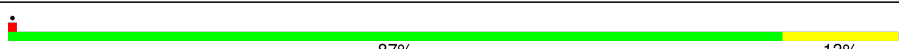





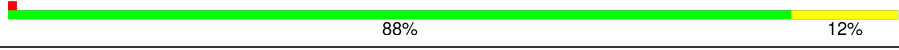
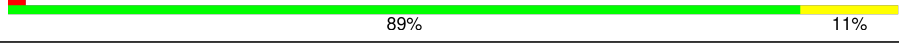



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Mol	Chain	Length	Quality of chain
1	LB	258	
1	LC	258	
1	LD	258	
1	M	258	
1	MA	258	
1	MB	258	
1	MC	258	
1	MD	258	
1	N	258	
1	NA	258	
1	NB	258	
1	NC	258	
1	ND	258	
1	O	258	
1	OA	258	
1	OB	258	
1	OC	258	
1	OD	258	
1	P	258	
1	PA	258	
1	PB	258	
1	PC	258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


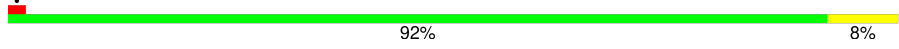
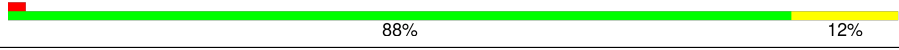


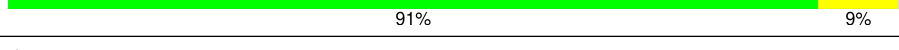
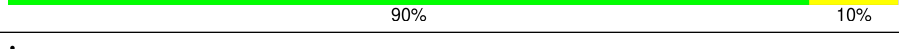
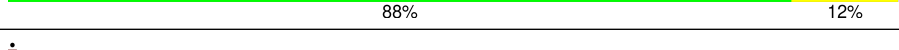
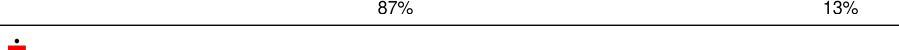
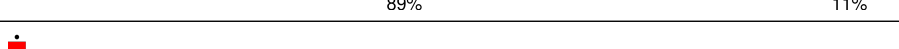

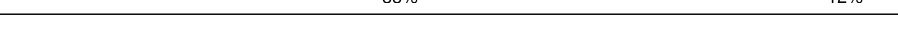
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Mol	Chain	Length	Quality of chain
1	QB	258	 89%11%
1	QC	258	 90%10%
1	R	258	 90%10%
1	RA	258	 88%12%
1	RB	258	 88%12%
1	RC	258	 89%11%
1	S	258	 90%10%
1	SA	258	 89%11%
1	SB	258	 88%12%
1	SC	258	 83%17%
1	T	258	 90%10%
1	TA	258	 90%10%
1	TB	258	 83%17%
1	TC	258	 86%14%
1	UA	258	 90%10%
1	UB	258	 87%13%
1	UC	258	 84%16%
1	V	258	 86%13%
1	VA	258	 91%9%
1	VB	258	 89%11%
1	VC	258	 87%13%
1	W	258	 88%12%
1	WA	258	 89%11%
1	WB	258	 87%13%
1	WC	258	 88%12%

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Mol	Chain	Length	Quality of chain
1	X	258	 85%15%
1	XA	258	 92%8%
1	XB	258	 88%12%
1	XC	258	 89%11%
1	Y	258	 87%13%
1	YA	258	 91%9%
1	YB	258	 90%10%
1	YC	258	 88%12%
1	Z	258	 87%13%
1	ZA	258	 89%11%
1	ZB	258	 90%10%
1	ZC	258	 88%12%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 236760 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Coat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Af	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	A	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	B	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	C	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	D	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	E	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	F	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	G	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	H	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	I	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	J	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	K	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	L	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	M	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	N	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	O	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	P	258	Total 1973	C 1226	N 352	O 391	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	R	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	S	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	T	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	V	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	W	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	X	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	Y	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	Z	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	AA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	BA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	CA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	DA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	EA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	FA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	GA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	HA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	IA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	JA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	KA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	LA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	MA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	NA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	OA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	PA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	QA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	RA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	SA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	TA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	UA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	VA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	WA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	XA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	YA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	ZA	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	AB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	BB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	CB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	DB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	EB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	FB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	GB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	HB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	IB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	JB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	KB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	LB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	MB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	NB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	OB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	PB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	QB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	RB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	SB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	TB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	UB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	VB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	WB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	XB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	YB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	ZB	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	AC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	BC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	DC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	EC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	FC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	GC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	HC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	IC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	JC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	KC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	LC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	MC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	NC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	OC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	PC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	QC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	RC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	SC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	TC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	UC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	VC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	WC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	XC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	YC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	ZC	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	AD	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	BD	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	CD	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	DD	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	ED	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	FD	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	GD	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	HD	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	ID	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	JD	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	KD	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	LD	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	MD	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	ND	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	OD	258	Total 1973	C 1226	N 352	O 391	S 4	0	0
1	PD	258	Total 1973	C 1226	N 352	O 391	S 4	0	0

There are 480 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Af	128	ALA	-	linker	UNP Q38062

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Chain	Residue	Modelled	Actual	Comment	Reference
Af	129	TYR	-	linker	UNP Q38062
Af	130	GLY	-	linker	UNP Q38062
Af	131	GLY	-	linker	UNP Q38062
A	128	ALA	-	linker	UNP Q38062
A	129	TYR	-	linker	UNP Q38062
A	130	GLY	-	linker	UNP Q38062
A	131	GLY	-	linker	UNP Q38062
B	128	ALA	-	linker	UNP Q38062
B	129	TYR	-	linker	UNP Q38062
B	130	GLY	-	linker	UNP Q38062
B	131	GLY	-	linker	UNP Q38062
C	128	ALA	-	linker	UNP Q38062
C	129	TYR	-	linker	UNP Q38062
C	130	GLY	-	linker	UNP Q38062
C	131	GLY	-	linker	UNP Q38062
D	128	ALA	-	linker	UNP Q38062
D	129	TYR	-	linker	UNP Q38062
D	130	GLY	-	linker	UNP Q38062
D	131	GLY	-	linker	UNP Q38062
E	128	ALA	-	linker	UNP Q38062
E	129	TYR	-	linker	UNP Q38062
E	130	GLY	-	linker	UNP Q38062
E	131	GLY	-	linker	UNP Q38062
F	128	ALA	-	linker	UNP Q38062
F	129	TYR	-	linker	UNP Q38062
F	130	GLY	-	linker	UNP Q38062
F	131	GLY	-	linker	UNP Q38062
G	128	ALA	-	linker	UNP Q38062
G	129	TYR	-	linker	UNP Q38062
G	130	GLY	-	linker	UNP Q38062
G	131	GLY	-	linker	UNP Q38062
H	128	ALA	-	linker	UNP Q38062
H	129	TYR	-	linker	UNP Q38062
H	130	GLY	-	linker	UNP Q38062
H	131	GLY	-	linker	UNP Q38062
I	128	ALA	-	linker	UNP Q38062
I	129	TYR	-	linker	UNP Q38062
I	130	GLY	-	linker	UNP Q38062
I	131	GLY	-	linker	UNP Q38062
J	128	ALA	-	linker	UNP Q38062
J	129	TYR	-	linker	UNP Q38062
J	130	GLY	-	linker	UNP Q38062

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Chain	Residue	Modelled	Actual	Comment	Reference
J	131	GLY	-	linker	UNP Q38062
K	128	ALA	-	linker	UNP Q38062
K	129	TYR	-	linker	UNP Q38062
K	130	GLY	-	linker	UNP Q38062
K	131	GLY	-	linker	UNP Q38062
L	128	ALA	-	linker	UNP Q38062
L	129	TYR	-	linker	UNP Q38062
L	130	GLY	-	linker	UNP Q38062
L	131	GLY	-	linker	UNP Q38062
M	128	ALA	-	linker	UNP Q38062
M	129	TYR	-	linker	UNP Q38062
M	130	GLY	-	linker	UNP Q38062
M	131	GLY	-	linker	UNP Q38062
N	128	ALA	-	linker	UNP Q38062
N	129	TYR	-	linker	UNP Q38062
N	130	GLY	-	linker	UNP Q38062
N	131	GLY	-	linker	UNP Q38062
O	128	ALA	-	linker	UNP Q38062
O	129	TYR	-	linker	UNP Q38062
O	130	GLY	-	linker	UNP Q38062
O	131	GLY	-	linker	UNP Q38062
P	128	ALA	-	linker	UNP Q38062
P	129	TYR	-	linker	UNP Q38062
P	130	GLY	-	linker	UNP Q38062
P	131	GLY	-	linker	UNP Q38062
Q	128	ALA	-	linker	UNP Q38062
Q	129	TYR	-	linker	UNP Q38062
Q	130	GLY	-	linker	UNP Q38062
Q	131	GLY	-	linker	UNP Q38062
R	128	ALA	-	linker	UNP Q38062
R	129	TYR	-	linker	UNP Q38062
R	130	GLY	-	linker	UNP Q38062
R	131	GLY	-	linker	UNP Q38062
S	128	ALA	-	linker	UNP Q38062
S	129	TYR	-	linker	UNP Q38062
S	130	GLY	-	linker	UNP Q38062
S	131	GLY	-	linker	UNP Q38062
T	128	ALA	-	linker	UNP Q38062
T	129	TYR	-	linker	UNP Q38062
T	130	GLY	-	linker	UNP Q38062
T	131	GLY	-	linker	UNP Q38062
V	128	ALA	-	linker	UNP Q38062

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Chain	Residue	Modelled	Actual	Comment	Reference
V	129	TYR	-	linker	UNP Q38062
V	130	GLY	-	linker	UNP Q38062
V	131	GLY	-	linker	UNP Q38062
W	128	ALA	-	linker	UNP Q38062
W	129	TYR	-	linker	UNP Q38062
W	130	GLY	-	linker	UNP Q38062
W	131	GLY	-	linker	UNP Q38062
X	128	ALA	-	linker	UNP Q38062
X	129	TYR	-	linker	UNP Q38062
X	130	GLY	-	linker	UNP Q38062
X	131	GLY	-	linker	UNP Q38062
Y	128	ALA	-	linker	UNP Q38062
Y	129	TYR	-	linker	UNP Q38062
Y	130	GLY	-	linker	UNP Q38062
Y	131	GLY	-	linker	UNP Q38062
Z	128	ALA	-	linker	UNP Q38062
Z	129	TYR	-	linker	UNP Q38062
Z	130	GLY	-	linker	UNP Q38062
Z	131	GLY	-	linker	UNP Q38062
AA	128	ALA	-	linker	UNP Q38062
AA	129	TYR	-	linker	UNP Q38062
AA	130	GLY	-	linker	UNP Q38062
AA	131	GLY	-	linker	UNP Q38062
BA	128	ALA	-	linker	UNP Q38062
BA	129	TYR	-	linker	UNP Q38062
BA	130	GLY	-	linker	UNP Q38062
BA	131	GLY	-	linker	UNP Q38062
CA	128	ALA	-	linker	UNP Q38062
CA	129	TYR	-	linker	UNP Q38062
CA	130	GLY	-	linker	UNP Q38062
CA	131	GLY	-	linker	UNP Q38062
DA	128	ALA	-	linker	UNP Q38062
DA	129	TYR	-	linker	UNP Q38062
DA	130	GLY	-	linker	UNP Q38062
DA	131	GLY	-	linker	UNP Q38062
EA	128	ALA	-	linker	UNP Q38062
EA	129	TYR	-	linker	UNP Q38062
EA	130	GLY	-	linker	UNP Q38062
EA	131	GLY	-	linker	UNP Q38062
FA	128	ALA	-	linker	UNP Q38062
FA	129	TYR	-	linker	UNP Q38062
FA	130	GLY	-	linker	UNP Q38062

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Chain	Residue	Modelled	Actual	Comment	Reference
FA	131	GLY	-	linker	UNP Q38062
GA	128	ALA	-	linker	UNP Q38062
GA	129	TYR	-	linker	UNP Q38062
GA	130	GLY	-	linker	UNP Q38062
GA	131	GLY	-	linker	UNP Q38062
HA	128	ALA	-	linker	UNP Q38062
HA	129	TYR	-	linker	UNP Q38062
HA	130	GLY	-	linker	UNP Q38062
HA	131	GLY	-	linker	UNP Q38062
IA	128	ALA	-	linker	UNP Q38062
IA	129	TYR	-	linker	UNP Q38062
IA	130	GLY	-	linker	UNP Q38062
IA	131	GLY	-	linker	UNP Q38062
JA	128	ALA	-	linker	UNP Q38062
JA	129	TYR	-	linker	UNP Q38062
JA	130	GLY	-	linker	UNP Q38062
JA	131	GLY	-	linker	UNP Q38062
KA	128	ALA	-	linker	UNP Q38062
KA	129	TYR	-	linker	UNP Q38062
KA	130	GLY	-	linker	UNP Q38062
KA	131	GLY	-	linker	UNP Q38062
LA	128	ALA	-	linker	UNP Q38062
LA	129	TYR	-	linker	UNP Q38062
LA	130	GLY	-	linker	UNP Q38062
LA	131	GLY	-	linker	UNP Q38062
MA	128	ALA	-	linker	UNP Q38062
MA	129	TYR	-	linker	UNP Q38062
MA	130	GLY	-	linker	UNP Q38062
MA	131	GLY	-	linker	UNP Q38062
NA	128	ALA	-	linker	UNP Q38062
NA	129	TYR	-	linker	UNP Q38062
NA	130	GLY	-	linker	UNP Q38062
NA	131	GLY	-	linker	UNP Q38062
OA	128	ALA	-	linker	UNP Q38062
OA	129	TYR	-	linker	UNP Q38062
OA	130	GLY	-	linker	UNP Q38062
OA	131	GLY	-	linker	UNP Q38062
PA	128	ALA	-	linker	UNP Q38062
PA	129	TYR	-	linker	UNP Q38062
PA	130	GLY	-	linker	UNP Q38062
PA	131	GLY	-	linker	UNP Q38062
QA	128	ALA	-	linker	UNP Q38062

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Chain	Residue	Modelled	Actual	Comment	Reference
QA	129	TYR	-	linker	UNP Q38062
QA	130	GLY	-	linker	UNP Q38062
QA	131	GLY	-	linker	UNP Q38062
RA	128	ALA	-	linker	UNP Q38062
RA	129	TYR	-	linker	UNP Q38062
RA	130	GLY	-	linker	UNP Q38062
RA	131	GLY	-	linker	UNP Q38062
SA	128	ALA	-	linker	UNP Q38062
SA	129	TYR	-	linker	UNP Q38062
SA	130	GLY	-	linker	UNP Q38062
SA	131	GLY	-	linker	UNP Q38062
TA	128	ALA	-	linker	UNP Q38062
TA	129	TYR	-	linker	UNP Q38062
TA	130	GLY	-	linker	UNP Q38062
TA	131	GLY	-	linker	UNP Q38062
UA	128	ALA	-	linker	UNP Q38062
UA	129	TYR	-	linker	UNP Q38062
UA	130	GLY	-	linker	UNP Q38062
UA	131	GLY	-	linker	UNP Q38062
VA	128	ALA	-	linker	UNP Q38062
VA	129	TYR	-	linker	UNP Q38062
VA	130	GLY	-	linker	UNP Q38062
VA	131	GLY	-	linker	UNP Q38062
WA	128	ALA	-	linker	UNP Q38062
WA	129	TYR	-	linker	UNP Q38062
WA	130	GLY	-	linker	UNP Q38062
WA	131	GLY	-	linker	UNP Q38062
XA	128	ALA	-	linker	UNP Q38062
XA	129	TYR	-	linker	UNP Q38062
XA	130	GLY	-	linker	UNP Q38062
XA	131	GLY	-	linker	UNP Q38062
YA	128	ALA	-	linker	UNP Q38062
YA	129	TYR	-	linker	UNP Q38062
YA	130	GLY	-	linker	UNP Q38062
YA	131	GLY	-	linker	UNP Q38062
ZA	128	ALA	-	linker	UNP Q38062
ZA	129	TYR	-	linker	UNP Q38062
ZA	130	GLY	-	linker	UNP Q38062
ZA	131	GLY	-	linker	UNP Q38062
AB	128	ALA	-	linker	UNP Q38062
AB	129	TYR	-	linker	UNP Q38062
AB	130	GLY	-	linker	UNP Q38062

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Chain	Residue	Modelled	Actual	Comment	Reference
AB	131	GLY	-	linker	UNP Q38062
BB	128	ALA	-	linker	UNP Q38062
BB	129	TYR	-	linker	UNP Q38062
BB	130	GLY	-	linker	UNP Q38062
BB	131	GLY	-	linker	UNP Q38062
CB	128	ALA	-	linker	UNP Q38062
CB	129	TYR	-	linker	UNP Q38062
CB	130	GLY	-	linker	UNP Q38062
CB	131	GLY	-	linker	UNP Q38062
DB	128	ALA	-	linker	UNP Q38062
DB	129	TYR	-	linker	UNP Q38062
DB	130	GLY	-	linker	UNP Q38062
DB	131	GLY	-	linker	UNP Q38062
EB	128	ALA	-	linker	UNP Q38062
EB	129	TYR	-	linker	UNP Q38062
EB	130	GLY	-	linker	UNP Q38062
EB	131	GLY	-	linker	UNP Q38062
FB	128	ALA	-	linker	UNP Q38062
FB	129	TYR	-	linker	UNP Q38062
FB	130	GLY	-	linker	UNP Q38062
FB	131	GLY	-	linker	UNP Q38062
GB	128	ALA	-	linker	UNP Q38062
GB	129	TYR	-	linker	UNP Q38062
GB	130	GLY	-	linker	UNP Q38062
GB	131	GLY	-	linker	UNP Q38062
HB	128	ALA	-	linker	UNP Q38062
HB	129	TYR	-	linker	UNP Q38062
HB	130	GLY	-	linker	UNP Q38062
HB	131	GLY	-	linker	UNP Q38062
IB	128	ALA	-	linker	UNP Q38062
IB	129	TYR	-	linker	UNP Q38062
IB	130	GLY	-	linker	UNP Q38062
IB	131	GLY	-	linker	UNP Q38062
JB	128	ALA	-	linker	UNP Q38062
JB	129	TYR	-	linker	UNP Q38062
JB	130	GLY	-	linker	UNP Q38062
JB	131	GLY	-	linker	UNP Q38062
KB	128	ALA	-	linker	UNP Q38062
KB	129	TYR	-	linker	UNP Q38062
KB	130	GLY	-	linker	UNP Q38062
KB	131	GLY	-	linker	UNP Q38062
LB	128	ALA	-	linker	UNP Q38062

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Chain	Residue	Modelled	Actual	Comment	Reference
LB	129	TYR	-	linker	UNP Q38062
LB	130	GLY	-	linker	UNP Q38062
LB	131	GLY	-	linker	UNP Q38062
MB	128	ALA	-	linker	UNP Q38062
MB	129	TYR	-	linker	UNP Q38062
MB	130	GLY	-	linker	UNP Q38062
MB	131	GLY	-	linker	UNP Q38062
NB	128	ALA	-	linker	UNP Q38062
NB	129	TYR	-	linker	UNP Q38062
NB	130	GLY	-	linker	UNP Q38062
NB	131	GLY	-	linker	UNP Q38062
OB	128	ALA	-	linker	UNP Q38062
OB	129	TYR	-	linker	UNP Q38062
OB	130	GLY	-	linker	UNP Q38062
OB	131	GLY	-	linker	UNP Q38062
PB	128	ALA	-	linker	UNP Q38062
PB	129	TYR	-	linker	UNP Q38062
PB	130	GLY	-	linker	UNP Q38062
PB	131	GLY	-	linker	UNP Q38062
QB	128	ALA	-	linker	UNP Q38062
QB	129	TYR	-	linker	UNP Q38062
QB	130	GLY	-	linker	UNP Q38062
QB	131	GLY	-	linker	UNP Q38062
RB	128	ALA	-	linker	UNP Q38062
RB	129	TYR	-	linker	UNP Q38062
RB	130	GLY	-	linker	UNP Q38062
RB	131	GLY	-	linker	UNP Q38062
SB	128	ALA	-	linker	UNP Q38062
SB	129	TYR	-	linker	UNP Q38062
SB	130	GLY	-	linker	UNP Q38062
SB	131	GLY	-	linker	UNP Q38062
TB	128	ALA	-	linker	UNP Q38062
TB	129	TYR	-	linker	UNP Q38062
TB	130	GLY	-	linker	UNP Q38062
TB	131	GLY	-	linker	UNP Q38062
UB	128	ALA	-	linker	UNP Q38062
UB	129	TYR	-	linker	UNP Q38062
UB	130	GLY	-	linker	UNP Q38062
UB	131	GLY	-	linker	UNP Q38062
VB	128	ALA	-	linker	UNP Q38062
VB	129	TYR	-	linker	UNP Q38062
VB	130	GLY	-	linker	UNP Q38062

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Chain	Residue	Modelled	Actual	Comment	Reference
VB	131	GLY	-	linker	UNP Q38062
WB	128	ALA	-	linker	UNP Q38062
WB	129	TYR	-	linker	UNP Q38062
WB	130	GLY	-	linker	UNP Q38062
WB	131	GLY	-	linker	UNP Q38062
XB	128	ALA	-	linker	UNP Q38062
XB	129	TYR	-	linker	UNP Q38062
XB	130	GLY	-	linker	UNP Q38062
XB	131	GLY	-	linker	UNP Q38062
YB	128	ALA	-	linker	UNP Q38062
YB	129	TYR	-	linker	UNP Q38062
YB	130	GLY	-	linker	UNP Q38062
YB	131	GLY	-	linker	UNP Q38062
ZB	128	ALA	-	linker	UNP Q38062
ZB	129	TYR	-	linker	UNP Q38062
ZB	130	GLY	-	linker	UNP Q38062
ZB	131	GLY	-	linker	UNP Q38062
AC	128	ALA	-	linker	UNP Q38062
AC	129	TYR	-	linker	UNP Q38062
AC	130	GLY	-	linker	UNP Q38062
AC	131	GLY	-	linker	UNP Q38062
BC	128	ALA	-	linker	UNP Q38062
BC	129	TYR	-	linker	UNP Q38062
BC	130	GLY	-	linker	UNP Q38062
BC	131	GLY	-	linker	UNP Q38062
CC	128	ALA	-	linker	UNP Q38062
CC	129	TYR	-	linker	UNP Q38062
CC	130	GLY	-	linker	UNP Q38062
CC	131	GLY	-	linker	UNP Q38062
DC	128	ALA	-	linker	UNP Q38062
DC	129	TYR	-	linker	UNP Q38062
DC	130	GLY	-	linker	UNP Q38062
DC	131	GLY	-	linker	UNP Q38062
EC	128	ALA	-	linker	UNP Q38062
EC	129	TYR	-	linker	UNP Q38062
EC	130	GLY	-	linker	UNP Q38062
EC	131	GLY	-	linker	UNP Q38062
FC	128	ALA	-	linker	UNP Q38062
FC	129	TYR	-	linker	UNP Q38062
FC	130	GLY	-	linker	UNP Q38062
FC	131	GLY	-	linker	UNP Q38062
GC	128	ALA	-	linker	UNP Q38062

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Chain	Residue	Modelled	Actual	Comment	Reference
GC	129	TYR	-	linker	UNP Q38062
GC	130	GLY	-	linker	UNP Q38062
GC	131	GLY	-	linker	UNP Q38062
HC	128	ALA	-	linker	UNP Q38062
HC	129	TYR	-	linker	UNP Q38062
HC	130	GLY	-	linker	UNP Q38062
HC	131	GLY	-	linker	UNP Q38062
IC	128	ALA	-	linker	UNP Q38062
IC	129	TYR	-	linker	UNP Q38062
IC	130	GLY	-	linker	UNP Q38062
IC	131	GLY	-	linker	UNP Q38062
JC	128	ALA	-	linker	UNP Q38062
JC	129	TYR	-	linker	UNP Q38062
JC	130	GLY	-	linker	UNP Q38062
JC	131	GLY	-	linker	UNP Q38062
KC	128	ALA	-	linker	UNP Q38062
KC	129	TYR	-	linker	UNP Q38062
KC	130	GLY	-	linker	UNP Q38062
KC	131	GLY	-	linker	UNP Q38062
LC	128	ALA	-	linker	UNP Q38062
LC	129	TYR	-	linker	UNP Q38062
LC	130	GLY	-	linker	UNP Q38062
LC	131	GLY	-	linker	UNP Q38062
MC	128	ALA	-	linker	UNP Q38062
MC	129	TYR	-	linker	UNP Q38062
MC	130	GLY	-	linker	UNP Q38062
MC	131	GLY	-	linker	UNP Q38062
NC	128	ALA	-	linker	UNP Q38062
NC	129	TYR	-	linker	UNP Q38062
NC	130	GLY	-	linker	UNP Q38062
NC	131	GLY	-	linker	UNP Q38062
OC	128	ALA	-	linker	UNP Q38062
OC	129	TYR	-	linker	UNP Q38062
OC	130	GLY	-	linker	UNP Q38062
OC	131	GLY	-	linker	UNP Q38062
PC	128	ALA	-	linker	UNP Q38062
PC	129	TYR	-	linker	UNP Q38062
PC	130	GLY	-	linker	UNP Q38062
PC	131	GLY	-	linker	UNP Q38062
QC	128	ALA	-	linker	UNP Q38062
QC	129	TYR	-	linker	UNP Q38062
QC	130	GLY	-	linker	UNP Q38062

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Chain	Residue	Modelled	Actual	Comment	Reference
QC	131	GLY	-	linker	UNP Q38062
RC	128	ALA	-	linker	UNP Q38062
RC	129	TYR	-	linker	UNP Q38062
RC	130	GLY	-	linker	UNP Q38062
RC	131	GLY	-	linker	UNP Q38062
SC	128	ALA	-	linker	UNP Q38062
SC	129	TYR	-	linker	UNP Q38062
SC	130	GLY	-	linker	UNP Q38062
SC	131	GLY	-	linker	UNP Q38062
TC	128	ALA	-	linker	UNP Q38062
TC	129	TYR	-	linker	UNP Q38062
TC	130	GLY	-	linker	UNP Q38062
TC	131	GLY	-	linker	UNP Q38062
UC	128	ALA	-	linker	UNP Q38062
UC	129	TYR	-	linker	UNP Q38062
UC	130	GLY	-	linker	UNP Q38062
UC	131	GLY	-	linker	UNP Q38062
VC	128	ALA	-	linker	UNP Q38062
VC	129	TYR	-	linker	UNP Q38062
VC	130	GLY	-	linker	UNP Q38062
VC	131	GLY	-	linker	UNP Q38062
WC	128	ALA	-	linker	UNP Q38062
WC	129	TYR	-	linker	UNP Q38062
WC	130	GLY	-	linker	UNP Q38062
WC	131	GLY	-	linker	UNP Q38062
XC	128	ALA	-	linker	UNP Q38062
XC	129	TYR	-	linker	UNP Q38062
XC	130	GLY	-	linker	UNP Q38062
XC	131	GLY	-	linker	UNP Q38062
YC	128	ALA	-	linker	UNP Q38062
YC	129	TYR	-	linker	UNP Q38062
YC	130	GLY	-	linker	UNP Q38062
YC	131	GLY	-	linker	UNP Q38062
ZC	128	ALA	-	linker	UNP Q38062
ZC	129	TYR	-	linker	UNP Q38062
ZC	130	GLY	-	linker	UNP Q38062
ZC	131	GLY	-	linker	UNP Q38062
AD	128	ALA	-	linker	UNP Q38062
AD	129	TYR	-	linker	UNP Q38062
AD	130	GLY	-	linker	UNP Q38062
AD	131	GLY	-	linker	UNP Q38062
BD	128	ALA	-	linker	UNP Q38062

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Chain	Residue	Modelled	Actual	Comment	Reference
BD	129	TYR	-	linker	UNP Q38062
BD	130	GLY	-	linker	UNP Q38062
BD	131	GLY	-	linker	UNP Q38062
CD	128	ALA	-	linker	UNP Q38062
CD	129	TYR	-	linker	UNP Q38062
CD	130	GLY	-	linker	UNP Q38062
CD	131	GLY	-	linker	UNP Q38062
DD	128	ALA	-	linker	UNP Q38062
DD	129	TYR	-	linker	UNP Q38062
DD	130	GLY	-	linker	UNP Q38062
DD	131	GLY	-	linker	UNP Q38062
ED	128	ALA	-	linker	UNP Q38062
ED	129	TYR	-	linker	UNP Q38062
ED	130	GLY	-	linker	UNP Q38062
ED	131	GLY	-	linker	UNP Q38062
FD	128	ALA	-	linker	UNP Q38062
FD	129	TYR	-	linker	UNP Q38062
FD	130	GLY	-	linker	UNP Q38062
FD	131	GLY	-	linker	UNP Q38062
GD	128	ALA	-	linker	UNP Q38062
GD	129	TYR	-	linker	UNP Q38062
GD	130	GLY	-	linker	UNP Q38062
GD	131	GLY	-	linker	UNP Q38062
HD	128	ALA	-	linker	UNP Q38062
HD	129	TYR	-	linker	UNP Q38062
HD	130	GLY	-	linker	UNP Q38062
HD	131	GLY	-	linker	UNP Q38062
ID	128	ALA	-	linker	UNP Q38062
ID	129	TYR	-	linker	UNP Q38062
ID	130	GLY	-	linker	UNP Q38062
ID	131	GLY	-	linker	UNP Q38062
JD	128	ALA	-	linker	UNP Q38062
JD	129	TYR	-	linker	UNP Q38062
JD	130	GLY	-	linker	UNP Q38062
JD	131	GLY	-	linker	UNP Q38062
KD	128	ALA	-	linker	UNP Q38062
KD	129	TYR	-	linker	UNP Q38062
KD	130	GLY	-	linker	UNP Q38062
KD	131	GLY	-	linker	UNP Q38062
LD	128	ALA	-	linker	UNP Q38062
LD	129	TYR	-	linker	UNP Q38062
LD	130	GLY	-	linker	UNP Q38062

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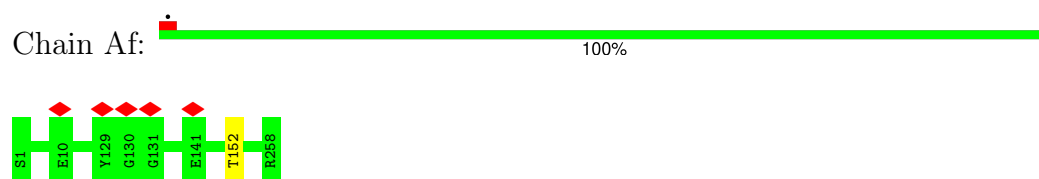
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Chain	Residue	Modelled	Actual	Comment	Reference
LD	131	GLY	-	linker	UNP Q38062
MD	128	ALA	-	linker	UNP Q38062
MD	129	TYR	-	linker	UNP Q38062
MD	130	GLY	-	linker	UNP Q38062
MD	131	GLY	-	linker	UNP Q38062
ND	128	ALA	-	linker	UNP Q38062
ND	129	TYR	-	linker	UNP Q38062
ND	130	GLY	-	linker	UNP Q38062
ND	131	GLY	-	linker	UNP Q38062
OD	128	ALA	-	linker	UNP Q38062
OD	129	TYR	-	linker	UNP Q38062
OD	130	GLY	-	linker	UNP Q38062
OD	131	GLY	-	linker	UNP Q38062
PD	128	ALA	-	linker	UNP Q38062
PD	129	TYR	-	linker	UNP Q38062
PD	130	GLY	-	linker	UNP Q38062
PD	131	GLY	-	linker	UNP Q38062

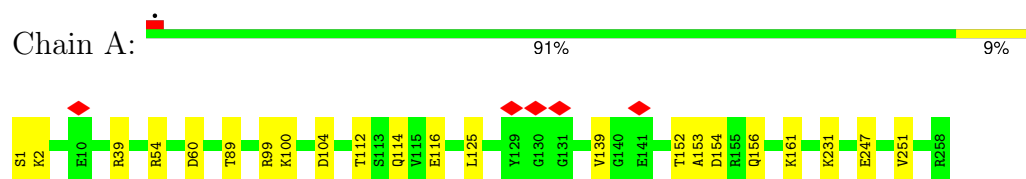
3 Residue-property plots [i](#)

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

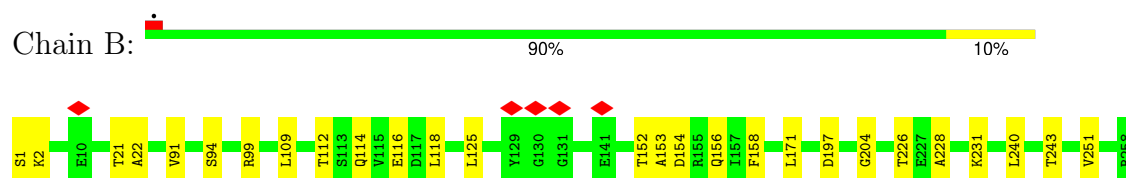
- Molecule 1: Coat protein



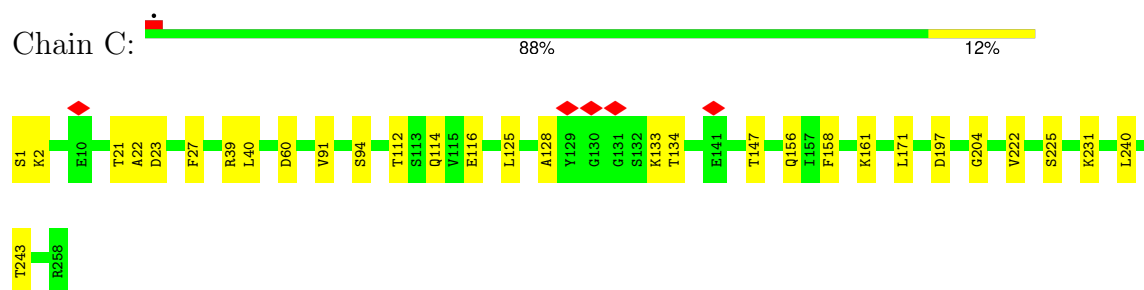
- Molecule 1: Coat protein



- Molecule 1: Coat protein

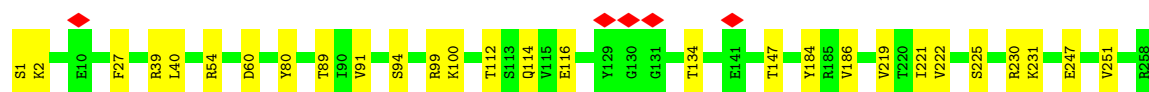


- Molecule 1: Coat protein

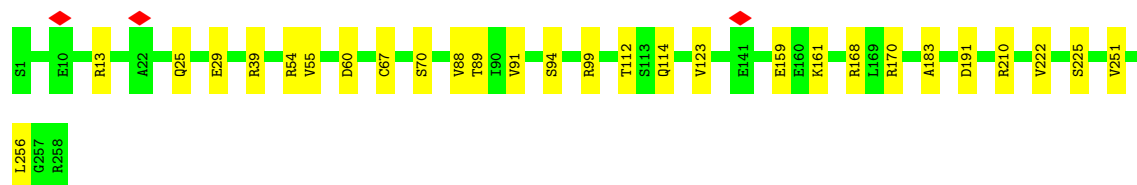
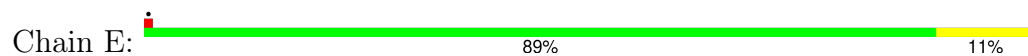


- Molecule 1: Coat protein

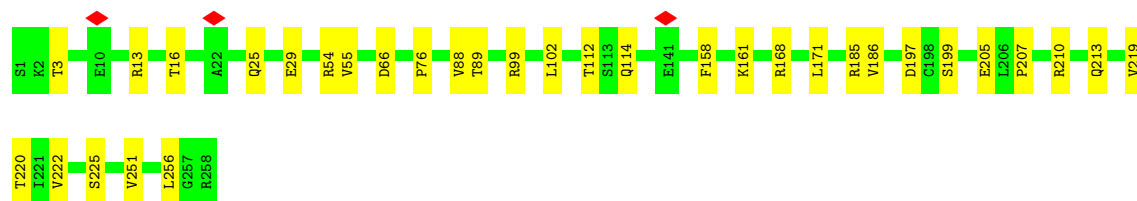
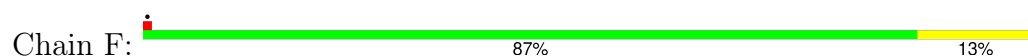




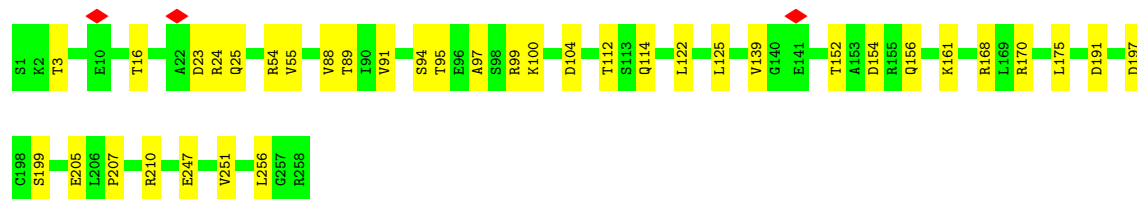
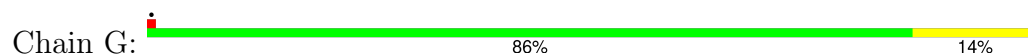
- Molecule 1: Coat protein



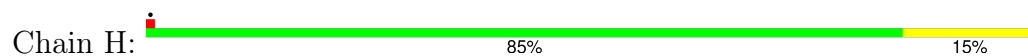
- Molecule 1: Coat protein



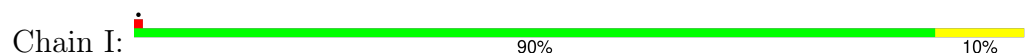
- Molecule 1: Coat protein

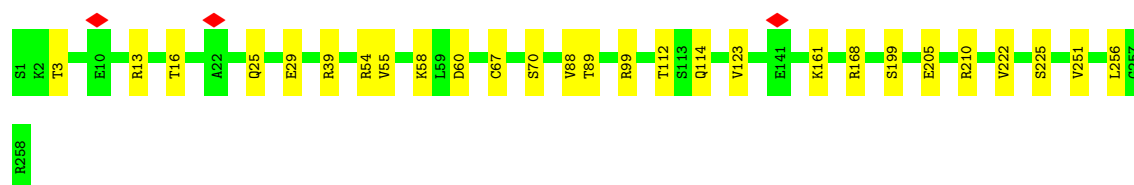


- Molecule 1: Coat protein

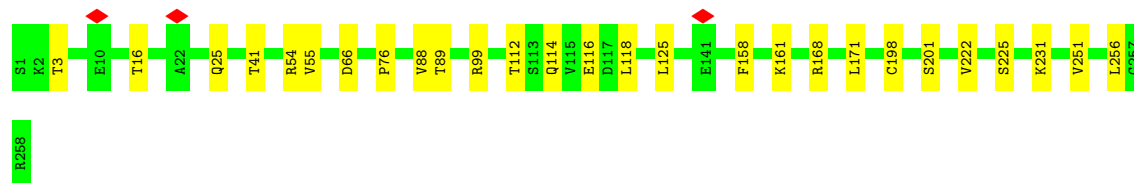


- Molecule 1: Coat protein

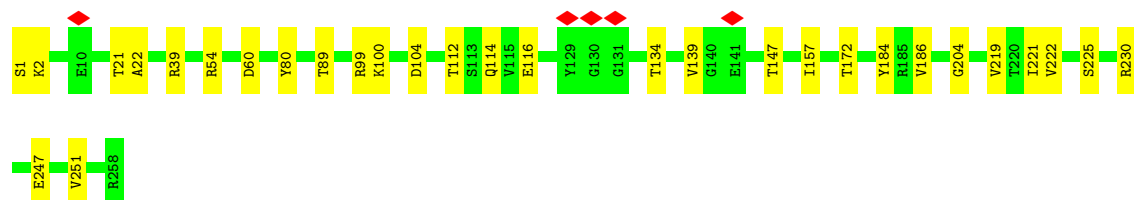
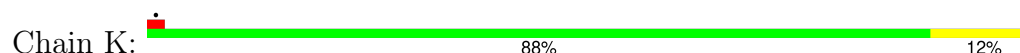




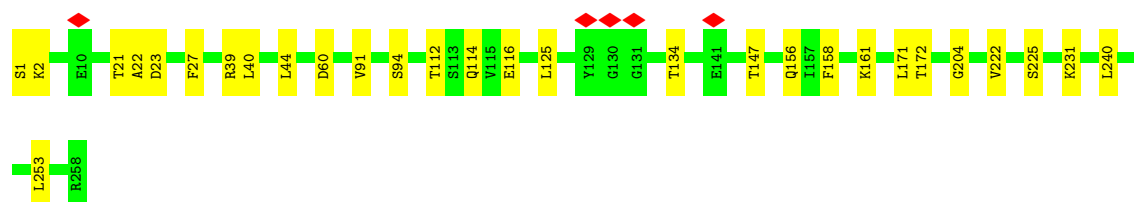
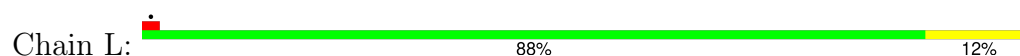
- Molecule 1: Coat protein



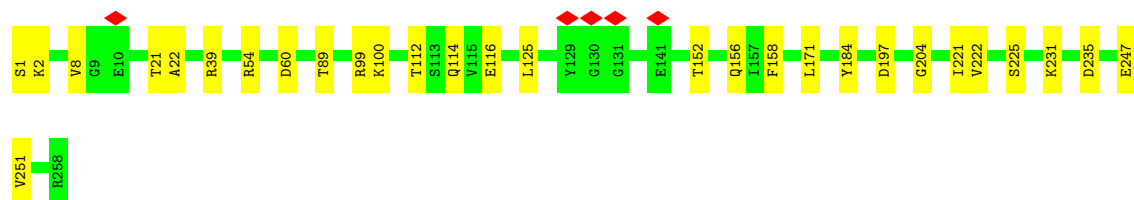
- Molecule 1: Coat protein



- Molecule 1: Coat protein

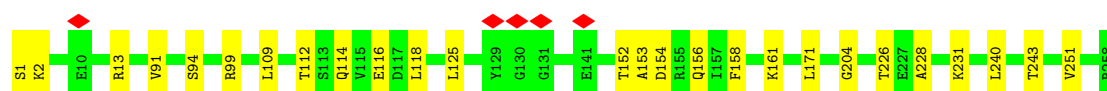


- Molecule 1: Coat protein




- Molecule 1: Coat protein

Chain N:  90% 10%




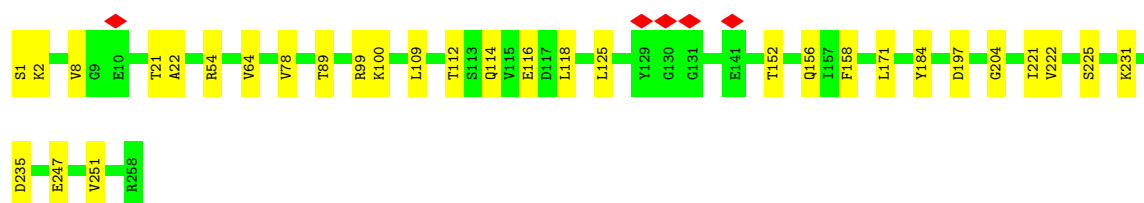
• Molecule 1: Coat protein

Chain O:  91% 9%



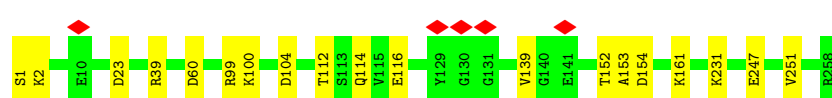
• Molecule 1: Coat protein

Chain P:  88% 12%




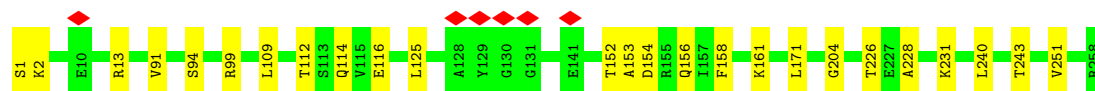
• Molecule 1: Coat protein

Chain Q:  93% 7%




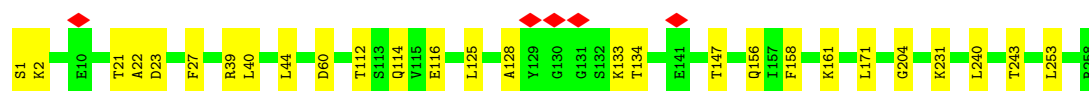
• Molecule 1: Coat protein

Chain R:  90% 10%



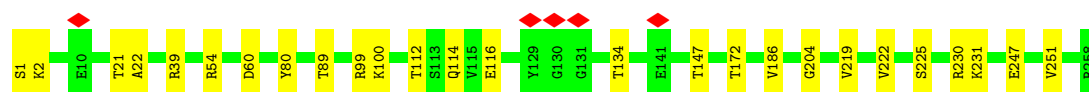
• Molecule 1: Coat protein

Chain S:  90% 10%

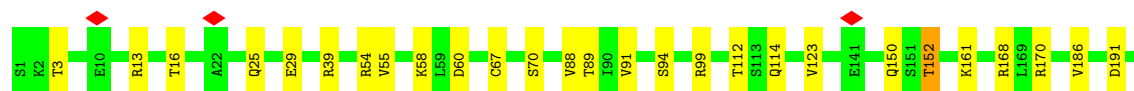
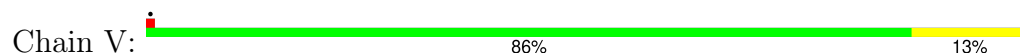


• Molecule 1: Coat protein

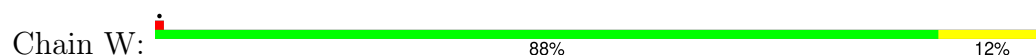
Chain T:  90% 10%



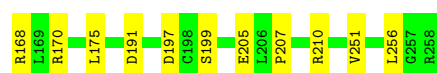
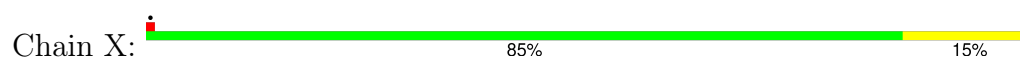
- Molecule 1: Coat protein



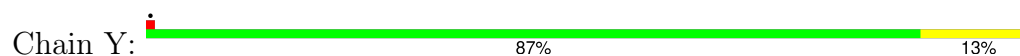
- Molecule 1: Coat protein



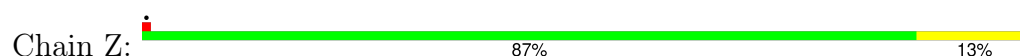
- Molecule 1: Coat protein

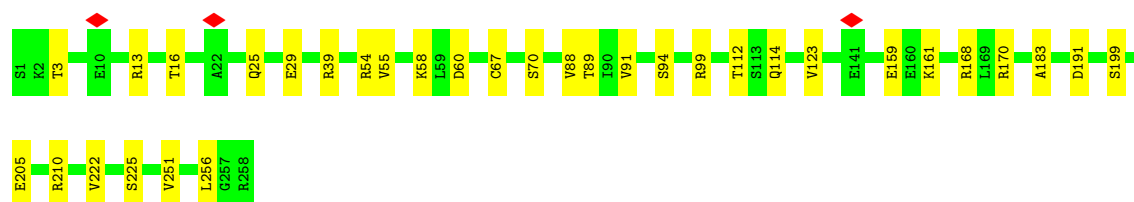


- Molecule 1: Coat protein



- Molecule 1: Coat protein

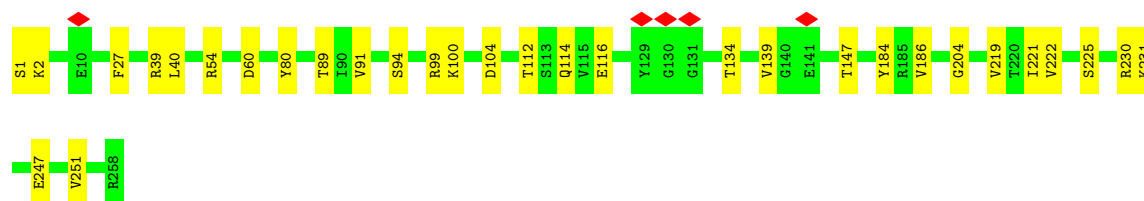




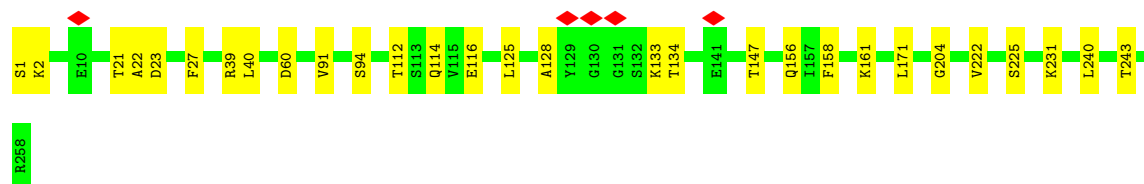
- Molecule 1: Coat protein



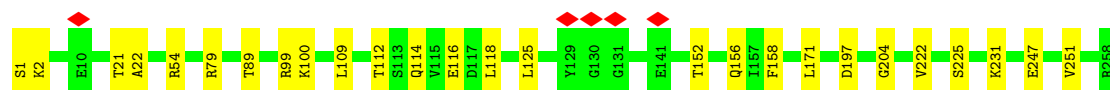
- Molecule 1: Coat protein



- Molecule 1: Coat protein

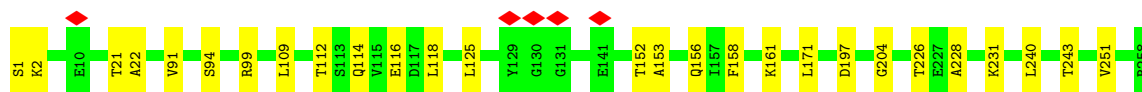


- Molecule 1: Coat protein

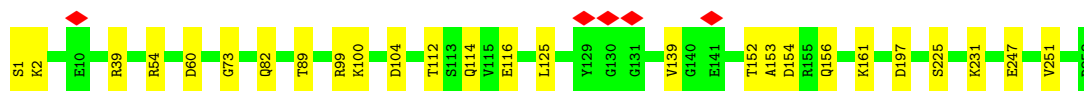
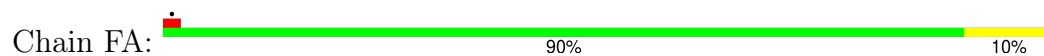


- Molecule 1: Coat protein

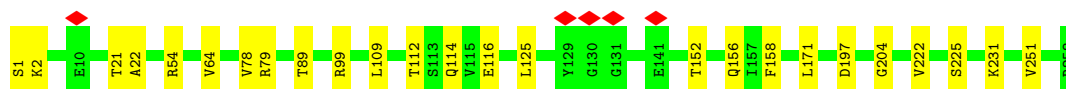




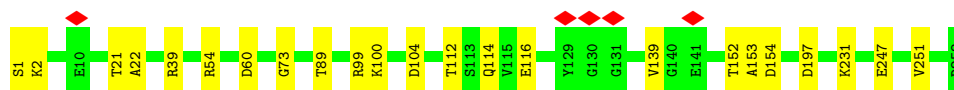
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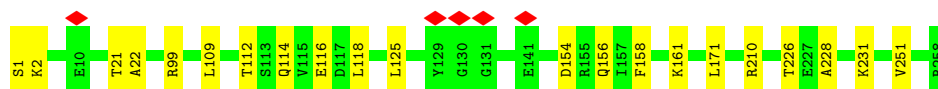
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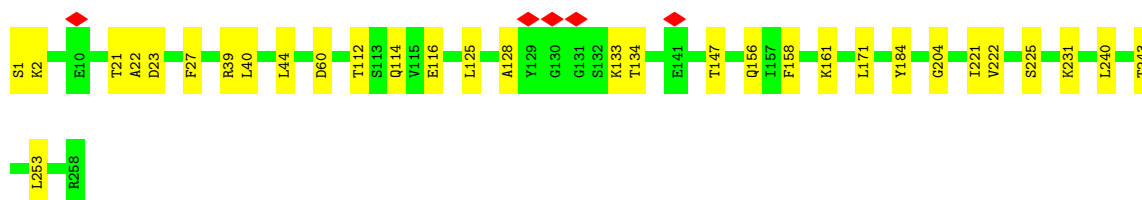
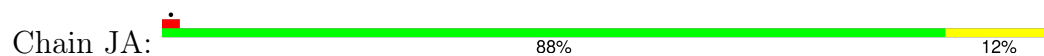
- Molecule 1: Coat protein



- Molecule 1: Coat protein

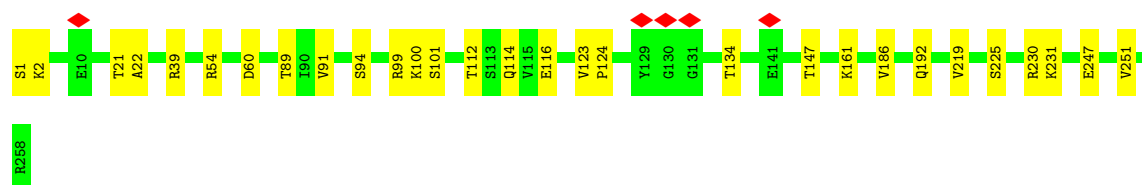


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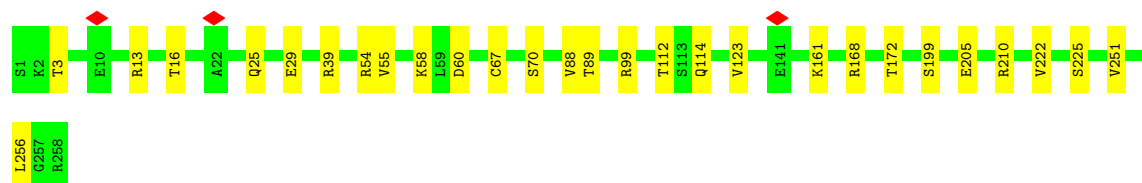


- Molecule 1: Coat protein





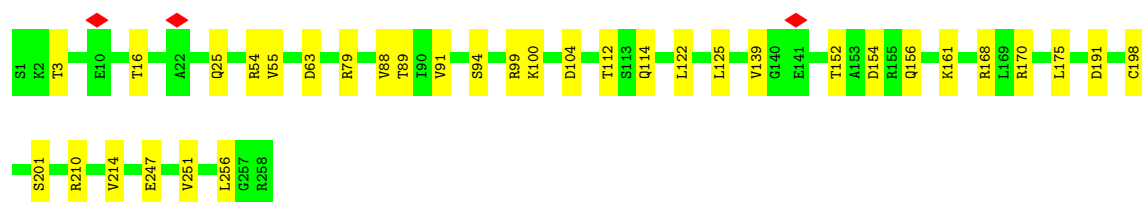
- Molecule 1: Coat protein



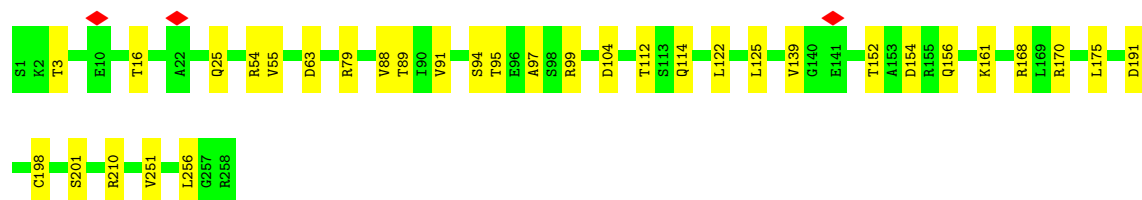
- Molecule 1: Coat protein



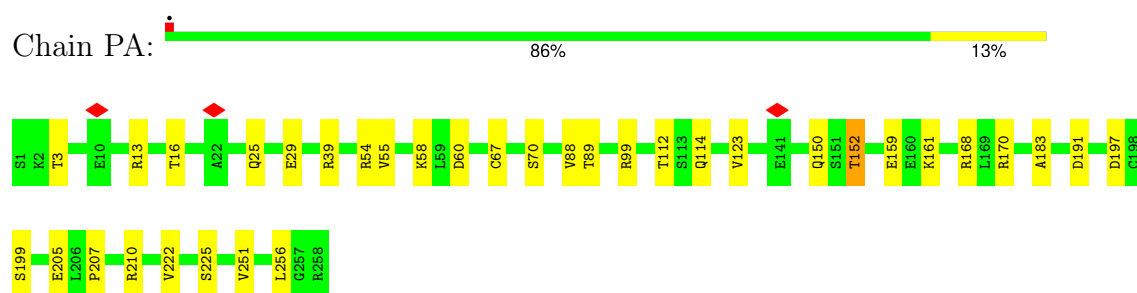
- Molecule 1: Coat protein



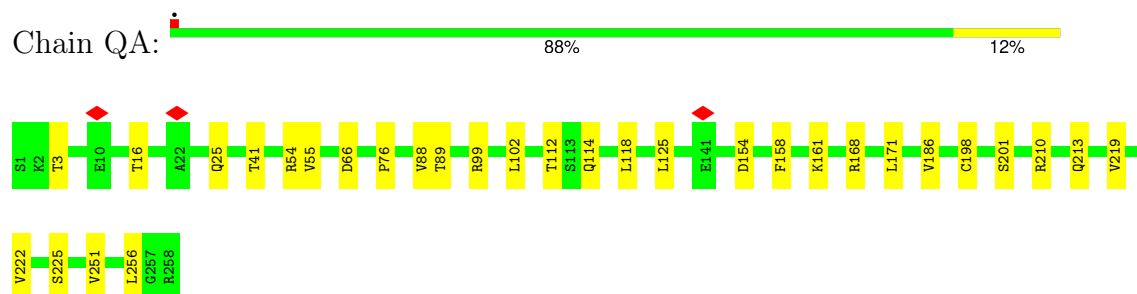
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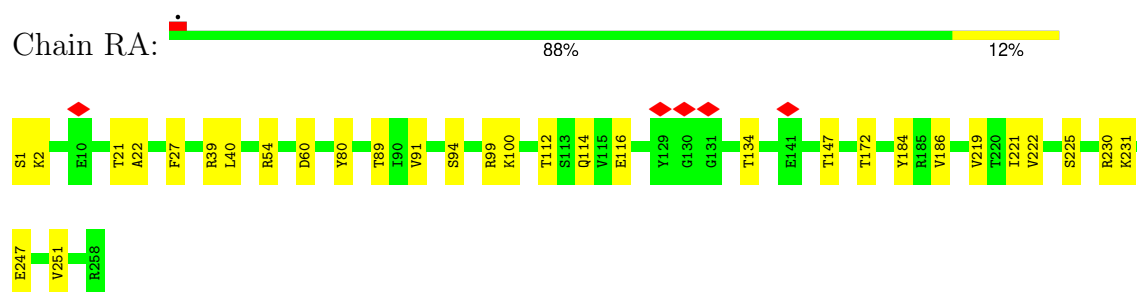
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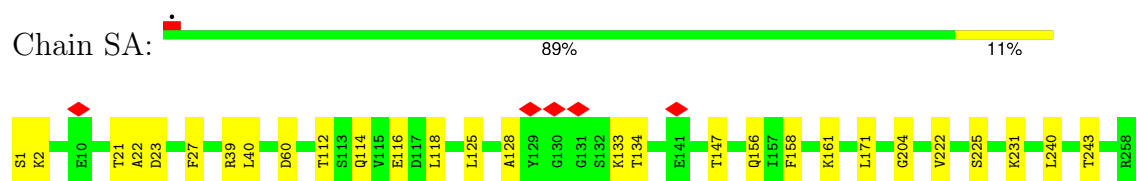
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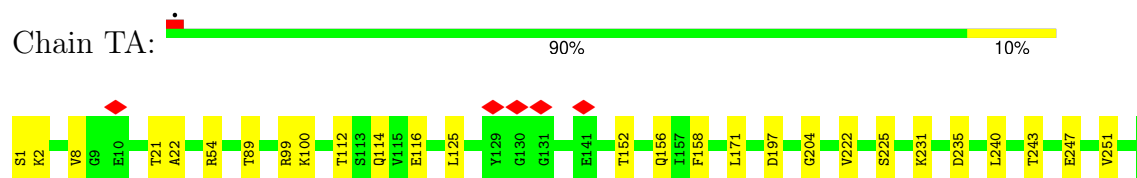
- Molecule 1: Coat protein



- Molecule 1: Coat protein

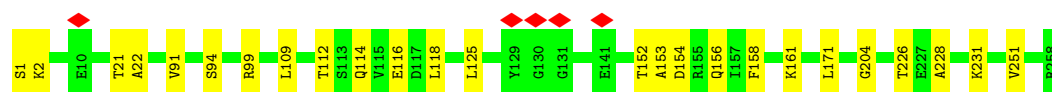


- Molecule 1: Coat protein



- Molecule 1: Coat protein

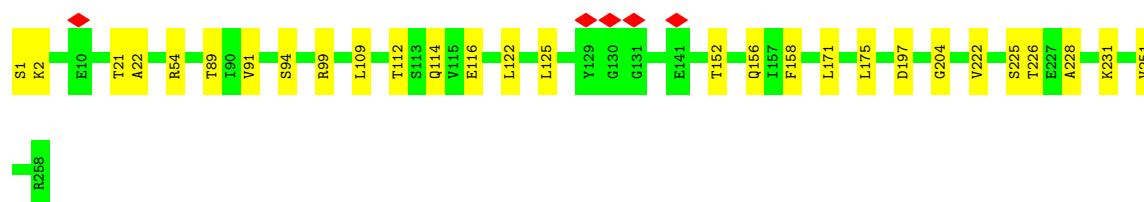




- Molecule 1: Coat protein



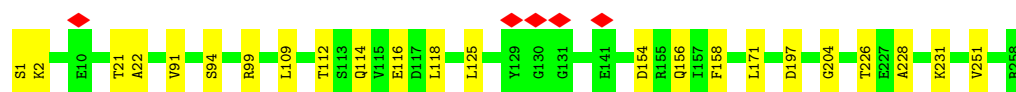
- Molecule 1: Coat protein



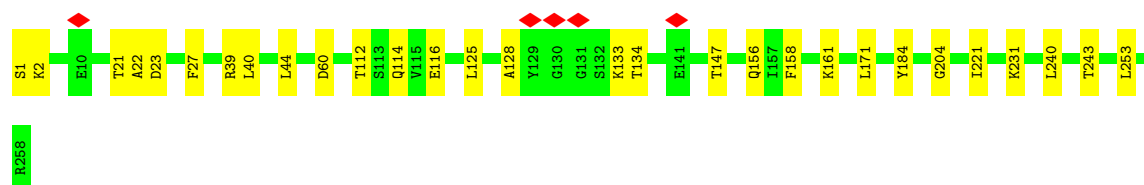
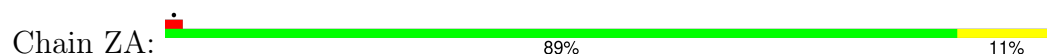
- Molecule 1: Coat protein



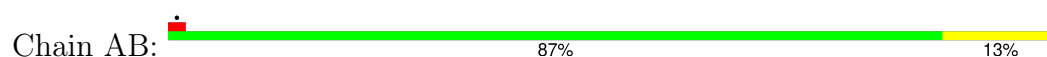
- Molecule 1: Coat protein

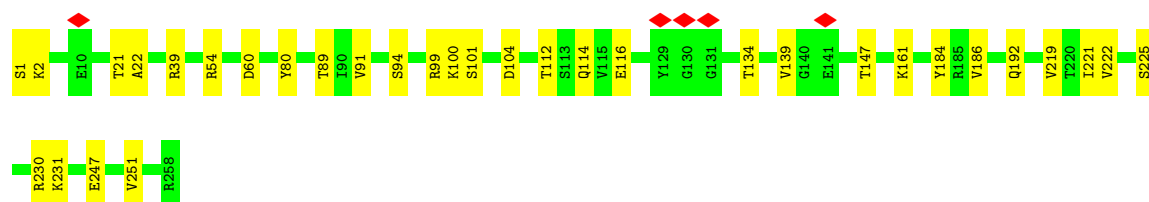


- Molecule 1: Coat protein

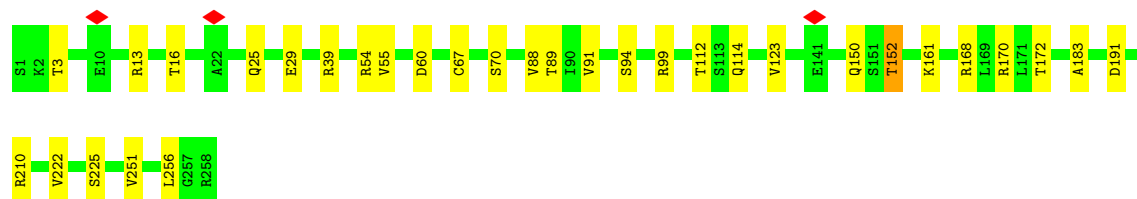


- Molecule 1: Coat protein

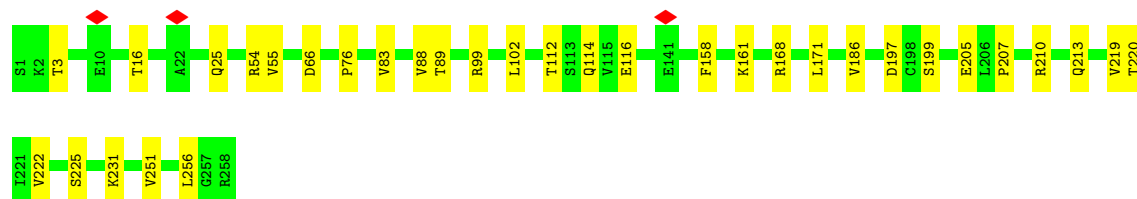




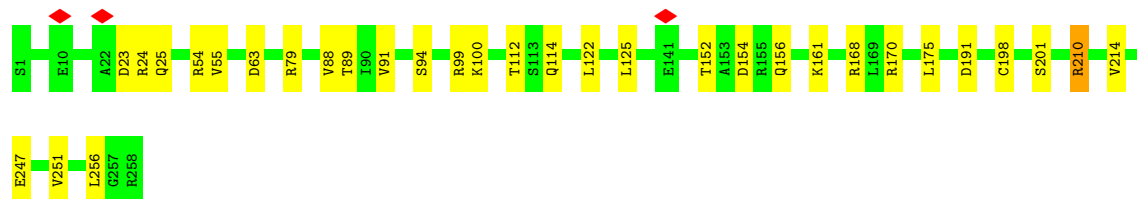
- Molecule 1: Coat protein



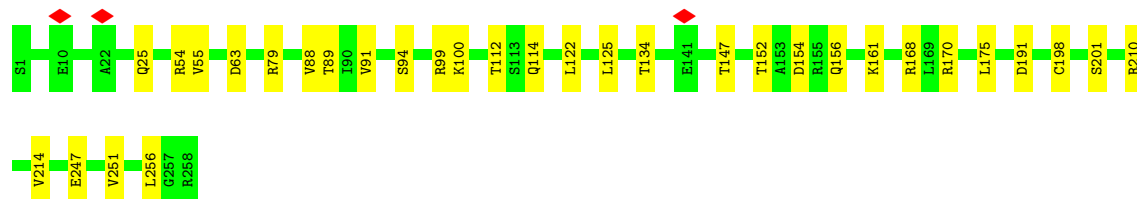
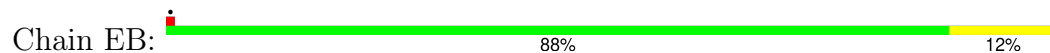
- Molecule 1: Coat protein



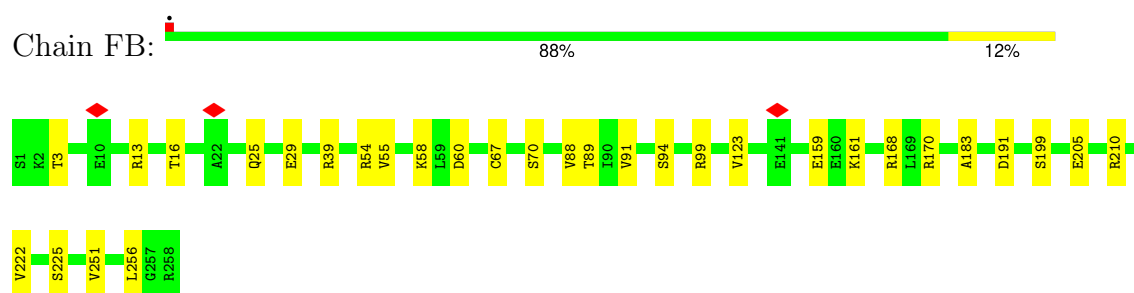
- Molecule 1: Coat protein



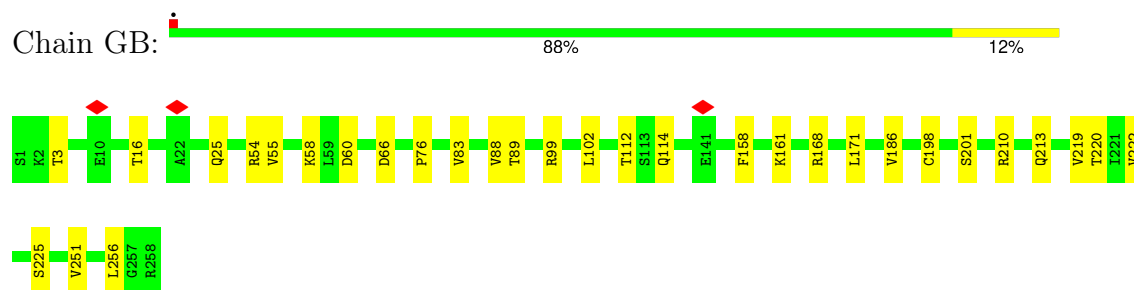
- Molecule 1: Coat protein



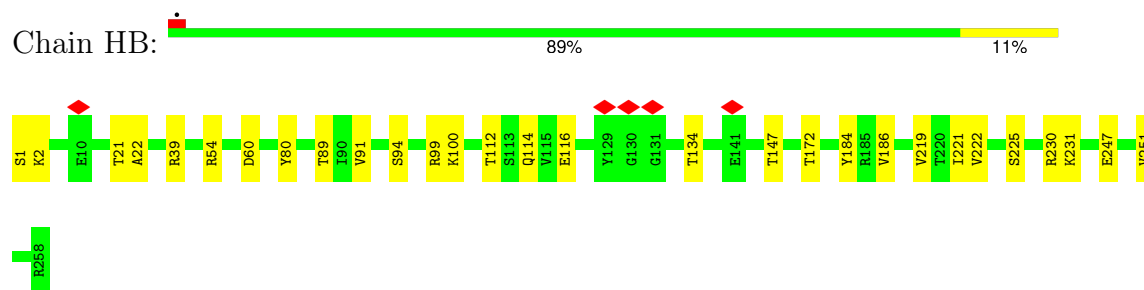
- Molecule 1: Coat protein



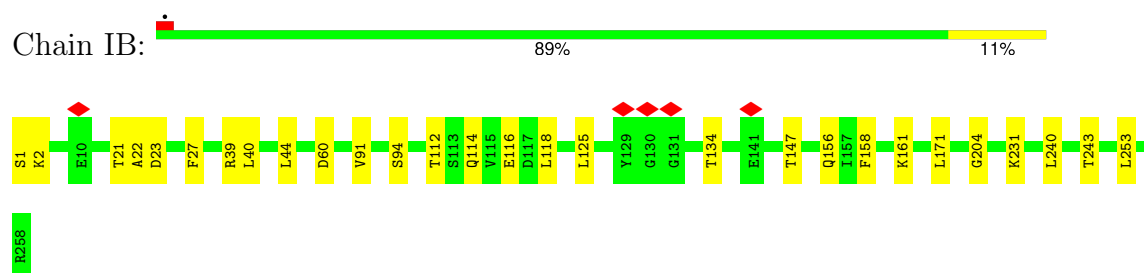
- Molecule 1: Coat protein



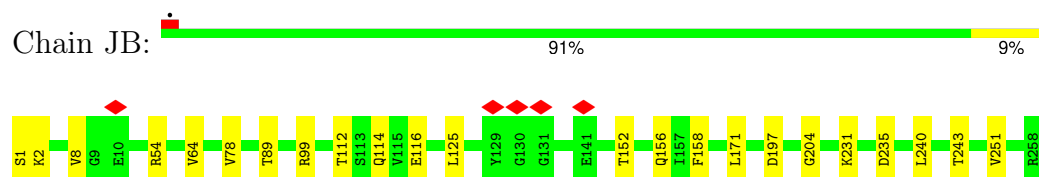
- Molecule 1: Coat protein



- Molecule 1: Coat protein

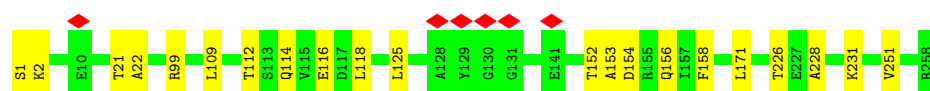


- Molecule 1: Coat protein



- Molecule 1: Coat protein

Chain KB:  92% 8%



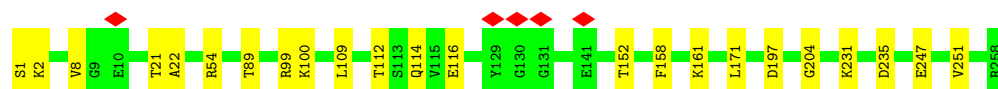
• Molecule 1: Coat protein

Chain LB:  91% 9%



• Molecule 1: Coat protein

Chain MB:  91% 9%



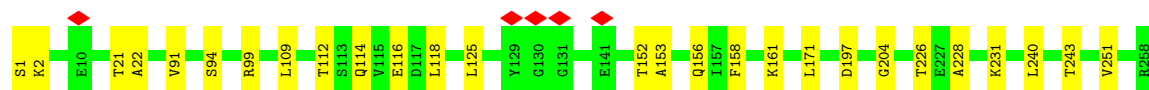
• Molecule 1: Coat protein

Chain NB:  91% 9%



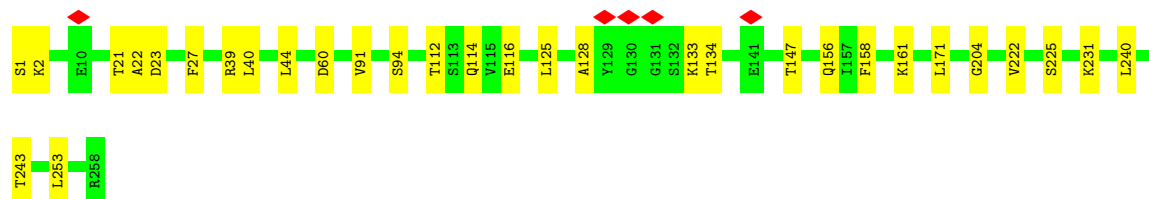
• Molecule 1: Coat protein

Chain OB:  90% 10%



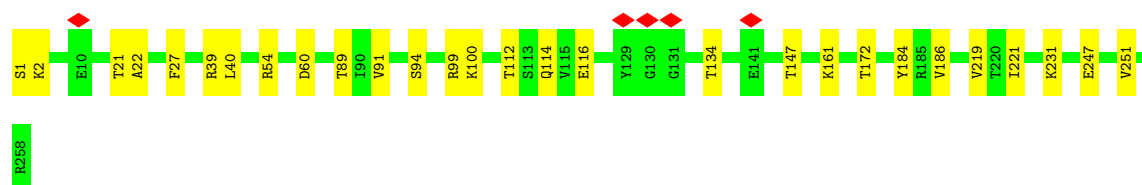
• Molecule 1: Coat protein

Chain PB:  88% 12%

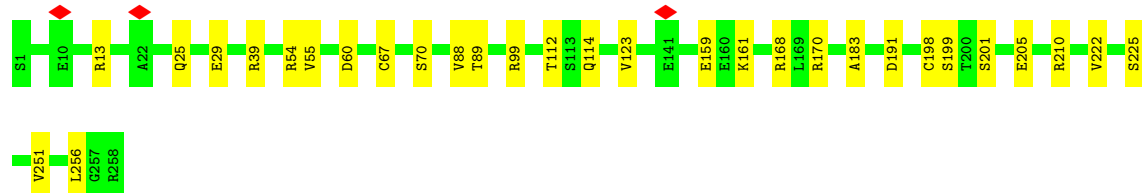


• Molecule 1: Coat protein

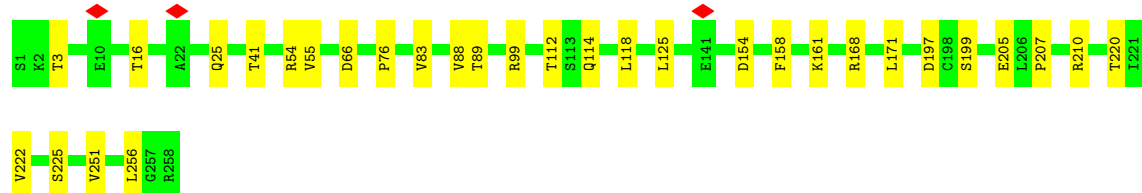
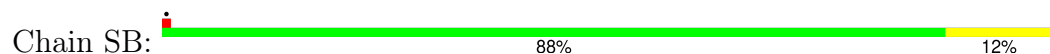
Chain QB:  89% 11%



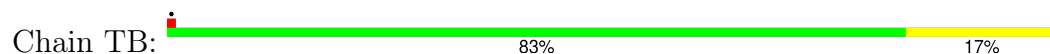
- Molecule 1: Coat protein



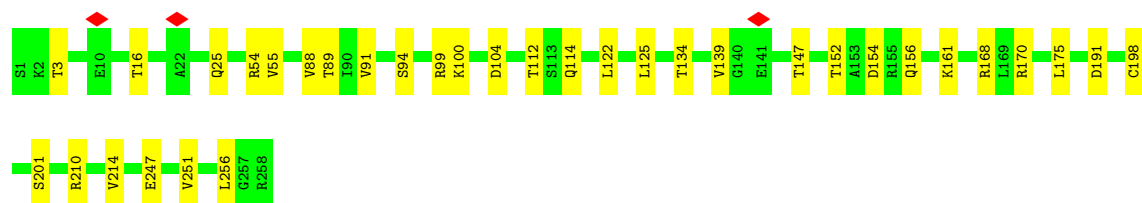
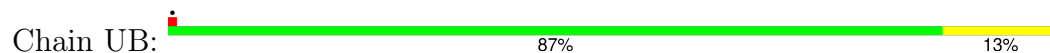
- Molecule 1: Coat protein



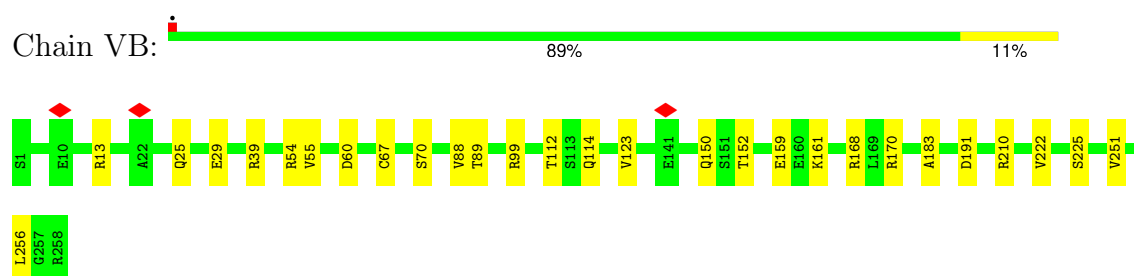
- Molecule 1: Coat protein



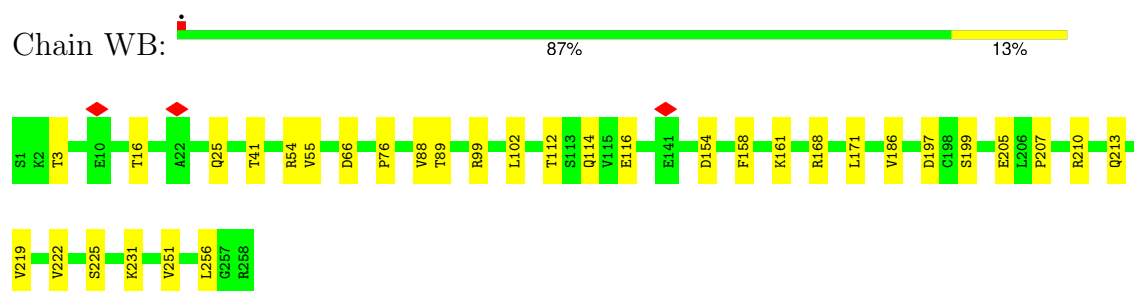
- Molecule 1: Coat protein



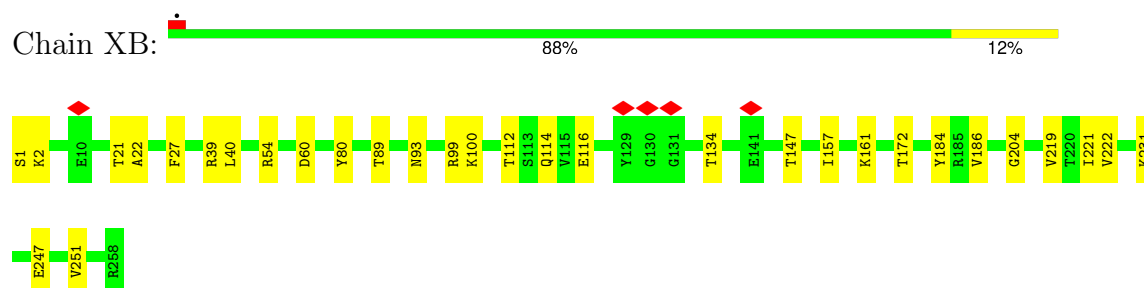
- Molecule 1: Coat protein



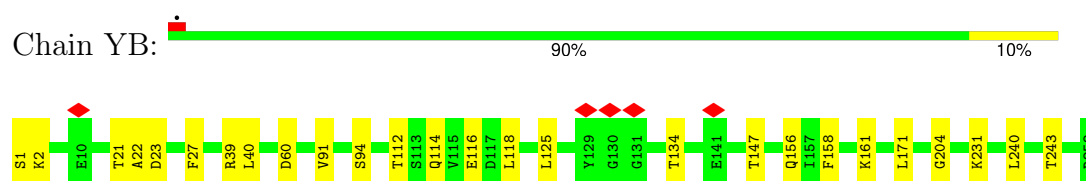
- Molecule 1: Coat protein



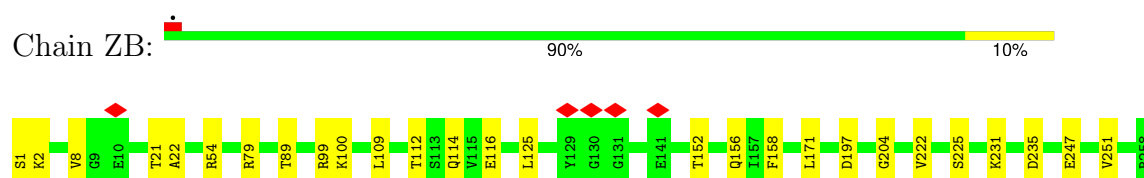
- Molecule 1: Coat protein



- Molecule 1: Coat protein

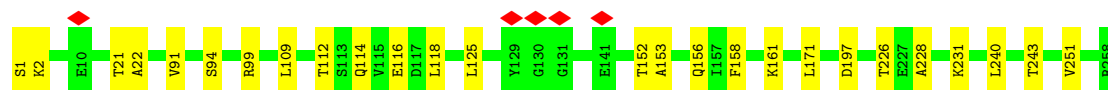


- Molecule 1: Coat protein

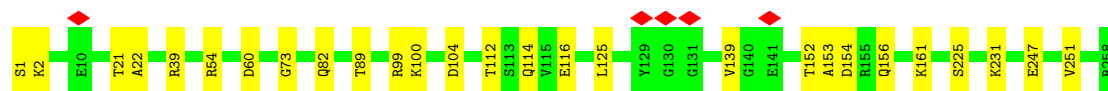


- Molecule 1: Coat protein

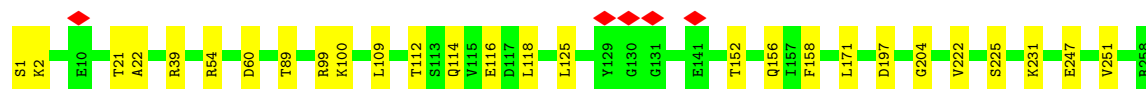




- Molecule 1: Coat protein



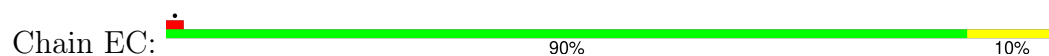
- Molecule 1: Coat protein



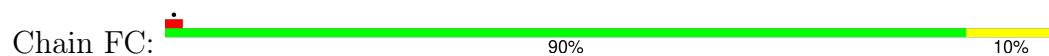
- Molecule 1: Coat protein



- Molecule 1: Coat protein

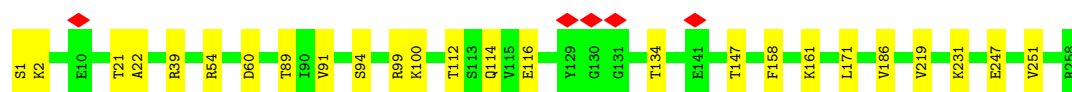


- Molecule 1: Coat protein

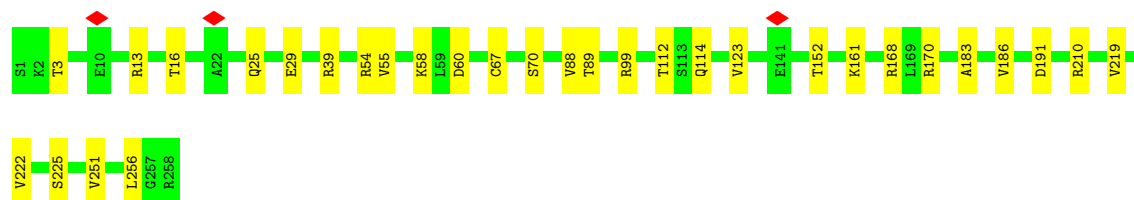


- Molecule 1: Coat protein

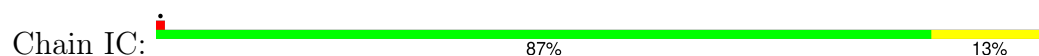




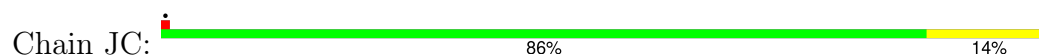
- Molecule 1: Coat protein



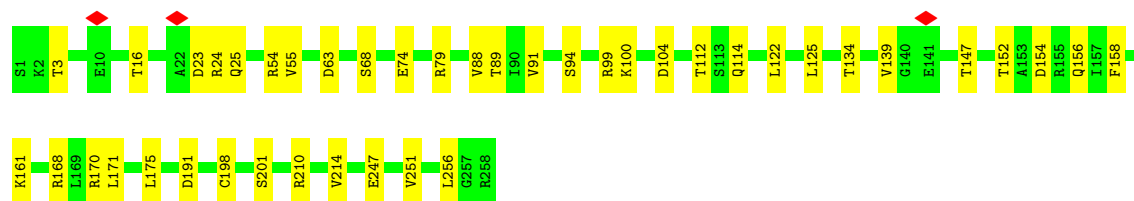
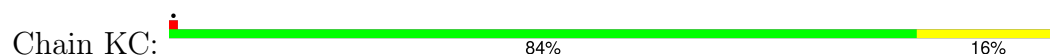
- Molecule 1: Coat protein



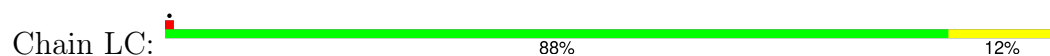
- Molecule 1: Coat protein

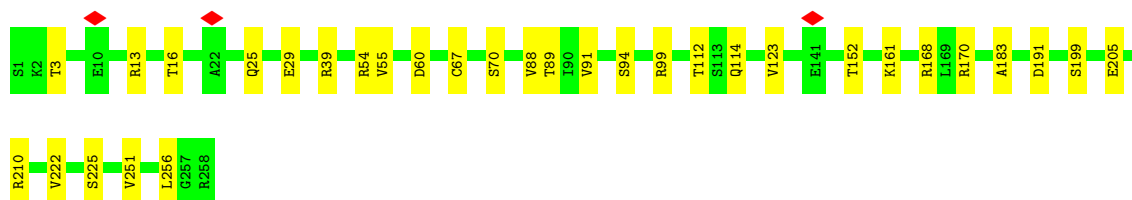


- Molecule 1: Coat protein

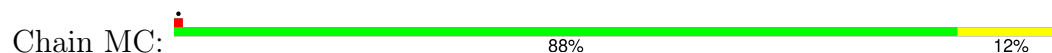


- Molecule 1: Coat protein





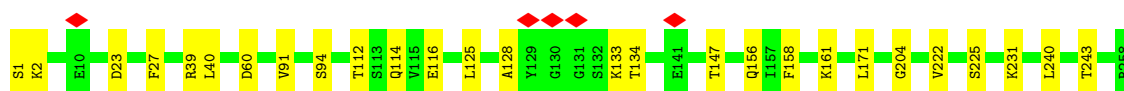
- Molecule 1: Coat protein



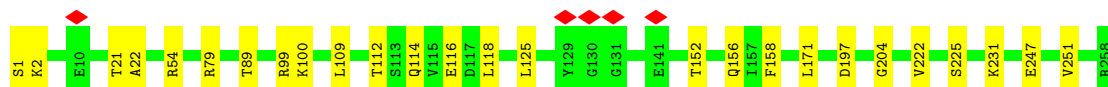
- Molecule 1: Coat protein



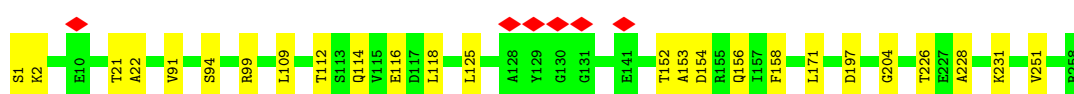
- Molecule 1: Coat protein



- Molecule 1: Coat protein

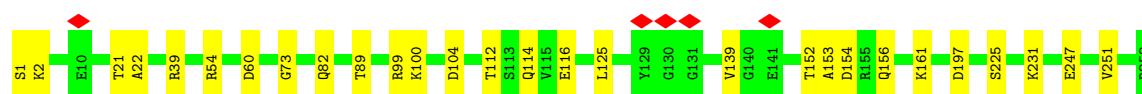


- Molecule 1: Coat protein




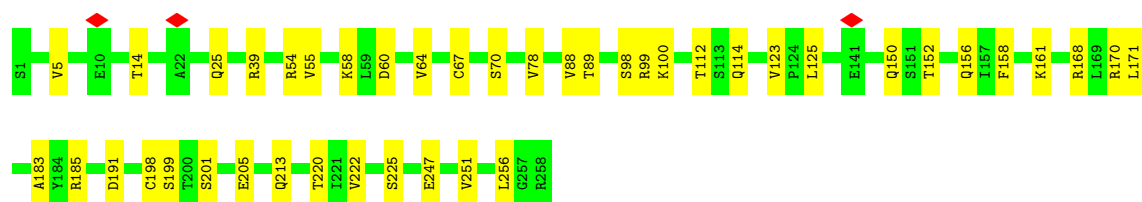
- Molecule 1: Coat protein

Chain RC:  89% 11%




- Molecule 1: Coat protein

Chain SC:  83% 17%




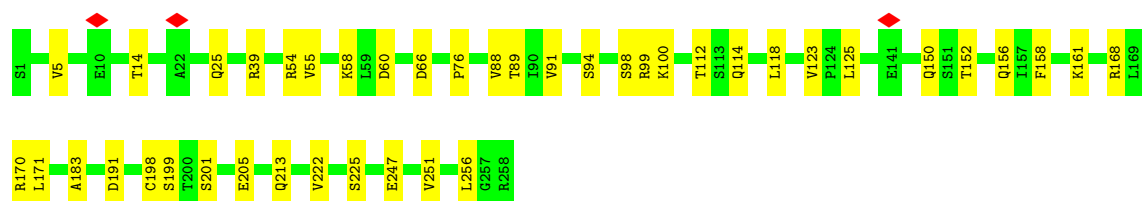
- Molecule 1: Coat protein

Chain TC:  86% 14%




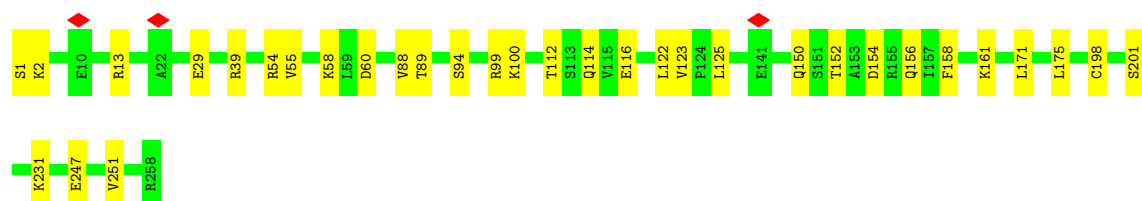
- Molecule 1: Coat protein

Chain UC:  84% 16%




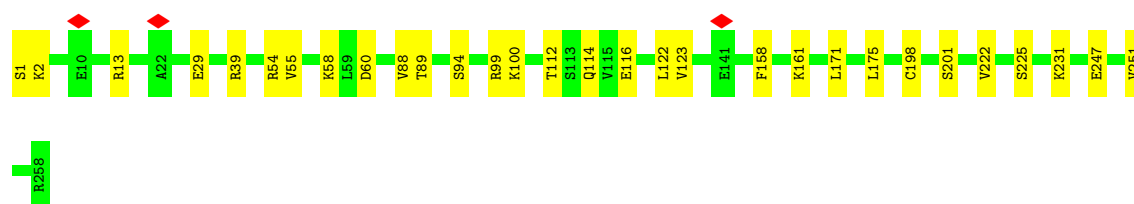
- Molecule 1: Coat protein

Chain VC:  87% 13%



- Molecule 1: Coat protein

Chain WC:  88% 12%




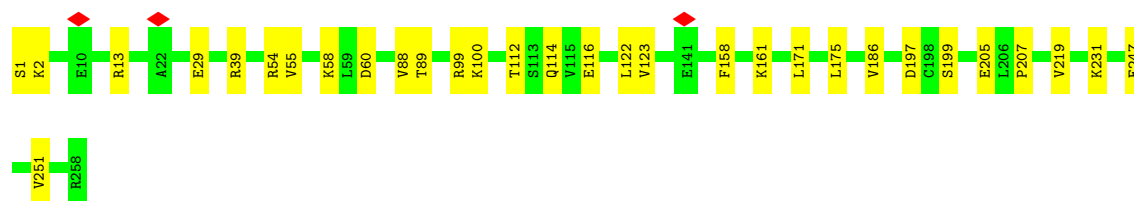
- Molecule 1: Coat protein

Chain XC:  89% 11%




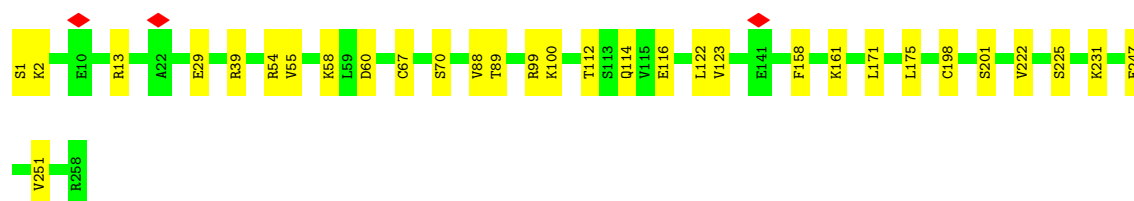
- Molecule 1: Coat protein

Chain YC:  88% 12%




- Molecule 1: Coat protein

Chain ZC:  88% 12%




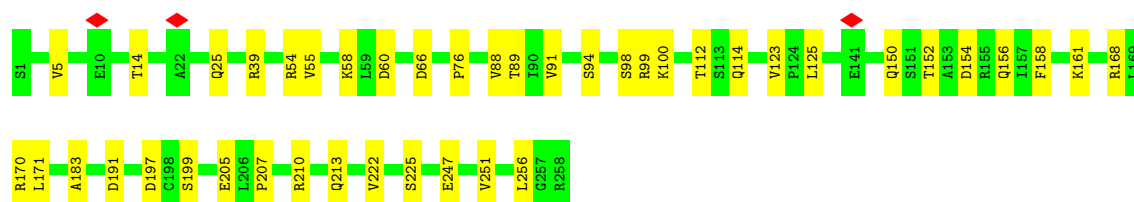
- Molecule 1: Coat protein

Chain AD:  89% 11%

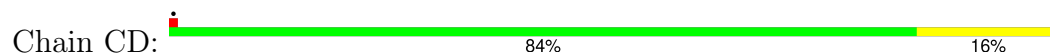


- Molecule 1: Coat protein

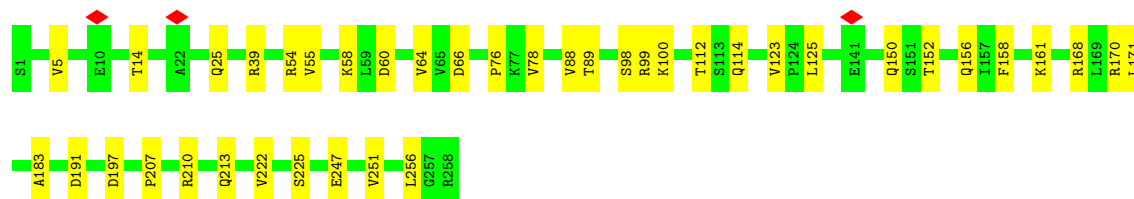
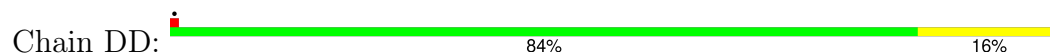
Chain BD:  83% 17%



- Molecule 1: Coat protein



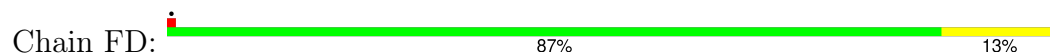
- Molecule 1: Coat protein



- Molecule 1: Coat protein

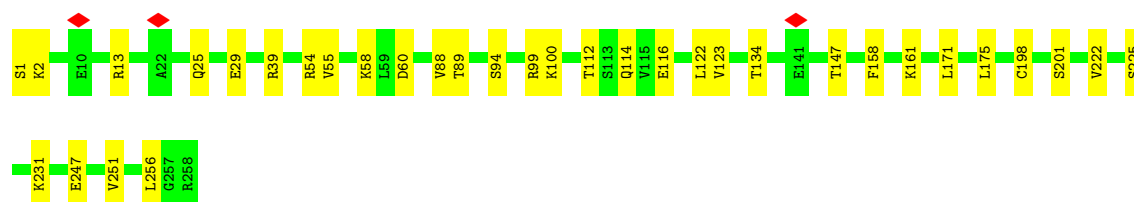


- Molecule 1: Coat protein

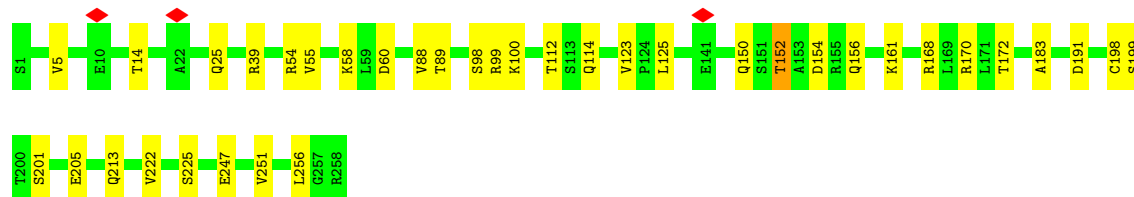


- Molecule 1: Coat protein

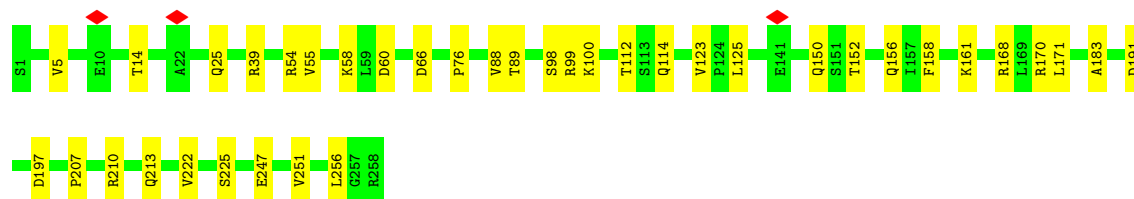
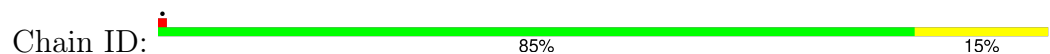




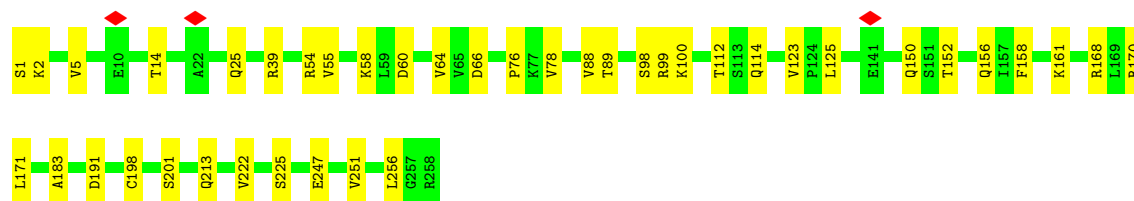
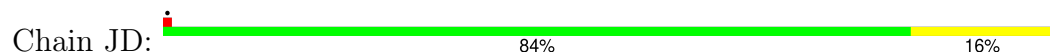
- Molecule 1: Coat protein



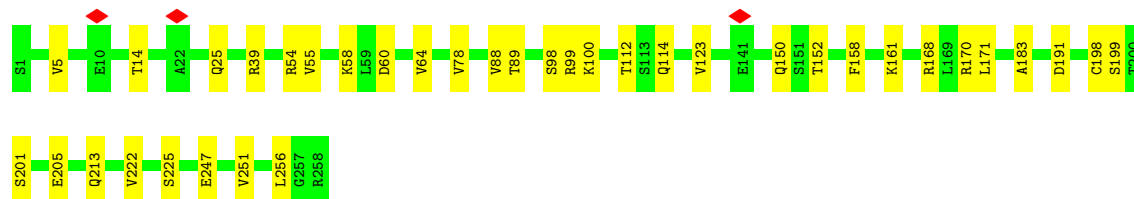
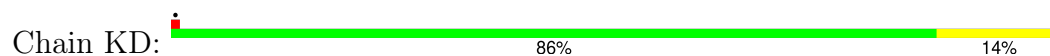
- Molecule 1: Coat protein




- Molecule 1: Coat protein

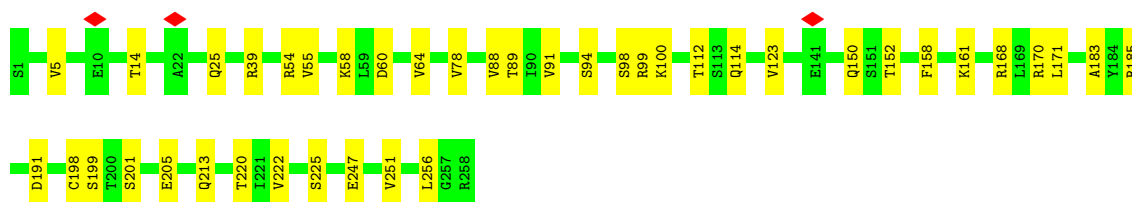


- Molecule 1: Coat protein




- Molecule 1: Coat protein

Chain LD:  84% 16%



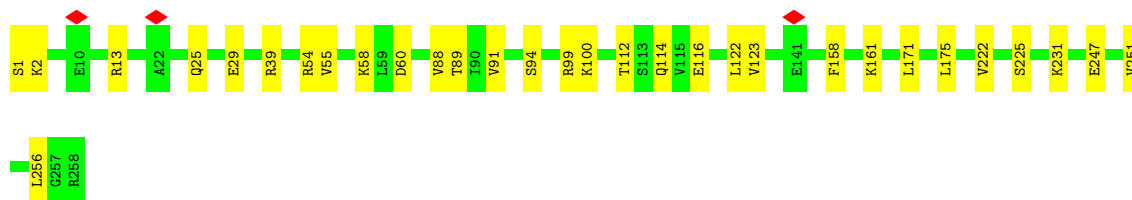
- Molecule 1: Coat protein

Chain MD:  84% 16%



- Molecule 1: Coat protein

Chain ND:  88% 12%



- Molecule 1: Coat protein

Chain OD:  88% 12%



- Molecule 1: Coat protein

Chain PD:  89% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	33224	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	2	Depositor
Maximum defocus (nm)	Not provided	
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.605	Depositor
Minimum map value	-1.490	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.149	Depositor
Recommended contour level	0.496	Depositor
Map size (Å)	549.5296, 549.5296, 549.5296	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0733, 1.0733, 1.0733	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.30	0/1993	0.53	0/2708
1	AA	0.28	0/1993	0.51	0/2708
1	AB	0.30	0/1993	0.53	0/2708
1	AC	0.29	0/1993	0.52	0/2708
1	AD	0.28	0/1993	0.52	0/2708
1	Af	0.30	0/1993	0.52	0/2708
1	B	0.29	0/1993	0.52	0/2708
1	BA	0.30	0/1993	0.52	0/2708
1	BB	0.28	0/1993	0.53	0/2708
1	BC	0.30	0/1993	0.53	0/2708
1	BD	0.28	0/1993	0.52	0/2708
1	C	0.30	0/1993	0.52	0/2708
1	CA	0.30	0/1993	0.52	0/2708
1	CB	0.28	0/1993	0.52	0/2708
1	CC	0.29	0/1993	0.52	0/2708
1	CD	0.28	0/1993	0.52	0/2708
1	D	0.30	0/1993	0.52	0/2708
1	DA	0.30	0/1993	0.52	0/2708
1	DB	0.28	0/1993	0.53	0/2708
1	DC	0.30	0/1993	0.53	0/2708
1	DD	0.28	0/1993	0.52	0/2708
1	E	0.28	0/1993	0.53	0/2708
1	EA	0.30	0/1993	0.52	0/2708
1	EB	0.29	0/1993	0.53	0/2708
1	EC	0.29	0/1993	0.51	0/2708
1	ED	0.28	0/1993	0.52	0/2708
1	F	0.28	0/1993	0.52	0/2708
1	FA	0.30	0/1993	0.53	0/2708
1	FB	0.28	0/1993	0.52	0/2708
1	FC	0.29	0/1993	0.52	0/2708
1	FD	0.28	0/1993	0.51	0/2708
1	G	0.28	0/1993	0.53	0/2708
1	GA	0.30	0/1993	0.52	0/2708
1	GB	0.28	0/1993	0.52	0/2708

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	GC	0.30	0/1993	0.52	0/2708
1	GD	0.28	0/1993	0.52	0/2708
1	H	0.29	0/1993	0.53	0/2708
1	HA	0.30	0/1993	0.53	0/2708
1	HB	0.30	0/1993	0.52	0/2708
1	HC	0.28	0/1993	0.54	0/2708
1	HD	0.28	0/1993	0.52	0/2708
1	I	0.28	0/1993	0.53	0/2708
1	IA	0.29	0/1993	0.51	0/2708
1	IB	0.29	0/1993	0.52	0/2708
1	IC	0.28	0/1993	0.52	0/2708
1	ID	0.28	0/1993	0.52	0/2708
1	J	0.28	0/1993	0.51	0/2708
1	JA	0.30	0/1993	0.53	0/2708
1	JB	0.30	0/1993	0.52	0/2708
1	JC	0.28	0/1993	0.53	0/2708
1	JD	0.28	0/1993	0.52	0/2708
1	K	0.29	0/1993	0.53	0/2708
1	KA	0.30	0/1993	0.52	0/2708
1	KB	0.29	0/1993	0.52	0/2708
1	KC	0.28	0/1993	0.53	0/2708
1	KD	0.28	0/1993	0.52	0/2708
1	L	0.29	0/1993	0.52	0/2708
1	LA	0.28	0/1993	0.53	0/2708
1	LB	0.30	0/1993	0.53	0/2708
1	LC	0.28	0/1993	0.52	0/2708
1	LD	0.28	0/1993	0.52	0/2708
1	M	0.30	0/1993	0.52	0/2708
1	MA	0.28	0/1993	0.52	0/2708
1	MB	0.29	0/1993	0.52	0/2708
1	MC	0.28	0/1993	0.52	0/2708
1	MD	0.28	0/1993	0.52	0/2708
1	N	0.30	0/1993	0.52	0/2708
1	NA	0.29	0/1993	0.53	0/2708
1	NB	0.30	0/1993	0.53	0/2708
1	NC	0.30	0/1993	0.52	0/2708
1	ND	0.28	0/1993	0.52	0/2708
1	O	0.30	0/1993	0.53	0/2708
1	OA	0.29	0/1993	0.53	0/2708
1	OB	0.29	0/1993	0.51	0/2708
1	OC	0.30	0/1993	0.52	0/2708
1	OD	0.28	0/1993	0.52	0/2708
1	P	0.30	0/1993	0.52	0/2708

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	PA	0.28	0/1993	0.53	0/2708
1	PB	0.30	0/1993	0.53	0/2708
1	PC	0.30	0/1993	0.52	0/2708
1	PD	0.28	0/1993	0.52	0/2708
1	Q	0.30	0/1993	0.53	0/2708
1	QA	0.28	0/1993	0.52	0/2708
1	QB	0.30	0/1993	0.52	0/2708
1	QC	0.29	0/1993	0.52	0/2708
1	R	0.30	0/1993	0.52	0/2708
1	RA	0.30	0/1993	0.52	0/2708
1	RB	0.28	0/1993	0.53	0/2708
1	RC	0.29	0/1993	0.53	0/2708
1	S	0.30	0/1993	0.52	0/2708
1	SA	0.30	0/1993	0.52	0/2708
1	SB	0.28	0/1993	0.51	0/2708
1	SC	0.28	0/1993	0.52	0/2708
1	T	0.30	0/1993	0.52	0/2708
1	TA	0.30	0/1993	0.52	0/2708
1	TB	0.28	0/1993	0.53	0/2708
1	TC	0.28	0/1993	0.52	0/2708
1	UA	0.30	0/1993	0.52	0/2708
1	UB	0.28	0/1993	0.53	0/2708
1	UC	0.28	0/1993	0.52	0/2708
1	V	0.28	0/1993	0.52	0/2708
1	VA	0.30	0/1993	0.53	0/2708
1	VB	0.28	0/1993	0.53	0/2708
1	VC	0.28	0/1993	0.51	0/2708
1	W	0.28	0/1993	0.51	0/2708
1	WA	0.30	0/1993	0.52	0/2708
1	WB	0.28	0/1993	0.52	0/2708
1	WC	0.28	0/1993	0.52	0/2708
1	X	0.29	0/1993	0.52	0/2708
1	XA	0.29	0/1993	0.53	0/2708
1	XB	0.30	0/1993	0.52	0/2708
1	XC	0.28	0/1993	0.52	0/2708
1	Y	0.28	0/1993	0.53	0/2708
1	YA	0.29	0/1993	0.51	0/2708
1	YB	0.29	0/1993	0.52	0/2708
1	YC	0.28	0/1993	0.51	0/2708
1	Z	0.28	0/1993	0.53	0/2708
1	ZA	0.30	0/1993	0.53	0/2708
1	ZB	0.30	0/1993	0.52	0/2708
1	ZC	0.28	0/1993	0.51	0/2708

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.29	0/239160	0.52	0/324960

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1973	0	2041	12	0
1	AA	1973	0	2039	16	0
1	AB	1973	0	2041	17	0
1	AC	1973	0	2041	15	0
1	AD	1973	0	2039	16	0
1	Af	1973	0	2041	0	0
1	B	1973	0	2041	16	0
1	BA	1973	0	2041	16	0
1	BB	1973	0	2039	18	0
1	BC	1973	0	2041	15	0
1	BD	1973	0	2039	25	0
1	C	1973	0	2041	17	0
1	CA	1973	0	2041	16	0
1	CB	1973	0	2039	18	0
1	CC	1973	0	2041	15	0
1	CD	1973	0	2039	24	0
1	D	1973	0	2041	14	0
1	DA	1973	0	2041	15	0
1	DB	1973	0	2039	17	0
1	DC	1973	0	2041	16	0
1	DD	1973	0	2039	23	0
1	E	1973	0	2039	16	0
1	EA	1973	0	2041	16	0
1	EB	1973	0	2039	17	0
1	EC	1973	0	2041	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	ED	1973	0	2039	16	0
1	F	1973	0	2039	18	0
1	FA	1973	0	2041	15	0
1	FB	1973	0	2039	18	0
1	FC	1973	0	2041	16	0
1	FD	1973	0	2039	18	0
1	G	1973	0	2039	19	0
1	GA	1973	0	2041	14	0
1	GB	1973	0	2039	17	0
1	GC	1973	0	2041	13	0
1	GD	1973	0	2039	19	0
1	H	1973	0	2039	21	0
1	HA	1973	0	2041	13	0
1	HB	1973	0	2041	15	0
1	HC	1973	0	2039	17	0
1	HD	1973	0	2039	23	0
1	I	1973	0	2039	15	0
1	IA	1973	0	2041	12	0
1	IB	1973	0	2041	16	0
1	IC	1973	0	2039	19	0
1	ID	1973	0	2039	22	0
1	J	1973	0	2039	15	0
1	JA	1973	0	2041	17	0
1	JB	1973	0	2041	12	0
1	JC	1973	0	2039	18	0
1	JD	1973	0	2039	23	0
1	K	1973	0	2041	16	0
1	KA	1973	0	2041	15	0
1	KB	1973	0	2041	12	0
1	KC	1973	0	2039	22	0
1	KD	1973	0	2039	21	0
1	L	1973	0	2041	18	0
1	LA	1973	0	2039	16	0
1	LB	1973	0	2041	13	0
1	LC	1973	0	2039	18	0
1	LD	1973	0	2039	23	0
1	M	1973	0	2041	16	0
1	MA	1973	0	2039	19	0
1	MB	1973	0	2041	13	0
1	MC	1973	0	2039	18	0
1	MD	1973	0	2039	23	0
1	N	1973	0	2041	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	NA	1973	0	2039	18	0
1	NB	1973	0	2041	13	0
1	NC	1973	0	2041	13	0
1	ND	1973	0	2039	17	0
1	O	1973	0	2041	12	0
1	OA	1973	0	2039	17	0
1	OB	1973	0	2041	16	0
1	OC	1973	0	2041	15	0
1	OD	1973	0	2039	18	0
1	P	1973	0	2041	18	0
1	PA	1973	0	2039	20	0
1	PB	1973	0	2041	17	0
1	PC	1973	0	2041	15	0
1	PD	1973	0	2039	16	0
1	Q	1973	0	2041	11	0
1	QA	1973	0	2039	18	0
1	QB	1973	0	2041	15	0
1	QC	1973	0	2041	15	0
1	R	1973	0	2041	15	0
1	RA	1973	0	2041	16	0
1	RB	1973	0	2039	17	0
1	RC	1973	0	2041	16	0
1	S	1973	0	2041	16	0
1	SA	1973	0	2041	16	0
1	SB	1973	0	2039	18	0
1	SC	1973	0	2039	24	0
1	T	1973	0	2041	14	0
1	TA	1973	0	2041	14	0
1	TB	1973	0	2039	22	0
1	TC	1973	0	2039	21	0
1	UA	1973	0	2041	15	0
1	UB	1973	0	2039	18	0
1	UC	1973	0	2039	24	0
1	V	1973	0	2039	19	0
1	VA	1973	0	2041	12	0
1	VB	1973	0	2039	16	0
1	VC	1973	0	2039	19	0
1	W	1973	0	2039	17	0
1	WA	1973	0	2041	15	0
1	WB	1973	0	2039	19	0
1	WC	1973	0	2039	17	0
1	X	1973	0	2039	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	XA	1973	0	2041	11	0
1	XB	1973	0	2041	17	0
1	XC	1973	0	2039	16	0
1	Y	1973	0	2039	17	0
1	YA	1973	0	2041	14	0
1	YB	1973	0	2041	15	0
1	YC	1973	0	2039	17	0
1	Z	1973	0	2039	19	0
1	ZA	1973	0	2041	16	0
1	ZB	1973	0	2041	15	0
1	ZC	1973	0	2039	17	0
All	All	236760	0	244800	1929	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1929) 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:MB:204:GLY:HA2	1:WB:210:ARG:HH21	1.60	0.67
1:SB:210:ARG:HH21	1:ZB:204:GLY:HA2	1.60	0.67
1:W:210:ARG:HH21	1:DA:204:GLY:HA2	1.61	0.66
1:MA:210:ARG:HH21	1:TA:204:GLY:HA2	1.60	0.66
1:CB:210:ARG:HH21	1:JB:204:GLY:HA2	1.60	0.66
1:CC:204:GLY:HA2	1:MC:210:ARG:HH21	1.60	0.66
1:VC:150:GLN:HE21	1:VC:152:THR:HG1	1.44	0.64
1:C:204:GLY:HA2	1:E:210:ARG:HH21	1.62	0.64
1:F:210:ARG:HH21	1:M:204:GLY:HA2	1.60	0.64
1:FB:210:ARG:HH21	1:IB:204:GLY:HA2	1.63	0.64
1:IC:210:ARG:HH21	1:PC:204:GLY:HA2	1.61	0.64
1:OD:150:GLN:HE21	1:OD:152:THR:HG1	1.45	0.64
1:X:210:ARG:HH21	1:OB:204:GLY:HA2	1.63	0.63
1:FC:204:GLY:HA2	1:HC:210:ARG:HH21	1.63	0.63
1:TC:198:CYS:HB3	1:TC:201:SER:HB3	1.81	0.63
1:PA:210:ARG:HH21	1:SA:204:GLY:HA2	1.63	0.63
1:I:210:ARG:HH21	1:L:204:GLY:HA2	1.62	0.63
1:CD:170:ARG:HB2	1:CD:191:ASP:HB2	1.81	0.62
1:CD:198:CYS:HB3	1:CD:201:SER:HB3	1.81	0.62
1:HD:198:CYS:HB3	1:HD:201:SER:HB3	1.81	0.62
1:JD:198:CYS:HB3	1:JD:201:SER:HB3	1.81	0.62
1:SC:198:CYS:HB3	1:SC:201:SER:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LD:198:CYS:HB3	1:LD:201:SER:HB3	1.81	0.62
1:LC:210:ARG:HH21	1:OC:204:GLY:HA2	1.63	0.62
1:Z:210:ARG:HH21	1:CA:204:GLY:HA2	1.64	0.62
1:TC:170:ARG:HB2	1:TC:191:ASP:HB2	1.82	0.62
1:DD:170:ARG:HB2	1:DD:191:ASP:HB2	1.82	0.62
1:HD:170:ARG:HB2	1:HD:191:ASP:HB2	1.82	0.62
1:SC:170:ARG:HB2	1:SC:191:ASP:HB2	1.81	0.62
1:BD:170:ARG:HB2	1:BD:191:ASP:HB2	1.82	0.62
1:LD:170:ARG:HB2	1:LD:191:ASP:HB2	1.81	0.62
1:MD:170:ARG:HB2	1:MD:191:ASP:HB2	1.82	0.62
1:G:210:ARG:HH21	1:QC:204:GLY:HA2	1.65	0.61
1:VB:210:ARG:HH21	1:YB:204:GLY:HA2	1.65	0.61
1:ID:170:ARG:HB2	1:ID:191:ASP:HB2	1.82	0.61
1:UC:170:ARG:HB2	1:UC:191:ASP:HB2	1.82	0.61
1:KD:170:ARG:HB2	1:KD:191:ASP:HB2	1.82	0.61
1:JD:170:ARG:HB2	1:JD:191:ASP:HB2	1.82	0.61
1:E:39:ARG:HB3	1:E:60:ASP:HB2	1.83	0.61
1:LA:39:ARG:HB3	1:LA:60:ASP:HB2	1.83	0.61
1:BB:39:ARG:HB3	1:BB:60:ASP:HB2	1.83	0.61
1:GB:198:CYS:HB3	1:GB:201:SER:HB3	1.83	0.61
1:RB:39:ARG:HB3	1:RB:60:ASP:HB2	1.83	0.60
1:PA:39:ARG:HB3	1:PA:60:ASP:HB2	1.83	0.60
1:KD:198:CYS:HB3	1:KD:201:SER:HB3	1.81	0.60
1:Z:39:ARG:HB3	1:Z:60:ASP:HB2	1.84	0.60
1:UC:198:CYS:HB3	1:UC:201:SER:HB3	1.81	0.60
1:QA:198:CYS:HB3	1:QA:201:SER:HB3	1.84	0.60
1:FB:39:ARG:HB3	1:FB:60:ASP:HB2	1.83	0.60
1:J:198:CYS:HB3	1:J:201:SER:HB3	1.83	0.60
1:HC:39:ARG:HB3	1:HC:60:ASP:HB2	1.83	0.59
1:LC:39:ARG:HB3	1:LC:60:ASP:HB2	1.83	0.59
1:B:204:GLY:HA2	1:OA:210:ARG:HH21	1.65	0.59
1:AA:198:CYS:HB3	1:AA:201:SER:HB3	1.83	0.59
1:V:39:ARG:HB3	1:V:60:ASP:HB2	1.83	0.59
1:PA:150:GLN:HE21	1:PA:152:THR:HG1	1.48	0.59
1:VB:39:ARG:HB3	1:VB:60:ASP:HB2	1.84	0.59
1:HD:150:GLN:HE21	1:HD:152:THR:HG1	1.50	0.59
1:I:39:ARG:HB3	1:I:60:ASP:HB2	1.83	0.59
1:H:197:ASP:HB3	1:H:207:PRO:HG3	1.86	0.58
1:Q:112:THR:HG23	1:Q:114:GLN:H	1.70	0.57
1:XB:204:GLY:HA2	1:BD:210:ARG:HH21	1.69	0.57
1:BA:204:GLY:HA2	1:MD:210:ARG:HH21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NB:112:THR:HG23	1:NB:114:GLN:H	1.69	0.57
1:K:204:GLY:HA2	1:DD:210:ARG:HH21	1.69	0.57
1:H:170:ARG:HB2	1:H:191:ASP:HB2	1.85	0.57
1:SA:1:SER:OG	1:SA:2:LYS:N	2.37	0.57
1:YB:1:SER:OG	1:YB:2:LYS:N	2.37	0.57
1:RB:198:CYS:HB3	1:RB:201:SER:HB3	1.86	0.56
1:O:112:THR:HG23	1:O:114:GLN:H	1.71	0.56
1:S:204:GLY:HA2	1:V:210:ARG:HH21	1.70	0.56
1:T:204:GLY:HA2	1:ID:210:ARG:HH21	1.69	0.56
1:YB:39:ARG:HB3	1:YB:60:ASP:HB2	1.88	0.56
1:XA:112:THR:HG23	1:XA:114:GLN:H	1.70	0.56
1:JC:197:ASP:HB3	1:JC:207:PRO:HG3	1.86	0.56
1:BC:112:THR:HG23	1:BC:114:GLN:H	1.71	0.56
1:GA:112:THR:HG23	1:GA:114:GLN:H	1.72	0.55
1:HA:112:THR:HG23	1:HA:114:GLN:H	1.71	0.55
1:RC:112:THR:HG23	1:RC:114:GLN:H	1.70	0.55
1:WA:112:THR:HG23	1:WA:114:GLN:H	1.72	0.55
1:ID:197:ASP:HB3	1:ID:207:PRO:HG3	1.89	0.55
1:EA:1:SER:OG	1:EA:2:LYS:N	2.39	0.55
1:DC:112:THR:HG23	1:DC:114:GLN:H	1.71	0.55
1:BB:150:GLN:HE21	1:BB:152:THR:HG1	1.53	0.55
1:KB:1:SER:OG	1:KB:2:LYS:N	2.39	0.55
1:O:1:SER:OG	1:O:2:LYS:N	2.40	0.54
1:DA:112:THR:HG23	1:DA:114:GLN:H	1.72	0.54
1:FA:112:THR:HG23	1:FA:114:GLN:H	1.71	0.54
1:QA:112:THR:HG23	1:QA:114:GLN:H	1.73	0.54
1:PD:39:ARG:HB3	1:PD:60:ASP:HB2	1.90	0.54
1:N:1:SER:OG	1:N:2:LYS:N	2.39	0.54
1:LB:112:THR:HG23	1:LB:114:GLN:H	1.71	0.54
1:PC:112:THR:HG23	1:PC:114:GLN:H	1.72	0.54
1:F:112:THR:HG23	1:F:114:GLN:H	1.72	0.54
1:GB:112:THR:HG23	1:GB:114:GLN:H	1.73	0.54
1:ZB:112:THR:HG23	1:ZB:114:GLN:H	1.72	0.54
1:PA:197:ASP:HB3	1:PA:207:PRO:HG3	1.89	0.54
1:VA:112:THR:HG23	1:VA:114:GLN:H	1.71	0.54
1:NB:1:SER:OG	1:NB:2:LYS:N	2.40	0.54
1:CC:112:THR:HG23	1:CC:114:GLN:H	1.72	0.54
1:A:112:THR:HG23	1:A:114:GLN:H	1.71	0.54
1:FA:1:SER:OG	1:FA:2:LYS:N	2.40	0.54
1:MB:112:THR:HG23	1:MB:114:GLN:H	1.72	0.54
1:OB:1:SER:OG	1:OB:2:LYS:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ED:39:ARG:HB3	1:ED:60:ASP:HB2	1.90	0.54
1:VA:1:SER:OG	1:VA:2:LYS:N	2.41	0.54
1:ZC:39:ARG:HB3	1:ZC:60:ASP:HB2	1.90	0.54
1:LA:25:GLN:NE2	1:LA:256:LEU:O	2.40	0.54
1:JB:112:THR:HG23	1:JB:114:GLN:H	1.73	0.54
1:LB:1:SER:OG	1:LB:2:LYS:N	2.41	0.54
1:AA:112:THR:HG23	1:AA:114:GLN:H	1.73	0.54
1:TA:112:THR:HG23	1:TA:114:GLN:H	1.73	0.54
1:BB:25:GLN:NE2	1:BB:256:LEU:O	2.40	0.54
1:KB:99:ARG:NH1	1:KB:251:VAL:O	2.41	0.54
1:BD:99:ARG:NH1	1:BD:251:VAL:O	2.41	0.54
1:GD:39:ARG:HB3	1:GD:60:ASP:HB2	1.90	0.54
1:HD:99:ARG:NH1	1:HD:251:VAL:O	2.41	0.54
1:MD:197:ASP:HB3	1:MD:207:PRO:HG3	1.90	0.54
1:Q:1:SER:OG	1:Q:2:LYS:N	2.41	0.54
1:MA:112:THR:HG23	1:MA:114:GLN:H	1.72	0.54
1:WB:112:THR:HG23	1:WB:114:GLN:H	1.73	0.54
1:NC:112:THR:HG23	1:NC:114:GLN:H	1.73	0.54
1:XC:39:ARG:HB3	1:XC:60:ASP:HB2	1.90	0.54
1:B:1:SER:OG	1:B:2:LYS:N	2.40	0.53
1:K:112:THR:HG23	1:K:114:GLN:H	1.73	0.53
1:N:204:GLY:HA2	1:DB:210:ARG:HH21	1.73	0.53
1:SB:112:THR:HG23	1:SB:114:GLN:H	1.73	0.53
1:VC:116:GLU:OE2	1:VC:231:LYS:NZ	2.41	0.53
1:WC:39:ARG:HB3	1:WC:60:ASP:HB2	1.90	0.53
1:YC:39:ARG:HB3	1:YC:60:ASP:HB2	1.90	0.53
1:R:204:GLY:HA2	1:NA:210:ARG:HH21	1.73	0.53
1:Z:99:ARG:NH1	1:Z:251:VAL:O	2.42	0.53
1:QB:112:THR:HG23	1:QB:114:GLN:H	1.73	0.53
1:UC:99:ARG:NH1	1:UC:251:VAL:O	2.42	0.53
1:KD:99:ARG:NH1	1:KD:251:VAL:O	2.42	0.53
1:E:99:ARG:NH1	1:E:251:VAL:O	2.42	0.53
1:R:1:SER:OG	1:R:2:LYS:N	2.40	0.53
1:CB:112:THR:HG23	1:CB:114:GLN:H	1.73	0.53
1:AC:1:SER:OG	1:AC:2:LYS:N	2.40	0.53
1:LC:99:ARG:NH1	1:LC:251:VAL:O	2.42	0.53
1:BD:197:ASP:HB3	1:BD:207:PRO:HG3	1.91	0.53
1:CD:99:ARG:NH1	1:CD:251:VAL:O	2.42	0.53
1:ID:99:ARG:NH1	1:ID:251:VAL:O	2.42	0.53
1:JD:99:ARG:NH1	1:JD:251:VAL:O	2.42	0.53
1:BC:1:SER:OG	1:BC:2:LYS:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HC:25:GLN:NE2	1:HC:256:LEU:O	2.40	0.53
1:HC:99:ARG:NH1	1:HC:251:VAL:O	2.42	0.53
1:DD:99:ARG:NH1	1:DD:251:VAL:O	2.42	0.53
1:V:91:VAL:HG23	1:V:94:SER:HB3	1.90	0.53
1:PA:99:ARG:NH1	1:PA:251:VAL:O	2.41	0.53
1:GC:112:THR:HG23	1:GC:114:GLN:H	1.74	0.53
1:AD:39:ARG:HB3	1:AD:60:ASP:HB2	1.91	0.53
1:ND:39:ARG:HB3	1:ND:60:ASP:HB2	1.90	0.53
1:OD:39:ARG:HB3	1:OD:60:ASP:HB2	1.90	0.53
1:D:112:THR:HG23	1:D:114:GLN:H	1.73	0.53
1:FB:25:GLN:NE2	1:FB:256:LEU:O	2.40	0.53
1:LC:25:GLN:NE2	1:LC:256:LEU:O	2.40	0.53
1:VC:39:ARG:HB3	1:VC:60:ASP:HB2	1.90	0.53
1:A:1:SER:OG	1:A:2:LYS:N	2.41	0.53
1:I:99:ARG:NH1	1:I:251:VAL:O	2.41	0.53
1:V:25:GLN:NE2	1:V:256:LEU:O	2.40	0.53
1:KA:112:THR:HG23	1:KA:114:GLN:H	1.74	0.53
1:H:63:ASP:OD2	1:H:79:ARG:NH1	2.42	0.53
1:T:112:THR:HG23	1:T:114:GLN:H	1.74	0.53
1:BA:112:THR:HG23	1:BA:114:GLN:H	1.73	0.53
1:XB:112:THR:HG23	1:XB:114:GLN:H	1.74	0.53
1:I:25:GLN:NE2	1:I:256:LEU:O	2.40	0.53
1:P:112:THR:HG23	1:P:114:GLN:H	1.72	0.53
1:EA:204:GLY:HA2	1:EB:210:ARG:HH21	1.74	0.53
1:YA:204:GLY:HA2	1:UB:210:ARG:HH21	1.74	0.53
1:KC:63:ASP:OD2	1:KC:79:ARG:NH1	2.42	0.53
1:RA:112:THR:HG23	1:RA:114:GLN:H	1.73	0.53
1:BB:99:ARG:NH1	1:BB:251:VAL:O	2.42	0.53
1:HB:112:THR:HG23	1:HB:114:GLN:H	1.73	0.53
1:BB:13:ARG:NH2	1:BB:29:GLU:OE1	2.42	0.52
1:LC:161:LYS:O	1:LC:168:ARG:NH2	2.42	0.52
1:MC:99:ARG:NH1	1:MC:251:VAL:O	2.42	0.52
1:SC:99:ARG:NH1	1:SC:251:VAL:O	2.42	0.52
1:M:112:THR:HG23	1:M:114:GLN:H	1.73	0.52
1:V:13:ARG:NH2	1:V:29:GLU:OE1	2.42	0.52
1:Y:170:ARG:HB2	1:Y:191:ASP:HB2	1.92	0.52
1:LA:99:ARG:NH1	1:LA:251:VAL:O	2.42	0.52
1:EB:63:ASP:OD2	1:EB:79:ARG:NH1	2.42	0.52
1:FB:99:ARG:NH1	1:FB:251:VAL:O	2.42	0.52
1:WC:116:GLU:OE2	1:WC:231:LYS:NZ	2.42	0.52
1:DB:63:ASP:OD2	1:DB:79:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ND:116:GLU:OE2	1:ND:231:LYS:NZ	2.42	0.52
1:Y:63:ASP:OD2	1:Y:79:ARG:NH1	2.42	0.52
1:AB:112:THR:HG23	1:AB:114:GLN:H	1.75	0.52
1:HC:161:LYS:O	1:HC:168:ARG:NH2	2.43	0.52
1:IC:112:THR:HG23	1:IC:114:GLN:H	1.73	0.52
1:I:161:LYS:O	1:I:168:ARG:NH2	2.42	0.52
1:W:112:THR:HG23	1:W:114:GLN:H	1.73	0.52
1:PA:25:GLN:NE2	1:PA:256:LEU:O	2.40	0.52
1:UA:204:GLY:HA2	1:KC:210:ARG:HH21	1.74	0.52
1:RB:161:LYS:O	1:RB:168:ARG:NH2	2.43	0.52
1:VB:161:LYS:O	1:VB:168:ARG:NH2	2.43	0.52
1:F:99:ARG:NH1	1:F:251:VAL:O	2.43	0.52
1:J:112:THR:HG23	1:J:114:GLN:H	1.73	0.52
1:X:197:ASP:HB3	1:X:207:PRO:HG3	1.92	0.52
1:Y:99:ARG:NH1	1:Y:251:VAL:O	2.43	0.52
1:PA:161:LYS:O	1:PA:168:ARG:NH2	2.43	0.52
1:FB:161:LYS:O	1:FB:168:ARG:NH2	2.43	0.52
1:HB:99:ARG:NH1	1:HB:251:VAL:O	2.41	0.52
1:MC:112:THR:HG23	1:MC:114:GLN:H	1.73	0.52
1:LD:99:ARG:NH1	1:LD:251:VAL:O	2.42	0.52
1:G:170:ARG:HB2	1:G:191:ASP:HB2	1.92	0.52
1:Y:25:GLN:NE2	1:Y:256:LEU:O	2.43	0.52
1:AA:99:ARG:NH1	1:AA:251:VAL:O	2.42	0.52
1:LA:13:ARG:NH2	1:LA:29:GLU:OE1	2.42	0.52
1:RA:99:ARG:NH1	1:RA:251:VAL:O	2.41	0.52
1:BB:161:LYS:O	1:BB:168:ARG:NH2	2.42	0.52
1:RB:25:GLN:NE2	1:RB:256:LEU:O	2.40	0.52
1:VB:25:GLN:NE2	1:VB:256:LEU:O	2.40	0.52
1:WB:99:ARG:NH1	1:WB:251:VAL:O	2.42	0.52
1:AD:198:CYS:HB2	1:AD:201:SER:HB3	1.92	0.52
1:LA:161:LYS:O	1:LA:168:ARG:NH2	2.43	0.52
1:J:25:GLN:NE2	1:J:256:LEU:O	2.42	0.52
1:V:161:LYS:O	1:V:168:ARG:NH2	2.43	0.52
1:W:25:GLN:NE2	1:W:256:LEU:O	2.42	0.52
1:X:170:ARG:HB2	1:X:191:ASP:HB2	1.92	0.52
1:Z:161:LYS:O	1:Z:168:ARG:NH2	2.43	0.52
1:EC:1:SER:OG	1:EC:2:LYS:N	2.40	0.52
1:E:161:LYS:O	1:E:168:ARG:NH2	2.43	0.52
1:G:25:GLN:NE2	1:G:256:LEU:O	2.43	0.52
1:NA:91:VAL:O	1:NA:94:SER:OG	2.27	0.52
1:CB:99:ARG:NH1	1:CB:251:VAL:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:91:VAL:O	1:DB:94:SER:OG	2.27	0.52
1:FB:91:VAL:HG23	1:FB:94:SER:HB3	1.92	0.52
1:SB:99:ARG:NH1	1:SB:251:VAL:O	2.43	0.52
1:QC:1:SER:OG	1:QC:2:LYS:N	2.40	0.52
1:TC:99:ARG:NH1	1:TC:251:VAL:O	2.42	0.52
1:ED:116:GLU:OE2	1:ED:231:LYS:NZ	2.42	0.52
1:MD:99:ARG:NH1	1:MD:251:VAL:O	2.42	0.52
1:C:1:SER:OG	1:C:2:LYS:N	2.42	0.51
1:CA:1:SER:OG	1:CA:2:LYS:N	2.42	0.51
1:XA:1:SER:OG	1:XA:2:LYS:N	2.41	0.51
1:IB:1:SER:OG	1:IB:2:LYS:N	2.42	0.51
1:AD:1:SER:OG	1:AD:2:LYS:N	2.43	0.51
1:ED:1:SER:OG	1:ED:2:LYS:N	2.43	0.51
1:E:25:GLN:NE2	1:E:256:LEU:O	2.40	0.51
1:SA:116:GLU:OE2	1:SA:231:LYS:NZ	2.43	0.51
1:GB:99:ARG:NH1	1:GB:251:VAL:O	2.42	0.51
1:KC:99:ARG:NH1	1:KC:251:VAL:O	2.43	0.51
1:VC:198:CYS:HB2	1:VC:201:SER:HB3	1.92	0.51
1:KA:99:ARG:NH1	1:KA:251:VAL:O	2.41	0.51
1:MA:99:ARG:NH1	1:MA:251:VAL:O	2.43	0.51
1:IB:116:GLU:OE2	1:IB:231:LYS:NZ	2.43	0.51
1:PB:1:SER:OG	1:PB:2:LYS:N	2.42	0.51
1:RB:123:VAL:HG22	1:SB:161:LYS:HG3	1.93	0.51
1:IC:25:GLN:NE2	1:IC:256:LEU:O	2.42	0.51
1:MC:25:GLN:NE2	1:MC:256:LEU:O	2.42	0.51
1:XC:99:ARG:NH1	1:XC:251:VAL:O	2.44	0.51
1:DD:197:ASP:HB3	1:DD:207:PRO:HG3	1.92	0.51
1:FD:39:ARG:HB3	1:FD:60:ASP:HB2	1.91	0.51
1:GD:198:CYS:HB2	1:GD:201:SER:HB3	1.91	0.51
1:ND:99:ARG:NH1	1:ND:251:VAL:O	2.44	0.51
1:F:25:GLN:NE2	1:F:256:LEU:O	2.42	0.51
1:L:1:SER:OG	1:L:2:LYS:N	2.42	0.51
1:S:1:SER:OG	1:S:2:LYS:N	2.42	0.51
1:GA:1:SER:OG	1:GA:2:LYS:N	2.42	0.51
1:QA:99:ARG:NH1	1:QA:251:VAL:O	2.43	0.51
1:ZA:116:GLU:OE2	1:ZA:231:LYS:NZ	2.43	0.51
1:XC:58:LYS:NZ	1:XC:60:ASP:OD1	2.43	0.51
1:AD:116:GLU:OE2	1:AD:231:LYS:NZ	2.42	0.51
1:AA:25:GLN:NE2	1:AA:256:LEU:O	2.42	0.51
1:HA:1:SER:OG	1:HA:2:LYS:N	2.41	0.51
1:VB:13:ARG:NH2	1:VB:29:GLU:OE1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ND:58:LYS:NZ	1:ND:60:ASP:OD1	2.44	0.51
1:G:99:ARG:NH1	1:G:251:VAL:O	2.44	0.51
1:S:116:GLU:OE2	1:S:231:LYS:NZ	2.43	0.51
1:JA:116:GLU:OE2	1:JA:231:LYS:NZ	2.43	0.51
1:AB:99:ARG:NH1	1:AB:251:VAL:O	2.42	0.51
1:RB:13:ARG:NH2	1:RB:29:GLU:OE1	2.42	0.51
1:VC:99:ARG:NH1	1:VC:251:VAL:O	2.43	0.51
1:ZC:116:GLU:OE2	1:ZC:231:LYS:NZ	2.42	0.51
1:Y:91:VAL:O	1:Y:94:SER:OG	2.27	0.51
1:Z:25:GLN:NE2	1:Z:256:LEU:O	2.40	0.51
1:EB:99:ARG:NH1	1:EB:251:VAL:O	2.43	0.51
1:TB:99:ARG:NH1	1:TB:251:VAL:O	2.44	0.51
1:UB:99:ARG:NH1	1:UB:251:VAL:O	2.44	0.51
1:JC:99:ARG:NH1	1:JC:251:VAL:O	2.44	0.51
1:WC:1:SER:OG	1:WC:2:LYS:N	2.44	0.51
1:XC:198:CYS:HB2	1:XC:201:SER:HB3	1.93	0.51
1:GD:1:SER:OG	1:GD:2:LYS:N	2.44	0.51
1:GD:116:GLU:OE2	1:GD:231:LYS:NZ	2.42	0.51
1:GB:25:GLN:NE2	1:GB:256:LEU:O	2.42	0.51
1:IC:222:VAL:O	1:IC:225:SER:OG	2.29	0.51
1:FD:198:CYS:HB2	1:FD:201:SER:HB3	1.92	0.51
1:OD:58:LYS:NZ	1:OD:60:ASP:OD1	2.43	0.51
1:OD:116:GLU:OE2	1:OD:231:LYS:NZ	2.44	0.51
1:K:99:ARG:NH1	1:K:251:VAL:O	2.42	0.51
1:QA:25:GLN:NE2	1:QA:256:LEU:O	2.42	0.51
1:GB:158:PHE:HB2	1:GB:171:LEU:HB3	1.93	0.51
1:WB:158:PHE:HB2	1:WB:171:LEU:HB3	1.93	0.51
1:FD:1:SER:OG	1:FD:2:LYS:N	2.43	0.51
1:PD:58:LYS:NZ	1:PD:60:ASP:OD1	2.44	0.51
1:S:39:ARG:HB3	1:S:60:ASP:HB2	1.93	0.51
1:W:158:PHE:HB2	1:W:171:LEU:HB3	1.93	0.51
1:MD:39:ARG:HB3	1:MD:60:ASP:HB2	1.93	0.51
1:W:222:VAL:O	1:W:225:SER:OG	2.29	0.50
1:NA:25:GLN:NE2	1:NA:256:LEU:O	2.43	0.50
1:PB:204:GLY:HA2	1:RB:210:ARG:HH21	1.77	0.50
1:NC:1:SER:OG	1:NC:2:LYS:N	2.43	0.50
1:PC:1:SER:OG	1:PC:2:LYS:N	2.42	0.50
1:UC:39:ARG:HB3	1:UC:60:ASP:HB2	1.93	0.50
1:WC:58:LYS:NZ	1:WC:60:ASP:OD1	2.44	0.50
1:ED:58:LYS:NZ	1:ED:60:ASP:OD1	2.44	0.50
1:G:197:ASP:HB3	1:G:207:PRO:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:99:ARG:NH1	1:T:251:VAL:O	2.41	0.50
1:V:99:ARG:NH1	1:V:251:VAL:O	2.44	0.50
1:Z:123:VAL:HG22	1:AA:161:LYS:HG3	1.93	0.50
1:QC:154:ASP:OD2	1:QC:154:ASP:N	2.44	0.50
1:ED:198:CYS:HB2	1:ED:201:SER:HB3	1.94	0.50
1:F:185:ARG:HH21	1:F:220:THR:HG1	1.59	0.50
1:J:222:VAL:O	1:J:225:SER:OG	2.29	0.50
1:OA:170:ARG:HB2	1:OA:191:ASP:HB2	1.92	0.50
1:WA:204:GLY:HA2	1:GB:210:ARG:HH21	1.76	0.50
1:HB:54:ARG:NH2	1:HB:89:THR:OG1	2.44	0.50
1:JB:1:SER:OG	1:JB:2:LYS:N	2.43	0.50
1:EC:154:ASP:OD2	1:EC:154:ASP:N	2.44	0.50
1:GC:1:SER:OG	1:GC:2:LYS:N	2.43	0.50
1:VC:58:LYS:NZ	1:VC:60:ASP:OD1	2.44	0.50
1:P:204:GLY:HA2	1:AA:210:ARG:HH21	1.76	0.50
1:CA:116:GLU:OE2	1:CA:231:LYS:NZ	2.43	0.50
1:SB:25:GLN:NE2	1:SB:256:LEU:O	2.42	0.50
1:MC:222:VAL:O	1:MC:225:SER:OG	2.29	0.50
1:E:13:ARG:NH2	1:E:29:GLU:OE1	2.42	0.50
1:Z:13:ARG:NH2	1:Z:29:GLU:OE1	2.42	0.50
1:GA:204:GLY:HA2	1:QA:210:ARG:HH21	1.76	0.50
1:KA:1:SER:OG	1:KA:2:LYS:N	2.43	0.50
1:QA:222:VAL:O	1:QA:225:SER:OG	2.29	0.50
1:RA:54:ARG:NH2	1:RA:89:THR:OG1	2.44	0.50
1:WA:1:SER:OG	1:WA:2:LYS:N	2.43	0.50
1:DB:25:GLN:NE2	1:DB:256:LEU:O	2.43	0.50
1:FB:222:VAL:O	1:FB:225:SER:OG	2.30	0.50
1:VB:99:ARG:NH1	1:VB:251:VAL:O	2.41	0.50
1:CC:1:SER:OG	1:CC:2:LYS:N	2.43	0.50
1:KC:25:GLN:NE2	1:KC:256:LEU:O	2.43	0.50
1:VC:1:SER:OG	1:VC:2:LYS:N	2.44	0.50
1:AD:58:LYS:NZ	1:AD:60:ASP:OD1	2.44	0.50
1:H:99:ARG:NH1	1:H:251:VAL:O	2.44	0.50
1:I:222:VAL:O	1:I:225:SER:OG	2.30	0.50
1:J:158:PHE:HB2	1:J:171:LEU:HB3	1.94	0.50
1:L:116:GLU:OE2	1:L:231:LYS:NZ	2.43	0.50
1:X:99:ARG:NH1	1:X:251:VAL:O	2.43	0.50
1:NA:99:ARG:NH1	1:NA:251:VAL:O	2.44	0.50
1:QA:158:PHE:HB2	1:QA:171:LEU:HB3	1.93	0.50
1:WB:25:GLN:NE2	1:WB:256:LEU:O	2.42	0.50
1:IC:158:PHE:HB2	1:IC:171:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JC:25:GLN:NE2	1:JC:256:LEU:O	2.43	0.50
1:ZC:1:SER:OG	1:ZC:2:LYS:N	2.45	0.50
1:D:99:ARG:NH1	1:D:251:VAL:O	2.41	0.50
1:OA:99:ARG:NH1	1:OA:251:VAL:O	2.44	0.50
1:DB:99:ARG:NH1	1:DB:251:VAL:O	2.44	0.50
1:GB:222:VAL:O	1:GB:225:SER:OG	2.30	0.50
1:RB:99:ARG:NH1	1:RB:251:VAL:O	2.41	0.50
1:SB:222:VAL:O	1:SB:225:SER:OG	2.30	0.50
1:UB:25:GLN:NE2	1:UB:256:LEU:O	2.43	0.50
1:WC:99:ARG:NH1	1:WC:251:VAL:O	2.43	0.50
1:YC:58:LYS:NZ	1:YC:60:ASP:OD1	2.44	0.50
1:FD:58:LYS:NZ	1:FD:60:ASP:OD1	2.44	0.50
1:OD:1:SER:OG	1:OD:2:LYS:N	2.44	0.50
1:C:116:GLU:OE2	1:C:231:LYS:NZ	2.43	0.50
1:H:25:GLN:NE2	1:H:256:LEU:O	2.43	0.50
1:M:1:SER:OG	1:M:2:LYS:N	2.43	0.50
1:BA:54:ARG:NH2	1:BA:89:THR:OG1	2.44	0.50
1:MA:58:LYS:NZ	1:MA:60:ASP:OD1	2.42	0.50
1:AB:1:SER:OG	1:AB:2:LYS:N	2.43	0.50
1:CB:158:PHE:HB2	1:CB:171:LEU:HB3	1.93	0.50
1:TB:25:GLN:NE2	1:TB:256:LEU:O	2.43	0.50
1:PD:99:ARG:NH1	1:PD:251:VAL:O	2.43	0.50
1:IA:1:SER:OG	1:IA:2:LYS:N	2.39	0.50
1:OA:25:GLN:NE2	1:OA:256:LEU:O	2.43	0.50
1:SA:39:ARG:HB3	1:SA:60:ASP:HB2	1.94	0.50
1:EB:25:GLN:NE2	1:EB:256:LEU:O	2.43	0.50
1:QB:99:ARG:NH1	1:QB:251:VAL:O	2.41	0.50
1:LC:123:VAL:HG22	1:MC:161:LYS:HG3	1.93	0.50
1:ZC:198:CYS:HB2	1:ZC:201:SER:HB3	1.93	0.50
1:B:116:GLU:OE2	1:B:231:LYS:NZ	2.45	0.49
1:J:99:ARG:NH1	1:J:251:VAL:O	2.43	0.49
1:MA:158:PHE:HB2	1:MA:171:LEU:HB3	1.93	0.49
1:TA:1:SER:OG	1:TA:2:LYS:N	2.43	0.49
1:UA:1:SER:OG	1:UA:2:LYS:N	2.40	0.49
1:TB:91:VAL:O	1:TB:94:SER:OG	2.28	0.49
1:WB:222:VAL:O	1:WB:225:SER:OG	2.30	0.49
1:D:1:SER:OG	1:D:2:LYS:N	2.43	0.49
1:F:158:PHE:HB2	1:F:171:LEU:HB3	1.93	0.49
1:G:161:LYS:O	1:G:168:ARG:NH2	2.45	0.49
1:W:99:ARG:NH1	1:W:251:VAL:O	2.42	0.49
1:X:25:GLN:NE2	1:X:256:LEU:O	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:161:LYS:O	1:X:168:ARG:NH2	2.45	0.49
1:QB:116:GLU:OE2	1:QB:231:LYS:NZ	2.43	0.49
1:ZB:99:ARG:NH1	1:ZB:251:VAL:O	2.44	0.49
1:P:1:SER:OG	1:P:2:LYS:N	2.43	0.49
1:BA:99:ARG:NH1	1:BA:251:VAL:O	2.42	0.49
1:JA:204:GLY:HA2	1:LA:210:ARG:HH21	1.77	0.49
1:NA:100:LYS:NZ	1:NA:247:GLU:OE2	2.44	0.49
1:OA:161:LYS:O	1:OA:168:ARG:NH2	2.45	0.49
1:RA:1:SER:OG	1:RA:2:LYS:N	2.43	0.49
1:CB:25:GLN:NE2	1:CB:256:LEU:O	2.42	0.49
1:DB:198:CYS:HB2	1:DB:201:SER:HB3	1.94	0.49
1:HB:1:SER:OG	1:HB:2:LYS:N	2.43	0.49
1:XB:54:ARG:NH2	1:XB:89:THR:OG1	2.44	0.49
1:GC:54:ARG:NH2	1:GC:89:THR:OG1	2.45	0.49
1:MA:25:GLN:NE2	1:MA:256:LEU:O	2.42	0.49
1:AB:54:ARG:NH2	1:AB:89:THR:OG1	2.44	0.49
1:CB:222:VAL:O	1:CB:225:SER:OG	2.29	0.49
1:UB:91:VAL:O	1:UB:94:SER:OG	2.28	0.49
1:KC:161:LYS:O	1:KC:168:ARG:NH2	2.45	0.49
1:XC:1:SER:OG	1:XC:2:LYS:N	2.43	0.49
1:D:54:ARG:NH2	1:D:89:THR:OG1	2.45	0.49
1:KA:54:ARG:NH2	1:KA:89:THR:OG1	2.44	0.49
1:TA:99:ARG:NH1	1:TA:251:VAL:O	2.44	0.49
1:SB:197:ASP:HB3	1:SB:207:PRO:HG3	1.95	0.49
1:FC:1:SER:OG	1:FC:2:LYS:N	2.42	0.49
1:JC:63:ASP:OD2	1:JC:79:ARG:NH2	2.46	0.49
1:UC:222:VAL:O	1:UC:225:SER:OG	2.30	0.49
1:XC:116:GLU:OE2	1:XC:231:LYS:NZ	2.44	0.49
1:HD:39:ARG:HB3	1:HD:60:ASP:HB2	1.95	0.49
1:T:1:SER:OG	1:T:2:LYS:N	2.43	0.49
1:BA:1:SER:OG	1:BA:2:LYS:N	2.43	0.49
1:EA:116:GLU:OE2	1:EA:231:LYS:NZ	2.45	0.49
1:EA:226:THR:HG22	1:EA:228:ALA:H	1.78	0.49
1:NA:161:LYS:O	1:NA:168:ARG:NH2	2.46	0.49
1:YA:125:LEU:O	1:YA:156:GLN:NE2	2.46	0.49
1:FC:116:GLU:OE2	1:FC:231:LYS:NZ	2.43	0.49
1:NC:54:ARG:NH2	1:NC:89:THR:OG1	2.45	0.49
1:OC:1:SER:OG	1:OC:2:LYS:N	2.42	0.49
1:WC:198:CYS:HB2	1:WC:201:SER:HB3	1.93	0.49
1:GD:99:ARG:NH1	1:GD:251:VAL:O	2.44	0.49
1:F:197:ASP:HB3	1:F:207:PRO:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:116:GLU:OE2	1:AB:231:LYS:NZ	2.43	0.49
1:UB:161:LYS:O	1:UB:168:ARG:NH2	2.46	0.49
1:VB:222:VAL:O	1:VB:225:SER:OG	2.29	0.49
1:FC:222:VAL:O	1:FC:225:SER:OG	2.31	0.49
1:GA:222:VAL:O	1:GA:225:SER:OG	2.31	0.49
1:MA:222:VAL:O	1:MA:225:SER:OG	2.29	0.49
1:YA:116:GLU:OE2	1:YA:231:LYS:NZ	2.45	0.49
1:DB:161:LYS:O	1:DB:168:ARG:NH2	2.46	0.49
1:EB:161:LYS:O	1:EB:168:ARG:NH2	2.46	0.49
1:SB:158:PHE:HB2	1:SB:171:LEU:HB3	1.95	0.49
1:TB:161:LYS:O	1:TB:168:ARG:NH2	2.46	0.49
1:XB:116:GLU:OE2	1:XB:231:LYS:NZ	2.44	0.49
1:JC:161:LYS:O	1:JC:168:ARG:NH2	2.46	0.49
1:SC:39:ARG:HB3	1:SC:60:ASP:HB2	1.94	0.49
1:ZC:99:ARG:NH1	1:ZC:251:VAL:O	2.44	0.49
1:OD:99:ARG:NH1	1:OD:251:VAL:O	2.43	0.49
1:PD:1:SER:OG	1:PD:2:LYS:N	2.46	0.49
1:UA:99:ARG:NH1	1:UA:251:VAL:O	2.43	0.49
1:DB:100:LYS:NZ	1:DB:247:GLU:OE2	2.45	0.49
1:KB:112:THR:HG23	1:KB:114:GLN:H	1.78	0.49
1:NB:99:ARG:NH1	1:NB:251:VAL:O	2.46	0.49
1:TB:197:ASP:HB3	1:TB:207:PRO:HG3	1.95	0.49
1:DC:100:LYS:NZ	1:DC:247:GLU:OE2	2.46	0.49
1:YC:116:GLU:OE2	1:YC:231:LYS:NZ	2.44	0.49
1:PD:116:GLU:OE2	1:PD:231:LYS:NZ	2.44	0.49
1:B:226:THR:HG22	1:B:228:ALA:H	1.78	0.49
1:K:1:SER:OG	1:K:2:LYS:N	2.44	0.49
1:DA:1:SER:OG	1:DA:2:LYS:N	2.43	0.49
1:KA:116:GLU:OE2	1:KA:231:LYS:NZ	2.43	0.49
1:QA:161:LYS:O	1:QA:168:ARG:NH2	2.46	0.49
1:YA:1:SER:OG	1:YA:2:LYS:N	2.40	0.49
1:QB:54:ARG:NH2	1:QB:89:THR:OG1	2.45	0.49
1:UB:198:CYS:HB2	1:UB:201:SER:HB3	1.95	0.49
1:IC:99:ARG:NH1	1:IC:251:VAL:O	2.42	0.49
1:OC:116:GLU:OE2	1:OC:231:LYS:NZ	2.43	0.49
1:OC:222:VAL:O	1:OC:225:SER:OG	2.31	0.49
1:Y:161:LYS:O	1:Y:168:ARG:NH2	2.46	0.48
1:XA:100:LYS:NZ	1:XA:247:GLU:OE2	2.46	0.48
1:KB:226:THR:HG22	1:KB:228:ALA:H	1.78	0.48
1:OB:112:THR:HG23	1:OB:114:GLN:H	1.78	0.48
1:OB:226:THR:HG22	1:OB:228:ALA:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KC:198:CYS:HB2	1:KC:201:SER:HB3	1.94	0.48
1:RC:1:SER:OG	1:RC:2:LYS:N	2.41	0.48
1:RC:100:LYS:NZ	1:RC:247:GLU:OE2	2.46	0.48
1:ID:39:ARG:HB3	1:ID:60:ASP:HB2	1.95	0.48
1:ND:1:SER:OG	1:ND:2:LYS:N	2.44	0.48
1:PD:198:CYS:HB2	1:PD:201:SER:HB3	1.94	0.48
1:B:99:ARG:NH1	1:B:251:VAL:O	2.44	0.48
1:C:158:PHE:HB2	1:C:171:LEU:HB2	1.95	0.48
1:F:222:VAL:O	1:F:225:SER:OG	2.29	0.48
1:L:39:ARG:HB3	1:L:60:ASP:HB2	1.95	0.48
1:Y:197:ASP:HB3	1:Y:207:PRO:HG3	1.94	0.48
1:CA:158:PHE:HB2	1:CA:171:LEU:HB2	1.95	0.48
1:UA:226:THR:HG22	1:UA:228:ALA:H	1.78	0.48
1:BC:99:ARG:NH1	1:BC:251:VAL:O	2.46	0.48
1:DD:39:ARG:HB3	1:DD:60:ASP:HB2	1.95	0.48
1:JD:39:ARG:HB3	1:JD:60:ASP:HB2	1.95	0.48
1:S:125:LEU:O	1:S:156:GLN:NE2	2.43	0.48
1:IA:116:GLU:OE2	1:IA:231:LYS:NZ	2.45	0.48
1:JA:158:PHE:HB2	1:JA:171:LEU:HB2	1.95	0.48
1:DC:1:SER:OG	1:DC:2:LYS:N	2.41	0.48
1:EC:112:THR:HG23	1:EC:114:GLN:H	1.78	0.48
1:TC:39:ARG:HB3	1:TC:60:ASP:HB2	1.95	0.48
1:HD:154:ASP:OD1	1:HD:154:ASP:N	2.46	0.48
1:MD:161:LYS:O	1:MD:168:ARG:NH2	2.46	0.48
1:H:161:LYS:O	1:H:168:ARG:NH2	2.46	0.48
1:L:158:PHE:HB2	1:L:171:LEU:HB2	1.94	0.48
1:IA:226:THR:HG22	1:IA:228:ALA:H	1.78	0.48
1:SA:158:PHE:HB2	1:SA:171:LEU:HB2	1.95	0.48
1:YA:112:THR:HG23	1:YA:114:GLN:H	1.78	0.48
1:YA:226:THR:HG22	1:YA:228:ALA:H	1.78	0.48
1:LB:99:ARG:NH1	1:LB:251:VAL:O	2.46	0.48
1:NC:99:ARG:NH1	1:NC:251:VAL:O	2.41	0.48
1:BD:39:ARG:HB3	1:BD:60:ASP:HB2	1.96	0.48
1:CD:39:ARG:HB3	1:CD:60:ASP:HB2	1.96	0.48
1:FD:116:GLU:OE2	1:FD:231:LYS:NZ	2.44	0.48
1:JD:150:GLN:NE2	1:JD:152:THR:OG1	2.43	0.48
1:AA:158:PHE:HB2	1:AA:171:LEU:HB3	1.95	0.48
1:EA:91:VAL:HG23	1:EA:94:SER:HB3	1.96	0.48
1:EA:99:ARG:NH1	1:EA:251:VAL:O	2.44	0.48
1:HA:99:ARG:NH1	1:HA:251:VAL:O	2.46	0.48
1:IA:112:THR:HG23	1:IA:114:GLN:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NA:198:CYS:HB2	1:NA:201:SER:HB3	1.95	0.48
1:XA:39:ARG:HB3	1:XA:60:ASP:HB2	1.95	0.48
1:EB:198:CYS:HB2	1:EB:201:SER:HB3	1.95	0.48
1:AC:112:THR:HG23	1:AC:114:GLN:H	1.79	0.48
1:AC:226:THR:HG22	1:AC:228:ALA:H	1.78	0.48
1:EC:91:VAL:HG23	1:EC:94:SER:HB3	1.95	0.48
1:MC:158:PHE:HB2	1:MC:171:LEU:HB3	1.95	0.48
1:DD:25:GLN:NE2	1:DD:256:LEU:O	2.44	0.48
1:HD:222:VAL:O	1:HD:225:SER:OG	2.30	0.48
1:A:116:GLU:OE2	1:A:231:LYS:NZ	2.43	0.48
1:V:123:VAL:HG22	1:W:161:LYS:HG3	1.95	0.48
1:EA:112:THR:HG23	1:EA:114:GLN:H	1.78	0.48
1:HA:100:LYS:NZ	1:HA:247:GLU:OE2	2.46	0.48
1:VA:99:ARG:NH1	1:VA:251:VAL:O	2.46	0.48
1:IB:158:PHE:HB2	1:IB:171:LEU:HB2	1.95	0.48
1:FC:125:LEU:O	1:FC:156:GLN:NE2	2.42	0.48
1:GC:99:ARG:NH1	1:GC:251:VAL:O	2.41	0.48
1:GC:116:GLU:OE2	1:GC:231:LYS:NZ	2.43	0.48
1:NC:116:GLU:OE2	1:NC:231:LYS:NZ	2.44	0.48
1:YC:1:SER:OG	1:YC:2:LYS:N	2.46	0.48
1:ZC:58:LYS:NZ	1:ZC:60:ASP:OD1	2.44	0.48
1:UA:112:THR:HG23	1:UA:114:GLN:H	1.78	0.48
1:CB:197:ASP:HB3	1:CB:207:PRO:HG3	1.96	0.48
1:EB:55:VAL:HB	1:EB:88:VAL:HB	1.96	0.48
1:FB:123:VAL:HG22	1:GB:161:LYS:HG3	1.94	0.48
1:XB:100:LYS:NZ	1:XB:247:GLU:OE2	2.43	0.48
1:LC:13:ARG:NH2	1:LC:29:GLU:OE1	2.42	0.48
1:GD:58:LYS:NZ	1:GD:60:ASP:OD1	2.43	0.48
1:AA:222:VAL:O	1:AA:225:SER:OG	2.30	0.48
1:YA:154:ASP:OD2	1:YA:154:ASP:N	2.44	0.48
1:GB:161:LYS:O	1:GB:168:ARG:NH2	2.47	0.48
1:RB:199:SER:OG	1:RB:205:GLU:O	2.32	0.48
1:TB:63:ASP:OD2	1:TB:79:ARG:NH2	2.46	0.48
1:QC:91:VAL:HG23	1:QC:94:SER:HB3	1.96	0.48
1:SC:25:GLN:NE2	1:SC:256:LEU:O	2.44	0.48
1:E:123:VAL:HG22	1:F:161:LYS:HG3	1.96	0.48
1:V:150:GLN:HE21	1:V:152:THR:HG1	1.57	0.48
1:PA:3:THR:HG22	1:PA:16:THR:HG22	1.95	0.48
1:RB:222:VAL:O	1:RB:225:SER:OG	2.31	0.48
1:VB:54:ARG:NH2	1:VB:89:THR:OG1	2.43	0.48
1:KC:100:LYS:NZ	1:KC:247:GLU:OE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CD:222:VAL:O	1:CD:225:SER:OG	2.30	0.48
1:JD:161:LYS:O	1:JD:168:ARG:NH2	2.47	0.48
1:D:186:VAL:HB	1:D:219:VAL:HB	1.96	0.48
1:X:63:ASP:OD2	1:X:79:ARG:NH2	2.46	0.48
1:BA:116:GLU:OE2	1:BA:231:LYS:NZ	2.43	0.48
1:IA:154:ASP:OD2	1:IA:154:ASP:N	2.44	0.48
1:AC:116:GLU:OE2	1:AC:231:LYS:NZ	2.45	0.48
1:QC:112:THR:HG23	1:QC:114:GLN:H	1.79	0.48
1:KD:161:LYS:HG3	1:MD:123:VAL:HG22	1.96	0.48
1:H:91:VAL:O	1:H:94:SER:OG	2.28	0.47
1:O:99:ARG:NH1	1:O:251:VAL:O	2.46	0.47
1:Y:55:VAL:HB	1:Y:88:VAL:HB	1.96	0.47
1:BA:186:VAL:HB	1:BA:219:VAL:HB	1.96	0.47
1:GA:64:VAL:HG22	1:GA:78:VAL:HG12	1.95	0.47
1:NA:55:VAL:HB	1:NA:88:VAL:HB	1.96	0.47
1:QA:154:ASP:OD1	1:QA:154:ASP:N	2.46	0.47
1:DB:55:VAL:HB	1:DB:88:VAL:HB	1.96	0.47
1:RB:54:ARG:NH2	1:RB:89:THR:OG1	2.43	0.47
1:YB:158:PHE:HB2	1:YB:171:LEU:HB2	1.96	0.47
1:BC:100:LYS:NZ	1:BC:247:GLU:OE2	2.46	0.47
1:EC:226:THR:HG22	1:EC:228:ALA:H	1.78	0.47
1:UC:5:VAL:HG12	1:UC:14:THR:HG22	1.96	0.47
1:CD:150:GLN:NE2	1:CD:152:THR:OG1	2.43	0.47
1:B:112:THR:HG23	1:B:114:GLN:H	1.78	0.47
1:R:116:GLU:OE2	1:R:231:LYS:NZ	2.45	0.47
1:R:125:LEU:O	1:R:156:GLN:NE2	2.47	0.47
1:T:186:VAL:HB	1:T:219:VAL:HB	1.97	0.47
1:PA:170:ARG:HB2	1:PA:191:ASP:HB2	1.96	0.47
1:ZA:158:PHE:HB2	1:ZA:171:LEU:HB2	1.96	0.47
1:OB:116:GLU:OE2	1:OB:231:LYS:NZ	2.45	0.47
1:FC:158:PHE:HB2	1:FC:171:LEU:HB2	1.95	0.47
1:QC:226:THR:HG22	1:QC:228:ALA:H	1.78	0.47
1:VC:13:ARG:NH2	1:VC:29:GLU:OE1	2.48	0.47
1:ID:25:GLN:NE2	1:ID:256:LEU:O	2.45	0.47
1:KD:39:ARG:HB3	1:KD:60:ASP:HB2	1.96	0.47
1:K:186:VAL:HB	1:K:219:VAL:HB	1.97	0.47
1:N:116:GLU:OE2	1:N:231:LYS:NZ	2.45	0.47
1:Q:99:ARG:NH1	1:Q:251:VAL:O	2.46	0.47
1:X:91:VAL:O	1:X:94:SER:OG	2.28	0.47
1:X:112:THR:HG23	1:X:114:GLN:H	1.80	0.47
1:KA:100:LYS:NZ	1:KA:247:GLU:OE2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NB:100:LYS:NZ	1:NB:247:GLU:OE2	2.46	0.47
1:OB:91:VAL:HG23	1:OB:94:SER:HB3	1.97	0.47
1:WB:197:ASP:HB3	1:WB:207:PRO:HG3	1.96	0.47
1:ZB:1:SER:OG	1:ZB:2:LYS:N	2.43	0.47
1:HC:13:ARG:NH2	1:HC:29:GLU:OE1	2.42	0.47
1:BD:150:GLN:NE2	1:BD:152:THR:OG1	2.43	0.47
1:GD:13:ARG:NH2	1:GD:29:GLU:OE1	2.48	0.47
1:D:116:GLU:OE2	1:D:231:LYS:NZ	2.44	0.47
1:G:54:ARG:NH2	1:G:89:THR:OG1	2.44	0.47
1:N:91:VAL:HG23	1:N:94:SER:HB3	1.96	0.47
1:Z:170:ARG:HB2	1:Z:191:ASP:HB2	1.97	0.47
1:UA:158:PHE:HB2	1:UA:171:LEU:HB2	1.96	0.47
1:PB:222:VAL:O	1:PB:225:SER:OG	2.31	0.47
1:QB:100:LYS:NZ	1:QB:247:GLU:OE2	2.44	0.47
1:KC:55:VAL:HB	1:KC:88:VAL:HB	1.96	0.47
1:LC:3:THR:HG22	1:LC:16:THR:HG22	1.95	0.47
1:SC:161:LYS:O	1:SC:168:ARG:NH2	2.48	0.47
1:TC:161:LYS:O	1:TC:168:ARG:NH2	2.48	0.47
1:ZC:13:ARG:NH2	1:ZC:29:GLU:OE1	2.48	0.47
1:ID:161:LYS:O	1:ID:168:ARG:NH2	2.47	0.47
1:OD:13:ARG:NH2	1:OD:29:GLU:OE1	2.48	0.47
1:W:161:LYS:O	1:W:168:ARG:NH2	2.48	0.47
1:CA:222:VAL:O	1:CA:225:SER:OG	2.31	0.47
1:JA:125:LEU:O	1:JA:156:GLN:NE2	2.42	0.47
1:OA:55:VAL:HB	1:OA:88:VAL:HB	1.97	0.47
1:TA:222:VAL:O	1:TA:225:SER:OG	2.31	0.47
1:UA:91:VAL:HG23	1:UA:94:SER:HB3	1.96	0.47
1:UA:116:GLU:OE2	1:UA:231:LYS:NZ	2.45	0.47
1:FB:170:ARG:HB2	1:FB:191:ASP:HB2	1.97	0.47
1:PB:158:PHE:HB2	1:PB:171:LEU:HB2	1.96	0.47
1:OC:125:LEU:O	1:OC:156:GLN:NE2	2.43	0.47
1:WC:123:VAL:HG22	1:XC:161:LYS:HG3	1.97	0.47
1:ZC:112:THR:HG23	1:ZC:114:GLN:H	1.80	0.47
1:G:55:VAL:HB	1:G:88:VAL:HB	1.97	0.47
1:R:226:THR:HG22	1:R:228:ALA:H	1.78	0.47
1:DA:116:GLU:OE2	1:DA:231:LYS:NZ	2.48	0.47
1:LA:199:SER:OG	1:LA:205:GLU:O	2.32	0.47
1:OA:91:VAL:O	1:OA:94:SER:OG	2.28	0.47
1:VA:39:ARG:HB3	1:VA:60:ASP:HB2	1.97	0.47
1:WA:54:ARG:NH2	1:WA:89:THR:OG1	2.47	0.47
1:AB:100:LYS:NZ	1:AB:247:GLU:OE2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:186:VAL:HB	1:AB:219:VAL:HB	1.96	0.47
1:EB:152:THR:OG1	1:EB:154:ASP:OD1	2.33	0.47
1:NB:39:ARG:HB3	1:NB:60:ASP:HB2	1.97	0.47
1:ZB:54:ARG:NH2	1:ZB:89:THR:OG1	2.47	0.47
1:BC:39:ARG:HB3	1:BC:60:ASP:HB2	1.97	0.47
1:EC:116:GLU:OE2	1:EC:231:LYS:NZ	2.45	0.47
1:HC:3:THR:HG22	1:HC:16:THR:HG22	1.95	0.47
1:KC:152:THR:OG1	1:KC:154:ASP:OD1	2.33	0.47
1:OC:158:PHE:HB2	1:OC:171:LEU:HB2	1.95	0.47
1:UC:161:LYS:O	1:UC:168:ARG:NH2	2.47	0.47
1:CD:161:LYS:O	1:CD:168:ARG:NH2	2.48	0.47
1:ED:13:ARG:NH2	1:ED:29:GLU:OE1	2.48	0.47
1:LD:161:LYS:O	1:LD:168:ARG:NH2	2.48	0.47
1:A:39:ARG:HB3	1:A:60:ASP:HB2	1.97	0.47
1:E:170:ARG:HB2	1:E:191:ASP:HB2	1.97	0.47
1:F:161:LYS:O	1:F:168:ARG:NH2	2.48	0.47
1:N:226:THR:HG22	1:N:228:ALA:H	1.78	0.47
1:P:222:VAL:O	1:P:225:SER:OG	2.31	0.47
1:S:158:PHE:HB2	1:S:171:LEU:HB2	1.96	0.47
1:T:54:ARG:NH2	1:T:89:THR:OG1	2.44	0.47
1:W:197:ASP:HB3	1:W:207:PRO:HG3	1.96	0.47
1:DA:197:ASP:OD1	1:DA:197:ASP:N	2.48	0.47
1:GA:54:ARG:NH2	1:GA:89:THR:OG1	2.47	0.47
1:HA:39:ARG:HB3	1:HA:60:ASP:HB2	1.97	0.47
1:IA:125:LEU:O	1:IA:156:GLN:NE2	2.48	0.47
1:PA:13:ARG:NH2	1:PA:29:GLU:OE1	2.42	0.47
1:QA:41:THR:O	1:QA:41:THR:OG1	2.33	0.47
1:ZA:125:LEU:O	1:ZA:156:GLN:NE2	2.42	0.47
1:BB:123:VAL:HG22	1:CB:161:LYS:HG3	1.96	0.47
1:BB:170:ARG:HB2	1:BB:191:ASP:HB2	1.97	0.47
1:LB:39:ARG:HB3	1:LB:60:ASP:HB2	1.97	0.47
1:MB:1:SER:OG	1:MB:2:LYS:N	2.43	0.47
1:VB:123:VAL:HG22	1:WB:161:LYS:HG3	1.96	0.47
1:AC:91:VAL:HG23	1:AC:94:SER:HB3	1.97	0.47
1:HC:123:VAL:HG22	1:IC:161:LYS:HG3	1.97	0.47
1:JC:55:VAL:HB	1:JC:88:VAL:HB	1.97	0.47
1:PC:54:ARG:NH2	1:PC:89:THR:OG1	2.47	0.47
1:QC:158:PHE:HB2	1:QC:171:LEU:HB2	1.97	0.47
1:RC:39:ARG:HB3	1:RC:60:ASP:HB2	1.96	0.47
1:XC:13:ARG:NH2	1:XC:29:GLU:OE1	2.48	0.47
1:YC:99:ARG:NH1	1:YC:251:VAL:O	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:5:VAL:HG12	1:BD:14:THR:HG22	1.97	0.47
1:BD:161:LYS:O	1:BD:168:ARG:NH2	2.48	0.47
1:DD:5:VAL:HG12	1:DD:14:THR:HG22	1.97	0.47
1:DD:161:LYS:O	1:DD:168:ARG:NH2	2.48	0.47
1:ED:99:ARG:NH1	1:ED:251:VAL:O	2.44	0.47
1:ID:5:VAL:HG12	1:ID:14:THR:HG22	1.97	0.47
1:KD:5:VAL:HG12	1:KD:14:THR:HG22	1.97	0.47
1:ND:91:VAL:O	1:ND:94:SER:OG	2.29	0.47
1:C:161:LYS:HD3	1:C:161:LYS:HA	1.73	0.47
1:H:152:THR:OG1	1:H:154:ASP:OD1	2.33	0.47
1:LA:123:VAL:HG22	1:MA:161:LYS:HG3	1.96	0.47
1:SA:23:ASP:OD2	1:SA:23:ASP:N	2.48	0.47
1:YA:91:VAL:HG23	1:YA:94:SER:HB3	1.97	0.47
1:CB:161:LYS:O	1:CB:168:ARG:NH2	2.48	0.47
1:EB:91:VAL:O	1:EB:94:SER:OG	2.28	0.47
1:FB:3:THR:HG22	1:FB:16:THR:HG22	1.96	0.47
1:IB:23:ASP:OD2	1:IB:23:ASP:N	2.48	0.47
1:LB:100:LYS:NZ	1:LB:247:GLU:OE2	2.46	0.47
1:SB:41:THR:O	1:SB:41:THR:OG1	2.33	0.47
1:WB:116:GLU:OE2	1:WB:231:LYS:NZ	2.46	0.47
1:OC:23:ASP:OD2	1:OC:23:ASP:N	2.48	0.47
1:WC:13:ARG:NH2	1:WC:29:GLU:OE1	2.48	0.47
1:WC:100:LYS:NZ	1:WC:247:GLU:OE2	2.45	0.47
1:AD:13:ARG:NH2	1:AD:29:GLU:OE1	2.48	0.47
1:AD:99:ARG:NH1	1:AD:251:VAL:O	2.44	0.47
1:JD:5:VAL:HG12	1:JD:14:THR:HG22	1.97	0.47
1:C:222:VAL:O	1:C:225:SER:OG	2.32	0.47
1:L:23:ASP:N	1:L:23:ASP:OD2	2.48	0.47
1:S:23:ASP:OD2	1:S:23:ASP:N	2.48	0.47
1:X:152:THR:OG1	1:X:154:ASP:OD1	2.33	0.47
1:KA:186:VAL:HB	1:KA:219:VAL:HB	1.97	0.47
1:LA:222:VAL:O	1:LA:225:SER:OG	2.30	0.47
1:MA:161:LYS:O	1:MA:168:ARG:NH2	2.48	0.47
1:XA:116:GLU:OE2	1:XA:231:LYS:NZ	2.43	0.47
1:WB:41:THR:O	1:WB:41:THR:OG1	2.33	0.47
1:DC:99:ARG:NH1	1:DC:251:VAL:O	2.46	0.47
1:FC:23:ASP:OD2	1:FC:23:ASP:N	2.48	0.47
1:GC:91:VAL:O	1:GC:94:SER:OG	2.30	0.47
1:NC:186:VAL:HB	1:NC:219:VAL:HB	1.96	0.47
1:QC:116:GLU:OE2	1:QC:231:LYS:NZ	2.45	0.47
1:FD:13:ARG:NH2	1:FD:29:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FD:91:VAL:O	1:FD:94:SER:OG	2.29	0.47
1:GD:112:THR:HG23	1:GD:114:GLN:H	1.80	0.47
1:LD:25:GLN:NE2	1:LD:256:LEU:O	2.45	0.47
1:ND:13:ARG:NH2	1:ND:29:GLU:OE1	2.48	0.47
1:PD:13:ARG:NH2	1:PD:29:GLU:OE1	2.48	0.47
1:PD:100:LYS:NZ	1:PD:247:GLU:OE2	2.46	0.47
1:I:123:VAL:HG22	1:J:161:LYS:HG3	1.96	0.47
1:K:54:ARG:NH2	1:K:89:THR:OG1	2.44	0.47
1:HA:116:GLU:OE2	1:HA:231:LYS:NZ	2.43	0.47
1:UA:161:LYS:HA	1:UA:161:LYS:HD3	1.75	0.47
1:ZA:204:GLY:HA2	1:BB:210:ARG:HH21	1.80	0.47
1:BB:222:VAL:O	1:BB:225:SER:OG	2.30	0.47
1:GB:54:ARG:NH2	1:GB:89:THR:OG1	2.47	0.47
1:KB:116:GLU:OE2	1:KB:231:LYS:NZ	2.45	0.47
1:KB:158:PHE:HB2	1:KB:171:LEU:HB2	1.97	0.47
1:MB:197:ASP:OD1	1:MB:197:ASP:N	2.48	0.47
1:ZB:222:VAL:O	1:ZB:225:SER:OG	2.31	0.47
1:FC:161:LYS:HA	1:FC:161:LYS:HD3	1.72	0.47
1:GC:186:VAL:HB	1:GC:219:VAL:HB	1.97	0.47
1:IC:161:LYS:O	1:IC:168:ARG:NH2	2.48	0.47
1:SC:55:VAL:HB	1:SC:88:VAL:HB	1.97	0.47
1:HD:25:GLN:NE2	1:HD:256:LEU:O	2.44	0.47
1:ID:55:VAL:HB	1:ID:88:VAL:HB	1.97	0.47
1:C:125:LEU:O	1:C:156:GLN:NE2	2.42	0.46
1:F:186:VAL:HB	1:F:219:VAL:HB	1.97	0.46
1:M:222:VAL:O	1:M:225:SER:OG	2.31	0.46
1:Z:199:SER:OG	1:Z:205:GLU:O	2.33	0.46
1:MA:197:ASP:HB3	1:MA:207:PRO:HG3	1.98	0.46
1:PA:123:VAL:HG22	1:QA:161:LYS:HG3	1.97	0.46
1:RA:186:VAL:HB	1:RA:219:VAL:HB	1.96	0.46
1:JC:125:LEU:O	1:JC:156:GLN:NE2	2.47	0.46
1:MC:197:ASP:HB3	1:MC:207:PRO:HG3	1.95	0.46
1:SC:5:VAL:HG12	1:SC:14:THR:HG22	1.96	0.46
1:YC:13:ARG:NH2	1:YC:29:GLU:OE1	2.48	0.46
1:ZC:123:VAL:HG22	1:AD:161:LYS:HG3	1.97	0.46
1:BD:25:GLN:NE2	1:BD:256:LEU:O	2.45	0.46
1:DD:64:VAL:HA	1:DD:78:VAL:HA	1.98	0.46
1:HD:5:VAL:HG12	1:HD:14:THR:HG22	1.96	0.46
1:MD:5:VAL:HG12	1:MD:14:THR:HG22	1.97	0.46
1:OD:112:THR:HG23	1:OD:114:GLN:H	1.80	0.46
1:A:99:ARG:NH1	1:A:251:VAL:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:VAL:HG23	1:B:94:SER:HB3	1.98	0.46
1:H:112:THR:HG23	1:H:114:GLN:H	1.81	0.46
1:EA:125:LEU:O	1:EA:156:GLN:NE2	2.46	0.46
1:TA:158:PHE:HB2	1:TA:171:LEU:HB2	1.98	0.46
1:BB:3:THR:HG22	1:BB:16:THR:HG22	1.95	0.46
1:HB:186:VAL:HB	1:HB:219:VAL:HB	1.97	0.46
1:RB:170:ARG:HB2	1:RB:191:ASP:HB2	1.97	0.46
1:YC:161:LYS:HG3	1:AD:123:VAL:HG22	1.97	0.46
1:BD:199:SER:OG	1:BD:205:GLU:O	2.34	0.46
1:HD:55:VAL:HB	1:HD:88:VAL:HB	1.97	0.46
1:HD:98:SER:OG	1:HD:213:GLN:OE1	2.33	0.46
1:HD:161:LYS:O	1:HD:168:ARG:NH2	2.48	0.46
1:JD:25:GLN:NE2	1:JD:256:LEU:O	2.45	0.46
1:LD:100:LYS:NZ	1:LD:247:GLU:OE2	2.49	0.46
1:D:100:LYS:NZ	1:D:247:GLU:OE2	2.44	0.46
1:N:125:LEU:O	1:N:156:GLN:NE2	2.48	0.46
1:FA:99:ARG:NH1	1:FA:251:VAL:O	2.46	0.46
1:JB:158:PHE:HB2	1:JB:171:LEU:HB2	1.98	0.46
1:VB:170:ARG:HB2	1:VB:191:ASP:HB2	1.97	0.46
1:AC:109:LEU:HD11	1:AC:171:LEU:HD21	1.97	0.46
1:AC:125:LEU:O	1:AC:156:GLN:NE2	2.47	0.46
1:AC:158:PHE:HB2	1:AC:171:LEU:HB2	1.97	0.46
1:OC:161:LYS:HA	1:OC:161:LYS:HD3	1.72	0.46
1:RC:99:ARG:NH1	1:RC:251:VAL:O	2.46	0.46
1:BD:222:VAL:O	1:BD:225:SER:OG	2.30	0.46
1:FD:99:ARG:NH1	1:FD:251:VAL:O	2.43	0.46
1:JD:222:VAL:O	1:JD:225:SER:OG	2.30	0.46
1:G:199:SER:OG	1:G:205:GLU:O	2.33	0.46
1:H:100:LYS:NZ	1:H:247:GLU:OE2	2.48	0.46
1:EA:158:PHE:HB2	1:EA:171:LEU:HB2	1.97	0.46
1:OA:112:THR:HG23	1:OA:114:GLN:H	1.80	0.46
1:OA:152:THR:OG1	1:OA:154:ASP:OD1	2.34	0.46
1:QA:54:ARG:NH2	1:QA:89:THR:OG1	2.47	0.46
1:DB:112:THR:HG23	1:DB:114:GLN:H	1.81	0.46
1:OB:125:LEU:O	1:OB:156:GLN:NE2	2.47	0.46
1:UB:55:VAL:HB	1:UB:88:VAL:HB	1.96	0.46
1:HC:170:ARG:HB2	1:HC:191:ASP:HB2	1.96	0.46
1:XC:112:THR:HG23	1:XC:114:GLN:H	1.80	0.46
1:LD:39:ARG:HB3	1:LD:60:ASP:HB2	1.96	0.46
1:LD:55:VAL:HB	1:LD:88:VAL:HB	1.98	0.46
1:LD:150:GLN:NE2	1:LD:152:THR:OG1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ND:112:THR:HG23	1:ND:114:GLN:H	1.80	0.46
1:C:112:THR:HG23	1:C:114:GLN:H	1.81	0.46
1:H:55:VAL:HB	1:H:88:VAL:HB	1.97	0.46
1:R:112:THR:HG23	1:R:114:GLN:H	1.80	0.46
1:BA:100:LYS:NZ	1:BA:247:GLU:OE2	2.44	0.46
1:CA:161:LYS:HD3	1:CA:161:LYS:HA	1.72	0.46
1:FA:161:LYS:HA	1:FA:161:LYS:HD3	1.72	0.46
1:FB:13:ARG:NH2	1:FB:29:GLU:OE1	2.42	0.46
1:OB:158:PHE:HB2	1:OB:171:LEU:HB2	1.97	0.46
1:WB:3:THR:HG22	1:WB:16:THR:HG22	1.98	0.46
1:CD:25:GLN:NE2	1:CD:256:LEU:O	2.45	0.46
1:JD:64:VAL:HA	1:JD:78:VAL:HA	1.98	0.46
1:F:3:THR:HG22	1:F:16:THR:HG22	1.98	0.46
1:J:161:LYS:O	1:J:168:ARG:NH2	2.49	0.46
1:N:99:ARG:NH1	1:N:251:VAL:O	2.44	0.46
1:CA:125:LEU:O	1:CA:156:GLN:NE2	2.42	0.46
1:NA:112:THR:HG23	1:NA:114:GLN:H	1.81	0.46
1:KB:125:LEU:O	1:KB:156:GLN:NE2	2.48	0.46
1:PB:125:LEU:O	1:PB:156:GLN:NE2	2.42	0.46
1:WB:186:VAL:HB	1:WB:219:VAL:HB	1.98	0.46
1:YB:125:LEU:O	1:YB:156:GLN:NE2	2.42	0.46
1:EC:158:PHE:HB2	1:EC:171:LEU:HB2	1.97	0.46
1:JC:91:VAL:O	1:JC:94:SER:OG	2.28	0.46
1:PC:116:GLU:OE2	1:PC:231:LYS:NZ	2.48	0.46
1:QC:99:ARG:NH1	1:QC:251:VAL:O	2.43	0.46
1:BD:154:ASP:OD1	1:BD:154:ASP:N	2.45	0.46
1:DD:98:SER:OG	1:DD:213:GLN:OE1	2.34	0.46
1:O:39:ARG:HB3	1:O:60:ASP:HB2	1.96	0.46
1:Y:100:LYS:NZ	1:Y:247:GLU:OE2	2.48	0.46
1:IA:158:PHE:HB2	1:IA:171:LEU:HB2	1.97	0.46
1:TA:116:GLU:OE2	1:TA:231:LYS:NZ	2.48	0.46
1:VA:100:LYS:NZ	1:VA:247:GLU:OE2	2.46	0.46
1:CB:3:THR:HG22	1:CB:16:THR:HG22	1.98	0.46
1:EB:112:THR:HG23	1:EB:114:GLN:H	1.81	0.46
1:MB:54:ARG:NH2	1:MB:89:THR:OG1	2.47	0.46
1:UB:125:LEU:O	1:UB:156:GLN:NE2	2.47	0.46
1:CC:197:ASP:OD1	1:CC:197:ASP:N	2.48	0.46
1:EC:109:LEU:HD11	1:EC:171:LEU:HD21	1.98	0.46
1:IC:3:THR:HG22	1:IC:16:THR:HG22	1.98	0.46
1:JC:152:THR:OG1	1:JC:154:ASP:OD1	2.34	0.46
1:MC:3:THR:HG22	1:MC:16:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OD:122:LEU:HD12	1:OD:175:LEU:HD11	1.98	0.46
1:B:158:PHE:HB2	1:B:171:LEU:HB2	1.97	0.46
1:E:54:ARG:NH2	1:E:89:THR:OG1	2.43	0.46
1:V:58:LYS:NZ	1:V:60:ASP:OD1	2.46	0.46
1:W:116:GLU:OE2	1:W:231:LYS:NZ	2.48	0.46
1:AA:3:THR:HG22	1:AA:16:THR:HG22	1.98	0.46
1:RA:134:THR:HG22	1:RA:147:THR:HG22	1.98	0.46
1:OB:109:LEU:HD11	1:OB:171:LEU:HD21	1.98	0.46
1:SB:3:THR:HG22	1:SB:16:THR:HG22	1.98	0.46
1:TB:112:THR:HG23	1:TB:114:GLN:H	1.81	0.46
1:PC:197:ASP:OD1	1:PC:197:ASP:N	2.49	0.46
1:SC:150:GLN:NE2	1:SC:152:THR:OG1	2.43	0.46
1:TC:5:VAL:HG12	1:TC:14:THR:HG22	1.97	0.46
1:AD:122:LEU:HD12	1:AD:175:LEU:HD11	1.98	0.46
1:CD:55:VAL:HB	1:CD:88:VAL:HB	1.98	0.46
1:DD:54:ARG:NH2	1:DD:89:THR:OG1	2.46	0.46
1:ED:54:ARG:NH2	1:ED:89:THR:OG1	2.46	0.46
1:ED:122:LEU:HD12	1:ED:175:LEU:HD11	1.98	0.46
1:MD:222:VAL:O	1:MD:225:SER:OG	2.30	0.46
1:OD:197:ASP:HB3	1:OD:207:PRO:HG3	1.96	0.46
1:PD:112:THR:HG23	1:PD:114:GLN:H	1.80	0.46
1:E:222:VAL:O	1:E:225:SER:OG	2.30	0.46
1:R:91:VAL:HG23	1:R:94:SER:HB3	1.97	0.46
1:Z:222:VAL:O	1:Z:225:SER:OG	2.30	0.46
1:QA:3:THR:HG22	1:QA:16:THR:HG22	1.98	0.46
1:QB:1:SER:OG	1:QB:2:LYS:N	2.43	0.46
1:TB:125:LEU:O	1:TB:156:GLN:NE2	2.47	0.46
1:UB:112:THR:HG23	1:UB:114:GLN:H	1.81	0.46
1:ZB:197:ASP:OD1	1:ZB:197:ASP:N	2.49	0.46
1:CC:116:GLU:OE2	1:CC:231:LYS:NZ	2.48	0.46
1:TC:222:VAL:O	1:TC:225:SER:OG	2.30	0.46
1:WC:112:THR:HG23	1:WC:114:GLN:H	1.80	0.46
1:DD:55:VAL:HB	1:DD:88:VAL:HB	1.98	0.46
1:FD:112:THR:HG23	1:FD:114:GLN:H	1.80	0.46
1:MD:150:GLN:NE2	1:MD:152:THR:OG1	2.43	0.46
1:FA:100:LYS:NZ	1:FA:247:GLU:OE2	2.46	0.46
1:NA:152:THR:OG1	1:NA:154:ASP:OD1	2.33	0.46
1:SA:125:LEU:O	1:SA:156:GLN:NE2	2.42	0.46
1:DB:152:THR:OG1	1:DB:154:ASP:OD1	2.33	0.46
1:DC:39:ARG:HB3	1:DC:60:ASP:HB2	1.97	0.46
1:SC:100:LYS:NZ	1:SC:247:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TC:150:GLN:NE2	1:TC:152:THR:OG1	2.43	0.46
1:YC:112:THR:HG23	1:YC:114:GLN:H	1.81	0.46
1:ED:112:THR:HG23	1:ED:114:GLN:H	1.80	0.46
1:JD:100:LYS:NZ	1:JD:247:GLU:OE2	2.49	0.46
1:A:100:LYS:NZ	1:A:247:GLU:OE2	2.46	0.45
1:T:116:GLU:OE2	1:T:231:LYS:NZ	2.43	0.45
1:Y:199:SER:OG	1:Y:205:GLU:O	2.34	0.45
1:Z:54:ARG:NH2	1:Z:89:THR:OG1	2.43	0.45
1:CA:112:THR:HG23	1:CA:114:GLN:H	1.82	0.45
1:FA:39:ARG:HB3	1:FA:60:ASP:HB2	1.98	0.45
1:YA:158:PHE:HB2	1:YA:171:LEU:HB2	1.98	0.45
1:DB:170:ARG:HB2	1:DB:191:ASP:HB2	1.98	0.45
1:FB:58:LYS:NZ	1:FB:60:ASP:OD1	2.46	0.45
1:FB:199:SER:OG	1:FB:205:GLU:O	2.34	0.45
1:GB:3:THR:HG22	1:GB:16:THR:HG22	1.98	0.45
1:JB:116:GLU:OE2	1:JB:231:LYS:NZ	2.48	0.45
1:WB:161:LYS:O	1:WB:168:ARG:NH2	2.48	0.45
1:JC:112:THR:HG23	1:JC:114:GLN:H	1.81	0.45
1:WC:54:ARG:NH2	1:WC:89:THR:OG1	2.46	0.45
1:AD:54:ARG:NH2	1:AD:89:THR:OG1	2.47	0.45
1:FD:123:VAL:HG22	1:GD:161:LYS:HG3	1.98	0.45
1:ID:54:ARG:NH2	1:ID:89:THR:OG1	2.46	0.45
1:KD:183:ALA:HA	1:KD:222:VAL:HA	1.98	0.45
1:LD:183:ALA:HA	1:LD:222:VAL:HA	1.98	0.45
1:ND:123:VAL:HG22	1:OD:161:LYS:HG3	1.97	0.45
1:D:134:THR:HG22	1:D:147:THR:HG22	1.98	0.45
1:K:116:GLU:OE2	1:K:231:LYS:NZ	2.44	0.45
1:K:134:THR:HG22	1:K:147:THR:HG22	1.98	0.45
1:TA:54:ARG:NH2	1:TA:89:THR:OG1	2.47	0.45
1:UA:125:LEU:O	1:UA:156:GLN:NE2	2.48	0.45
1:PB:116:GLU:OE2	1:PB:231:LYS:NZ	2.43	0.45
1:EC:99:ARG:NH1	1:EC:251:VAL:O	2.43	0.45
1:KC:91:VAL:O	1:KC:94:SER:OG	2.27	0.45
1:KC:112:THR:HG23	1:KC:114:GLN:H	1.81	0.45
1:NC:134:THR:HG22	1:NC:147:THR:HG22	1.98	0.45
1:QC:109:LEU:HD11	1:QC:171:LEU:HD21	1.99	0.45
1:UC:125:LEU:O	1:UC:156:GLN:NE2	2.46	0.45
1:YC:122:LEU:HD12	1:YC:175:LEU:HD11	1.98	0.45
1:AD:112:THR:HG23	1:AD:114:GLN:H	1.80	0.45
1:BD:100:LYS:NZ	1:BD:247:GLU:OE2	2.49	0.45
1:MD:25:GLN:NE2	1:MD:256:LEU:O	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3:THR:HG22	1:G:16:THR:HG22	1.99	0.45
1:J:116:GLU:OE2	1:J:231:LYS:NZ	2.48	0.45
1:N:112:THR:HG23	1:N:114:GLN:H	1.80	0.45
1:T:134:THR:HG22	1:T:147:THR:HG22	1.98	0.45
1:W:3:THR:HG22	1:W:16:THR:HG22	1.98	0.45
1:QB:186:VAL:HB	1:QB:219:VAL:HB	1.97	0.45
1:UB:152:THR:OG1	1:UB:154:ASP:OD1	2.34	0.45
1:XB:99:ARG:NH1	1:XB:251:VAL:O	2.44	0.45
1:GC:134:THR:HG22	1:GC:147:THR:HG22	1.98	0.45
1:TC:25:GLN:NE2	1:TC:256:LEU:O	2.45	0.45
1:UC:183:ALA:HA	1:UC:222:VAL:HA	1.99	0.45
1:BD:55:VAL:HB	1:BD:88:VAL:HB	1.98	0.45
1:DD:183:ALA:HA	1:DD:222:VAL:HA	1.98	0.45
1:GD:122:LEU:HD12	1:GD:175:LEU:HD11	1.98	0.45
1:KD:55:VAL:HB	1:KD:88:VAL:HB	1.97	0.45
1:ND:161:LYS:HG3	1:PD:123:VAL:HG22	1.99	0.45
1:OD:123:VAL:HG22	1:PD:161:LYS:HG3	1.97	0.45
1:B:125:LEU:O	1:B:156:GLN:NE2	2.48	0.45
1:G:91:VAL:O	1:G:94:SER:OG	2.28	0.45
1:I:13:ARG:NH2	1:I:29:GLU:OE1	2.42	0.45
1:M:197:ASP:OD1	1:M:197:ASP:N	2.48	0.45
1:Y:152:THR:OG1	1:Y:154:ASP:OD1	2.33	0.45
1:IB:125:LEU:O	1:IB:156:GLN:NE2	2.42	0.45
1:JB:197:ASP:OD1	1:JB:197:ASP:N	2.48	0.45
1:TB:55:VAL:HB	1:TB:88:VAL:HB	1.97	0.45
1:YB:116:GLU:OE2	1:YB:231:LYS:NZ	2.43	0.45
1:KC:170:ARG:HB2	1:KC:191:ASP:HB2	1.99	0.45
1:UC:55:VAL:HB	1:UC:88:VAL:HB	1.98	0.45
1:VC:123:VAL:HG22	1:WC:161:LYS:HG3	1.97	0.45
1:ZC:122:LEU:HD12	1:ZC:175:LEU:HD11	1.99	0.45
1:CD:5:VAL:HG12	1:CD:14:THR:HG22	1.97	0.45
1:JD:55:VAL:HB	1:JD:88:VAL:HB	1.98	0.45
1:MD:64:VAL:HA	1:MD:78:VAL:HA	1.98	0.45
1:F:199:SER:OG	1:F:205:GLU:O	2.34	0.45
1:N:109:LEU:HD11	1:N:171:LEU:HD21	1.98	0.45
1:Q:161:LYS:HA	1:Q:161:LYS:HD3	1.72	0.45
1:R:158:PHE:HB2	1:R:171:LEU:HB2	1.97	0.45
1:S:112:THR:HG23	1:S:114:GLN:H	1.81	0.45
1:V:170:ARG:HB2	1:V:191:ASP:HB2	1.97	0.45
1:X:154:ASP:OD1	1:X:154:ASP:N	2.45	0.45
1:GA:125:LEU:O	1:GA:156:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PA:67:CYS:HB3	1:PA:70:SER:HB3	1.98	0.45
1:HB:134:THR:HG22	1:HB:147:THR:HG22	1.99	0.45
1:TB:152:THR:OG1	1:TB:154:ASP:OD1	2.34	0.45
1:LC:199:SER:OG	1:LC:205:GLU:O	2.32	0.45
1:SC:183:ALA:HA	1:SC:222:VAL:HA	1.98	0.45
1:VC:122:LEU:HD12	1:VC:175:LEU:HD11	1.99	0.45
1:XC:122:LEU:HD12	1:XC:175:LEU:HD11	1.98	0.45
1:ZC:67:CYS:HB3	1:ZC:70:SER:HB3	1.99	0.45
1:HD:123:VAL:HG22	1:ID:161:LYS:HG3	1.99	0.45
1:LD:123:VAL:HG22	1:MD:161:LYS:HG3	1.99	0.45
1:ND:122:LEU:HD12	1:ND:175:LEU:HD11	1.98	0.45
1:G:100:LYS:NZ	1:G:247:GLU:OE2	2.49	0.45
1:O:100:LYS:NZ	1:O:247:GLU:OE2	2.46	0.45
1:Q:39:ARG:HB3	1:Q:60:ASP:HB2	1.97	0.45
1:Q:100:LYS:NZ	1:Q:247:GLU:OE2	2.46	0.45
1:ZA:161:LYS:HA	1:ZA:161:LYS:HD3	1.72	0.45
1:QB:134:THR:HG22	1:QB:147:THR:HG22	1.98	0.45
1:XB:1:SER:OG	1:XB:2:LYS:N	2.44	0.45
1:FC:197:ASP:N	1:FC:197:ASP:OD1	2.50	0.45
1:TC:125:LEU:O	1:TC:156:GLN:NE2	2.47	0.45
1:CD:123:VAL:HG22	1:DD:161:LYS:HG3	1.99	0.45
1:ID:183:ALA:HA	1:ID:222:VAL:HA	1.98	0.45
1:JD:183:ALA:HA	1:JD:222:VAL:HA	1.99	0.45
1:KD:161:LYS:O	1:KD:168:ARG:NH2	2.49	0.45
1:MD:55:VAL:HB	1:MD:88:VAL:HB	1.97	0.45
1:B:109:LEU:HD11	1:B:171:LEU:HD21	1.98	0.45
1:Y:112:THR:HG23	1:Y:114:GLN:H	1.81	0.45
1:BA:134:THR:HG22	1:BA:147:THR:HG22	1.99	0.45
1:MA:66:ASP:HB2	1:MA:76:PRO:HB3	1.99	0.45
1:QA:186:VAL:HB	1:QA:219:VAL:HB	1.98	0.45
1:UA:154:ASP:OD2	1:UA:154:ASP:N	2.44	0.45
1:WA:197:ASP:OD1	1:WA:197:ASP:N	2.50	0.45
1:ZA:27:PHE:HB2	1:ZA:40:LEU:HB3	1.99	0.45
1:ZA:112:THR:HG23	1:ZA:114:GLN:H	1.81	0.45
1:NB:116:GLU:OE2	1:NB:231:LYS:NZ	2.43	0.45
1:XB:186:VAL:HB	1:XB:219:VAL:HB	1.97	0.45
1:KC:125:LEU:O	1:KC:156:GLN:NE2	2.49	0.45
1:SC:98:SER:OG	1:SC:213:GLN:OE1	2.35	0.45
1:MD:125:LEU:O	1:MD:156:GLN:NE2	2.47	0.45
1:F:54:ARG:NH2	1:F:89:THR:OG1	2.47	0.45
1:G:112:THR:HG23	1:G:114:GLN:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3:THR:HG22	1:J:16:THR:HG22	1.98	0.45
1:N:154:ASP:OD2	1:N:154:ASP:N	2.44	0.45
1:V:54:ARG:NH2	1:V:89:THR:OG1	2.43	0.45
1:AA:161:LYS:O	1:AA:168:ARG:NH2	2.50	0.45
1:GA:197:ASP:OD1	1:GA:197:ASP:N	2.50	0.45
1:JA:112:THR:HG23	1:JA:114:GLN:H	1.81	0.45
1:MA:3:THR:HG22	1:MA:16:THR:HG22	1.99	0.45
1:MA:39:ARG:HB3	1:MA:60:ASP:HB2	1.98	0.45
1:SA:27:PHE:HB2	1:SA:40:LEU:HB3	1.99	0.45
1:UA:109:LEU:HD11	1:UA:171:LEU:HD21	1.99	0.45
1:KB:109:LEU:HD11	1:KB:171:LEU:HD21	1.99	0.45
1:FC:27:PHE:HB2	1:FC:40:LEU:HB3	1.99	0.45
1:OC:27:PHE:HB2	1:OC:40:LEU:HB3	1.99	0.45
1:OC:112:THR:HG23	1:OC:114:GLN:H	1.82	0.45
1:YC:197:ASP:HB3	1:YC:207:PRO:HG3	1.98	0.45
1:BD:91:VAL:O	1:BD:94:SER:OG	2.32	0.45
1:ID:100:LYS:NZ	1:ID:247:GLU:OE2	2.49	0.45
1:LD:5:VAL:HG12	1:LD:14:THR:HG22	1.97	0.45
1:A:161:LYS:HA	1:A:161:LYS:HD3	1.73	0.45
1:M:54:ARG:NH2	1:M:89:THR:OG1	2.47	0.45
1:M:158:PHE:HB2	1:M:171:LEU:HB2	1.97	0.45
1:R:109:LEU:HD11	1:R:171:LEU:HD21	1.99	0.45
1:JA:23:ASP:OD2	1:JA:23:ASP:N	2.48	0.45
1:FB:67:CYS:HB3	1:FB:70:SER:HB3	1.98	0.45
1:LC:170:ARG:HB2	1:LC:191:ASP:HB2	1.98	0.45
1:TC:55:VAL:HB	1:TC:88:VAL:HB	1.98	0.45
1:TC:183:ALA:HA	1:TC:222:VAL:HA	1.98	0.45
1:VC:112:THR:HG23	1:VC:114:GLN:H	1.82	0.45
1:BD:183:ALA:HA	1:BD:222:VAL:HA	1.99	0.45
1:CD:98:SER:OG	1:CD:213:GLN:OE1	2.35	0.45
1:DD:100:LYS:NZ	1:DD:247:GLU:OE2	2.50	0.45
1:ED:161:LYS:HG3	1:GD:123:VAL:HG22	1.99	0.45
1:JD:54:ARG:NH2	1:JD:89:THR:OG1	2.45	0.45
1:C:27:PHE:HB2	1:C:40:LEU:HB3	1.99	0.45
1:L:27:PHE:HB2	1:L:40:LEU:HB3	1.99	0.45
1:CA:27:PHE:HB2	1:CA:40:LEU:HB3	1.99	0.45
1:JA:1:SER:OG	1:JA:2:LYS:N	2.42	0.45
1:JA:27:PHE:HB2	1:JA:40:LEU:HB3	1.99	0.45
1:SA:222:VAL:O	1:SA:225:SER:OG	2.31	0.45
1:WA:222:VAL:O	1:WA:225:SER:OG	2.31	0.45
1:BB:67:CYS:HB3	1:BB:70:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KB:154:ASP:OD2	1:KB:154:ASP:N	2.45	0.45
1:SB:161:LYS:O	1:SB:168:ARG:NH2	2.50	0.45
1:IC:66:ASP:HB2	1:IC:76:PRO:HB3	1.99	0.45
1:BD:123:VAL:HG22	1:CD:161:LYS:HG3	1.99	0.45
1:ED:123:VAL:HG22	1:FD:161:LYS:HG3	1.99	0.45
1:HD:161:LYS:HG3	1:JD:123:VAL:HG22	1.99	0.45
1:E:67:CYS:HB3	1:E:70:SER:HB3	1.98	0.44
1:G:122:LEU:HD12	1:G:175:LEU:HD11	1.99	0.44
1:S:27:PHE:HB2	1:S:40:LEU:HB3	1.99	0.44
1:Z:67:CYS:HB3	1:Z:70:SER:HB3	1.99	0.44
1:TA:197:ASP:OD1	1:TA:197:ASP:N	2.49	0.44
1:ZA:23:ASP:OD2	1:ZA:23:ASP:N	2.48	0.44
1:AB:91:VAL:O	1:AB:94:SER:OG	2.30	0.44
1:AB:134:THR:HG22	1:AB:147:THR:HG22	1.98	0.44
1:CB:66:ASP:HB2	1:CB:76:PRO:HB3	2.00	0.44
1:EB:170:ARG:HB2	1:EB:191:ASP:HB2	1.99	0.44
1:HB:100:LYS:NZ	1:HB:247:GLU:OE2	2.44	0.44
1:MB:158:PHE:HB2	1:MB:171:LEU:HB2	1.99	0.44
1:FC:112:THR:HG23	1:FC:114:GLN:H	1.83	0.44
1:LC:222:VAL:O	1:LC:225:SER:OG	2.30	0.44
1:MC:161:LYS:O	1:MC:168:ARG:NH2	2.50	0.44
1:PC:222:VAL:O	1:PC:225:SER:OG	2.31	0.44
1:UC:98:SER:OG	1:UC:213:GLN:OE1	2.35	0.44
1:FD:122:LEU:HD12	1:FD:175:LEU:HD11	1.99	0.44
1:KD:98:SER:OG	1:KD:213:GLN:OE1	2.35	0.44
1:B:154:ASP:OD1	1:B:154:ASP:N	2.49	0.44
1:F:55:VAL:HB	1:F:88:VAL:HB	2.00	0.44
1:I:54:ARG:NH2	1:I:89:THR:OG1	2.42	0.44
1:R:99:ARG:NH1	1:R:251:VAL:O	2.43	0.44
1:LA:67:CYS:HB3	1:LA:70:SER:HB3	1.99	0.44
1:CB:199:SER:OG	1:CB:205:GLU:O	2.35	0.44
1:RB:67:CYS:HB3	1:RB:70:SER:HB3	1.99	0.44
1:SB:55:VAL:HB	1:SB:88:VAL:HB	1.99	0.44
1:IC:197:ASP:HB3	1:IC:207:PRO:HG3	1.99	0.44
1:JC:54:ARG:NH2	1:JC:89:THR:OG1	2.44	0.44
1:LC:91:VAL:O	1:LC:94:SER:OG	2.31	0.44
1:SC:123:VAL:HG22	1:TC:161:LYS:HG3	1.99	0.44
1:SC:125:LEU:O	1:SC:156:GLN:NE2	2.46	0.44
1:TC:100:LYS:NZ	1:TC:247:GLU:OE2	2.49	0.44
1:UC:25:GLN:NE2	1:UC:256:LEU:O	2.44	0.44
1:LD:64:VAL:HA	1:LD:78:VAL:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:158:PHE:HB2	1:N:171:LEU:HB2	1.97	0.44
1:P:54:ARG:NH2	1:P:89:THR:OG1	2.47	0.44
1:X:122:LEU:HD12	1:X:175:LEU:HD11	2.00	0.44
1:Y:122:LEU:HD12	1:Y:175:LEU:HD11	1.99	0.44
1:AA:54:ARG:NH2	1:AA:89:THR:OG1	2.47	0.44
1:AA:55:VAL:HB	1:AA:88:VAL:HB	2.00	0.44
1:FA:116:GLU:OE2	1:FA:231:LYS:NZ	2.42	0.44
1:KA:134:THR:HG22	1:KA:147:THR:HG22	1.98	0.44
1:NA:170:ARG:HB2	1:NA:191:ASP:HB2	1.99	0.44
1:SA:112:THR:HG23	1:SA:114:GLN:H	1.82	0.44
1:YA:109:LEU:HD11	1:YA:171:LEU:HD21	1.98	0.44
1:CB:186:VAL:HB	1:CB:219:VAL:HB	1.98	0.44
1:HB:116:GLU:OE2	1:HB:231:LYS:NZ	2.44	0.44
1:NB:125:LEU:O	1:NB:156:GLN:NE2	2.50	0.44
1:NB:161:LYS:HA	1:NB:161:LYS:HD3	1.72	0.44
1:UB:170:ARG:HB2	1:UB:191:ASP:HB2	1.98	0.44
1:VB:67:CYS:HB3	1:VB:70:SER:HB3	1.99	0.44
1:EC:125:LEU:O	1:EC:156:GLN:NE2	2.48	0.44
1:BD:54:ARG:NH2	1:BD:89:THR:OG1	2.46	0.44
1:CD:183:ALA:HA	1:CD:222:VAL:HA	1.98	0.44
1:JD:98:SER:OG	1:JD:213:GLN:OE1	2.35	0.44
1:JD:125:LEU:O	1:JD:156:GLN:NE2	2.46	0.44
1:KD:123:VAL:HG22	1:LD:161:LYS:HG3	1.99	0.44
1:H:125:LEU:O	1:H:156:GLN:NE2	2.47	0.44
1:R:154:ASP:OD1	1:R:154:ASP:N	2.49	0.44
1:S:128:ALA:HB2	1:S:133:LYS:HG2	1.98	0.44
1:V:67:CYS:HB3	1:V:70:SER:HB3	1.98	0.44
1:Z:91:VAL:O	1:Z:94:SER:OG	2.31	0.44
1:EA:109:LEU:HD11	1:EA:171:LEU:HD21	1.98	0.44
1:RA:100:LYS:NZ	1:RA:247:GLU:OE2	2.44	0.44
1:CB:116:GLU:OE2	1:CB:231:LYS:NZ	2.48	0.44
1:JB:54:ARG:NH2	1:JB:89:THR:OG1	2.47	0.44
1:XB:134:THR:HG22	1:XB:147:THR:HG22	1.99	0.44
1:ZB:100:LYS:NZ	1:ZB:247:GLU:OE2	2.46	0.44
1:ZB:158:PHE:HB2	1:ZB:171:LEU:HB2	2.00	0.44
1:CC:222:VAL:O	1:CC:225:SER:OG	2.31	0.44
1:GC:100:LYS:NZ	1:GC:247:GLU:OE2	2.44	0.44
1:HC:222:VAL:O	1:HC:225:SER:OG	2.31	0.44
1:QC:125:LEU:O	1:QC:156:GLN:NE2	2.48	0.44
1:TC:123:VAL:HG22	1:UC:161:LYS:HG3	1.99	0.44
1:ZC:55:VAL:HB	1:ZC:88:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:125:LEU:O	1:BD:156:GLN:NE2	2.47	0.44
1:E:91:VAL:O	1:E:94:SER:OG	2.31	0.44
1:G:125:LEU:O	1:G:156:GLN:NE2	2.47	0.44
1:Y:125:LEU:O	1:Y:156:GLN:NE2	2.47	0.44
1:KA:91:VAL:O	1:KA:94:SER:OG	2.30	0.44
1:OA:54:ARG:NH2	1:OA:89:THR:OG1	2.44	0.44
1:WA:125:LEU:O	1:WA:156:GLN:NE2	2.51	0.44
1:IB:27:PHE:HB2	1:IB:40:LEU:HB3	1.99	0.44
1:KC:54:ARG:NH2	1:KC:89:THR:OG1	2.44	0.44
1:DD:222:VAL:O	1:DD:225:SER:OG	2.30	0.44
1:ED:100:LYS:NZ	1:ED:247:GLU:OE2	2.45	0.44
1:MD:98:SER:OG	1:MD:213:GLN:OE1	2.35	0.44
1:MD:183:ALA:HA	1:MD:222:VAL:HA	1.99	0.44
1:ZA:1:SER:OG	1:ZA:2:LYS:N	2.42	0.44
1:WB:66:ASP:HB2	1:WB:76:PRO:HB3	1.99	0.44
1:BC:116:GLU:OE2	1:BC:231:LYS:NZ	2.43	0.44
1:RC:154:ASP:OD2	1:RC:154:ASP:N	2.51	0.44
1:VC:161:LYS:HG3	1:XC:123:VAL:HG22	1.99	0.44
1:YC:54:ARG:NH2	1:YC:89:THR:OG1	2.46	0.44
1:CD:64:VAL:HA	1:CD:78:VAL:HA	1.98	0.44
1:CD:100:LYS:NZ	1:CD:247:GLU:OE2	2.49	0.44
1:DD:112:THR:HG23	1:DD:114:GLN:H	1.82	0.44
1:KD:25:GLN:NE2	1:KD:256:LEU:O	2.45	0.44
1:C:197:ASP:N	1:C:197:ASP:OD1	2.50	0.44
1:D:184:TYR:N	1:D:221:ILE:O	2.47	0.44
1:H:199:SER:OG	1:H:205:GLU:O	2.34	0.44
1:DA:125:LEU:O	1:DA:156:GLN:NE2	2.49	0.44
1:JA:161:LYS:HA	1:JA:161:LYS:HD3	1.72	0.44
1:RA:91:VAL:O	1:RA:94:SER:OG	2.30	0.44
1:GB:186:VAL:HB	1:GB:219:VAL:HB	1.99	0.44
1:SB:66:ASP:HB2	1:SB:76:PRO:HB3	2.00	0.44
1:SB:199:SER:OG	1:SB:205:GLU:O	2.35	0.44
1:TB:170:ARG:HB2	1:TB:191:ASP:HB2	1.99	0.44
1:YB:112:THR:HG23	1:YB:114:GLN:H	1.82	0.44
1:JC:3:THR:HG22	1:JC:16:THR:HG22	2.00	0.44
1:JC:122:LEU:HD12	1:JC:175:LEU:HD11	1.99	0.44
1:RC:104:ASP:HB3	1:RC:139:VAL:HG13	2.00	0.44
1:VC:54:ARG:NH2	1:VC:89:THR:OG1	2.46	0.44
1:VC:55:VAL:HB	1:VC:88:VAL:HB	1.99	0.44
1:WC:122:LEU:HD12	1:WC:175:LEU:HD11	1.98	0.44
1:HD:199:SER:OG	1:HD:205:GLU:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ID:98:SER:OG	1:ID:213:GLN:OE1	2.36	0.44
1:ID:222:VAL:O	1:ID:225:SER:OG	2.30	0.44
1:G:152:THR:OG1	1:G:154:ASP:OD1	2.34	0.44
1:L:125:LEU:O	1:L:156:GLN:NE2	2.43	0.44
1:O:104:ASP:HB3	1:O:139:VAL:HG13	1.99	0.44
1:BA:184:TYR:N	1:BA:221:ILE:O	2.47	0.44
1:IA:161:LYS:HD3	1:IA:161:LYS:HA	1.74	0.44
1:JA:222:VAL:O	1:JA:225:SER:OG	2.32	0.44
1:RA:116:GLU:OE2	1:RA:231:LYS:NZ	2.44	0.44
1:WA:158:PHE:HB2	1:WA:171:LEU:HB2	2.00	0.44
1:HB:91:VAL:O	1:HB:94:SER:OG	2.30	0.44
1:IB:112:THR:HG23	1:IB:114:GLN:H	1.83	0.44
1:NB:154:ASP:OD1	1:NB:154:ASP:N	2.51	0.44
1:BC:154:ASP:OD2	1:BC:154:ASP:N	2.51	0.44
1:DC:154:ASP:OD1	1:DC:154:ASP:N	2.51	0.44
1:TC:98:SER:OG	1:TC:213:GLN:OE1	2.35	0.44
1:UC:100:LYS:NZ	1:UC:247:GLU:OE2	2.49	0.44
1:YC:123:VAL:HG22	1:ZC:161:LYS:HG3	1.99	0.44
1:FD:54:ARG:NH2	1:FD:89:THR:OG1	2.46	0.44
1:HD:125:LEU:O	1:HD:156:GLN:NE2	2.48	0.44
1:L:161:LYS:HA	1:L:161:LYS:HD3	1.72	0.44
1:P:197:ASP:OD1	1:P:197:ASP:N	2.50	0.44
1:W:66:ASP:HB2	1:W:76:PRO:HB3	1.99	0.44
1:GA:116:GLU:OE2	1:GA:231:LYS:NZ	2.48	0.44
1:HA:154:ASP:OD2	1:HA:154:ASP:N	2.51	0.44
1:YB:27:PHE:HB2	1:YB:40:LEU:HB3	1.99	0.44
1:YB:161:LYS:HA	1:YB:161:LYS:HD3	1.73	0.44
1:NC:100:LYS:NZ	1:NC:247:GLU:OE2	2.44	0.44
1:RC:116:GLU:OE2	1:RC:231:LYS:NZ	2.42	0.44
1:WC:55:VAL:HB	1:WC:88:VAL:HB	1.99	0.44
1:GD:55:VAL:HB	1:GD:88:VAL:HB	2.00	0.44
1:ID:123:VAL:HG22	1:JD:161:LYS:HG3	1.99	0.44
1:LD:98:SER:OG	1:LD:213:GLN:OE1	2.36	0.44
1:L:112:THR:HG23	1:L:114:GLN:H	1.83	0.43
1:O:154:ASP:OD2	1:O:154:ASP:N	2.51	0.43
1:W:199:SER:OG	1:W:205:GLU:O	2.35	0.43
1:GA:158:PHE:HB2	1:GA:171:LEU:HB2	2.00	0.43
1:BB:91:VAL:O	1:BB:94:SER:OG	2.31	0.43
1:EB:54:ARG:NH2	1:EB:89:THR:OG1	2.44	0.43
1:IB:161:LYS:HD3	1:IB:161:LYS:HA	1.72	0.43
1:PB:27:PHE:HB2	1:PB:40:LEU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PB:112:THR:HG23	1:PB:114:GLN:H	1.82	0.43
1:WB:55:VAL:HB	1:WB:88:VAL:HB	2.00	0.43
1:MC:66:ASP:HB2	1:MC:76:PRO:HB3	2.00	0.43
1:FD:158:PHE:HB2	1:FD:171:LEU:HB3	2.00	0.43
1:PD:122:LEU:HD12	1:PD:175:LEU:HD11	1.99	0.43
1:D:91:VAL:O	1:D:94:SER:OG	2.30	0.43
1:N:161:LYS:HA	1:N:161:LYS:HD3	1.74	0.43
1:P:109:LEU:HD11	1:P:171:LEU:HD21	2.00	0.43
1:Q:154:ASP:OD2	1:Q:154:ASP:N	2.51	0.43
1:T:100:LYS:NZ	1:T:247:GLU:OE2	2.44	0.43
1:OA:3:THR:HG22	1:OA:16:THR:HG22	2.00	0.43
1:XA:154:ASP:OD1	1:XA:154:ASP:N	2.51	0.43
1:QB:91:VAL:O	1:QB:94:SER:OG	2.30	0.43
1:BC:54:ARG:HH21	1:BC:89:THR:HG1	1.64	0.43
1:IC:186:VAL:HB	1:IC:219:VAL:HB	1.99	0.43
1:JC:170:ARG:HB2	1:JC:191:ASP:HB2	1.99	0.43
1:KC:3:THR:HG22	1:KC:16:THR:HG22	2.00	0.43
1:LC:67:CYS:HB3	1:LC:70:SER:HB3	1.99	0.43
1:PC:158:PHE:HB2	1:PC:171:LEU:HB2	2.00	0.43
1:KD:100:LYS:NZ	1:KD:247:GLU:OE2	2.49	0.43
1:H:122:LEU:HD12	1:H:175:LEU:HD11	2.01	0.43
1:K:100:LYS:NZ	1:K:247:GLU:OE2	2.44	0.43
1:X:125:LEU:O	1:X:156:GLN:NE2	2.47	0.43
1:LA:55:VAL:HB	1:LA:88:VAL:HB	2.00	0.43
1:NA:125:LEU:O	1:NA:156:GLN:NE2	2.47	0.43
1:DC:116:GLU:OE2	1:DC:231:LYS:NZ	2.43	0.43
1:DC:161:LYS:HA	1:DC:161:LYS:HD3	1.72	0.43
1:HC:67:CYS:HB3	1:HC:70:SER:HB3	1.99	0.43
1:OC:128:ALA:HB2	1:OC:133:LYS:HG2	1.99	0.43
1:UC:54:ARG:NH2	1:UC:89:THR:OG1	2.46	0.43
1:XC:100:LYS:NZ	1:XC:247:GLU:OE2	2.45	0.43
1:ND:100:LYS:NZ	1:ND:247:GLU:OE2	2.46	0.43
1:E:159:GLU:OE1	1:E:170:ARG:NE	2.45	0.43
1:I:55:VAL:HB	1:I:88:VAL:HB	2.00	0.43
1:J:41:THR:O	1:J:41:THR:OG1	2.33	0.43
1:M:116:GLU:OE2	1:M:231:LYS:NZ	2.48	0.43
1:UB:122:LEU:HD12	1:UB:175:LEU:HD11	1.99	0.43
1:XB:161:LYS:HD3	1:XB:161:LYS:HA	1.85	0.43
1:BC:161:LYS:HA	1:BC:161:LYS:HD3	1.72	0.43
1:CC:158:PHE:HB2	1:CC:171:LEU:HB2	2.00	0.43
1:FD:100:LYS:NZ	1:FD:247:GLU:OE2	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HD:150:GLN:NE2	1:HD:152:THR:OG1	2.42	0.43
1:MD:100:LYS:NZ	1:MD:247:GLU:OE2	2.50	0.43
1:M:99:ARG:NH1	1:M:251:VAL:O	2.51	0.43
1:Z:55:VAL:HB	1:Z:88:VAL:HB	2.01	0.43
1:IA:109:LEU:HD11	1:IA:171:LEU:HD21	1.99	0.43
1:PA:222:VAL:O	1:PA:225:SER:OG	2.30	0.43
1:QA:66:ASP:HB2	1:QA:76:PRO:HB3	2.00	0.43
1:TB:3:THR:HG22	1:TB:16:THR:HG22	2.00	0.43
1:IC:55:VAL:HB	1:IC:88:VAL:HB	2.00	0.43
1:IC:102:LEU:HD22	1:IC:213:GLN:HB3	2.01	0.43
1:IC:199:SER:OG	1:IC:205:GLU:O	2.35	0.43
1:RC:161:LYS:HA	1:RC:161:LYS:HD3	1.72	0.43
1:SC:199:SER:OG	1:SC:205:GLU:O	2.36	0.43
1:AD:100:LYS:NZ	1:AD:247:GLU:OE2	2.45	0.43
1:BD:98:SER:OG	1:BD:213:GLN:OE1	2.36	0.43
1:HD:183:ALA:HA	1:HD:222:VAL:HA	1.99	0.43
1:KD:64:VAL:HA	1:KD:78:VAL:HA	2.00	0.43
1:ND:55:VAL:HB	1:ND:88:VAL:HB	2.00	0.43
1:K:39:ARG:HB3	1:K:60:ASP:HB2	2.01	0.43
1:O:116:GLU:OE2	1:O:231:LYS:NZ	2.42	0.43
1:P:158:PHE:HB2	1:P:171:LEU:HB2	2.00	0.43
1:W:55:VAL:HB	1:W:88:VAL:HB	2.00	0.43
1:Z:159:GLU:OE1	1:Z:170:ARG:NE	2.45	0.43
1:PB:161:LYS:HA	1:PB:161:LYS:HD3	1.73	0.43
1:TB:122:LEU:HD12	1:TB:175:LEU:HD11	1.99	0.43
1:WB:154:ASP:OD1	1:WB:154:ASP:N	2.46	0.43
1:CC:99:ARG:NH1	1:CC:251:VAL:O	2.51	0.43
1:OC:39:ARG:HB3	1:OC:60:ASP:HB2	2.01	0.43
1:SC:161:LYS:HG3	1:UC:123:VAL:HG22	1.99	0.43
1:TC:54:ARG:NH2	1:TC:89:THR:OG1	2.46	0.43
1:XC:54:ARG:NH2	1:XC:89:THR:OG1	2.47	0.43
1:AD:55:VAL:HB	1:AD:88:VAL:HB	2.00	0.43
1:ID:125:LEU:O	1:ID:156:GLN:NE2	2.47	0.43
1:ND:54:ARG:NH2	1:ND:89:THR:OG1	2.46	0.43
1:E:55:VAL:HB	1:E:88:VAL:HB	2.01	0.43
1:P:99:ARG:NH1	1:P:251:VAL:O	2.52	0.43
1:Q:116:GLU:OE2	1:Q:231:LYS:NZ	2.43	0.43
1:S:161:LYS:HA	1:S:161:LYS:HD3	1.72	0.43
1:X:199:SER:OG	1:X:205:GLU:O	2.34	0.43
1:SA:128:ALA:HB2	1:SA:133:LYS:HG2	2.00	0.43
1:VA:54:ARG:NH2	1:VA:89:THR:OG1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:55:VAL:HB	1:GB:88:VAL:HB	2.00	0.43
1:MB:99:ARG:NH1	1:MB:251:VAL:O	2.52	0.43
1:AC:99:ARG:NH1	1:AC:251:VAL:O	2.43	0.43
1:ED:55:VAL:HB	1:ED:88:VAL:HB	2.00	0.43
1:KD:150:GLN:NE2	1:KD:152:THR:OG1	2.43	0.43
1:OD:55:VAL:HB	1:OD:88:VAL:HB	2.00	0.43
1:I:67:CYS:HB3	1:I:70:SER:HB3	1.99	0.43
1:P:116:GLU:OE2	1:P:231:LYS:NZ	2.48	0.43
1:Y:3:THR:HG22	1:Y:16:THR:HG22	2.01	0.43
1:CA:23:ASP:OD2	1:CA:23:ASP:N	2.48	0.43
1:OA:122:LEU:HD12	1:OA:175:LEU:HD11	1.99	0.43
1:CB:54:ARG:NH2	1:CB:89:THR:OG1	2.47	0.43
1:EB:125:LEU:O	1:EB:156:GLN:NE2	2.47	0.43
1:GB:66:ASP:HB2	1:GB:76:PRO:HB3	2.00	0.43
1:MB:109:LEU:HD11	1:MB:171:LEU:HD21	2.00	0.43
1:NB:54:ARG:HH21	1:NB:89:THR:HG1	1.64	0.43
1:BC:104:ASP:HB3	1:BC:139:VAL:HG13	2.00	0.43
1:MC:55:VAL:HB	1:MC:88:VAL:HB	2.01	0.43
1:SC:64:VAL:HA	1:SC:78:VAL:HA	2.01	0.43
1:SC:112:THR:HG23	1:SC:114:GLN:H	1.83	0.43
1:TC:112:THR:HG23	1:TC:114:GLN:H	1.83	0.43
1:ID:158:PHE:HB2	1:ID:171:LEU:HB3	2.01	0.43
1:JD:112:THR:HG23	1:JD:114:GLN:H	1.84	0.43
1:MD:112:THR:HG23	1:MD:114:GLN:H	1.83	0.43
1:C:128:ALA:HB2	1:C:133:LYS:HG2	1.99	0.43
1:F:66:ASP:HB2	1:F:76:PRO:HB3	1.99	0.43
1:J:55:VAL:HB	1:J:88:VAL:HB	2.00	0.43
1:IA:99:ARG:NH1	1:IA:251:VAL:O	2.43	0.43
1:ZA:128:ALA:HB2	1:ZA:133:LYS:HG2	2.00	0.43
1:AB:39:ARG:HB3	1:AB:60:ASP:HB2	2.01	0.43
1:DB:54:ARG:NH2	1:DB:89:THR:OG1	2.44	0.43
1:MB:100:LYS:NZ	1:MB:247:GLU:OE2	2.48	0.43
1:SB:154:ASP:OD1	1:SB:154:ASP:N	2.46	0.43
1:YB:23:ASP:OD2	1:YB:23:ASP:N	2.48	0.43
1:GC:161:LYS:HD3	1:GC:161:LYS:HA	1.86	0.43
1:UC:66:ASP:HB2	1:UC:76:PRO:HB3	2.00	0.43
1:XC:55:VAL:HB	1:XC:88:VAL:HB	2.00	0.43
1:BD:161:LYS:HG3	1:DD:123:VAL:HG22	1.99	0.43
1:CD:58:LYS:NZ	1:CD:60:ASP:OD1	2.52	0.43
1:HD:58:LYS:NZ	1:HD:60:ASP:OD1	2.52	0.43
1:OD:54:ARG:NH2	1:OD:89:THR:OG1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:134:THR:HG22	1:S:147:THR:HG22	2.01	0.43
1:T:39:ARG:HB3	1:T:60:ASP:HB2	2.01	0.43
1:X:68:SER:OG	1:X:74:GLU:O	2.32	0.43
1:BA:91:VAL:O	1:BA:94:SER:OG	2.31	0.43
1:KA:101:SER:OG	1:KA:192:GLN:NE2	2.42	0.43
1:MA:54:ARG:NH2	1:MA:89:THR:OG1	2.47	0.43
1:MA:55:VAL:HB	1:MA:88:VAL:HB	2.00	0.43
1:MA:83:VAL:HG22	1:MA:220:THR:HB	2.01	0.43
1:WA:109:LEU:HD11	1:WA:171:LEU:HD21	2.00	0.43
1:FB:54:ARG:NH2	1:FB:89:THR:OG1	2.43	0.43
1:JB:125:LEU:O	1:JB:156:GLN:NE2	2.51	0.43
1:LB:54:ARG:NH2	1:LB:89:THR:OG1	2.46	0.43
1:OB:99:ARG:NH1	1:OB:251:VAL:O	2.44	0.43
1:UB:100:LYS:NZ	1:UB:247:GLU:OE2	2.48	0.43
1:ZB:109:LEU:HD11	1:ZB:171:LEU:HD21	2.00	0.43
1:PC:109:LEU:HD11	1:PC:171:LEU:HD21	2.00	0.43
1:UC:112:THR:HG23	1:UC:114:GLN:H	1.83	0.43
1:YC:100:LYS:NZ	1:YC:247:GLU:OE2	2.45	0.43
1:DD:58:LYS:NZ	1:DD:60:ASP:OD1	2.52	0.43
1:ED:158:PHE:HB2	1:ED:171:LEU:HB3	2.00	0.43
1:FD:55:VAL:HB	1:FD:88:VAL:HB	2.00	0.43
1:KD:199:SER:OG	1:KD:205:GLU:O	2.37	0.43
1:LD:54:ARG:NH2	1:LD:89:THR:OG1	2.45	0.43
1:MD:54:ARG:NH2	1:MD:89:THR:OG1	2.46	0.43
1:C:23:ASP:OD2	1:C:23:ASP:N	2.48	0.42
1:J:54:ARG:NH2	1:J:89:THR:OG1	2.46	0.42
1:DA:99:ARG:NH1	1:DA:251:VAL:O	2.51	0.42
1:FA:54:ARG:NH2	1:FA:89:THR:OG1	2.46	0.42
1:FA:104:ASP:HB3	1:FA:139:VAL:HG13	2.00	0.42
1:KA:39:ARG:HB3	1:KA:60:ASP:HB2	2.01	0.42
1:MA:186:VAL:HB	1:MA:219:VAL:HB	2.00	0.42
1:PA:159:GLU:OE1	1:PA:170:ARG:NE	2.45	0.42
1:QA:55:VAL:HB	1:QA:88:VAL:HB	2.00	0.42
1:VA:116:GLU:OE2	1:VA:231:LYS:NZ	2.43	0.42
1:EB:89:THR:HB	1:EB:214:VAL:HG22	2.01	0.42
1:LB:116:GLU:OE2	1:LB:231:LYS:NZ	2.43	0.42
1:YC:55:VAL:HB	1:YC:88:VAL:HB	2.00	0.42
1:HD:100:LYS:NZ	1:HD:247:GLU:OE2	2.50	0.42
1:JD:66:ASP:HB2	1:JD:76:PRO:HB3	2.01	0.42
1:KD:158:PHE:HB2	1:KD:171:LEU:HB3	2.01	0.42
1:PD:55:VAL:HB	1:PD:88:VAL:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LEU:O	1:B:243:THR:OG1	2.36	0.42
1:J:66:ASP:HB2	1:J:76:PRO:HB3	1.99	0.42
1:K:157:ILE:HG12	1:K:172:THR:HG22	2.01	0.42
1:M:100:LYS:NZ	1:M:247:GLU:OE2	2.47	0.42
1:P:100:LYS:NZ	1:P:247:GLU:OE2	2.47	0.42
1:P:125:LEU:O	1:P:156:GLN:NE2	2.50	0.42
1:BA:80:TYR:HB2	1:BA:222:VAL:HG21	2.02	0.42
1:GA:109:LEU:HD11	1:GA:171:LEU:HD21	2.00	0.42
1:RA:184:TYR:N	1:RA:221:ILE:O	2.47	0.42
1:ZA:184:TYR:N	1:ZA:221:ILE:O	2.47	0.42
1:BB:55:VAL:HB	1:BB:88:VAL:HB	2.01	0.42
1:FB:159:GLU:OE1	1:FB:170:ARG:NE	2.45	0.42
1:QB:161:LYS:HD3	1:QB:161:LYS:HA	1.87	0.42
1:UB:3:THR:HG22	1:UB:16:THR:HG22	2.00	0.42
1:HC:186:VAL:HB	1:HC:219:VAL:HB	2.01	0.42
1:JC:89:THR:HB	1:JC:214:VAL:HG22	2.02	0.42
1:TC:58:LYS:NZ	1:TC:60:ASP:OD1	2.51	0.42
1:UC:150:GLN:NE2	1:UC:152:THR:OG1	2.43	0.42
1:UC:158:PHE:HB2	1:UC:171:LEU:HB3	2.01	0.42
1:XC:222:VAL:HG23	1:XC:225:SER:HB3	2.01	0.42
1:ZC:100:LYS:NZ	1:ZC:247:GLU:OE2	2.46	0.42
1:CD:112:THR:HG23	1:CD:114:GLN:H	1.85	0.42
1:KD:58:LYS:NZ	1:KD:60:ASP:OD1	2.52	0.42
1:A:54:ARG:NH2	1:A:89:THR:OG1	2.46	0.42
1:D:80:TYR:HB2	1:D:222:VAL:HG21	2.02	0.42
1:F:102:LEU:HD22	1:F:213:GLN:HB3	2.01	0.42
1:H:3:THR:HG22	1:H:16:THR:HG22	2.00	0.42
1:K:104:ASP:HB3	1:K:139:VAL:HG13	2.01	0.42
1:L:172:THR:O	1:L:172:THR:OG1	2.36	0.42
1:L:222:VAL:O	1:L:225:SER:OG	2.32	0.42
1:R:161:LYS:HA	1:R:161:LYS:HD3	1.75	0.42
1:T:80:TYR:HB2	1:T:222:VAL:HG21	2.02	0.42
1:X:3:THR:HG22	1:X:16:THR:HG22	2.00	0.42
1:DA:158:PHE:HB2	1:DA:171:LEU:HB2	2.00	0.42
1:OA:125:LEU:O	1:OA:156:GLN:NE2	2.47	0.42
1:PA:112:THR:HG23	1:PA:114:GLN:H	1.84	0.42
1:RA:80:TYR:HB2	1:RA:222:VAL:HG21	2.01	0.42
1:WA:116:GLU:OE2	1:WA:231:LYS:NZ	2.50	0.42
1:EB:122:LEU:HD12	1:EB:175:LEU:HD11	1.99	0.42
1:JB:99:ARG:NH1	1:JB:251:VAL:O	2.52	0.42
1:PB:134:THR:HG22	1:PB:147:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TB:199:SER:OG	1:TB:205:GLU:O	2.34	0.42
1:CC:109:LEU:HD11	1:CC:171:LEU:HD21	2.00	0.42
1:KC:89:THR:HB	1:KC:214:VAL:HG22	2.02	0.42
1:LC:55:VAL:HB	1:LC:88:VAL:HB	2.01	0.42
1:OC:134:THR:HG22	1:OC:147:THR:HG22	2.01	0.42
1:PC:99:ARG:NH1	1:PC:251:VAL:O	2.51	0.42
1:HD:112:THR:HG23	1:HD:114:GLN:H	1.85	0.42
1:L:134:THR:HG22	1:L:147:THR:HG22	2.02	0.42
1:LA:172:THR:O	1:LA:172:THR:OG1	2.37	0.42
1:MA:199:SER:OG	1:MA:205:GLU:O	2.36	0.42
1:NA:54:ARG:NH2	1:NA:89:THR:OG1	2.44	0.42
1:PA:58:LYS:NZ	1:PA:60:ASP:OD1	2.49	0.42
1:PA:199:SER:OG	1:PA:205:GLU:O	2.34	0.42
1:YA:99:ARG:NH1	1:YA:251:VAL:O	2.44	0.42
1:AB:101:SER:OG	1:AB:192:GLN:NE2	2.42	0.42
1:FB:55:VAL:HB	1:FB:88:VAL:HB	2.02	0.42
1:HB:80:TYR:HB2	1:HB:222:VAL:HG21	2.01	0.42
1:MB:116:GLU:OE2	1:MB:231:LYS:NZ	2.47	0.42
1:TB:134:THR:HG22	1:TB:147:THR:HG22	2.02	0.42
1:WB:199:SER:OG	1:WB:205:GLU:O	2.37	0.42
1:KC:122:LEU:HD12	1:KC:175:LEU:HD11	2.01	0.42
1:MC:199:SER:OG	1:MC:205:GLU:O	2.37	0.42
1:PC:100:LYS:NZ	1:PC:247:GLU:OE2	2.47	0.42
1:SC:54:ARG:NH2	1:SC:89:THR:OG1	2.46	0.42
1:VC:158:PHE:HB2	1:VC:171:LEU:HB3	2.00	0.42
1:MD:158:PHE:HB2	1:MD:171:LEU:HB3	2.01	0.42
1:E:183:ALA:HA	1:E:222:VAL:HA	2.02	0.42
1:Q:104:ASP:HB3	1:Q:139:VAL:HG13	2.00	0.42
1:S:240:LEU:O	1:S:243:THR:OG1	2.36	0.42
1:VA:104:ASP:HB3	1:VA:139:VAL:HG13	2.00	0.42
1:VA:125:LEU:O	1:VA:156:GLN:NE2	2.52	0.42
1:CB:55:VAL:HB	1:CB:88:VAL:HB	2.00	0.42
1:LB:104:ASP:HB3	1:LB:139:VAL:HG13	2.00	0.42
1:PB:23:ASP:OD2	1:PB:23:ASP:N	2.48	0.42
1:CC:125:LEU:O	1:CC:156:GLN:NE2	2.50	0.42
1:DC:125:LEU:O	1:DC:156:GLN:NE2	2.51	0.42
1:NC:161:LYS:HD3	1:NC:161:LYS:HA	1.87	0.42
1:PC:125:LEU:O	1:PC:156:GLN:NE2	2.50	0.42
1:UC:91:VAL:O	1:UC:94:SER:OG	2.32	0.42
1:FD:222:VAL:HG23	1:FD:225:SER:HB3	2.01	0.42
1:ID:58:LYS:NZ	1:ID:60:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JD:58:LYS:NZ	1:JD:60:ASP:OD1	2.53	0.42
1:LD:58:LYS:NZ	1:LD:60:ASP:OD1	2.51	0.42
1:K:80:TYR:HB2	1:K:222:VAL:HG21	2.02	0.42
1:CA:39:ARG:HB3	1:CA:60:ASP:HB2	2.01	0.42
1:DA:109:LEU:HD11	1:DA:171:LEU:HD21	2.00	0.42
1:GA:99:ARG:NH1	1:GA:251:VAL:O	2.52	0.42
1:JA:39:ARG:HB3	1:JA:60:ASP:HB2	2.01	0.42
1:PA:55:VAL:HB	1:PA:88:VAL:HB	2.02	0.42
1:PA:183:ALA:HA	1:PA:222:VAL:HA	2.02	0.42
1:SA:118:LEU:HD22	1:SA:125:LEU:HG	2.02	0.42
1:BB:54:ARG:NH2	1:BB:89:THR:OG1	2.43	0.42
1:BB:172:THR:O	1:BB:172:THR:OG1	2.37	0.42
1:DB:125:LEU:O	1:DB:156:GLN:NE2	2.48	0.42
1:GB:83:VAL:HG22	1:GB:220:THR:HB	2.02	0.42
1:HB:184:TYR:N	1:HB:221:ILE:O	2.47	0.42
1:CC:100:LYS:NZ	1:CC:247:GLU:OE2	2.47	0.42
1:IC:41:THR:O	1:IC:41:THR:OG1	2.33	0.42
1:IC:58:LYS:NZ	1:IC:60:ASP:OD1	2.50	0.42
1:MC:58:LYS:NZ	1:MC:60:ASP:OD1	2.50	0.42
1:NC:80:TYR:HB2	1:NC:222:VAL:HG21	2.02	0.42
1:TC:64:VAL:HA	1:TC:78:VAL:HA	2.02	0.42
1:VC:125:LEU:O	1:VC:156:GLN:NE2	2.49	0.42
1:YC:158:PHE:HB2	1:YC:171:LEU:HB3	2.02	0.42
1:BD:112:THR:HG23	1:BD:114:GLN:H	1.85	0.42
1:FD:125:LEU:O	1:FD:156:GLN:NE2	2.49	0.42
1:KD:222:VAL:O	1:KD:225:SER:OG	2.30	0.42
1:MD:1:SER:HB3	1:MD:2:LYS:H	1.68	0.42
1:A:104:ASP:HB3	1:A:139:VAL:HG13	2.01	0.42
1:L:171:LEU:HD23	1:L:171:LEU:HA	1.94	0.42
1:V:186:VAL:HB	1:V:219:VAL:HB	2.02	0.42
1:AA:66:ASP:HB2	1:AA:76:PRO:HB3	2.00	0.42
1:DA:222:VAL:O	1:DA:225:SER:OG	2.32	0.42
1:JA:134:THR:HG22	1:JA:147:THR:HG22	2.01	0.42
1:LA:54:ARG:NH2	1:LA:89:THR:OG1	2.43	0.42
1:ZA:134:THR:HG22	1:ZA:147:THR:HG22	2.01	0.42
1:DB:122:LEU:HD12	1:DB:175:LEU:HD11	2.01	0.42
1:NB:104:ASP:HB3	1:NB:139:VAL:HG13	2.01	0.42
1:SB:83:VAL:HG22	1:SB:220:THR:HB	2.02	0.42
1:CC:54:ARG:NH2	1:CC:89:THR:OG1	2.47	0.42
1:HC:55:VAL:HB	1:HC:88:VAL:HB	2.02	0.42
1:LD:91:VAL:O	1:LD:94:SER:OG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104:ASP:HB3	1:G:139:VAL:HG13	2.02	0.42
1:X:54:ARG:NH2	1:X:89:THR:OG1	2.44	0.42
1:OA:198:CYS:HB2	1:OA:201:SER:HB3	2.01	0.42
1:RA:39:ARG:HB3	1:RA:60:ASP:HB2	2.01	0.42
1:SA:161:LYS:HD3	1:SA:161:LYS:HA	1.73	0.42
1:XA:54:ARG:NH2	1:XA:89:THR:OG1	2.46	0.42
1:AB:104:ASP:HB3	1:AB:139:VAL:HG13	2.02	0.42
1:RB:55:VAL:HB	1:RB:88:VAL:HB	2.01	0.42
1:UB:54:ARG:NH2	1:UB:89:THR:OG1	2.44	0.42
1:XB:157:ILE:HG12	1:XB:172:THR:HG22	2.01	0.42
1:BC:125:LEU:O	1:BC:156:GLN:NE2	2.53	0.42
1:HC:54:ARG:NH2	1:HC:89:THR:OG1	2.43	0.42
1:LC:54:ARG:NH2	1:LC:89:THR:OG1	2.43	0.42
1:NC:225:SER:HB2	1:NC:230:ARG:HH11	1.85	0.42
1:QC:152:THR:HG22	1:QC:153:ALA:H	1.85	0.42
1:ZC:158:PHE:HB2	1:ZC:171:LEU:HB3	2.00	0.42
1:BD:158:PHE:HB2	1:BD:171:LEU:HB3	2.01	0.42
1:JD:1:SER:HB3	1:JD:2:LYS:H	1.67	0.42
1:ND:158:PHE:HB2	1:ND:171:LEU:HB3	2.01	0.42
1:W:41:THR:O	1:W:41:THR:OG1	2.36	0.42
1:PA:54:ARG:NH2	1:PA:89:THR:OG1	2.43	0.42
1:WA:99:ARG:NH1	1:WA:251:VAL:O	2.52	0.42
1:IB:240:LEU:O	1:IB:243:THR:OG1	2.37	0.42
1:PB:128:ALA:HB2	1:PB:133:LYS:HG2	2.01	0.42
1:RB:159:GLU:OE1	1:RB:170:ARG:NE	2.45	0.42
1:YB:134:THR:HG22	1:YB:147:THR:HG22	2.02	0.42
1:AC:240:LEU:O	1:AC:243:THR:OG1	2.37	0.42
1:MC:41:THR:O	1:MC:41:THR:OG1	2.33	0.42
1:MC:118:LEU:HD22	1:MC:125:LEU:HG	2.02	0.42
1:NC:39:ARG:HB3	1:NC:60:ASP:HB2	2.01	0.42
1:SC:158:PHE:HB2	1:SC:171:LEU:HB3	2.02	0.42
1:XC:158:PHE:HB2	1:XC:171:LEU:HB3	2.01	0.42
1:ZC:54:ARG:NH2	1:ZC:89:THR:OG1	2.46	0.42
1:ID:112:THR:HG23	1:ID:114:GLN:H	1.84	0.42
1:LD:158:PHE:HB2	1:LD:171:LEU:HB3	2.02	0.42
1:C:39:ARG:HB3	1:C:60:ASP:HB2	2.02	0.42
1:I:112:THR:HG23	1:I:114:GLN:H	1.85	0.42
1:L:240:LEU:O	1:L:243:THR:OG1	2.37	0.42
1:O:152:THR:HG22	1:O:153:ALA:H	1.85	0.42
1:P:64:VAL:HG22	1:P:78:VAL:HG12	2.02	0.42
1:V:55:VAL:HB	1:V:88:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:102:LEU:HD22	1:AA:213:GLN:HB3	2.02	0.42
1:DA:79:ARG:HH21	1:FA:73:GLY:HA2	1.85	0.42
1:SA:240:LEU:O	1:SA:243:THR:OG1	2.37	0.42
1:TA:125:LEU:O	1:TA:156:GLN:NE2	2.52	0.42
1:ZA:39:ARG:HB3	1:ZA:60:ASP:HB2	2.02	0.42
1:IB:39:ARG:HB3	1:IB:60:ASP:HB2	2.01	0.42
1:IB:118:LEU:HD22	1:IB:125:LEU:HG	2.02	0.42
1:QB:184:TYR:N	1:QB:221:ILE:O	2.46	0.42
1:TB:54:ARG:NH2	1:TB:89:THR:OG1	2.44	0.42
1:TB:100:LYS:NZ	1:TB:247:GLU:OE2	2.49	0.42
1:VB:159:GLU:OE1	1:VB:170:ARG:NE	2.45	0.42
1:ZB:125:LEU:O	1:ZB:156:GLN:NE2	2.51	0.42
1:IC:83:VAL:HG22	1:IC:220:THR:HB	2.02	0.42
1:MC:83:VAL:HG22	1:MC:220:THR:HB	2.02	0.42
1:RC:54:ARG:NH2	1:RC:89:THR:OG1	2.46	0.42
1:VC:154:ASP:OD1	1:VC:154:ASP:N	2.47	0.42
1:WC:158:PHE:HB2	1:WC:171:LEU:HB3	2.01	0.42
1:ZC:222:VAL:HG23	1:ZC:225:SER:HB3	2.01	0.42
1:BD:58:LYS:NZ	1:BD:60:ASP:OD1	2.53	0.42
1:DD:125:LEU:O	1:DD:156:GLN:NE2	2.47	0.42
1:MD:66:ASP:HB2	1:MD:76:PRO:HB3	2.01	0.42
1:C:134:THR:HG22	1:C:147:THR:HG22	2.01	0.41
1:I:3:THR:HG22	1:I:16:THR:HG22	2.02	0.41
1:M:125:LEU:O	1:M:156:GLN:NE2	2.51	0.41
1:N:13:ARG:HE	1:N:13:ARG:HB3	1.75	0.41
1:Q:152:THR:HG22	1:Q:153:ALA:H	1.85	0.41
1:R:240:LEU:O	1:R:243:THR:OG1	2.36	0.41
1:Y:104:ASP:HB3	1:Y:139:VAL:HG13	2.02	0.41
1:EA:240:LEU:O	1:EA:243:THR:OG1	2.37	0.41
1:JA:184:TYR:N	1:JA:221:ILE:O	2.47	0.41
1:KA:161:LYS:HA	1:KA:161:LYS:HD3	1.86	0.41
1:NA:3:THR:HG22	1:NA:16:THR:HG22	2.02	0.41
1:HB:39:ARG:HB3	1:HB:60:ASP:HB2	2.01	0.41
1:OB:240:LEU:O	1:OB:243:THR:OG1	2.37	0.41
1:QB:39:ARG:HB3	1:QB:60:ASP:HB2	2.01	0.41
1:RB:112:THR:HG23	1:RB:114:GLN:H	1.85	0.41
1:VB:55:VAL:HB	1:VB:88:VAL:HB	2.02	0.41
1:XB:39:ARG:HB3	1:XB:60:ASP:HB2	2.01	0.41
1:CC:39:ARG:HB3	1:CC:60:ASP:HB2	2.02	0.41
1:DC:54:ARG:NH2	1:DC:89:THR:OG1	2.46	0.41
1:FC:39:ARG:HB3	1:FC:60:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FC:134:THR:HG22	1:FC:147:THR:HG22	2.02	0.41
1:JC:100:LYS:NZ	1:JC:247:GLU:OE2	2.48	0.41
1:ND:222:VAL:HG23	1:ND:225:SER:HB3	2.02	0.41
1:OD:222:VAL:HG23	1:OD:225:SER:HB3	2.02	0.41
1:PD:222:VAL:HG23	1:PD:225:SER:HB3	2.01	0.41
1:E:112:THR:HG23	1:E:114:GLN:H	1.85	0.41
1:I:58:LYS:NZ	1:I:60:ASP:OD1	2.50	0.41
1:P:21:THR:HG22	1:P:22:ALA:H	1.85	0.41
1:XA:104:ASP:HB3	1:XA:139:VAL:HG13	2.00	0.41
1:LB:125:LEU:O	1:LB:156:GLN:NE2	2.53	0.41
1:LB:154:ASP:OD1	1:LB:154:ASP:N	2.51	0.41
1:UB:134:THR:HG22	1:UB:147:THR:HG22	2.02	0.41
1:VB:150:GLN:NE2	1:VB:152:THR:OG1	2.43	0.41
1:CC:21:THR:HG22	1:CC:22:ALA:H	1.85	0.41
1:EC:118:LEU:HD22	1:EC:125:LEU:HG	2.02	0.41
1:EC:240:LEU:O	1:EC:243:THR:OG1	2.37	0.41
1:PC:21:THR:HG22	1:PC:22:ALA:H	1.85	0.41
1:SC:58:LYS:NZ	1:SC:60:ASP:OD1	2.52	0.41
1:TC:158:PHE:HB2	1:TC:171:LEU:HB3	2.02	0.41
1:CD:172:THR:O	1:CD:172:THR:OG1	2.38	0.41
1:GD:222:VAL:HG23	1:GD:225:SER:HB3	2.01	0.41
1:HD:172:THR:O	1:HD:172:THR:OG1	2.37	0.41
1:LD:222:VAL:O	1:LD:225:SER:OG	2.30	0.41
1:K:225:SER:HB2	1:K:230:ARG:HH11	1.85	0.41
1:M:21:THR:HG22	1:M:22:ALA:H	1.85	0.41
1:M:171:LEU:HD23	1:M:171:LEU:HA	1.95	0.41
1:P:171:LEU:HD23	1:P:171:LEU:HA	1.93	0.41
1:V:112:THR:HG23	1:V:114:GLN:H	1.85	0.41
1:W:118:LEU:HD22	1:W:125:LEU:HG	2.02	0.41
1:Z:58:LYS:NZ	1:Z:60:ASP:OD1	2.47	0.41
1:Z:183:ALA:HA	1:Z:222:VAL:HA	2.03	0.41
1:CA:21:THR:HG22	1:CA:22:ALA:H	1.86	0.41
1:FA:154:ASP:OD2	1:FA:154:ASP:N	2.51	0.41
1:GA:21:THR:HG22	1:GA:22:ALA:H	1.85	0.41
1:HA:104:ASP:HB3	1:HA:139:VAL:HG13	2.00	0.41
1:UA:118:LEU:HD22	1:UA:125:LEU:HG	2.03	0.41
1:VA:154:ASP:OD1	1:VA:154:ASP:N	2.51	0.41
1:BB:112:THR:HG23	1:BB:114:GLN:H	1.85	0.41
1:RB:183:ALA:HA	1:RB:222:VAL:HA	2.02	0.41
1:UB:89:THR:HB	1:UB:214:VAL:HG22	2.01	0.41
1:MC:13:ARG:NH2	1:MC:29:GLU:OE1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SC:222:VAL:O	1:SC:225:SER:OG	2.30	0.41
1:AD:158:PHE:HB2	1:AD:171:LEU:HB3	2.01	0.41
1:GD:158:PHE:HB2	1:GD:171:LEU:HB3	2.01	0.41
1:OD:154:ASP:OD1	1:OD:154:ASP:N	2.46	0.41
1:OD:158:PHE:HB2	1:OD:171:LEU:HB3	2.02	0.41
1:G:95:THR:HG22	1:G:97:ALA:H	1.86	0.41
1:P:118:LEU:HD22	1:P:125:LEU:HG	2.03	0.41
1:R:13:ARG:HE	1:R:13:ARG:HB3	1.75	0.41
1:CA:134:THR:HG22	1:CA:147:THR:HG22	2.01	0.41
1:KA:21:THR:HG22	1:KA:22:ALA:H	1.86	0.41
1:LA:112:THR:HG23	1:LA:114:GLN:H	1.85	0.41
1:TA:100:LYS:NZ	1:TA:247:GLU:OE2	2.47	0.41
1:UA:21:THR:HG22	1:UA:22:ALA:H	1.86	0.41
1:OB:118:LEU:HD22	1:OB:125:LEU:HG	2.02	0.41
1:XB:184:TYR:N	1:XB:221:ILE:O	2.47	0.41
1:YB:240:LEU:O	1:YB:243:THR:OG1	2.36	0.41
1:DC:104:ASP:HB3	1:DC:139:VAL:HG13	2.01	0.41
1:DC:152:THR:HG22	1:DC:153:ALA:H	1.85	0.41
1:RC:125:LEU:O	1:RC:156:GLN:NE2	2.52	0.41
1:WC:222:VAL:HG23	1:WC:225:SER:HB3	2.02	0.41
1:BD:66:ASP:HB2	1:BD:76:PRO:HB3	2.02	0.41
1:DD:150:GLN:NE2	1:DD:152:THR:OG1	2.43	0.41
1:GD:54:ARG:NH2	1:GD:89:THR:OG1	2.47	0.41
1:ID:150:GLN:NE2	1:ID:152:THR:OG1	2.43	0.41
1:KD:112:THR:HG23	1:KD:114:GLN:H	1.84	0.41
1:D:39:ARG:HB3	1:D:60:ASP:HB2	2.01	0.41
1:L:21:THR:HG22	1:L:22:ALA:H	1.86	0.41
1:S:21:THR:HG22	1:S:22:ALA:H	1.86	0.41
1:W:54:ARG:NH2	1:W:89:THR:OG1	2.47	0.41
1:Z:3:THR:HG22	1:Z:16:THR:HG22	2.03	0.41
1:BA:39:ARG:HB3	1:BA:60:ASP:HB2	2.01	0.41
1:EA:152:THR:HG22	1:EA:153:ALA:H	1.85	0.41
1:LA:3:THR:HG22	1:LA:16:THR:HG22	2.03	0.41
1:WA:21:THR:HG22	1:WA:22:ALA:H	1.85	0.41
1:KB:21:THR:HG22	1:KB:22:ALA:H	1.86	0.41
1:KB:118:LEU:HD22	1:KB:125:LEU:HG	2.03	0.41
1:PB:240:LEU:O	1:PB:243:THR:OG1	2.36	0.41
1:XB:80:TYR:HB2	1:XB:222:VAL:HG21	2.03	0.41
1:ZB:79:ARG:HH21	1:BC:73:GLY:HA2	1.86	0.41
1:ZB:116:GLU:OE2	1:ZB:231:LYS:NZ	2.48	0.41
1:IC:13:ARG:NH2	1:IC:29:GLU:OE1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KC:134:THR:HG22	1:KC:147:THR:HG22	2.02	0.41
1:RC:152:THR:HG22	1:RC:153:ALA:H	1.85	0.41
1:UC:58:LYS:NZ	1:UC:60:ASP:OD1	2.54	0.41
1:WC:94:SER:HB2	1:WC:99:ARG:HE	1.85	0.41
1:JD:158:PHE:HB2	1:JD:171:LEU:HB3	2.01	0.41
1:LD:199:SER:OG	1:LD:205:GLU:O	2.38	0.41
1:D:225:SER:HB2	1:D:230:ARG:HH11	1.85	0.41
1:H:54:ARG:NH2	1:H:89:THR:OG1	2.45	0.41
1:J:118:LEU:HD22	1:J:125:LEU:HG	2.02	0.41
1:K:21:THR:HG22	1:K:22:ALA:H	1.85	0.41
1:P:8:VAL:HG13	1:P:235:ASP:HB3	2.03	0.41
1:V:199:SER:OG	1:V:205:GLU:O	2.38	0.41
1:FA:82:GLN:NE2	1:FA:225:SER:OG	2.54	0.41
1:HA:54:ARG:NH2	1:HA:89:THR:OG1	2.46	0.41
1:RA:172:THR:O	1:RA:172:THR:OG1	2.37	0.41
1:SA:134:THR:HG22	1:SA:147:THR:HG22	2.02	0.41
1:AB:21:THR:HG22	1:AB:22:ALA:H	1.86	0.41
1:LB:152:THR:HG22	1:LB:153:ALA:H	1.85	0.41
1:NB:152:THR:HG22	1:NB:153:ALA:H	1.85	0.41
1:PB:39:ARG:HB3	1:PB:60:ASP:HB2	2.01	0.41
1:CC:118:LEU:HD22	1:CC:125:LEU:HG	2.03	0.41
1:JC:68:SER:OG	1:JC:74:GLU:O	2.34	0.41
1:YC:199:SER:OG	1:YC:205:GLU:O	2.38	0.41
1:GD:100:LYS:NZ	1:GD:247:GLU:OE2	2.45	0.41
1:LD:112:THR:HG23	1:LD:114:GLN:H	1.84	0.41
1:A:154:ASP:OD1	1:A:154:ASP:N	2.51	0.41
1:C:21:THR:HG22	1:C:22:ALA:H	1.86	0.41
1:H:23:ASP:OD2	1:H:24:ARG:N	2.54	0.41
1:Q:23:ASP:OD2	1:Q:23:ASP:N	2.54	0.41
1:V:3:THR:HG22	1:V:16:THR:HG22	2.03	0.41
1:BA:104:ASP:HB3	1:BA:139:VAL:HG13	2.01	0.41
1:DA:100:LYS:NZ	1:DA:247:GLU:OE2	2.47	0.41
1:LA:58:LYS:NZ	1:LA:60:ASP:OD1	2.45	0.41
1:NA:63:ASP:OD2	1:NA:79:ARG:NH2	2.54	0.41
1:OB:197:ASP:OD1	1:OB:197:ASP:N	2.53	0.41
1:XB:93:ASN:OD1	1:XB:93:ASN:N	2.54	0.41
1:LC:112:THR:HG23	1:LC:114:GLN:H	1.85	0.41
1:QC:118:LEU:HD22	1:QC:125:LEU:HG	2.03	0.41
1:RC:21:THR:HG22	1:RC:22:ALA:H	1.86	0.41
1:CD:199:SER:OG	1:CD:205:GLU:O	2.39	0.41
1:DD:158:PHE:HB2	1:DD:171:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OD:100:LYS:NZ	1:OD:247:GLU:OE2	2.45	0.41
1:PD:94:SER:HB2	1:PD:99:ARG:HE	1.86	0.41
1:PD:158:PHE:HB2	1:PD:171:LEU:HB3	2.02	0.41
1:A:125:LEU:O	1:A:156:GLN:NE2	2.51	0.41
1:H:134:THR:HG22	1:H:147:THR:HG22	2.02	0.41
1:N:240:LEU:O	1:N:243:THR:OG1	2.37	0.41
1:S:44:LEU:HD11	1:S:253:LEU:HD22	2.03	0.41
1:T:21:THR:HG22	1:T:22:ALA:H	1.86	0.41
1:T:225:SER:HB2	1:T:230:ARG:HH11	1.86	0.41
1:X:23:ASP:OD2	1:X:24:ARG:N	2.54	0.41
1:BA:225:SER:HB2	1:BA:230:ARG:HH11	1.85	0.41
1:IA:21:THR:HG22	1:IA:22:ALA:H	1.86	0.41
1:KA:225:SER:HB2	1:KA:230:ARG:HH11	1.86	0.41
1:NA:122:LEU:HD12	1:NA:175:LEU:HD11	2.02	0.41
1:VA:82:GLN:NE2	1:VA:225:SER:OG	2.53	0.41
1:XA:197:ASP:OD1	1:XA:197:ASP:N	2.54	0.41
1:GB:58:LYS:NZ	1:GB:60:ASP:OD1	2.50	0.41
1:TB:89:THR:HB	1:TB:214:VAL:HG22	2.02	0.41
1:VB:112:THR:HG23	1:VB:114:GLN:H	1.86	0.41
1:AC:197:ASP:OD1	1:AC:197:ASP:N	2.54	0.41
1:BC:82:GLN:NE2	1:BC:225:SER:OG	2.54	0.41
1:BC:152:THR:HG22	1:BC:153:ALA:H	1.85	0.41
1:EC:152:THR:HG22	1:EC:153:ALA:H	1.86	0.41
1:KC:158:PHE:HB2	1:KC:171:LEU:HB3	2.03	0.41
1:NC:21:THR:HG22	1:NC:22:ALA:H	1.85	0.41
1:VC:94:SER:HB2	1:VC:99:ARG:HE	1.85	0.41
1:ED:94:SER:HB2	1:ED:99:ARG:HE	1.86	0.41
1:B:21:THR:HG22	1:B:22:ALA:H	1.86	0.41
1:B:118:LEU:HD22	1:B:125:LEU:HG	2.03	0.41
1:B:152:THR:HG22	1:B:153:ALA:H	1.85	0.41
1:H:89:THR:HB	1:H:214:VAL:HG22	2.03	0.41
1:H:95:THR:HG22	1:H:97:ALA:H	1.86	0.41
1:L:44:LEU:HD11	1:L:253:LEU:HD22	2.03	0.41
1:O:21:THR:HG22	1:O:22:ALA:H	1.86	0.41
1:O:23:ASP:OD2	1:O:23:ASP:N	2.54	0.41
1:X:95:THR:HG22	1:X:97:ALA:H	1.86	0.41
1:X:134:THR:HG22	1:X:147:THR:HG22	2.03	0.41
1:Y:89:THR:HB	1:Y:214:VAL:HG22	2.03	0.41
1:Z:112:THR:HG23	1:Z:114:GLN:H	1.85	0.41
1:AA:118:LEU:HD22	1:AA:125:LEU:HG	2.02	0.41
1:DA:118:LEU:HD22	1:DA:125:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:21:THR:HG22	1:EA:22:ALA:H	1.86	0.41
1:EA:161:LYS:HA	1:EA:161:LYS:HD3	1.74	0.41
1:FA:197:ASP:OD1	1:FA:197:ASP:N	2.54	0.41
1:GA:79:ARG:HH21	1:HA:73:GLY:HA2	1.85	0.41
1:HA:21:THR:HG22	1:HA:22:ALA:H	1.86	0.41
1:JA:44:LEU:HD11	1:JA:253:LEU:HD22	2.03	0.41
1:JA:128:ALA:HB2	1:JA:133:LYS:HG2	2.02	0.41
1:JA:240:LEU:O	1:JA:243:THR:OG1	2.36	0.41
1:KA:123:VAL:HA	1:KA:124:PRO:HD3	1.96	0.41
1:NA:89:THR:HB	1:NA:214:VAL:HG22	2.01	0.41
1:OA:63:ASP:OD2	1:OA:79:ARG:NH2	2.48	0.41
1:RA:225:SER:HB2	1:RA:230:ARG:HH11	1.85	0.41
1:UA:152:THR:HG22	1:UA:153:ALA:H	1.85	0.41
1:VA:152:THR:HG22	1:VA:153:ALA:H	1.85	0.41
1:XA:21:THR:HG22	1:XA:22:ALA:H	1.86	0.41
1:YA:21:THR:HG22	1:YA:22:ALA:H	1.86	0.41
1:ZA:240:LEU:O	1:ZA:243:THR:OG1	2.36	0.41
1:AB:80:TYR:HB2	1:AB:222:VAL:HG21	2.02	0.41
1:DB:89:THR:HB	1:DB:214:VAL:HG22	2.01	0.41
1:HB:172:THR:O	1:HB:172:THR:OG1	2.37	0.41
1:IB:91:VAL:HG23	1:IB:94:SER:HB2	2.03	0.41
1:MB:161:LYS:HD3	1:MB:161:LYS:HA	1.90	0.41
1:OB:21:THR:HG22	1:OB:22:ALA:H	1.86	0.41
1:OB:152:THR:HG22	1:OB:153:ALA:H	1.85	0.41
1:PB:91:VAL:HG23	1:PB:94:SER:HB2	2.02	0.41
1:QB:27:PHE:HB2	1:QB:40:LEU:HB3	2.03	0.41
1:TB:68:SER:OG	1:TB:74:GLU:O	2.34	0.41
1:VB:183:ALA:HA	1:VB:222:VAL:HA	2.03	0.41
1:WB:102:LEU:HD22	1:WB:213:GLN:HB3	2.03	0.41
1:YB:91:VAL:HG23	1:YB:94:SER:HB2	2.02	0.41
1:AC:118:LEU:HD22	1:AC:125:LEU:HG	2.03	0.41
1:FC:91:VAL:HG23	1:FC:94:SER:HB2	2.02	0.41
1:GC:21:THR:HG22	1:GC:22:ALA:H	1.86	0.41
1:GC:39:ARG:HB3	1:GC:60:ASP:HB2	2.02	0.41
1:KC:68:SER:OG	1:KC:74:GLU:O	2.35	0.41
1:LC:183:ALA:HA	1:LC:222:VAL:HA	2.02	0.41
1:PC:118:LEU:HD22	1:PC:125:LEU:HG	2.03	0.41
1:QC:197:ASP:OD1	1:QC:197:ASP:N	2.54	0.41
1:ID:66:ASP:HB2	1:ID:76:PRO:HB3	2.03	0.41
1:C:91:VAL:HG23	1:C:94:SER:HB2	2.03	0.41
1:D:27:PHE:HB2	1:D:40:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:154:ASP:OD1	1:H:154:ASP:N	2.45	0.41
1:O:54:ARG:NH2	1:O:89:THR:OG1	2.45	0.41
1:P:184:TYR:N	1:P:221:ILE:O	2.52	0.41
1:T:172:THR:O	1:T:172:THR:OG1	2.36	0.41
1:BA:27:PHE:HB2	1:BA:40:LEU:HB3	2.03	0.41
1:CA:91:VAL:HG23	1:CA:94:SER:HB2	2.03	0.41
1:EA:118:LEU:HD22	1:EA:125:LEU:HG	2.03	0.41
1:JA:21:THR:HG22	1:JA:22:ALA:H	1.86	0.41
1:YA:197:ASP:OD1	1:YA:197:ASP:N	2.54	0.41
1:FB:183:ALA:HA	1:FB:222:VAL:HA	2.03	0.41
1:IB:134:THR:HG22	1:IB:147:THR:HG22	2.03	0.41
1:LB:82:GLN:NE2	1:LB:225:SER:OG	2.54	0.41
1:OB:161:LYS:HA	1:OB:161:LYS:HD3	1.75	0.41
1:QB:172:THR:O	1:QB:172:THR:OG1	2.37	0.41
1:SB:118:LEU:HD22	1:SB:125:LEU:HG	2.02	0.41
1:TB:104:ASP:HB3	1:TB:139:VAL:HG13	2.03	0.41
1:ZB:21:THR:HG22	1:ZB:22:ALA:H	1.85	0.41
1:AC:21:THR:HG22	1:AC:22:ALA:H	1.86	0.41
1:AC:161:LYS:HD3	1:AC:161:LYS:HA	1.75	0.41
1:EC:197:ASP:OD1	1:EC:197:ASP:N	2.54	0.41
1:HC:112:THR:HG23	1:HC:114:GLN:H	1.85	0.41
1:KC:104:ASP:HB3	1:KC:139:VAL:HG13	2.02	0.41
1:OC:91:VAL:HG23	1:OC:94:SER:HB2	2.03	0.41
1:PC:79:ARG:HH21	1:RC:73:GLY:HA2	1.86	0.41
1:RC:197:ASP:OD1	1:RC:197:ASP:N	2.54	0.41
1:CD:1:SER:HB3	1:CD:2:LYS:H	1.67	0.41
1:HD:54:ARG:NH2	1:HD:89:THR:OG1	2.46	0.41
1:G:23:ASP:OD2	1:G:24:ARG:N	2.54	0.40
1:N:152:THR:HG22	1:N:153:ALA:H	1.85	0.40
1:S:171:LEU:HD23	1:S:171:LEU:HA	1.95	0.40
1:X:104:ASP:HB3	1:X:139:VAL:HG13	2.02	0.40
1:CA:128:ALA:HB2	1:CA:133:LYS:HG2	2.01	0.40
1:HA:152:THR:HG22	1:HA:153:ALA:H	1.85	0.40
1:HA:197:ASP:OD1	1:HA:197:ASP:N	2.54	0.40
1:IA:118:LEU:HD22	1:IA:125:LEU:HG	2.03	0.40
1:TA:8:VAL:HG13	1:TA:235:ASP:HB3	2.03	0.40
1:TA:240:LEU:O	1:TA:243:THR:OG1	2.38	0.40
1:ZA:44:LEU:HD11	1:ZA:253:LEU:HD22	2.03	0.40
1:AB:225:SER:HB2	1:AB:230:ARG:HH11	1.86	0.40
1:CB:102:LEU:HD22	1:CB:213:GLN:HB3	2.03	0.40
1:KB:152:THR:HG22	1:KB:153:ALA:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MB:8:VAL:HG13	1:MB:235:ASP:HB3	2.03	0.40
1:MB:21:THR:HG22	1:MB:22:ALA:H	1.85	0.40
1:PB:21:THR:HG22	1:PB:22:ALA:H	1.86	0.40
1:FC:118:LEU:HD22	1:FC:125:LEU:HG	2.02	0.40
1:LC:161:LYS:HD3	1:LC:161:LYS:HA	1.90	0.40
1:CD:158:PHE:HB2	1:CD:171:LEU:HB3	2.02	0.40
1:M:8:VAL:HG13	1:M:235:ASP:HB3	2.03	0.40
1:M:184:TYR:N	1:M:221:ILE:O	2.52	0.40
1:CA:240:LEU:O	1:CA:243:THR:OG1	2.36	0.40
1:DA:54:ARG:NH2	1:DA:89:THR:OG1	2.47	0.40
1:OA:95:THR:HG22	1:OA:97:ALA:H	1.86	0.40
1:SA:21:THR:HG22	1:SA:22:ALA:H	1.86	0.40
1:XA:152:THR:HG22	1:XA:153:ALA:H	1.85	0.40
1:YA:118:LEU:HD22	1:YA:125:LEU:HG	2.03	0.40
1:ZA:21:THR:HG22	1:ZA:22:ALA:H	1.86	0.40
1:GB:102:LEU:HD22	1:GB:213:GLN:HB3	2.03	0.40
1:HB:225:SER:HB2	1:HB:230:ARG:HH11	1.85	0.40
1:IB:21:THR:HG22	1:IB:22:ALA:H	1.86	0.40
1:JB:64:VAL:HG22	1:JB:78:VAL:HG12	2.03	0.40
1:QB:21:THR:HG22	1:QB:22:ALA:H	1.86	0.40
1:XB:21:THR:HG22	1:XB:22:ALA:H	1.86	0.40
1:XB:27:PHE:HB2	1:XB:40:LEU:HB3	2.04	0.40
1:ZB:8:VAL:HG13	1:ZB:235:ASP:HB3	2.03	0.40
1:AC:152:THR:HG22	1:AC:153:ALA:H	1.85	0.40
1:DC:197:ASP:OD1	1:DC:197:ASP:N	2.54	0.40
1:OC:240:LEU:O	1:OC:243:THR:OG1	2.36	0.40
1:QC:21:THR:HG22	1:QC:22:ALA:H	1.86	0.40
1:SC:67:CYS:HB3	1:SC:70:SER:HB3	2.04	0.40
1:UC:199:SER:OG	1:UC:205:GLU:O	2.38	0.40
1:AD:222:VAL:HG23	1:AD:225:SER:HB3	2.01	0.40
1:CD:118:LEU:HD22	1:CD:125:LEU:HG	2.03	0.40
1:ND:25:GLN:NE2	1:ND:256:LEU:O	2.53	0.40
1:A:152:THR:HG22	1:A:153:ALA:H	1.85	0.40
1:L:91:VAL:HG23	1:L:94:SER:HB2	2.02	0.40
1:R:152:THR:HG22	1:R:153:ALA:H	1.85	0.40
1:AA:83:VAL:HG22	1:AA:220:THR:HB	2.02	0.40
1:QA:118:LEU:HD22	1:QA:125:LEU:HG	2.04	0.40
1:RA:21:THR:HG22	1:RA:22:ALA:H	1.85	0.40
1:RA:27:PHE:HB2	1:RA:40:LEU:HB3	2.03	0.40
1:WA:91:VAL:HG23	1:WA:94:SER:HB3	2.03	0.40
1:EB:134:THR:HG22	1:EB:147:THR:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HB:21:THR:HG22	1:HB:22:ALA:H	1.86	0.40
1:IB:44:LEU:HD11	1:IB:253:LEU:HD22	2.03	0.40
1:JB:8:VAL:HG13	1:JB:235:ASP:HB3	2.03	0.40
1:YB:21:THR:HG22	1:YB:22:ALA:H	1.86	0.40
1:YB:118:LEU:HD22	1:YB:125:LEU:HG	2.03	0.40
1:BC:21:THR:HG22	1:BC:22:ALA:H	1.86	0.40
1:DC:82:GLN:NE2	1:DC:225:SER:OG	2.54	0.40
1:GC:158:PHE:HB2	1:GC:171:LEU:HB3	2.04	0.40
1:HC:58:LYS:NZ	1:HC:60:ASP:OD1	2.48	0.40
1:GD:94:SER:HB2	1:GD:99:ARG:HE	1.86	0.40
1:GD:134:THR:HG22	1:GD:147:THR:HG22	2.04	0.40
1:B:197:ASP:OD1	1:B:197:ASP:N	2.54	0.40
1:C:240:LEU:O	1:C:243:THR:OG1	2.36	0.40
1:F:13:ARG:NH2	1:F:29:GLU:OE1	2.45	0.40
1:DA:21:THR:HG22	1:DA:22:ALA:H	1.86	0.40
1:EA:197:ASP:OD1	1:EA:197:ASP:N	2.54	0.40
1:MA:102:LEU:HD22	1:MA:213:GLN:HB3	2.03	0.40
1:OA:104:ASP:HB3	1:OA:139:VAL:HG13	2.02	0.40
1:QA:102:LEU:HD22	1:QA:213:GLN:HB3	2.03	0.40
1:AB:184:TYR:N	1:AB:221:ILE:O	2.47	0.40
1:BB:183:ALA:HA	1:BB:222:VAL:HA	2.02	0.40
1:DB:23:ASP:OD2	1:DB:24:ARG:N	2.55	0.40
1:EB:100:LYS:NZ	1:EB:247:GLU:OE2	2.48	0.40
1:JB:240:LEU:O	1:JB:243:THR:OG1	2.38	0.40
1:SB:54:ARG:NH2	1:SB:89:THR:OG1	2.47	0.40
1:DC:21:THR:HG22	1:DC:22:ALA:H	1.86	0.40
1:EC:21:THR:HG22	1:EC:22:ALA:H	1.86	0.40
1:JC:104:ASP:HB3	1:JC:139:VAL:HG13	2.03	0.40
1:RC:82:GLN:NE2	1:RC:225:SER:OG	2.54	0.40
1:SC:185:ARG:HH21	1:SC:220:THR:HG1	1.62	0.40
1:VC:100:LYS:NZ	1:VC:247:GLU:OE2	2.46	0.40
1:CD:54:ARG:NH2	1:CD:89:THR:OG1	2.45	0.40
1:GD:25:GLN:NE2	1:GD:256:LEU:O	2.54	0.40
1:I:199:SER:OG	1:I:205:GLU:O	2.37	0.40
1:K:184:TYR:N	1:K:221:ILE:O	2.47	0.40
1:M:39:ARG:HB3	1:M:60:ASP:HB2	2.04	0.40
1:N:118:LEU:HD22	1:N:125:LEU:HG	2.03	0.40
1:V:222:VAL:O	1:V:225:SER:OG	2.30	0.40
1:FA:125:LEU:O	1:FA:156:GLN:NE2	2.52	0.40
1:FA:152:THR:HG22	1:FA:153:ALA:H	1.85	0.40
1:NA:104:ASP:HB3	1:NA:139:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TA:21:THR:HG22	1:TA:22:ALA:H	1.85	0.40
1:WA:122:LEU:HD12	1:WA:175:LEU:HD21	2.04	0.40
1:WA:226:THR:HG22	1:WA:228:ALA:H	1.87	0.40
1:AB:161:LYS:HD3	1:AB:161:LYS:HA	1.87	0.40
1:CB:83:VAL:HG22	1:CB:220:THR:HB	2.04	0.40
1:LB:197:ASP:OD1	1:LB:197:ASP:N	2.54	0.40
1:NB:82:GLN:NE2	1:NB:225:SER:OG	2.55	0.40
1:PB:44:LEU:HD11	1:PB:253:LEU:HD22	2.03	0.40
1:TB:95:THR:HG22	1:TB:97:ALA:H	1.86	0.40
1:TB:183:ALA:HA	1:TB:222:VAL:HA	2.03	0.40
1:UB:104:ASP:HB3	1:UB:139:VAL:HG13	2.03	0.40
1:WB:54:ARG:NH2	1:WB:89:THR:OG1	2.47	0.40
1:DC:23:ASP:OD2	1:DC:23:ASP:N	2.54	0.40
1:FC:240:LEU:O	1:FC:243:THR:OG1	2.36	0.40
1:HC:183:ALA:HA	1:HC:222:VAL:HA	2.03	0.40
1:KC:23:ASP:OD2	1:KC:24:ARG:N	2.54	0.40
1:UC:118:LEU:HD22	1:UC:125:LEU:HG	2.03	0.40
1:YC:186:VAL:HB	1:YC:219:VAL:HB	2.04	0.40
1:DD:66:ASP:HB2	1:DD:76:PRO:HB3	2.03	0.40
1:KD:54:ARG:NH2	1:KD:89:THR:OG1	2.46	0.40
1:LD:185:ARG:HH21	1:LD:220:THR:HG1	1.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	AA	256/258 (99%)	239 (93%)	17 (7%)	0	100	100
1	AB	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	AC	256/258 (99%)	244 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AD	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	Af	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	B	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	BA	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	BB	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	BC	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	BD	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	C	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	CA	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	CB	256/258 (99%)	238 (93%)	18 (7%)	0	100	100
1	CC	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	CD	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	D	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	DA	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
1	DB	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	DC	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	DD	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	E	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	EA	256/258 (99%)	245 (96%)	11 (4%)	0	100	100
1	EB	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	EC	256/258 (99%)	245 (96%)	11 (4%)	0	100	100
1	ED	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	F	256/258 (99%)	240 (94%)	16 (6%)	0	100	100
1	FA	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
1	FB	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
1	FC	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	FD	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	G	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	GA	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
1	GB	256/258 (99%)	239 (93%)	17 (7%)	0	100	100
1	GC	256/258 (99%)	243 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GD	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	H	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	HA	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	HB	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	HC	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	HD	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	I	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	IA	256/258 (99%)	245 (96%)	11 (4%)	0	100	100
1	IB	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	IC	256/258 (99%)	239 (93%)	17 (7%)	0	100	100
1	ID	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	J	256/258 (99%)	238 (93%)	18 (7%)	0	100	100
1	JA	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	JB	256/258 (99%)	245 (96%)	11 (4%)	0	100	100
1	JC	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	JD	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	K	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
1	KA	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	KB	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	KC	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	KD	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	L	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	LA	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	LB	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	LC	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
1	LD	256/258 (99%)	240 (94%)	16 (6%)	0	100	100
1	M	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	MA	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	MB	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	MC	256/258 (99%)	239 (93%)	17 (7%)	0	100	100
1	MD	256/258 (99%)	242 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
1	NA	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
1	NB	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	NC	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	ND	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	O	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	OA	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	OB	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
1	OC	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	OD	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	P	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	PA	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	PB	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	PC	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	PD	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	Q	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
1	QA	256/258 (99%)	239 (93%)	17 (7%)	0	100	100
1	QB	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	QC	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
1	R	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
1	RA	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
1	RB	256/258 (99%)	240 (94%)	16 (6%)	0	100	100
1	RC	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	S	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	SA	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	SB	256/258 (99%)	240 (94%)	16 (6%)	0	100	100
1	SC	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	T	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	TA	256/258 (99%)	245 (96%)	11 (4%)	0	100	100
1	TB	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	TC	256/258 (99%)	242 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UA	256/258 (99%)	245 (96%)	11 (4%)	0	100	100
1	UB	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	UC	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	V	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
1	VA	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	VB	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	VC	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	W	256/258 (99%)	238 (93%)	18 (7%)	0	100	100
1	WA	256/258 (99%)	245 (96%)	11 (4%)	0	100	100
1	WB	256/258 (99%)	240 (94%)	16 (6%)	0	100	100
1	WC	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	X	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	XA	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	XB	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	XC	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	Y	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	YA	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	YB	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	YC	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	Z	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	ZA	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
1	ZB	256/258 (99%)	244 (95%)	12 (5%)	0	100	100
1	ZC	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
All	All	30720/30960 (99%)	29056 (95%)	1664 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	225/225 (100%)	225 (100%)	0	100	100
1	AA	225/225 (100%)	225 (100%)	0	100	100
1	AB	225/225 (100%)	225 (100%)	0	100	100
1	AC	225/225 (100%)	225 (100%)	0	100	100
1	AD	225/225 (100%)	225 (100%)	0	100	100
1	Af	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	B	225/225 (100%)	225 (100%)	0	100	100
1	BA	225/225 (100%)	225 (100%)	0	100	100
1	BB	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	BC	225/225 (100%)	225 (100%)	0	100	100
1	BD	225/225 (100%)	225 (100%)	0	100	100
1	C	225/225 (100%)	225 (100%)	0	100	100
1	CA	225/225 (100%)	225 (100%)	0	100	100
1	CB	225/225 (100%)	225 (100%)	0	100	100
1	CC	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	CD	225/225 (100%)	225 (100%)	0	100	100
1	D	225/225 (100%)	225 (100%)	0	100	100
1	DA	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	DB	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	DC	225/225 (100%)	225 (100%)	0	100	100
1	DD	225/225 (100%)	225 (100%)	0	100	100
1	E	225/225 (100%)	225 (100%)	0	100	100
1	EA	225/225 (100%)	225 (100%)	0	100	100
1	EB	225/225 (100%)	225 (100%)	0	100	100
1	EC	225/225 (100%)	225 (100%)	0	100	100
1	ED	225/225 (100%)	225 (100%)	0	100	100
1	F	225/225 (100%)	225 (100%)	0	100	100
1	FA	225/225 (100%)	225 (100%)	0	100	100
1	FB	225/225 (100%)	225 (100%)	0	100	100
1	FC	225/225 (100%)	225 (100%)	0	100	100
1	FD	225/225 (100%)	225 (100%)	0	100	100
1	G	225/225 (100%)	225 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GA	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	GB	225/225 (100%)	225 (100%)	0	100	100
1	GC	225/225 (100%)	225 (100%)	0	100	100
1	GD	225/225 (100%)	225 (100%)	0	100	100
1	H	225/225 (100%)	225 (100%)	0	100	100
1	HA	225/225 (100%)	225 (100%)	0	100	100
1	HB	225/225 (100%)	225 (100%)	0	100	100
1	HC	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	HD	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	I	225/225 (100%)	225 (100%)	0	100	100
1	IA	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	IB	225/225 (100%)	225 (100%)	0	100	100
1	IC	225/225 (100%)	225 (100%)	0	100	100
1	ID	225/225 (100%)	225 (100%)	0	100	100
1	J	225/225 (100%)	225 (100%)	0	100	100
1	JA	225/225 (100%)	225 (100%)	0	100	100
1	JB	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	JC	225/225 (100%)	225 (100%)	0	100	100
1	JD	225/225 (100%)	225 (100%)	0	100	100
1	K	225/225 (100%)	225 (100%)	0	100	100
1	KA	225/225 (100%)	225 (100%)	0	100	100
1	KB	225/225 (100%)	225 (100%)	0	100	100
1	KC	225/225 (100%)	225 (100%)	0	100	100
1	KD	225/225 (100%)	225 (100%)	0	100	100
1	L	225/225 (100%)	225 (100%)	0	100	100
1	LA	225/225 (100%)	225 (100%)	0	100	100
1	LB	225/225 (100%)	225 (100%)	0	100	100
1	LC	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	LD	225/225 (100%)	225 (100%)	0	100	100
1	M	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	MA	225/225 (100%)	225 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	MB	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	MC	225/225 (100%)	225 (100%)	0	100	100
1	MD	225/225 (100%)	225 (100%)	0	100	100
1	N	225/225 (100%)	225 (100%)	0	100	100
1	NA	225/225 (100%)	225 (100%)	0	100	100
1	NB	225/225 (100%)	225 (100%)	0	100	100
1	NC	225/225 (100%)	225 (100%)	0	100	100
1	ND	225/225 (100%)	225 (100%)	0	100	100
1	O	225/225 (100%)	225 (100%)	0	100	100
1	OA	225/225 (100%)	225 (100%)	0	100	100
1	OB	225/225 (100%)	225 (100%)	0	100	100
1	OC	225/225 (100%)	225 (100%)	0	100	100
1	OD	225/225 (100%)	225 (100%)	0	100	100
1	P	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	PA	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	PB	225/225 (100%)	225 (100%)	0	100	100
1	PC	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	PD	225/225 (100%)	225 (100%)	0	100	100
1	Q	225/225 (100%)	225 (100%)	0	100	100
1	QA	225/225 (100%)	225 (100%)	0	100	100
1	QB	225/225 (100%)	225 (100%)	0	100	100
1	QC	225/225 (100%)	225 (100%)	0	100	100
1	R	225/225 (100%)	225 (100%)	0	100	100
1	RA	225/225 (100%)	225 (100%)	0	100	100
1	RB	225/225 (100%)	225 (100%)	0	100	100
1	RC	225/225 (100%)	225 (100%)	0	100	100
1	S	225/225 (100%)	225 (100%)	0	100	100
1	SA	225/225 (100%)	225 (100%)	0	100	100
1	SB	225/225 (100%)	225 (100%)	0	100	100
1	SC	225/225 (100%)	225 (100%)	0	100	100
1	T	225/225 (100%)	225 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	TA	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	TB	225/225 (100%)	225 (100%)	0	100	100
1	TC	225/225 (100%)	225 (100%)	0	100	100
1	UA	225/225 (100%)	225 (100%)	0	100	100
1	UB	225/225 (100%)	225 (100%)	0	100	100
1	UC	225/225 (100%)	225 (100%)	0	100	100
1	V	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	VA	225/225 (100%)	225 (100%)	0	100	100
1	VB	225/225 (100%)	225 (100%)	0	100	100
1	VC	225/225 (100%)	225 (100%)	0	100	100
1	W	225/225 (100%)	225 (100%)	0	100	100
1	WA	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	WB	225/225 (100%)	225 (100%)	0	100	100
1	WC	225/225 (100%)	225 (100%)	0	100	100
1	X	225/225 (100%)	225 (100%)	0	100	100
1	XA	225/225 (100%)	225 (100%)	0	100	100
1	XB	225/225 (100%)	225 (100%)	0	100	100
1	XC	225/225 (100%)	225 (100%)	0	100	100
1	Y	225/225 (100%)	225 (100%)	0	100	100
1	YA	225/225 (100%)	225 (100%)	0	100	100
1	YB	225/225 (100%)	225 (100%)	0	100	100
1	YC	225/225 (100%)	225 (100%)	0	100	100
1	Z	225/225 (100%)	225 (100%)	0	100	100
1	ZA	225/225 (100%)	225 (100%)	0	100	100
1	ZB	225/225 (100%)	224 (100%)	1 (0%)	89	95
1	ZC	225/225 (100%)	225 (100%)	0	100	100
All	All	27000/27000 (100%)	26980 (100%)	20 (0%)	92	98

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Af	152	THR
1	M	152	THR

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Mol	Chain	Res	Type
1	P	152	THR
1	V	152	THR
1	DA	152	THR
1	GA	152	THR
1	IA	210	ARG
1	PA	152	THR
1	TA	152	THR
1	WA	152	THR
1	BB	152	THR
1	DB	210	ARG
1	JB	152	THR
1	MB	152	THR
1	ZB	152	THR
1	CC	152	THR
1	HC	152	THR
1	LC	152	THR
1	PC	152	THR
1	HD	152	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	D	192	GLN
1	E	213	GLN
1	G	82	GLN
1	H	82	GLN
1	I	213	GLN
1	O	82	GLN
1	Q	82	GLN
1	S	82	GLN
1	X	82	GLN
1	Y	82	GLN
1	Z	213	GLN
1	BA	192	GLN
1	FA	82	GLN
1	HA	82	GLN
1	KA	192	GLN
1	LA	213	GLN
1	NA	82	GLN
1	OA	82	GLN
1	PA	213	GLN

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Mol	Chain	Res	Type
1	RA	192	GLN
1	SA	213	GLN
1	VA	82	GLN
1	XA	82	GLN
1	ZA	82	GLN
1	BB	213	GLN
1	DB	82	GLN
1	EB	82	GLN
1	IB	82	GLN
1	KB	213	GLN
1	LB	82	GLN
1	NB	82	GLN
1	RB	213	GLN
1	TB	82	GLN
1	UB	82	GLN
1	VB	213	GLN
1	YB	82	GLN
1	BC	82	GLN
1	DC	82	GLN
1	HC	213	GLN
1	JC	82	GLN
1	KC	82	GLN
1	LC	213	GLN
1	RC	82	GLN
1	VC	150	GLN
1	HD	150	GLN
1	JD	178	ASN
1	OD	150	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

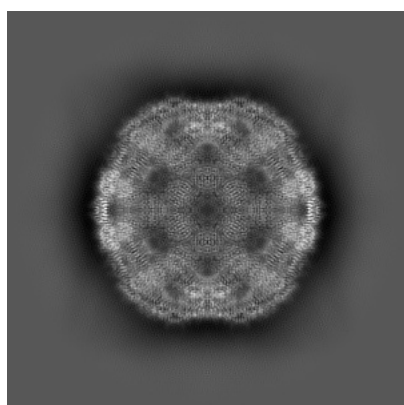
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0344. These allow visual inspection of the internal detail of the map and identification of artifacts.

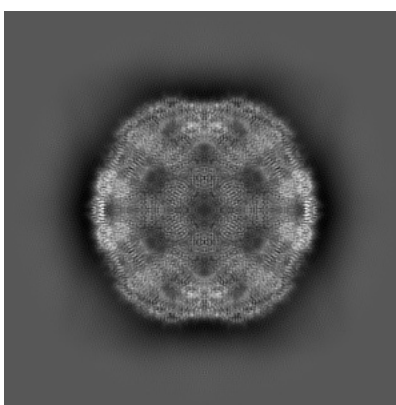
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

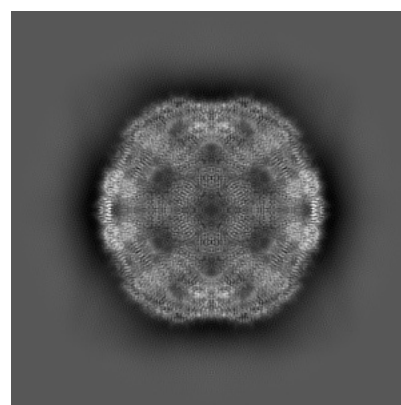
6.1.1 Primary map



X



Y

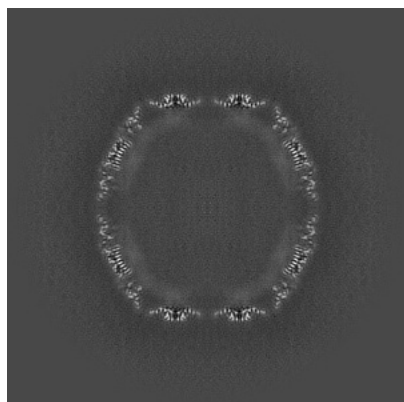


Z

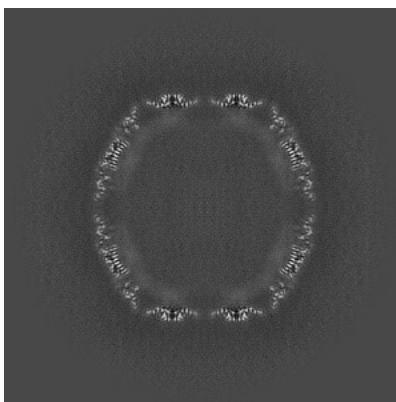
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

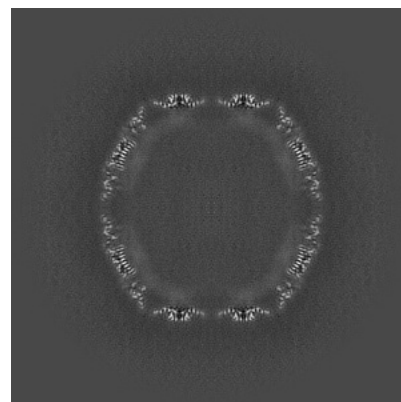
6.2.1 Primary map



X Index: 256



Y Index: 256

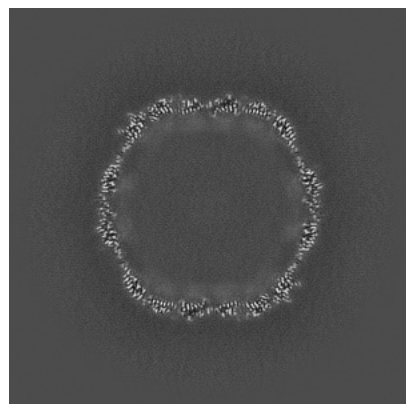


Z Index: 256

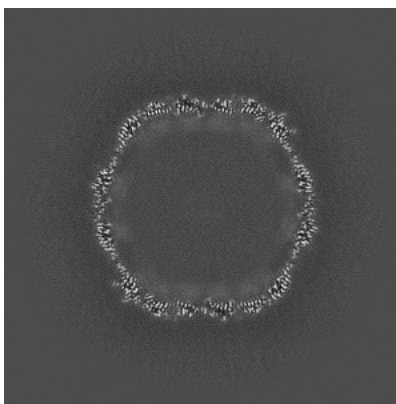
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

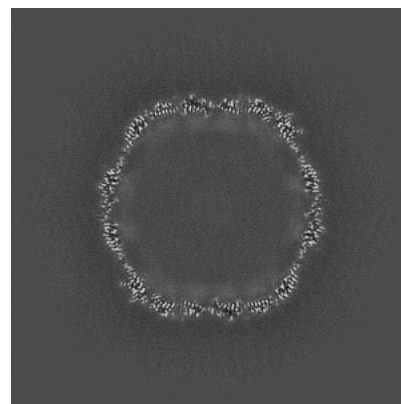
6.3.1 Primary map



X Index: 230



Y Index: 282

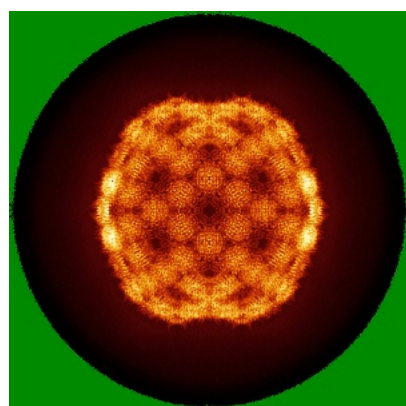


Z Index: 282

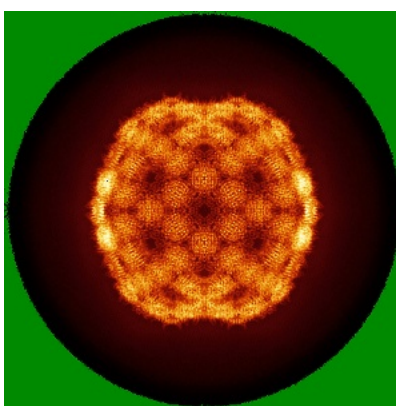
The images above show the largest variance slices of the map in three orthogonal directions.

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

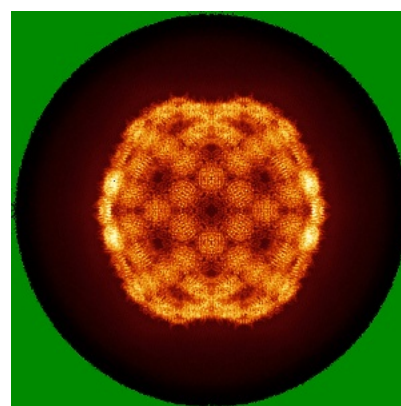
6.4.1 Primary map



X



Y

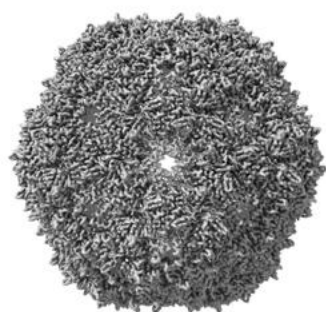


Z

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

6.5 Orthogonal surface views [i](#)

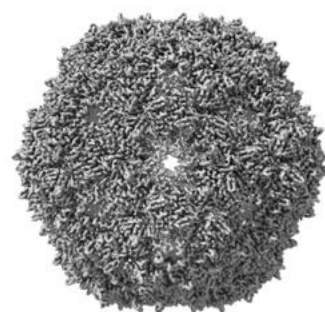
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.496. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

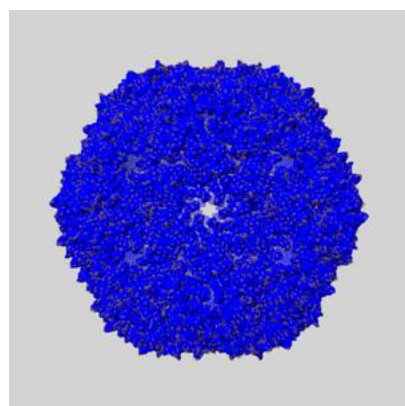
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

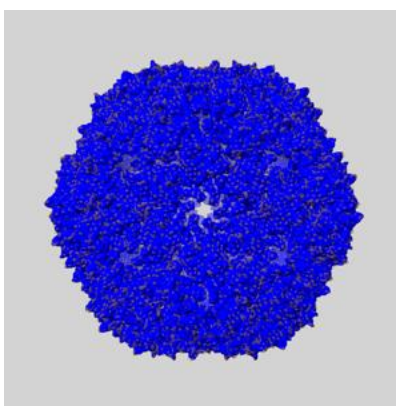
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

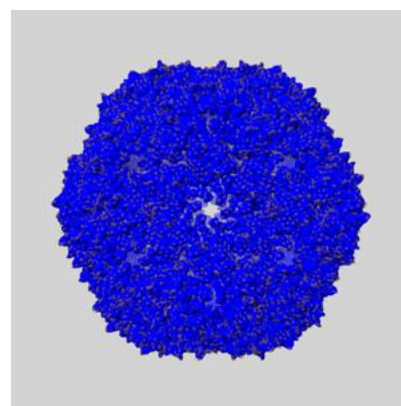
6.6.1 emd_0344_msk_1.map [i](#)



X



Y

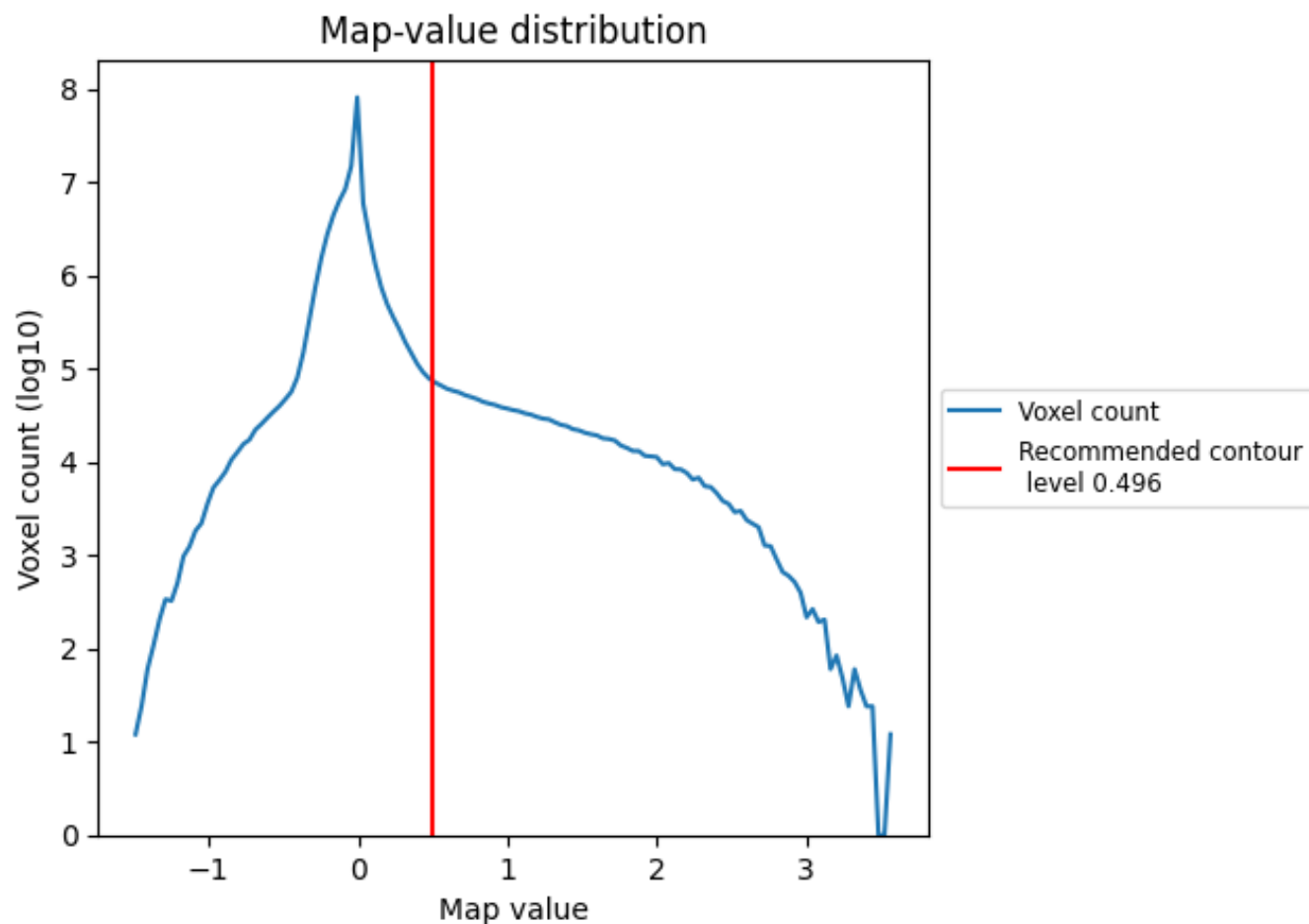


Z

7 Map analysis [i](#)

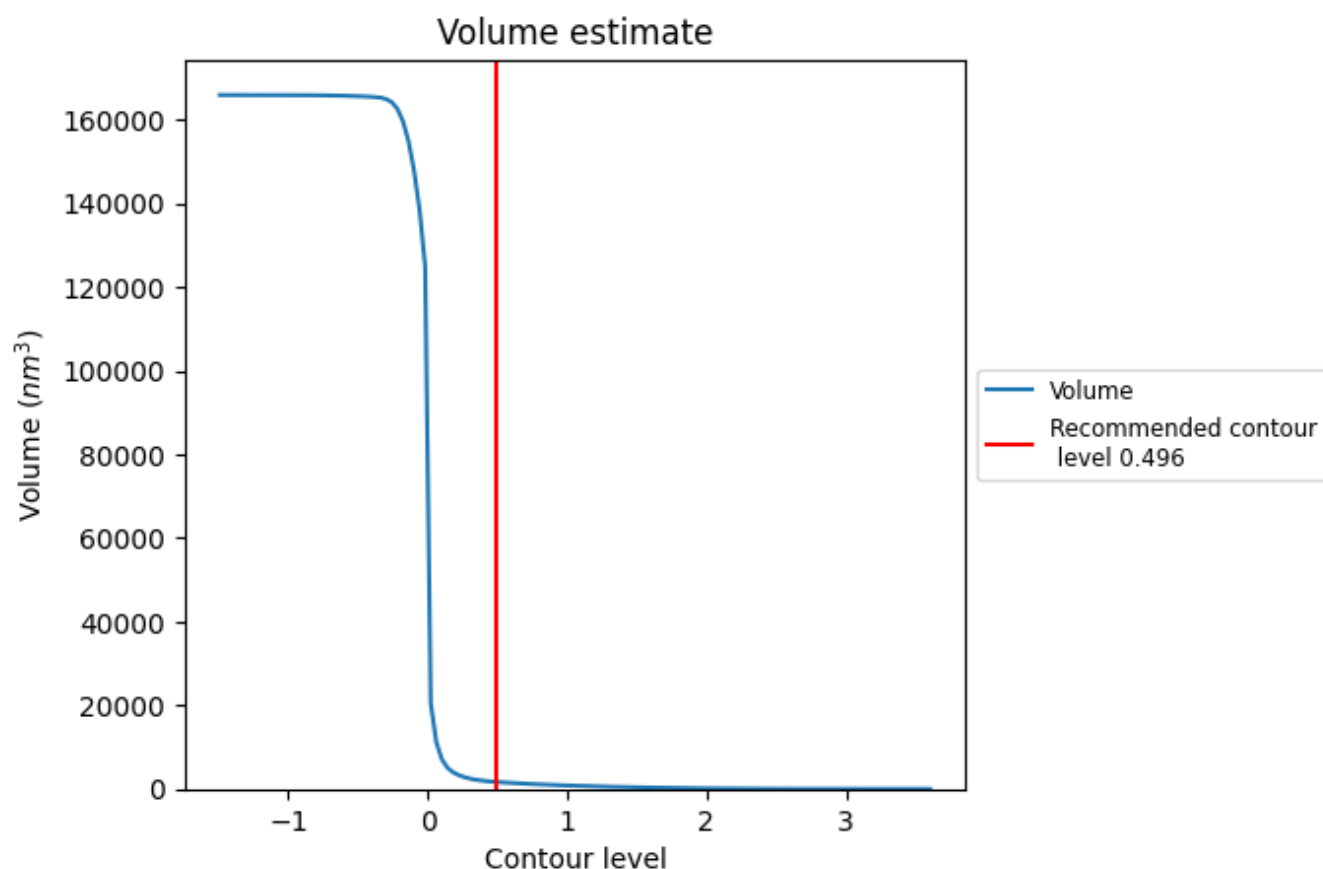
This section contains the results of statistical analysis of the map.

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.

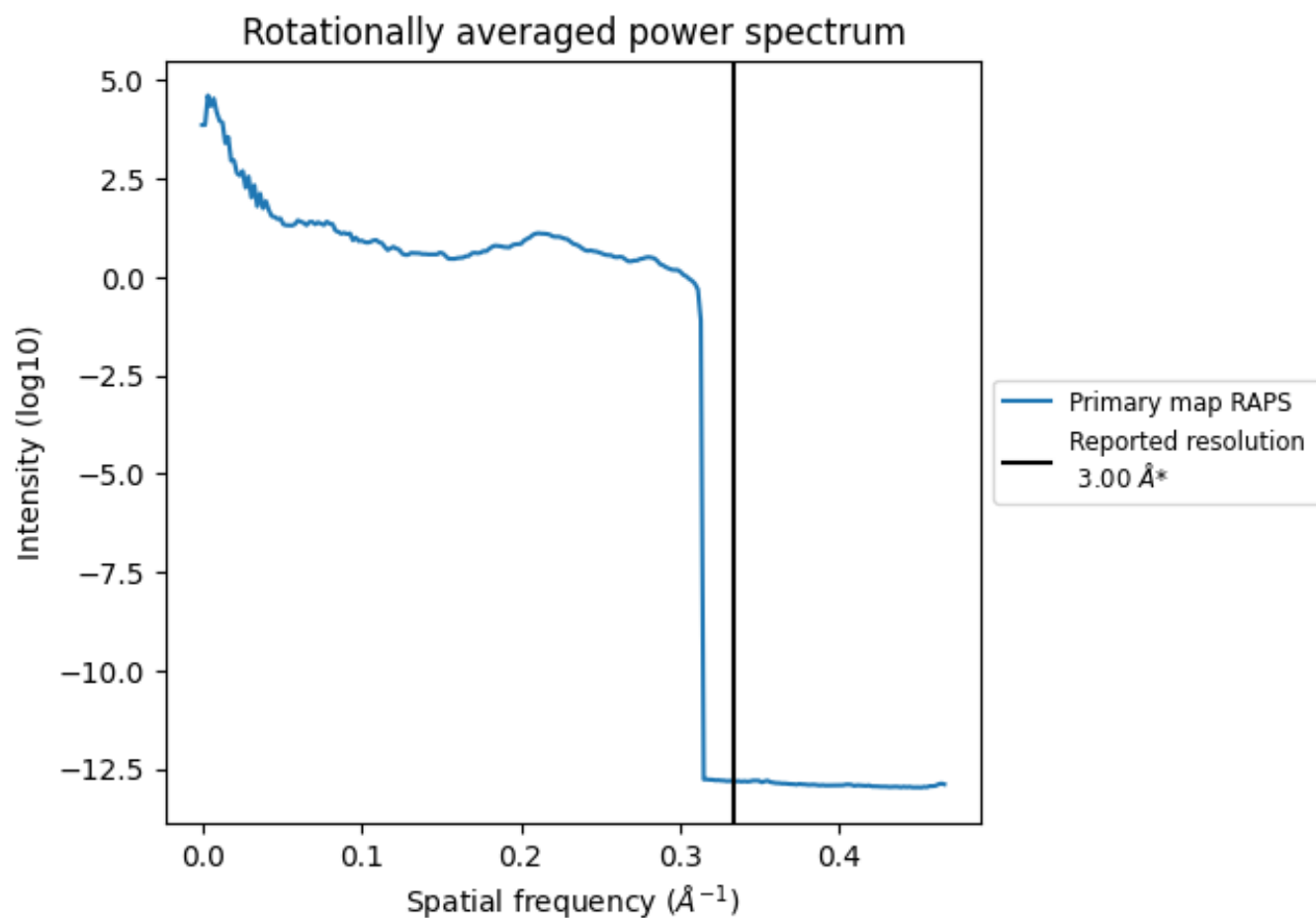
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1662 nm³; this corresponds to an approximate mass of 1501 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

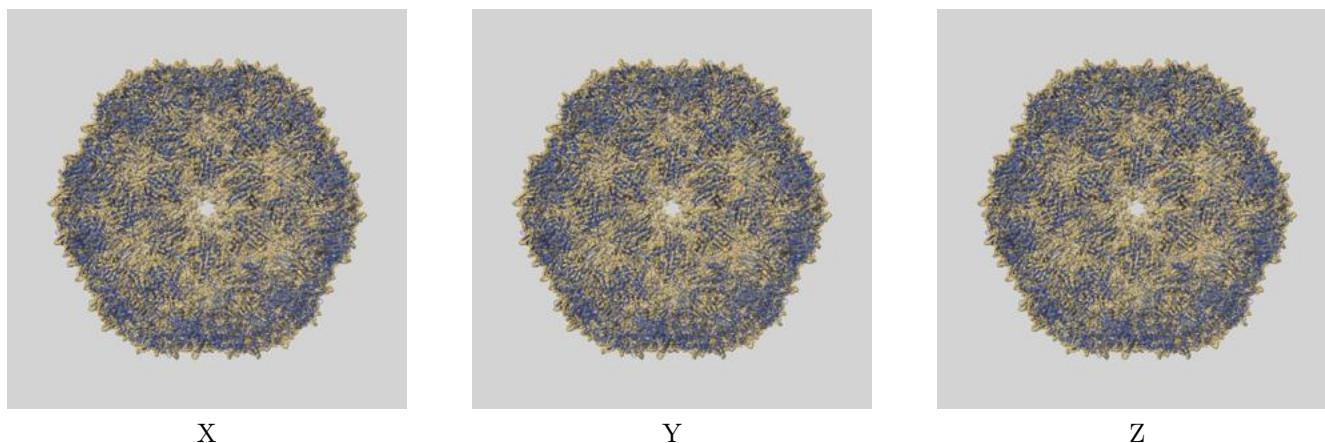
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

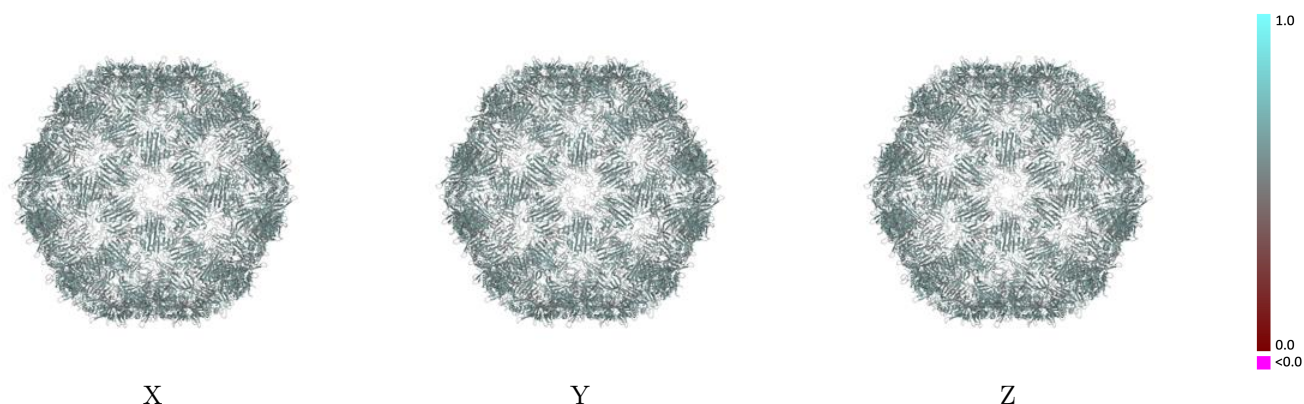
This section contains information regarding the fit between EMDB map EMD-0344 and PDB model 6N4V. Per-residue inclusion information can be found in section [3](#) on page [26](#).

9.1 Map-model overlay [i](#)



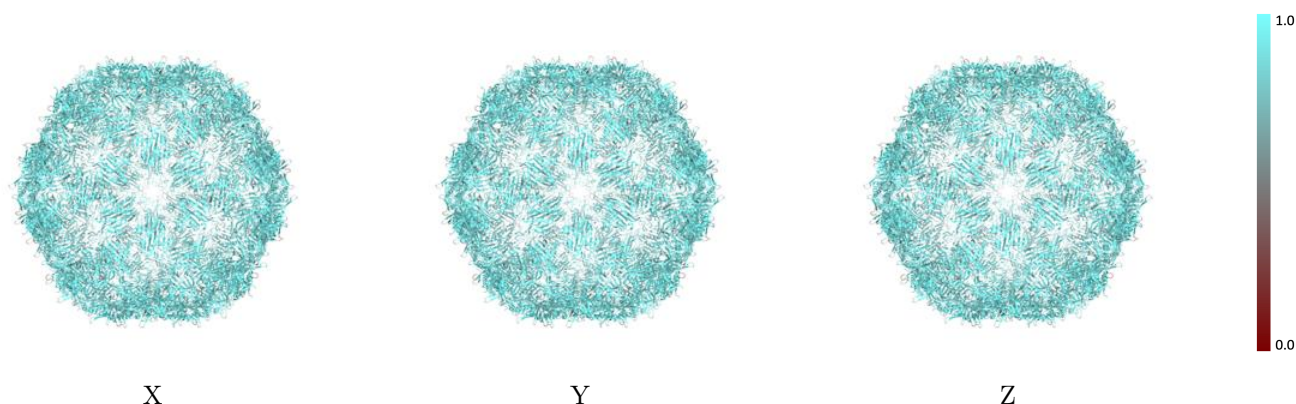
The images above show the 3D surface view of the map at the recommended contour level 0.496 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



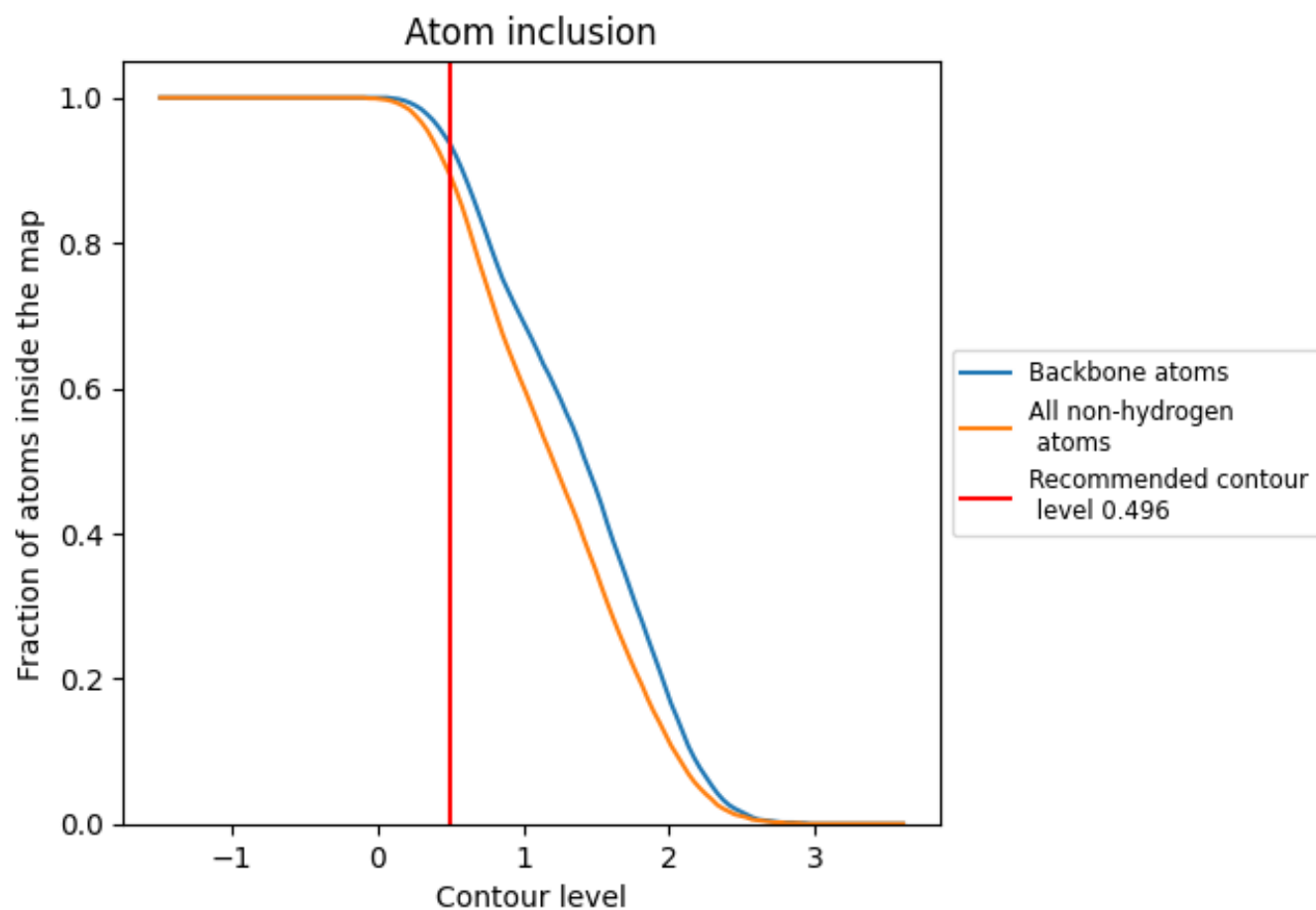
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.496).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 89% 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 (0.496) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8940	 0.5530
A	 0.8940	 0.5530
AA	 0.8920	 0.5450
AB	 0.8990	 0.5560
AC	 0.8970	 0.5540
AD	 0.8880	 0.5540
Af	 0.9010	 0.5510
B	 0.8970	 0.5550
BA	 0.8980	 0.5530
BB	 0.8910	 0.5520
BC	 0.8930	 0.5550
BD	 0.8940	 0.5510
C	 0.8960	 0.5490
CA	 0.9010	 0.5500
CB	 0.8940	 0.5520
CC	 0.9000	 0.5530
CD	 0.8920	 0.5520
D	 0.8960	 0.5540
DA	 0.9010	 0.5500
DB	 0.8900	 0.5520
DC	 0.8940	 0.5560
DD	 0.8950	 0.5520
E	 0.8940	 0.5520
EA	 0.8970	 0.5530
EB	 0.8870	 0.5530
EC	 0.8990	 0.5530
ED	 0.8900	 0.5530
F	 0.8920	 0.5490
FA	 0.8950	 0.5560
FB	 0.8920	 0.5540
FC	 0.8980	 0.5520
FD	 0.8880	 0.5520
G	 0.8870	 0.5510
GA	 0.9000	 0.5560
GB	 0.8890	 0.5510























































































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Chain	Atom inclusion	Q-score
GC	 0.8970	 0.5530
GD	 0.8890	 0.5520
H	 0.8910	 0.5490
HA	 0.8930	 0.5550
HB	 0.8970	 0.5550
HC	 0.8930	 0.5550
HD	 0.8940	 0.5540
I	 0.8910	 0.5500
IA	 0.8970	 0.5550
IB	 0.9020	 0.5500
IC	 0.8930	 0.5550
ID	 0.8930	 0.5560
J	 0.8880	 0.5460
JA	 0.8980	 0.5510
JB	 0.9000	 0.5570
JC	 0.8910	 0.5540
JD	 0.8940	 0.5530
K	 0.8990	 0.5530
KA	 0.8950	 0.5570
KB	 0.8980	 0.5570
KC	 0.8900	 0.5520
KD	 0.8950	 0.5500
L	 0.8990	 0.5510
LA	 0.8920	 0.5540
LB	 0.8920	 0.5550
LC	 0.8910	 0.5570
LD	 0.8950	 0.5530
M	 0.8980	 0.5520
MA	 0.8920	 0.5500
MB	 0.8990	 0.5540
MC	 0.8930	 0.5530
MD	 0.8920	 0.5510
N	 0.8970	 0.5540
NA	 0.8870	 0.5530
NB	 0.8930	 0.5560
NC	 0.9000	 0.5540
ND	 0.8870	 0.5540
O	 0.8940	 0.5550
OA	 0.8850	 0.5540
OB	 0.8980	 0.5570
OC	 0.8990	 0.5550
OD	 0.8900	 0.5560





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Chain	Atom inclusion	Q-score
P	 0.8980	 0.5500
PA	 0.8910	 0.5550
PB	 0.8980	 0.5550
PC	 0.8970	 0.5540
PD	 0.8920	 0.5530
Q	 0.8970	 0.5510
QA	 0.8880	 0.5490
QB	 0.8990	 0.5560
QC	 0.8990	 0.5560
R	 0.8960	 0.5550
RA	 0.8990	 0.5570
RB	 0.8910	 0.5540
RC	 0.8950	 0.5580
S	 0.8950	 0.5510
SA	 0.8970	 0.5520
SB	 0.8920	 0.5530
SC	 0.8940	 0.5530
T	 0.9000	 0.5540
TA	 0.8970	 0.5570
TB	 0.8880	 0.5540
TC	 0.8950	 0.5530
UA	 0.8970	 0.5550
UB	 0.8880	 0.5510
UC	 0.8910	 0.5520
V	 0.8890	 0.5500
VA	 0.8940	 0.5550
VB	 0.8930	 0.5550
VC	 0.8890	 0.5520
W	 0.8930	 0.5510
WA	 0.8950	 0.5560
WB	 0.8940	 0.5530
WC	 0.8890	 0.5510
X	 0.8910	 0.5530
XA	 0.8950	 0.5540
XB	 0.8950	 0.5540
XC	 0.8880	 0.5510
Y	 0.8890	 0.5480
YA	 0.8980	 0.5560
YB	 0.9000	 0.5540
YC	 0.8910	 0.5550
Z	 0.8920	 0.5510
ZA	 0.8980	 0.5510

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Chain	Atom inclusion	Q-score
ZB	 0.8990	 0.5540
ZC	 0.8910	 0.5540