Full wwPDB EM Validation Report ⓘ

May 16, 2024 – 01:10 PM EDT

PDB ID	:	8UEJ
EMDB ID	:	EMD-42163
Title	:	ssRNA phage PhiCb5 virion
Authors	:	Wang, Y.; Zhang, J.
Deposited on	:	2023-10-01
Resolution	:	2.70 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:

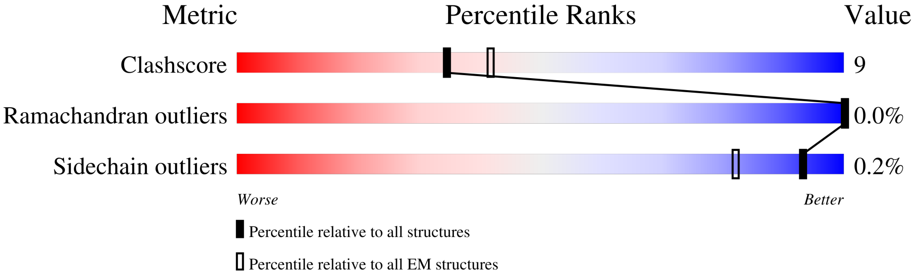
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	AA	122	 73% 27%
1	AB	122	 82% 17% •
1	AC	122	 79% 21%
1	AG	122	 78% 22%
1	AH	122	 86% 14%
1	AI	122	 75% 25%
1	AM	122	 83% 17%
1	AN	122	 76% 24%

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Mol	Chain	Length	Quality of chain
1	AO	122	
1	AS	122	
1	AT	122	
1	AU	122	
1	AY	122	
1	AZ	122	
1	BA	122	
1	BE	122	
1	BF	122	
1	BG	122	
1	BK	122	
1	BL	122	
1	BM	122	
1	BQ	122	
1	BR	122	
1	BS	122	
1	BW	122	
1	BX	122	
1	BY	122	
1	CC	122	
1	CD	122	
1	CE	122	
1	CI	122	
1	CJ	122	
1	CK	122	

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Mol	Chain	Length	Quality of chain
1	CO	122	
1	CP	122	
1	CQ	122	
1	CU	122	
1	CV	122	
1	CW	122	
1	DA	122	
1	DB	122	
1	DC	122	
1	DG	122	
1	DH	122	
1	DI	122	
1	DM	122	
1	DN	122	
1	DO	122	
1	DS	122	
1	DT	122	
1	DU	122	
1	DY	122	
1	DZ	122	
1	EA	122	
1	EE	122	
1	EF	122	
1	EG	122	
1	EK	122	

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Mol	Chain	Length	Quality of chain
1	EL	122	
1	EM	122	
1	EQ	122	
1	ER	122	
1	ES	122	
1	EW	122	
1	EX	122	
1	EY	122	
1	FC	122	
1	FD	122	
1	FE	122	
1	FI	122	
1	FJ	122	
1	FK	122	
1	FO	122	
1	FP	122	
1	FQ	122	
1	FU	122	
1	FV	122	
1	FW	122	
1	GA	122	
1	GB	122	
1	GC	122	
1	GG	122	
1	GH	122	

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Mol	Chain	Length	Quality of chain
1	GI	122	84% 16%
1	GM	122	80% 20%
1	GN	122	82% 18%
1	GO	122	74% 26%
1	GS	122	84% 16%
1	GT	122	75% 25%
1	GU	122	84% 16%
1	GY	122	• 77% 23%
1	GZ	122	74% 26%
1	HC	122	75% 25%
1	HD	122	• 79% 21%
1	HE	122	70% 30%
1	HI	122	83% 17%
1	HJ	122	• 84% 16%
1	HK	122	75% 25%
1	HO	122	80% 20%
1	HP	122	85% 15%
1	HQ	122	73% 27%
1	HU	122	81% 18% •
1	HV	122	84% 16%
1	HW	122	78% 22%
1	IA	122	89% 11%
1	IB	122	87% 13%
1	IC	122	85% 15%
1	IG	122	77% 23%

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Mol	Chain	Length	Quality of chain
1	IH	122	
1	II	122	
1	IM	122	
1	IN	122	
1	IO	122	
1	IS	122	
1	IT	122	
1	IU	122	
1	IY	122	
1	IZ	122	
1	JA	122	
1	JE	122	
1	JF	122	
1	JG	122	
1	JK	122	
1	JL	122	
1	JM	122	
1	JQ	122	
1	JR	122	
1	JS	122	
1	JW	122	
1	JX	122	
1	JY	122	
1	KC	122	
1	KD	122	

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Mol	Chain	Length	Quality of chain
1	KE	122	 75% 25%
1	KI	122	 75% 25%
1	KJ	122	 74% 26%
1	KK	122	 75% 25%
1	KO	122	 83% 17%
1	KP	122	 81% 19%
1	KQ	122	 84% 16%
1	KU	122	 84% 16%
1	KV	122	 75% 25%
1	KW	122	 77% 23%
1	LA	122	 81% 19%
1	LB	122	 80% 20%
1	LC	122	 76% 24%
1	LG	122	 82% 18%
1	LH	122	 84% 16%
1	LI	122	 84% 16%
1	LM	122	 78% 22%
1	LN	122	 81% 19%
1	LO	122	 82% 18%
1	LS	122	 79% 21%
1	LT	122	 79% 21%
1	LU	122	 75% 25%
1	LY	122	 74% 26%
1	LZ	122	 76% 24%
1	MA	122	 82% 18%

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Mol	Chain	Length	Quality of chain
1	ME	122	80% 20%
1	MF	122	79% 21%
1	MG	122	76% 24%
1	MK	122	77% 23%
1	ML	122	81% 19%
1	MM	122	79% 21%
1	MQ	122	84% 16%
1	MR	122	72% 28%
1	MS	122	80% 20%
1	MW	122	75% 25%
1	MX	122	76% 24%
1	NA	122	77% 22%
1	NB	122	79% 21%
1	NC	122	66% 34%
1	NG	122	86% 14%
1	NH	122	80% 20%
1	NI	122	80% 20%
1	NM	122	81% 19%
1	NN	122	75% 24%
1	NO	122	80% 20%
2	M	372	30% 83% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 172913 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	AA	122	Total 954	C 602	N 162	O 190	0	0
1	AB	122	Total 954	C 602	N 162	O 190	0	0
1	AC	122	Total 954	C 602	N 162	O 190	0	0
1	AG	122	Total 954	C 602	N 162	O 190	0	0
1	AH	122	Total 954	C 602	N 162	O 190	0	0
1	AI	122	Total 954	C 602	N 162	O 190	0	0
1	AM	122	Total 954	C 602	N 162	O 190	0	0
1	AN	122	Total 954	C 602	N 162	O 190	0	0
1	AO	122	Total 954	C 602	N 162	O 190	0	0
1	AS	122	Total 954	C 602	N 162	O 190	0	0
1	AT	122	Total 954	C 602	N 162	O 190	0	0
1	AU	122	Total 954	C 602	N 162	O 190	0	0
1	AY	122	Total 954	C 602	N 162	O 190	0	0
1	AZ	122	Total 954	C 602	N 162	O 190	0	0
1	BA	122	Total 954	C 602	N 162	O 190	0	0
1	BE	122	Total 954	C 602	N 162	O 190	0	0
1	BF	122	Total 954	C 602	N 162	O 190	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	BG	122	Total 954	C 602	N 162	O 190	0	0
1	BK	122	Total 954	C 602	N 162	O 190	0	0
1	BL	122	Total 954	C 602	N 162	O 190	0	0
1	BM	122	Total 954	C 602	N 162	O 190	0	0
1	BQ	122	Total 954	C 602	N 162	O 190	0	0
1	BR	122	Total 954	C 602	N 162	O 190	0	0
1	BS	122	Total 954	C 602	N 162	O 190	0	0
1	BW	122	Total 954	C 602	N 162	O 190	0	0
1	BX	122	Total 954	C 602	N 162	O 190	0	0
1	BY	122	Total 954	C 602	N 162	O 190	0	0
1	CC	122	Total 954	C 602	N 162	O 190	0	0
1	CD	122	Total 954	C 602	N 162	O 190	0	0
1	CE	122	Total 954	C 602	N 162	O 190	0	0
1	CI	122	Total 954	C 602	N 162	O 190	0	0
1	CJ	122	Total 954	C 602	N 162	O 190	0	0
1	CK	122	Total 954	C 602	N 162	O 190	0	0
1	CO	122	Total 954	C 602	N 162	O 190	0	0
1	CP	122	Total 954	C 602	N 162	O 190	0	0
1	CQ	122	Total 954	C 602	N 162	O 190	0	0
1	CU	122	Total 954	C 602	N 162	O 190	0	0
1	CV	122	Total 954	C 602	N 162	O 190	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	CW	122	Total C N O 954 602 162 190	0	0
1	DA	122	Total C N O 954 602 162 190	0	0
1	DB	122	Total C N O 954 602 162 190	0	0
1	DC	122	Total C N O 954 602 162 190	0	0
1	DG	122	Total C N O 954 602 162 190	0	0
1	DH	122	Total C N O 954 602 162 190	0	0
1	DI	122	Total C N O 954 602 162 190	0	0
1	DM	122	Total C N O 954 602 162 190	0	0
1	DN	122	Total C N O 954 602 162 190	0	0
1	DO	122	Total C N O 954 602 162 190	0	0
1	DS	122	Total C N O 954 602 162 190	0	0
1	DT	122	Total C N O 954 602 162 190	0	0
1	DU	122	Total C N O 954 602 162 190	0	0
1	DY	122	Total C N O 954 602 162 190	0	0
1	DZ	122	Total C N O 954 602 162 190	0	0
1	EA	122	Total C N O 954 602 162 190	0	0
1	EE	122	Total C N O 954 602 162 190	0	0
1	EF	122	Total C N O 954 602 162 190	0	0
1	EG	122	Total C N O 954 602 162 190	0	0
1	EK	122	Total C N O 954 602 162 190	0	0
1	EL	122	Total C N O 954 602 162 190	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	EM	122	Total C N O 954 602 162 190	0	0
1	EQ	122	Total C N O 954 602 162 190	0	0
1	ER	122	Total C N O 954 602 162 190	0	0
1	ES	122	Total C N O 954 602 162 190	0	0
1	EW	122	Total C N O 954 602 162 190	0	0
1	EX	122	Total C N O 954 602 162 190	0	0
1	EY	122	Total C N O 954 602 162 190	0	0
1	FC	122	Total C N O 954 602 162 190	0	0
1	FD	122	Total C N O 954 602 162 190	0	0
1	FE	122	Total C N O 954 602 162 190	0	0
1	FI	122	Total C N O 954 602 162 190	0	0
1	FJ	122	Total C N O 954 602 162 190	0	0
1	FK	122	Total C N O 954 602 162 190	0	0
1	FO	122	Total C N O 954 602 162 190	0	0
1	FP	122	Total C N O 954 602 162 190	0	0
1	FQ	122	Total C N O 954 602 162 190	0	0
1	FU	122	Total C N O 954 602 162 190	0	0
1	FV	122	Total C N O 954 602 162 190	0	0
1	FW	122	Total C N O 954 602 162 190	0	0
1	GA	122	Total C N O 954 602 162 190	0	0
1	GB	122	Total C N O 954 602 162 190	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	GC	122	Total 954	C 602	N 162	O 190	0	0
1	GG	122	Total 954	C 602	N 162	O 190	0	0
1	GH	122	Total 954	C 602	N 162	O 190	0	0
1	GI	122	Total 954	C 602	N 162	O 190	0	0
1	GM	122	Total 954	C 602	N 162	O 190	0	0
1	GN	122	Total 954	C 602	N 162	O 190	0	0
1	GO	122	Total 954	C 602	N 162	O 190	0	0
1	GS	122	Total 954	C 602	N 162	O 190	0	0
1	GT	122	Total 954	C 602	N 162	O 190	0	0
1	GU	122	Total 954	C 602	N 162	O 190	0	0
1	GY	122	Total 954	C 602	N 162	O 190	0	0
1	GZ	122	Total 954	C 602	N 162	O 190	0	0
1	HC	122	Total 954	C 602	N 162	O 190	0	0
1	HD	122	Total 954	C 602	N 162	O 190	0	0
1	HE	122	Total 954	C 602	N 162	O 190	0	0
1	HI	122	Total 954	C 602	N 162	O 190	0	0
1	HJ	122	Total 954	C 602	N 162	O 190	0	0
1	HK	122	Total 954	C 602	N 162	O 190	0	0
1	HO	122	Total 954	C 602	N 162	O 190	0	0
1	HP	122	Total 954	C 602	N 162	O 190	0	0
1	HQ	122	Total 954	C 602	N 162	O 190	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	HU	122	Total 954	C 602	N 162	O 190	0	0
1	HV	122	Total 954	C 602	N 162	O 190	0	0
1	HW	122	Total 954	C 602	N 162	O 190	0	0
1	IA	122	Total 954	C 602	N 162	O 190	0	0
1	IB	122	Total 954	C 602	N 162	O 190	0	0
1	IC	122	Total 954	C 602	N 162	O 190	0	0
1	IG	122	Total 954	C 602	N 162	O 190	0	0
1	IH	122	Total 954	C 602	N 162	O 190	0	0
1	II	122	Total 954	C 602	N 162	O 190	0	0
1	IM	122	Total 954	C 602	N 162	O 190	0	0
1	IN	122	Total 954	C 602	N 162	O 190	0	0
1	IO	122	Total 954	C 602	N 162	O 190	0	0
1	IS	122	Total 954	C 602	N 162	O 190	0	0
1	IT	122	Total 954	C 602	N 162	O 190	0	0
1	IU	122	Total 954	C 602	N 162	O 190	0	0
1	IY	122	Total 954	C 602	N 162	O 190	0	0
1	IZ	122	Total 954	C 602	N 162	O 190	0	0
1	JA	122	Total 954	C 602	N 162	O 190	0	0
1	JE	122	Total 954	C 602	N 162	O 190	0	0
1	JF	122	Total 954	C 602	N 162	O 190	0	0
1	JG	122	Total 954	C 602	N 162	O 190	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	JK	122	Total 954	C 602	N 162	O 190	0	0
1	JL	122	Total 954	C 602	N 162	O 190	0	0
1	JM	122	Total 954	C 602	N 162	O 190	0	0
1	JQ	122	Total 954	C 602	N 162	O 190	0	0
1	JR	122	Total 954	C 602	N 162	O 190	0	0
1	JS	122	Total 954	C 602	N 162	O 190	0	0
1	JW	122	Total 954	C 602	N 162	O 190	0	0
1	JX	122	Total 954	C 602	N 162	O 190	0	0
1	JY	122	Total 954	C 602	N 162	O 190	0	0
1	KC	122	Total 954	C 602	N 162	O 190	0	0
1	KD	122	Total 954	C 602	N 162	O 190	0	0
1	KE	122	Total 954	C 602	N 162	O 190	0	0
1	KI	122	Total 954	C 602	N 162	O 190	0	0
1	KJ	122	Total 954	C 602	N 162	O 190	0	0
1	KK	122	Total 954	C 602	N 162	O 190	0	0
1	KO	122	Total 954	C 602	N 162	O 190	0	0
1	KP	122	Total 954	C 602	N 162	O 190	0	0
1	KQ	122	Total 954	C 602	N 162	O 190	0	0
1	KU	122	Total 954	C 602	N 162	O 190	0	0
1	KV	122	Total 954	C 602	N 162	O 190	0	0
1	KW	122	Total 954	C 602	N 162	O 190	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	LA	122	Total 954	C 602	N 162	O 190	0	0
1	LB	122	Total 954	C 602	N 162	O 190	0	0
1	LC	122	Total 954	C 602	N 162	O 190	0	0
1	LG	122	Total 954	C 602	N 162	O 190	0	0
1	LH	122	Total 954	C 602	N 162	O 190	0	0
1	LI	122	Total 954	C 602	N 162	O 190	0	0
1	LM	122	Total 954	C 602	N 162	O 190	0	0
1	LN	122	Total 954	C 602	N 162	O 190	0	0
1	LO	122	Total 954	C 602	N 162	O 190	0	0
1	LS	122	Total 954	C 602	N 162	O 190	0	0
1	LT	122	Total 954	C 602	N 162	O 190	0	0
1	LU	122	Total 954	C 602	N 162	O 190	0	0
1	LY	122	Total 954	C 602	N 162	O 190	0	0
1	LZ	122	Total 954	C 602	N 162	O 190	0	0
1	MA	122	Total 954	C 602	N 162	O 190	0	0
1	ME	122	Total 954	C 602	N 162	O 190	0	0
1	MF	122	Total 954	C 602	N 162	O 190	0	0
1	MG	122	Total 954	C 602	N 162	O 190	0	0
1	MK	122	Total 954	C 602	N 162	O 190	0	0
1	ML	122	Total 954	C 602	N 162	O 190	0	0
1	MM	122	Total 954	C 602	N 162	O 190	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	MQ	122	Total 954	C 602	N 162	O 190	0	0
1	MR	122	Total 954	C 602	N 162	O 190	0	0
1	MS	122	Total 954	C 602	N 162	O 190	0	0
1	MW	122	Total 954	C 602	N 162	O 190	0	0
1	MX	122	Total 954	C 602	N 162	O 190	0	0
1	NA	122	Total 954	C 602	N 162	O 190	0	0
1	NB	122	Total 954	C 602	N 162	O 190	0	0
1	NC	122	Total 954	C 602	N 162	O 190	0	0
1	NG	122	Total 954	C 602	N 162	O 190	0	0
1	NH	122	Total 954	C 602	N 162	O 190	0	0
1	NI	122	Total 954	C 602	N 162	O 190	0	0
1	NM	122	Total 954	C 602	N 162	O 190	0	0
1	NN	122	Total 954	C 602	N 162	O 190	0	0
1	NO	122	Total 954	C 602	N 162	O 190	0	0

- Molecule 2 is a protein called Maturation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	372	Total 2865	C 1805	N 522	O 527	S 11	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	AA	2	Total 2	Ca 2	0
3	AB	2	Total 2	Ca 2	0

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Mol	Chain	Residues	Atoms	AltConf
3	AC	2	Total Ca 2 2	0
3	AH	2	Total Ca 2 2	0
3	AI	2	Total Ca 2 2	0
3	AM	1	Total Ca 1 1	0
3	AN	2	Total Ca 2 2	0
3	AO	2	Total Ca 2 2	0
3	AS	1	Total Ca 1 1	0
3	AT	3	Total Ca 3 3	0
3	AU	1	Total Ca 1 1	0
3	AY	2	Total Ca 2 2	0
3	AZ	3	Total Ca 3 3	0
3	BA	1	Total Ca 1 1	0
3	BE	1	Total Ca 1 1	0
3	BG	1	Total Ca 1 1	0
3	BK	3	Total Ca 3 3	0
3	BM	1	Total Ca 1 1	0
3	BQ	3	Total Ca 3 3	0
3	BR	1	Total Ca 1 1	0
3	BS	1	Total Ca 1 1	0
3	BW	1	Total Ca 1 1	0
3	BX	1	Total Ca 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
3	BY	2	Total Ca 2 2	0
3	CC	2	Total Ca 2 2	0
3	CD	1	Total Ca 1 1	0
3	CE	2	Total Ca 2 2	0
3	CI	3	Total Ca 3 3	0
3	CK	2	Total Ca 2 2	0
3	CO	3	Total Ca 3 3	0
3	CP	1	Total Ca 1 1	0
3	CQ	1	Total Ca 1 1	0
3	CU	1	Total Ca 1 1	0
3	CV	2	Total Ca 2 2	0
3	CW	1	Total Ca 1 1	0
3	DB	1	Total Ca 1 1	0
3	DG	2	Total Ca 2 2	0
3	DH	1	Total Ca 1 1	0
3	DM	1	Total Ca 1 1	0
3	DN	1	Total Ca 1 1	0
3	DO	2	Total Ca 2 2	0
3	DS	2	Total Ca 2 2	0
3	DT	1	Total Ca 1 1	0
3	DY	2	Total Ca 2 2	0

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Mol	Chain	Residues	Atoms	AltConf
3	DZ	1	Total Ca 1 1	0
3	EE	2	Total Ca 2 2	0
3	EF	1	Total Ca 1 1	0
3	EG	1	Total Ca 1 1	0
3	EK	1	Total Ca 1 1	0
3	EM	2	Total Ca 2 2	0
3	EQ	2	Total Ca 2 2	0
3	ER	2	Total Ca 2 2	0
3	ES	2	Total Ca 2 2	0
3	EW	1	Total Ca 1 1	0
3	EX	2	Total Ca 2 2	0
3	FC	2	Total Ca 2 2	0
3	FD	1	Total Ca 1 1	0
3	FI	1	Total Ca 1 1	0
3	FJ	3	Total Ca 3 3	0
3	FK	2	Total Ca 2 2	0
3	FO	3	Total Ca 3 3	0
3	FP	1	Total Ca 1 1	0
3	FU	2	Total Ca 2 2	0
3	FV	1	Total Ca 1 1	0
3	FW	1	Total Ca 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
3	GA	1	Total Ca 1 1	0
3	GB	2	Total Ca 2 2	0
3	GC	2	Total Ca 2 2	0
3	GH	1	Total Ca 1 1	0
3	GI	2	Total Ca 2 2	0
3	GM	3	Total Ca 3 3	0
3	GO	2	Total Ca 2 2	0
3	GS	1	Total Ca 1 1	0
3	GT	1	Total Ca 1 1	0
3	GY	1	Total Ca 1 1	0
3	HC	2	Total Ca 2 2	0
3	HD	2	Total Ca 2 2	0
3	HE	1	Total Ca 1 1	0
3	HI	2	Total Ca 2 2	0
3	HK	1	Total Ca 1 1	0
3	HO	3	Total Ca 3 3	0
3	HP	2	Total Ca 2 2	0
3	HU	3	Total Ca 3 3	0
3	HV	1	Total Ca 1 1	0
3	HW	2	Total Ca 2 2	0
3	IA	1	Total Ca 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
3	IB	2	Total Ca 2 2	0
3	IC	1	Total Ca 1 1	0
3	IG	1	Total Ca 1 1	0
3	IH	1	Total Ca 1 1	0
3	II	1	Total Ca 1 1	0
3	IM	2	Total Ca 2 2	0
3	IO	1	Total Ca 1 1	0
3	IS	3	Total Ca 3 3	0
3	IU	1	Total Ca 1 1	0
3	IY	1	Total Ca 1 1	0
3	IZ	3	Total Ca 3 3	0
3	JA	2	Total Ca 2 2	0
3	JE	1	Total Ca 1 1	0
3	JF	1	Total Ca 1 1	0
3	JK	2	Total Ca 2 2	0
3	JL	1	Total Ca 1 1	0
3	JQ	1	Total Ca 1 1	0
3	JR	2	Total Ca 2 2	0
3	JW	2	Total Ca 2 2	0
3	JX	1	Total Ca 1 1	0
3	JY	2	Total Ca 2 2	0

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Mol	Chain	Residues	Atoms	AltConf
3	KC	3	Total Ca 3 3	0
3	KD	2	Total Ca 2 2	0
3	KI	1	Total Ca 1 1	0
3	KJ	1	Total Ca 1 1	0
3	KK	1	Total Ca 1 1	0
3	KO	2	Total Ca 2 2	0
3	KQ	1	Total Ca 1 1	0
3	KU	3	Total Ca 3 3	0
3	KV	1	Total Ca 1 1	0
3	KW	2	Total Ca 2 2	0
3	LA	1	Total Ca 1 1	0
3	LB	1	Total Ca 1 1	0
3	LG	2	Total Ca 2 2	0
3	LH	1	Total Ca 1 1	0
3	LI	3	Total Ca 3 3	0
3	LM	2	Total Ca 2 2	0
3	LN	2	Total Ca 2 2	0
3	LO	2	Total Ca 2 2	0
3	LS	1	Total Ca 1 1	0
3	LT	1	Total Ca 1 1	0
3	LU	1	Total Ca 1 1	0

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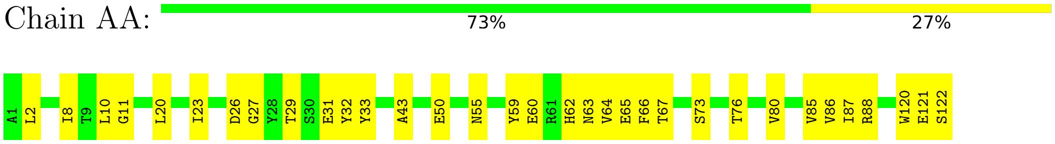
Mol	Chain	Residues	Atoms	AltConf
3	LY	2	Total Ca 2 2	0
3	ME	2	Total Ca 2 2	0
3	MG	2	Total Ca 2 2	0
3	MK	3	Total Ca 3 3	0
3	MQ	2	Total Ca 2 2	0
3	MR	2	Total Ca 2 2	0
3	MS	2	Total Ca 2 2	0
3	MX	1	Total Ca 1 1	0
3	NA	2	Total Ca 2 2	0
3	NC	1	Total Ca 1 1	0
3	NG	3	Total Ca 3 3	0
3	NI	2	Total Ca 2 2	0
3	NM	1	Total Ca 1 1	0
3	NN	1	Total Ca 1 1	0
3	NO	1	Total Ca 1 1	0

3 Residue-property plots ⓘ

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.

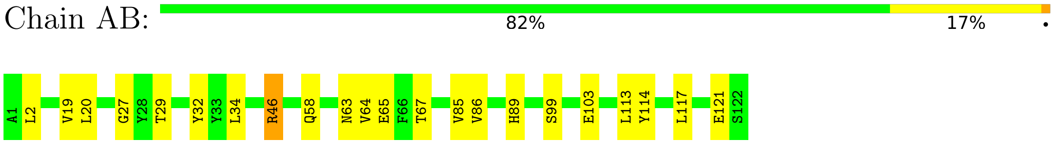
- Molecule 1: Coat protein

Chain AA:



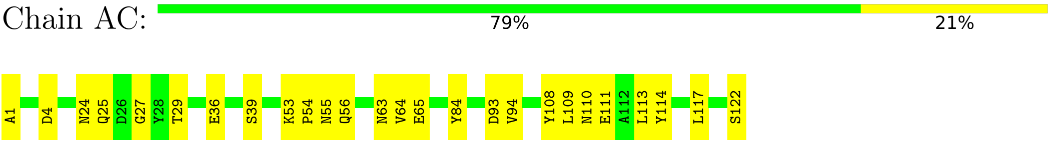
- Molecule 1: Coat protein

Chain AB:



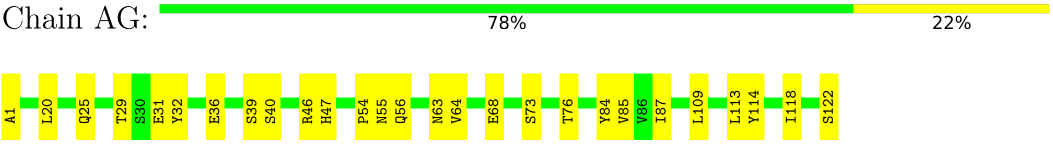
- Molecule 1: Coat protein

Chain AC:



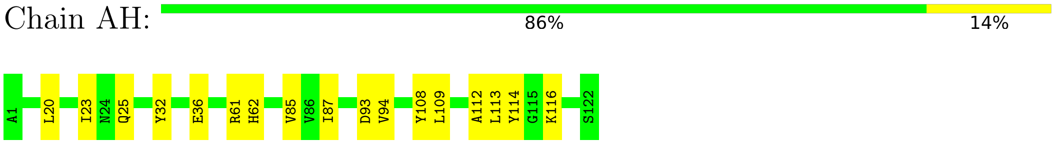
- Molecule 1: Coat protein

Chain AG:



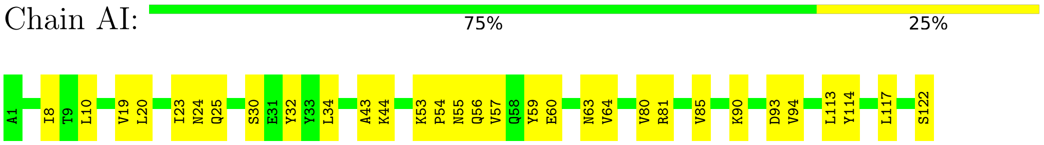
- Molecule 1: Coat protein

Chain AH:



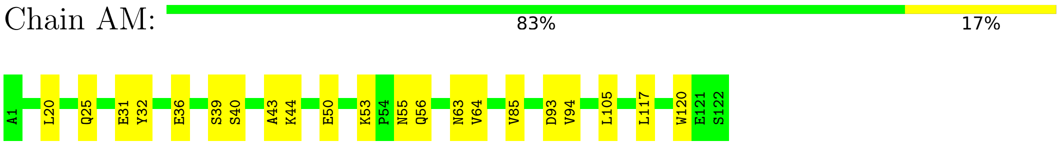
- Molecule 1: Coat protein

Chain AI:



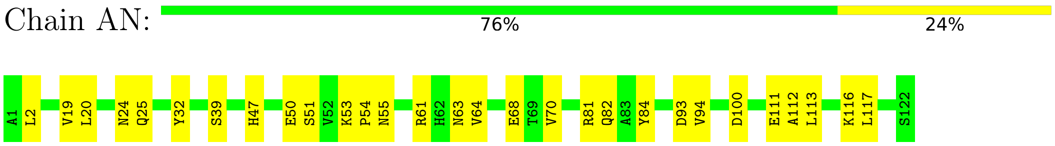
- Molecule 1: Coat protein

Chain AM:



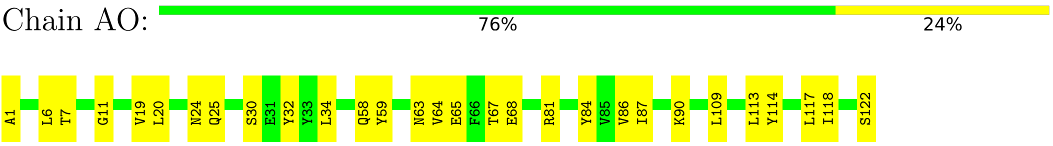
- Molecule 1: Coat protein

Chain AN:



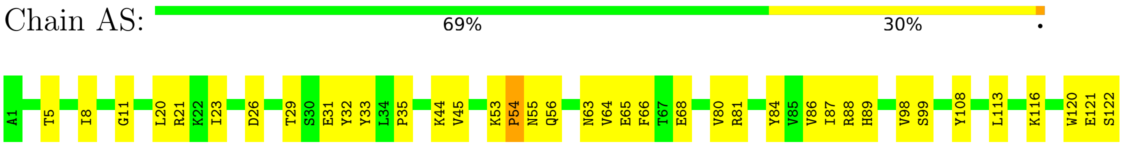
- Molecule 1: Coat protein

Chain AO:



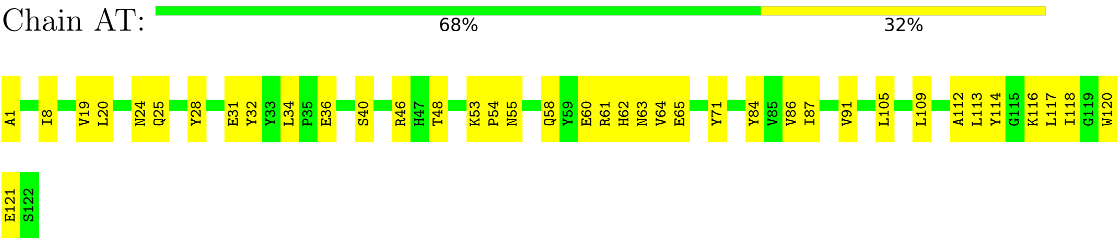
- Molecule 1: Coat protein

Chain AS:



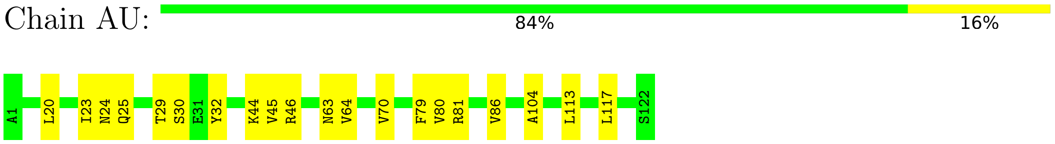
- Molecule 1: Coat protein

Chain AT:



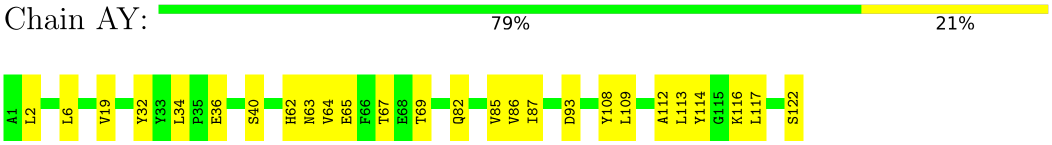
- Molecule 1: Coat protein

Chain AU:



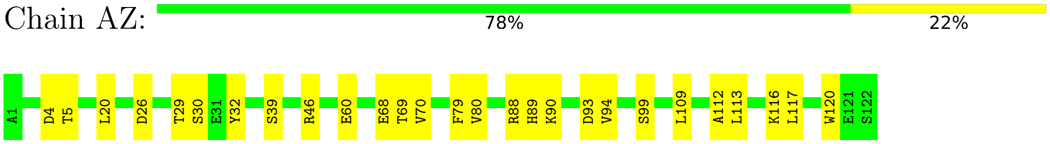
- Molecule 1: Coat protein

Chain AY:



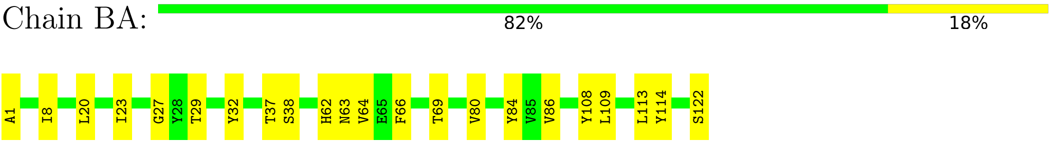
- Molecule 1: Coat protein

Chain AZ:



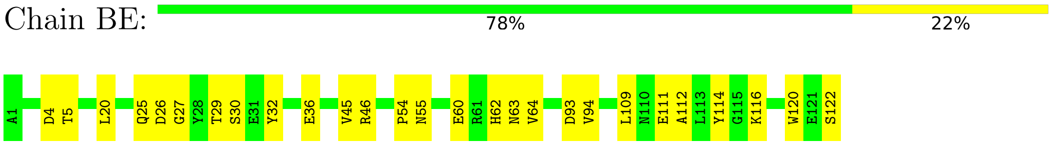
- Molecule 1: Coat protein

Chain BA:



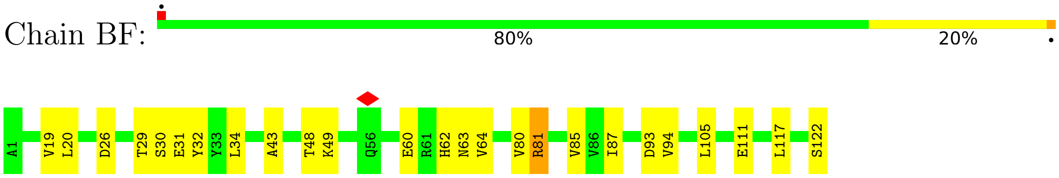
- Molecule 1: Coat protein

Chain BE:



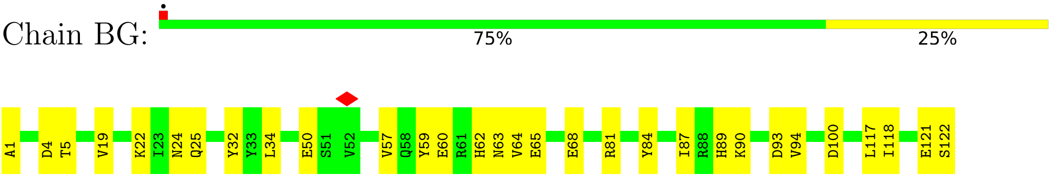
- Molecule 1: Coat protein

Chain BF:



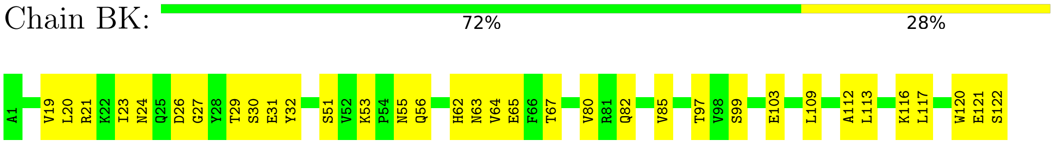
- Molecule 1: Coat protein

Chain BG:



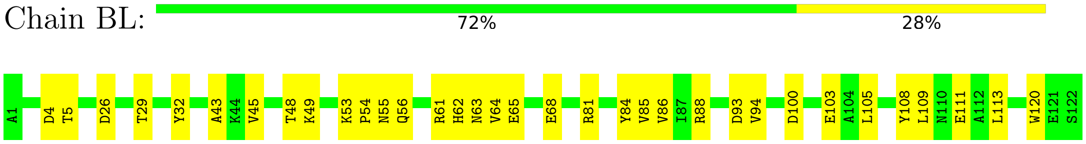
- Molecule 1: Coat protein

Chain BK:



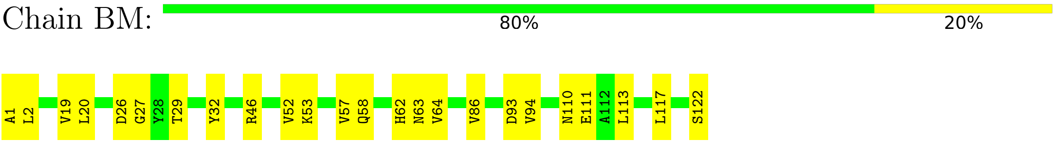
- Molecule 1: Coat protein

Chain BL:



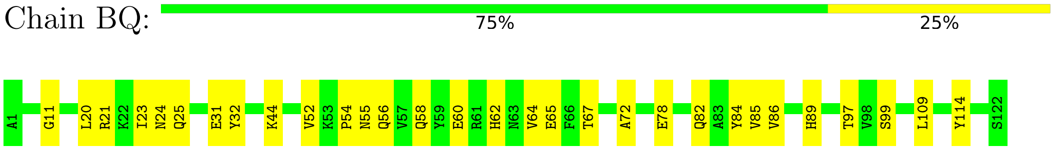
- Molecule 1: Coat protein

Chain BM:



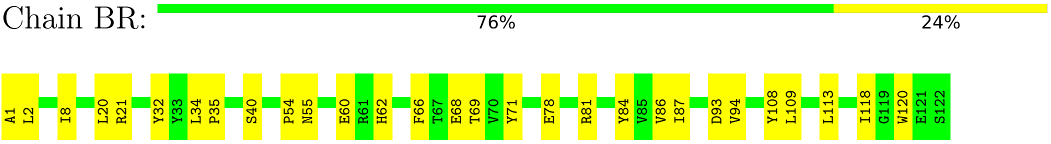
- Molecule 1: Coat protein

Chain BQ:



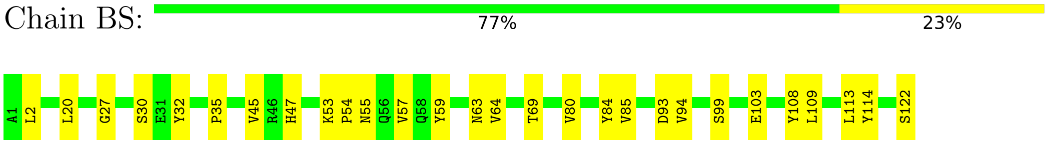
- Molecule 1: Coat protein

Chain BR:



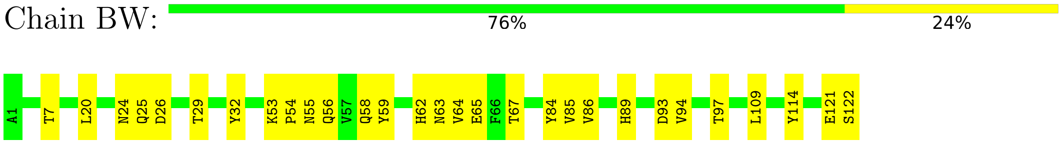
- Molecule 1: Coat protein

Chain BS:



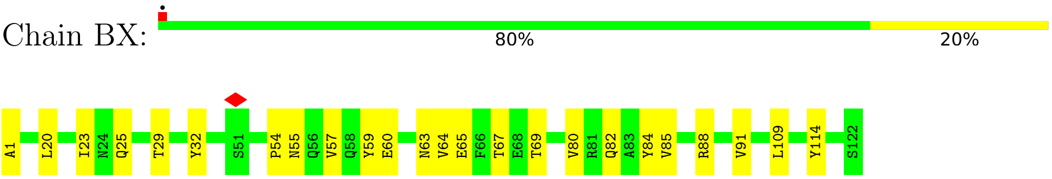
- Molecule 1: Coat protein

Chain BW:

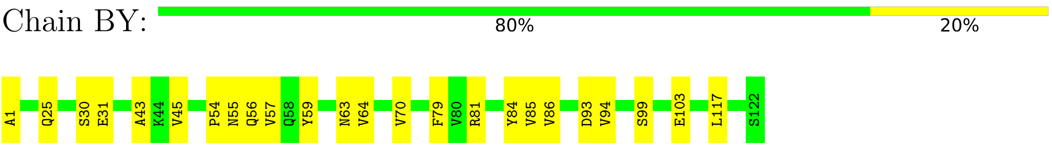


- Molecule 1: Coat protein

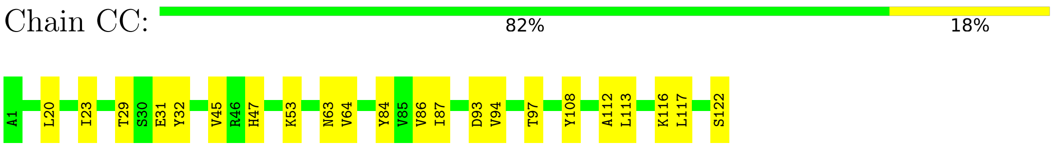
Chain BX:



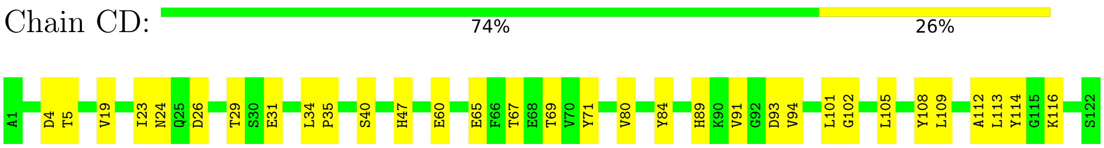
- Molecule 1: Coat protein



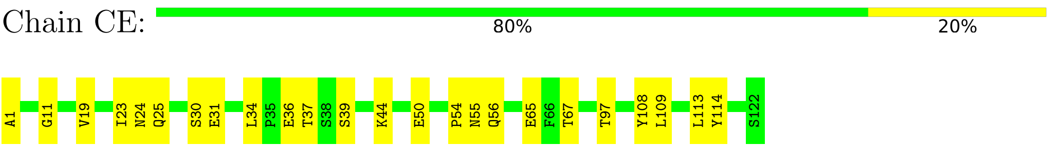
- Molecule 1: Coat protein



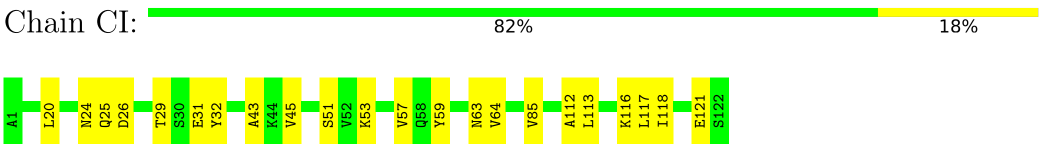
- Molecule 1: Coat protein



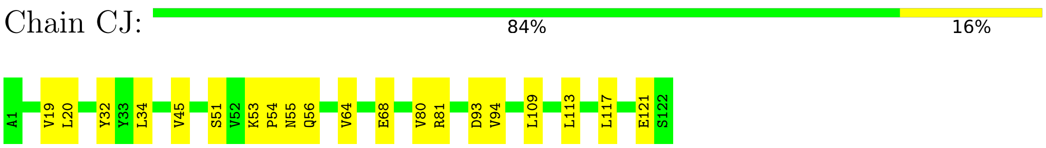
- Molecule 1: Coat protein



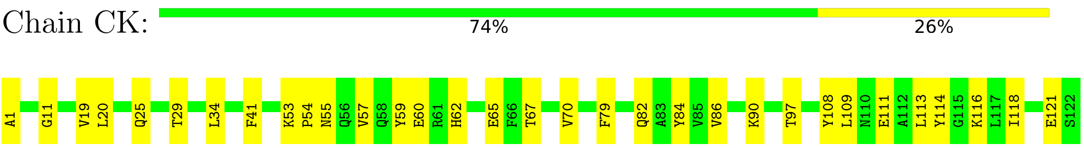
- Molecule 1: Coat protein



- Molecule 1: Coat protein

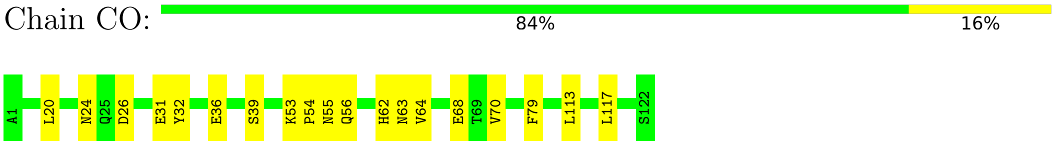


- Molecule 1: Coat protein



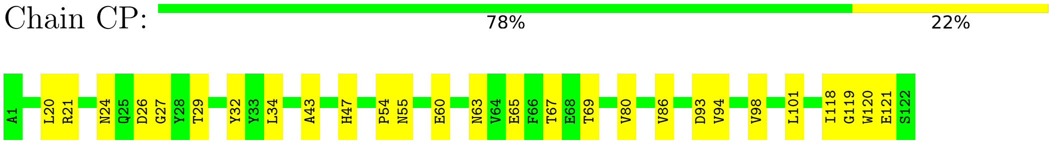
- Molecule 1: Coat protein

Chain CO:



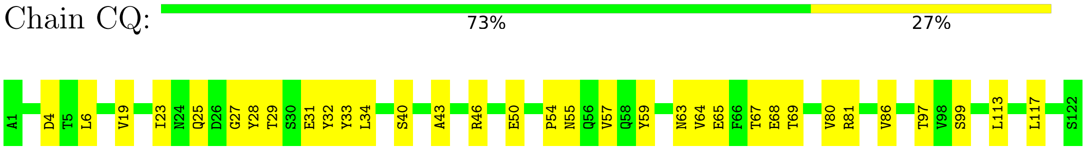
- Molecule 1: Coat protein

Chain CP:



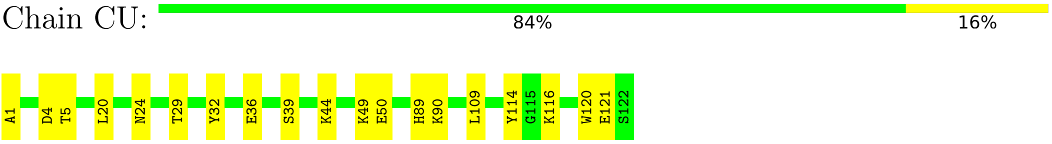
- Molecule 1: Coat protein

Chain CQ:



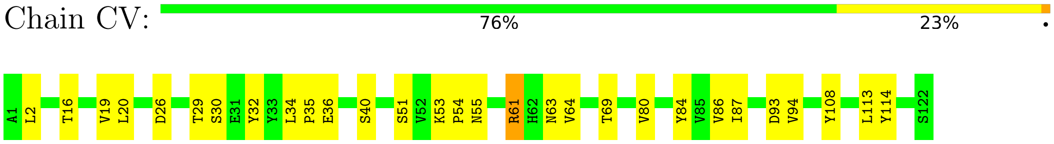
- Molecule 1: Coat protein

Chain CU:



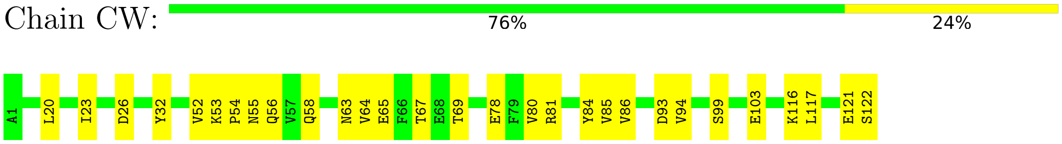
- Molecule 1: Coat protein

Chain CV:



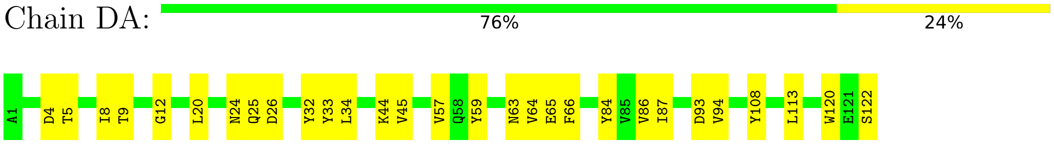
- Molecule 1: Coat protein

Chain CW:



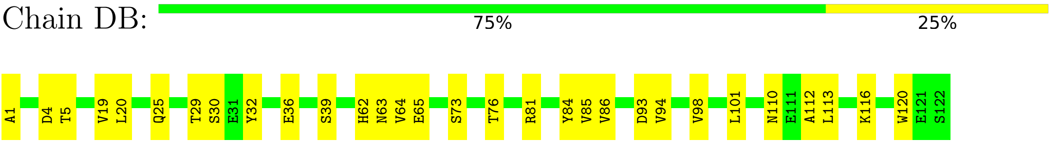
- Molecule 1: Coat protein

Chain DA:



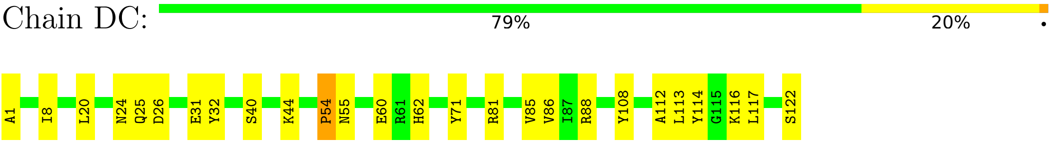
- Molecule 1: Coat protein

Chain DB:



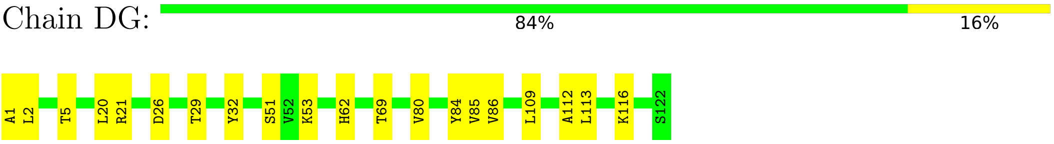
- Molecule 1: Coat protein

Chain DC:



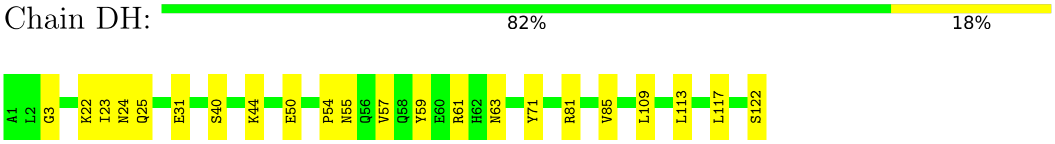
- Molecule 1: Coat protein

Chain DG:



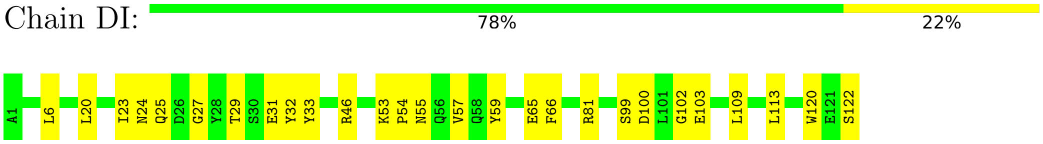
- Molecule 1: Coat protein

Chain DH:



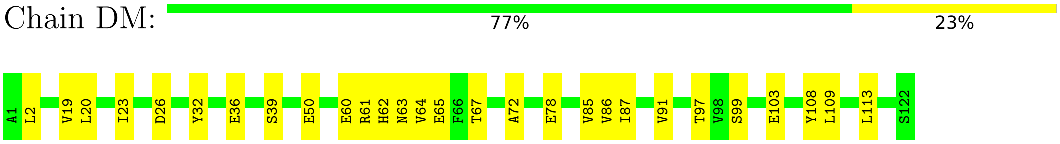
- Molecule 1: Coat protein

Chain DI:



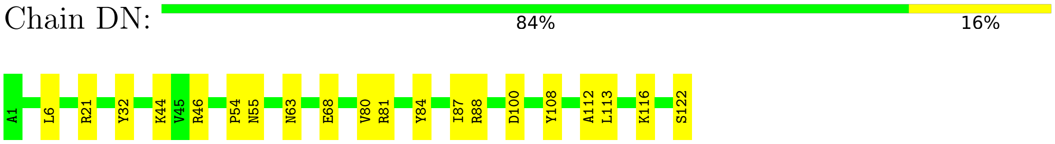
- Molecule 1: Coat protein

Chain DM:



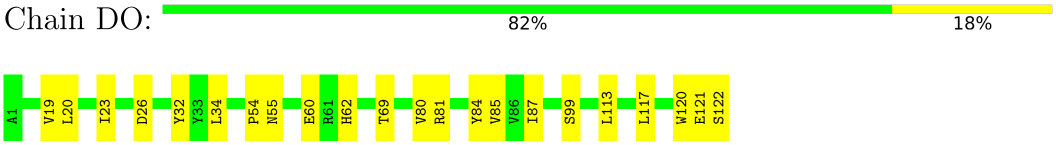
- Molecule 1: Coat protein

Chain DN:



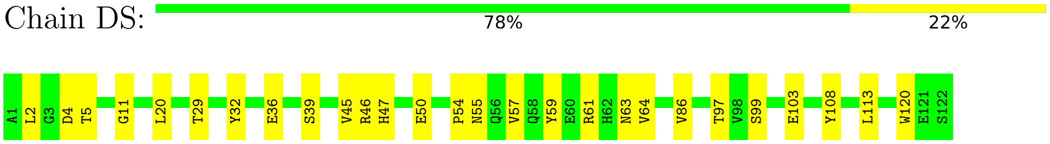
- Molecule 1: Coat protein

Chain DO:



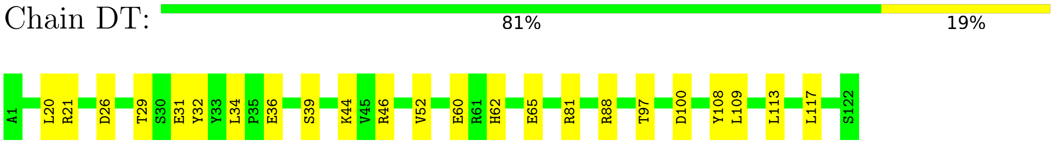
- Molecule 1: Coat protein

Chain DS:



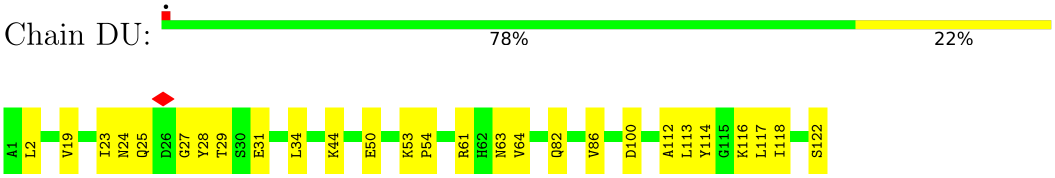
- Molecule 1: Coat protein

Chain DT:



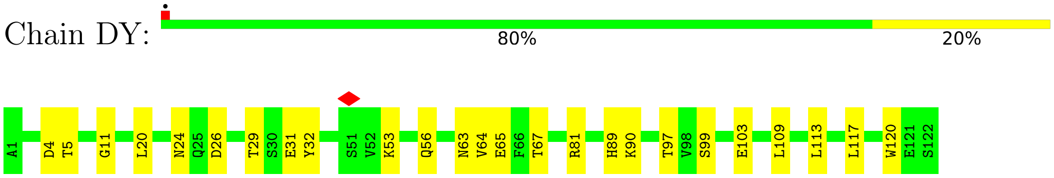
- Molecule 1: Coat protein

Chain DU:



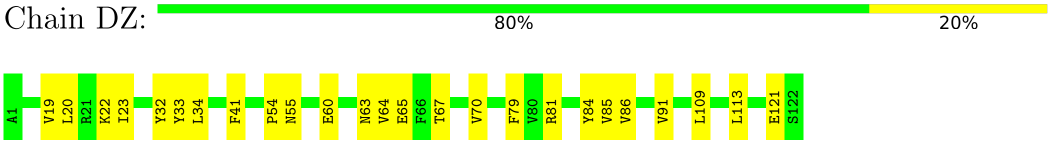
- Molecule 1: Coat protein

Chain DY:



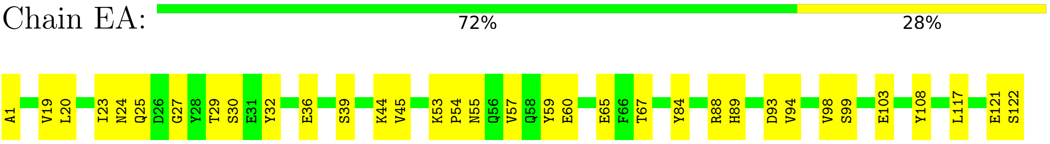
- Molecule 1: Coat protein

Chain DZ:



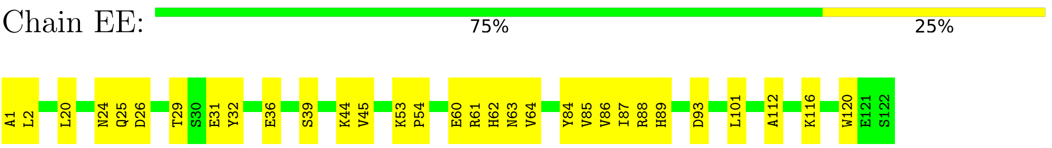
- Molecule 1: Coat protein

Chain EA:



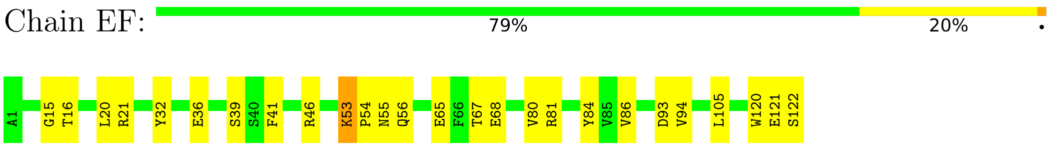
- Molecule 1: Coat protein

Chain EE:



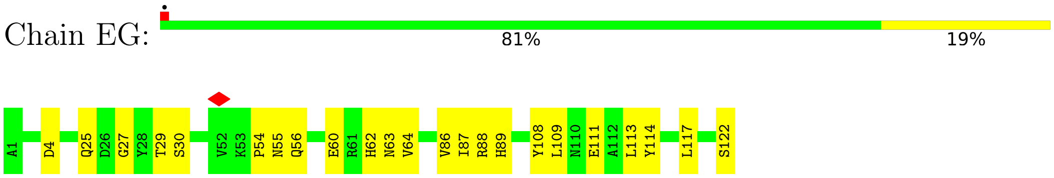
- Molecule 1: Coat protein

Chain EF:



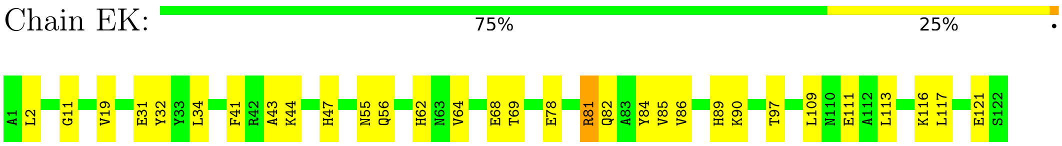
- Molecule 1: Coat protein

Chain EG:



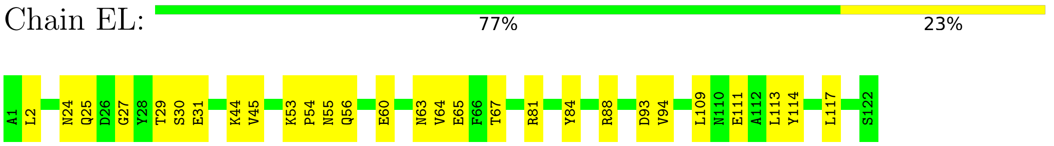
- Molecule 1: Coat protein

Chain EK:



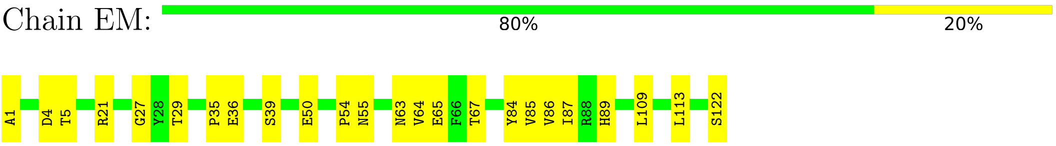
- Molecule 1: Coat protein

Chain EL:



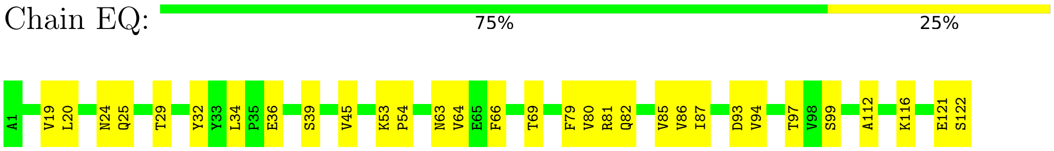
- Molecule 1: Coat protein

Chain EM:



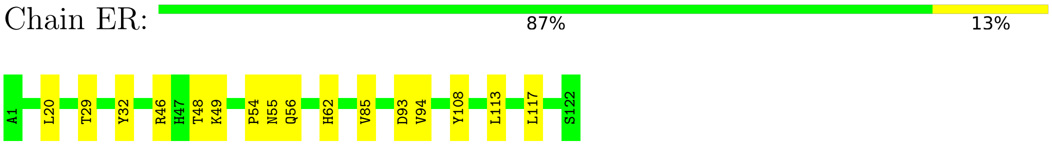
- Molecule 1: Coat protein

Chain EQ:



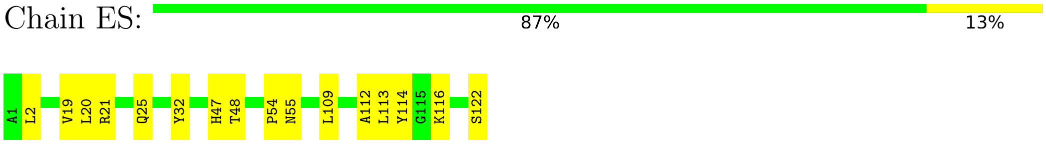
- Molecule 1: Coat protein

Chain ER:



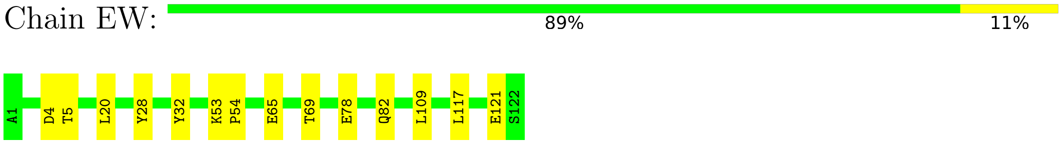
- Molecule 1: Coat protein

Chain ES:



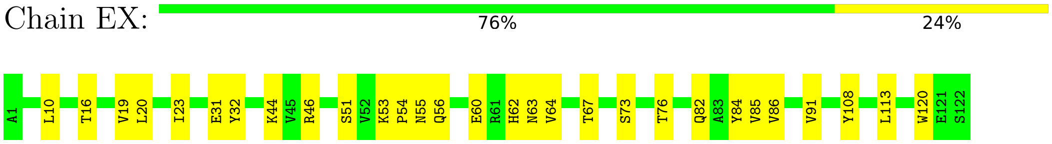
- Molecule 1: Coat protein

Chain EW:



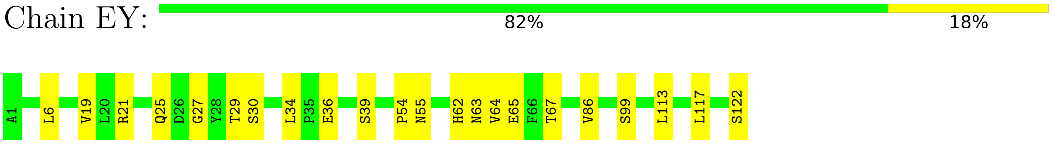
- Molecule 1: Coat protein

Chain EX:



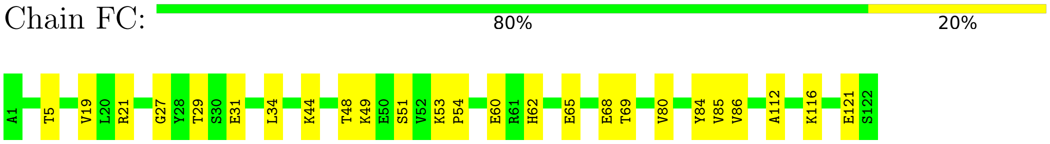
- Molecule 1: Coat protein

Chain EY:



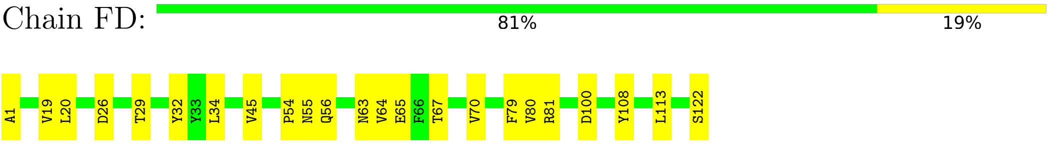
- Molecule 1: Coat protein

Chain FC:



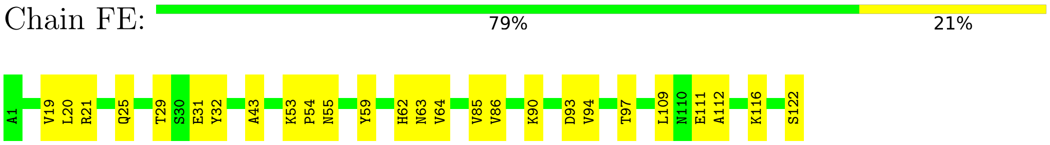
- Molecule 1: Coat protein

Chain FD:



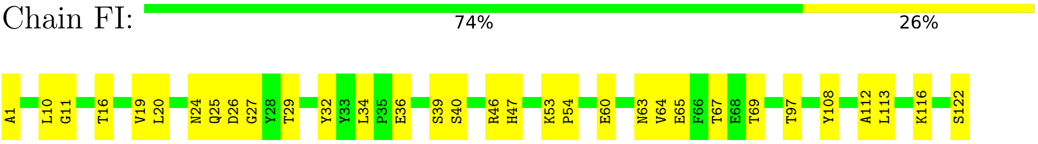
- Molecule 1: Coat protein

Chain FE:



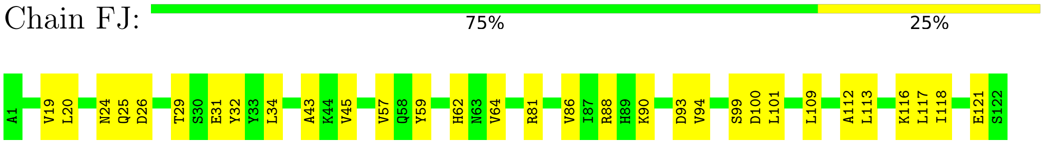
- Molecule 1: Coat protein

Chain FI:



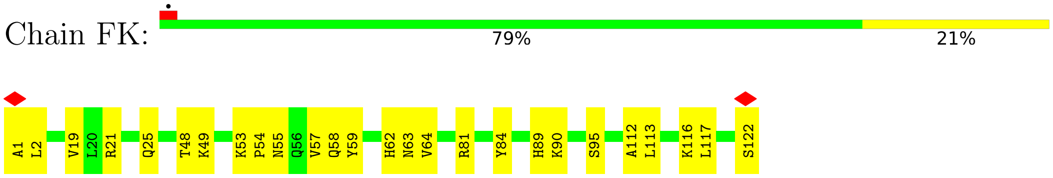
- Molecule 1: Coat protein

Chain FJ:



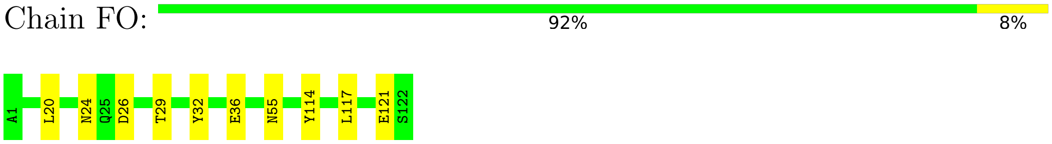
- Molecule 1: Coat protein

Chain FK:



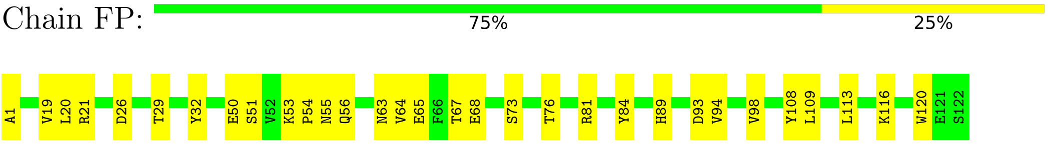
- Molecule 1: Coat protein

Chain FO:



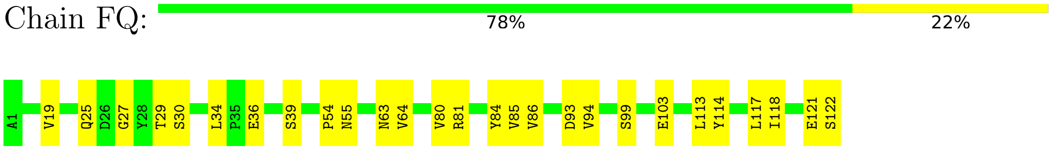
- Molecule 1: Coat protein

Chain FP:



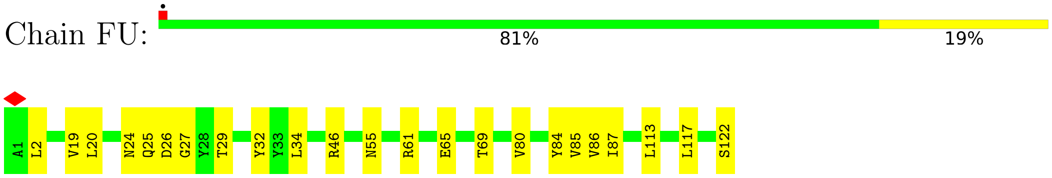
- Molecule 1: Coat protein

Chain FQ:



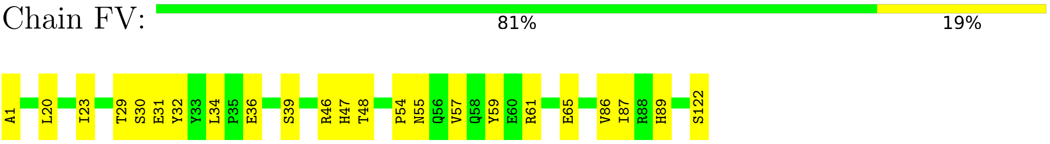
- Molecule 1: Coat protein

Chain FU:



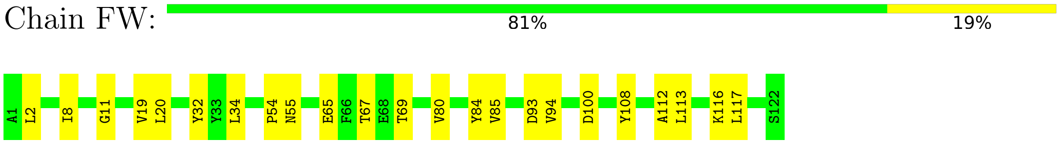
- Molecule 1: Coat protein

Chain FV:



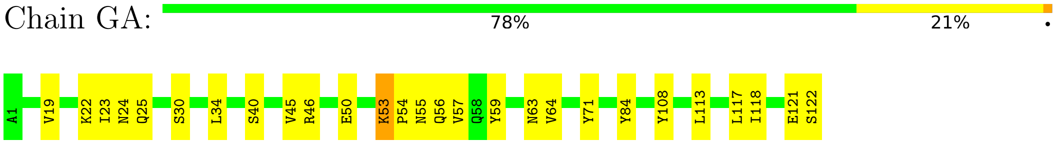
- Molecule 1: Coat protein

Chain FW:



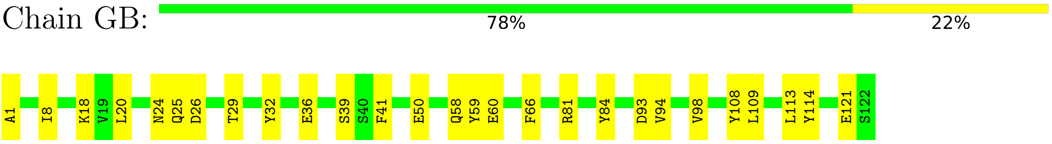
- Molecule 1: Coat protein

Chain GA:



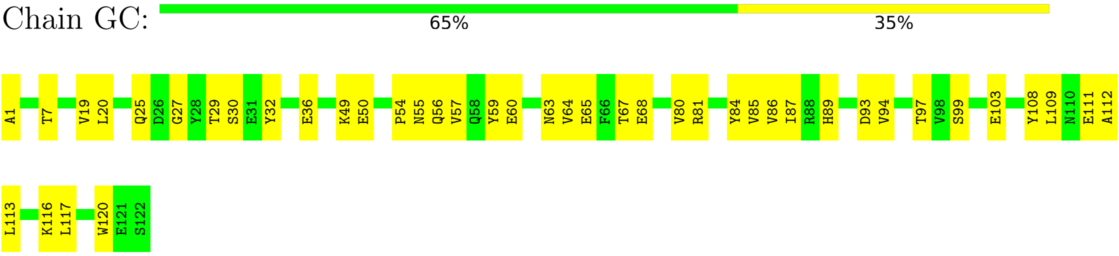
- Molecule 1: Coat protein

Chain GB:



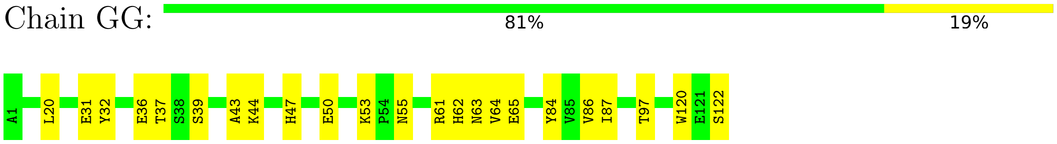
- Molecule 1: Coat protein

Chain GC:



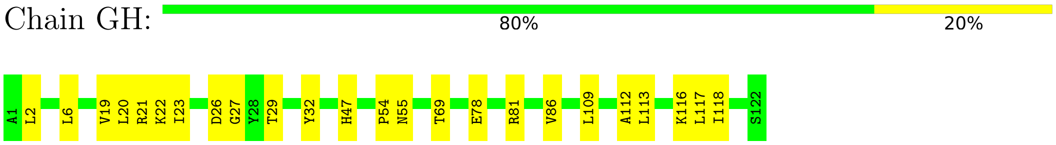
- Molecule 1: Coat protein

Chain GG:



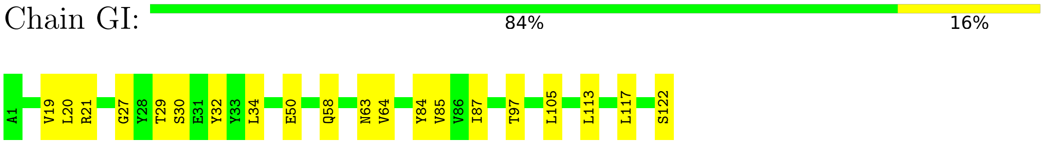
- Molecule 1: Coat protein

Chain GH:



- Molecule 1: Coat protein

Chain GI:



- Molecule 1: Coat protein

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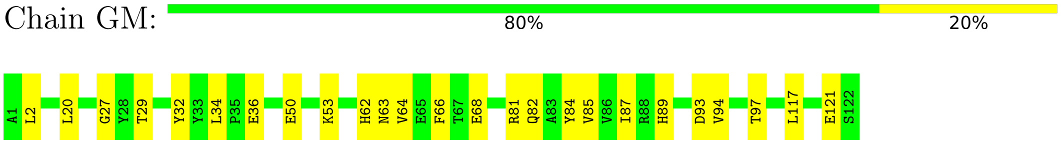

- Molecule 1: Coat protein

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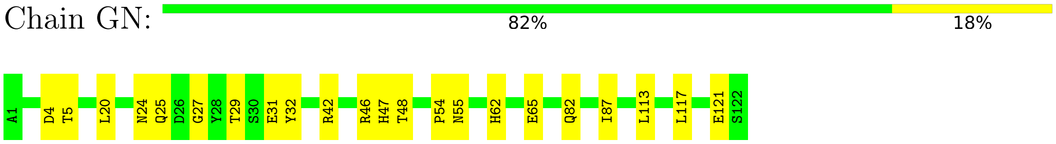

- Molecule 1: Coat protein

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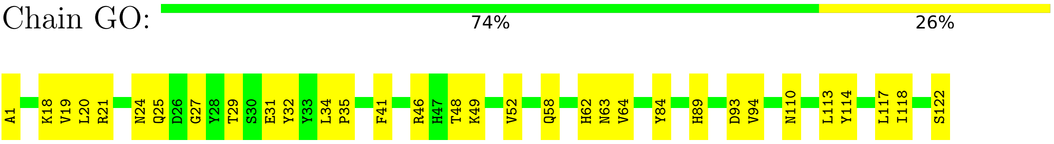
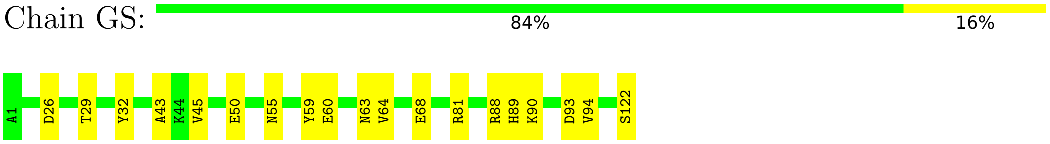


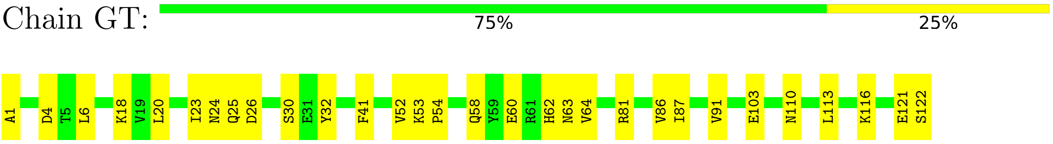
- Molecule 1: Coat protein

Chain GS:



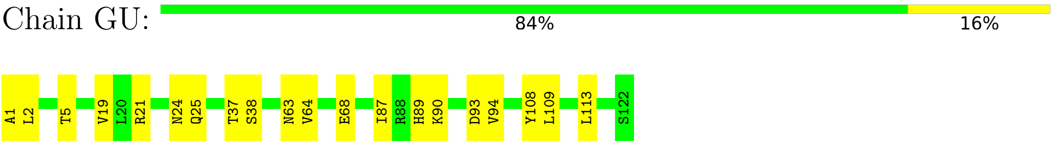
- Molecule 1: Coat protein

Chain GT:



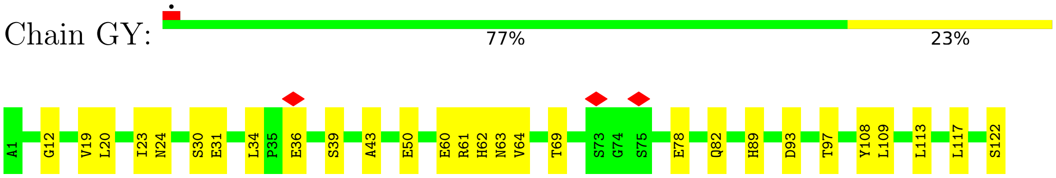
- Molecule 1: Coat protein

Chain GU:



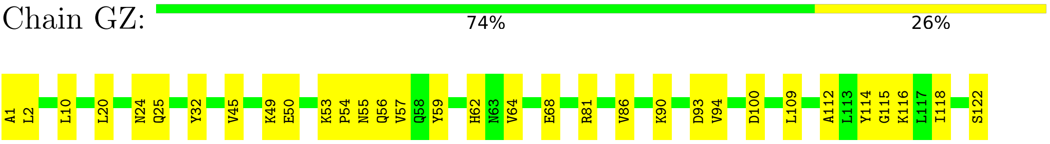
- Molecule 1: Coat protein

Chain GY:



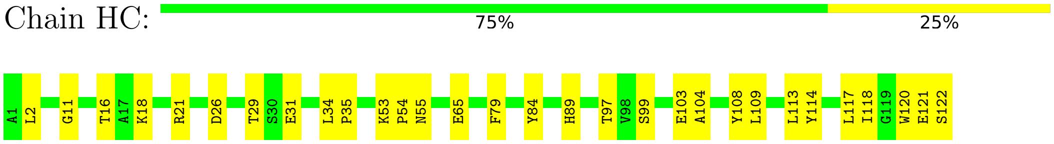
- Molecule 1: Coat protein

Chain GZ:



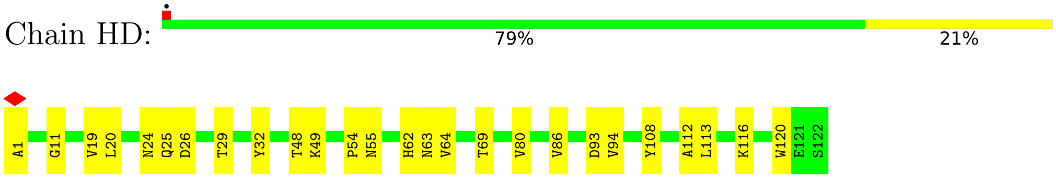
- Molecule 1: Coat protein

Chain HC:



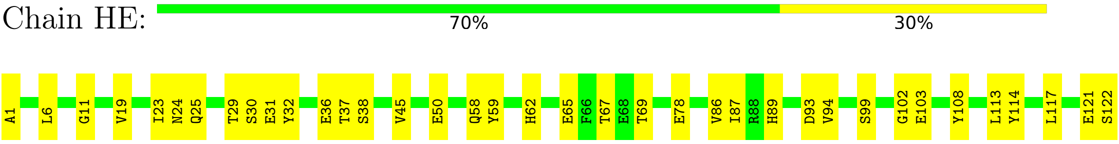
- Molecule 1: Coat protein

Chain HD:



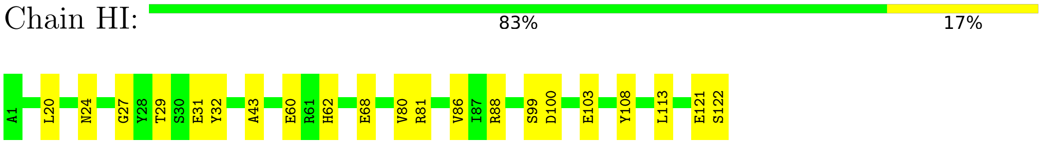
- Molecule 1: Coat protein

Chain HE:



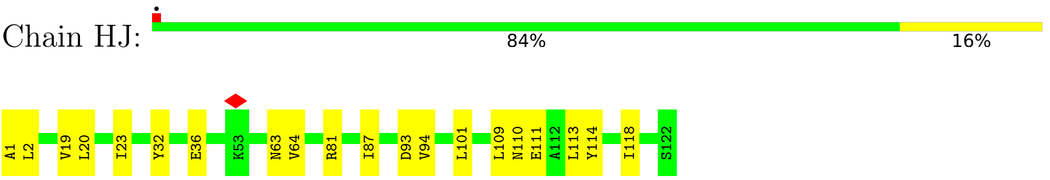
- Molecule 1: Coat protein

Chain HI:



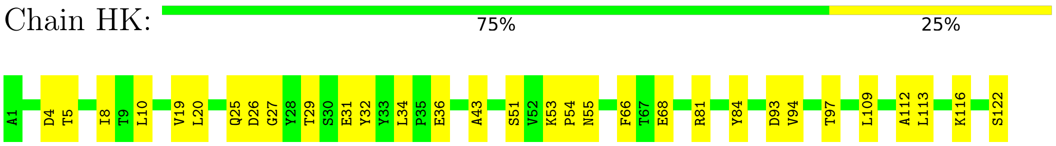
- Molecule 1: Coat protein

Chain HJ:



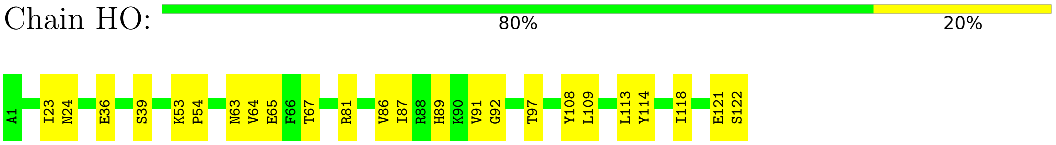
• Molecule 1: Coat protein

Chain HK:



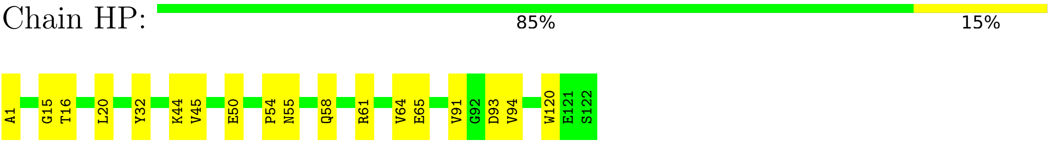
• Molecule 1: Coat protein

Chain HO:



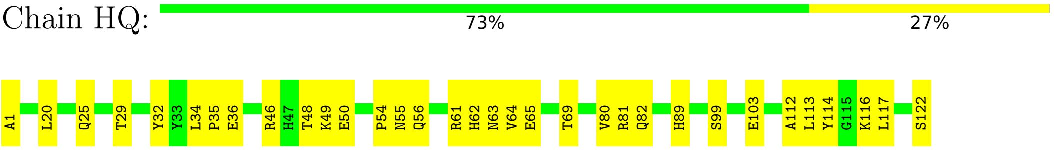
• Molecule 1: Coat protein

Chain HP:



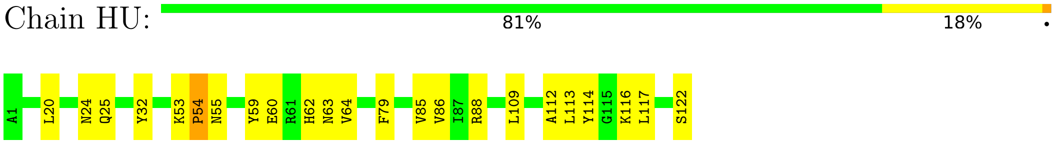
• Molecule 1: Coat protein

Chain HQ:



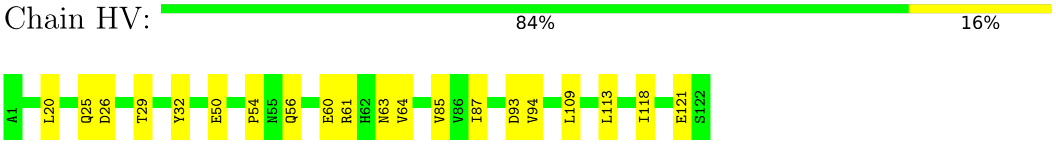
• Molecule 1: Coat protein

Chain HU:



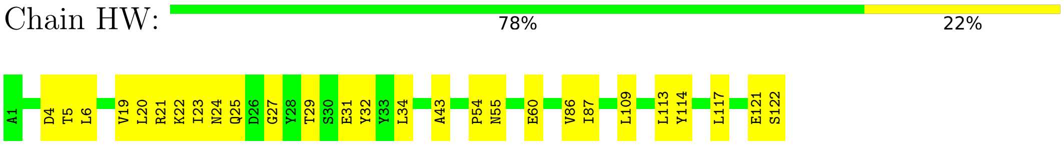
• Molecule 1: Coat protein

Chain HV:



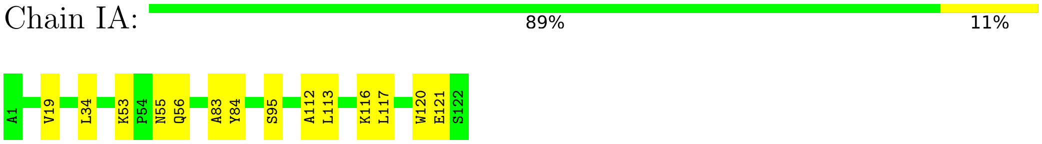
• Molecule 1: Coat protein

Chain HW:



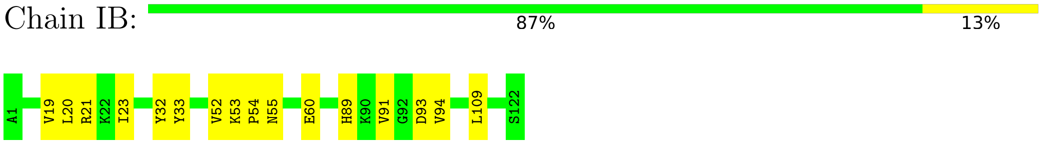
- Molecule 1: Coat protein

Chain IA:



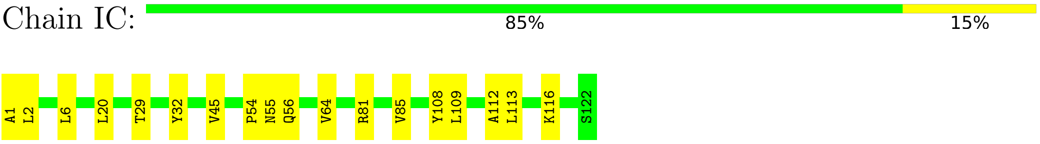
- Molecule 1: Coat protein

Chain IB:



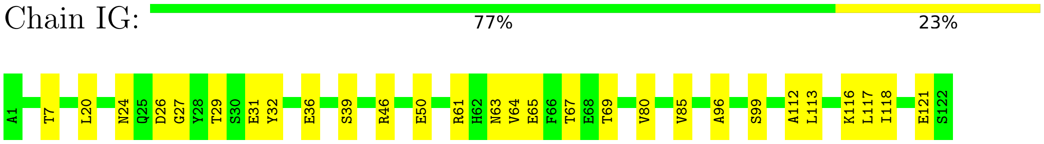
- Molecule 1: Coat protein

Chain IC:



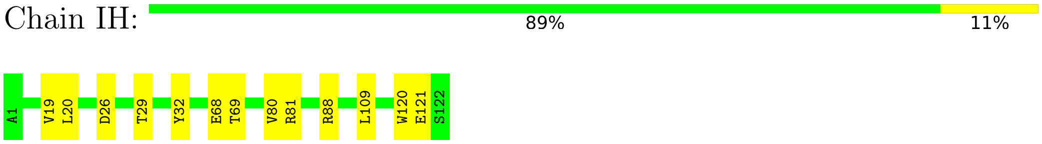
- Molecule 1: Coat protein

Chain IG:



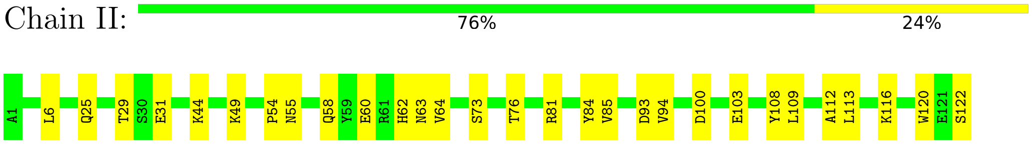
- Molecule 1: Coat protein

Chain IH:



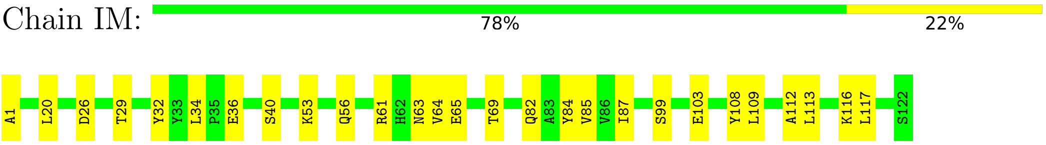
- Molecule 1: Coat protein

Chain II:



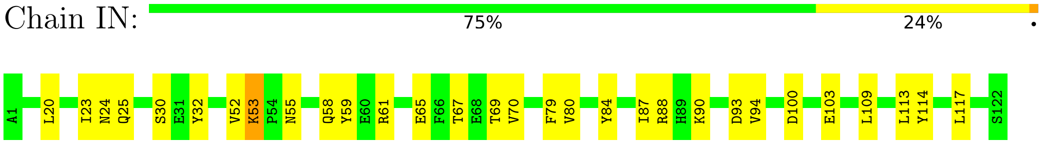
- Molecule 1: Coat protein

Chain IM:



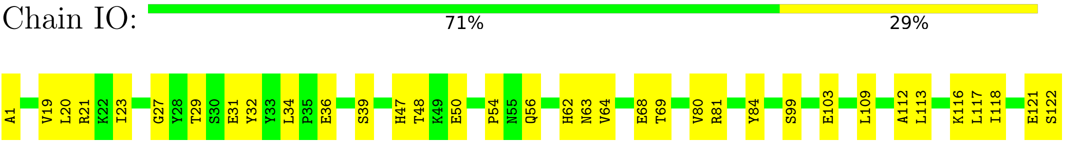
- Molecule 1: Coat protein

Chain IN:



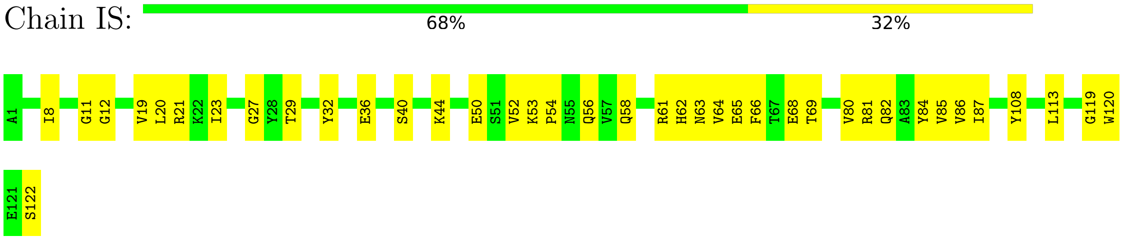
- Molecule 1: Coat protein

Chain IO:



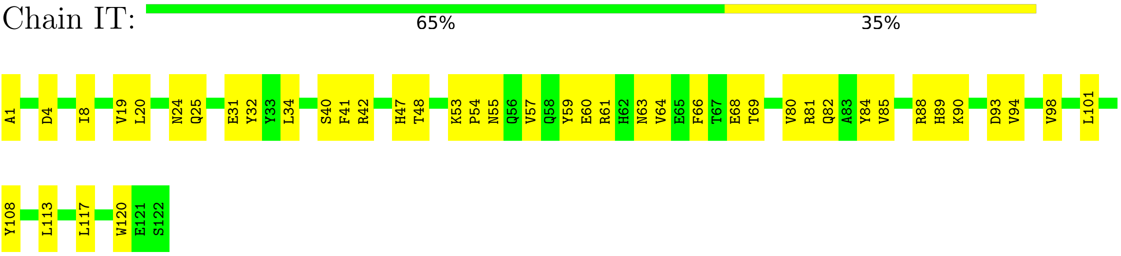
- Molecule 1: Coat protein

Chain IS:



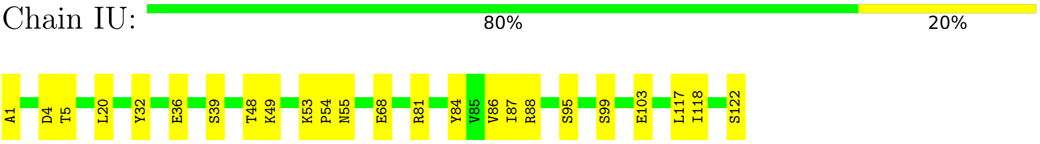
- Molecule 1: Coat protein

Chain IT:



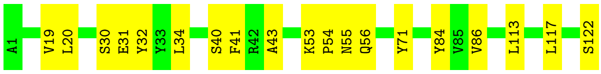
- Molecule 1: Coat protein

Chain IU:



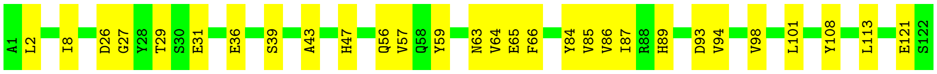
- Molecule 1: Coat protein

Chain IY:



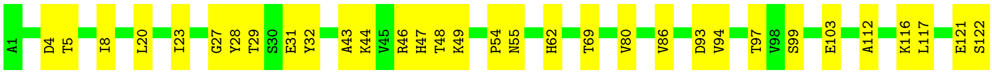
- Molecule 1: Coat protein

Chain IZ:



- Molecule 1: Coat protein

Chain JA:

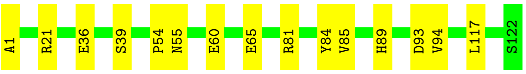


- Molecule 1: Coat protein

Chain JE:

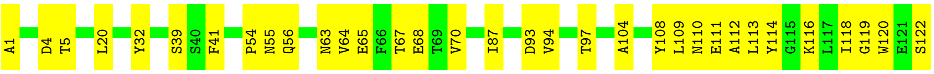
- Molecule 1: Coat protein

Chain JF:



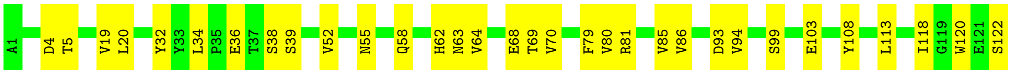
- Molecule 1: Coat protein

Chain JG:



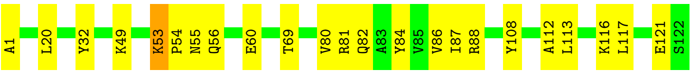
- Molecule 1: Coat protein

Chain JK:



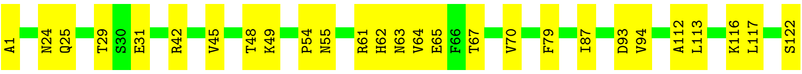
- Molecule 1: Coat protein

Chain JL:



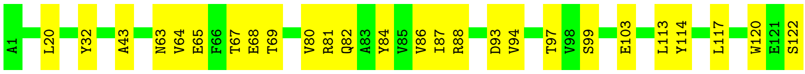
- Molecule 1: Coat protein

Chain JM:



- Molecule 1: Coat protein

Chain JQ:

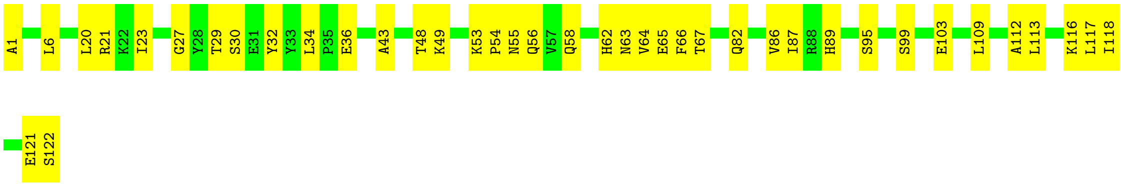


- Molecule 1: Coat protein

Chain JR:

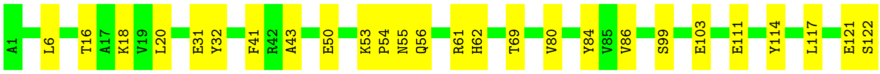
- Molecule 1: Coat protein

Chain JS:



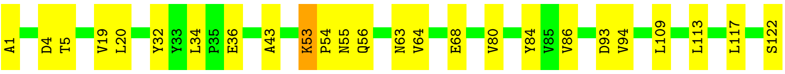
- Molecule 1: Coat protein

Chain JW:



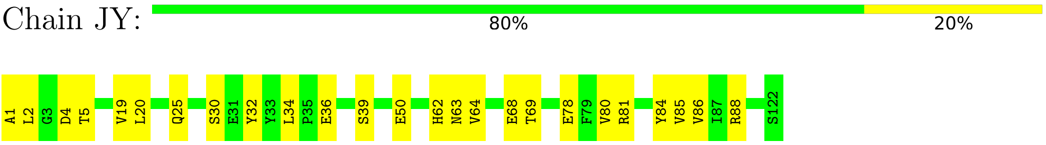
- Molecule 1: Coat protein

Chain JX:



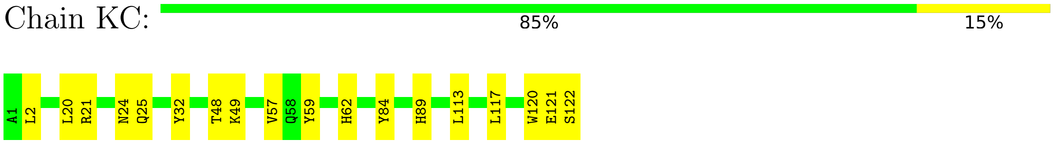
- Molecule 1: Coat protein

Chain JY:



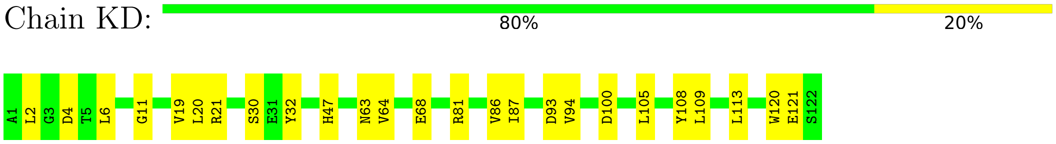
- Molecule 1: Coat protein

Chain KC:



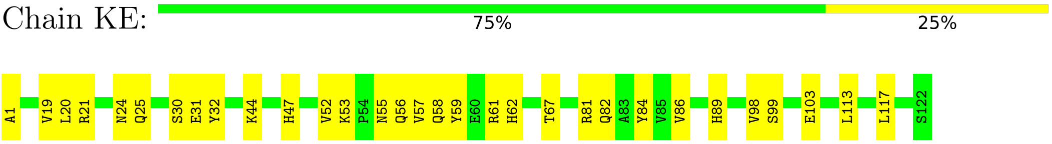
- Molecule 1: Coat protein

Chain KD:



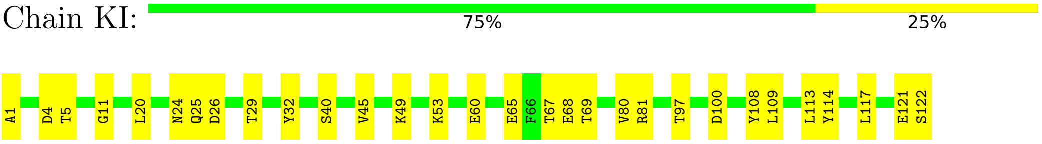
- Molecule 1: Coat protein

Chain KE:



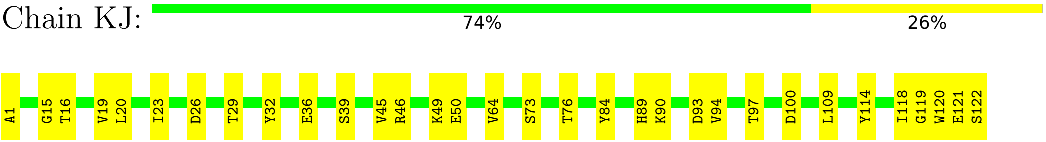
- Molecule 1: Coat protein

Chain KI:



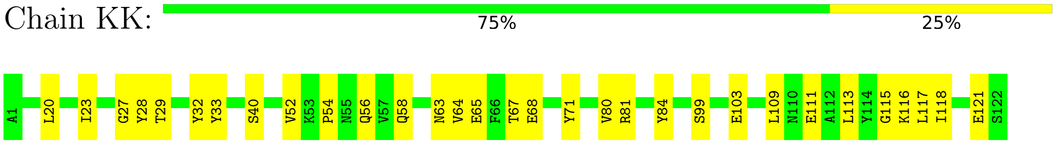
- Molecule 1: Coat protein

Chain KJ:



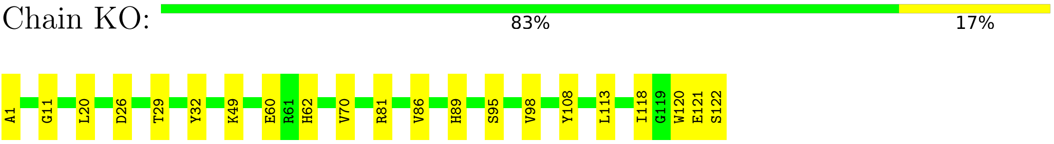
- Molecule 1: Coat protein

Chain KK:



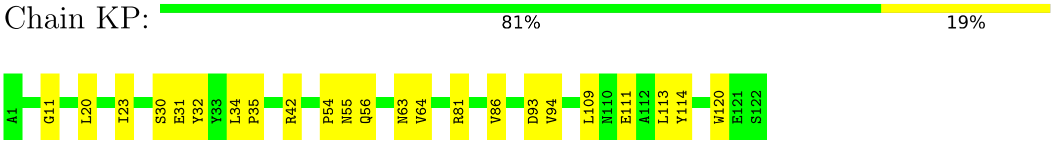
- Molecule 1: Coat protein

Chain KO:



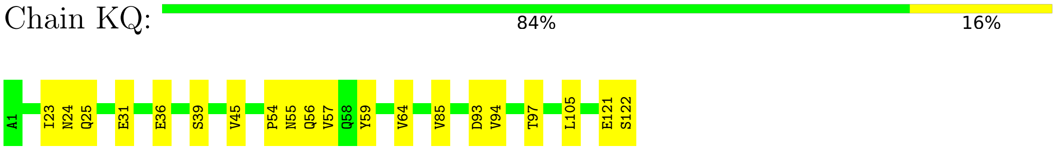
- Molecule 1: Coat protein

Chain KP:



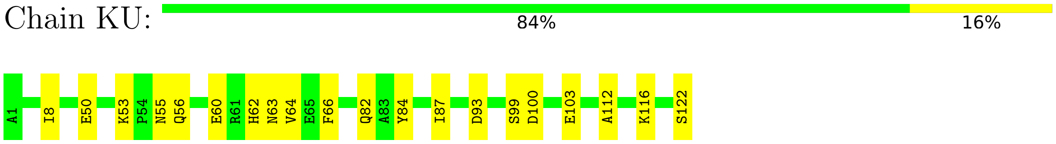
- Molecule 1: Coat protein

Chain KQ:



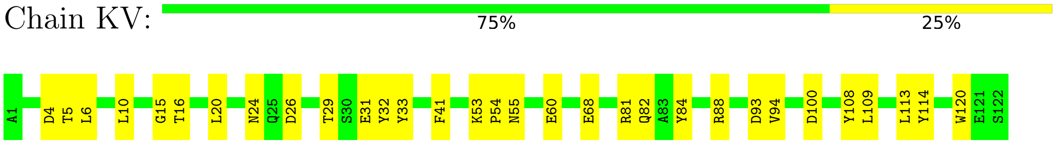
- Molecule 1: Coat protein

Chain KU:



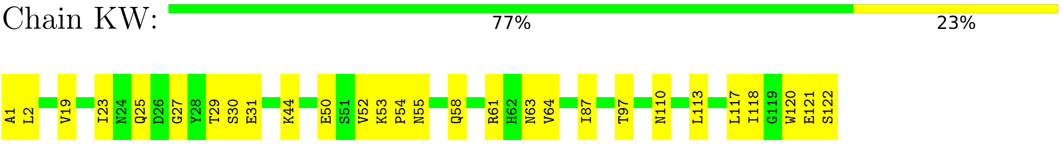
- Molecule 1: Coat protein

Chain KV:



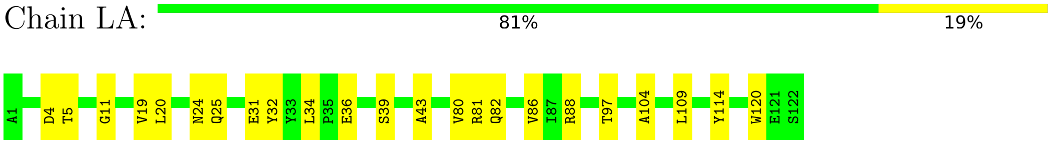
- Molecule 1: Coat protein

Chain KW:



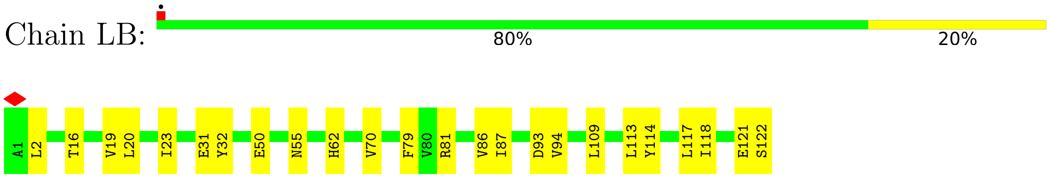
- Molecule 1: Coat protein

Chain LA:



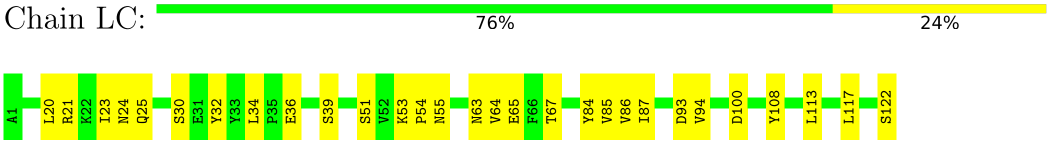
- Molecule 1: Coat protein

Chain LB:



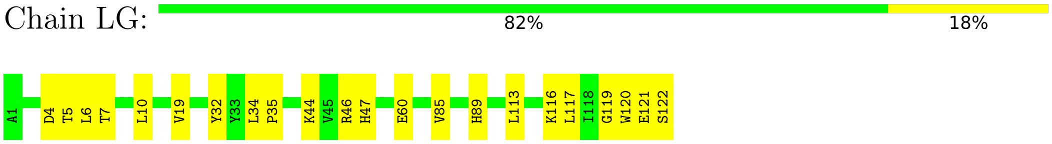
- Molecule 1: Coat protein

Chain LC:



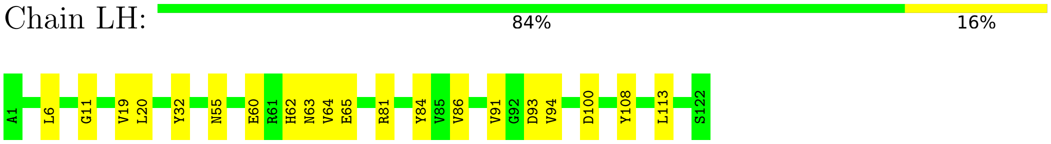
- Molecule 1: Coat protein

Chain LG:



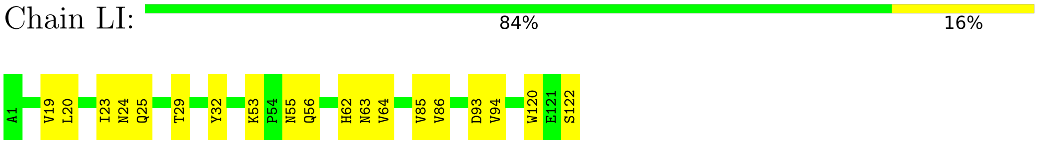
- Molecule 1: Coat protein

Chain LH:



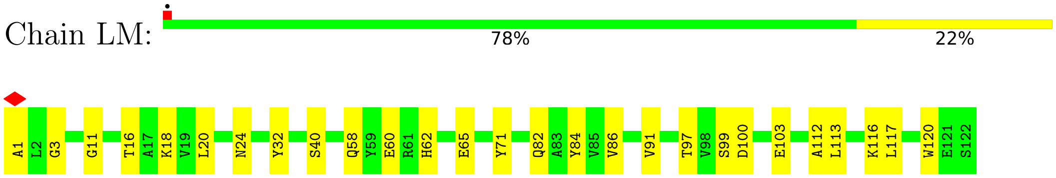
- Molecule 1: Coat protein

Chain LI:



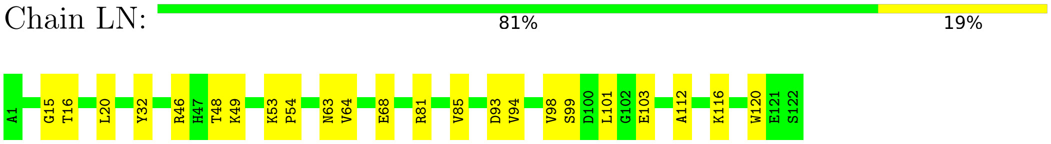
- Molecule 1: Coat protein

Chain LM:

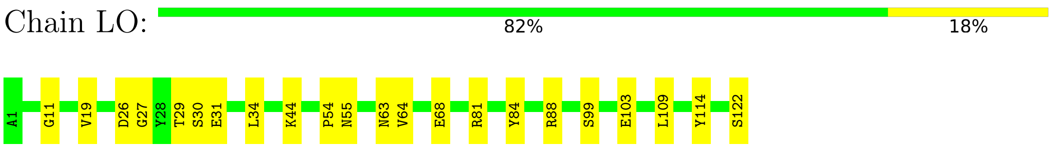


- Molecule 1: Coat protein

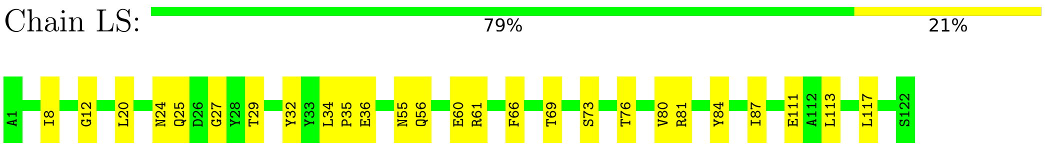
Chain LN:



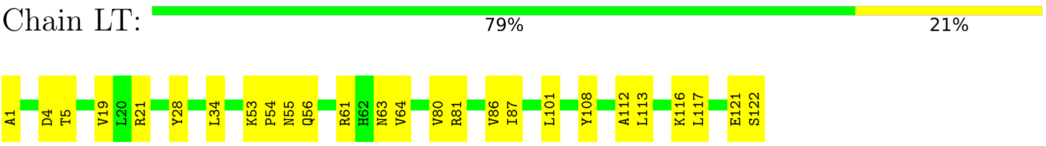
- Molecule 1: Coat protein



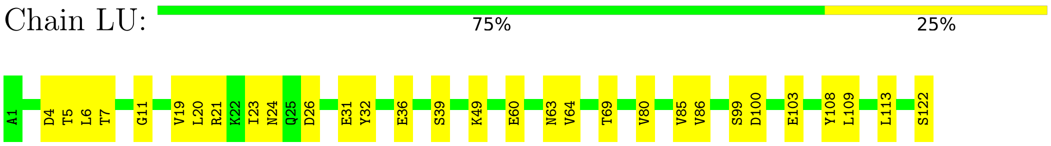
- Molecule 1: Coat protein



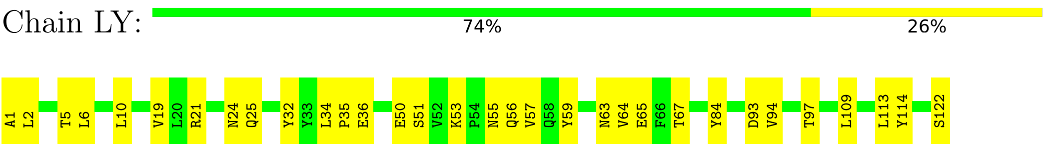
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein



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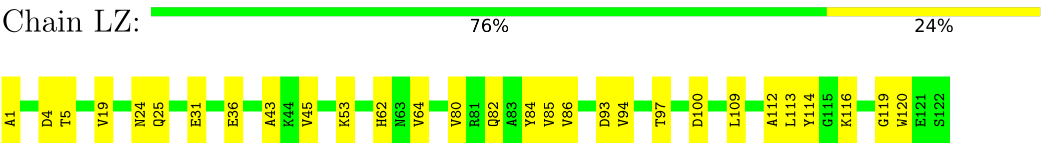
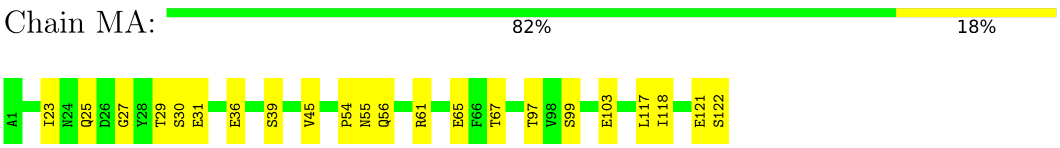
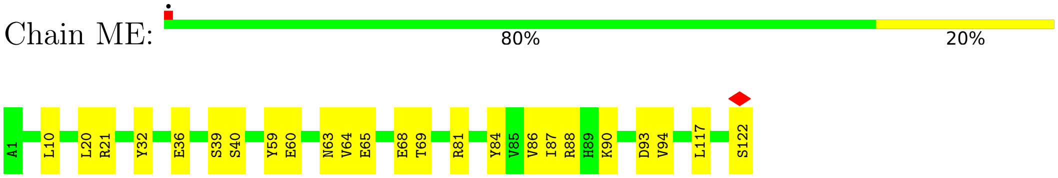


- Molecule 1: Coat protein



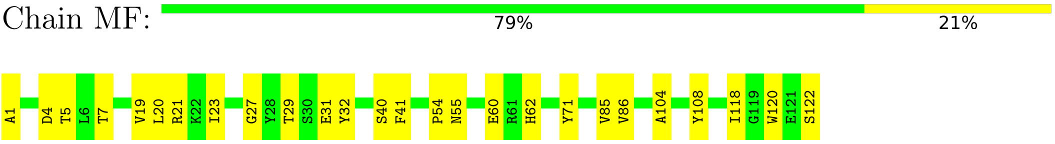
- Molecule 1: Coat protein

Chain ME:



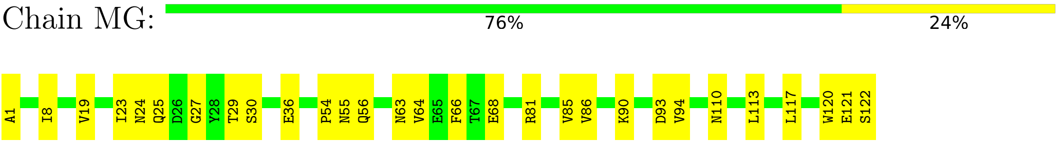
- Molecule 1: Coat protein

Chain MF:



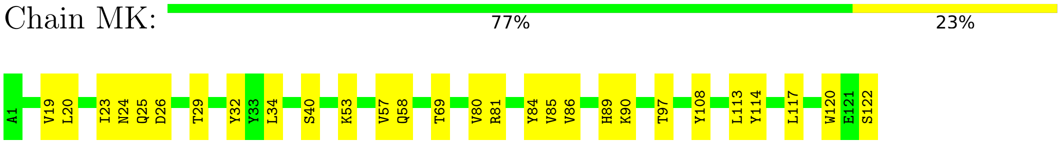
- Molecule 1: Coat protein

Chain MG:



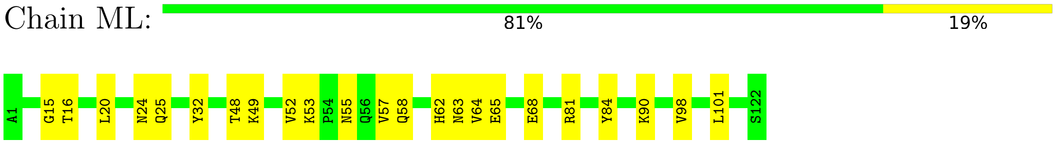
- Molecule 1: Coat protein

Chain MK:



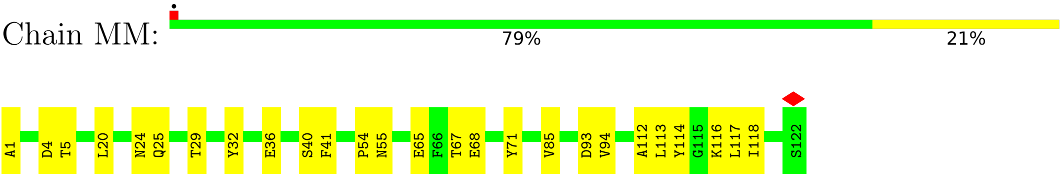
- Molecule 1: Coat protein

Chain ML:



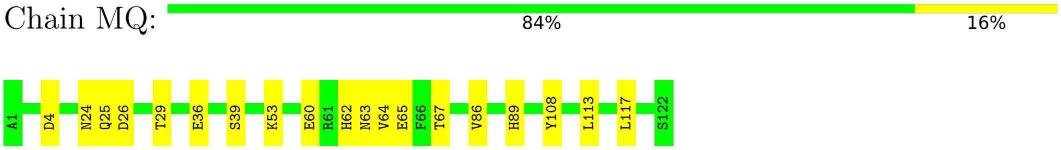
- Molecule 1: Coat protein

Chain MM:

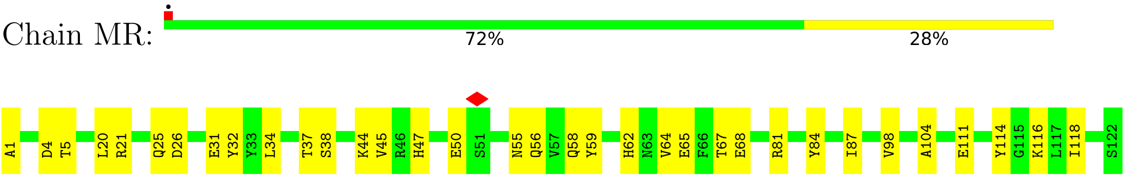


- Molecule 1: Coat protein

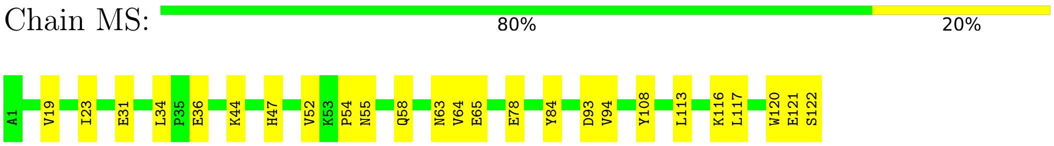
Chain MQ:



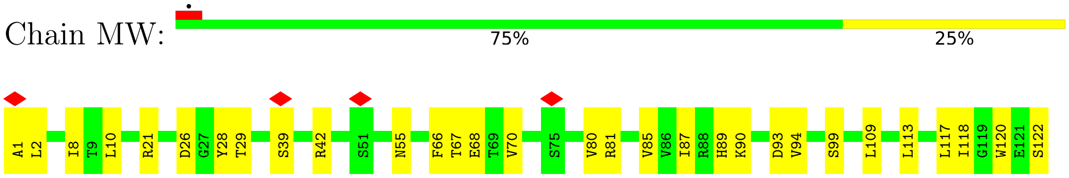
- Molecule 1: Coat protein



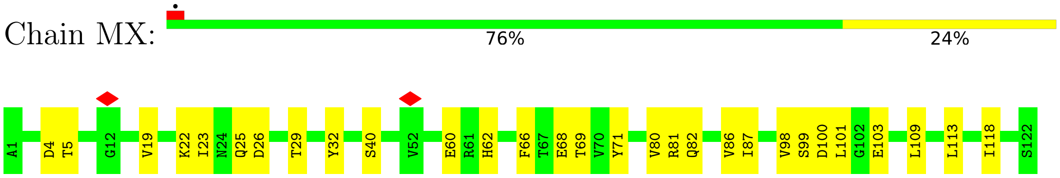
- Molecule 1: Coat protein



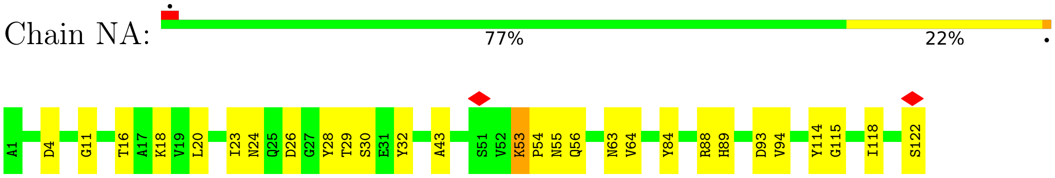
- Molecule 1: Coat protein



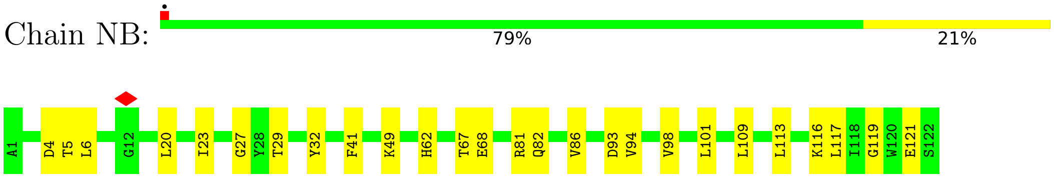
- Molecule 1: Coat protein



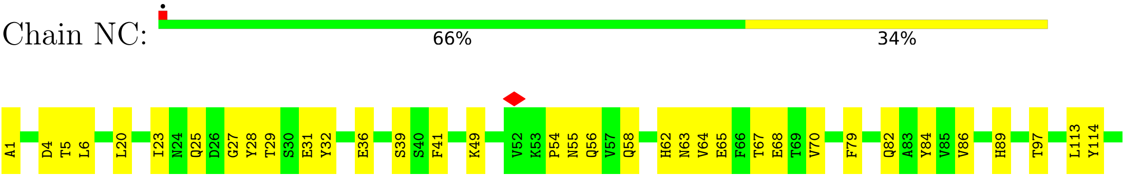
- Molecule 1: Coat protein

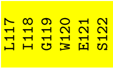


- Molecule 1: Coat protein



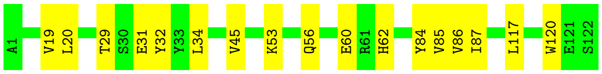
- Molecule 1: Coat protein





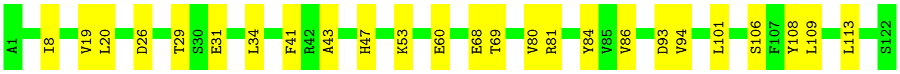
- Molecule 1: Coat protein

Chain NG:



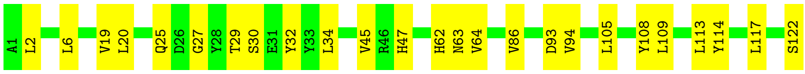
- Molecule 1: Coat protein

Chain NH:



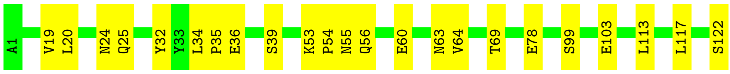
- Molecule 1: Coat protein

Chain NI:



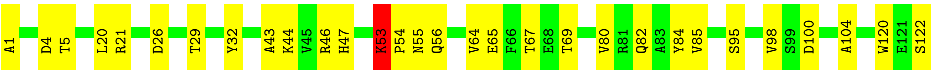
- Molecule 1: Coat protein

Chain NM:



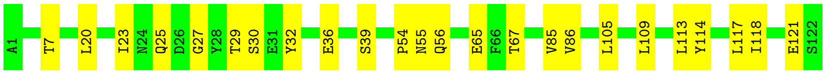
- Molecule 1: Coat protein

Chain NN:



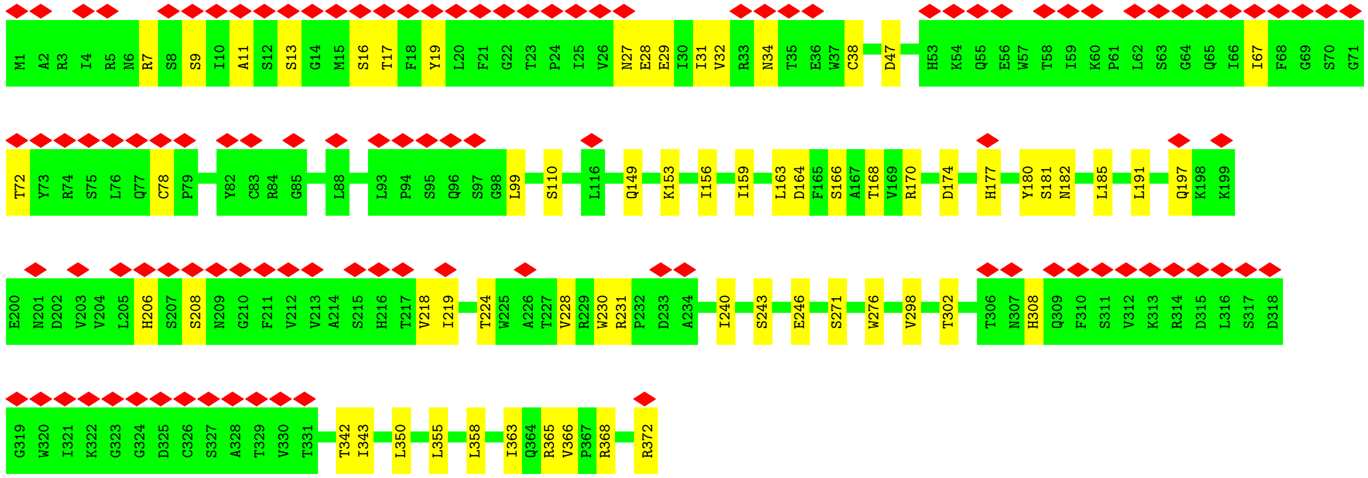
- Molecule 1: Coat protein

Chain NO:



- Molecule 2: Maturation protein

Chain M:


M1 A2 R3 I4 R5 N6 R7 S8 S9 I10 A11 S12 S13 G14 M15 S16 T17 F18 Y19 L20 F21 G22 T23 P24 I25 V26 N27 E28 E29 I30 I31 V32 R33 N34 T35 E36 W37 C38 D47 H53 K54 Q55 E56 W57 T58 I59 K60 P61 L62 S63 G64 Q65 I66 I67 F68 G69 S70 G71
T72 Y73 R74 S75 L76 Q77 C78 P79 Y82 C83 R84 G85 L88 L93 P94 S95 Q96 S97 G98 L99 S110 L116 Q149 K153 I156 I159 L163 D164 F165 S166 A167 T168 V169 R170 D174 H177 Y180 S181 N182 L185 L191 Q197 K198 K199
E200 N201 D202 V203 V204 L205 H206 S207 S208 N209 G210 F211 V212 V213 A214 S215 H216 T217 V218 I219 T224 W225 A226 T227 V228 R229 W230 R231 P232 D233 A234 I240 S243 E246 S271 W276 V298 T302 T306 N307 H308 Q309 F310 S311 V312 K313 R314 D315 L316 S317 D318
G319 W320 I321 K322 G323 G324 D325 C326 S327 A328 T329 V330 T331 T342 I343 L350 L355 L358 I363 Q364 R365 V366 P367 R368 R372

4 Experimental information

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	272204	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 ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.794	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.0334	Depositor
Map size (Å)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	AA	0.30	0/973	0.58	0/1317
1	AB	0.29	0/973	0.55	0/1317
1	AC	0.29	0/973	0.55	0/1317
1	AG	0.28	0/973	0.55	0/1317
1	AH	0.29	0/973	0.53	0/1317
1	AI	0.27	0/973	0.55	0/1317
1	AM	0.28	0/973	0.56	0/1317
1	AN	0.29	0/973	0.57	0/1317
1	AO	0.28	0/973	0.54	0/1317
1	AS	0.30	0/973	0.59	0/1317
1	AT	0.28	0/973	0.56	0/1317
1	AU	0.29	0/973	0.58	0/1317
1	AY	0.29	0/973	0.55	0/1317
1	AZ	0.28	0/973	0.55	0/1317
1	BA	0.32	0/973	0.55	0/1317
1	BE	0.31	0/973	0.60	0/1317
1	BF	0.29	0/973	0.54	0/1317
1	BG	0.29	0/973	0.53	0/1317
1	BK	0.29	0/973	0.56	0/1317
1	BL	0.30	0/973	0.57	0/1317
1	BM	0.28	0/973	0.54	0/1317
1	BQ	0.31	0/973	0.59	0/1317
1	BR	0.28	0/973	0.56	0/1317
1	BS	0.32	0/973	0.60	1/1317 (0.1%)
1	BW	0.29	0/973	0.56	0/1317
1	BX	0.28	0/973	0.57	0/1317
1	BY	0.28	0/973	0.54	0/1317
1	CC	0.29	0/973	0.57	0/1317
1	CD	0.31	0/973	0.60	0/1317
1	CE	0.28	0/973	0.55	0/1317
1	CI	0.29	0/973	0.57	0/1317
1	CJ	0.28	0/973	0.54	0/1317

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	CK	0.30	0/973	0.57	0/1317
1	CO	0.29	0/973	0.58	0/1317
1	CP	0.28	0/973	0.56	0/1317
1	CQ	0.28	0/973	0.55	0/1317
1	CU	0.28	0/973	0.54	0/1317
1	CV	0.28	0/973	0.56	0/1317
1	CW	0.29	0/973	0.59	0/1317
1	DA	0.30	0/973	0.58	0/1317
1	DB	0.29	0/973	0.58	0/1317
1	DC	0.29	0/973	0.59	2/1317 (0.2%)
1	DG	0.29	0/973	0.56	0/1317
1	DH	0.29	0/973	0.58	0/1317
1	DI	0.29	0/973	0.57	0/1317
1	DM	0.29	0/973	0.54	0/1317
1	DN	0.29	0/973	0.56	0/1317
1	DO	0.28	0/973	0.55	0/1317
1	DS	0.30	0/973	0.54	0/1317
1	DT	0.31	0/973	0.56	0/1317
1	DU	0.28	0/973	0.58	0/1317
1	DY	0.28	0/973	0.55	0/1317
1	DZ	0.30	0/973	0.56	0/1317
1	EA	0.30	0/973	0.58	0/1317
1	EE	0.30	0/973	0.60	0/1317
1	EF	0.30	0/973	0.57	0/1317
1	EG	0.27	0/973	0.55	0/1317
1	EK	0.29	0/973	0.53	0/1317
1	EL	0.29	0/973	0.56	0/1317
1	EM	0.33	0/973	0.62	2/1317 (0.2%)
1	EQ	0.29	0/973	0.55	0/1317
1	ER	0.28	0/973	0.51	0/1317
1	ES	0.27	0/973	0.52	0/1317
1	EW	0.28	0/973	0.55	0/1317
1	EX	0.28	0/973	0.55	0/1317
1	EY	0.27	0/973	0.54	0/1317
1	FC	0.30	0/973	0.58	0/1317
1	FD	0.28	0/973	0.52	0/1317
1	FE	0.30	0/973	0.56	0/1317
1	FI	0.29	0/973	0.58	0/1317
1	FJ	0.29	0/973	0.55	0/1317
1	FK	0.30	0/973	0.55	0/1317
1	FO	0.30	0/973	0.58	0/1317
1	FP	0.29	0/973	0.55	0/1317
1	FQ	0.28	0/973	0.55	0/1317

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	FU	0.31	0/973	0.55	0/1317
1	FV	0.29	0/973	0.56	0/1317
1	FW	0.29	0/973	0.55	0/1317
1	GA	0.29	0/973	0.55	0/1317
1	GB	0.29	0/973	0.58	0/1317
1	GC	0.30	0/973	0.57	0/1317
1	GG	0.29	0/973	0.56	0/1317
1	GH	0.28	0/973	0.55	0/1317
1	GI	0.29	0/973	0.53	0/1317
1	GM	0.29	0/973	0.55	0/1317
1	GN	0.31	0/973	0.57	0/1317
1	GO	0.30	0/973	0.58	0/1317
1	GS	0.30	0/973	0.58	0/1317
1	GT	0.29	0/973	0.55	0/1317
1	GU	0.28	0/973	0.54	0/1317
1	GY	0.29	0/973	0.54	0/1317
1	GZ	0.28	0/973	0.54	0/1317
1	HC	0.31	0/973	0.57	0/1317
1	HD	0.29	0/973	0.56	0/1317
1	HE	0.30	0/973	0.57	0/1317
1	HI	0.29	0/973	0.57	0/1317
1	HJ	0.28	0/973	0.54	0/1317
1	HK	0.30	0/973	0.56	0/1317
1	HO	0.29	0/973	0.56	0/1317
1	HP	0.29	0/973	0.58	0/1317
1	HQ	0.29	0/973	0.56	0/1317
1	HU	0.30	0/973	0.59	1/1317 (0.1%)
1	HV	0.28	0/973	0.54	0/1317
1	HW	0.29	0/973	0.54	0/1317
1	IA	0.30	0/973	0.60	0/1317
1	IB	0.29	0/973	0.57	0/1317
1	IC	0.28	0/973	0.54	0/1317
1	IG	0.28	0/973	0.55	0/1317
1	IH	0.28	0/973	0.54	0/1317
1	II	0.30	0/973	0.56	0/1317
1	IM	0.31	0/973	0.59	0/1317
1	IN	0.29	0/973	0.59	0/1317
1	IO	0.30	0/973	0.56	0/1317
1	IS	0.32	0/973	0.58	0/1317
1	IT	0.30	0/973	0.57	0/1317
1	IU	0.29	0/973	0.58	0/1317
1	IY	0.29	0/973	0.57	0/1317
1	IZ	0.29	0/973	0.57	0/1317

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	JA	0.29	0/973	0.55	0/1317
1	JE	0.28	0/973	0.55	0/1317
1	JF	0.29	0/973	0.54	0/1317
1	JG	0.29	0/973	0.55	0/1317
1	JK	0.31	0/973	0.57	0/1317
1	JL	0.29	0/973	0.57	0/1317
1	JM	0.30	0/973	0.57	0/1317
1	JQ	0.29	0/973	0.56	0/1317
1	JR	0.30	0/973	0.58	0/1317
1	JS	0.29	0/973	0.58	0/1317
1	JW	0.28	0/973	0.56	0/1317
1	JX	0.30	0/973	0.59	0/1317
1	JY	0.29	0/973	0.56	0/1317
1	KC	0.29	0/973	0.57	0/1317
1	KD	0.28	0/973	0.55	0/1317
1	KE	0.29	0/973	0.60	0/1317
1	KI	0.30	0/973	0.55	0/1317
1	KJ	0.31	0/973	0.56	0/1317
1	KK	0.30	0/973	0.57	0/1317
1	KO	0.31	0/973	0.55	0/1317
1	KP	0.29	0/973	0.55	0/1317
1	KQ	0.27	0/973	0.52	0/1317
1	KU	0.28	0/973	0.55	0/1317
1	KV	0.30	0/973	0.57	0/1317
1	KW	0.29	0/973	0.57	0/1317
1	LA	0.28	0/973	0.56	0/1317
1	LB	0.30	0/973	0.57	0/1317
1	LC	0.28	0/973	0.55	0/1317
1	LG	0.28	0/973	0.55	0/1317
1	LH	0.29	0/973	0.53	0/1317
1	LI	0.29	0/973	0.55	0/1317
1	LM	0.28	0/973	0.55	0/1317
1	LN	0.29	0/973	0.54	0/1317
1	LO	0.29	0/973	0.55	0/1317
1	LS	0.28	0/973	0.57	0/1317
1	LT	0.28	0/973	0.54	0/1317
1	LU	0.28	0/973	0.57	0/1317
1	LY	0.30	0/973	0.54	0/1317
1	LZ	0.30	0/973	0.55	0/1317
1	MA	0.29	0/973	0.55	0/1317
1	ME	0.31	0/973	0.55	0/1317
1	MF	0.28	0/973	0.55	0/1317
1	MG	0.28	0/973	0.54	0/1317

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	MK	0.29	0/973	0.55	0/1317
1	ML	0.28	0/973	0.54	0/1317
1	MM	0.30	0/973	0.57	0/1317
1	MQ	0.29	0/973	0.54	0/1317
1	MR	0.28	0/973	0.56	0/1317
1	MS	0.28	0/973	0.57	0/1317
1	MW	0.29	0/973	0.56	0/1317
1	MX	0.28	0/973	0.55	0/1317
1	NA	0.33	0/973	0.60	0/1317
1	NB	0.30	0/973	0.55	0/1317
1	NC	0.33	0/973	0.59	0/1317
1	NG	0.29	0/973	0.57	0/1317
1	NH	0.31	0/973	0.59	0/1317
1	NI	0.28	0/973	0.54	0/1317
1	NM	0.28	0/973	0.56	0/1317
1	NN	0.30	0/973	0.59	0/1317
1	NO	0.28	0/973	0.54	0/1317
2	M	0.27	0/2932	0.55	0/3980
All	All	0.29	0/176126	0.56	6/238406 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	EE	0	1
1	GA	0	1
1	IA	0	1
1	IN	0	1
1	JL	0	1
1	JX	0	1
1	MK	0	1
1	NA	0	1
1	NH	0	1
1	NN	0	1
All	All	0	10

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EM	35	PRO	CA-N-CD	-6.85	101.91	111.50
1	EM	35	PRO	N-CD-CG	-6.57	93.34	103.20
1	BS	35	PRO	CA-N-CD	-6.10	102.96	111.50
1	HU	54	PRO	CA-N-CD	-6.05	103.03	111.50
1	DC	54	PRO	CA-N-CD	-5.42	103.91	111.50
1	DC	54	PRO	N-CD-CG	-5.15	95.47	103.20

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	EE	53	LYS	Peptide
1	GA	53	LYS	Peptide
1	IA	53	LYS	Peptide
1	IN	53	LYS	Peptide
1	JL	53	LYS	Peptide
1	JX	53	LYS	Peptide
1	MK	53	LYS	Peptide
1	NA	53	LYS	Peptide
1	NH	53	LYS	Peptide
1	NN	53	LYS	Peptide

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	AA	954	0	935	28	0
1	AB	954	0	935	17	0
1	AC	954	0	935	22	0
1	AG	954	0	935	22	0
1	AH	954	0	935	14	0
1	AI	954	0	935	26	0
1	AM	954	0	935	19	0
1	AN	954	0	935	21	0
1	AO	954	0	935	20	0
1	AS	954	0	935	29	0
1	AT	954	0	935	30	0
1	AU	954	0	935	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AY	954	0	935	23	0
1	AZ	954	0	935	20	0
1	BA	954	0	935	14	0
1	BE	954	0	935	21	0
1	BF	954	0	935	19	0
1	BG	954	0	935	28	0
1	BK	954	0	935	30	0
1	BL	954	0	935	26	0
1	BM	954	0	935	16	0
1	BQ	954	0	935	27	0
1	BR	954	0	935	21	0
1	BS	954	0	935	20	0
1	BW	954	0	935	19	0
1	BX	954	0	935	16	0
1	BY	954	0	935	22	0
1	CC	954	0	935	23	0
1	CD	954	0	935	23	0
1	CE	954	0	935	24	0
1	CI	954	0	935	14	0
1	CJ	954	0	935	17	0
1	CK	954	0	935	25	0
1	CO	954	0	935	14	0
1	CP	954	0	935	18	0
1	CQ	954	0	935	23	0
1	CU	954	0	935	14	0
1	CV	954	0	935	21	0
1	CW	954	0	935	23	0
1	DA	954	0	935	25	0
1	DB	954	0	935	26	0
1	DC	954	0	935	21	0
1	DG	954	0	935	13	0
1	DH	954	0	935	18	0
1	DI	954	0	935	23	0
1	DM	954	0	935	21	0
1	DN	954	0	935	17	0
1	DO	954	0	935	18	0
1	DS	954	0	935	19	0
1	DT	954	0	935	21	0
1	DU	954	0	935	18	0
1	DY	954	0	935	20	0
1	DZ	954	0	935	19	0
1	EA	954	0	935	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EE	954	0	935	21	0
1	EF	954	0	935	25	0
1	EG	954	0	935	20	0
1	EK	954	0	935	26	0
1	EL	954	0	935	20	0
1	EM	954	0	935	19	0
1	EQ	954	0	935	23	0
1	ER	954	0	935	11	0
1	ES	954	0	935	12	0
1	EW	954	0	935	11	0
1	EX	954	0	935	20	0
1	EY	954	0	935	15	0
1	FC	954	0	935	18	0
1	FD	954	0	935	15	0
1	FE	954	0	935	24	0
1	FI	954	0	935	22	0
1	FJ	954	0	935	26	0
1	FK	954	0	935	22	0
1	FO	954	0	935	11	0
1	FP	954	0	935	22	0
1	FQ	954	0	935	20	0
1	FU	954	0	935	15	0
1	FV	954	0	935	18	0
1	FW	954	0	935	15	0
1	GA	954	0	935	19	0
1	GB	954	0	935	21	0
1	GC	954	0	935	34	0
1	GG	954	0	935	18	0
1	GH	954	0	935	22	0
1	GI	954	0	935	16	0
1	GM	954	0	935	20	0
1	GN	954	0	935	14	0
1	GO	954	0	935	26	0
1	GS	954	0	935	12	0
1	GT	954	0	935	22	0
1	GU	954	0	935	16	0
1	GY	954	0	935	24	0
1	GZ	954	0	935	30	0
1	HC	954	0	935	29	0
1	HD	954	0	935	18	0
1	HE	954	0	935	31	0
1	HI	954	0	935	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	HJ	954	0	935	17	0
1	HK	954	0	935	21	0
1	HO	954	0	935	20	0
1	HP	954	0	935	10	0
1	HQ	954	0	935	28	0
1	HU	954	0	935	23	0
1	HV	954	0	935	13	0
1	HW	954	0	935	23	0
1	IA	954	0	935	10	0
1	IB	954	0	935	10	0
1	IC	954	0	935	15	0
1	IG	954	0	935	18	0
1	IH	954	0	935	10	0
1	II	954	0	935	21	0
1	IM	954	0	935	16	0
1	IN	954	0	935	24	0
1	IO	954	0	935	25	0
1	IS	954	0	935	31	0
1	IT	954	0	935	36	0
1	IU	954	0	935	24	0
1	IY	954	0	935	13	0
1	IZ	954	0	935	21	0
1	JA	954	0	934	30	0
1	JE	954	0	935	21	0
1	JF	954	0	935	13	0
1	JG	954	0	935	27	0
1	JK	954	0	935	25	0
1	JL	954	0	935	19	0
1	JM	954	0	935	17	0
1	JQ	954	0	935	18	0
1	JR	954	0	935	18	0
1	JS	954	0	935	31	0
1	JW	954	0	935	18	0
1	JX	954	0	935	20	0
1	JY	954	0	935	23	0
1	KC	954	0	935	13	0
1	KD	954	0	935	22	0
1	KE	954	0	935	26	0
1	KI	954	0	935	24	0
1	KJ	954	0	935	28	0
1	KK	954	0	935	22	0
1	KO	954	0	935	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	KP	954	0	935	18	0
1	KQ	954	0	935	16	0
1	KU	954	0	935	18	0
1	KV	954	0	935	25	0
1	KW	954	0	935	28	0
1	LA	954	0	935	18	0
1	LB	954	0	935	23	0
1	LC	954	0	935	22	0
1	LG	954	0	935	21	0
1	LH	954	0	935	16	0
1	LI	954	0	935	15	0
1	LM	954	0	935	18	0
1	LN	954	0	935	16	0
1	LO	954	0	935	15	0
1	LS	954	0	935	18	0
1	LT	954	0	935	23	0
1	LU	954	0	935	23	0
1	LY	954	0	935	27	0
1	LZ	954	0	935	23	0
1	MA	954	0	935	21	0
1	ME	954	0	935	21	0
1	MF	954	0	935	27	0
1	MG	954	0	935	24	0
1	MK	954	0	935	20	0
1	ML	954	0	935	13	0
1	MM	954	0	935	19	0
1	MQ	954	0	935	13	0
1	MR	954	0	935	30	0
1	MS	954	0	935	24	0
1	MW	954	0	935	32	0
1	MX	954	0	935	22	0
1	NA	954	0	935	22	0
1	NB	954	0	935	21	0
1	NC	954	0	935	35	0
1	NG	954	0	935	12	0
1	NH	954	0	935	21	0
1	NI	954	0	935	21	0
1	NM	954	0	935	15	0
1	NN	954	0	935	25	0
1	NO	954	0	935	16	0
2	M	2865	0	2877	40	0
3	AA	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AB	2	0	0	0	0
3	AC	2	0	0	0	0
3	AH	2	0	0	0	0
3	AI	2	0	0	0	0
3	AM	1	0	0	0	0
3	AN	2	0	0	0	0
3	AO	2	0	0	0	0
3	AS	1	0	0	0	0
3	AT	3	0	0	0	0
3	AU	1	0	0	0	0
3	AY	2	0	0	0	0
3	AZ	3	0	0	0	0
3	BA	1	0	0	0	0
3	BE	1	0	0	0	0
3	BG	1	0	0	0	0
3	BK	3	0	0	0	0
3	BM	1	0	0	0	0
3	BQ	3	0	0	0	0
3	BR	1	0	0	0	0
3	BS	1	0	0	0	0
3	BW	1	0	0	0	0
3	BX	1	0	0	0	0
3	BY	2	0	0	0	0
3	CC	2	0	0	0	0
3	CD	1	0	0	0	0
3	CE	2	0	0	0	0
3	CI	3	0	0	0	0
3	CK	2	0	0	0	0
3	CO	3	0	0	0	0
3	CP	1	0	0	0	0
3	CQ	1	0	0	0	0
3	CU	1	0	0	0	0
3	CV	2	0	0	0	0
3	CW	1	0	0	0	0
3	DB	1	0	0	0	0
3	DG	2	0	0	0	0
3	DH	1	0	0	0	0
3	DM	1	0	0	0	0
3	DN	1	0	0	0	0
3	DO	2	0	0	0	0
3	DS	2	0	0	0	0
3	DT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	DY	2	0	0	0	0
3	DZ	1	0	0	0	0
3	EE	2	0	0	0	0
3	EF	1	0	0	0	0
3	EG	1	0	0	0	0
3	EK	1	0	0	0	0
3	EM	2	0	0	0	0
3	EQ	2	0	0	0	0
3	ER	2	0	0	0	0
3	ES	2	0	0	0	0
3	EW	1	0	0	0	0
3	EX	2	0	0	0	0
3	FC	2	0	0	0	0
3	FD	1	0	0	0	0
3	FI	1	0	0	0	0
3	FJ	3	0	0	0	0
3	FK	2	0	0	0	0
3	FO	3	0	0	0	0
3	FP	1	0	0	0	0
3	FU	2	0	0	0	0
3	FV	1	0	0	0	0
3	FW	1	0	0	0	0
3	GA	1	0	0	0	0
3	GB	2	0	0	0	0
3	GC	2	0	0	0	0
3	GH	1	0	0	0	0
3	GI	2	0	0	0	0
3	GM	3	0	0	0	0
3	GO	2	0	0	0	0
3	GS	1	0	0	0	0
3	GT	1	0	0	0	0
3	GY	1	0	0	0	0
3	HC	2	0	0	0	0
3	HD	2	0	0	0	0
3	HE	1	0	0	0	0
3	HI	2	0	0	0	0
3	HK	1	0	0	0	0
3	HO	3	0	0	0	0
3	HP	2	0	0	0	0
3	HU	3	0	0	0	0
3	HV	1	0	0	0	0
3	HW	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	IA	1	0	0	0	0
3	IB	2	0	0	0	0
3	IC	1	0	0	0	0
3	IG	1	0	0	0	0
3	IH	1	0	0	0	0
3	II	1	0	0	0	0
3	IM	2	0	0	0	0
3	IO	1	0	0	0	0
3	IS	3	0	0	0	0
3	IU	1	0	0	0	0
3	IY	1	0	0	0	0
3	IZ	3	0	0	0	0
3	JA	2	0	0	0	0
3	JE	1	0	0	0	0
3	JF	1	0	0	0	0
3	JK	2	0	0	0	0
3	JL	1	0	0	0	0
3	JQ	1	0	0	0	0
3	JR	2	0	0	0	0
3	JW	2	0	0	0	0
3	JX	1	0	0	0	0
3	JY	2	0	0	0	0
3	KC	3	0	0	0	0
3	KD	2	0	0	0	0
3	KI	1	0	0	0	0
3	KJ	1	0	0	0	0
3	KK	1	0	0	0	0
3	KO	2	0	0	0	0
3	KQ	1	0	0	0	0
3	KU	3	0	0	0	0
3	KV	1	0	0	0	0
3	KW	2	0	0	0	0
3	LA	1	0	0	0	0
3	LB	1	0	0	0	0
3	LG	2	0	0	0	0
3	LH	1	0	0	0	0
3	LI	3	0	0	0	0
3	LM	2	0	0	0	0
3	LN	2	0	0	0	0
3	LO	2	0	0	0	0
3	LS	1	0	0	0	0
3	LT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	LU	1	0	0	0	0
3	LY	2	0	0	0	0
3	ME	2	0	0	0	0
3	MG	2	0	0	0	0
3	MK	3	0	0	0	0
3	MQ	2	0	0	0	0
3	MR	2	0	0	0	0
3	MS	2	0	0	0	0
3	MX	1	0	0	0	0
3	NA	2	0	0	0	0
3	NC	1	0	0	0	0
3	NG	3	0	0	0	0
3	NI	2	0	0	0	0
3	NM	1	0	0	0	0
3	NN	1	0	0	0	0
3	NO	1	0	0	0	0
All	All	172913	0	169306	3023	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 9.

All (3023) 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:EM:85:VAL:HG12	1:FQ:85:VAL:HG12	1.42	1.01
1:NN:53:LYS:NZ	1:NN:56:GLN:OE1	1.99	0.95
1:MA:54:PRO:O	1:MA:56:GLN:NE2	2.02	0.93
1:KP:11:GLY:N	1:KU:100:ASP:OD1	2.02	0.92
1:NN:67:THR:OG1	1:NN:82:GLN:OE1	1.87	0.92
1:CK:11:GLY:N	1:II:100:ASP:OD1	2.04	0.91
1:BL:26:ASP:O	1:BL:29:THR:OG1	1.88	0.91
1:IC:54:PRO:O	1:IC:56:GLN:NE2	2.04	0.90
1:IU:1:ALA:N	1:NC:122:SER:OXT	2.02	0.90
1:BL:100:ASP:OD1	1:BQ:11:GLY:N	2.05	0.90
1:EX:54:PRO:O	1:EX:56:GLN:NE2	2.04	0.90
1:HQ:1:ALA:N	1:KW:122:SER:OXT	2.04	0.90
1:BS:30:SER:OG	1:MG:122:SER:O	1.90	0.89
1:AZ:26:ASP:O	1:AZ:29:THR:OG1	1.89	0.89
1:FV:122:SER:HG	1:GA:30:SER:HG	1.09	0.89
1:FW:100:ASP:OD1	1:LU:11:GLY:N	2.05	0.89
1:GZ:56:GLN:NE2	1:GZ:57:VAL:O	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BL:85:VAL:HG12	1:BQ:85:VAL:HG12	1.56	0.88
1:FD:26:ASP:O	1:FD:29:THR:OG1	1.91	0.88
1:GC:54:PRO:O	1:GC:56:GLN:NE2	2.06	0.88
1:MS:93:ASP:OD1	1:MS:94:VAL:N	2.08	0.87
1:HU:85:VAL:HG22	1:IT:85:VAL:HG12	1.56	0.87
1:JM:65:GLU:OE2	1:JM:67:THR:OG1	1.91	0.87
1:EE:29:THR:OG1	1:EE:45:VAL:O	1.92	0.87
1:MQ:65:GLU:OE2	1:MQ:67:THR:OG1	1.90	0.87
1:MX:40:SER:OG	1:MX:71:TYR:OH	1.91	0.87
1:GC:93:ASP:OD1	1:GC:94:VAL:N	2.08	0.87
1:CK:1:ALA:N	1:II:122:SER:OXT	2.07	0.87
1:HQ:54:PRO:O	1:HQ:56:GLN:NE2	2.07	0.87
1:JQ:65:GLU:OE2	1:JQ:67:THR:OG1	1.91	0.87
1:KD:11:GLY:N	1:KI:100:ASP:OD1	2.08	0.87
1:BE:26:ASP:O	1:BE:29:THR:OG1	1.93	0.86
1:DY:26:ASP:O	1:DY:29:THR:OG1	1.92	0.86
1:IG:26:ASP:O	1:IG:29:THR:OG1	1.93	0.86
1:KK:54:PRO:O	1:KK:56:GLN:NE2	2.08	0.86
1:HO:65:GLU:OE2	1:HO:67:THR:OG1	1.92	0.86
1:CV:40:SER:OG	1:CV:69:THR:OG1	1.94	0.86
1:IH:88:ARG:NH2	1:IM:82:GLN:OE1	2.09	0.86
1:HV:26:ASP:O	1:HV:29:THR:OG1	1.95	0.85
1:JG:93:ASP:OD1	1:JG:94:VAL:N	2.10	0.85
1:HE:69:THR:OG1	1:HE:78:GLU:OE2	1.94	0.85
1:AO:11:GLY:N	1:LC:100:ASP:OD1	2.10	0.85
1:BK:65:GLU:OE2	1:BK:67:THR:OG1	1.95	0.85
1:DN:100:ASP:OD1	1:DS:11:GLY:N	2.10	0.85
1:EX:85:VAL:HG12	1:FC:85:VAL:HG12	1.56	0.85
1:IM:26:ASP:O	1:IM:29:THR:OG1	1.94	0.85
1:BF:60:GLU:OE2	1:BK:120:TRP:NE1	2.10	0.84
1:CW:122:SER:O	1:JY:30:SER:OG	1.93	0.84
1:JE:26:ASP:O	1:JE:29:THR:HG22	1.76	0.84
1:HE:65:GLU:OE2	1:HE:67:THR:OG1	1.93	0.84
1:LH:11:GLY:N	1:LM:100:ASP:OD1	2.10	0.84
1:HC:26:ASP:O	1:HC:29:THR:OG1	1.95	0.84
1:FW:85:VAL:HG12	1:LU:85:VAL:HG12	1.60	0.83
1:JF:60:GLU:OE2	1:JK:120:TRP:NE1	2.12	0.83
1:DM:36:GLU:OE1	1:DM:39:SER:OG	1.97	0.83
1:LZ:62:HIS:HB3	1:ME:117:LEU:HD21	1.59	0.83
1:AT:25:GLN:NE2	1:AU:23:ILE:O	2.12	0.82
1:EY:65:GLU:OE2	1:EY:67:THR:OG1	1.96	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BX:65:GLU:OE2	1:BX:82:GLN:NE2	2.12	0.82
1:NN:69:THR:HG22	1:NN:80:VAL:HG12	1.60	0.82
1:AS:29:THR:OG1	1:AS:45:VAL:O	1.97	0.82
1:CD:24:ASN:N	1:CD:31:GLU:OE2	2.13	0.82
1:GU:93:ASP:OD1	1:GU:94:VAL:N	2.13	0.82
1:KP:93:ASP:OD1	1:KP:94:VAL:N	2.11	0.82
1:BA:1:ALA:N	1:NO:121:GLU:OE2	2.12	0.82
1:IZ:26:ASP:O	1:IZ:29:THR:OG1	1.96	0.82
1:LT:122:SER:OXT	1:LY:1:ALA:N	2.13	0.82
1:KV:26:ASP:O	1:KV:29:THR:OG1	1.96	0.82
1:LY:65:GLU:OE2	1:LY:67:THR:OG1	1.96	0.82
1:GY:60:GLU:OE1	1:GY:62:HIS:NE2	2.13	0.82
1:LU:36:GLU:OE2	1:LU:39:SER:OG	1.98	0.82
1:IN:65:GLU:OE2	1:IN:67:THR:OG1	1.98	0.81
1:LA:36:GLU:OE2	1:LA:39:SER:OG	1.97	0.81
1:AI:53:LYS:NZ	1:AI:55:ASN:OD1	2.13	0.81
1:GO:89:HIS:NE2	1:JS:118:ILE:HD11	1.95	0.81
1:KI:26:ASP:O	1:KI:29:THR:HG22	1.81	0.81
1:DO:99:SER:OG	1:GC:111:GLU:OE1	1.99	0.80
1:KK:40:SER:OG	1:KK:71:TYR:OH	2.00	0.80
1:LI:85:VAL:HG12	1:MM:85:VAL:HG22	1.62	0.80
2:M:16:SER:OG	2:M:78:CYS:SG	2.33	0.80
1:CW:65:GLU:OE2	1:CW:67:THR:OG1	1.97	0.80
1:DU:100:ASP:OD1	1:LO:11:GLY:N	2.13	0.80
1:NH:26:ASP:O	1:NH:29:THR:OG1	1.99	0.80
1:GS:29:THR:OG1	1:GS:45:VAL:O	2.00	0.80
1:GU:1:ALA:N	1:HW:122:SER:OXT	2.14	0.80
1:KJ:1:ALA:N	1:KO:122:SER:OXT	2.15	0.80
1:CD:65:GLU:OE2	1:CD:67:THR:OG1	1.99	0.79
1:HQ:65:GLU:OE2	1:HQ:82:GLN:NE2	2.14	0.79
1:IU:99:SER:OG	1:IU:103:GLU:OE2	1.99	0.79
1:DA:24:ASN:ND2	1:DC:26:ASP:O	2.16	0.79
1:DB:63:ASN:ND2	1:DB:65:GLU:OE2	2.14	0.79
1:IB:60:GLU:OE2	1:IB:91:VAL:HG12	1.83	0.79
1:JL:121:GLU:OE2	1:JR:21:ARG:NH1	2.16	0.79
1:MM:40:SER:OG	1:MM:71:TYR:OH	2.01	0.79
1:CV:26:ASP:O	1:CV:29:THR:OG1	2.01	0.79
1:BL:55:ASN:OD1	1:BL:56:GLN:NE2	2.15	0.79
1:BR:93:ASP:OD1	1:BR:94:VAL:N	2.16	0.78
1:IN:100:ASP:OD1	1:IS:11:GLY:N	2.16	0.78
1:JY:69:THR:OG1	1:JY:78:GLU:OE2	2.00	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LI:122:SER:OXT	1:MM:1:ALA:N	2.16	0.78
1:CJ:54:PRO:O	1:CJ:56:GLN:NE2	2.16	0.78
1:CP:65:GLU:OE2	1:CP:67:THR:OG1	2.00	0.78
1:FW:65:GLU:OE2	1:FW:67:THR:OG1	2.02	0.78
1:AH:93:ASP:OD2	1:AH:94:VAL:N	2.16	0.78
1:HD:11:GLY:N	1:HI:100:ASP:OD1	2.16	0.78
1:FW:19:VAL:O	1:FW:34:LEU:HD22	1.84	0.78
1:FD:65:GLU:OE2	1:FD:67:THR:OG1	2.00	0.78
1:CE:65:GLU:OE2	1:CE:67:THR:OG1	2.02	0.78
1:DM:65:GLU:OE2	1:DM:67:THR:OG1	2.01	0.78
1:BQ:65:GLU:OE2	1:BQ:82:GLN:NE2	2.16	0.77
1:JL:69:THR:HG22	1:JL:80:VAL:HG12	1.65	0.77
1:NI:109:LEU:HD13	1:NI:113:LEU:HD11	1.65	0.77
1:HV:93:ASP:OD2	1:HV:94:VAL:N	2.16	0.77
1:EQ:19:VAL:O	1:EQ:34:LEU:HD12	1.85	0.77
1:BS:93:ASP:OD1	1:BS:94:VAL:N	2.16	0.77
1:DM:60:GLU:OE2	1:DM:91:VAL:HG12	1.84	0.77
1:KJ:100:ASP:OD1	1:KO:11:GLY:N	2.17	0.77
1:KP:120:TRP:NE1	1:KU:60:GLU:OE2	2.17	0.77
1:NO:65:GLU:OE2	1:NO:67:THR:OG1	2.01	0.77
1:DG:26:ASP:O	1:DG:29:THR:OG1	2.01	0.76
1:ES:122:SER:OXT	1:JM:1:ALA:N	2.18	0.76
1:DG:1:ALA:N	1:EF:122:SER:OXT	2.17	0.76
1:HQ:1:ALA:N	1:KW:121:GLU:OE2	2.14	0.76
1:CK:60:GLU:OE2	1:II:120:TRP:NE1	2.19	0.76
1:EA:1:ALA:N	1:NI:122:SER:OXT	2.19	0.76
1:FC:51:SER:O	1:FC:53:LYS:NZ	2.18	0.76
1:AI:30:SER:OG	1:JG:122:SER:O	2.03	0.76
1:BF:85:VAL:HG12	1:BK:85:VAL:HG22	1.67	0.76
1:EA:25:GLN:OE1	1:EA:30:SER:OG	2.02	0.76
1:EF:93:ASP:OD2	1:EF:94:VAL:N	2.18	0.76
1:LM:24:ASN:ND2	1:LO:26:ASP:O	2.17	0.76
1:HU:60:GLU:OE2	1:IT:120:TRP:NE1	2.19	0.76
1:LZ:4:ASP:OD1	1:LZ:5:THR:HG23	1.86	0.76
1:MF:40:SER:OG	1:MF:71:TYR:OH	2.03	0.76
1:ML:62:HIS:HB3	1:MQ:117:LEU:HD21	1.68	0.76
1:NA:16:THR:OG1	1:NA:18:LYS:NZ	2.19	0.75
1:AT:40:SER:OG	1:AT:71:TYR:OH	2.03	0.75
1:DT:36:GLU:OE2	1:DT:39:SER:OG	2.00	0.75
1:DH:3:GLY:O	1:DH:22:LYS:NZ	2.20	0.75
1:LC:24:ASN:OD1	1:LC:25:GLN:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MX:100:ASP:OD1	1:NA:11:GLY:N	2.19	0.75
1:IT:19:VAL:O	1:IT:34:LEU:HD22	1.87	0.75
1:AO:65:GLU:OE2	1:AO:67:THR:OG1	2.03	0.75
1:MG:93:ASP:OD1	1:MG:94:VAL:N	2.20	0.75
1:CC:23:ILE:HD11	1:DI:120:TRP:HB3	1.69	0.74
1:II:31:GLU:OE1	1:II:44:LYS:NZ	2.20	0.74
1:EK:32:TYR:HB2	1:EK:43:ALA:HB3	1.68	0.74
1:AI:85:VAL:HG11	1:JG:109:LEU:HD11	1.68	0.74
1:GM:50:GLU:OE2	1:GM:53:LYS:NZ	2.20	0.74
1:BG:117:LEU:HD21	1:HE:62:HIS:HB3	1.69	0.74
1:IU:122:SER:OXT	1:NC:1:ALA:N	2.21	0.74
1:JR:99:SER:OG	1:JW:111:GLU:OE1	2.06	0.74
1:LT:121:GLU:OE2	1:LY:1:ALA:N	2.18	0.74
1:NN:4:ASP:OD1	1:NN:5:THR:HG23	1.88	0.74
1:EM:65:GLU:OE2	1:EM:67:THR:OG1	2.05	0.74
1:IC:85:VAL:HG22	1:KQ:85:VAL:HG12	1.70	0.74
1:IZ:93:ASP:OD1	1:IZ:94:VAL:N	2.20	0.74
1:KI:29:THR:OG1	1:KI:45:VAL:O	2.00	0.73
1:MX:82:GLN:OE1	1:NA:88:ARG:NH2	2.20	0.73
1:DT:20:LEU:HB3	1:DT:32:TYR:HB3	1.70	0.73
1:AO:19:VAL:O	1:AO:34:LEU:HD22	1.88	0.73
1:GY:23:ILE:HD11	1:GY:31:GLU:OE2	1.88	0.73
1:ME:68:GLU:OE2	1:ME:81:ARG:NH2	2.21	0.73
1:HE:24:ASN:OD1	1:HE:25:GLN:N	2.22	0.73
1:HW:24:ASN:OD1	1:HW:25:GLN:N	2.21	0.73
1:MR:111:GLU:OE1	1:MW:99:SER:OG	2.07	0.73
1:AB:29:THR:HG22	1:AB:46:ARG:HB2	1.69	0.73
1:CO:55:ASN:OD1	1:CO:56:GLN:NE2	2.22	0.73
1:JW:50:GLU:OE2	1:JW:61:ARG:NH2	2.21	0.73
1:LG:4:ASP:OD1	1:LG:5:THR:HG23	1.89	0.73
1:BF:26:ASP:O	1:BF:29:THR:OG1	2.04	0.72
1:HD:69:THR:HG22	1:HD:80:VAL:HG12	1.70	0.72
1:CE:11:GLY:N	1:DI:100:ASP:OD1	2.21	0.72
1:JY:4:ASP:OD1	1:JY:5:THR:HG23	1.89	0.72
1:AA:60:GLU:OE2	1:NN:120:TRP:NE1	2.22	0.72
1:DT:62:HIS:HB3	1:DY:117:LEU:HD21	1.71	0.72
1:FK:62:HIS:HB3	1:MA:117:LEU:HD21	1.71	0.72
1:IB:93:ASP:OD2	1:IB:94:VAL:N	2.23	0.72
1:EX:120:TRP:NE1	1:FC:60:GLU:OE2	2.22	0.72
1:BG:50:GLU:N	1:BG:50:GLU:OE2	2.23	0.72
1:CV:93:ASP:OD1	1:CV:94:VAL:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FO:117:LEU:HD21	1:GN:62:HIS:CB	2.20	0.72
1:FU:26:ASP:O	1:FU:29:THR:OG1	2.05	0.72
1:KQ:55:ASN:OD1	1:KQ:56:GLN:NE2	2.23	0.72
1:GZ:62:HIS:HB3	1:HC:117:LEU:HD21	1.71	0.72
1:BG:122:SER:O	1:HE:30:SER:OG	2.04	0.72
1:BQ:52:VAL:HG22	1:BQ:58:GLN:NE2	2.04	0.72
1:KD:109:LEU:HD13	1:KD:113:LEU:HD22	1.72	0.72
1:AM:93:ASP:OD1	1:AM:94:VAL:N	2.22	0.72
1:HQ:122:SER:O	1:KW:30:SER:OG	2.04	0.72
1:NC:65:GLU:OE2	1:NC:67:THR:OG1	2.07	0.72
1:GN:31:GLU:OE2	1:GN:42:ARG:NH1	2.23	0.71
1:JE:19:VAL:O	1:JE:34:LEU:HD22	1.89	0.71
1:JK:5:THR:OG1	1:JK:20:LEU:O	2.05	0.71
1:BS:85:VAL:HG12	1:MG:85:VAL:HG22	1.72	0.71
1:GA:40:SER:OG	1:GA:71:TYR:OH	2.07	0.71
1:AC:122:SER:O	1:EY:30:SER:OG	2.05	0.71
1:BS:122:SER:OXT	1:MG:1:ALA:N	2.23	0.71
1:DT:60:GLU:OE2	1:DY:120:TRP:NE1	2.23	0.71
1:GY:50:GLU:OE2	1:GY:61:ARG:NH1	2.22	0.71
1:HJ:1:ALA:N	1:HO:122:SER:OXT	2.23	0.71
1:HV:50:GLU:OE2	1:HV:61:ARG:NH2	2.24	0.71
1:JF:85:VAL:HG22	1:JK:85:VAL:HG12	1.71	0.71
1:NI:109:LEU:HD12	1:NI:114:TYR:HE1	1.54	0.71
1:GS:68:GLU:OE1	1:GS:81:ARG:NE	2.24	0.71
1:KJ:118:ILE:HD11	1:KO:89:HIS:HE2	1.54	0.71
1:MX:26:ASP:O	1:MX:29:THR:OG1	2.07	0.71
1:KK:65:GLU:OE2	1:KK:67:THR:OG1	2.08	0.71
1:AI:60:GLU:OE2	1:JG:120:TRP:NE1	2.24	0.70
1:BG:19:VAL:O	1:BG:34:LEU:HD22	1.91	0.70
1:CE:24:ASN:OD1	1:CE:25:GLN:N	2.24	0.70
1:MX:81:ARG:NH1	1:NA:93:ASP:OD2	2.24	0.70
1:AA:11:GLY:N	1:NN:100:ASP:OD1	2.25	0.70
1:EM:1:ALA:N	1:FQ:122:SER:OXT	2.24	0.70
1:MF:31:GLU:N	1:MF:31:GLU:OE1	2.25	0.70
1:CW:116:LYS:NZ	1:JY:2:LEU:HD23	2.06	0.70
1:DT:100:ASP:OD1	1:DY:11:GLY:N	2.24	0.70
1:GB:36:GLU:OE2	1:GB:39:SER:OG	2.06	0.70
1:MR:65:GLU:OE2	1:MR:67:THR:OG1	2.07	0.70
1:BW:65:GLU:OE2	1:BW:67:THR:OG1	2.10	0.70
1:DS:99:SER:OG	1:DS:103:GLU:OE2	2.08	0.70
1:IC:1:ALA:N	1:KQ:122:SER:OXT	2.25	0.70

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:LO:19:VAL:O	1:LO:34:LEU:HD22	1.92	0.70
1:AG:25:GLN:NE2	1:AH:23:ILE:O	2.25	0.70
1:DO:19:VAL:O	1:DO:34:LEU:HD22	1.92	0.70
1:JW:16:THR:OG1	1:JW:18:LYS:NZ	2.25	0.70
1:AO:30:SER:OG	1:LC:122:SER:O	2.06	0.69
1:GB:1:ALA:N	1:GG:122:SER:OXT	2.25	0.69
1:GU:24:ASN:OD1	1:GU:25:GLN:N	2.25	0.69
1:JY:50:GLU:OE1	1:JY:88:ARG:NH1	2.24	0.69
1:GG:36:GLU:OE2	1:GG:39:SER:N	2.25	0.69
1:IO:23:ILE:HG22	1:IO:31:GLU:O	1.92	0.69
1:KV:4:ASP:OD1	1:KV:5:THR:HG23	1.92	0.69
1:CQ:65:GLU:OE2	1:CQ:67:THR:OG1	2.09	0.69
1:DO:85:VAL:HG11	1:GC:109:LEU:HD11	1.72	0.69
1:BW:58:GLN:NE2	1:BW:59:TYR:O	2.25	0.69
1:BY:85:VAL:HG11	1:FE:109:LEU:HD11	1.75	0.69
1:KI:109:LEU:HD13	1:KI:113:LEU:HD22	1.74	0.69
1:CI:26:ASP:O	1:CI:29:THR:HG22	1.93	0.69
1:JA:31:GLU:OE1	1:JA:44:LYS:NZ	2.26	0.69
1:KC:89:HIS:NE2	1:LB:118:ILE:HD11	2.08	0.69
1:LC:34:LEU:HD21	1:LC:36:GLU:OE2	1.93	0.69
1:LT:55:ASN:OD1	1:LT:56:GLN:NE2	2.25	0.69
1:MQ:24:ASN:OD1	1:MQ:25:GLN:N	2.26	0.69
1:BX:67:THR:HG23	1:BX:82:GLN:OE1	1.93	0.69
1:BY:93:ASP:OD1	1:BY:94:VAL:N	2.25	0.69
1:EK:47:HIS:NE2	1:FJ:121:GLU:O	2.26	0.69
1:GO:122:SER:O	1:JS:30:SER:OG	2.10	0.69
1:LH:100:ASP:OD1	1:LM:11:GLY:N	2.26	0.69
1:GS:122:SER:OXT	1:HP:1:ALA:N	2.26	0.68
1:CJ:68:GLU:OE1	1:CJ:81:ARG:NE	2.26	0.68
1:KV:60:GLU:OE2	1:LA:120:TRP:NE1	2.25	0.68
1:GZ:1:ALA:N	1:HC:122:SER:OXT	2.26	0.68
1:KO:60:GLU:OE2	1:KO:89:HIS:NE2	2.27	0.68
1:JF:93:ASP:OD1	1:JF:94:VAL:N	2.26	0.68
1:MW:26:ASP:OD1	1:MW:29:THR:OG1	2.11	0.68
1:DH:40:SER:OG	1:DH:71:TYR:OH	2.11	0.68
1:EK:89:HIS:NE2	1:FJ:118:ILE:HD11	2.07	0.68
1:FK:1:ALA:N	1:MA:122:SER:OXT	2.14	0.68
1:HJ:2:LEU:HD22	1:HO:121:GLU:OE2	1.93	0.68
1:LN:99:SER:OG	1:LS:111:GLU:OE1	2.11	0.68
1:AI:19:VAL:O	1:AI:34:LEU:HD12	1.94	0.68
1:IN:117:LEU:HD21	1:IS:62:HIS:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JL:54:PRO:O	1:JL:56:GLN:NE2	2.26	0.68
1:GB:60:GLU:OE2	1:GG:120:TRP:NE1	2.26	0.68
1:GO:117:LEU:HD21	1:JS:62:HIS:HB3	1.74	0.68
1:JK:55:ASN:OD1	1:JK:55:ASN:O	2.12	0.68
1:LN:120:TRP:NE1	1:LS:60:GLU:OE2	2.26	0.68
1:GH:109:LEU:HD11	1:GM:85:VAL:HG11	1.76	0.68
1:JR:62:HIS:CB	1:JW:117:LEU:HD21	2.23	0.68
1:LU:24:ASN:ND2	1:LU:26:ASP:OD2	2.27	0.68
1:BE:4:ASP:OD1	1:BE:5:THR:HG23	1.94	0.68
1:HO:114:TYR:O	1:HO:118:ILE:HD12	1.94	0.68
1:KV:20:LEU:HB3	1:KV:32:TYR:HB3	1.76	0.68
1:AC:1:ALA:N	1:EY:122:SER:OXT	2.27	0.68
1:AI:30:SER:OG	1:JG:122:SER:OG	2.12	0.68
1:FD:19:VAL:O	1:FD:34:LEU:HD22	1.94	0.68
1:GB:36:GLU:OE2	1:GB:39:SER:N	2.27	0.68
1:LT:19:VAL:O	1:LT:34:LEU:HD22	1.94	0.68
1:LO:109:LEU:HD12	1:LO:114:TYR:CZ	2.29	0.67
1:HP:45:VAL:HG22	1:HP:64:VAL:HG12	1.76	0.67
1:NG:29:THR:OG1	1:NG:45:VAL:O	2.08	0.67
1:JE:65:GLU:OE2	1:JE:67:THR:OG1	2.11	0.67
1:EK:11:GLY:N	1:FJ:100:ASP:OD1	2.28	0.67
1:AZ:120:TRP:NE1	1:BE:60:GLU:OE2	2.27	0.67
1:LS:8:ILE:HD13	1:LS:66:PHE:CE2	2.29	0.67
1:CJ:45:VAL:HG12	1:CJ:64:VAL:HG23	1.77	0.67
1:KV:68:GLU:OE1	1:KV:81:ARG:NE	2.27	0.67
1:DZ:109:LEU:HD13	1:DZ:113:LEU:HD22	1.75	0.67
1:EE:26:ASP:O	1:EE:29:THR:HG22	1.94	0.67
1:EX:108:TYR:OH	1:EX:113:LEU:HD11	1.95	0.67
1:HE:29:THR:OG1	1:HE:45:VAL:O	2.05	0.67
1:EK:121:GLU:OE2	1:FK:21:ARG:NE	2.28	0.66
1:IH:120:TRP:O	1:IN:23:ILE:HD11	1.96	0.66
1:MX:4:ASP:OD1	1:MX:5:THR:HG23	1.95	0.66
1:BR:69:THR:OG1	1:BR:78:GLU:OE2	2.13	0.66
1:BW:55:ASN:OD1	1:BW:55:ASN:O	2.13	0.66
1:LU:20:LEU:HB3	1:LU:32:TYR:HB3	1.75	0.66
1:BY:30:SER:OG	1:FE:122:SER:O	2.11	0.66
1:DY:65:GLU:OE1	1:DY:67:THR:HG23	1.95	0.66
1:KO:26:ASP:O	1:KO:29:THR:HG22	1.95	0.66
1:LZ:45:VAL:HG22	1:LZ:64:VAL:HG22	1.77	0.66
2:M:243:SER:OG	2:M:246:GLU:OE2	2.13	0.66
1:BG:60:GLU:OE1	1:BG:62:HIS:NE2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CE:36:GLU:OE2	1:CE:39:SER:OG	2.10	0.66
1:GA:24:ASN:OD1	1:GA:25:GLN:N	2.29	0.66
1:IY:40:SER:OG	1:IY:71:TYR:OH	2.12	0.66
1:JR:32:TYR:HB2	1:JR:43:ALA:HB3	1.76	0.66
1:DA:24:ASN:OD1	1:DA:25:GLN:N	2.29	0.66
1:DU:24:ASN:OD1	1:DU:25:GLN:N	2.29	0.66
1:FK:113:LEU:O	1:FK:117:LEU:HD23	1.95	0.66
1:AY:108:TYR:CE2	1:AY:113:LEU:HD21	2.30	0.66
1:CJ:117:LEU:HD21	1:CO:62:HIS:CB	2.25	0.66
1:IC:2:LEU:HD22	1:KQ:121:GLU:OE2	1.95	0.66
1:BK:51:SER:OG	1:BK:53:LYS:NZ	2.29	0.66
1:GS:26:ASP:O	1:GS:29:THR:HG22	1.96	0.66
1:HD:1:ALA:N	1:HI:122:SER:OXT	2.16	0.66
1:IN:52:VAL:HG22	1:IN:58:GLN:NE2	2.11	0.66
1:AO:122:SER:O	1:LC:30:SER:OG	2.09	0.66
1:AT:60:GLU:OE2	1:AT:91:VAL:HG22	1.96	0.66
1:FP:109:LEU:HD23	1:FP:113:LEU:HD23	1.78	0.65
1:MF:4:ASP:OD1	1:MF:21:ARG:NH2	2.28	0.65
1:AB:19:VAL:O	1:AB:34:LEU:HD22	1.96	0.65
1:BG:117:LEU:HD21	1:HE:62:HIS:CB	2.26	0.65
1:EM:50:GLU:OE1	1:EM:50:GLU:N	2.29	0.65
1:AT:40:SER:HG	1:AT:71:TYR:HH	1.42	0.65
1:CD:93:ASP:OD1	1:CD:94:VAL:N	2.29	0.65
1:DC:122:SER:O	1:GI:30:SER:OG	2.14	0.65
1:DU:114:TYR:O	1:DU:118:ILE:HD12	1.96	0.65
1:HD:1:ALA:N	1:HI:121:GLU:OE2	2.29	0.65
1:HJ:2:LEU:HD23	1:HO:122:SER:O	1.96	0.65
1:MM:4:ASP:OD1	1:MM:5:THR:HG23	1.95	0.65
1:BF:117:LEU:HD21	1:BK:62:HIS:HB3	1.79	0.65
1:MK:120:TRP:NE1	1:NH:60:GLU:OE2	2.29	0.65
1:GC:63:ASN:OD1	1:GC:64:VAL:N	2.30	0.65
1:MR:58:GLN:NE2	1:MR:59:TYR:O	2.30	0.65
1:DG:2:LEU:N	1:EF:121:GLU:OE2	2.30	0.65
1:GZ:2:LEU:HD12	1:HC:121:GLU:OE2	1.96	0.65
1:HU:122:SER:OXT	1:IT:1:ALA:N	2.30	0.65
1:JK:36:GLU:OE1	1:JK:39:SER:N	2.30	0.65
1:JS:21:ARG:NH1	1:JW:121:GLU:OE2	2.30	0.65
1:AN:51:SER:OG	1:AN:53:LYS:NZ	2.30	0.65
1:AZ:99:SER:OG	1:BE:111:GLU:OE2	2.12	0.65
1:ER:62:HIS:CG	1:EW:117:LEU:HD21	2.31	0.65
1:KV:100:ASP:OD1	1:LA:11:GLY:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CP:26:ASP:O	1:CP:29:THR:OG1	2.12	0.65
1:HW:109:LEU:HD12	1:HW:114:TYR:CZ	2.32	0.65
1:KJ:122:SER:OXT	1:KO:1:ALA:N	2.29	0.65
1:AS:26:ASP:O	1:AS:29:THR:HG22	1.97	0.64
1:GT:62:HIS:N	1:GT:87:ILE:O	2.27	0.64
1:CP:60:GLU:OE2	1:CU:120:TRP:NE1	2.28	0.64
1:DN:68:GLU:OE1	1:DN:81:ARG:NE	2.30	0.64
1:HE:58:GLN:NE2	1:HE:59:TYR:O	2.30	0.64
1:KI:49:LYS:NZ	1:KI:60:GLU:OE2	2.29	0.64
1:NI:109:LEU:HD12	1:NI:114:TYR:CE1	2.31	0.64
1:ER:108:TYR:CE2	1:ER:113:LEU:HD21	2.33	0.64
1:LM:65:GLU:OE2	1:LM:82:GLN:NE2	2.30	0.64
1:GS:93:ASP:OD1	1:GS:94:VAL:N	2.30	0.64
1:JE:24:ASN:OD1	1:JE:25:GLN:N	2.30	0.64
1:KD:100:ASP:OD1	1:KI:11:GLY:N	2.30	0.64
1:BQ:67:THR:HG23	1:BQ:82:GLN:OE1	1.97	0.64
1:BW:93:ASP:OD1	1:BW:94:VAL:N	2.31	0.64
1:EG:109:LEU:HD12	1:EG:114:TYR:CZ	2.32	0.64
1:LI:85:VAL:CG1	1:MM:85:VAL:HG22	2.27	0.64
1:MM:113:LEU:O	1:MM:117:LEU:HD23	1.98	0.64
1:DO:122:SER:O	1:GC:30:SER:OG	2.16	0.64
1:DS:50:GLU:OE2	1:DS:61:ARG:NH1	2.31	0.64
1:JQ:32:TYR:HB2	1:JQ:43:ALA:HB3	1.80	0.64
1:CD:47:HIS:NE2	1:CI:121:GLU:O	2.31	0.64
1:ES:21:ARG:NE	1:EW:121:GLU:OE2	2.29	0.64
1:GC:60:GLU:OE1	1:GC:89:HIS:NE2	2.31	0.64
1:HU:59:TYR:OH	1:IT:80:VAL:HG22	1.97	0.64
1:HW:19:VAL:O	1:HW:34:LEU:HD12	1.98	0.64
1:NC:4:ASP:OD1	1:NC:5:THR:N	2.31	0.64
1:AC:24:ASN:OD1	1:AC:25:GLN:N	2.31	0.64
1:DU:31:GLU:OE1	1:DU:44:LYS:NZ	2.28	0.64
1:FD:108:TYR:OH	1:FD:113:LEU:HD11	1.98	0.64
1:IU:1:ALA:N	1:NC:121:GLU:OE2	2.30	0.64
1:JL:82:GLN:OE1	1:JQ:88:ARG:NH1	2.30	0.64
1:MK:19:VAL:O	1:MK:34:LEU:HD22	1.98	0.64
1:NB:20:LEU:HB3	1:NB:32:TYR:HB3	1.78	0.64
1:FK:122:SER:O	1:MA:30:SER:OG	2.16	0.63
1:GT:24:ASN:OD1	1:GT:25:GLN:N	2.31	0.63
1:KJ:118:ILE:HD11	1:KO:89:HIS:NE2	2.13	0.63
1:CI:24:ASN:OD1	1:CI:25:GLN:N	2.30	0.63
1:IT:113:LEU:O	1:IT:117:LEU:HD23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EM:4:ASP:OD1	1:EM:5:THR:HG23	1.98	0.63
1:NN:26:ASP:O	1:NN:29:THR:OG1	2.09	0.63
1:HP:93:ASP:OD1	1:HP:94:VAL:N	2.31	0.63
1:AM:36:GLU:OE2	1:AM:39:SER:N	2.31	0.63
1:GT:52:VAL:HG22	1:GT:58:GLN:NE2	2.13	0.63
1:KI:65:GLU:OE2	1:KI:67:THR:OG1	2.15	0.63
1:AC:110:ASN:OD1	1:AC:111:GLU:N	2.30	0.63
1:CW:117:LEU:HD21	1:JY:62:HIS:HB3	1.81	0.63
1:DG:85:VAL:HG23	1:EF:105:LEU:HD21	1.80	0.63
1:ME:36:GLU:OE1	1:ME:39:SER:N	2.32	0.63
1:MK:122:SER:OG	1:NH:47:HIS:NE2	2.31	0.63
1:DC:24:ASN:OD1	1:DC:25:GLN:N	2.32	0.63
1:AC:117:LEU:HD21	1:EY:62:HIS:CB	2.29	0.63
1:LC:65:GLU:OE2	1:LC:67:THR:OG1	2.13	0.63
1:AT:113:LEU:O	1:AT:117:LEU:HD23	1.99	0.63
1:BF:19:VAL:O	1:BF:34:LEU:HD22	1.98	0.63
1:EQ:93:ASP:OD1	1:EQ:94:VAL:N	2.31	0.63
1:LB:93:ASP:OD1	1:LB:94:VAL:N	2.32	0.63
1:FP:1:ALA:N	1:FU:122:SER:OXT	2.31	0.62
1:GU:5:THR:HG22	1:GU:21:ARG:HD3	1.81	0.62
1:HJ:87:ILE:HD11	1:HO:114:TYR:HE2	1.62	0.62
1:JE:108:TYR:CZ	1:JE:113:LEU:HD11	2.34	0.62
1:JK:108:TYR:CE2	1:JK:113:LEU:HD11	2.34	0.62
1:MR:45:VAL:HG22	1:MR:64:VAL:HG23	1.81	0.62
1:CW:117:LEU:HD21	1:JY:62:HIS:CB	2.28	0.62
1:LY:50:GLU:OE2	1:LY:53:LYS:NZ	2.27	0.62
1:LZ:19:VAL:HG23	1:LZ:19:VAL:O	1.99	0.62
1:BA:109:LEU:HD12	1:BA:114:TYR:CE1	2.35	0.62
1:BF:122:SER:O	1:BK:30:SER:OG	2.13	0.62
1:BK:19:VAL:HG23	1:BK:19:VAL:O	1.99	0.62
1:DB:112:ALA:O	1:DB:116:LYS:HG3	1.99	0.62
1:EA:23:ILE:HD11	1:EE:120:TRP:HB3	1.82	0.62
1:KC:62:HIS:HB3	1:LB:117:LEU:HD21	1.81	0.62
1:LA:36:GLU:OE2	1:LA:39:SER:N	2.32	0.62
1:BG:100:ASP:OD1	1:HE:11:GLY:N	2.32	0.62
2:M:164:ASP:O	2:M:168:THR:HG23	1.98	0.62
1:CD:40:SER:OG	1:CD:71:TYR:OH	2.07	0.62
1:BR:40:SER:OG	1:BR:71:TYR:OH	2.17	0.62
1:CD:26:ASP:O	1:CD:29:THR:OG1	2.09	0.62
1:CO:36:GLU:OE2	1:CO:39:SER:N	2.32	0.62
1:DA:65:GLU:CB	1:DA:84:TYR:HB3	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DC:60:GLU:OE1	1:DC:62:HIS:NE2	2.33	0.62
1:DC:113:LEU:O	1:DC:117:LEU:HD23	1.99	0.62
1:EA:122:SER:O	1:NI:30:SER:OG	2.04	0.62
1:HD:120:TRP:NE1	1:HI:60:GLU:OE2	2.33	0.62
1:GN:24:ASN:OD1	1:GN:25:GLN:N	2.32	0.62
1:BW:24:ASN:OD1	1:BW:25:GLN:N	2.32	0.62
1:HE:108:TYR:CZ	1:HE:113:LEU:HD11	2.35	0.62
1:IO:19:VAL:O	1:IO:34:LEU:HD22	1.99	0.62
1:IO:54:PRO:O	1:IO:56:GLN:NE2	2.33	0.62
1:JE:113:LEU:HD23	1:JE:117:LEU:HD23	1.81	0.62
1:LI:55:ASN:OD1	1:LI:56:GLN:N	2.32	0.62
1:AZ:69:THR:HG22	1:AZ:80:VAL:HG12	1.82	0.62
1:JE:40:SER:OG	1:JE:71:TYR:OH	2.14	0.62
1:LN:85:VAL:HG23	1:LS:84:TYR:O	1.98	0.62
1:CQ:40:SER:HG	1:CQ:69:THR:HG1	1.46	0.62
1:ER:85:VAL:HG11	1:EW:109:LEU:HD11	1.82	0.62
1:HD:19:VAL:HG23	1:HD:19:VAL:O	2.00	0.62
1:IT:24:ASN:OD1	1:IT:25:GLN:N	2.33	0.62
2:M:29:GLU:OE1	2:M:31:ILE:HG23	2.00	0.62
1:JG:65:GLU:OE2	1:JG:67:THR:OG1	2.18	0.61
1:MR:68:GLU:O	1:MR:81:ARG:N	2.28	0.61
1:MX:118:ILE:HD11	1:NA:89:HIS:CE1	2.35	0.61
1:NH:19:VAL:HG23	1:NH:19:VAL:O	2.00	0.61
1:GN:113:LEU:O	1:GN:117:LEU:HD23	2.01	0.61
1:IU:118:ILE:HD11	1:NC:89:HIS:NE2	2.14	0.61
1:JA:117:LEU:HD21	1:KE:62:HIS:CB	2.30	0.61
1:AY:65:GLU:OE2	1:AY:82:GLN:NE2	2.33	0.61
1:IU:117:LEU:HD21	1:NC:62:HIS:CB	2.30	0.61
1:KC:120:TRP:O	1:LC:23:ILE:HD11	2.00	0.61
1:AI:10:LEU:HA	1:JG:104:ALA:HB2	1.82	0.61
1:DZ:20:LEU:HB3	1:DZ:32:TYR:HB3	1.81	0.61
1:LB:19:VAL:O	1:LB:19:VAL:HG23	2.00	0.61
1:DM:50:GLU:OE2	1:DM:61:ARG:NE	2.32	0.61
1:HE:36:GLU:OE1	1:HE:38:SER:N	2.32	0.61
1:JR:24:ASN:ND2	1:JR:26:ASP:OD2	2.32	0.61
1:EL:63:ASN:OD1	1:EL:64:VAL:N	2.33	0.61
1:BW:53:LYS:HG2	1:BW:54:PRO:HD2	1.82	0.61
1:EQ:24:ASN:OD1	1:EQ:25:GLN:N	2.33	0.61
1:FE:93:ASP:OD1	1:FE:94:VAL:N	2.33	0.61
1:CJ:19:VAL:O	1:CJ:34:LEU:HD22	2.01	0.61
1:FJ:109:LEU:HD13	1:FJ:113:LEU:HD22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:117:LEU:HD21	1:DB:62:HIS:CB	2.30	0.61
1:IH:120:TRP:C	1:IN:23:ILE:HD11	2.21	0.61
1:JM:31:GLU:OE2	1:JM:42:ARG:NH1	2.34	0.61
1:LH:19:VAL:HG23	1:LH:19:VAL:O	2.01	0.61
1:AA:26:ASP:O	1:AA:29:THR:OG1	2.14	0.61
1:BL:45:VAL:HG22	1:BL:64:VAL:HG12	1.82	0.61
1:CC:108:TYR:CE2	1:CC:113:LEU:HD21	2.35	0.61
1:DN:108:TYR:CE1	1:DN:113:LEU:HD21	2.36	0.61
1:KP:31:GLU:OE2	1:KP:42:ARG:NH1	2.33	0.61
1:AB:63:ASN:OD1	1:AB:64:VAL:N	2.34	0.60
1:AC:117:LEU:HD21	1:EY:62:HIS:HB3	1.83	0.60
1:ER:113:LEU:O	1:ER:117:LEU:HD23	2.00	0.60
1:HV:60:GLU:OE2	1:IA:120:TRP:NE1	2.31	0.60
1:KV:120:TRP:HB3	1:LB:23:ILE:HD11	1.83	0.60
1:DC:31:GLU:OE1	1:DC:44:LYS:NZ	2.33	0.60
1:EM:63:ASN:OD1	1:EM:64:VAL:N	2.34	0.60
1:FO:55:ASN:OD1	1:FO:55:ASN:O	2.19	0.60
1:GC:19:VAL:HG23	1:GC:19:VAL:O	2.01	0.60
1:IC:20:LEU:HB3	1:IC:32:TYR:HB3	1.83	0.60
2:M:368:ARG:O	2:M:372:ARG:N	2.30	0.60
1:BK:21:ARG:NH1	1:MS:121:GLU:OE2	2.34	0.60
1:FE:19:VAL:HG23	1:FE:19:VAL:O	2.00	0.60
1:FP:109:LEU:HD11	1:FU:85:VAL:HG11	1.84	0.60
1:HQ:62:HIS:CB	1:KW:117:LEU:HD21	2.31	0.60
1:NM:24:ASN:OD1	1:NM:25:GLN:N	2.33	0.60
1:EK:69:THR:OG1	1:EK:78:GLU:OE2	2.20	0.60
1:ER:62:HIS:CB	1:EW:117:LEU:HD21	2.32	0.60
1:FE:20:LEU:HB3	1:FE:32:TYR:HB3	1.83	0.60
1:GO:117:LEU:HD21	1:JS:62:HIS:CB	2.31	0.60
1:HE:99:SER:O	1:HE:103:GLU:OE1	2.19	0.60
1:IY:113:LEU:O	1:IY:117:LEU:HD23	2.01	0.60
1:AH:62:HIS:CB	1:AM:117:LEU:HD21	2.31	0.60
1:HJ:110:ASN:OD1	1:HJ:111:GLU:N	2.34	0.60
1:JF:117:LEU:HD21	1:JK:62:HIS:CB	2.31	0.60
1:BG:87:ILE:HD11	1:HE:114:TYR:HE1	1.66	0.60
1:DU:122:SER:O	1:LO:30:SER:OG	2.15	0.60
1:LM:16:THR:OG1	1:LM:18:LYS:NZ	2.34	0.60
1:AZ:30:SER:OG	1:BE:122:SER:O	2.17	0.60
1:BQ:24:ASN:OD1	1:BQ:25:GLN:N	2.35	0.60
1:CD:101:LEU:HD12	1:CD:102:GLY:H	1.65	0.60
1:FP:116:LYS:HE3	1:FU:2:LEU:HD23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JR:51:SER:OG	1:JR:53:LYS:NZ	2.32	0.60
1:JR:93:ASP:OD1	1:JR:94:VAL:N	2.34	0.60
1:CE:109:LEU:HA	1:CE:113:LEU:HD23	1.84	0.60
1:HE:36:GLU:OE1	1:HE:37:THR:N	2.35	0.60
1:BS:47:HIS:NE2	1:MG:121:GLU:O	2.33	0.60
1:EA:24:ASN:OD1	1:EA:25:GLN:N	2.35	0.60
1:EX:51:SER:OG	1:EX:53:LYS:NZ	2.28	0.60
1:FW:113:LEU:O	1:FW:117:LEU:HD13	2.02	0.60
1:HD:48:THR:HG22	1:HD:49:LYS:O	2.02	0.60
1:CC:122:SER:O	1:DB:30:SER:OG	2.16	0.59
1:FJ:24:ASN:OD1	1:FJ:25:GLN:N	2.35	0.59
1:FP:26:ASP:O	1:FP:29:THR:OG1	2.14	0.59
1:IH:19:VAL:O	1:IH:19:VAL:HG23	2.02	0.59
1:IN:117:LEU:HD21	1:IS:62:HIS:CB	2.32	0.59
1:JS:56:GLN:O	1:JS:58:GLN:NE2	2.35	0.59
1:BG:24:ASN:OD1	1:BG:25:GLN:N	2.35	0.59
1:CI:113:LEU:O	1:CI:117:LEU:HD23	2.01	0.59
1:GI:19:VAL:HG23	1:GI:19:VAL:O	2.02	0.59
1:AY:67:THR:HG22	1:AY:82:GLN:HG3	1.84	0.59
1:CQ:99:SER:OG	1:KK:111:GLU:OE1	2.19	0.59
1:FO:117:LEU:HD21	1:GN:62:HIS:HB3	1.82	0.59
1:GH:69:THR:OG1	1:GH:78:GLU:OE2	2.21	0.59
1:KJ:89:HIS:NE2	1:KO:118:ILE:HD11	2.18	0.59
1:LB:2:LEU:HD23	1:LB:2:LEU:H	1.68	0.59
1:LC:113:LEU:O	1:LC:117:LEU:HD23	2.03	0.59
1:LG:7:THR:HG22	1:LG:19:VAL:HG12	1.84	0.59
1:AS:8:ILE:HD13	1:AS:66:PHE:CE2	2.37	0.59
1:GZ:93:ASP:OD1	1:GZ:94:VAL:N	2.34	0.59
1:JS:65:GLU:OE2	1:JS:67:THR:OG1	2.20	0.59
1:CQ:23:ILE:HG23	1:CU:120:TRP:O	2.02	0.59
1:DA:4:ASP:OD1	1:DA:5:THR:HG23	2.03	0.59
1:FV:1:ALA:N	1:GA:121:GLU:OE1	2.35	0.59
1:GB:58:GLN:NE2	1:GB:59:TYR:O	2.36	0.59
1:LG:122:SER:OXT	1:MF:1:ALA:N	2.35	0.59
1:ML:24:ASN:OD1	1:ML:25:GLN:N	2.36	0.59
1:FK:89:HIS:CD2	1:MA:118:ILE:HD11	2.37	0.59
1:AI:113:LEU:O	1:AI:117:LEU:HD23	2.01	0.59
1:BS:69:THR:HG22	1:BS:80:VAL:HG12	1.84	0.59
1:CK:109:LEU:HD11	1:II:85:VAL:HG11	1.84	0.59
1:EG:117:LEU:HD21	1:IO:62:HIS:HB3	1.83	0.59
1:JR:65:GLU:OE2	1:JR:82:GLN:NE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JX:113:LEU:O	1:JX:117:LEU:HD23	2.02	0.59
1:JY:63:ASN:OD1	1:JY:64:VAL:N	2.35	0.59
1:AN:82:GLN:OE1	1:AS:88:ARG:NH2	2.31	0.59
1:CE:108:TYR:OH	1:DI:6:LEU:HD11	2.03	0.59
1:CQ:50:GLU:N	1:CQ:50:GLU:OE2	2.35	0.59
1:JY:68:GLU:O	1:JY:80:VAL:HA	2.01	0.59
1:CW:69:THR:OG1	1:CW:78:GLU:OE2	2.21	0.59
1:GU:109:LEU:HD13	1:GU:113:LEU:HD22	1.83	0.59
1:NG:19:VAL:O	1:NG:34:LEU:HD12	2.03	0.59
1:AY:122:SER:OXT	1:BX:1:ALA:N	2.35	0.59
1:MS:19:VAL:HG23	1:MS:19:VAL:O	2.03	0.59
1:FD:1:ALA:N	1:FI:122:SER:OXT	2.35	0.58
1:GO:62:HIS:NE2	1:JS:118:ILE:HD12	2.17	0.58
1:LZ:1:ALA:N	1:ME:122:SER:OXT	2.36	0.58
1:NC:20:LEU:HB3	1:NC:32:TYR:HB3	1.83	0.58
1:CV:2:LEU:HD23	1:DA:122:SER:C	2.23	0.58
1:HE:23:ILE:HB	1:HE:31:GLU:OE1	2.03	0.58
1:MA:23:ILE:HG22	1:MA:31:GLU:HB2	1.84	0.58
2:M:99:LEU:HD22	2:M:191:LEU:HD22	1.85	0.58
1:AT:1:ALA:N	1:NM:122:SER:OXT	2.36	0.58
1:CE:19:VAL:HG13	1:CE:19:VAL:O	2.03	0.58
1:IS:52:VAL:HG22	1:IS:58:GLN:HE22	1.67	0.58
1:MX:19:VAL:HG23	1:MX:19:VAL:O	2.02	0.58
1:LG:6:LEU:HD11	1:MF:108:TYR:CE1	2.38	0.58
1:BA:8:ILE:HD13	1:BA:66:PHE:CE2	2.38	0.58
1:CC:86:VAL:O	1:CC:87:ILE:HD13	2.03	0.58
1:CP:121:GLU:OE2	1:CU:1:ALA:N	2.23	0.58
1:GI:113:LEU:O	1:GI:117:LEU:HD23	2.03	0.58
1:HC:55:ASN:OD1	1:HC:55:ASN:O	2.21	0.58
1:HV:20:LEU:HB3	1:HV:32:TYR:HB3	1.85	0.58
1:IA:113:LEU:O	1:IA:117:LEU:HD23	2.03	0.58
1:MG:24:ASN:OD1	1:MG:25:GLN:N	2.35	0.58
1:ER:93:ASP:OD1	1:ER:94:VAL:N	2.33	0.58
1:EW:20:LEU:HB3	1:EW:32:TYR:HB3	1.85	0.58
1:IH:68:GLU:OE2	1:IH:81:ARG:NH1	2.35	0.58
1:JL:113:LEU:O	1:JL:117:LEU:HD12	2.03	0.58
1:KE:89:HIS:CD2	1:KE:98:VAL:HG11	2.38	0.58
1:MM:114:TYR:O	1:MM:118:ILE:HD12	2.03	0.58
1:BM:1:ALA:N	1:MS:122:SER:OXT	2.37	0.58
1:BR:86:VAL:HG21	1:BW:84:TYR:CZ	2.39	0.58
1:EL:111:GLU:OE1	1:EQ:99:SER:OG	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FD:63:ASN:OD1	1:FD:64:VAL:N	2.36	0.58
1:HQ:62:HIS:HB3	1:KW:117:LEU:HD21	1.85	0.58
1:HQ:114:TYR:CE1	1:KW:87:ILE:HD11	2.39	0.58
1:HU:109:LEU:HD13	1:HU:113:LEU:HD22	1.86	0.58
1:IO:68:GLU:O	1:IO:81:ARG:N	2.32	0.58
1:IU:117:LEU:HD21	1:NC:62:HIS:HB3	1.85	0.58
1:JK:113:LEU:O	1:JK:113:LEU:HD23	2.04	0.58
1:JR:26:ASP:O	1:JR:29:THR:OG1	2.16	0.58
1:KC:113:LEU:O	1:KC:117:LEU:HD23	2.03	0.58
1:LZ:24:ASN:OD1	1:LZ:25:GLN:N	2.36	0.58
1:HQ:63:ASN:OD1	1:HQ:64:VAL:N	2.37	0.58
1:HW:4:ASP:OD1	1:HW:5:THR:N	2.37	0.58
1:IB:109:LEU:HD11	1:IG:85:VAL:HG11	1.85	0.58
1:IG:36:GLU:OE1	1:IG:39:SER:N	2.36	0.58
1:IT:60:GLU:O	1:IT:88:ARG:HG3	2.04	0.58
1:IY:30:SER:OG	1:JX:122:SER:O	2.21	0.58
1:JL:49:LYS:HA	1:JL:49:LYS:HE3	1.86	0.58
1:KV:10:LEU:HA	1:LA:104:ALA:HB2	1.86	0.58
1:NG:20:LEU:HB3	1:NG:32:TYR:HB3	1.85	0.58
1:EE:24:ASN:OD1	1:EE:25:GLN:N	2.37	0.58
1:HQ:114:TYR:HE1	1:KW:87:ILE:HD11	1.68	0.58
1:HV:54:PRO:O	1:HV:56:GLN:NE2	2.37	0.58
1:JK:99:SER:O	1:JK:103:GLU:HG3	2.04	0.58
1:CP:47:HIS:NE2	1:CU:121:GLU:O	2.36	0.57
1:EA:19:VAL:O	1:EA:19:VAL:HG23	2.04	0.57
1:EF:55:ASN:O	1:EF:56:GLN:NE2	2.37	0.57
1:EL:109:LEU:HD11	1:EQ:85:VAL:HG11	1.85	0.57
1:HJ:19:VAL:HG23	1:HJ:19:VAL:O	2.04	0.57
1:II:60:GLU:OE2	1:II:62:HIS:NE2	2.36	0.57
1:KU:60:GLU:OE2	1:KU:62:HIS:NE2	2.37	0.57
1:LU:36:GLU:OE2	1:LU:39:SER:N	2.37	0.57
1:MR:62:HIS:N	1:MR:87:ILE:O	2.35	0.57
1:KD:19:VAL:HG23	1:KD:19:VAL:O	2.02	0.57
1:AY:6:LEU:HD23	1:AY:32:TYR:CE2	2.39	0.57
1:BS:63:ASN:OD1	1:BS:64:VAL:N	2.37	0.57
1:FJ:57:VAL:HG23	1:FJ:59:TYR:CE1	2.40	0.57
1:FV:23:ILE:HG22	1:FV:31:GLU:O	2.05	0.57
1:GZ:109:LEU:HD12	1:GZ:114:TYR:CE1	2.40	0.57
1:JA:117:LEU:HD21	1:KE:62:HIS:HB3	1.85	0.57
1:NC:113:LEU:O	1:NC:117:LEU:HD23	2.04	0.57
2:M:17:THR:OG1	2:M:27:ASN:OD1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CQ:68:GLU:OE2	1:CQ:81:ARG:NE	2.37	0.57
1:FI:65:GLU:OE2	1:FI:67:THR:OG1	2.21	0.57
1:AO:114:TYR:O	1:AO:118:ILE:HD12	2.04	0.57
1:EK:55:ASN:O	1:EK:56:GLN:NE2	2.37	0.57
1:GO:118:ILE:HD11	1:JS:89:HIS:NE2	2.20	0.57
1:KC:24:ASN:OD1	1:KC:25:GLN:N	2.37	0.57
1:KK:20:LEU:CD2	1:KK:32:TYR:HB3	2.34	0.57
1:AB:27:GLY:O	1:AB:29:THR:HG23	2.04	0.57
1:DM:19:VAL:O	1:DM:19:VAL:HG23	2.05	0.57
1:HP:50:GLU:OE2	1:HP:61:ARG:NH2	2.34	0.57
1:NI:113:LEU:O	1:NI:117:LEU:HD23	2.04	0.57
1:JK:93:ASP:OD1	1:JK:94:VAL:N	2.37	0.57
1:KE:19:VAL:HG23	1:KE:19:VAL:O	2.04	0.57
1:AZ:117:LEU:HD21	1:BE:62:HIS:CB	2.34	0.57
1:BW:20:LEU:HB3	1:BW:32:TYR:HB3	1.86	0.57
1:GZ:50:GLU:OE2	1:GZ:59:TYR:N	2.37	0.57
1:KK:27:GLY:O	1:KK:29:THR:HG23	2.04	0.57
1:AN:50:GLU:OE2	1:AN:61:ARG:NH2	2.38	0.57
1:DU:63:ASN:OD1	1:DU:64:VAL:N	2.38	0.57
1:FU:113:LEU:O	1:FU:117:LEU:HD23	2.05	0.57
1:GU:19:VAL:O	1:GU:19:VAL:HG23	2.03	0.57
1:KV:82:GLN:OE1	1:LA:88:ARG:NH1	2.38	0.57
1:KW:23:ILE:HD11	1:LA:120:TRP:C	2.25	0.57
1:LU:69:THR:HG22	1:LU:80:VAL:HG12	1.85	0.57
1:BG:57:VAL:HG23	1:BG:59:TYR:CE2	2.40	0.57
1:CK:108:TYR:CE2	1:CK:113:LEU:HD21	2.39	0.57
1:HU:24:ASN:OD1	1:HU:25:GLN:N	2.37	0.57
1:IT:20:LEU:HB3	1:IT:32:TYR:HB3	1.87	0.57
1:AA:120:TRP:HB3	1:NO:23:ILE:HD11	1.86	0.56
1:BQ:54:PRO:O	1:BQ:56:GLN:OE1	2.23	0.56
1:NA:55:ASN:O	1:NA:56:GLN:OE1	2.22	0.56
1:NB:113:LEU:O	1:NB:117:LEU:HD23	2.05	0.56
1:NM:20:LEU:HB3	1:NM:32:TYR:HB3	1.86	0.56
1:BE:93:ASP:OD1	1:BE:94:VAL:N	2.34	0.56
1:BX:69:THR:HG22	1:BX:80:VAL:HG12	1.86	0.56
1:DH:24:ASN:OD1	1:DH:25:GLN:N	2.37	0.56
1:DH:122:SER:C	1:DM:2:LEU:HD13	2.24	0.56
1:EM:122:SER:O	1:FQ:30:SER:OG	2.10	0.56
1:EX:19:VAL:HG23	1:EX:19:VAL:O	2.03	0.56
1:FP:20:LEU:HB3	1:FP:32:TYR:HB3	1.87	0.56
1:IZ:63:ASN:OD1	1:IZ:64:VAL:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KW:23:ILE:HD11	1:LA:120:TRP:O	2.05	0.56
1:LB:117:LEU:O	1:LB:117:LEU:HD23	2.06	0.56
1:MX:40:SER:HG	1:MX:71:TYR:HH	1.32	0.56
1:AA:10:LEU:HA	1:NN:104:ALA:HB2	1.86	0.56
1:AN:93:ASP:OD2	1:AS:81:ARG:NH1	2.39	0.56
1:AS:20:LEU:HB3	1:AS:32:TYR:HB3	1.88	0.56
1:AT:112:ALA:O	1:AT:116:LYS:HG2	2.05	0.56
1:BL:63:ASN:HB3	1:BL:86:VAL:HG12	1.86	0.56
1:BM:122:SER:OG	1:MS:47:HIS:NE2	2.33	0.56
1:BS:108:TYR:CZ	1:BS:113:LEU:HD11	2.39	0.56
1:HJ:87:ILE:HD11	1:HO:114:TYR:CE2	2.41	0.56
1:IO:69:THR:OG1	1:IO:80:VAL:HG12	2.05	0.56
1:KD:120:TRP:HB3	1:KJ:23:ILE:HD11	1.87	0.56
1:LZ:93:ASP:OD1	1:LZ:94:VAL:N	2.36	0.56
1:MW:109:LEU:HA	1:MW:113:LEU:HD23	1.86	0.56
1:NM:69:THR:OG1	1:NM:78:GLU:OE2	2.22	0.56
1:BK:55:ASN:OD1	1:BK:56:GLN:NE2	2.39	0.56
1:BR:34:LEU:HD12	1:BR:35:PRO:HD2	1.88	0.56
1:EE:20:LEU:HB3	1:EE:32:TYR:HB3	1.88	0.56
1:FW:108:TYR:CE2	1:FW:113:LEU:HD21	2.40	0.56
1:IO:36:GLU:OE2	1:IO:39:SER:OG	2.22	0.56
1:IT:40:SER:OG	1:IT:69:THR:OG1	2.17	0.56
1:ME:93:ASP:OD1	1:ME:94:VAL:N	2.38	0.56
1:MS:113:LEU:O	1:MS:117:LEU:HD23	2.06	0.56
1:EK:111:GLU:OE2	1:FJ:99:SER:OG	2.21	0.56
1:FD:20:LEU:HB3	1:FD:32:TYR:HB3	1.88	0.56
1:IH:26:ASP:O	1:IH:29:THR:OG1	2.17	0.56
1:JL:88:ARG:NH2	1:JQ:82:GLN:OE1	2.34	0.56
1:KV:88:ARG:NH2	1:LA:82:GLN:OE1	2.37	0.56
1:LI:120:TRP:CE3	1:MK:23:ILE:HD11	2.41	0.56
1:LZ:82:GLN:OE1	1:ME:88:ARG:NH2	2.27	0.56
1:MX:25:GLN:NE2	1:NA:122:SER:OXT	2.38	0.56
1:NA:93:ASP:OD1	1:NA:94:VAL:N	2.39	0.56
1:EE:63:ASN:OD1	1:EE:64:VAL:N	2.38	0.56
1:FJ:20:LEU:HB3	1:FJ:32:TYR:HB3	1.86	0.56
1:HQ:99:SER:O	1:HQ:103:GLU:OE1	2.22	0.56
1:LY:5:THR:HG22	1:LY:21:ARG:HE	1.71	0.56
1:AY:109:LEU:HD21	1:BX:85:VAL:HG11	1.86	0.56
1:BG:121:GLU:OE2	1:HC:21:ARG:NH2	2.34	0.56
1:DT:62:HIS:CB	1:DY:117:LEU:HD21	2.34	0.56
1:GS:32:TYR:HB2	1:GS:43:ALA:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GU:1:ALA:HB3	1:HW:121:GLU:HG3	1.86	0.56
1:HU:54:PRO:HD2	1:HU:55:ASN:H	1.71	0.56
1:IT:54:PRO:O	1:IT:55:ASN:OD1	2.24	0.56
1:KW:63:ASN:OD1	1:KW:64:VAL:N	2.39	0.56
1:BA:108:TYR:OH	1:BA:113:LEU:HD11	2.05	0.56
1:CQ:27:GLY:O	1:CQ:29:THR:HG23	2.05	0.56
1:JA:4:ASP:OD1	1:JA:5:THR:N	2.39	0.56
1:KW:54:PRO:O	1:KW:55:ASN:OD1	2.24	0.56
1:LY:109:LEU:HD23	1:LY:113:LEU:HD23	1.87	0.56
1:NB:62:HIS:HB3	1:NG:117:LEU:HD21	1.86	0.56
1:NB:68:GLU:N	1:NB:81:ARG:O	2.38	0.56
1:AA:20:LEU:HB3	1:AA:32:TYR:HB3	1.86	0.56
1:AU:20:LEU:HB3	1:AU:32:TYR:HB3	1.88	0.56
1:CJ:117:LEU:HD21	1:CO:62:HIS:HB3	1.87	0.56
1:DZ:65:GLU:OE2	1:DZ:67:THR:OG1	2.24	0.56
1:EY:19:VAL:O	1:EY:34:LEU:HD22	2.05	0.56
1:FV:57:VAL:HG23	1:FV:59:TYR:HE1	1.70	0.56
1:HQ:113:LEU:O	1:HQ:117:LEU:HD23	2.04	0.56
1:JK:69:THR:HG22	1:JK:80:VAL:HG12	1.88	0.56
1:JL:54:PRO:O	1:JL:55:ASN:OD1	2.24	0.56
1:LB:20:LEU:HB3	1:LB:32:TYR:HB3	1.88	0.56
1:LT:122:SER:O	1:LY:2:LEU:HD13	2.06	0.56
1:BF:93:ASP:OD2	1:BF:94:VAL:N	2.39	0.56
1:GH:19:VAL:HG23	1:GH:19:VAL:O	2.06	0.56
1:IU:68:GLU:O	1:IU:81:ARG:N	2.36	0.56
1:JA:69:THR:HG22	1:JA:80:VAL:HG12	1.88	0.56
1:AB:89:HIS:NE2	1:AG:118:ILE:HD11	2.21	0.55
1:AN:19:VAL:HG23	1:AN:19:VAL:O	2.05	0.55
1:DA:63:ASN:OD1	1:DA:64:VAL:N	2.40	0.55
1:GC:108:TYR:CE2	1:GC:113:LEU:HD21	2.40	0.55
1:GI:21:ARG:NE	1:GM:121:GLU:OE1	2.39	0.55
1:MA:36:GLU:OE2	1:MA:39:SER:OG	2.16	0.55
1:BF:105:LEU:HD21	1:BK:85:VAL:HG23	1.88	0.55
1:BF:117:LEU:HD21	1:BK:62:HIS:CB	2.36	0.55
1:CE:30:SER:OG	1:DI:122:SER:O	2.25	0.55
1:FI:24:ASN:OD1	1:FI:25:GLN:N	2.39	0.55
1:FK:84:TYR:OH	1:MA:61:ARG:NH2	2.40	0.55
1:LM:99:SER:O	1:LM:103:GLU:HG3	2.06	0.55
1:MR:20:LEU:HD23	1:MR:32:TYR:O	2.05	0.55
1:BM:2:LEU:HD23	1:MS:122:SER:C	2.26	0.55
1:GA:19:VAL:O	1:GA:34:LEU:HD12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:24:ASN:OD1	1:LA:25:GLN:N	2.39	0.55
1:LH:93:ASP:OD1	1:LH:94:VAL:N	2.36	0.55
1:LY:55:ASN:O	1:LY:55:ASN:OD1	2.24	0.55
1:DH:40:SER:HG	1:DH:71:TYR:HH	1.48	0.55
1:EL:24:ASN:OD1	1:EL:25:GLN:N	2.39	0.55
1:FV:57:VAL:HG23	1:FV:59:TYR:CE1	2.42	0.55
1:GC:113:LEU:O	1:GC:117:LEU:HD23	2.06	0.55
1:HJ:63:ASN:OD1	1:HJ:64:VAL:N	2.39	0.55
1:IZ:27:GLY:O	1:IZ:29:THR:HG23	2.05	0.55
1:KJ:109:LEU:HD13	1:KJ:114:TYR:OH	2.07	0.55
1:LI:20:LEU:HB3	1:LI:32:TYR:HB3	1.88	0.55
1:LT:1:ALA:N	1:LY:122:SER:OXT	2.39	0.55
1:BF:20:LEU:HB3	1:BF:32:TYR:HB3	1.88	0.55
1:BR:120:TRP:HB3	1:BX:23:ILE:HD11	1.87	0.55
1:DN:54:PRO:O	1:DN:55:ASN:OD1	2.25	0.55
1:EA:121:GLU:O	1:NI:47:HIS:NE2	2.39	0.55
1:EE:86:VAL:O	1:EE:87:ILE:HD13	2.07	0.55
1:FI:19:VAL:O	1:FI:34:LEU:HD12	2.06	0.55
1:IB:19:VAL:HG23	1:IB:19:VAL:O	2.06	0.55
1:JS:113:LEU:O	1:JS:117:LEU:HD23	2.07	0.55
2:M:177:HIS:CD2	2:M:240:ILE:HD13	2.42	0.55
1:DI:99:SER:O	1:DI:103:GLU:OE1	2.24	0.55
1:DS:57:VAL:HG23	1:DS:59:TYR:CE2	2.41	0.55
2:M:185:LEU:O	2:M:230:TRP:N	2.35	0.55
1:CI:57:VAL:HG23	1:CI:59:TYR:CE1	2.41	0.55
1:CJ:51:SER:OG	1:CJ:53:LYS:NZ	2.35	0.55
1:II:73:SER:O	1:II:76:THR:OG1	2.24	0.55
1:KC:2:LEU:HD12	1:LB:122:SER:OXT	2.07	0.55
1:LI:24:ASN:OD1	1:LI:25:GLN:N	2.39	0.55
1:LY:19:VAL:O	1:LY:34:LEU:HD22	2.07	0.55
1:MR:98:VAL:HG12	1:MW:81:ARG:CD	2.36	0.55
1:BF:111:GLU:OE1	1:BK:99:SER:OG	2.24	0.55
1:BM:63:ASN:OD1	1:BM:64:VAL:N	2.39	0.55
1:CC:86:VAL:HG21	1:DB:84:TYR:CZ	2.42	0.55
1:CV:114:TYR:HE1	1:DA:87:ILE:HD11	1.72	0.55
1:DS:4:ASP:OD1	1:DS:5:THR:HG23	2.07	0.55
1:EF:68:GLU:N	1:EF:81:ARG:O	2.35	0.55
1:IO:63:ASN:OD1	1:IO:64:VAL:N	2.38	0.55
1:KE:31:GLU:HB3	1:KE:44:LYS:HG2	1.88	0.55
1:BG:87:ILE:HD11	1:HE:114:TYR:CE1	2.42	0.55
1:EA:20:LEU:HB3	1:EA:32:TYR:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:53:LYS:HG2	1:EA:54:PRO:HD2	1.89	0.55
1:EX:67:THR:OG1	1:EX:82:GLN:OE1	2.24	0.55
1:GY:108:TYR:CZ	1:GY:113:LEU:HD11	2.42	0.55
1:JQ:93:ASP:OD1	1:JQ:94:VAL:N	2.38	0.55
1:KJ:15:GLY:O	1:KJ:16:THR:OG1	2.24	0.55
1:KQ:57:VAL:HG23	1:KQ:59:TYR:CE2	2.42	0.55
1:CW:53:LYS:HG2	1:CW:54:PRO:HD2	1.88	0.55
1:DG:112:ALA:O	1:DG:116:LYS:HG2	2.06	0.55
1:DM:72:ALA:N	1:DM:78:GLU:OE2	2.40	0.55
1:IO:69:THR:CB	1:IO:80:VAL:HG12	2.37	0.55
1:IY:20:LEU:HB3	1:IY:32:TYR:HB3	1.88	0.55
1:JX:63:ASN:OD1	1:JX:64:VAL:N	2.39	0.55
1:KE:24:ASN:OD1	1:KE:25:GLN:N	2.39	0.55
1:AZ:29:THR:HG22	1:AZ:46:ARG:HG3	1.88	0.54
1:EL:114:TYR:HE1	1:EQ:87:ILE:HD11	1.72	0.54
1:GB:84:TYR:CZ	1:GG:86:VAL:HG11	2.42	0.54
1:GG:32:TYR:HB2	1:GG:43:ALA:HB3	1.88	0.54
1:IZ:121:GLU:OE2	1:JF:21:ARG:NE	2.40	0.54
1:LY:63:ASN:OD1	1:LY:64:VAL:N	2.40	0.54
1:MK:26:ASP:O	1:MK:29:THR:OG1	2.10	0.54
1:ML:62:HIS:CB	1:MQ:117:LEU:HD21	2.37	0.54
1:MQ:63:ASN:OD1	1:MQ:64:VAL:N	2.40	0.54
1:CD:4:ASP:OD1	1:CD:5:THR:N	2.40	0.54
1:ES:54:PRO:O	1:ES:55:ASN:OD1	2.24	0.54
1:GC:65:GLU:OE1	1:GC:84:TYR:HB3	2.07	0.54
1:GS:55:ASN:O	1:GS:55:ASN:OD1	2.24	0.54
1:IG:69:THR:HG22	1:IG:80:VAL:HG12	1.88	0.54
1:IT:40:SER:HG	1:IT:69:THR:HG1	1.43	0.54
1:IZ:89:HIS:CD2	1:IZ:98:VAL:HG11	2.42	0.54
1:LG:113:LEU:O	1:LG:117:LEU:HD23	2.08	0.54
1:CP:20:LEU:HB3	1:CP:32:TYR:HB3	1.88	0.54
1:CQ:57:VAL:HG23	1:CQ:59:TYR:CE2	2.43	0.54
1:DT:113:LEU:O	1:DT:117:LEU:HD23	2.07	0.54
1:FO:121:GLU:OE2	1:GO:21:ARG:NH1	2.41	0.54
1:GH:2:LEU:HD23	1:GH:2:LEU:H	1.73	0.54
1:GT:122:SER:O	1:GY:30:SER:OG	2.17	0.54
1:GZ:81:ARG:NH2	1:HC:97:THR:HG21	2.22	0.54
1:HW:113:LEU:O	1:HW:117:LEU:HD23	2.08	0.54
1:IH:20:LEU:HB3	1:IH:32:TYR:HB3	1.89	0.54
1:JQ:113:LEU:O	1:JQ:117:LEU:HD23	2.06	0.54
1:KD:86:VAL:O	1:KD:87:ILE:HD13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KK:113:LEU:O	1:KK:117:LEU:HD23	2.08	0.54
1:KO:108:TYR:CE2	1:KO:113:LEU:HD21	2.42	0.54
1:MS:52:VAL:HG22	1:MS:58:GLN:OE1	2.06	0.54
1:BY:117:LEU:HD21	1:FE:62:HIS:HB3	1.90	0.54
1:ES:114:TYR:HE1	1:JM:87:ILE:HD11	1.72	0.54
1:KC:20:LEU:HB3	1:KC:32:TYR:HB3	1.89	0.54
1:AA:63:ASN:OD1	1:AA:64:VAL:N	2.41	0.54
1:AI:93:ASP:OD1	1:AI:94:VAL:N	2.39	0.54
1:AT:19:VAL:HG23	1:AT:19:VAL:O	2.07	0.54
1:CD:40:SER:HG	1:CD:71:TYR:HH	1.47	0.54
1:CO:70:VAL:HG11	1:CO:79:PHE:CZ	2.42	0.54
1:DB:19:VAL:O	1:DB:19:VAL:HG23	2.07	0.54
1:EL:27:GLY:O	1:EL:29:THR:HG23	2.08	0.54
1:IS:19:VAL:O	1:IS:19:VAL:HG23	2.08	0.54
2:M:67:ILE:HA	2:M:72:THR:HG22	1.90	0.54
1:CE:1:ALA:N	1:DI:122:SER:OXT	2.41	0.54
1:DO:20:LEU:HB3	1:DO:32:TYR:HB3	1.89	0.54
1:MM:54:PRO:O	1:MM:55:ASN:OD1	2.25	0.54
1:MM:112:ALA:O	1:MM:116:LYS:HG2	2.07	0.54
1:BL:93:ASP:OD1	1:BL:94:VAL:N	2.39	0.54
1:BM:19:VAL:HG23	1:BM:19:VAL:O	2.08	0.54
1:HJ:109:LEU:HD12	1:HJ:114:TYR:CZ	2.42	0.54
1:IN:114:TYR:HE2	1:IS:87:ILE:HD11	1.72	0.54
1:NB:4:ASP:OD1	1:NB:5:THR:HG23	2.07	0.54
1:NM:113:LEU:O	1:NM:117:LEU:HD23	2.07	0.54
1:AU:29:THR:HG22	1:AU:30:SER:N	2.23	0.54
1:BK:63:ASN:OD1	1:BK:64:VAL:N	2.41	0.54
1:HO:108:TYR:CE2	1:HO:113:LEU:HD21	2.43	0.54
1:KW:19:VAL:HG23	1:KW:19:VAL:O	2.07	0.54
1:LG:60:GLU:OE2	1:MF:120:TRP:NE1	2.40	0.54
1:MR:114:TYR:HE1	1:MW:87:ILE:HD11	1.72	0.54
1:MR:116:LYS:NZ	1:MW:2:LEU:HD22	2.23	0.54
1:NM:36:GLU:OE1	1:NM:36:GLU:HA	2.08	0.54
1:AY:62:HIS:O	1:AY:87:ILE:N	2.37	0.54
1:CQ:63:ASN:OD1	1:CQ:64:VAL:N	2.40	0.54
1:DC:40:SER:OG	1:DC:71:TYR:OH	2.12	0.54
1:DU:112:ALA:O	1:DU:116:LYS:HG2	2.08	0.54
1:HO:23:ILE:HD11	1:KW:120:TRP:CE3	2.43	0.54
1:HV:63:ASN:OD1	1:HV:64:VAL:N	2.41	0.54
2:M:358:LEU:HD23	2:M:358:LEU:H	1.72	0.54
1:CC:117:LEU:HD21	1:DB:62:HIS:CG	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CI:29:THR:OG1	1:CI:45:VAL:O	2.16	0.54
1:EG:117:LEU:HD23	1:EG:117:LEU:O	2.08	0.54
1:LY:57:VAL:HG23	1:LY:59:TYR:CE1	2.44	0.54
1:BM:113:LEU:O	1:BM:117:LEU:HD23	2.08	0.53
1:FE:25:GLN:HG3	1:FE:25:GLN:O	2.08	0.53
1:GI:63:ASN:OD1	1:GI:64:VAL:N	2.41	0.53
1:IY:55:ASN:O	1:IY:55:ASN:OD1	2.26	0.53
1:JA:20:LEU:HB3	1:JA:32:TYR:HB3	1.90	0.53
1:MX:68:GLU:N	1:MX:81:ARG:O	2.39	0.53
1:AU:113:LEU:O	1:AU:117:LEU:HD23	2.08	0.53
1:BM:110:ASN:OD1	1:BM:111:GLU:N	2.39	0.53
1:DA:65:GLU:HB2	1:DA:84:TYR:HB3	1.90	0.53
1:ER:20:LEU:HB3	1:ER:32:TYR:HB3	1.91	0.53
1:JX:19:VAL:HG23	1:JX:19:VAL:O	2.07	0.53
1:MG:8:ILE:HD12	1:MG:66:PHE:CE2	2.43	0.53
1:AG:54:PRO:O	1:AG:56:GLN:OE1	2.26	0.53
1:DH:109:LEU:CD2	1:DH:113:LEU:HD23	2.39	0.53
1:DT:108:TYR:CE2	1:DT:113:LEU:HD21	2.44	0.53
1:IU:4:ASP:OD1	1:IU:5:THR:N	2.41	0.53
1:JM:24:ASN:OD1	1:JM:25:GLN:N	2.41	0.53
1:LY:24:ASN:OD1	1:LY:25:GLN:N	2.42	0.53
1:LZ:109:LEU:HD23	1:LZ:113:LEU:HD23	1.89	0.53
1:ME:36:GLU:OE1	1:ME:39:SER:OG	2.15	0.53
1:MG:54:PRO:O	1:MG:55:ASN:OD1	2.27	0.53
2:M:166:SER:OG	2:M:246:GLU:OE1	2.25	0.53
1:AG:54:PRO:O	1:AG:55:ASN:OD1	2.26	0.53
1:BW:109:LEU:HD12	1:BW:114:TYR:CE1	2.44	0.53
1:DC:1:ALA:N	1:GI:122:SER:OXT	2.42	0.53
1:IB:20:LEU:HB3	1:IB:32:TYR:HB3	1.90	0.53
1:IG:29:THR:HG22	1:IG:46:ARG:HG2	1.90	0.53
1:IO:68:GLU:N	1:IO:81:ARG:O	2.37	0.53
2:M:180:TYR:O	2:M:231:ARG:NE	2.36	0.53
1:DZ:85:VAL:HG22	1:EE:85:VAL:HG12	1.89	0.53
1:HI:68:GLU:HB3	1:HI:81:ARG:HB2	1.90	0.53
1:LC:63:ASN:OD1	1:LC:64:VAL:N	2.41	0.53
1:LH:60:GLU:HG3	1:LH:91:VAL:HG22	1.90	0.53
1:LS:20:LEU:HB3	1:LS:32:TYR:HB3	1.91	0.53
1:LT:108:TYR:CZ	1:LT:113:LEU:HD11	2.44	0.53
1:NO:54:PRO:O	1:NO:56:GLN:OE1	2.26	0.53
1:AZ:93:ASP:OD1	1:AZ:94:VAL:N	2.39	0.53
1:CU:4:ASP:OD1	1:CU:5:THR:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DM:36:GLU:OE1	1:DM:39:SER:N	2.42	0.53
1:LH:81:ARG:NH2	1:LM:97:THR:HG21	2.23	0.53
1:LO:109:LEU:HD12	1:LO:114:TYR:CE1	2.42	0.53
1:LS:36:GLU:OE1	1:LS:36:GLU:HA	2.09	0.53
1:NO:54:PRO:O	1:NO:55:ASN:OD1	2.27	0.53
1:BK:23:ILE:HD12	1:MS:120:TRP:HB3	1.90	0.53
1:DH:109:LEU:HD11	1:DM:85:VAL:HG11	1.90	0.53
1:EW:65:GLU:OE2	1:EW:82:GLN:NE2	2.41	0.53
1:GB:121:GLU:O	1:GG:47:HIS:NE2	2.41	0.53
1:GO:20:LEU:HB3	1:GO:32:TYR:HB3	1.90	0.53
1:JA:62:HIS:HB3	1:KE:117:LEU:HD21	1.91	0.53
1:MG:19:VAL:HG23	1:MG:19:VAL:O	2.09	0.53
1:NB:93:ASP:OD1	1:NB:94:VAL:N	2.40	0.53
1:NO:113:LEU:O	1:NO:117:LEU:HD23	2.07	0.53
1:BK:113:LEU:O	1:BK:117:LEU:HD23	2.08	0.53
1:DG:84:TYR:CZ	1:EF:86:VAL:HG21	2.43	0.53
1:DI:24:ASN:OD1	1:DI:25:GLN:N	2.42	0.53
1:EE:60:GLU:OE2	1:EE:89:HIS:NE2	2.41	0.53
1:FE:54:PRO:O	1:FE:55:ASN:OD1	2.27	0.53
1:FU:24:ASN:OD1	1:FU:25:GLN:N	2.39	0.53
1:GC:36:GLU:OE1	1:GC:36:GLU:HA	2.09	0.53
1:GO:63:ASN:OD1	1:GO:64:VAL:N	2.42	0.53
1:HE:19:VAL:HG23	1:HE:19:VAL:O	2.07	0.53
1:HW:22:LYS:O	1:HW:23:ILE:HD13	2.08	0.53
1:JW:99:SER:OG	1:JW:103:GLU:OE2	2.21	0.53
1:KD:93:ASP:OD1	1:KD:94:VAL:N	2.40	0.53
1:LN:68:GLU:N	1:LN:81:ARG:O	2.42	0.53
1:MG:36:GLU:OE1	1:MG:36:GLU:HA	2.09	0.53
1:EA:54:PRO:O	1:EA:55:ASN:OD1	2.26	0.53
1:FK:19:VAL:O	1:FK:19:VAL:HG23	2.07	0.53
1:GB:81:ARG:NH2	1:GG:97:THR:HG21	2.23	0.53
1:HK:93:ASP:OD1	1:HK:94:VAL:N	2.42	0.53
1:LO:54:PRO:C	1:LO:55:ASN:OD1	2.47	0.53
1:MW:93:ASP:OD1	1:MW:94:VAL:N	2.42	0.53
1:NI:19:VAL:O	1:NI:34:LEU:HD22	2.09	0.53
1:AO:68:GLU:O	1:AO:81:ARG:N	2.40	0.53
1:BA:122:SER:O	1:NO:30:SER:OG	2.15	0.53
1:CK:19:VAL:HG23	1:CK:19:VAL:O	2.08	0.53
1:CK:109:LEU:HD13	1:CK:114:TYR:OH	2.08	0.53
1:CW:20:LEU:HB3	1:CW:32:TYR:HB3	1.91	0.53
1:DI:65:GLU:OE1	1:DI:66:PHE:N	2.42	0.53

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:GN:20:LEU:HB3	1:GN:32:TYR:HB3	1.91	0.53
1:HK:54:PRO:O	1:HK:55:ASN:OD1	2.27	0.53
1:LC:20:LEU:HB3	1:LC:32:TYR:HB3	1.91	0.53
1:NH:93:ASP:OD1	1:NH:94:VAL:N	2.40	0.53
1:AO:58:GLN:NE2	1:AO:59:TYR:O	2.39	0.52
1:BK:31:GLU:OE2	1:BK:32:TYR:N	2.42	0.52
1:BY:54:PRO:O	1:BY:55:ASN:OD1	2.27	0.52
1:CV:19:VAL:O	1:CV:34:LEU:HD22	2.09	0.52
1:DZ:81:ARG:HB3	1:EE:101:LEU:CD1	2.39	0.52
1:EF:53:LYS:HB2	1:EF:54:PRO:HD2	1.92	0.52
1:FC:5:THR:HG22	1:FC:21:ARG:HE	1.73	0.52
1:GB:24:ASN:OD1	1:GB:25:GLN:N	2.41	0.52
1:LT:63:ASN:OD1	1:LT:64:VAL:N	2.42	0.52
1:MM:4:ASP:OD1	1:MM:5:THR:N	2.41	0.52
1:NB:20:LEU:HD21	1:NB:41:PHE:CB	2.38	0.52
1:CE:97:THR:HG21	1:DI:81:ARG:NH1	2.25	0.52
1:DB:93:ASP:OD1	1:DB:94:VAL:N	2.38	0.52
1:ES:47:HIS:O	1:ES:48:THR:HG23	2.09	0.52
1:GB:121:GLU:OE2	1:GH:21:ARG:NH2	2.37	0.52
1:KD:20:LEU:HB3	1:KD:32:TYR:HB3	1.90	0.52
1:LI:23:ILE:HD11	1:LM:120:TRP:O	2.08	0.52
1:LY:93:ASP:OD1	1:LY:94:VAL:N	2.43	0.52
2:M:350:LEU:HB2	2:M:355:LEU:HD11	1.90	0.52
1:CD:84:TYR:O	1:CI:85:VAL:HG23	2.09	0.52
1:CJ:20:LEU:HB3	1:CJ:32:TYR:HB3	1.90	0.52
1:GZ:53:LYS:O	1:GZ:55:ASN:N	2.42	0.52
1:HE:93:ASP:OD1	1:HE:94:VAL:N	2.42	0.52
1:II:93:ASP:OD2	1:II:94:VAL:N	2.43	0.52
1:JE:108:TYR:CE2	1:JE:113:LEU:HD11	2.45	0.52
1:JR:4:ASP:OD1	1:JR:5:THR:N	2.42	0.52
1:KD:68:GLU:N	1:KD:81:ARG:O	2.41	0.52
2:M:13:SER:OG	2:M:29:GLU:OE2	2.25	0.52
1:AA:121:GLU:O	1:NN:47:HIS:NE2	2.38	0.52
1:BA:69:THR:HG22	1:BA:80:VAL:HG12	1.91	0.52
1:DO:84:TYR:O	1:GC:85:VAL:HG23	2.10	0.52
1:FK:63:ASN:OD1	1:FK:64:VAL:N	2.42	0.52
1:LB:113:LEU:O	1:LB:117:LEU:N	2.29	0.52
1:MK:84:TYR:CZ	1:NH:86:VAL:HG21	2.43	0.52
1:MR:118:ILE:HD11	1:MW:89:HIS:NE2	2.24	0.52
1:AG:63:ASN:OD1	1:AG:64:VAL:N	2.43	0.52
1:AH:20:LEU:HB3	1:AH:32:TYR:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AT:63:ASN:OD1	1:AT:64:VAL:N	2.43	0.52
1:CC:122:SER:OXT	1:DB:1:ALA:N	2.39	0.52
1:DU:23:ILE:HD11	1:DY:120:TRP:O	2.09	0.52
1:DY:109:LEU:HD23	1:DY:113:LEU:HD23	1.90	0.52
1:FU:69:THR:HG22	1:FU:80:VAL:HG12	1.92	0.52
1:IS:53:LYS:HD2	1:IS:54:PRO:HD2	1.92	0.52
1:JA:46:ARG:O	1:JA:47:HIS:ND1	2.43	0.52
1:DS:36:GLU:OE1	1:DS:39:SER:N	2.43	0.52
1:GG:44:LYS:HA	1:GG:44:LYS:HE3	1.90	0.52
1:GT:18:LYS:HZ2	1:GT:41:PHE:HE2	1.57	0.52
1:HQ:36:GLU:OE1	1:HQ:36:GLU:HA	2.10	0.52
1:HV:121:GLU:OE2	1:IB:21:ARG:NE	2.43	0.52
1:IA:55:ASN:OD1	1:IA:55:ASN:O	2.28	0.52
1:IS:20:LEU:HB3	1:IS:32:TYR:HB3	1.89	0.52
1:MW:42:ARG:HH11	1:MW:67:THR:HG21	1.75	0.52
1:CK:57:VAL:HG23	1:CK:59:TYR:CE2	2.44	0.52
1:DC:54:PRO:O	1:DC:55:ASN:OD1	2.28	0.52
1:DH:117:LEU:HD21	1:DM:62:HIS:HB3	1.92	0.52
1:DI:109:LEU:HD23	1:DI:113:LEU:HD23	1.92	0.52
1:DZ:19:VAL:O	1:DZ:34:LEU:HD22	2.09	0.52
1:EA:65:GLU:HB3	1:EA:84:TYR:HB3	1.90	0.52
1:EK:62:HIS:CB	1:FJ:117:LEU:HD21	2.40	0.52
1:EL:93:ASP:OD1	1:EL:94:VAL:N	2.41	0.52
1:FP:54:PRO:O	1:FP:55:ASN:OD1	2.27	0.52
1:GU:87:ILE:HD11	1:HW:114:TYR:HE1	1.74	0.52
1:JX:19:VAL:O	1:JX:34:LEU:HD12	2.09	0.52
1:DB:110:ASN:OD1	1:DB:113:LEU:HD23	2.10	0.52
1:EQ:63:ASN:OD1	1:EQ:64:VAL:N	2.43	0.52
1:EX:31:GLU:OE2	1:EX:44:LYS:NZ	2.33	0.52
1:HQ:122:SER:OXT	1:KW:1:ALA:N	2.42	0.52
1:JM:113:LEU:O	1:JM:117:LEU:HD23	2.09	0.52
1:BK:24:ASN:ND2	1:BM:27:GLY:O	2.41	0.52
1:BL:109:LEU:HD23	1:BL:113:LEU:HD23	1.91	0.52
1:CD:60:GLU:CD	1:CD:91:VAL:HG22	2.30	0.52
1:CI:112:ALA:O	1:CI:116:LYS:HG2	2.10	0.52
1:DN:108:TYR:CZ	1:DN:113:LEU:HD21	2.45	0.52
1:EG:89:HIS:NE2	1:IO:118:ILE:HD11	2.24	0.52
1:EW:4:ASP:OD1	1:EW:5:THR:HG23	2.10	0.52
1:FJ:45:VAL:HG22	1:FJ:64:VAL:HG22	1.91	0.52
1:GZ:122:SER:C	1:HC:2:LEU:HD12	2.30	0.52
1:JR:62:HIS:HB3	1:JW:117:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KK:20:LEU:HD23	1:KK:32:TYR:HB3	1.92	0.52
1:AT:114:TYR:O	1:AT:118:ILE:HD12	2.10	0.52
1:BS:122:SER:O	1:MG:30:SER:OG	2.23	0.52
1:DM:109:LEU:HD23	1:DM:113:LEU:HD23	1.92	0.52
1:EG:30:SER:OG	1:IO:122:SER:O	2.28	0.52
1:ES:109:LEU:HA	1:ES:113:LEU:HD23	1.91	0.52
1:IT:8:ILE:HD11	1:IT:66:PHE:CE1	2.45	0.52
1:LC:86:VAL:O	1:LC:87:ILE:HD13	2.10	0.52
1:AB:2:LEU:HD23	1:AG:122:SER:C	2.31	0.51
1:BQ:72:ALA:N	1:BQ:78:GLU:OE1	2.43	0.51
1:CD:19:VAL:HG23	1:CD:19:VAL:O	2.10	0.51
1:FJ:57:VAL:HG23	1:FJ:59:TYR:HE1	1.74	0.51
1:IS:44:LYS:HB2	1:IS:65:GLU:HB3	1.91	0.51
1:JK:52:VAL:HG22	1:JK:58:GLN:OE1	2.10	0.51
1:CW:93:ASP:OD1	1:CW:94:VAL:N	2.41	0.51
1:DC:85:VAL:HG22	1:GI:85:VAL:HG12	1.92	0.51
1:EL:53:LYS:HG2	1:EL:54:PRO:HD2	1.92	0.51
1:FJ:19:VAL:O	1:FJ:34:LEU:HD22	2.09	0.51
1:HD:93:ASP:OD1	1:HD:94:VAL:N	2.44	0.51
1:IA:112:ALA:O	1:IA:116:LYS:HG2	2.10	0.51
1:IC:54:PRO:O	1:IC:55:ASN:OD1	2.29	0.51
1:IG:113:LEU:HD23	1:IG:117:LEU:HD23	1.91	0.51
1:IN:30:SER:OG	1:IS:122:SER:O	2.27	0.51
1:IT:31:GLU:OE2	1:IT:42:ARG:NH1	2.44	0.51
1:IU:54:PRO:O	1:IU:55:ASN:OD1	2.28	0.51
1:IC:112:ALA:O	1:IC:116:LYS:HG2	2.10	0.51
1:IN:70:VAL:HG21	1:IN:79:PHE:CZ	2.45	0.51
1:KI:68:GLU:HB3	1:KI:81:ARG:HB2	1.91	0.51
1:MW:39:SER:HB3	1:MW:70:VAL:HG12	1.92	0.51
1:NI:63:ASN:OD1	1:NI:64:VAL:N	2.43	0.51
1:NM:19:VAL:HG23	1:NM:19:VAL:O	2.09	0.51
2:M:11:ALA:HB2	2:M:34:ASN:OD1	2.11	0.51
1:DB:63:ASN:OD1	1:DB:64:VAL:N	2.42	0.51
1:EG:60:GLU:OE1	1:EG:60:GLU:N	2.43	0.51
1:EK:89:HIS:ND1	1:EK:90:LYS:O	2.43	0.51
1:IN:109:LEU:HD11	1:IS:85:VAL:HG11	1.92	0.51
1:IT:63:ASN:OD1	1:IT:64:VAL:N	2.44	0.51
1:LZ:53:LYS:HE2	1:LZ:53:LYS:HA	1.92	0.51
1:MM:36:GLU:HA	1:MM:36:GLU:OE1	2.10	0.51
1:MW:42:ARG:HB3	1:MW:67:THR:HB	1.92	0.51
1:AI:63:ASN:OD1	1:AI:64:VAL:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AM:20:LEU:HB3	1:AM:32:TYR:HB3	1.93	0.51
1:AM:50:GLU:OE1	1:AM:50:GLU:N	2.43	0.51
1:AN:2:LEU:HD23	1:AS:122:SER:HA	1.93	0.51
1:BR:20:LEU:HB3	1:BR:32:TYR:HB3	1.93	0.51
1:BR:68:GLU:N	1:BR:81:ARG:O	2.39	0.51
1:DM:63:ASN:OD1	1:DM:64:VAL:N	2.44	0.51
1:EX:10:LEU:O	1:EX:16:THR:OG1	2.29	0.51
1:FV:34:LEU:HD21	1:FV:36:GLU:OE2	2.11	0.51
1:IC:2:LEU:HD23	1:KQ:122:SER:O	2.10	0.51
1:LT:80:VAL:HG12	1:LY:59:TYR:OH	2.10	0.51
1:AG:36:GLU:OE1	1:AG:36:GLU:N	2.43	0.51
1:BE:36:GLU:HA	1:BE:36:GLU:OE1	2.10	0.51
1:EA:65:GLU:CB	1:EA:84:TYR:HB3	2.40	0.51
1:EG:63:ASN:OD1	1:EG:64:VAL:N	2.44	0.51
1:FI:40:SER:HG	1:FI:69:THR:HG1	1.58	0.51
1:GZ:49:LYS:HZ1	1:HC:120:TRP:HH2	1.58	0.51
1:HU:59:TYR:HH	1:IT:80:VAL:HG22	1.74	0.51
1:II:63:ASN:OD1	1:II:64:VAL:N	2.43	0.51
1:IO:27:GLY:O	1:IO:29:THR:HG23	2.10	0.51
1:IU:36:GLU:OE1	1:IU:36:GLU:HA	2.10	0.51
1:JS:109:LEU:HA	1:JS:113:LEU:HD23	1.92	0.51
1:KD:6:LEU:HD11	1:KI:108:TYR:OH	2.09	0.51
1:LC:51:SER:OG	1:LC:53:LYS:NZ	2.39	0.51
1:LZ:97:THR:HG22	1:ME:81:ARG:NH1	2.26	0.51
1:MG:113:LEU:O	1:MG:117:LEU:HD23	2.10	0.51
1:NA:20:LEU:HB3	1:NA:32:TYR:HB3	1.93	0.51
1:NI:109:LEU:HD13	1:NI:113:LEU:CD1	2.40	0.51
1:AS:68:GLU:N	1:AS:81:ARG:O	2.43	0.51
1:CV:69:THR:HG22	1:CV:80:VAL:HG12	1.93	0.51
1:HJ:20:LEU:HB3	1:HJ:32:TYR:HB3	1.93	0.51
1:HK:4:ASP:OD1	1:HK:5:THR:N	2.44	0.51
1:JF:54:PRO:O	1:JF:55:ASN:OD1	2.28	0.51
1:LC:36:GLU:HA	1:LC:36:GLU:OE1	2.10	0.51
1:AG:109:LEU:HD13	1:AG:113:LEU:HD23	1.92	0.51
1:BR:109:LEU:HD23	1:BR:113:LEU:HD23	1.93	0.51
1:CI:20:LEU:HB3	1:CI:32:TYR:HB3	1.93	0.51
1:DS:63:ASN:OD1	1:DS:64:VAL:N	2.44	0.51
1:FC:69:THR:HG22	1:FC:80:VAL:HG12	1.91	0.51
1:GM:2:LEU:O	1:GM:2:LEU:HD23	2.11	0.51
1:GZ:62:HIS:O	1:GZ:86:VAL:HA	2.11	0.51
1:KU:63:ASN:OD1	1:KU:64:VAL:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MS:116:LYS:O	1:MS:121:GLU:OE1	2.29	0.51
1:CD:69:THR:HG22	1:CD:80:VAL:HG12	1.93	0.51
1:CP:118:ILE:HD11	1:CU:89:HIS:NE2	2.26	0.51
1:DH:109:LEU:HD23	1:DH:113:LEU:HD23	1.91	0.51
1:GY:113:LEU:HD23	1:GY:117:LEU:HD13	1.92	0.51
1:JK:20:LEU:HB3	1:JK:32:TYR:HB3	1.91	0.51
1:KJ:119:GLY:O	1:KJ:120:TRP:HB2	2.11	0.51
1:KP:54:PRO:O	1:KP:56:GLN:OE1	2.28	0.51
1:BQ:20:LEU:CB	1:BQ:32:TYR:HB3	2.41	0.51
1:DM:20:LEU:HB3	1:DM:32:TYR:HB3	1.93	0.51
1:FP:21:ARG:NH1	1:GN:121:GLU:OE2	2.44	0.51
1:FP:120:TRP:HB3	1:FV:23:ILE:HD11	1.93	0.51
1:GG:63:ASN:OD1	1:GG:64:VAL:N	2.44	0.51
1:GU:108:TYR:CZ	1:HW:6:LEU:HD11	2.46	0.51
1:JY:20:LEU:HB3	1:JY:32:TYR:HB3	1.93	0.51
1:KP:114:TYR:HE1	1:KU:87:ILE:HD11	1.76	0.51
1:LI:63:ASN:OD1	1:LI:64:VAL:N	2.43	0.51
1:NB:116:LYS:O	1:NB:119:GLY:N	2.44	0.51
1:NC:54:PRO:O	1:NC:56:GLN:NE2	2.44	0.51
1:BS:54:PRO:O	1:BS:55:ASN:OD1	2.30	0.50
1:BY:54:PRO:O	1:BY:56:GLN:OE1	2.28	0.50
1:CC:53:LYS:HE2	1:CC:53:LYS:HA	1.93	0.50
1:EA:65:GLU:OE1	1:EA:67:THR:OG1	2.21	0.50
1:EX:20:LEU:HB3	1:EX:32:TYR:HB3	1.92	0.50
1:HI:20:LEU:HB3	1:HI:32:TYR:HB3	1.93	0.50
1:HP:20:LEU:HB3	1:HP:32:TYR:HB3	1.93	0.50
1:IG:63:ASN:OD1	1:IG:64:VAL:N	2.43	0.50
1:IM:20:LEU:HB3	1:IM:32:TYR:HB3	1.92	0.50
1:JG:55:ASN:OD1	1:JG:56:GLN:NE2	2.44	0.50
1:KJ:118:ILE:HD12	1:KO:62:HIS:NE2	2.26	0.50
1:LG:4:ASP:OD1	1:LG:5:THR:N	2.44	0.50
1:AH:85:VAL:HG22	1:AM:85:VAL:HG12	1.93	0.50
1:DB:4:ASP:OD1	1:DB:5:THR:HG23	2.11	0.50
1:FU:20:LEU:HB3	1:FU:32:TYR:HB3	1.93	0.50
1:GB:94:VAL:O	1:GB:98:VAL:HG23	2.12	0.50
1:GM:27:GLY:O	1:GM:29:THR:HG23	2.11	0.50
1:HK:51:SER:OG	1:HK:53:LYS:NZ	2.44	0.50
1:KW:23:ILE:HG22	1:KW:31:GLU:CG	2.41	0.50
1:MX:118:ILE:HD11	1:NA:89:HIS:NE2	2.26	0.50
1:AI:32:TYR:N	1:AI:43:ALA:O	2.38	0.50
1:AY:109:LEU:HD23	1:AY:114:TYR:OH	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:117:LEU:O	1:EA:117:LEU:HD23	2.11	0.50
1:FQ:19:VAL:O	1:FQ:34:LEU:HD12	2.11	0.50
1:HI:68:GLU:N	1:HI:81:ARG:O	2.43	0.50
1:IA:55:ASN:O	1:IA:56:GLN:OE1	2.29	0.50
1:IN:88:ARG:HH22	1:IS:80:VAL:HG21	1.77	0.50
1:IS:23:ILE:HD11	1:NC:120:TRP:O	2.11	0.50
1:JY:68:GLU:N	1:JY:81:ARG:O	2.44	0.50
1:KJ:121:GLU:OE1	1:KO:1:ALA:N	2.42	0.50
1:MK:114:TYR:OH	1:NH:106:SER:OG	2.28	0.50
1:AI:122:SER:OXT	1:JG:1:ALA:N	2.34	0.50
1:AO:1:ALA:N	1:LC:122:SER:OXT	2.44	0.50
1:CW:84:TYR:OH	1:JY:86:VAL:HG21	2.11	0.50
1:DZ:63:ASN:OD1	1:DZ:64:VAL:N	2.44	0.50
1:FD:70:VAL:HG11	1:FD:79:PHE:CZ	2.47	0.50
1:FD:122:SER:OXT	1:FI:1:ALA:N	2.42	0.50
1:FI:36:GLU:HA	1:FI:36:GLU:OE1	2.12	0.50
1:FJ:26:ASP:O	1:FJ:29:THR:OG1	2.19	0.50
1:GB:20:LEU:HB3	1:GB:32:TYR:HB3	1.92	0.50
1:GO:48:THR:HG22	1:GO:49:LYS:O	2.12	0.50
1:GT:103:GLU:OE2	1:GY:12:GLY:N	2.44	0.50
1:HI:68:GLU:O	1:HI:80:VAL:HG13	2.11	0.50
1:HO:23:ILE:HD11	1:KW:120:TRP:HE3	1.75	0.50
1:IM:63:ASN:OD1	1:IM:64:VAL:N	2.44	0.50
1:KC:89:HIS:CE1	1:LB:118:ILE:HD11	2.45	0.50
1:LG:47:HIS:ND1	1:MF:122:SER:OG	2.44	0.50
1:AT:20:LEU:HB3	1:AT:32:TYR:HB3	1.93	0.50
1:BE:30:SER:HB3	1:BE:45:VAL:HG22	1.93	0.50
1:BY:70:VAL:HG21	1:BY:79:PHE:CZ	2.47	0.50
1:CO:20:LEU:HB3	1:CO:32:TYR:HB3	1.92	0.50
1:CQ:97:THR:HG21	1:KK:81:ARG:NH2	2.26	0.50
1:CU:116:LYS:HB3	1:CU:121:GLU:OE2	2.11	0.50
1:CV:34:LEU:HD12	1:CV:35:PRO:HD2	1.92	0.50
1:CV:36:GLU:OE1	1:CV:36:GLU:HA	2.12	0.50
1:EK:117:LEU:HD11	1:FJ:62:HIS:HB3	1.94	0.50
1:GA:50:GLU:OE1	1:GA:50:GLU:N	2.44	0.50
1:GO:93:ASP:OD1	1:GO:94:VAL:N	2.43	0.50
1:AU:30:SER:OG	1:HK:122:SER:O	2.24	0.50
1:BY:117:LEU:HD23	1:BY:117:LEU:O	2.12	0.50
1:CK:86:VAL:HG21	1:II:84:TYR:CZ	2.47	0.50
1:DI:23:ILE:HD11	1:DI:33:TYR:HB3	1.93	0.50
1:HD:24:ASN:OD1	1:HD:25:GLN:N	2.44	0.50

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:JK:19:VAL:O	1:JK:34:LEU:HD12	2.11	0.50
1:ML:65:GLU:CB	1:ML:84:TYR:HB3	2.41	0.50
2:M:181:SER:O	2:M:182:ASN:OD1	2.29	0.50
1:BQ:109:LEU:HD13	1:BQ:114:TYR:OH	2.11	0.50
1:DN:81:ARG:NH2	1:DS:97:THR:HG21	2.26	0.50
1:EL:65:GLU:OE1	1:EL:67:THR:OG1	2.24	0.50
1:EX:54:PRO:O	1:EX:55:ASN:OD1	2.30	0.50
1:FE:112:ALA:O	1:FE:116:LYS:HG2	2.11	0.50
1:GH:20:LEU:HB3	1:GH:32:TYR:HB3	1.93	0.50
1:HE:99:SER:O	1:HE:102:GLY:N	2.45	0.50
1:IG:27:GLY:O	1:IG:29:THR:HG23	2.11	0.50
1:JA:62:HIS:CB	1:KE:117:LEU:HD21	2.42	0.50
1:JF:81:ARG:NH1	1:JK:93:ASP:OD2	2.41	0.50
1:JM:93:ASP:OD1	1:JM:94:VAL:N	2.42	0.50
1:KE:20:LEU:HB3	1:KE:32:TYR:HB3	1.93	0.50
1:KE:99:SER:OG	1:KE:103:GLU:OE2	2.25	0.50
1:LG:6:LEU:HD22	1:LG:32:TYR:CE2	2.45	0.50
1:NH:20:LEU:HD21	1:NH:41:PHE:HB2	1.93	0.50
1:CC:23:ILE:HD11	1:DI:120:TRP:CB	2.41	0.50
1:CC:86:VAL:HG21	1:DB:84:TYR:CE2	2.47	0.50
1:CJ:121:GLU:OE2	1:CP:21:ARG:NH1	2.45	0.50
1:DC:108:TYR:CE2	1:DC:113:LEU:HD21	2.47	0.50
1:DM:108:TYR:CE2	1:DM:113:LEU:HD21	2.46	0.50
1:FW:54:PRO:O	1:FW:55:ASN:OD1	2.30	0.50
1:GA:113:LEU:HD23	1:GA:117:LEU:HD13	1.93	0.50
1:GY:82:GLN:OE1	1:GY:82:GLN:N	2.44	0.50
1:JM:112:ALA:O	1:JM:116:LYS:HG2	2.12	0.50
1:KW:110:ASN:OD1	1:KW:113:LEU:HD23	2.11	0.50
1:LN:93:ASP:OD1	1:LN:94:VAL:N	2.45	0.50
1:MM:20:LEU:HB3	1:MM:32:TYR:HB3	1.93	0.50
2:M:149:GLN:O	2:M:365:ARG:NH2	2.40	0.50
1:GB:109:LEU:HD12	1:GB:114:TYR:CE1	2.46	0.50
1:GT:110:ASN:OD1	1:GT:113:LEU:HD23	2.11	0.50
1:HV:109:LEU:HD23	1:HV:113:LEU:HD23	1.94	0.50
1:IY:122:SER:OXT	1:JX:1:ALA:N	2.45	0.50
1:KD:81:ARG:NH2	1:KI:97:THR:HG21	2.27	0.50
1:KW:27:GLY:O	1:KW:29:THR:HG23	2.11	0.50
1:LN:53:LYS:HG2	1:LN:54:PRO:HD2	1.94	0.50
1:LY:36:GLU:HA	1:LY:36:GLU:OE1	2.12	0.50
1:MF:5:THR:HG22	1:MF:21:ARG:HH22	1.76	0.50
1:MW:68:GLU:N	1:MW:81:ARG:O	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CE:108:TYR:CE1	1:CE:113:LEU:HD21	2.47	0.49
1:CU:20:LEU:HB3	1:CU:32:TYR:HB3	1.93	0.49
1:DS:20:LEU:HB3	1:DS:32:TYR:HB3	1.94	0.49
1:DZ:70:VAL:HG21	1:DZ:79:PHE:CZ	2.46	0.49
1:EX:73:SER:O	1:EX:76:THR:OG1	2.24	0.49
1:FK:54:PRO:O	1:FK:55:ASN:OD1	2.30	0.49
1:HV:87:ILE:HD13	1:IA:83:ALA:HB2	1.94	0.49
1:JA:122:SER:OXT	1:KE:1:ALA:N	2.44	0.49
1:KP:109:LEU:HD23	1:KP:113:LEU:HD23	1.93	0.49
1:LT:101:LEU:HD12	1:LY:10:LEU:HD11	1.94	0.49
1:NN:44:LYS:HB3	1:NN:65:GLU:HB2	1.93	0.49
2:M:7:ARG:NH2	2:M:38:CYS:SG	2.84	0.49
1:DU:27:GLY:O	1:DU:29:THR:HG23	2.12	0.49
1:EE:112:ALA:O	1:EE:116:LYS:HG2	2.13	0.49
1:JQ:63:ASN:OD1	1:JQ:64:VAL:N	2.45	0.49
1:MF:21:ARG:HA	1:MF:21:ARG:CZ	2.42	0.49
1:MR:62:HIS:O	1:MR:87:ILE:N	2.41	0.49
1:AN:54:PRO:O	1:AN:55:ASN:OD1	2.30	0.49
1:DA:8:ILE:HD12	1:DA:66:PHE:CE2	2.47	0.49
1:FQ:63:ASN:OD1	1:FQ:64:VAL:N	2.45	0.49
1:GO:1:ALA:N	1:JS:122:SER:OXT	2.45	0.49
1:GT:1:ALA:N	1:GY:122:SER:OXT	2.44	0.49
1:GT:20:LEU:HG	1:GT:32:TYR:HB3	1.95	0.49
1:IS:40:SER:OG	1:IS:69:THR:HG22	2.12	0.49
1:KD:47:HIS:NE2	1:KI:121:GLU:O	2.37	0.49
1:LB:20:LEU:HD23	1:LB:32:TYR:C	2.33	0.49
1:LN:15:GLY:O	1:LN:16:THR:OG1	2.22	0.49
1:LO:31:GLU:HB3	1:LO:44:LYS:HG3	1.94	0.49
1:AA:8:ILE:HD12	1:AA:66:PHE:CE2	2.48	0.49
1:AT:65:GLU:HB3	1:AT:84:TYR:HB3	1.93	0.49
1:BQ:24:ASN:ND2	1:BS:27:GLY:O	2.46	0.49
1:EA:36:GLU:N	1:EA:39:SER:O	2.44	0.49
1:EM:54:PRO:O	1:EM:55:ASN:OD1	2.29	0.49
1:FP:68:GLU:N	1:FP:81:ARG:O	2.40	0.49
1:HU:112:ALA:O	1:HU:116:LYS:HG2	2.12	0.49
1:IC:108:TYR:CE2	1:IC:113:LEU:HD21	2.48	0.49
1:JR:50:GLU:OE1	1:JR:50:GLU:N	2.45	0.49
1:KK:68:GLU:O	1:KK:80:VAL:HG23	2.12	0.49
1:LH:20:LEU:HB3	1:LH:32:TYR:HB3	1.94	0.49
1:CK:70:VAL:HG21	1:CK:79:PHE:CZ	2.48	0.49
1:FK:2:LEU:HD23	1:MA:122:SER:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FO:117:LEU:HD21	1:GN:62:HIS:CG	2.47	0.49
1:FW:2:LEU:HD23	1:LU:122:SER:C	2.33	0.49
1:JA:122:SER:O	1:KE:30:SER:OG	2.21	0.49
1:KQ:93:ASP:OD1	1:KQ:94:VAL:N	2.38	0.49
1:LB:50:GLU:OE1	1:LB:50:GLU:N	2.45	0.49
1:NG:53:LYS:HB3	1:NG:56:GLN:OE1	2.12	0.49
1:AC:55:ASN:OD1	1:AC:56:GLN:N	2.46	0.49
1:AG:20:LEU:HB3	1:AG:32:TYR:HB3	1.94	0.49
1:AH:109:LEU:HD13	1:AH:114:TYR:OH	2.12	0.49
1:AN:113:LEU:O	1:AN:117:LEU:HD13	2.12	0.49
1:BE:54:PRO:O	1:BE:55:ASN:OD1	2.29	0.49
1:DS:46:ARG:O	1:DS:47:HIS:ND1	2.44	0.49
1:DT:108:TYR:CZ	1:DT:113:LEU:HD21	2.48	0.49
1:EE:1:ALA:C	1:EE:2:LEU:HD12	2.33	0.49
1:HK:36:GLU:OE1	1:HK:36:GLU:HA	2.13	0.49
1:JG:114:TYR:O	1:JG:118:ILE:HD12	2.12	0.49
1:KI:53:LYS:HE2	1:KI:53:LYS:HA	1.95	0.49
1:LT:81:ARG:HH22	1:LY:97:THR:HG21	1.78	0.49
1:ML:68:GLU:O	1:ML:81:ARG:N	2.43	0.49
1:AA:62:HIS:N	1:AA:87:ILE:O	2.41	0.49
1:CE:55:ASN:OD1	1:CE:55:ASN:O	2.31	0.49
1:CU:49:LYS:HG3	1:CU:50:GLU:H	1.77	0.49
1:DI:54:PRO:O	1:DI:55:ASN:OD1	2.30	0.49
1:GZ:100:ASP:OD1	1:HC:11:GLY:N	2.46	0.49
1:HC:53:LYS:HD2	1:HC:54:PRO:HD2	1.95	0.49
1:IU:88:ARG:HB3	1:NC:82:GLN:HB2	1.95	0.49
1:JL:112:ALA:O	1:JL:116:LYS:HG2	2.13	0.49
1:JM:48:THR:HG22	1:JM:49:LYS:O	2.13	0.49
1:LG:89:HIS:CE1	1:MF:118:ILE:HD11	2.48	0.49
1:LH:6:LEU:HD23	1:LH:32:TYR:CE2	2.47	0.49
1:MX:69:THR:HG22	1:MX:80:VAL:HG12	1.94	0.49
1:CK:54:PRO:O	1:CK:55:ASN:OD1	2.30	0.49
1:EF:65:GLU:OE1	1:EF:84:TYR:HB3	2.12	0.49
1:FE:21:ARG:CZ	1:FE:21:ARG:HB2	2.42	0.49
1:FW:93:ASP:OD1	1:FW:94:VAL:N	2.44	0.49
1:GM:93:ASP:OD1	1:GM:94:VAL:N	2.37	0.49
1:HJ:36:GLU:HA	1:HJ:36:GLU:OE1	2.12	0.49
1:II:112:ALA:O	1:II:116:LYS:HG3	2.13	0.49
1:JA:121:GLU:O	1:KE:47:HIS:NE2	2.37	0.49
1:KP:54:PRO:O	1:KP:55:ASN:OD1	2.30	0.49
1:LZ:36:GLU:OE1	1:LZ:36:GLU:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AI:53:LYS:HB2	1:AI:54:PRO:HD2	1.95	0.49
1:BS:108:TYR:CE1	1:BS:113:LEU:HD11	2.47	0.49
1:CD:101:LEU:HD12	1:CD:102:GLY:N	2.28	0.49
1:FI:27:GLY:O	1:FI:29:THR:HG23	2.13	0.49
1:GH:26:ASP:O	1:GH:29:THR:OG1	2.14	0.49
1:HK:5:THR:HG23	1:HK:19:VAL:HG13	1.95	0.49
1:JS:54:PRO:O	1:JS:55:ASN:OD1	2.31	0.49
1:LG:47:HIS:CE1	1:MF:122:SER:HG	2.30	0.49
1:AY:36:GLU:OE1	1:AY:36:GLU:HA	2.13	0.49
1:BE:112:ALA:O	1:BE:116:LYS:HG2	2.12	0.49
1:CK:65:GLU:CB	1:CK:84:TYR:HB3	2.42	0.49
1:CQ:69:THR:HG22	1:CQ:80:VAL:HG12	1.95	0.49
1:CW:85:VAL:HG22	1:JY:85:VAL:HG22	1.95	0.49
1:DG:109:LEU:HD23	1:DG:113:LEU:HD23	1.95	0.49
1:DH:54:PRO:O	1:DH:55:ASN:OD1	2.31	0.49
1:FI:63:ASN:OD1	1:FI:64:VAL:N	2.46	0.49
1:FJ:112:ALA:O	1:FJ:116:LYS:HG3	2.13	0.49
1:FK:1:ALA:N	1:MA:121:GLU:OE1	2.45	0.49
1:FQ:113:LEU:O	1:FQ:117:LEU:HD23	2.13	0.49
1:GZ:24:ASN:OD1	1:GZ:25:GLN:N	2.46	0.49
1:JX:55:ASN:OD1	1:JX:56:GLN:NE2	2.45	0.49
1:LM:40:SER:HG	1:LM:71:TYR:HH	1.59	0.49
1:LT:122:SER:C	1:LY:2:LEU:HD13	2.32	0.49
1:ME:63:ASN:OD1	1:ME:64:VAL:N	2.45	0.49
1:MQ:53:LYS:HE2	1:MQ:53:LYS:HA	1.94	0.49
1:AA:85:VAL:HG23	1:NN:85:VAL:HG12	1.95	0.48
1:AI:81:ARG:CZ	1:JG:97:THR:HG21	2.43	0.48
1:DN:122:SER:C	1:DS:2:LEU:HD13	2.33	0.48
1:EF:15:GLY:O	1:EF:16:THR:OG1	2.27	0.48
1:EG:109:LEU:HD12	1:EG:114:TYR:CE1	2.48	0.48
1:EL:113:LEU:HD23	1:EL:117:LEU:HD23	1.95	0.48
1:FO:26:ASP:O	1:FO:29:THR:OG1	2.14	0.48
1:FV:54:PRO:O	1:FV:55:ASN:OD1	2.31	0.48
1:GY:69:THR:OG1	1:GY:78:GLU:OE2	2.31	0.48
1:HW:25:GLN:O	1:HW:25:GLN:HG3	2.12	0.48
1:IY:55:ASN:O	1:IY:56:GLN:HG2	2.12	0.48
1:JF:65:GLU:CB	1:JF:84:TYR:HB3	2.43	0.48
1:JX:20:LEU:HB3	1:JX:32:TYR:HB3	1.95	0.48
1:KD:2:LEU:HD22	1:KI:121:GLU:HB3	1.95	0.48
1:LS:27:GLY:O	1:LS:29:THR:HG23	2.13	0.48
1:MK:20:LEU:HB3	1:MK:32:TYR:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MK:24:ASN:OD1	1:MK:25:GLN:N	2.46	0.48
1:NB:68:GLU:O	1:NB:81:ARG:N	2.38	0.48
1:CC:20:LEU:HB3	1:CC:32:TYR:HB3	1.95	0.48
1:CD:109:LEU:HD13	1:CD:113:LEU:HD22	1.95	0.48
1:CW:121:GLU:OE1	1:JY:1:ALA:HB3	2.13	0.48
1:FP:65:GLU:OE1	1:FP:67:THR:OG1	2.26	0.48
1:IC:109:LEU:HD23	1:IC:113:LEU:HD23	1.95	0.48
1:JG:20:LEU:HB3	1:JG:32:TYR:HB3	1.95	0.48
1:JM:61:ARG:O	1:JM:62:HIS:ND1	2.46	0.48
1:KV:54:PRO:O	1:KV:55:ASN:OD1	2.31	0.48
1:AH:62:HIS:CG	1:AM:117:LEU:HD21	2.49	0.48
1:AO:113:LEU:O	1:AO:117:LEU:HD23	2.13	0.48
1:AZ:109:LEU:HD13	1:AZ:113:LEU:HD23	1.96	0.48
1:DN:122:SER:OXT	1:DS:2:LEU:HD13	2.13	0.48
1:DT:81:ARG:NH2	1:DY:97:THR:HG21	2.28	0.48
1:DU:23:ILE:HD11	1:DY:120:TRP:HB3	1.94	0.48
1:EY:113:LEU:O	1:EY:117:LEU:HD13	2.13	0.48
1:IS:50:GLU:OE2	1:IS:61:ARG:NH2	2.47	0.48
1:IU:4:ASP:OD1	1:IU:5:THR:HG23	2.12	0.48
1:JL:60:GLU:OE2	1:JQ:120:TRP:NE1	2.32	0.48
2:M:206:HIS:ND1	2:M:208:SER:O	2.46	0.48
1:AZ:99:SER:HG	1:BE:111:GLU:CD	2.15	0.48
1:FC:31:GLU:HG3	1:FC:44:LYS:NZ	2.29	0.48
1:GB:26:ASP:O	1:GB:29:THR:OG1	2.21	0.48
1:II:54:PRO:O	1:II:55:ASN:OD1	2.30	0.48
1:IT:68:GLU:HB2	1:IT:81:ARG:HB2	1.94	0.48
1:JL:87:ILE:HD11	1:JQ:114:TYR:HE1	1.78	0.48
1:JW:6:LEU:HD22	1:JW:32:TYR:HE2	1.79	0.48
1:LA:20:LEU:HB3	1:LA:32:TYR:HB3	1.95	0.48
1:LM:1:ALA:O	1:LM:3:GLY:N	2.43	0.48
1:ME:65:GLU:CB	1:ME:84:TYR:HB3	2.43	0.48
1:AA:31:GLU:HA	1:AA:43:ALA:O	2.14	0.48
1:AT:24:ASN:ND2	1:AT:31:GLU:OE1	2.46	0.48
1:BF:30:SER:OG	1:BK:122:SER:OG	2.25	0.48
1:BQ:60:GLU:HG2	1:BQ:89:HIS:O	2.13	0.48
1:CO:55:ASN:O	1:CO:56:GLN:NE2	2.46	0.48
1:DA:93:ASP:OD1	1:DA:94:VAL:N	2.44	0.48
1:EM:113:LEU:O	1:EM:113:LEU:HD23	2.13	0.48
1:GT:62:HIS:O	1:GT:86:VAL:HA	2.13	0.48
1:GU:87:ILE:HD11	1:HW:114:TYR:CE1	2.48	0.48
1:HK:109:LEU:HA	1:HK:113:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HV:25:GLN:HG2	1:HV:29:THR:O	2.14	0.48
1:JL:1:ALA:N	1:JQ:122:SER:OXT	2.46	0.48
1:KW:31:GLU:OE1	1:KW:44:LYS:HG2	2.13	0.48
1:LC:93:ASP:OD1	1:LC:94:VAL:N	2.43	0.48
1:LO:63:ASN:OD1	1:LO:64:VAL:N	2.47	0.48
1:MR:31:GLU:HB3	1:MR:44:LYS:HB3	1.96	0.48
2:M:363:ILE:O	2:M:366:VAL:HG12	2.13	0.48
1:AY:19:VAL:O	1:AY:34:LEU:HD12	2.14	0.48
1:BY:84:TYR:CZ	1:FE:86:VAL:HG21	2.48	0.48
1:CQ:19:VAL:O	1:CQ:19:VAL:HG23	2.13	0.48
1:CW:116:LYS:HZ1	1:JY:2:LEU:HD23	1.76	0.48
1:EQ:66:PHE:O	1:EQ:82:GLN:HB2	2.13	0.48
1:FI:53:LYS:HG3	1:FI:54:PRO:HD2	1.96	0.48
1:FO:20:LEU:HB3	1:FO:32:TYR:HB3	1.95	0.48
1:GG:31:GLU:OE1	1:GG:32:TYR:N	2.46	0.48
1:GS:63:ASN:OD1	1:GS:64:VAL:N	2.47	0.48
1:GY:36:GLU:OE1	1:GY:39:SER:OG	2.27	0.48
1:GY:60:GLU:OE2	1:GY:89:HIS:NE2	2.47	0.48
1:HP:54:PRO:O	1:HP:55:ASN:OD1	2.31	0.48
1:IN:88:ARG:NH2	1:IS:82:GLN:OE1	2.45	0.48
1:IS:65:GLU:OE1	1:IS:84:TYR:HB3	2.13	0.48
1:IZ:87:ILE:HD11	1:JE:114:TYR:HE1	1.79	0.48
1:KI:113:LEU:O	1:KI:117:LEU:HD23	2.12	0.48
1:KV:93:ASP:OD1	1:KV:94:VAL:N	2.45	0.48
1:KW:52:VAL:HG21	1:KW:58:GLN:HA	1.94	0.48
1:LG:6:LEU:HD11	1:MF:108:TYR:HE1	1.77	0.48
2:M:197:GLN:OE1	2:M:219:ILE:HG23	2.14	0.48
1:AA:60:GLU:O	1:AA:88:ARG:HA	2.13	0.48
1:BQ:54:PRO:O	1:BQ:55:ASN:OD1	2.32	0.48
1:DC:8:ILE:HD12	1:DC:20:LEU:HD11	1.95	0.48
1:DH:50:GLU:OE2	1:DH:61:ARG:NH2	2.46	0.48
1:DN:112:ALA:O	1:DN:116:LYS:HG3	2.13	0.48
1:EG:27:GLY:O	1:EG:29:THR:HG23	2.14	0.48
1:FQ:54:PRO:O	1:FQ:55:ASN:OD1	2.32	0.48
1:HU:113:LEU:HD23	1:HU:117:LEU:HD23	1.95	0.48
1:IH:69:THR:HG22	1:IH:80:VAL:HG12	1.95	0.48
1:JW:69:THR:HG22	1:JW:80:VAL:HG12	1.96	0.48
1:KK:68:GLU:CB	1:KK:81:ARG:HB2	2.44	0.48
1:LC:54:PRO:O	1:LC:55:ASN:OD1	2.31	0.48
1:AH:112:ALA:O	1:AH:116:LYS:HG2	2.14	0.48
1:AM:53:LYS:HE2	1:AM:53:LYS:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BK:109:LEU:HD23	1:BK:113:LEU:HD23	1.96	0.48
1:DG:62:HIS:O	1:DG:86:VAL:HG23	2.13	0.48
1:FU:29:THR:HG22	1:FU:46:ARG:HG2	1.96	0.48
1:FV:29:THR:HG23	1:FV:46:ARG:HG2	1.96	0.48
1:GO:27:GLY:O	1:GO:29:THR:HG23	2.13	0.48
1:JE:113:LEU:HD23	1:JE:117:LEU:CD2	2.42	0.48
1:KI:40:SER:OG	1:KI:69:THR:OG1	2.28	0.48
1:KJ:93:ASP:OD1	1:KJ:94:VAL:N	2.45	0.48
1:LZ:112:ALA:O	1:LZ:116:LYS:HG3	2.13	0.48
1:AY:63:ASN:HA	1:AY:85:VAL:O	2.13	0.48
1:BG:63:ASN:OD1	1:BG:64:VAL:N	2.47	0.48
1:CC:112:ALA:O	1:CC:116:LYS:HG2	2.13	0.48
1:CK:59:TYR:HA	1:CK:90:LYS:HA	1.95	0.48
1:CO:63:ASN:OD1	1:CO:64:VAL:N	2.46	0.48
1:CV:54:PRO:O	1:CV:55:ASN:OD1	2.32	0.48
1:EQ:112:ALA:O	1:EQ:116:LYS:HG2	2.13	0.48
1:GH:118:ILE:HD11	1:GM:89:HIS:NE2	2.29	0.48
1:GT:62:HIS:HB2	1:GT:87:ILE:HB	1.96	0.48
1:HJ:93:ASP:OD1	1:HJ:94:VAL:N	2.47	0.48
1:HO:36:GLU:OE2	1:HO:39:SER:N	2.47	0.48
1:HU:62:HIS:O	1:HU:86:VAL:HA	2.13	0.48
1:IT:89:HIS:CD2	1:IT:98:VAL:HG11	2.49	0.48
1:JA:116:LYS:HE2	1:JA:121:GLU:OE1	2.14	0.48
1:LY:34:LEU:HD12	1:LY:35:PRO:HD2	1.94	0.48
1:AG:46:ARG:O	1:AG:47:HIS:ND1	2.47	0.48
1:DB:73:SER:O	1:DB:76:THR:OG1	2.27	0.48
1:DO:54:PRO:O	1:DO:55:ASN:OD1	2.31	0.48
1:DT:109:LEU:HD23	1:DT:113:LEU:HD23	1.95	0.48
1:EQ:20:LEU:HB3	1:EQ:32:TYR:HB3	1.96	0.48
1:EY:54:PRO:O	1:EY:55:ASN:OD1	2.32	0.48
1:FV:30:SER:HG	1:GA:122:SER:HG	1.59	0.48
1:GO:122:SER:OXT	1:JS:1:ALA:N	2.45	0.48
1:HE:62:HIS:O	1:HE:86:VAL:HA	2.14	0.48
1:IC:85:VAL:HG23	1:KQ:105:LEU:HD21	1.95	0.48
1:IG:20:LEU:HB3	1:IG:32:TYR:HB3	1.95	0.48
1:IY:84:TYR:CZ	1:JX:86:VAL:HG21	2.49	0.48
1:JA:54:PRO:O	1:JA:55:ASN:OD1	2.31	0.48
1:JF:36:GLU:OE1	1:JF:36:GLU:HA	2.14	0.48
1:KJ:73:SER:O	1:KJ:76:THR:OG1	2.31	0.48
1:KV:15:GLY:O	1:KV:16:THR:OG1	2.23	0.48
1:LS:113:LEU:O	1:LS:117:LEU:HD13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NC:121:GLU:OE1	1:NC:121:GLU:HA	2.14	0.48
1:AA:65:GLU:OE2	1:AA:67:THR:OG1	2.26	0.47
1:AO:63:ASN:OD1	1:AO:64:VAL:N	2.47	0.47
1:HI:68:GLU:O	1:HI:80:VAL:HA	2.14	0.47
1:HU:20:LEU:HB3	1:HU:32:TYR:HB3	1.96	0.47
1:IN:103:GLU:OE1	1:IS:12:GLY:N	2.47	0.47
1:LG:120:TRP:NE1	1:MF:60:GLU:OE2	2.47	0.47
1:MR:84:TYR:O	1:MW:85:VAL:HG23	2.14	0.47
1:AZ:20:LEU:HB3	1:AZ:32:TYR:HB3	1.96	0.47
1:BQ:21:ARG:HD2	1:MG:121:GLU:OE2	2.14	0.47
1:CK:108:TYR:CZ	1:II:6:LEU:HD11	2.48	0.47
1:CQ:6:LEU:HD22	1:CQ:32:TYR:CE2	2.49	0.47
1:HW:4:ASP:OD1	1:HW:5:THR:HG23	2.14	0.47
1:IM:99:SER:O	1:IM:103:GLU:HG3	2.14	0.47
1:IU:81:ARG:NH2	1:NC:97:THR:HG21	2.28	0.47
1:JY:19:VAL:HG23	1:JY:19:VAL:O	2.13	0.47
1:LG:116:LYS:O	1:LG:119:GLY:N	2.48	0.47
1:NN:95:SER:O	1:NN:98:VAL:HG12	2.13	0.47
1:DZ:19:VAL:O	1:DZ:19:VAL:HG23	2.15	0.47
1:DZ:33:TYR:CD1	1:DZ:34:LEU:N	2.82	0.47
1:EE:36:GLU:OE1	1:EE:39:SER:OG	2.15	0.47
1:EK:62:HIS:HB3	1:FJ:117:LEU:HD21	1.96	0.47
1:FC:62:HIS:O	1:FC:86:VAL:HA	2.14	0.47
1:FC:121:GLU:OE1	1:FC:121:GLU:N	2.46	0.47
1:FP:54:PRO:O	1:FP:56:GLN:OE1	2.32	0.47
1:GA:46:ARG:NH1	1:GA:63:ASN:OD1	2.48	0.47
1:GG:53:LYS:HE2	1:GG:53:LYS:HA	1.95	0.47
1:JW:20:LEU:HB3	1:JW:32:TYR:HB3	1.97	0.47
1:LU:19:VAL:HG23	1:LU:19:VAL:O	2.15	0.47
1:NI:20:LEU:HB3	1:NI:32:TYR:HB3	1.95	0.47
1:NI:30:SER:HB2	1:NI:45:VAL:HG22	1.96	0.47
1:AN:20:LEU:HB3	1:AN:32:TYR:HB3	1.96	0.47
1:AU:81:ARG:NH2	1:HK:97:THR:HG21	2.29	0.47
1:CD:23:ILE:HB	1:CD:31:GLU:OE2	2.15	0.47
1:CU:109:LEU:HD13	1:CU:114:TYR:OH	2.14	0.47
1:GB:93:ASP:OD1	1:GB:94:VAL:N	2.47	0.47
1:GO:18:LYS:HZ2	1:GO:41:PHE:HE2	1.63	0.47
1:HC:114:TYR:O	1:HC:118:ILE:HG22	2.13	0.47
1:HQ:20:LEU:HB3	1:HQ:32:TYR:HB3	1.96	0.47
1:HQ:122:SER:C	1:KW:2:LEU:HD23	2.35	0.47
1:IO:113:LEU:O	1:IO:117:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:8:ILE:HD11	1:JA:20:LEU:HD11	1.96	0.47
1:JA:48:THR:HG22	1:JA:49:LYS:O	2.14	0.47
1:JE:20:LEU:HB3	1:JE:32:TYR:HB3	1.96	0.47
1:KI:109:LEU:HD12	1:KI:114:TYR:CZ	2.49	0.47
1:MM:24:ASN:OD1	1:MM:25:GLN:N	2.48	0.47
1:NC:63:ASN:OD1	1:NC:64:VAL:N	2.48	0.47
1:AY:86:VAL:HB	1:BX:84:TYR:CZ	2.49	0.47
1:BL:85:VAL:HG21	1:BQ:109:LEU:HD11	1.95	0.47
1:BM:20:LEU:HB3	1:BM:32:TYR:HB3	1.96	0.47
1:GI:20:LEU:HB3	1:GI:32:TYR:HB3	1.95	0.47
1:HD:20:LEU:HB3	1:HD:32:TYR:HB3	1.96	0.47
1:HW:20:LEU:HB3	1:HW:32:TYR:HB3	1.97	0.47
1:JA:23:ILE:HD11	1:JE:120:TRP:HB3	1.95	0.47
1:KV:109:LEU:HD13	1:KV:114:TYR:OH	2.13	0.47
1:NN:20:LEU:HB3	1:NN:32:TYR:HB3	1.97	0.47
2:M:159:ILE:O	2:M:163:LEU:HD23	2.14	0.47
1:AI:24:ASN:OD1	1:AI:25:GLN:N	2.47	0.47
1:AY:63:ASN:OD1	1:AY:64:VAL:N	2.47	0.47
1:BQ:64:VAL:O	1:BQ:84:TYR:HB2	2.14	0.47
1:BX:60:GLU:CD	1:BX:91:VAL:HG22	2.34	0.47
1:ER:54:PRO:O	1:ER:56:GLN:OE1	2.32	0.47
1:KE:57:VAL:HG23	1:KE:59:TYR:CE2	2.50	0.47
1:BA:20:LEU:HB3	1:BA:32:TYR:HB3	1.97	0.47
1:BX:20:LEU:HB3	1:BX:32:TYR:HB3	1.97	0.47
1:CD:105:LEU:O	1:CD:109:LEU:HD23	2.15	0.47
1:DZ:22:LYS:O	1:DZ:23:ILE:HD13	2.15	0.47
1:DZ:60:GLU:HG3	1:DZ:91:VAL:HG22	1.97	0.47
1:EF:53:LYS:CD	1:EF:54:PRO:HD2	2.45	0.47
1:EK:2:LEU:O	1:EK:2:LEU:HD23	2.14	0.47
1:EM:21:ARG:NH1	1:EQ:121:GLU:OE2	2.47	0.47
1:ES:114:TYR:CE1	1:JM:87:ILE:HD11	2.49	0.47
1:GU:108:TYR:CZ	1:GU:113:LEU:CD1	2.98	0.47
1:HW:54:PRO:O	1:HW:55:ASN:OD1	2.33	0.47
1:IC:29:THR:OG1	1:IC:45:VAL:O	2.17	0.47
1:II:108:TYR:CZ	1:II:113:LEU:HD22	2.48	0.47
1:JG:110:ASN:OD1	1:JG:111:GLU:N	2.47	0.47
1:JS:63:ASN:OD1	1:JS:64:VAL:N	2.48	0.47
1:KI:68:GLU:O	1:KI:80:VAL:HA	2.15	0.47
1:KJ:20:LEU:HB3	1:KJ:32:TYR:HB3	1.97	0.47
1:KK:23:ILE:HD12	1:KO:120:TRP:HD1	1.79	0.47
1:KQ:24:ASN:OD1	1:KQ:25:GLN:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LS:73:SER:O	1:LS:76:THR:OG1	2.28	0.47
1:ME:20:LEU:HB3	1:ME:32:TYR:HB3	1.96	0.47
1:MR:47:HIS:HE1	1:MW:117:LEU:HD12	1.79	0.47
1:NA:53:LYS:HD3	1:NA:54:PRO:HD2	1.96	0.47
1:CK:25:GLN:HB2	1:CK:29:THR:O	2.15	0.47
1:CU:24:ASN:ND2	1:CW:26:ASP:O	2.38	0.47
1:DY:20:LEU:HB3	1:DY:32:TYR:HB3	1.97	0.47
1:EK:116:LYS:NZ	1:EK:121:GLU:OE1	2.40	0.47
1:EQ:69:THR:HG22	1:EQ:80:VAL:HG12	1.96	0.47
1:FD:54:PRO:O	1:FD:55:ASN:OD1	2.32	0.47
1:HK:20:LEU:HB3	1:HK:32:TYR:HB3	1.97	0.47
1:IZ:84:TYR:CE1	1:JE:86:VAL:HB	2.50	0.47
1:JG:112:ALA:O	1:JG:116:LYS:NZ	2.48	0.47
1:KP:111:GLU:OE1	1:KU:99:SER:OG	2.32	0.47
1:LS:34:LEU:HD12	1:LS:35:PRO:HD2	1.96	0.47
1:MQ:108:TYR:CE2	1:MQ:113:LEU:HD21	2.50	0.47
1:MR:98:VAL:HG21	1:MW:118:ILE:HD12	1.97	0.47
1:NA:23:ILE:HG22	1:NC:28:TYR:HD1	1.79	0.47
1:AN:47:HIS:HB2	1:AS:120:TRP:CZ3	2.50	0.47
1:AZ:4:ASP:OD1	1:AZ:5:THR:HG23	2.15	0.47
1:BR:1:ALA:H2	1:BW:121:GLU:HG2	1.80	0.47
1:CP:119:GLY:O	1:CP:120:TRP:HB2	2.15	0.47
1:CV:51:SER:OG	1:CV:53:LYS:NZ	2.48	0.47
1:DO:62:HIS:HB2	1:DO:87:ILE:HG22	1.97	0.47
1:DO:81:ARG:NH2	1:GC:97:THR:HG21	2.30	0.47
1:DO:121:GLU:OE2	1:GC:1:ALA:N	2.30	0.47
1:HK:8:ILE:HD12	1:HK:66:PHE:CE2	2.50	0.47
1:HQ:89:HIS:CD2	1:KW:118:ILE:HD11	2.50	0.47
1:JK:62:HIS:O	1:JK:86:VAL:HA	2.14	0.47
1:KK:68:GLU:HB2	1:KK:81:ARG:HB2	1.97	0.47
1:KW:52:VAL:HG12	1:KW:53:LYS:O	2.14	0.47
1:LN:103:GLU:OE1	1:LS:111:GLU:OE2	2.32	0.47
1:LT:112:ALA:O	1:LT:116:LYS:HG2	2.15	0.47
1:MA:54:PRO:O	1:MA:55:ASN:OD1	2.33	0.47
1:AC:63:ASN:OD1	1:AC:64:VAL:N	2.48	0.47
1:CW:54:PRO:O	1:CW:55:ASN:OD1	2.33	0.47
1:DA:24:ASN:ND2	1:DA:26:ASP:OD2	2.48	0.47
1:DT:29:THR:HG23	1:DT:46:ARG:HG2	1.97	0.47
1:FK:48:THR:HG22	1:FK:49:LYS:N	2.29	0.47
1:FQ:80:VAL:HG22	1:FQ:81:ARG:N	2.30	0.47
1:GN:65:GLU:OE2	1:GN:82:GLN:NE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HD:54:PRO:O	1:HD:55:ASN:OD1	2.33	0.47
1:HU:60:GLU:O	1:HU:88:ARG:HA	2.15	0.47
1:IZ:85:VAL:HG11	1:JE:109:LEU:HD11	1.95	0.47
1:MS:63:ASN:OD1	1:MS:64:VAL:N	2.47	0.47
1:AH:25:GLN:NE2	1:AI:23:ILE:O	2.48	0.46
1:BL:65:GLU:CB	1:BL:84:TYR:HB3	2.45	0.46
1:DI:25:GLN:HG3	1:DI:25:GLN:O	2.15	0.46
1:EL:81:ARG:NH1	1:EQ:97:THR:HG21	2.30	0.46
1:EM:109:LEU:HD13	1:EM:113:LEU:HD22	1.97	0.46
1:FP:108:TYR:CE1	1:FP:113:LEU:HD21	2.50	0.46
1:GG:50:GLU:N	1:GG:50:GLU:OE2	2.48	0.46
1:GI:19:VAL:O	1:GI:34:LEU:HD12	2.15	0.46
1:HD:120:TRP:HB3	1:HJ:23:ILE:HD12	1.97	0.46
1:IN:69:THR:HG22	1:IN:80:VAL:HG12	1.97	0.46
1:JG:54:PRO:O	1:JG:55:ASN:OD1	2.32	0.46
1:JS:32:TYR:HD2	1:JS:43:ALA:HB3	1.79	0.46
1:MQ:26:ASP:O	1:MQ:29:THR:OG1	2.18	0.46
1:MS:108:TYR:CE2	1:MS:113:LEU:HD21	2.49	0.46
2:M:19:TYR:N	2:M:72:THR:O	2.39	0.46
1:AS:116:LYS:HB3	1:AS:121:GLU:OE2	2.15	0.46
1:BF:48:THR:HG22	1:BF:49:LYS:N	2.30	0.46
1:CV:108:TYR:CZ	1:CV:113:LEU:HD21	2.51	0.46
1:EX:63:ASN:OD1	1:EX:64:VAL:N	2.48	0.46
1:FC:19:VAL:O	1:FC:34:LEU:HD12	2.16	0.46
1:FW:112:ALA:O	1:FW:116:LYS:HG2	2.15	0.46
1:HU:53:LYS:HB3	1:HU:54:PRO:HD3	1.97	0.46
1:IG:7:THR:HG23	1:IG:7:THR:O	2.15	0.46
1:JK:62:HIS:O	1:JK:86:VAL:HG23	2.15	0.46
1:KI:4:ASP:OD1	1:KI:5:THR:HG23	2.15	0.46
1:KV:81:ARG:NH2	1:LA:97:THR:HG21	2.30	0.46
2:M:342:THR:O	2:M:343:ILE:HD13	2.15	0.46
1:AC:109:LEU:HD13	1:AC:113:LEU:HD22	1.96	0.46
1:CP:69:THR:HG22	1:CP:80:VAL:HG12	1.96	0.46
1:DZ:84:TYR:CZ	1:EE:86:VAL:HB	2.50	0.46
1:FC:112:ALA:O	1:FC:116:LYS:HG2	2.16	0.46
1:GA:53:LYS:HB2	1:GA:54:PRO:HD2	1.97	0.46
1:GA:55:ASN:O	1:GA:56:GLN:HG3	2.16	0.46
1:GI:50:GLU:O	1:GI:58:GLN:NE2	2.46	0.46
1:GS:90:LYS:HG2	1:GS:93:ASP:HB2	1.98	0.46
1:IC:6:LEU:HD22	1:IC:20:LEU:HD12	1.97	0.46
1:IU:86:VAL:HB	1:NC:84:TYR:CZ	2.50	0.46

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:IZ:2:LEU:HD23	1:JE:122:SER:OXT	2.15	0.46
1:JM:29:THR:HG23	1:JM:45:VAL:O	2.15	0.46
1:KO:121:GLU:OE1	1:KO:121:GLU:HA	2.16	0.46
1:NB:20:LEU:HD21	1:NB:41:PHE:HB3	1.96	0.46
1:BG:1:ALA:HB3	1:HE:121:GLU:HG2	1.98	0.46
1:DA:57:VAL:HG13	1:DA:59:TYR:CE2	2.51	0.46
1:DU:86:VAL:HG21	1:LO:84:TYR:CZ	2.51	0.46
1:EA:27:GLY:O	1:EA:29:THR:HG23	2.16	0.46
1:EK:84:TYR:CZ	1:FJ:86:VAL:HG21	2.51	0.46
1:FI:112:ALA:O	1:FI:116:LYS:HG2	2.16	0.46
1:FP:89:HIS:CD2	1:FP:98:VAL:HG21	2.51	0.46
1:IG:112:ALA:O	1:IG:116:LYS:HG2	2.15	0.46
1:IM:61:ARG:HA	1:IM:87:ILE:O	2.16	0.46
1:IT:93:ASP:OD1	1:IT:94:VAL:N	2.44	0.46
1:JM:63:ASN:OD1	1:JM:64:VAL:N	2.49	0.46
1:KP:114:TYR:CE1	1:KU:87:ILE:HD11	2.50	0.46
1:LM:20:LEU:HB3	1:LM:32:TYR:HB3	1.97	0.46
1:NC:49:LYS:NZ	1:NC:58:GLN:OE1	2.44	0.46
1:NI:105:LEU:O	1:NI:109:LEU:HD23	2.16	0.46
1:AA:55:ASN:OD1	1:AA:55:ASN:O	2.33	0.46
1:AB:114:TYR:HE1	1:AG:87:ILE:HD11	1.80	0.46
1:BG:59:TYR:HA	1:BG:90:LYS:HA	1.98	0.46
1:BY:63:ASN:OD1	1:BY:64:VAL:N	2.49	0.46
1:DI:29:THR:HG22	1:DI:46:ARG:HA	1.97	0.46
1:FW:20:LEU:HB3	1:FW:32:TYR:HB3	1.97	0.46
1:IU:53:LYS:HG2	1:IU:54:PRO:HD2	1.96	0.46
1:LM:113:LEU:O	1:LM:117:LEU:HD13	2.16	0.46
1:MG:63:ASN:OD1	1:MG:64:VAL:N	2.49	0.46
1:MR:20:LEU:HB3	1:MR:32:TYR:HB3	1.96	0.46
1:MS:54:PRO:O	1:MS:55:ASN:OD1	2.34	0.46
1:MS:64:VAL:O	1:MS:84:TYR:HB2	2.15	0.46
1:BK:27:GLY:O	1:BK:29:THR:HG23	2.15	0.46
1:BW:62:HIS:O	1:BW:86:VAL:HA	2.16	0.46
1:CC:23:ILE:HG22	1:CC:31:GLU:HB2	1.98	0.46
1:DA:108:TYR:CZ	1:DA:113:LEU:CD1	2.98	0.46
1:DC:114:TYR:HE1	1:GI:87:ILE:HD11	1.81	0.46
1:ER:54:PRO:O	1:ER:55:ASN:OD1	2.34	0.46
1:EX:108:TYR:CZ	1:EX:113:LEU:HD11	2.50	0.46
1:FV:47:HIS:O	1:FV:48:THR:HG23	2.16	0.46
1:HK:27:GLY:O	1:HK:29:THR:HG23	2.16	0.46
1:IO:20:LEU:HB3	1:IO:32:TYR:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IT:59:TYR:HA	1:IT:90:LYS:HA	1.98	0.46
1:IU:68:GLU:N	1:IU:81:ARG:O	2.42	0.46
1:JX:63:ASN:HB2	1:JX:86:VAL:HG12	1.97	0.46
1:KP:30:SER:OG	1:KU:122:SER:O	2.32	0.46
1:LH:62:HIS:O	1:LH:86:VAL:HA	2.15	0.46
1:LS:55:ASN:O	1:LS:56:GLN:OE1	2.34	0.46
1:MF:54:PRO:O	1:MF:55:ASN:OD1	2.33	0.46
1:MR:104:ALA:HB2	1:MW:10:LEU:HA	1.97	0.46
1:MW:89:HIS:ND1	1:MW:90:LYS:O	2.49	0.46
1:NM:99:SER:O	1:NM:103:GLU:HG3	2.15	0.46
1:AN:2:LEU:HD22	1:AS:121:GLU:HG3	1.98	0.46
1:AZ:117:LEU:HD21	1:BE:62:HIS:CG	2.51	0.46
1:BR:2:LEU:HD23	1:BW:122:SER:O	2.15	0.46
1:CV:114:TYR:CE1	1:DA:87:ILE:HD11	2.49	0.46
1:EG:122:SER:OXT	1:IO:1:ALA:N	2.37	0.46
1:FK:58:GLN:NE2	1:FK:59:TYR:O	2.49	0.46
1:FV:20:LEU:HB3	1:FV:32:TYR:HB3	1.98	0.46
1:GS:50:GLU:OE2	1:GS:59:TYR:N	2.41	0.46
1:HW:21:ARG:NH1	1:IA:121:GLU:OE2	2.49	0.46
1:IO:109:LEU:HD13	1:IO:113:LEU:HD23	1.98	0.46
1:LN:48:THR:HG22	1:LN:49:LYS:N	2.31	0.46
1:MF:62:HIS:O	1:MF:86:VAL:HA	2.16	0.46
1:AC:93:ASP:OD1	1:AC:94:VAL:N	2.44	0.46
1:CJ:109:LEU:HD23	1:CJ:113:LEU:HD23	1.98	0.46
1:DU:82:GLN:OE1	1:LO:88:ARG:NH1	2.49	0.46
1:EK:109:LEU:HA	1:EK:113:LEU:HD23	1.97	0.46
1:EM:89:HIS:CE1	1:FQ:118:ILE:HD12	2.51	0.46
1:FI:20:LEU:HB3	1:FI:32:TYR:HB3	1.98	0.46
1:GC:86:VAL:O	1:GC:87:ILE:HD13	2.16	0.46
1:GH:112:ALA:O	1:GH:116:LYS:HG2	2.16	0.46
1:GO:20:LEU:HD13	1:GO:34:LEU:HB2	1.98	0.46
1:GS:60:GLU:N	1:GS:89:HIS:O	2.48	0.46
1:HI:24:ASN:ND2	1:HK:26:ASP:O	2.47	0.46
1:IN:20:LEU:HB3	1:IN:32:TYR:HB3	1.97	0.46
1:JY:68:GLU:O	1:JY:81:ARG:N	2.41	0.46
1:KD:63:ASN:OD1	1:KD:64:VAL:N	2.49	0.46
1:LA:4:ASP:OD1	1:LA:5:THR:HG23	2.16	0.46
1:LZ:31:GLU:HA	1:LZ:43:ALA:O	2.15	0.46
1:ME:117:LEU:HD23	1:ME:117:LEU:C	2.37	0.46
1:MF:20:LEU:HB3	1:MF:32:TYR:HB3	1.97	0.46
1:NM:53:LYS:HB3	1:NM:54:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:19:VAL:O	1:AB:19:VAL:HG23	2.16	0.46
1:AU:104:ALA:HB2	1:HK:10:LEU:HA	1.98	0.46
1:BG:60:GLU:OE1	1:BG:89:HIS:NE2	2.48	0.46
1:BQ:62:HIS:O	1:BQ:86:VAL:HA	2.16	0.46
1:EF:20:LEU:HG	1:EF:32:TYR:HB3	1.97	0.46
1:FC:27:GLY:O	1:FC:29:THR:HG23	2.16	0.46
1:FE:59:TYR:HA	1:FE:90:LYS:HA	1.98	0.46
1:FK:57:VAL:HG13	1:FK:90:LYS:HE3	1.97	0.46
1:GC:67:THR:HA	1:GC:81:ARG:O	2.16	0.46
1:GY:19:VAL:O	1:GY:34:LEU:HD12	2.16	0.46
1:JR:28:TYR:CD1	1:JS:23:ILE:HG22	2.50	0.46
1:LH:63:ASN:OD1	1:LH:64:VAL:N	2.49	0.46
1:LU:109:LEU:HD22	1:LU:113:LEU:HD22	1.97	0.46
1:MX:86:VAL:HB	1:NA:84:TYR:CZ	2.50	0.46
1:NH:69:THR:CB	1:NH:80:VAL:HG12	2.46	0.46
1:AH:36:GLU:OE1	1:AH:36:GLU:HA	2.16	0.46
1:AO:7:THR:HG23	1:AO:7:THR:O	2.16	0.46
1:AZ:60:GLU:OE2	1:BE:120:TRP:NE1	2.49	0.46
1:BL:120:TRP:HZ2	1:BQ:60:GLU:OE1	1.99	0.46
1:BM:62:HIS:O	1:BM:86:VAL:HA	2.16	0.46
1:CV:20:LEU:HB3	1:CV:32:TYR:HB3	1.97	0.46
1:DH:81:ARG:CZ	1:DM:97:THR:HG21	2.46	0.46
1:FC:44:LYS:HG2	1:FC:65:GLU:OE2	2.15	0.46
1:FP:19:VAL:HG23	1:FP:19:VAL:O	2.15	0.46
1:GY:63:ASN:OD1	1:GY:64:VAL:N	2.49	0.46
1:IM:65:GLU:OE1	1:IM:84:TYR:HB3	2.16	0.46
1:JG:63:ASN:OD1	1:JG:64:VAL:N	2.48	0.46
1:KI:24:ASN:OD1	1:KI:25:GLN:N	2.47	0.46
1:LN:63:ASN:OD1	1:LN:64:VAL:N	2.49	0.46
1:NA:29:THR:HG22	1:NA:30:SER:N	2.30	0.46
1:NB:49:LYS:NZ	1:NG:120:TRP:CH2	2.84	0.46
1:NN:32:TYR:HB2	1:NN:43:ALA:HB3	1.98	0.46
1:CD:108:TYR:CZ	1:CD:113:LEU:CD1	3.00	0.45
1:CE:23:ILE:HG13	1:CE:31:GLU:OE2	2.16	0.45
1:DO:120:TRP:NE1	1:GC:60:GLU:OE2	2.46	0.45
1:DS:57:VAL:HG23	1:DS:59:TYR:HE2	1.81	0.45
1:DU:113:LEU:O	1:DU:117:LEU:HD23	2.16	0.45
1:EY:25:GLN:HG3	1:EY:25:GLN:O	2.16	0.45
1:IM:34:LEU:HD21	1:IM:36:GLU:OE2	2.16	0.45
1:IZ:108:TYR:CE1	1:IZ:113:LEU:HD12	2.51	0.45
1:JA:27:GLY:O	1:JA:29:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KQ:23:ILE:HG13	1:KQ:31:GLU:OE2	2.16	0.45
1:LI:93:ASP:OD1	1:LI:94:VAL:N	2.43	0.45
1:ML:57:VAL:HG11	1:ML:90:LYS:HD2	1.97	0.45
1:NB:109:LEU:HD11	1:NG:85:VAL:HG11	1.98	0.45
1:AT:28:TYR:CZ	1:AU:24:ASN:ND2	2.84	0.45
1:AT:60:GLU:CD	1:AT:91:VAL:HG22	2.37	0.45
1:AZ:60:GLU:O	1:AZ:88:ARG:HA	2.16	0.45
1:CC:47:HIS:CD2	1:DB:120:TRP:O	2.69	0.45
1:DA:45:VAL:HG22	1:DA:64:VAL:HG22	1.99	0.45
1:DB:20:LEU:HB3	1:DB:32:TYR:HB3	1.98	0.45
1:FD:81:ARG:CZ	1:FI:97:THR:HG21	2.46	0.45
1:FJ:62:HIS:O	1:FJ:86:VAL:HA	2.16	0.45
1:FJ:93:ASP:OD1	1:FJ:94:VAL:N	2.46	0.45
1:HI:60:GLU:O	1:HI:88:ARG:HA	2.16	0.45
1:IM:40:SER:OG	1:IM:69:THR:OG1	2.34	0.45
1:IO:50:GLU:OE1	1:IO:50:GLU:N	2.48	0.45
1:JE:53:LYS:HB3	1:JE:54:PRO:HD2	1.99	0.45
1:LI:53:LYS:HG2	1:LI:56:GLN:NE2	2.31	0.45
1:LU:6:LEU:HD23	1:LU:6:LEU:C	2.37	0.45
1:NA:32:TYR:HB2	1:NA:43:ALA:HB3	1.97	0.45
1:NA:115:GLY:O	1:NA:118:ILE:HG22	2.16	0.45
1:NC:36:GLU:HB2	1:NC:39:SER:O	2.17	0.45
1:NC:54:PRO:C	1:NC:55:ASN:OD1	2.55	0.45
1:AM:31:GLU:HA	1:AM:43:ALA:O	2.16	0.45
1:BK:99:SER:OG	1:BK:103:GLU:OE2	2.27	0.45
1:BL:61:ARG:O	1:BL:62:HIS:ND1	2.50	0.45
1:CC:122:SER:C	1:DB:30:SER:HG	2.15	0.45
1:CE:108:TYR:CZ	1:DI:6:LEU:HD11	2.52	0.45
1:EQ:19:VAL:O	1:EQ:19:VAL:HG23	2.16	0.45
1:GA:45:VAL:HG22	1:GA:64:VAL:HG23	1.97	0.45
1:GC:68:GLU:O	1:GC:80:VAL:HA	2.16	0.45
1:GM:66:PHE:O	1:GM:82:GLN:HB2	2.16	0.45
1:HI:27:GLY:O	1:HI:29:THR:HG23	2.16	0.45
1:HQ:34:LEU:HD12	1:HQ:35:PRO:HD2	1.99	0.45
1:JA:86:VAL:HG21	1:KE:84:TYR:CZ	2.51	0.45
1:KJ:120:TRP:HB3	1:KP:23:ILE:CD1	2.46	0.45
1:ML:63:ASN:OD1	1:ML:64:VAL:N	2.50	0.45
1:NI:93:ASP:OD1	1:NI:94:VAL:N	2.43	0.45
1:AS:116:LYS:HD2	1:AS:121:GLU:OE2	2.16	0.45
1:AY:113:LEU:O	1:AY:117:LEU:HD13	2.16	0.45
1:CJ:68:GLU:N	1:CJ:81:ARG:O	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DS:54:PRO:O	1:DS:55:ASN:OD1	2.34	0.45
1:EX:60:GLU:CG	1:EX:91:VAL:HG22	2.45	0.45
1:EX:86:VAL:HG21	1:FC:84:TYR:CZ	2.51	0.45
1:FO:36:GLU:OE1	1:FO:36:GLU:HA	2.17	0.45
1:FQ:36:GLU:OE2	1:FQ:39:SER:N	2.50	0.45
1:GC:20:LEU:HB3	1:GC:32:TYR:HB3	1.98	0.45
1:HC:65:GLU:CB	1:HC:84:TYR:HB3	2.47	0.45
1:JG:41:PHE:CE2	1:JG:68:GLU:OE1	2.70	0.45
1:JX:53:LYS:HG2	1:JX:54:PRO:HD2	1.99	0.45
1:KI:20:LEU:HB3	1:KI:32:TYR:HB3	1.98	0.45
1:KO:95:SER:O	1:KO:98:VAL:HG12	2.17	0.45
1:MR:50:GLU:O	1:MR:58:GLN:NE2	2.49	0.45
1:NB:27:GLY:O	1:NB:29:THR:HG23	2.17	0.45
1:NI:108:TYR:O	1:NI:113:LEU:HD21	2.16	0.45
1:NO:105:LEU:O	1:NO:109:LEU:HD23	2.16	0.45
2:M:11:ALA:HB3	2:M:32:VAL:CG1	2.46	0.45
1:AA:62:HIS:O	1:AA:86:VAL:HA	2.16	0.45
1:BK:20:LEU:HB3	1:BK:32:TYR:HB3	1.98	0.45
1:BY:31:GLU:HA	1:BY:43:ALA:O	2.17	0.45
1:DY:4:ASP:OD1	1:DY:5:THR:HG23	2.16	0.45
1:FW:84:TYR:CE1	1:LU:86:VAL:HB	2.52	0.45
1:IH:109:LEU:HD11	1:IM:85:VAL:HG11	1.98	0.45
1:JQ:99:SER:O	1:JQ:103:GLU:HG3	2.15	0.45
1:JX:32:TYR:N	1:JX:43:ALA:O	2.46	0.45
1:KJ:36:GLU:HB2	1:KJ:39:SER:O	2.17	0.45
1:LM:112:ALA:O	1:LM:116:LYS:HG2	2.16	0.45
1:LZ:100:ASP:OD2	1:ME:10:LEU:HB3	2.15	0.45
1:MK:40:SER:HG	1:MK:69:THR:HG1	1.64	0.45
1:MR:55:ASN:OD1	1:MR:56:GLN:NE2	2.50	0.45
1:AB:65:GLU:OE2	1:AB:67:THR:OG1	2.27	0.45
1:BM:52:VAL:HG13	1:BM:58:GLN:NE2	2.32	0.45
1:CD:23:ILE:HG23	1:DB:120:TRP:O	2.16	0.45
1:CJ:68:GLU:O	1:CJ:80:VAL:HA	2.16	0.45
1:CJ:93:ASP:OD1	1:CJ:94:VAL:N	2.45	0.45
1:CW:63:ASN:OD1	1:CW:64:VAL:N	2.50	0.45
1:DY:63:ASN:OD1	1:DY:64:VAL:N	2.49	0.45
1:EM:36:GLU:OE1	1:EM:39:SER:N	2.48	0.45
1:EQ:53:LYS:HB3	1:EQ:54:PRO:HD2	1.99	0.45
1:FK:81:ARG:NH2	1:MA:97:THR:HG21	2.32	0.45
1:FP:84:TYR:CZ	1:FU:86:VAL:HB	2.51	0.45
1:GO:24:ASN:HB3	1:GO:31:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IS:36:GLU:OE1	1:IS:36:GLU:HA	2.17	0.45
1:IZ:65:GLU:HG2	1:IZ:84:TYR:HB2	1.99	0.45
1:JR:87:ILE:HD11	1:JW:114:TYR:HE1	1.81	0.45
1:MG:25:GLN:O	1:MG:25:GLN:HG3	2.17	0.45
1:MS:54:PRO:C	1:MS:55:ASN:OD1	2.55	0.45
1:AA:2:LEU:HD12	1:NN:122:SER:O	2.17	0.45
1:AN:24:ASN:OD1	1:AN:25:GLN:N	2.49	0.45
1:BR:118:ILE:HD11	1:BW:89:HIS:CE1	2.52	0.45
1:CK:116:LYS:NZ	1:CK:121:GLU:OE1	2.45	0.45
1:EQ:116:LYS:HD2	1:EQ:121:GLU:OE1	2.16	0.45
1:GG:65:GLU:OE1	1:GG:84:TYR:HB3	2.17	0.45
1:GH:47:HIS:HE1	1:GM:117:LEU:HD12	1.82	0.45
1:GN:47:HIS:O	1:GN:48:THR:HG23	2.17	0.45
1:HU:59:TYR:CZ	1:IT:80:VAL:HG22	2.52	0.45
1:IN:114:TYR:CE2	1:IS:87:ILE:HD11	2.51	0.45
1:IZ:31:GLU:HA	1:IZ:43:ALA:O	2.16	0.45
1:IZ:36:GLU:OE2	1:IZ:39:SER:N	2.49	0.45
1:LS:61:ARG:HA	1:LS:87:ILE:O	2.17	0.45
1:LT:113:LEU:HD23	1:LT:117:LEU:HD13	1.99	0.45
1:LU:6:LEU:HD23	1:LU:7:THR:N	2.31	0.45
1:MW:8:ILE:HD12	1:MW:66:PHE:CE2	2.51	0.45
1:NB:116:LYS:O	1:NB:121:GLU:OE1	2.35	0.45
1:NC:119:GLY:O	1:NC:120:TRP:HB2	2.17	0.45
1:AN:112:ALA:O	1:AN:116:LYS:HG3	2.17	0.45
1:AT:58:GLN:O	1:AT:91:VAL:HG23	2.17	0.45
1:AT:61:ARG:HA	1:AT:87:ILE:O	2.17	0.45
1:BF:87:ILE:HD12	1:BK:82:GLN:O	2.16	0.45
1:BY:1:ALA:N	1:FE:122:SER:OXT	2.47	0.45
1:DY:56:GLN:OE1	1:DY:56:GLN:N	2.49	0.45
1:FE:63:ASN:OD1	1:FE:64:VAL:N	2.50	0.45
1:GC:54:PRO:C	1:GC:55:ASN:OD1	2.55	0.45
1:GM:20:LEU:HB3	1:GM:32:TYR:HB3	1.99	0.45
1:JR:105:LEU:HD21	1:JR:109:LEU:HD11	1.98	0.45
1:KQ:54:PRO:O	1:KQ:55:ASN:OD1	2.35	0.45
1:ML:52:VAL:HG22	1:ML:58:GLN:NE2	2.32	0.45
1:NB:86:VAL:HG21	1:NG:84:TYR:CZ	2.52	0.45
1:NM:34:LEU:HD23	1:NM:35:PRO:O	2.17	0.45
1:BL:26:ASP:HA	1:BM:26:ASP:OD1	2.17	0.45
1:BR:81:ARG:NH2	1:BW:97:THR:HG21	2.32	0.45
1:DU:19:VAL:O	1:DU:34:LEU:HD12	2.16	0.45
1:ES:25:GLN:HG3	1:ES:25:GLN:O	2.17	0.45

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:EX:84:TYR:CE1	1:FC:86:VAL:CG1	3.00	0.45
1:FD:100:ASP:OD1	1:FI:11:GLY:HA2	2.16	0.45
1:GZ:55:ASN:OD1	2:M:271:SER:OG	2.35	0.45
1:GZ:90:LYS:HE3	1:HC:79:PHE:CD2	2.52	0.45
1:HE:50:GLU:OE2	1:HE:59:TYR:N	2.40	0.45
1:HI:31:GLU:HA	1:HI:43:ALA:O	2.16	0.45
1:HQ:48:THR:HG22	1:HQ:49:LYS:N	2.32	0.45
1:JG:4:ASP:OD1	1:JG:5:THR:N	2.49	0.45
1:KE:24:ASN:HB3	1:KE:31:GLU:OE2	2.16	0.45
1:KK:115:GLY:O	1:KK:118:ILE:HG22	2.17	0.45
1:LZ:109:LEU:HD13	1:LZ:114:TYR:OH	2.16	0.45
1:MK:97:THR:HG21	1:NH:81:ARG:NH2	2.32	0.45
1:MR:98:VAL:HG12	1:MW:81:ARG:HD3	1.98	0.45
1:AI:30:SER:O	1:AI:44:LYS:HB2	2.17	0.45
1:AM:39:SER:OG	1:AM:40:SER:N	2.50	0.45
1:BK:112:ALA:O	1:BK:116:LYS:HG2	2.17	0.45
1:BR:86:VAL:O	1:BR:87:ILE:HD13	2.17	0.45
1:CO:54:PRO:O	1:CO:55:ASN:OD1	2.35	0.45
1:EA:117:LEU:HD21	1:NI:62:HIS:HB3	1.98	0.45
1:EF:20:LEU:HG	1:EF:32:TYR:CB	2.47	0.45
1:GO:114:TYR:HE1	1:JS:87:ILE:HD11	1.81	0.45
1:HC:109:LEU:HD23	1:HC:113:LEU:HD23	1.99	0.45
1:HD:62:HIS:O	1:HD:86:VAL:HA	2.17	0.45
1:JA:23:ILE:HD11	1:JE:120:TRP:O	2.17	0.45
1:JF:117:LEU:HD21	1:JK:62:HIS:HB3	1.99	0.45
1:JL:20:LEU:HB3	1:JL:32:TYR:HB3	1.98	0.45
1:KD:68:GLU:OE1	1:KD:68:GLU:HA	2.16	0.45
1:LA:19:VAL:O	1:LA:34:LEU:HD12	2.17	0.45
1:LT:61:ARG:HA	1:LT:87:ILE:O	2.17	0.45
1:LU:113:LEU:HD23	1:LU:113:LEU:C	2.37	0.45
1:AO:24:ASN:OD1	1:AO:25:GLN:N	2.51	0.44
1:BE:63:ASN:OD1	1:BE:64:VAL:N	2.50	0.44
1:BR:8:ILE:HD13	1:BR:66:PHE:CE2	2.52	0.44
1:CO:113:LEU:O	1:CO:117:LEU:HD12	2.17	0.44
1:EA:57:VAL:HG23	1:EA:59:TYR:HE1	1.81	0.44
1:EM:87:ILE:HD11	1:FQ:114:TYR:CE2	2.52	0.44
1:EW:69:THR:OG1	1:EW:78:GLU:OE2	2.34	0.44
1:FW:11:GLY:HA2	1:LU:100:ASP:OD1	2.17	0.44
1:GH:54:PRO:O	1:GH:55:ASN:OD1	2.35	0.44
1:GT:53:LYS:HB2	1:GT:54:PRO:HD2	1.98	0.44
1:HC:34:LEU:HD23	1:HC:35:PRO:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HK:68:GLU:OE2	1:HK:81:ARG:NH1	2.47	0.44
1:HQ:89:HIS:NE2	1:KW:118:ILE:HD11	2.31	0.44
1:HQ:112:ALA:O	1:HQ:116:LYS:HG2	2.17	0.44
1:JF:1:ALA:N	1:JK:122:SER:OXT	2.50	0.44
1:LB:16:THR:O	1:LB:16:THR:HG22	2.17	0.44
1:LY:109:LEU:HD13	1:LY:114:TYR:OH	2.16	0.44
1:CE:25:GLN:HG3	1:CE:25:GLN:O	2.17	0.44
1:CQ:54:PRO:C	1:CQ:55:ASN:OD1	2.55	0.44
1:EF:68:GLU:O	1:EF:81:ARG:N	2.45	0.44
1:EK:97:THR:HG21	1:FJ:81:ARG:NH2	2.32	0.44
1:EM:113:LEU:HD23	1:EM:113:LEU:C	2.37	0.44
1:EQ:81:ARG:HG3	1:EQ:81:ARG:O	2.17	0.44
1:FJ:113:LEU:C	1:FJ:113:LEU:HD23	2.37	0.44
1:IN:24:ASN:OD1	1:IN:25:GLN:N	2.50	0.44
1:IS:63:ASN:OD1	1:IS:64:VAL:N	2.49	0.44
1:IS:68:GLU:N	1:IS:81:ARG:O	2.49	0.44
1:JA:48:THR:HG22	1:JA:49:LYS:N	2.32	0.44
1:KD:105:LEU:O	1:KD:109:LEU:HD23	2.17	0.44
1:KK:99:SER:O	1:KK:103:GLU:HG3	2.17	0.44
1:KV:20:LEU:HD13	1:KV:32:TYR:HB2	1.99	0.44
1:LH:108:TYR:CE2	1:LH:113:LEU:HD11	2.51	0.44
1:NH:20:LEU:HD23	1:NH:34:LEU:HB3	1.98	0.44
1:AC:25:GLN:HB2	1:AC:29:THR:O	2.18	0.44
1:AI:8:ILE:HD12	1:AI:20:LEU:HD11	1.99	0.44
1:AS:23:ILE:HB	1:AS:31:GLU:OE2	2.18	0.44
1:AT:65:GLU:CB	1:AT:84:TYR:HB3	2.47	0.44
1:BS:53:LYS:HB2	1:BS:54:PRO:HD2	1.98	0.44
1:CD:112:ALA:O	1:CD:116:LYS:HG2	2.18	0.44
1:CE:36:GLU:OE2	1:CE:39:SER:N	2.50	0.44
1:EG:55:ASN:O	1:EG:56:GLN:HG3	2.18	0.44
1:EM:27:GLY:O	1:EM:29:THR:HG23	2.18	0.44
1:GG:20:LEU:HB3	1:GG:32:TYR:HB3	2.00	0.44
1:GO:110:ASN:OD1	1:GO:113:LEU:HD23	2.16	0.44
1:GZ:115:GLY:O	1:GZ:118:ILE:HG22	2.17	0.44
1:KO:49:LYS:HE3	1:KO:60:GLU:HB2	1.99	0.44
1:LG:10:LEU:HA	1:MF:104:ALA:HB2	1.99	0.44
1:NH:68:GLU:O	1:NH:81:ARG:N	2.38	0.44
1:AC:4:ASP:OD1	1:AC:4:ASP:O	2.35	0.44
1:AO:6:LEU:HD11	1:LC:108:TYR:OH	2.17	0.44
1:BS:99:SER:O	1:BS:103:GLU:HG3	2.17	0.44
1:BX:60:GLU:OE1	1:BX:91:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CK:67:THR:OG1	1:CK:82:GLN:NE2	2.44	0.44
1:DT:52:VAL:O	1:DT:52:VAL:HG13	2.18	0.44
1:GO:52:VAL:HG22	1:GO:58:GLN:OE1	2.17	0.44
1:GT:116:LYS:NZ	1:GT:121:GLU:OE1	2.48	0.44
1:GU:37:THR:HG23	1:GU:38:SER:N	2.32	0.44
1:HO:109:LEU:HD13	1:HO:114:TYR:OH	2.18	0.44
1:IM:109:LEU:HD13	1:IM:113:LEU:HD22	2.00	0.44
1:IT:66:PHE:O	1:IT:82:GLN:HG3	2.17	0.44
1:LN:68:GLU:O	1:LN:81:ARG:N	2.41	0.44
1:MA:23:ILE:CG2	1:MA:31:GLU:HB2	2.47	0.44
1:ME:86:VAL:O	1:ME:87:ILE:HD13	2.17	0.44
1:MM:65:GLU:OE2	1:MM:67:THR:HB	2.17	0.44
1:MQ:36:GLU:OE2	1:MQ:39:SER:N	2.50	0.44
1:MQ:62:HIS:O	1:MQ:86:VAL:HA	2.18	0.44
1:AB:99:SER:O	1:AB:103:GLU:HG3	2.18	0.44
1:AC:65:GLU:HG2	1:AC:84:TYR:HB3	2.00	0.44
1:BL:4:ASP:OD1	1:BL:5:THR:N	2.51	0.44
1:CQ:54:PRO:O	1:CQ:55:ASN:OD1	2.36	0.44
1:CW:55:ASN:O	1:CW:56:GLN:HG3	2.18	0.44
1:DB:98:VAL:O	1:DB:101:LEU:O	2.36	0.44
1:DN:6:LEU:HD23	1:DN:32:TYR:CE2	2.52	0.44
1:DY:89:HIS:ND1	1:DY:90:LYS:O	2.46	0.44
1:EW:117:LEU:C	1:EW:117:LEU:HD23	2.38	0.44
1:FI:46:ARG:O	1:FI:47:HIS:ND1	2.48	0.44
1:FI:60:GLU:OE1	1:FI:60:GLU:N	2.50	0.44
1:FP:51:SER:OG	1:FP:53:LYS:NZ	2.41	0.44
1:FP:63:ASN:OD1	1:FP:64:VAL:N	2.50	0.44
1:FU:55:ASN:OD1	1:FU:55:ASN:O	2.36	0.44
1:GG:62:HIS:O	1:GG:86:VAL:HA	2.17	0.44
1:GH:47:HIS:CE1	1:GM:117:LEU:HD12	2.53	0.44
1:GZ:10:LEU:HA	1:HC:104:ALA:HB2	2.00	0.44
1:HP:58:GLN:HB2	1:HP:91:VAL:HG11	2.00	0.44
1:JA:112:ALA:O	1:JA:116:LYS:HG2	2.17	0.44
1:JE:63:ASN:OD1	1:JE:64:VAL:N	2.50	0.44
1:JL:108:TYR:OH	1:JL:113:LEU:HD11	2.18	0.44
1:LG:44:LYS:NZ	1:LG:46:ARG:HE	2.16	0.44
1:ME:60:GLU:OE1	1:ME:60:GLU:HA	2.17	0.44
1:NB:109:LEU:HD23	1:NB:113:LEU:HD23	1.98	0.44
2:M:174:ASP:HA	2:M:240:ILE:HD11	1.98	0.44
1:AH:108:TYR:CE2	1:AH:113:LEU:HD21	2.53	0.44
1:AY:40:SER:OG	1:AY:69:THR:OG1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BM:93:ASP:OD1	1:BM:94:VAL:N	2.48	0.44
1:CU:89:HIS:ND1	1:CU:90:LYS:O	2.51	0.44
1:DN:44:LYS:HG3	1:DN:46:ARG:HH11	1.82	0.44
1:DS:108:TYR:CE1	1:DS:113:LEU:HD21	2.53	0.44
1:EF:68:GLU:O	1:EF:80:VAL:HA	2.18	0.44
1:EK:82:GLN:OE1	1:FJ:88:ARG:NH2	2.50	0.44
1:FI:26:ASP:O	1:FI:29:THR:OG1	2.21	0.44
1:FK:122:SER:O	1:MA:25:GLN:NE2	2.50	0.44
1:FQ:27:GLY:O	1:FQ:29:THR:HG23	2.17	0.44
1:GO:84:TYR:CE1	1:JS:86:VAL:HB	2.53	0.44
1:HO:23:ILE:HG23	1:HO:24:ASN:N	2.32	0.44
1:II:25:GLN:HB2	1:II:29:THR:O	2.18	0.44
1:IN:93:ASP:OD1	1:IN:94:VAL:N	2.45	0.44
1:KE:55:ASN:OD1	1:KE:56:GLN:N	2.50	0.44
1:LU:108:TYR:CE2	1:LU:113:LEU:HD11	2.53	0.44
1:MF:19:VAL:HG13	1:MF:19:VAL:O	2.17	0.44
1:NC:25:GLN:HA	1:NC:29:THR:O	2.17	0.44
1:AM:63:ASN:OD1	1:AM:64:VAL:N	2.50	0.44
1:AS:31:GLU:HB3	1:AS:44:LYS:HG2	2.00	0.44
1:AT:53:LYS:HG2	1:AT:54:PRO:HD2	2.00	0.44
1:AZ:89:HIS:ND1	1:AZ:90:LYS:O	2.49	0.44
1:BG:100:ASP:OD1	1:HE:11:GLY:CA	2.66	0.44
1:DY:4:ASP:OD1	1:DY:5:THR:N	2.50	0.44
1:EF:36:GLU:N	1:EF:39:SER:O	2.42	0.44
1:EL:2:LEU:HD23	1:EQ:122:SER:C	2.37	0.44
1:FD:45:VAL:HG22	1:FD:64:VAL:HG12	1.98	0.44
1:FE:31:GLU:HA	1:FE:43:ALA:O	2.18	0.44
1:FI:53:LYS:HD2	1:FI:54:PRO:HD3	1.99	0.44
1:FI:108:TYR:CZ	1:FI:113:LEU:HD21	2.52	0.44
1:FK:1:ALA:H3	1:MA:121:GLU:CD	2.19	0.44
1:FK:112:ALA:O	1:FK:116:LYS:HG3	2.18	0.44
1:GU:63:ASN:OD1	1:GU:64:VAL:N	2.51	0.44
1:HQ:54:PRO:O	1:HQ:55:ASN:OD1	2.36	0.44
1:HW:109:LEU:HD13	1:HW:113:LEU:HD23	1.98	0.44
1:IT:47:HIS:O	1:IT:48:THR:OG1	2.31	0.44
1:JA:97:THR:HG21	1:KE:81:ARG:NH2	2.33	0.44
1:JS:20:LEU:C	1:JS:21:ARG:HD2	2.38	0.44
1:KE:52:VAL:HG22	1:KE:58:GLN:HE22	1.83	0.44
1:KE:113:LEU:HD23	1:KE:113:LEU:C	2.39	0.44
1:LH:113:LEU:HD23	1:LH:113:LEU:C	2.38	0.44
1:LM:60:GLU:OE2	1:LM:91:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LS:24:ASN:OD1	1:LS:25:GLN:N	2.48	0.44
1:MG:27:GLY:O	1:MG:29:THR:HG23	2.18	0.44
1:NI:27:GLY:O	1:NI:29:THR:HG23	2.17	0.44
1:AT:109:LEU:HD12	1:AT:114:TYR:CE1	2.53	0.44
1:BK:23:ILE:HD12	1:MS:120:TRP:CB	2.47	0.44
1:BS:20:LEU:HB3	1:BS:32:TYR:HB3	1.99	0.44
1:CE:109:LEU:HD13	1:CE:113:LEU:HD23	1.99	0.44
1:CV:30:SER:OG	1:DA:122:SER:O	2.21	0.44
1:EA:89:HIS:CD2	1:EA:98:VAL:HG11	2.53	0.44
1:FE:25:GLN:HB2	1:FE:29:THR:O	2.18	0.44
1:FQ:36:GLU:HG3	1:FQ:39:SER:O	2.18	0.44
1:GA:19:VAL:O	1:GA:19:VAL:HG23	2.18	0.44
1:GC:112:ALA:O	1:GC:116:LYS:HG2	2.17	0.44
1:HP:44:LYS:HG2	1:HP:65:GLU:OE2	2.18	0.44
1:IT:48:THR:HG21	1:IT:61:ARG:NH2	2.31	0.44
1:JX:93:ASP:OD1	1:JX:94:VAL:N	2.47	0.44
1:KD:4:ASP:OD1	1:KD:4:ASP:N	2.50	0.44
1:NM:63:ASN:OD1	1:NM:64:VAL:N	2.50	0.44
1:NO:36:GLU:HB2	1:NO:39:SER:O	2.17	0.44
1:AS:55:ASN:O	1:AS:56:GLN:OE1	2.36	0.44
1:BG:65:GLU:CB	1:BG:84:TYR:HB3	2.48	0.44
1:BQ:20:LEU:HB2	1:BQ:32:TYR:HB3	1.99	0.44
1:BX:54:PRO:O	1:BX:55:ASN:OD1	2.35	0.44
1:CI:63:ASN:OD1	1:CI:64:VAL:N	2.51	0.44
1:DH:57:VAL:HG23	1:DH:59:TYR:CE2	2.52	0.44
1:DO:81:ARG:NH1	1:GC:93:ASP:OD2	2.50	0.44
1:EG:62:HIS:O	1:EG:87:ILE:N	2.43	0.44
1:FO:114:TYR:HE1	1:GN:87:ILE:HD11	1.82	0.44
1:FV:86:VAL:HB	1:GA:84:TYR:CZ	2.52	0.44
1:GM:63:ASN:OD1	1:GM:64:VAL:N	2.51	0.44
1:GT:25:GLN:O	1:GT:26:ASP:OD1	2.36	0.44
1:HJ:118:ILE:HD11	1:HO:89:HIS:NE2	2.33	0.44
1:JK:70:VAL:HG21	1:JK:79:PHE:CZ	2.53	0.44
1:JL:113:LEU:O	1:JL:117:LEU:CD1	2.66	0.44
1:MF:60:GLU:OE2	1:MF:62:HIS:NE2	2.51	0.44
1:ML:48:THR:HG22	1:ML:49:LYS:O	2.18	0.44
1:MR:1:ALA:N	1:MW:122:SER:OXT	2.41	0.44
1:MR:25:GLN:O	1:MR:26:ASP:OD2	2.36	0.44
1:NB:6:LEU:HB2	1:NB:32:TYR:CE2	2.53	0.44
1:NO:25:GLN:HG3	1:NO:25:GLN:O	2.18	0.44
1:AS:63:ASN:OD1	1:AS:64:VAL:N	2.51	0.43

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:AU:45:VAL:HG22	1:AU:64:VAL:HG22	2.00	0.43
1:AY:19:VAL:O	1:AY:19:VAL:HG13	2.18	0.43
1:BY:81:ARG:NH2	1:FE:97:THR:HG21	2.33	0.43
1:CJ:20:LEU:HD13	1:CJ:34:LEU:HB3	2.00	0.43
1:DG:51:SER:OG	1:DG:53:LYS:NZ	2.49	0.43
1:DH:23:ILE:HD11	1:EF:120:TRP:C	2.38	0.43
1:DI:20:LEU:HB3	1:DI:32:TYR:HB3	1.99	0.43
1:EG:62:HIS:N	1:EG:87:ILE:O	2.39	0.43
1:EL:54:PRO:O	1:EL:55:ASN:OD1	2.36	0.43
1:FJ:59:TYR:HA	1:FJ:90:LYS:HA	1.99	0.43
1:GM:68:GLU:N	1:GM:81:ARG:O	2.51	0.43
1:IO:23:ILE:HD11	1:IS:120:TRP:O	2.18	0.43
1:JA:27:GLY:O	1:JA:28:TYR:HB2	2.18	0.43
1:JG:108:TYR:O	1:JG:110:ASN:N	2.50	0.43
1:JS:116:LYS:HD2	1:JS:121:GLU:OE2	2.18	0.43
1:LB:70:VAL:HG11	1:LB:79:PHE:CZ	2.53	0.43
1:LZ:97:THR:HG22	1:ME:81:ARG:HH12	1.83	0.43
1:MM:93:ASP:OD1	1:MM:94:VAL:N	2.46	0.43
1:NH:20:LEU:HD21	1:NH:41:PHE:CB	2.46	0.43
2:M:11:ALA:HB2	2:M:34:ASN:CG	2.37	0.43
1:AA:2:LEU:HD12	1:NN:122:SER:C	2.38	0.43
1:AA:59:TYR:OH	1:NN:80:VAL:HG22	2.18	0.43
1:AA:67:THR:HG23	1:AA:80:VAL:CG2	2.48	0.43
1:AA:122:SER:OXT	1:NN:1:ALA:N	2.50	0.43
1:BE:109:LEU:HG	1:BE:114:TYR:CZ	2.53	0.43
1:BR:54:PRO:O	1:BR:55:ASN:OD1	2.36	0.43
1:BR:60:GLU:OE2	1:BR:62:HIS:NE2	2.51	0.43
1:BW:7:THR:O	1:BW:7:THR:HG23	2.17	0.43
1:BY:25:GLN:HG3	1:BY:25:GLN:O	2.18	0.43
1:CO:113:LEU:HD23	1:CO:117:LEU:CD1	2.49	0.43
1:CP:54:PRO:O	1:CP:55:ASN:OD1	2.36	0.43
1:DA:64:VAL:O	1:DA:84:TYR:HB2	2.19	0.43
1:DN:21:ARG:NH1	1:DN:21:ARG:HB2	2.32	0.43
1:EE:24:ASN:HB3	1:EE:31:GLU:OE2	2.18	0.43
1:EE:61:ARG:HG3	1:EE:88:ARG:HB3	1.99	0.43
1:EQ:29:THR:HG23	1:EQ:45:VAL:O	2.18	0.43
1:ES:19:VAL:HG23	1:ES:19:VAL:O	2.18	0.43
1:FK:25:GLN:HG3	1:FK:25:GLN:O	2.18	0.43
1:FU:65:GLU:CB	1:FU:84:TYR:HB3	2.47	0.43
1:FV:36:GLU:HB2	1:FV:39:SER:O	2.18	0.43
1:GA:57:VAL:HG23	1:GA:59:TYR:CE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:109:LEU:HA	1:GB:113:LEU:HD23	2.00	0.43
1:GT:4:ASP:OD1	1:GT:4:ASP:N	2.51	0.43
1:HD:108:TYR:CE2	1:HD:113:LEU:HD21	2.53	0.43
1:IZ:87:ILE:HD11	1:JE:114:TYR:CE1	2.53	0.43
1:JG:4:ASP:OD1	1:JG:5:THR:HG23	2.18	0.43
1:JK:63:ASN:OD1	1:JK:64:VAL:N	2.51	0.43
1:JL:84:TYR:CZ	1:JQ:86:VAL:HB	2.53	0.43
1:JS:99:SER:O	1:JS:103:GLU:HG3	2.18	0.43
1:JX:109:LEU:HD23	1:JX:113:LEU:HD23	2.00	0.43
1:KE:20:LEU:CB	1:KE:32:TYR:HB3	2.49	0.43
1:KV:68:GLU:N	1:KV:81:ARG:O	2.48	0.43
1:LC:25:GLN:HG3	1:LC:25:GLN:O	2.18	0.43
1:LT:101:LEU:CD1	1:LY:10:LEU:HD11	2.48	0.43
1:NM:20:LEU:HD13	1:NM:34:LEU:HB2	2.00	0.43
1:NN:4:ASP:OD1	1:NN:4:ASP:C	2.57	0.43
1:AH:85:VAL:CG2	1:AM:105:LEU:HD21	2.48	0.43
1:AN:68:GLU:N	1:AN:81:ARG:O	2.52	0.43
1:CK:20:LEU:HD21	1:CK:41:PHE:HB3	2.00	0.43
1:DB:36:GLU:OE1	1:DB:36:GLU:HA	2.17	0.43
1:DO:60:GLU:OE2	1:GC:120:TRP:NE1	2.51	0.43
1:EG:108:TYR:OH	1:EG:113:LEU:HD11	2.18	0.43
1:HD:112:ALA:O	1:HD:116:LYS:HG3	2.18	0.43
1:IS:119:GLY:O	1:IS:120:TRP:HB2	2.18	0.43
1:IY:31:GLU:HA	1:IY:43:ALA:O	2.17	0.43
1:JY:68:GLU:HB3	1:JY:81:ARG:HB2	2.01	0.43
1:KQ:45:VAL:HG22	1:KQ:64:VAL:HG22	2.00	0.43
1:KV:24:ASN:HB3	1:KV:31:GLU:OE1	2.18	0.43
1:LN:112:ALA:O	1:LN:116:LYS:HG2	2.19	0.43
1:LT:81:ARG:NH2	1:LY:97:THR:HG21	2.33	0.43
1:ME:90:LYS:HG2	1:ME:93:ASP:HB2	1.99	0.43
1:MS:34:LEU:HD21	1:MS:36:GLU:OE2	2.18	0.43
1:NC:54:PRO:O	1:NC:55:ASN:OD1	2.35	0.43
1:NN:29:THR:HG22	1:NN:46:ARG:HG3	2.00	0.43
1:AC:113:LEU:HD23	1:AC:113:LEU:C	2.39	0.43
1:AT:62:HIS:O	1:AT:86:VAL:HA	2.17	0.43
1:BE:20:LEU:HB3	1:BE:32:TYR:HB3	2.01	0.43
1:BE:29:THR:HG22	1:BE:46:ARG:HG2	2.00	0.43
1:BX:63:ASN:OD1	1:BX:64:VAL:N	2.50	0.43
1:DI:57:VAL:HB	1:DI:59:TYR:HE1	1.84	0.43
1:ES:20:LEU:HB3	1:ES:32:TYR:HB3	1.99	0.43
1:GU:2:LEU:HD22	1:HW:121:GLU:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HD:69:THR:HG22	1:HD:80:VAL:CG1	2.44	0.43
1:HJ:109:LEU:HD13	1:HJ:113:LEU:HD23	1.99	0.43
1:HK:25:GLN:HG3	1:HK:25:GLN:O	2.18	0.43
1:IO:112:ALA:O	1:IO:116:LYS:HG2	2.18	0.43
1:JQ:69:THR:HA	1:JQ:80:VAL:HG12	2.00	0.43
1:JS:54:PRO:C	1:JS:55:ASN:OD1	2.56	0.43
1:KJ:49:LYS:HA	1:KJ:49:LYS:HD3	1.79	0.43
1:KV:120:TRP:C	1:LB:23:ILE:HD11	2.38	0.43
1:NA:24:ASN:ND2	1:NA:26:ASP:OD2	2.51	0.43
2:M:153:LYS:HA	2:M:156:ILE:HG12	2.01	0.43
1:AC:111:GLU:OE1	1:EY:99:SER:OG	2.35	0.43
1:AT:105:LEU:O	1:AT:109:LEU:HD23	2.19	0.43
1:AU:63:ASN:OD1	1:AU:64:VAL:N	2.52	0.43
1:BY:85:VAL:HG22	1:BY:86:VAL:N	2.33	0.43
1:CD:34:LEU:HD12	1:CD:35:PRO:HD2	2.00	0.43
1:CE:54:PRO:O	1:CE:55:ASN:OD1	2.37	0.43
1:CK:118:ILE:HD13	1:II:62:HIS:CE1	2.54	0.43
1:DI:100:ASP:HA	1:DI:103:GLU:OE2	2.17	0.43
1:DM:61:ARG:HA	1:DM:87:ILE:O	2.18	0.43
1:DT:20:LEU:HD23	1:DT:34:LEU:HB3	2.00	0.43
1:FP:73:SER:O	1:FP:76:THR:OG1	2.31	0.43
1:GH:117:LEU:HD21	1:GM:62:HIS:CB	2.48	0.43
1:IM:108:TYR:CZ	1:IM:113:LEU:HD11	2.53	0.43
1:IO:47:HIS:O	1:IO:48:THR:HG23	2.18	0.43
1:JS:27:GLY:O	1:JS:29:THR:HG23	2.19	0.43
1:JS:53:LYS:HG2	1:JS:54:PRO:HD2	1.99	0.43
1:KJ:84:TYR:CE1	1:KO:86:VAL:HB	2.53	0.43
1:KK:116:LYS:O	1:KK:121:GLU:OE1	2.36	0.43
1:KU:112:ALA:O	1:KU:116:LYS:HG2	2.19	0.43
1:KV:6:LEU:HD22	1:KV:20:LEU:HD12	2.00	0.43
1:LU:99:SER:O	1:LU:103:GLU:HG3	2.19	0.43
1:MG:110:ASN:OD1	1:MG:113:LEU:HD23	2.18	0.43
1:NO:20:LEU:HB3	1:NO:32:TYR:HB3	2.00	0.43
1:AB:85:VAL:HG22	1:AG:85:VAL:HG22	2.01	0.43
1:AG:73:SER:O	1:AG:76:THR:OG1	2.35	0.43
1:AT:120:TRP:HZ2	1:NM:60:GLU:HG2	1.84	0.43
1:AZ:112:ALA:O	1:AZ:116:LYS:HG2	2.18	0.43
1:BA:23:ILE:HD11	1:BE:120:TRP:HB3	2.00	0.43
1:BA:27:GLY:O	1:BA:29:THR:HG23	2.19	0.43
1:BR:84:TYR:O	1:BW:85:VAL:HG23	2.19	0.43
1:CQ:25:GLN:O	1:CQ:25:GLN:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CQ:113:LEU:HD23	1:CQ:117:LEU:HD23	2.00	0.43
1:DH:117:LEU:HD21	1:DM:62:HIS:CB	2.48	0.43
1:DS:99:SER:O	1:DS:103:GLU:HG3	2.18	0.43
1:EK:41:PHE:CE1	1:EK:68:GLU:OE2	2.71	0.43
1:HO:63:ASN:OD1	1:HO:64:VAL:N	2.52	0.43
1:HQ:54:PRO:C	1:HQ:55:ASN:OD1	2.56	0.43
1:IM:53:LYS:HB3	1:IM:56:GLN:OE1	2.19	0.43
1:JA:31:GLU:HA	1:JA:43:ALA:O	2.18	0.43
1:JA:46:ARG:HH11	1:JA:46:ARG:HG3	1.84	0.43
1:KC:48:THR:HG22	1:KC:49:LYS:N	2.34	0.43
1:KC:57:VAL:HG23	1:KC:59:TYR:CE2	2.53	0.43
1:KI:69:THR:HG22	1:KI:80:VAL:HG12	2.00	0.43
1:KJ:50:GLU:N	1:KJ:50:GLU:OE1	2.51	0.43
1:KJ:118:ILE:HD12	1:KO:62:HIS:HE2	1.82	0.43
1:KJ:121:GLU:OE1	1:KJ:122:SER:N	2.52	0.43
1:LB:109:LEU:HG	1:LB:114:TYR:CE1	2.54	0.43
1:MA:30:SER:HB2	1:MA:45:VAL:HG12	2.00	0.43
1:ML:53:LYS:NZ	1:ML:55:ASN:OD1	2.52	0.43
1:MS:19:VAL:O	1:MS:34:LEU:HD12	2.19	0.43
1:MX:87:ILE:HD11	1:NA:114:TYR:HE1	1.84	0.43
2:M:47:ASP:OD1	2:M:47:ASP:N	2.49	0.43
1:AB:20:LEU:HB3	1:AB:32:TYR:HB3	2.00	0.43
1:BA:63:ASN:OD1	1:BA:64:VAL:N	2.52	0.43
1:BK:24:ASN:ND2	1:BK:26:ASP:OD2	2.46	0.43
1:BS:57:VAL:HG23	1:BS:59:TYR:CE2	2.54	0.43
1:CO:68:GLU:OE1	1:CO:68:GLU:HA	2.19	0.43
1:CV:54:PRO:C	1:CV:55:ASN:OD1	2.57	0.43
1:DU:2:LEU:HD23	1:LO:122:SER:C	2.38	0.43
1:EM:86:VAL:HB	1:FQ:84:TYR:CZ	2.53	0.43
1:FI:108:TYR:CE1	1:FI:113:LEU:HD21	2.54	0.43
1:FK:95:SER:OG	1:MA:118:ILE:HG21	2.19	0.43
1:FO:117:LEU:HD23	1:FO:117:LEU:C	2.38	0.43
1:GI:27:GLY:O	1:GI:29:THR:HG23	2.18	0.43
1:HO:53:LYS:HG3	1:HO:54:PRO:HD2	1.99	0.43
1:IG:50:GLU:OE2	1:IG:61:ARG:NH2	2.51	0.43
1:IT:57:VAL:HG23	1:IT:59:TYR:CE2	2.54	0.43
1:JA:93:ASP:OD1	1:JA:94:VAL:N	2.42	0.43
1:JX:63:ASN:CB	1:JX:86:VAL:HG12	2.48	0.43
1:KD:30:SER:OG	1:KI:122:SER:O	2.36	0.43
1:LM:58:GLN:O	1:LM:91:VAL:HG23	2.19	0.43
1:ML:15:GLY:O	1:ML:16:THR:OG1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:224:THR:HG23	2:M:302:THR:HG22	1.99	0.43
1:AY:2:LEU:HD12	1:AY:2:LEU:N	2.33	0.43
1:BF:81:ARG:HH12	1:BK:97:THR:HG21	1.84	0.43
1:BG:122:SER:OXT	1:HE:1:ALA:N	2.51	0.43
1:BW:63:ASN:OD1	1:BW:64:VAL:N	2.51	0.43
1:BX:109:LEU:HD12	1:BX:114:TYR:CE1	2.53	0.43
1:CK:25:GLN:HG3	1:CK:25:GLN:O	2.18	0.43
1:DZ:109:LEU:CD1	1:DZ:113:LEU:HD22	2.47	0.43
1:EA:99:SER:O	1:EA:103:GLU:HG3	2.19	0.43
1:EK:68:GLU:HB2	1:EK:81:ARG:HB2	2.01	0.43
1:EW:53:LYS:HD2	1:EW:54:PRO:HD2	2.00	0.43
1:FC:53:LYS:HB3	1:FC:54:PRO:HD2	2.01	0.43
1:FE:62:HIS:O	1:FE:86:VAL:HA	2.19	0.43
1:FK:89:HIS:NE2	1:MA:118:ILE:HD11	2.34	0.43
1:FO:24:ASN:ND2	1:FO:26:ASP:OD2	2.50	0.43
1:GZ:118:ILE:HD11	1:HC:89:HIS:CE1	2.54	0.43
1:HE:113:LEU:HD23	1:HE:117:LEU:HD13	2.00	0.43
1:IS:27:GLY:O	1:IS:29:THR:HG23	2.19	0.43
1:JS:66:PHE:O	1:JS:82:GLN:HB2	2.19	0.43
1:KP:86:VAL:HB	1:KU:84:TYR:CZ	2.54	0.43
1:LM:62:HIS:O	1:LM:86:VAL:HA	2.18	0.43
1:LO:99:SER:O	1:LO:103:GLU:HG3	2.19	0.43
1:MA:65:GLU:OE1	1:MA:67:THR:OG1	2.28	0.43
1:MK:89:HIS:ND1	1:MK:90:LYS:O	2.51	0.43
1:MS:78:GLU:OE1	1:MS:78:GLU:HA	2.18	0.43
1:AM:53:LYS:HB2	1:AM:56:GLN:OE1	2.19	0.43
1:AS:86:VAL:O	1:AS:87:ILE:HD13	2.18	0.43
1:AU:70:VAL:HG21	1:AU:79:PHE:CZ	2.54	0.43
1:BR:21:ARG:N	1:BR:21:ARG:HD2	2.34	0.43
1:BY:45:VAL:HG22	1:BY:64:VAL:HG22	2.01	0.43
1:CI:57:VAL:HG23	1:CI:59:TYR:HE1	1.84	0.43
1:CW:23:ILE:HD12	1:DA:120:TRP:O	2.19	0.43
1:DB:36:GLU:HB2	1:DB:39:SER:O	2.19	0.43
1:DG:69:THR:HG22	1:DG:80:VAL:HG12	2.01	0.43
1:DI:27:GLY:O	1:DI:29:THR:HG23	2.19	0.43
1:DO:23:ILE:HD12	1:DS:120:TRP:O	2.19	0.43
1:DS:29:THR:HG23	1:DS:45:VAL:O	2.19	0.43
1:DT:31:GLU:HB3	1:DT:44:LYS:HD2	2.01	0.43
1:DZ:54:PRO:O	1:DZ:55:ASN:OD1	2.37	0.43
1:EG:25:GLN:O	1:EG:25:GLN:HG3	2.19	0.43
1:EY:63:ASN:OD1	1:EY:64:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FV:61:ARG:HA	1:FV:87:ILE:O	2.19	0.43
1:GB:108:TYR:CD1	1:GB:113:LEU:HD21	2.53	0.43
1:GH:22:LYS:O	1:GH:23:ILE:HD13	2.19	0.43
1:GH:109:LEU:HD22	1:GH:113:LEU:HD22	2.01	0.43
1:GZ:86:VAL:HG11	1:HC:84:TYR:CZ	2.54	0.43
1:HI:68:GLU:CB	1:HI:81:ARG:HB2	2.48	0.43
1:IU:48:THR:HG22	1:IU:49:LYS:N	2.34	0.43
1:KK:63:ASN:OD1	1:KK:64:VAL:N	2.51	0.43
1:LB:62:HIS:HB2	1:LB:87:ILE:HG22	2.00	0.43
1:LU:63:ASN:OD1	1:LU:64:VAL:N	2.52	0.43
1:AA:10:LEU:HB2	1:NN:100:ASP:OD1	2.19	0.43
1:AA:23:ILE:HD11	1:AA:33:TYR:HB3	2.01	0.43
1:BL:32:TYR:HB2	1:BL:43:ALA:HB3	2.00	0.43
1:BL:111:GLU:OE1	1:BQ:99:SER:OG	2.29	0.43
1:CD:109:LEU:HD12	1:CD:114:TYR:CE1	2.54	0.43
1:DY:53:LYS:H	1:DY:56:GLN:HE22	1.67	0.43
1:EL:45:VAL:HG22	1:EL:64:VAL:HG23	2.00	0.43
1:FQ:25:GLN:O	1:FQ:25:GLN:HG3	2.19	0.43
1:FW:69:THR:HG22	1:FW:80:VAL:HG23	2.01	0.43
1:GH:27:GLY:O	1:GH:29:THR:HG23	2.19	0.43
1:GH:81:ARG:CZ	1:GM:97:THR:HG21	2.49	0.43
1:JR:30:SER:OG	1:JW:122:SER:O	2.28	0.43
1:KE:21:ARG:HD3	1:KI:121:GLU:OE2	2.18	0.43
1:KV:33:TYR:HA	1:KV:41:PHE:O	2.19	0.43
1:LU:4:ASP:OD1	1:LU:5:THR:N	2.52	0.43
1:LZ:119:GLY:O	1:LZ:120:TRP:HB2	2.19	0.43
1:AO:86:VAL:HG21	1:LC:84:TYR:CZ	2.54	0.42
1:AU:25:GLN:HG3	1:AU:25:GLN:O	2.18	0.42
1:AU:80:VAL:HG12	1:AU:81:ARG:N	2.34	0.42
1:BG:1:ALA:N	1:HE:122:SER:OXT	2.51	0.42
1:CK:19:VAL:O	1:CK:34:LEU:HD12	2.18	0.42
1:CO:24:ASN:ND2	1:CO:26:ASP:OD2	2.48	0.42
1:CP:93:ASP:OD1	1:CP:94:VAL:N	2.49	0.42
1:DA:65:GLU:HB3	1:DA:84:TYR:HB3	2.00	0.42
1:DU:50:GLU:OE2	1:DU:61:ARG:HB2	2.19	0.42
1:FU:19:VAL:O	1:FU:34:LEU:HD12	2.19	0.42
1:FU:61:ARG:HA	1:FU:87:ILE:O	2.18	0.42
1:FW:8:ILE:HG23	1:FW:8:ILE:O	2.18	0.42
1:GZ:109:LEU:HD12	1:GZ:114:TYR:CZ	2.54	0.42
1:HE:86:VAL:O	1:HE:87:ILE:HD13	2.19	0.42
1:HQ:50:GLU:OE2	1:HQ:61:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IN:55:ASN:N	1:IN:55:ASN:OD1	2.52	0.42
1:IU:20:LEU:HB3	1:IU:32:TYR:HB3	2.00	0.42
1:IY:19:VAL:O	1:IY:34:LEU:HD22	2.19	0.42
1:JF:89:HIS:NE2	1:JK:118:ILE:HD11	2.33	0.42
1:JW:53:LYS:HG2	1:JW:54:PRO:HD2	2.01	0.42
1:KJ:89:HIS:ND1	1:KJ:90:LYS:O	2.52	0.42
1:LT:53:LYS:HD2	1:LT:54:PRO:HD2	2.00	0.42
1:LT:113:LEU:O	1:LT:117:LEU:HD12	2.19	0.42
1:MK:57:VAL:HG12	1:MK:58:GLN:N	2.34	0.42
1:ML:20:LEU:HB3	1:ML:32:TYR:HB3	2.00	0.42
1:MR:34:LEU:HD23	1:MR:34:LEU:C	2.40	0.42
1:MW:10:LEU:HD12	1:MW:10:LEU:O	2.19	0.42
1:AG:39:SER:HB3	1:AG:68:GLU:OE2	2.19	0.42
1:AN:100:ASP:OD1	1:AS:11:GLY:HA2	2.18	0.42
1:AO:84:TYR:CZ	1:LC:86:VAL:HB	2.53	0.42
1:AZ:39:SER:HB2	1:AZ:68:GLU:OE2	2.18	0.42
1:CC:84:TYR:O	1:DB:85:VAL:HG23	2.20	0.42
1:CE:55:ASN:OD1	1:CE:56:GLN:NE2	2.53	0.42
1:DC:114:TYR:CE1	1:GI:87:ILE:HD11	2.54	0.42
1:EG:60:GLU:O	1:EG:88:ARG:HA	2.18	0.42
1:EL:30:SER:N	1:EQ:122:SER:OG	2.52	0.42
1:GN:27:GLY:O	1:GN:29:THR:HG23	2.19	0.42
1:GU:68:GLU:OE1	1:GU:68:GLU:HA	2.19	0.42
1:GZ:112:ALA:O	1:GZ:116:LYS:HG2	2.19	0.42
1:HD:63:ASN:OD1	1:HD:64:VAL:N	2.52	0.42
1:HU:54:PRO:HD2	1:HU:55:ASN:N	2.34	0.42
1:IA:19:VAL:O	1:IA:34:LEU:HD12	2.19	0.42
1:IH:121:GLU:OE1	1:IM:1:ALA:N	2.50	0.42
1:IT:60:GLU:N	1:IT:89:HIS:O	2.43	0.42
1:JG:108:TYR:CE2	1:JG:113:LEU:HD21	2.54	0.42
1:JW:62:HIS:O	1:JW:86:VAL:HA	2.19	0.42
1:KE:67:THR:HG22	1:KE:82:GLN:HG2	2.01	0.42
1:LU:21:ARG:O	1:LU:32:TYR:HA	2.19	0.42
1:MG:54:PRO:O	1:MG:56:GLN:OE1	2.36	0.42
1:NC:23:ILE:HB	1:NC:31:GLU:OE1	2.19	0.42
1:AM:117:LEU:C	1:AM:117:LEU:HD23	2.39	0.42
1:AS:108:TYR:CE2	1:AS:113:LEU:HD21	2.54	0.42
1:AT:53:LYS:CG	1:AT:54:PRO:HD2	2.50	0.42
1:BS:84:TYR:CZ	1:MG:86:VAL:HB	2.55	0.42
1:BX:57:VAL:HG23	1:BX:59:TYR:CE2	2.55	0.42
1:BY:103:GLU:OE2	1:FE:111:GLU:OE1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CP:24:ASN:ND2	1:CP:26:ASP:OD2	2.52	0.42
1:CP:32:TYR:HB2	1:CP:43:ALA:HB3	2.01	0.42
1:DG:20:LEU:HB3	1:DG:32:TYR:HB3	2.01	0.42
1:DT:60:GLU:O	1:DT:88:ARG:HA	2.18	0.42
1:FI:10:LEU:O	1:FI:16:THR:N	2.52	0.42
1:FJ:31:GLU:HA	1:FJ:43:ALA:O	2.18	0.42
1:GC:109:LEU:HD23	1:GC:113:LEU:HD23	2.00	0.42
1:GZ:20:LEU:HB3	1:GZ:32:TYR:HB3	2.01	0.42
1:HW:27:GLY:O	1:HW:29:THR:HG23	2.18	0.42
1:IS:21:ARG:O	1:IS:32:TYR:HA	2.20	0.42
1:JR:22:LYS:O	1:JR:23:ILE:HD13	2.19	0.42
1:LN:20:LEU:HB3	1:LN:32:TYR:HB3	2.01	0.42
1:LO:27:GLY:O	1:LO:29:THR:HG23	2.18	0.42
1:NH:31:GLU:HA	1:NH:43:ALA:O	2.19	0.42
1:AB:58:GLN:N	1:AB:58:GLN:OE1	2.52	0.42
1:AC:25:GLN:HG3	1:AC:25:GLN:O	2.20	0.42
1:AS:65:GLU:CB	1:AS:84:TYR:HB3	2.50	0.42
1:AT:8:ILE:HD11	1:AT:20:LEU:HD11	2.01	0.42
1:BG:93:ASP:OD1	1:BG:94:VAL:N	2.52	0.42
1:BX:60:GLU:OE1	1:BX:60:GLU:N	2.53	0.42
1:CP:63:ASN:HB3	1:CP:86:VAL:HG22	2.01	0.42
1:CU:36:GLU:HB2	1:CU:39:SER:O	2.20	0.42
1:DC:81:ARG:NH1	1:GI:97:THR:HG21	2.34	0.42
1:DO:84:TYR:CZ	1:GC:86:VAL:HG21	2.55	0.42
1:DY:24:ASN:HB3	1:DY:31:GLU:OE2	2.18	0.42
1:EA:30:SER:O	1:EA:45:VAL:HG22	2.20	0.42
1:EK:81:ARG:HB3	1:FJ:101:LEU:HD12	2.02	0.42
1:FC:68:GLU:O	1:FC:80:VAL:HA	2.20	0.42
1:FE:53:LYS:HG2	1:FE:54:PRO:HD2	2.01	0.42
1:GN:54:PRO:O	1:GN:55:ASN:OD1	2.37	0.42
1:HI:62:HIS:O	1:HI:86:VAL:HA	2.20	0.42
1:HU:86:VAL:HB	1:IT:84:TYR:CZ	2.55	0.42
1:IU:118:ILE:HD11	1:NC:89:HIS:CD2	2.53	0.42
1:JS:112:ALA:O	1:JS:116:LYS:HG2	2.20	0.42
1:JW:18:LYS:HG2	1:JW:41:PHE:CE2	2.54	0.42
1:LT:4:ASP:OD1	1:LT:5:THR:HG23	2.19	0.42
1:LT:113:LEU:HD23	1:LT:117:LEU:CD1	2.49	0.42
1:NO:114:TYR:O	1:NO:118:ILE:HG12	2.19	0.42
1:AC:36:GLU:HB2	1:AC:39:SER:O	2.18	0.42
1:AN:39:SER:OG	1:AN:70:VAL:HG12	2.20	0.42
1:AT:46:ARG:NH1	1:AT:48:THR:HG22	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:84:TYR:CZ	1:NO:86:VAL:CG2	3.02	0.42
1:BY:81:ARG:CZ	1:FE:97:THR:HG21	2.50	0.42
1:BY:117:LEU:HD23	1:BY:117:LEU:C	2.39	0.42
1:CD:89:HIS:CE1	1:CI:118:ILE:HD11	2.54	0.42
1:CJ:55:ASN:OD1	1:CJ:56:GLN:OE1	2.38	0.42
1:CK:118:ILE:HD13	1:II:62:HIS:HE1	1.84	0.42
1:DC:112:ALA:O	1:DC:116:LYS:HG3	2.19	0.42
1:DT:21:ARG:O	1:DT:32:TYR:HA	2.20	0.42
1:DU:53:LYS:HB3	1:DU:54:PRO:CD	2.50	0.42
1:DZ:121:GLU:O	1:EE:2:LEU:HD11	2.19	0.42
1:EK:55:ASN:O	1:EK:55:ASN:OD1	2.37	0.42
1:GC:57:VAL:HG23	1:GC:59:TYR:CE2	2.55	0.42
1:GT:23:ILE:HG23	1:HP:120:TRP:O	2.20	0.42
1:GT:81:ARG:HH12	1:GY:97:THR:HG21	1.85	0.42
1:GZ:1:ALA:N	1:HC:121:GLU:OE2	2.47	0.42
1:HK:19:VAL:O	1:HK:34:LEU:HD12	2.20	0.42
1:IB:54:PRO:O	1:IB:55:ASN:OD1	2.36	0.42
1:IM:112:ALA:O	1:IM:116:LYS:HG3	2.20	0.42
1:IU:84:TYR:CZ	1:NC:86:VAL:HB	2.54	0.42
1:IY:53:LYS:HB3	1:IY:54:PRO:CD	2.50	0.42
1:JA:99:SER:O	1:JA:103:GLU:HG2	2.19	0.42
1:KD:120:TRP:CB	1:KJ:23:ILE:HD11	2.47	0.42
1:KP:34:LEU:HD12	1:KP:35:PRO:HD2	2.01	0.42
1:LH:62:HIS:O	1:LH:86:VAL:HG23	2.20	0.42
1:LO:68:GLU:HB2	1:LO:81:ARG:HB2	2.02	0.42
1:LY:51:SER:OG	1:LY:53:LYS:NZ	2.52	0.42
1:AI:59:TYR:HA	1:AI:90:LYS:HA	2.01	0.42
1:AS:53:LYS:HB3	1:AS:54:PRO:HD2	2.01	0.42
1:AY:62:HIS:N	1:AY:87:ILE:O	2.40	0.42
1:BM:29:THR:HG22	1:BM:46:ARG:HA	2.01	0.42
1:CK:97:THR:HG21	1:II:81:ARG:NH1	2.34	0.42
1:CU:29:THR:CG2	1:CU:44:LYS:HE2	2.50	0.42
1:DA:33:TYR:CD1	1:DA:34:LEU:N	2.88	0.42
1:DC:60:GLU:O	1:DC:88:ARG:HA	2.19	0.42
1:DH:63:ASN:HB2	1:DH:85:VAL:O	2.20	0.42
1:EA:44:LYS:HG2	1:EA:65:GLU:OE2	2.20	0.42
1:EM:84:TYR:CE1	1:FQ:86:VAL:HB	2.54	0.42
1:EQ:79:PHE:HE2	1:EQ:81:ARG:HH21	1.67	0.42
1:FC:21:ARG:N	1:FC:21:ARG:HD2	2.35	0.42
1:GU:89:HIS:ND1	1:GU:90:LYS:O	2.51	0.42
1:HE:6:LEU:HB2	1:HE:32:TYR:CE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IG:65:GLU:OE1	1:IG:67:THR:OG1	2.25	0.42
1:IT:8:ILE:HD11	1:IT:66:PHE:CD1	2.54	0.42
1:IZ:57:VAL:HG23	1:IZ:59:TYR:CE2	2.55	0.42
1:IZ:98:VAL:O	1:IZ:101:LEU:O	2.37	0.42
1:JG:119:GLY:O	1:JG:120:TRP:HB2	2.18	0.42
1:KU:50:GLU:OE2	1:KU:50:GLU:N	2.52	0.42
1:KV:84:TYR:CE1	1:LA:86:VAL:HB	2.55	0.42
1:LB:55:ASN:N	1:LB:55:ASN:OD1	2.52	0.42
1:MX:109:LEU:HD22	1:MX:113:LEU:HD22	2.01	0.42
1:NM:36:GLU:HB2	1:NM:39:SER:O	2.19	0.42
1:AZ:70:VAL:HG21	1:AZ:79:PHE:CZ	2.54	0.42
1:BL:105:LEU:HD21	1:BQ:85:VAL:HG13	2.02	0.42
1:CV:16:THR:O	1:CV:16:THR:HG22	2.20	0.42
1:EL:31:GLU:HG2	1:EL:44:LYS:HB3	2.00	0.42
1:ER:29:THR:HG23	1:ER:46:ARG:HG2	2.00	0.42
1:ES:112:ALA:O	1:ES:116:LYS:HG3	2.19	0.42
1:FP:50:GLU:OE1	1:FP:50:GLU:HA	2.20	0.42
1:GM:62:HIS:N	1:GM:87:ILE:O	2.50	0.42
1:GM:64:VAL:O	1:GM:84:TYR:HB2	2.20	0.42
1:GS:60:GLU:O	1:GS:88:ARG:HA	2.19	0.42
1:HI:108:TYR:OH	1:HI:113:LEU:HD11	2.20	0.42
1:IC:45:VAL:HG12	1:IC:64:VAL:HG22	2.01	0.42
1:IM:113:LEU:O	1:IM:117:LEU:HD23	2.19	0.42
1:IT:68:GLU:N	1:IT:81:ARG:O	2.52	0.42
1:IZ:47:HIS:HB2	1:JE:120:TRP:CZ3	2.55	0.42
1:JQ:86:VAL:O	1:JQ:87:ILE:HD13	2.20	0.42
1:JX:4:ASP:OD1	1:JX:5:THR:N	2.52	0.42
1:JY:36:GLU:OE1	1:JY:36:GLU:HA	2.19	0.42
1:KP:81:ARG:NH1	1:KU:93:ASP:OD1	2.53	0.42
1:LN:93:ASP:OD2	1:LS:81:ARG:NH1	2.52	0.42
1:MS:23:ILE:HD12	1:MW:120:TRP:O	2.19	0.42
1:MW:113:LEU:HD12	1:MW:113:LEU:O	2.20	0.42
1:NN:54:PRO:O	1:NN:55:ASN:OD1	2.38	0.42
2:M:228:VAL:HG12	2:M:298:VAL:HA	2.01	0.42
1:AG:109:LEU:HD12	1:AG:114:TYR:CE1	2.54	0.42
1:AM:31:GLU:HB3	1:AM:44:LYS:HG2	2.01	0.42
1:AS:33:TYR:OH	1:AS:35:PRO:HB3	2.20	0.42
1:BG:84:TYR:CE1	1:HE:86:VAL:CG2	3.03	0.42
1:BL:84:TYR:CZ	1:BQ:86:VAL:HG11	2.55	0.42
1:DC:85:VAL:HG23	1:GI:105:LEU:HD21	2.02	0.42
1:DH:23:ILE:HD11	1:EF:120:TRP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EF:21:ARG:O	1:EF:32:TYR:HA	2.20	0.42
1:GC:25:GLN:HG3	1:GC:25:GLN:O	2.20	0.42
1:GH:54:PRO:C	1:GH:55:ASN:OD1	2.58	0.42
1:GH:117:LEU:HD21	1:GM:62:HIS:HB3	2.01	0.42
1:HO:86:VAL:O	1:HO:87:ILE:HD13	2.19	0.42
1:IU:36:GLU:N	1:IU:39:SER:O	2.53	0.42
1:JS:6:LEU:HD22	1:JS:32:TYR:CE2	2.55	0.42
1:JY:25:GLN:HG3	1:JY:25:GLN:O	2.20	0.42
1:KC:122:SER:HA	1:LB:2:LEU:HD22	2.02	0.42
1:LN:98:VAL:O	1:LN:101:LEU:O	2.38	0.42
1:LT:28:TYR:CD2	1:LU:23:ILE:HG22	2.55	0.42
1:MK:81:ARG:HB3	1:NH:101:LEU:HD23	2.02	0.42
1:MW:21:ARG:NH2	2:M:110:SER:OG	2.47	0.42
1:NG:31:GLU:OE1	1:NG:31:GLU:N	2.52	0.42
1:AG:29:THR:HG22	1:AG:46:ARG:HG3	2.00	0.42
1:AN:111:GLU:OE1	1:AS:99:SER:OG	2.33	0.42
1:BQ:20:LEU:HB3	1:BQ:32:TYR:HB3	1.99	0.42
1:BS:45:VAL:HG22	1:BS:64:VAL:HG23	2.01	0.42
1:DA:44:LYS:CG	1:DA:65:GLU:OE2	2.68	0.42
1:DN:21:ARG:HB2	1:DN:21:ARG:CZ	2.50	0.42
1:EK:31:GLU:OE1	1:EK:44:LYS:CD	2.68	0.42
1:EM:1:ALA:HB3	1:FQ:121:GLU:HG3	2.00	0.42
1:GH:86:VAL:HB	1:GM:84:TYR:CZ	2.55	0.42
1:GT:20:LEU:HG	1:GT:32:TYR:CB	2.50	0.42
1:IG:121:GLU:HG2	1:IG:121:GLU:O	2.20	0.42
1:JG:118:ILE:HD12	1:JG:118:ILE:H	1.85	0.42
1:JS:48:THR:HG22	1:JS:49:LYS:N	2.35	0.42
1:KK:52:VAL:HG22	1:KK:58:GLN:OE1	2.20	0.42
1:LG:121:GLU:HA	1:MG:23:ILE:HD13	2.02	0.42
1:LT:86:VAL:HB	1:LY:84:TYR:CZ	2.55	0.42
1:NM:55:ASN:O	1:NM:56:GLN:HB3	2.20	0.42
1:NN:64:VAL:O	1:NN:84:TYR:HB2	2.20	0.42
1:AY:6:LEU:HD23	1:AY:32:TYR:CD2	2.54	0.42
1:CE:34:LEU:HD23	1:CE:34:LEU:C	2.40	0.42
1:EA:25:GLN:O	1:EA:25:GLN:HG3	2.19	0.42
1:EX:60:GLU:HG3	1:EX:91:VAL:HG22	2.02	0.42
1:EY:27:GLY:O	1:EY:29:THR:HG23	2.20	0.42
1:FD:54:PRO:O	1:FD:56:GLN:NE2	2.48	0.42
1:GZ:45:VAL:HG22	1:GZ:64:VAL:HG12	2.02	0.42
1:HP:15:GLY:O	1:HP:16:THR:OG1	2.36	0.42
1:HU:85:VAL:HG12	1:HU:86:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IG:50:GLU:OE2	1:IG:61:ARG:NH1	2.53	0.42
1:IT:108:TYR:OH	1:IT:113:LEU:HD11	2.20	0.42
1:IZ:56:GLN:OE1	1:IZ:56:GLN:N	2.52	0.42
1:JM:70:VAL:HG21	1:JM:79:PHE:CZ	2.55	0.42
1:KQ:55:ASN:O	1:KQ:56:GLN:NE2	2.53	0.42
1:LI:62:HIS:O	1:LI:86:VAL:HA	2.20	0.42
1:LZ:120:TRP:HB3	1:MF:23:ILE:HD13	2.02	0.42
1:LZ:120:TRP:O	1:MF:23:ILE:CD1	2.68	0.42
1:MA:99:SER:O	1:MA:103:GLU:HG3	2.20	0.42
1:MK:113:LEU:O	1:MK:117:LEU:HD13	2.20	0.42
1:MM:25:GLN:HA	1:MM:29:THR:O	2.19	0.42
1:NG:62:HIS:O	1:NG:86:VAL:HA	2.20	0.42
1:AB:121:GLU:OE2	1:AG:1:ALA:N	2.43	0.41
1:AT:55:ASN:OD1	1:AT:55:ASN:N	2.53	0.41
1:BG:121:GLU:OE2	1:HC:21:ARG:NE	2.49	0.41
1:BK:116:LYS:HD2	1:BK:121:GLU:OE2	2.20	0.41
1:CC:93:ASP:OD2	1:CC:94:VAL:N	2.50	0.41
1:CE:109:LEU:HD12	1:CE:114:TYR:CE1	2.55	0.41
1:CW:99:SER:OG	1:CW:103:GLU:OE2	2.24	0.41
1:EL:53:LYS:O	1:EL:56:GLN:HG3	2.20	0.41
1:ES:2:LEU:HD23	1:JM:122:SER:C	2.41	0.41
1:FQ:99:SER:O	1:FQ:103:GLU:HG3	2.19	0.41
1:HC:108:TYR:CE2	1:HC:113:LEU:HD21	2.54	0.41
1:HU:63:ASN:OD1	1:HU:64:VAL:N	2.53	0.41
1:IS:108:TYR:CZ	1:IS:113:LEU:HD11	2.55	0.41
1:IT:4:ASP:N	1:IT:4:ASP:OD1	2.52	0.41
1:IU:87:ILE:HD11	1:NC:114:TYR:HE1	1.85	0.41
1:KC:84:TYR:CZ	1:LB:86:VAL:HB	2.54	0.41
1:KJ:45:VAL:HG22	1:KJ:64:VAL:HG12	2.01	0.41
1:KK:23:ILE:HG13	1:KK:33:TYR:HB3	2.02	0.41
1:KU:99:SER:O	1:KU:103:GLU:HG3	2.20	0.41
1:KV:4:ASP:OD1	1:KV:4:ASP:C	2.59	0.41
1:MF:27:GLY:O	1:MF:29:THR:HG23	2.20	0.41
1:MQ:4:ASP:OD1	1:MQ:4:ASP:C	2.58	0.41
1:MQ:117:LEU:C	1:MQ:117:LEU:HD23	2.39	0.41
1:MR:4:ASP:OD1	1:MR:5:THR:HG23	2.19	0.41
1:MR:59:TYR:OH	1:MW:80:VAL:HG12	2.20	0.41
1:MW:8:ILE:HD12	1:MW:66:PHE:CD2	2.55	0.41
1:MX:99:SER:O	1:MX:103:GLU:HG3	2.20	0.41
1:NI:2:LEU:N	1:NI:2:LEU:HD12	2.35	0.41
1:NN:21:ARG:O	1:NN:32:TYR:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NO:7:THR:O	1:NO:7:THR:HG23	2.20	0.41
1:AC:53:LYS:HB3	1:AC:54:PRO:HD2	2.01	0.41
1:AS:44:LYS:HB2	1:AS:65:GLU:OE2	2.19	0.41
1:AS:89:HIS:CG	1:AS:98:VAL:HG21	2.55	0.41
1:BA:37:THR:HG23	1:BA:38:SER:N	2.35	0.41
1:BL:81:ARG:NH1	1:BQ:97:THR:HG21	2.34	0.41
1:CJ:54:PRO:O	1:CJ:55:ASN:OD1	2.38	0.41
1:CV:63:ASN:OD1	1:CV:64:VAL:N	2.53	0.41
1:DB:25:GLN:HG2	1:DB:29:THR:O	2.19	0.41
1:DC:25:GLN:HG3	1:DC:25:GLN:O	2.19	0.41
1:DM:23:ILE:HG23	1:GC:120:TRP:O	2.20	0.41
1:FQ:93:ASP:OD1	1:FQ:94:VAL:N	2.50	0.41
1:GB:108:TYR:CE1	1:GB:113:LEU:HD21	2.55	0.41
1:GC:27:GLY:O	1:GC:29:THR:HG23	2.20	0.41
1:GO:34:LEU:HD23	1:GO:35:PRO:O	2.20	0.41
1:GT:60:GLU:OE1	1:GT:91:VAL:HG22	2.20	0.41
1:HW:5:THR:HG22	1:HW:21:ARG:HE	1.84	0.41
1:IB:52:VAL:O	1:IB:53:LYS:HE2	2.20	0.41
1:JL:20:LEU:HD23	1:JL:32:TYR:C	2.41	0.41
1:JM:25:GLN:O	1:JM:25:GLN:HG3	2.20	0.41
1:KQ:36:GLU:OE2	1:KQ:39:SER:OG	2.28	0.41
1:KW:50:GLU:OE2	1:KW:61:ARG:NH1	2.53	0.41
1:LA:109:LEU:HD12	1:LA:114:TYR:CE1	2.55	0.41
1:LG:116:LYS:HB3	1:LG:121:GLU:OE2	2.20	0.41
1:MK:86:VAL:HB	1:NH:84:TYR:CE1	2.55	0.41
1:MR:116:LYS:HZ1	1:MW:2:LEU:HD22	1.85	0.41
1:MX:60:GLU:OE2	1:MX:62:HIS:CE1	2.73	0.41
1:NA:4:ASP:C	1:NA:4:ASP:OD1	2.58	0.41
1:NA:28:TYR:HD1	1:NB:23:ILE:HG22	1.85	0.41
2:M:9:SER:O	2:M:34:ASN:N	2.52	0.41
2:M:28:GLU:OE1	2:M:28:GLU:N	2.51	0.41
1:AC:27:GLY:O	1:AC:29:THR:HG23	2.20	0.41
1:AH:85:VAL:HG23	1:AM:105:LEU:HD21	2.02	0.41
1:AS:5:THR:HG22	1:AS:21:ARG:HE	1.85	0.41
1:BG:4:ASP:OD1	1:BG:5:THR:N	2.53	0.41
1:BL:100:ASP:O	1:BL:103:GLU:HG3	2.20	0.41
1:CC:29:THR:HA	1:CC:45:VAL:O	2.20	0.41
1:CI:51:SER:OG	1:CI:53:LYS:NZ	2.40	0.41
1:CQ:86:VAL:HB	1:KK:84:TYR:CZ	2.56	0.41
1:CV:86:VAL:HB	1:DA:84:TYR:CE1	2.55	0.41
1:DG:86:VAL:CG1	1:EF:84:TYR:CZ	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DT:20:LEU:HD23	1:DT:34:LEU:CB	2.50	0.41
1:EG:111:GLU:OE2	1:IO:103:GLU:OE1	2.38	0.41
1:GN:4:ASP:OD1	1:GN:5:THR:N	2.53	0.41
1:IO:116:LYS:HE2	1:IO:121:GLU:OE1	2.20	0.41
1:KO:70:VAL:O	1:KO:70:VAL:HG23	2.20	0.41
1:NB:4:ASP:OD1	1:NB:5:THR:N	2.52	0.41
1:AA:8:ILE:HG23	1:AA:8:ILE:O	2.20	0.41
1:AA:50:GLU:OE1	1:AA:50:GLU:N	2.42	0.41
1:AI:114:TYR:CE1	1:JG:87:ILE:HD11	2.56	0.41
1:AY:67:THR:HG22	1:AY:82:GLN:CG	2.49	0.41
1:BF:31:GLU:HB2	1:BF:43:ALA:O	2.19	0.41
1:BS:109:LEU:HB3	1:BS:114:TYR:CE1	2.56	0.41
1:CK:62:HIS:O	1:CK:86:VAL:HA	2.21	0.41
1:CW:86:VAL:HB	1:JY:84:TYR:CZ	2.55	0.41
1:DC:20:LEU:HB3	1:DC:32:TYR:HB3	2.02	0.41
1:DI:99:SER:O	1:DI:102:GLY:N	2.53	0.41
1:DM:26:ASP:OD2	1:DO:26:ASP:O	2.38	0.41
1:DZ:81:ARG:NH2	1:EE:93:ASP:OD1	2.47	0.41
1:EA:57:VAL:HG23	1:EA:59:TYR:CE1	2.55	0.41
1:EK:64:VAL:O	1:EK:84:TYR:HB2	2.20	0.41
1:EL:60:GLU:O	1:EL:88:ARG:HA	2.21	0.41
1:GC:7:THR:HG22	1:GC:19:VAL:HG12	2.02	0.41
1:GY:20:LEU:HD13	1:GY:34:LEU:HB2	2.02	0.41
1:GY:31:GLU:HA	1:GY:43:ALA:O	2.20	0.41
1:GZ:122:SER:O	1:HC:2:LEU:HD12	2.19	0.41
1:HC:16:THR:OG1	1:HC:18:LYS:NZ	2.53	0.41
1:HQ:29:THR:HG22	1:HQ:46:ARG:HA	2.02	0.41
1:HV:85:VAL:HG23	1:IA:84:TYR:O	2.20	0.41
1:HW:86:VAL:HG22	1:HW:87:ILE:N	2.36	0.41
1:IN:61:ARG:HA	1:IN:87:ILE:O	2.21	0.41
1:IY:20:LEU:HD21	1:IY:41:PHE:HB3	2.03	0.41
1:JW:31:GLU:HA	1:JW:43:ALA:O	2.20	0.41
1:KJ:97:THR:HG21	1:KO:81:ARG:NH2	2.35	0.41
1:KU:55:ASN:OD1	1:KU:55:ASN:O	2.39	0.41
1:LS:69:THR:HG22	1:LS:80:VAL:HG12	2.01	0.41
1:LU:24:ASN:HB3	1:LU:31:GLU:OE2	2.20	0.41
1:MG:68:GLU:O	1:MG:81:ARG:N	2.40	0.41
1:NC:27:GLY:O	1:NC:29:THR:HG23	2.20	0.41
1:NH:108:TYR:CZ	1:NH:113:LEU:CD1	3.03	0.41
1:AN:63:ASN:OD1	1:AN:64:VAL:N	2.54	0.41
1:AY:112:ALA:O	1:AY:116:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BF:63:ASN:OD1	1:BF:64:VAL:N	2.53	0.41
1:BL:61:ARG:HH11	1:BL:61:ARG:HG2	1.85	0.41
1:CC:84:TYR:CZ	1:DB:86:VAL:HG21	2.56	0.41
1:DB:4:ASP:OD1	1:DB:4:ASP:C	2.58	0.41
1:DT:97:THR:HG21	1:DY:81:ARG:NH2	2.35	0.41
1:EX:62:HIS:O	1:EX:86:VAL:HA	2.20	0.41
1:FP:93:ASP:OD1	1:FP:94:VAL:N	2.47	0.41
1:GO:118:ILE:HG21	1:JS:95:SER:OG	2.21	0.41
1:GZ:68:GLU:N	1:GZ:81:ARG:O	2.52	0.41
1:HW:31:GLU:HA	1:HW:43:ALA:O	2.20	0.41
1:IZ:86:VAL:CG1	1:JE:84:TYR:CZ	3.03	0.41
1:JW:55:ASN:O	1:JW:56:GLN:HG3	2.20	0.41
1:JX:34:LEU:HD23	1:JX:34:LEU:C	2.41	0.41
1:KP:20:LEU:HB3	1:KP:32:TYR:HB3	2.01	0.41
1:LU:49:LYS:NZ	1:LU:60:GLU:OE2	2.46	0.41
1:MF:5:THR:HG22	1:MF:21:ARG:NH2	2.34	0.41
1:MW:28:TYR:HD1	1:MX:23:ILE:HG22	1.85	0.41
1:NH:108:TYR:CZ	1:NH:113:LEU:HD11	2.55	0.41
1:NO:27:GLY:O	1:NO:29:THR:HG23	2.21	0.41
1:AM:55:ASN:OD1	1:AM:55:ASN:O	2.39	0.41
1:AN:93:ASP:OD1	1:AN:94:VAL:N	2.53	0.41
1:AT:46:ARG:HH11	1:AT:48:THR:HG22	1.84	0.41
1:BA:84:TYR:O	1:NO:85:VAL:HG23	2.21	0.41
1:BW:26:ASP:O	1:BW:29:THR:OG1	2.20	0.41
1:CC:117:LEU:HD23	1:CC:117:LEU:C	2.40	0.41
1:CO:31:GLU:OE2	1:CO:32:TYR:N	2.51	0.41
1:DA:20:LEU:HB3	1:DA:32:TYR:HB3	2.03	0.41
1:DH:31:GLU:HB3	1:DH:44:LYS:HG2	2.03	0.41
1:DM:99:SER:O	1:DM:103:GLU:HG3	2.20	0.41
1:DY:99:SER:OG	1:DY:103:GLU:OE2	2.36	0.41
1:EF:41:PHE:CD2	1:EF:68:GLU:OE2	2.73	0.41
1:GC:49:LYS:HD2	1:GC:50:GLU:N	2.36	0.41
1:GY:23:ILE:HG13	1:GY:24:ASN:N	2.36	0.41
1:HJ:81:ARG:NH2	1:HO:97:THR:HG21	2.35	0.41
1:IB:89:HIS:NE2	1:IG:118:ILE:CD1	2.84	0.41
1:IN:109:LEU:HD22	1:IN:113:LEU:HD22	2.02	0.41
1:JX:36:GLU:N	1:JX:36:GLU:OE1	2.54	0.41
1:KP:63:ASN:OD1	1:KP:64:VAL:N	2.54	0.41
1:LA:31:GLU:HA	1:LA:43:ALA:O	2.20	0.41
1:MR:98:VAL:HG12	1:MW:81:ARG:HD2	2.01	0.41
1:MX:22:LYS:HA	1:MX:32:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NA:63:ASN:OD1	1:NA:64:VAL:N	2.54	0.41
1:AA:73:SER:O	1:AA:76:THR:OG1	2.34	0.41
1:AC:108:TYR:CZ	1:EY:6:LEU:HD11	2.55	0.41
1:AC:109:LEU:HD12	1:AC:114:TYR:CE1	2.56	0.41
1:AI:20:LEU:HB3	1:AI:32:TYR:HB3	2.02	0.41
1:AT:121:GLU:OE1	1:NN:21:ARG:HG2	2.21	0.41
1:BS:2:LEU:HD23	1:MG:122:SER:C	2.41	0.41
1:BY:99:SER:O	1:BY:103:GLU:HG3	2.20	0.41
1:CC:63:ASN:OD1	1:CC:64:VAL:N	2.54	0.41
1:CP:27:GLY:O	1:CP:29:THR:HG23	2.20	0.41
1:CP:98:VAL:O	1:CP:101:LEU:O	2.39	0.41
1:CW:52:VAL:HG22	1:CW:58:GLN:OE1	2.20	0.41
1:DC:86:VAL:HB	1:GI:84:TYR:CZ	2.56	0.41
1:DI:53:LYS:HG2	1:DI:54:PRO:HD2	2.03	0.41
1:DM:62:HIS:O	1:DM:86:VAL:HA	2.21	0.41
1:DN:87:ILE:HG22	1:DN:88:ARG:N	2.35	0.41
1:GH:6:LEU:HD13	1:GH:32:TYR:CZ	2.55	0.41
1:HQ:81:ARG:NH2	1:KW:97:THR:HG21	2.35	0.41
1:II:109:LEU:HD12	1:II:109:LEU:O	2.21	0.41
1:JY:36:GLU:HB2	1:JY:39:SER:O	2.20	0.41
1:KJ:19:VAL:HG23	1:KJ:19:VAL:O	2.21	0.41
1:KK:27:GLY:O	1:KK:28:TYR:HB2	2.19	0.41
1:KP:30:SER:HG	1:KU:122:SER:C	2.23	0.41
1:LH:55:ASN:OD1	1:LH:55:ASN:N	2.52	0.41
1:LM:62:HIS:O	1:LM:86:VAL:HG23	2.20	0.41
1:LZ:85:VAL:HG22	1:LZ:86:VAL:N	2.35	0.41
1:MM:20:LEU:HD21	1:MM:41:PHE:HB3	2.01	0.41
1:MR:37:THR:HG23	1:MR:38:SER:N	2.34	0.41
1:AG:36:GLU:OE1	1:AG:40:SER:HA	2.21	0.41
1:AI:25:GLN:HG3	1:AI:25:GLN:O	2.20	0.41
1:AN:84:TYR:CZ	1:AS:86:VAL:CG2	3.04	0.41
1:AU:86:VAL:HG21	1:HK:84:TYR:CZ	2.55	0.41
1:BG:22:LYS:HA	1:BG:32:TYR:CD1	2.56	0.41
1:BK:21:ARG:HD2	1:MS:121:GLU:OE2	2.20	0.41
1:BM:86:VAL:HG11	1:MS:84:TYR:CZ	2.56	0.41
1:BY:57:VAL:HG23	1:BY:59:TYR:CE2	2.56	0.41
1:CP:20:LEU:HD23	1:CP:34:LEU:HB3	2.02	0.41
1:DZ:86:VAL:HB	1:EE:84:TYR:CE1	2.56	0.41
1:EF:67:THR:HA	1:EF:81:ARG:O	2.21	0.41
1:GC:99:SER:O	1:GC:103:GLU:HG3	2.21	0.41
1:GH:113:LEU:HD23	1:GH:113:LEU:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GM:34:LEU:HD21	1:GM:36:GLU:OE2	2.20	0.41
1:GY:60:GLU:OE1	1:GY:62:HIS:CD2	2.74	0.41
1:HE:113:LEU:O	1:HE:117:LEU:HD13	2.21	0.41
1:HK:31:GLU:HA	1:HK:43:ALA:O	2.20	0.41
1:IB:23:ILE:HG13	1:IB:33:TYR:HB3	2.03	0.41
1:IS:53:LYS:HB3	1:IS:56:GLN:OE1	2.20	0.41
1:IT:20:LEU:HD21	1:IT:41:PHE:HB3	2.01	0.41
1:IY:86:VAL:HB	1:JX:84:TYR:CE2	2.56	0.41
1:JR:86:VAL:HB	1:JW:84:TYR:CZ	2.56	0.41
1:JX:68:GLU:O	1:JX:80:VAL:HA	2.20	0.41
1:KC:121:GLU:HA	1:KC:121:GLU:OE1	2.20	0.41
1:KJ:26:ASP:O	1:KJ:29:THR:HB	2.21	0.41
1:KU:8:ILE:HD12	1:KU:66:PHE:CE2	2.55	0.41
1:LH:65:GLU:CB	1:LH:84:TYR:HB3	2.51	0.41
1:MM:41:PHE:CD2	1:MM:68:GLU:OE2	2.74	0.41
1:MR:21:ARG:HH11	1:MR:21:ARG:HG2	1.86	0.41
1:NA:55:ASN:O	1:NA:55:ASN:OD1	2.38	0.41
1:NC:70:VAL:HG21	1:NC:79:PHE:CZ	2.56	0.41
1:NI:25:GLN:HA	1:NI:29:THR:O	2.21	0.41
2:M:218:VAL:HG12	2:M:308:HIS:ND1	2.36	0.41
1:AA:27:GLY:O	1:AA:29:THR:HG23	2.20	0.41
1:AC:84:TYR:CE1	1:EY:86:VAL:HB	2.56	0.41
1:AO:25:GLN:HG3	1:AO:25:GLN:O	2.20	0.41
1:AO:109:LEU:HD21	1:LC:85:VAL:HG11	2.01	0.41
1:AU:44:LYS:HB3	1:AU:46:ARG:HH11	1.86	0.41
1:BL:48:THR:HG22	1:BL:49:LYS:N	2.36	0.41
1:BM:57:VAL:HG12	1:BM:58:GLN:N	2.36	0.41
1:BW:55:ASN:O	1:BW:56:GLN:HB3	2.21	0.41
1:CC:97:THR:HG21	1:DB:81:ARG:NH2	2.35	0.41
1:CE:36:GLU:OE1	1:CE:37:THR:N	2.54	0.41
1:CE:44:LYS:HB2	1:CE:65:GLU:HB3	2.03	0.41
1:CQ:4:ASP:OD2	1:CQ:4:ASP:N	2.54	0.41
1:CQ:23:ILE:HB	1:CQ:31:GLU:OE2	2.21	0.41
1:CQ:31:GLU:HA	1:CQ:43:ALA:O	2.21	0.41
1:DO:113:LEU:O	1:DO:117:LEU:HD13	2.20	0.41
1:DT:44:LYS:HB2	1:DT:65:GLU:HB3	2.03	0.41
1:EA:84:TYR:CZ	1:NI:86:VAL:HB	2.56	0.41
1:EA:93:ASP:OD1	1:EA:94:VAL:N	2.40	0.41
1:EF:46:ARG:NH1	1:EF:46:ARG:HG3	2.36	0.41
1:EG:4:ASP:O	1:EG:4:ASP:OD1	2.39	0.41
1:EG:86:VAL:HB	1:IO:84:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EK:85:VAL:HG22	1:EK:86:VAL:N	2.36	0.41
1:EL:84:TYR:CZ	1:EQ:86:VAL:HB	2.56	0.41
1:ER:48:THR:HG22	1:ER:49:LYS:N	2.35	0.41
1:FC:48:THR:HG22	1:FC:49:LYS:N	2.36	0.41
1:FI:39:SER:HA	1:FI:69:THR:O	2.21	0.41
1:FJ:113:LEU:HD23	1:FJ:113:LEU:O	2.21	0.41
1:GB:18:LYS:HE2	1:GB:41:PHE:CE2	2.56	0.41
1:GB:50:GLU:OE1	1:GB:50:GLU:HA	2.20	0.41
1:GT:6:LEU:N	1:GT:20:LEU:O	2.45	0.41
1:GT:30:SER:OG	1:GY:122:SER:OG	2.29	0.41
1:GY:31:GLU:HB2	1:GY:43:ALA:O	2.20	0.41
1:HC:117:LEU:C	1:HC:117:LEU:HD23	2.41	0.41
1:HU:79:PHE:CD2	1:IT:90:LYS:HE3	2.56	0.41
1:HU:109:LEU:CD1	1:HU:113:LEU:HD22	2.51	0.41
1:HU:113:LEU:HD23	1:HU:113:LEU:C	2.41	0.41
1:HV:118:ILE:HG21	1:IA:95:SER:CB	2.51	0.41
1:IC:81:ARG:NH2	1:KQ:97:THR:HG21	2.35	0.41
1:IN:84:TYR:CZ	1:IS:86:VAL:HG21	2.56	0.41
1:IS:8:ILE:HG12	1:IS:66:PHE:CZ	2.56	0.41
1:IT:34:LEU:HB3	1:IT:41:PHE:HB2	2.02	0.41
1:IU:95:SER:OG	1:NC:118:ILE:HG21	2.21	0.41
1:IZ:8:ILE:HG12	1:IZ:66:PHE:CE2	2.56	0.41
1:JM:54:PRO:O	1:JM:55:ASN:OD1	2.38	0.41
1:KD:121:GLU:HB3	1:KI:1:ALA:HB3	2.03	0.41
1:KK:109:LEU:HD23	1:KK:113:LEU:HD23	2.03	0.41
1:KU:53:LYS:HB3	1:KU:56:GLN:OE1	2.21	0.41
1:KV:108:TYR:CZ	1:KV:113:LEU:HD11	2.56	0.41
1:KW:25:GLN:HB2	1:KW:29:THR:O	2.21	0.41
1:LB:23:ILE:HG22	1:LB:31:GLU:HB2	2.03	0.41
1:LG:89:HIS:NE2	1:MF:118:ILE:HD11	2.36	0.41
1:LI:19:VAL:HG23	1:LI:19:VAL:O	2.21	0.41
1:LI:25:GLN:O	1:LI:25:GLN:NE2	2.54	0.41
1:LY:6:LEU:HD22	1:LY:32:TYR:CD2	2.56	0.41
1:LY:55:ASN:O	1:LY:56:GLN:HG3	2.21	0.41
1:MF:7:THR:HG23	1:MF:7:THR:O	2.21	0.41
1:MK:20:LEU:HD23	1:MK:34:LEU:HB3	2.03	0.41
1:MK:69:THR:HG22	1:MK:80:VAL:HG12	2.03	0.41
1:ML:98:VAL:O	1:ML:101:LEU:O	2.39	0.41
1:MW:68:GLU:O	1:MW:81:ARG:N	2.31	0.41
1:NB:67:THR:HA	1:NB:82:GLN:HG2	2.03	0.41
1:NC:41:PHE:HA	1:NC:68:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NH:68:GLU:N	1:NH:81:ARG:O	2.48	0.41
1:AT:34:LEU:HG	1:AT:36:GLU:OE2	2.21	0.41
1:BQ:31:GLU:OE1	1:BQ:44:LYS:HE3	2.20	0.41
1:BR:68:GLU:O	1:BR:81:ARG:N	2.38	0.41
1:BR:108:TYR:CE2	1:BR:113:LEU:HD21	2.55	0.41
1:CW:117:LEU:C	1:CW:117:LEU:HD23	2.42	0.41
1:DN:68:GLU:O	1:DN:80:VAL:HA	2.21	0.41
1:DT:26:ASP:O	1:DT:29:THR:HB	2.21	0.41
1:EE:62:HIS:O	1:EE:86:VAL:HA	2.21	0.41
1:EF:36:GLU:HB2	1:EF:39:SER:O	2.21	0.41
1:FE:21:ARG:HB2	1:FE:21:ARG:NH1	2.36	0.41
1:GA:22:LYS:O	1:GA:23:ILE:HD13	2.20	0.41
1:GA:108:TYR:CZ	1:GA:113:LEU:HD11	2.56	0.41
1:GB:8:ILE:HG12	1:GB:66:PHE:CE2	2.56	0.41
1:GO:25:GLN:HB2	1:GO:29:THR:O	2.21	0.41
1:GY:109:LEU:HD23	1:GY:113:LEU:HD22	2.02	0.41
1:HD:26:ASP:O	1:HD:29:THR:OG1	2.33	0.41
1:JA:46:ARG:HG3	1:JA:46:ARG:NH1	2.36	0.41
1:JK:4:ASP:OD1	1:JK:4:ASP:C	2.58	0.41
1:JK:36:GLU:OE2	1:JK:38:SER:OG	2.27	0.41
1:JL:86:VAL:HB	1:JQ:84:TYR:CZ	2.56	0.41
1:KD:21:ARG:HD2	1:LB:121:GLU:OE2	2.19	0.41
1:KD:108:TYR:CE2	1:KD:113:LEU:HD11	2.56	0.41
1:KE:62:HIS:O	1:KE:86:VAL:HA	2.20	0.41
1:KW:53:LYS:HB3	1:KW:54:PRO:HD3	2.03	0.41
1:LA:80:VAL:HG22	1:LA:81:ARG:N	2.36	0.41
1:MX:98:VAL:O	1:MX:101:LEU:O	2.38	0.41
1:NB:98:VAL:O	1:NB:101:LEU:O	2.38	0.41
1:AI:81:ARG:NH2	1:JG:97:THR:HG21	2.36	0.40
1:AM:25:GLN:O	1:AM:25:GLN:HG3	2.21	0.40
1:AO:86:VAL:O	1:AO:87:ILE:HD13	2.21	0.40
1:AY:109:LEU:HD23	1:AY:114:TYR:CZ	2.56	0.40
1:BG:60:GLU:N	1:BG:89:HIS:O	2.52	0.40
1:BK:67:THR:HG23	1:BK:80:VAL:CG2	2.51	0.40
1:BL:53:LYS:HD2	1:BL:54:PRO:HD3	2.03	0.40
1:BX:25:GLN:HG2	1:BX:29:THR:O	2.20	0.40
1:CI:31:GLU:HA	1:CI:43:ALA:O	2.21	0.40
1:CV:84:TYR:CZ	1:DA:86:VAL:HB	2.56	0.40
1:DI:24:ASN:H	1:DI:31:GLU:HB3	1.85	0.40
1:DZ:33:TYR:HA	1:DZ:41:PHE:O	2.21	0.40
1:EA:108:TYR:CZ	1:NI:6:LEU:HD11	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EQ:36:GLU:HB2	1:EQ:39:SER:O	2.20	0.40
1:FQ:34:LEU:HD23	1:FQ:34:LEU:C	2.40	0.40
1:GC:68:GLU:N	1:GC:81:ARG:O	2.42	0.40
1:GG:36:GLU:OE1	1:GG:37:THR:N	2.54	0.40
1:GG:55:ASN:OD1	1:GG:55:ASN:O	2.40	0.40
1:GO:19:VAL:O	1:GO:34:LEU:HD12	2.20	0.40
1:HC:31:GLU:N	1:HC:31:GLU:OE1	2.54	0.40
1:HJ:101:LEU:HD23	1:HO:81:ARG:HB3	2.02	0.40
1:HU:109:LEU:HD12	1:HU:114:TYR:CE1	2.56	0.40
1:IG:96:ALA:O	1:IG:99:SER:OG	2.31	0.40
1:IN:59:TYR:HA	1:IN:90:LYS:HA	2.02	0.40
1:IO:99:SER:O	1:IO:103:GLU:HG3	2.22	0.40
1:JF:36:GLU:HB2	1:JF:39:SER:O	2.21	0.40
1:JK:68:GLU:HB2	1:JK:81:ARG:HB2	2.03	0.40
1:JQ:20:LEU:HB3	1:JQ:32:TYR:HB3	2.01	0.40
1:KE:67:THR:HA	1:KE:81:ARG:O	2.21	0.40
1:LI:25:GLN:HA	1:LI:29:THR:O	2.21	0.40
1:LZ:80:VAL:HG12	1:ME:59:TYR:OH	2.21	0.40
1:MQ:60:GLU:OE2	1:MQ:89:HIS:CE1	2.75	0.40
1:NC:5:THR:HA	1:NC:20:LEU:O	2.21	0.40
1:NG:60:GLU:N	1:NG:60:GLU:OE1	2.54	0.40
2:M:9:SER:O	2:M:34:ASN:HB2	2.21	0.40
1:AI:23:ILE:HD12	1:AM:120:TRP:O	2.22	0.40
1:AI:80:VAL:HG22	1:AI:81:ARG:N	2.36	0.40
1:AS:68:GLU:O	1:AS:80:VAL:HA	2.21	0.40
1:AZ:117:LEU:HD23	1:AZ:117:LEU:C	2.41	0.40
1:BF:62:HIS:ND1	1:BF:87:ILE:HG23	2.37	0.40
1:BG:118:ILE:HD12	1:HE:89:HIS:CE1	2.56	0.40
1:DA:9:THR:HG22	1:DA:12:GLY:O	2.22	0.40
1:EA:60:GLU:O	1:EA:88:ARG:HA	2.21	0.40
1:EE:31:GLU:HB3	1:EE:44:LYS:HG2	2.03	0.40
1:EL:113:LEU:CD2	1:EL:117:LEU:HD23	2.51	0.40
1:EW:28:TYR:HE2	1:EX:23:ILE:HD12	1.84	0.40
1:EY:36:GLU:HB3	1:EY:39:SER:O	2.21	0.40
1:GT:63:ASN:OD1	1:GT:64:VAL:N	2.55	0.40
1:GY:39:SER:HA	1:GY:69:THR:O	2.21	0.40
1:GZ:53:LYS:HG2	1:GZ:54:PRO:HD2	2.03	0.40
1:HK:112:ALA:O	1:HK:116:LYS:HG2	2.21	0.40
1:HQ:69:THR:HG22	1:HQ:80:VAL:HG12	2.03	0.40
1:II:49:LYS:HG3	1:II:58:GLN:HE22	1.85	0.40
1:JG:39:SER:HB3	1:JG:70:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JQ:68:GLU:N	1:JQ:81:ARG:O	2.42	0.40
1:KQ:25:GLN:O	1:KQ:25:GLN:HG3	2.21	0.40
1:KU:66:PHE:O	1:KU:82:GLN:HB2	2.21	0.40
1:LG:85:VAL:HG22	1:MF:85:VAL:HG23	2.03	0.40
1:LN:103:GLU:OE2	1:LS:12:GLY:HA3	2.21	0.40
1:ME:40:SER:HG	1:ME:69:THR:HG1	1.70	0.40
1:MK:85:VAL:HG11	1:NH:109:LEU:HD11	2.02	0.40
1:MS:31:GLU:OE1	1:MS:44:LYS:NZ	2.54	0.40
1:MS:65:GLU:HG2	1:MS:84:TYR:CB	2.51	0.40
1:MW:1:ALA:O	1:MW:2:LEU:HB2	2.21	0.40
1:MW:55:ASN:O	1:MW:55:ASN:OD1	2.40	0.40
1:MX:66:PHE:O	1:MX:82:GLN:HB2	2.22	0.40
1:AA:59:TYR:CD2	1:AA:88:ARG:NH2	2.89	0.40
1:AB:114:TYR:CE1	1:AG:87:ILE:HD11	2.56	0.40
1:AG:31:GLU:N	1:AG:31:GLU:OE1	2.55	0.40
1:AI:56:GLN:OE1	1:AI:57:VAL:O	2.39	0.40
1:BE:25:GLN:HG2	1:BE:29:THR:O	2.22	0.40
1:BE:27:GLY:O	1:BE:29:THR:HG23	2.21	0.40
1:BL:108:TYR:CE2	1:BL:113:LEU:HD21	2.57	0.40
1:BY:84:TYR:CE2	1:FE:86:VAL:HG21	2.56	0.40
1:CE:50:GLU:OE2	1:CE:50:GLU:N	2.53	0.40
1:CW:80:VAL:HG22	1:CW:81:ARG:N	2.37	0.40
1:DN:46:ARG:NH2	1:DN:63:ASN:ND2	2.69	0.40
1:DN:84:TYR:CE1	1:DS:86:VAL:HB	2.56	0.40
1:EG:54:PRO:O	1:EG:55:ASN:OD1	2.39	0.40
1:GO:29:THR:HG22	1:GO:46:ARG:HG3	2.04	0.40
1:GY:89:HIS:ND1	1:GY:93:ASP:OD1	2.52	0.40
1:HQ:25:GLN:O	1:HQ:25:GLN:HG3	2.21	0.40
1:HW:60:GLU:OE1	1:HW:60:GLU:N	2.53	0.40
1:IT:53:LYS:HG2	1:IT:54:PRO:HD2	2.04	0.40
1:JA:117:LEU:C	1:JA:117:LEU:HD23	2.41	0.40
1:JG:109:LEU:HD13	1:JG:114:TYR:OH	2.21	0.40
1:JL:81:ARG:NH1	1:JQ:97:THR:HG21	2.37	0.40
1:JS:34:LEU:HD21	1:JS:36:GLU:OE2	2.22	0.40
1:LS:113:LEU:O	1:LS:117:LEU:CD1	2.70	0.40
1:MA:27:GLY:O	1:MA:29:THR:HG23	2.20	0.40
1:MG:25:GLN:HB2	1:MG:29:THR:O	2.22	0.40
1:NC:55:ASN:O	1:NC:56:GLN:NE2	2.54	0.40
2:M:153:LYS:O	2:M:156:ILE:HG12	2.21	0.40
1:AB:86:VAL:HG21	1:AG:84:TYR:CZ	2.56	0.40
1:AG:64:VAL:O	1:AG:84:TYR:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AH:61:ARG:HA	1:AH:87:ILE:O	2.22	0.40
1:AO:20:LEU:HB3	1:AO:32:TYR:HB3	2.03	0.40
1:AY:93:ASP:OD1	1:AY:93:ASP:N	2.54	0.40
1:BL:68:GLU:OE1	1:BL:81:ARG:NH1	2.51	0.40
1:BL:84:TYR:CZ	1:BQ:86:VAL:CG1	3.04	0.40
1:CK:111:GLU:OE1	1:II:103:GLU:OE1	2.38	0.40
1:CQ:27:GLY:O	1:CQ:28:TYR:HB2	2.21	0.40
1:DO:69:THR:HG22	1:DO:80:VAL:HG12	2.03	0.40
1:DU:27:GLY:O	1:DU:28:TYR:HB2	2.22	0.40
1:EF:53:LYS:HD3	1:EF:54:PRO:HD2	2.03	0.40
1:EK:19:VAL:O	1:EK:34:LEU:HD12	2.21	0.40
1:FD:80:VAL:HG22	1:FD:81:ARG:N	2.37	0.40
1:FE:85:VAL:HG12	1:FE:86:VAL:N	2.37	0.40
1:FU:27:GLY:O	1:FU:29:THR:HG23	2.22	0.40
1:FV:89:HIS:NE2	1:GA:118:ILE:CD1	2.85	0.40
1:FV:122:SER:OG	1:GA:30:SER:OG	1.98	0.40
1:HC:99:SER:OG	1:HC:103:GLU:OE2	2.37	0.40
1:HI:99:SER:O	1:HI:103:GLU:HG3	2.22	0.40
1:HO:91:VAL:HG13	1:HO:92:GLY:N	2.37	0.40
1:IG:24:ASN:HB3	1:IG:31:GLU:OE2	2.22	0.40
1:IS:113:LEU:HD23	1:IS:113:LEU:O	2.21	0.40
1:IT:98:VAL:O	1:IT:101:LEU:O	2.40	0.40
1:ME:21:ARG:CZ	1:ME:21:ARG:HB2	2.52	0.40
1:MF:20:LEU:HD21	1:MF:41:PHE:HB3	2.04	0.40
1:NG:62:HIS:O	1:NG:87:ILE:N	2.47	0.40
1:NH:8:ILE:HG13	1:NH:8:ILE:O	2.21	0.40
2:M:170:ARG:HB2	2:M:276:TRP:CH2	2.56	0.40
1:AB:113:LEU:O	1:AB:117:LEU:HG	2.22	0.40
1:AN:100:ASP:OD2	1:AS:11:GLY:N	2.55	0.40
1:BA:62:HIS:O	1:BA:86:VAL:HA	2.21	0.40
1:BF:80:VAL:HG12	1:BF:81:ARG:N	2.37	0.40
1:BG:68:GLU:OE2	1:BG:81:ARG:HB2	2.22	0.40
1:BQ:23:ILE:HD12	1:MG:120:TRP:HB3	2.02	0.40
1:CJ:117:LEU:HD23	1:CJ:117:LEU:C	2.41	0.40
1:CQ:33:TYR:CD1	1:CQ:34:LEU:N	2.89	0.40
1:CV:61:ARG:HA	1:CV:87:ILE:O	2.22	0.40
1:DG:5:THR:HG22	1:DG:21:ARG:NH2	2.36	0.40
1:FP:109:LEU:CD2	1:FP:113:LEU:HD23	2.49	0.40
1:FV:65:GLU:OE1	1:FV:65:GLU:N	2.54	0.40
1:GG:61:ARG:HA	1:GG:87:ILE:O	2.21	0.40
1:GZ:62:HIS:CB	1:HC:117:LEU:HD21	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GZ:81:ARG:HH21	1:HC:97:THR:HG21	1.85	0.40
1:HK:32:TYR:N	1:HK:43:ALA:O	2.49	0.40
1:JY:34:LEU:HD23	1:JY:34:LEU:C	2.42	0.40
1:KE:53:LYS:HB3	1:KE:56:GLN:HE22	1.87	0.40
1:KO:20:LEU:HB3	1:KO:32:TYR:HB3	2.04	0.40
1:KV:53:LYS:HB3	1:KV:54:PRO:HD2	2.02	0.40
1:LC:36:GLU:HB2	1:LC:39:SER:O	2.21	0.40
1:LG:34:LEU:HD12	1:LG:35:PRO:HD2	2.03	0.40
1:LH:86:VAL:HG11	1:LM:84:TYR:CZ	2.57	0.40
1:LZ:84:TYR:CE1	1:ME:86:VAL:HG21	2.57	0.40
1:MK:108:TYR:CZ	1:MK:113:LEU:HD21	2.56	0.40
1:MM:114:TYR:O	1:MM:118:ILE:CD1	2.67	0.40
1:NC:6:LEU:HB2	1:NC:32:TYR:CE2	2.57	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	AA	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	AB	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	AC	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	AG	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	AH	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	AI	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	AM	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	AN	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	AO	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
1	AS	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AT	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	AU	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	AY	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	AZ	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	BA	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	BE	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	BF	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
1	BG	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	BK	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	BL	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	BM	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	BQ	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
1	BR	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	BS	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	BW	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	BX	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	BY	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	CC	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	CD	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	CE	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	CI	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	CJ	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	CK	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	CO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	CP	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	CQ	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	CU	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	CV	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	CW	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	DA	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	DB	120/122 (98%)	116 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DC	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	DG	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	DH	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	DI	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	DM	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	DN	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	DO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	DS	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	DT	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	DU	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	DY	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	DZ	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	EA	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	EE	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	19	43
1	EF	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	EG	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	EK	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	EL	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	EM	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	EQ	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	ER	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
1	ES	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	EW	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	EX	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
1	EY	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	FC	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
1	FD	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	FE	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	FI	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
1	FJ	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	FK	120/122 (98%)	113 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	FO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	FP	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	FQ	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	FU	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	FV	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	FW	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	GA	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	GB	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	GC	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	GG	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
1	GH	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	GI	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	GM	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	GN	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	GO	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	GS	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	GT	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	GU	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	GY	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
1	GZ	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	HC	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	HD	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	HE	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	HI	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	HJ	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	HK	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	HO	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
1	HP	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	HQ	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	HU	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	HV	120/122 (98%)	115 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	HW	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	IA	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
1	IB	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	IC	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	IG	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
1	IH	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	II	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	IM	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	IN	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	IO	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	IS	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	IT	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	IU	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	IY	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	IZ	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	JA	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	JE	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	JF	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	JG	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	JK	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
1	JL	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	JM	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
1	JQ	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	JR	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
1	JS	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
1	JW	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
1	JX	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
1	JY	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	KC	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	KD	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	KE	120/122 (98%)	117 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	KI	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	KJ	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	KK	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	KO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	KP	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	KQ	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	KU	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	KV	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	KW	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	LA	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	LB	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	LC	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	LG	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	LH	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	LI	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	LM	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	LN	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	LO	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
1	LS	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	LT	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	LU	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	LY	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	LZ	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	MA	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	ME	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
1	MF	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	MG	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	MK	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	ML	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	MM	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	MQ	120/122 (98%)	113 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	MR	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	MS	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	MW	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
1	MX	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	NA	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	NB	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	NC	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	NG	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	NH	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
1	NI	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	NM	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	NN	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
1	NO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
2	M	370/372 (100%)	359 (97%)	11 (3%)	0	100	100
All	All	21730/22088 (98%)	20647 (95%)	1081 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	EE	54	PRO
1	AS	54	PRO

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	AA	103/103 (100%)	103 (100%)	0	100	100
1	AB	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	AC	103/103 (100%)	103 (100%)	0	100	100
1	AG	103/103 (100%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AH	103/103 (100%)	103 (100%)	0	100	100
1	AI	103/103 (100%)	103 (100%)	0	100	100
1	AM	103/103 (100%)	103 (100%)	0	100	100
1	AN	103/103 (100%)	103 (100%)	0	100	100
1	AO	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	AS	103/103 (100%)	103 (100%)	0	100	100
1	AT	103/103 (100%)	103 (100%)	0	100	100
1	AU	103/103 (100%)	103 (100%)	0	100	100
1	AY	103/103 (100%)	103 (100%)	0	100	100
1	AZ	103/103 (100%)	103 (100%)	0	100	100
1	BA	103/103 (100%)	103 (100%)	0	100	100
1	BE	103/103 (100%)	103 (100%)	0	100	100
1	BF	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	BG	103/103 (100%)	103 (100%)	0	100	100
1	BK	103/103 (100%)	103 (100%)	0	100	100
1	BL	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	BM	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	BQ	103/103 (100%)	103 (100%)	0	100	100
1	BR	103/103 (100%)	103 (100%)	0	100	100
1	BS	103/103 (100%)	103 (100%)	0	100	100
1	BW	103/103 (100%)	103 (100%)	0	100	100
1	BX	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	BY	103/103 (100%)	103 (100%)	0	100	100
1	CC	103/103 (100%)	103 (100%)	0	100	100
1	CD	103/103 (100%)	103 (100%)	0	100	100
1	CE	103/103 (100%)	103 (100%)	0	100	100
1	CI	103/103 (100%)	103 (100%)	0	100	100
1	CJ	103/103 (100%)	103 (100%)	0	100	100
1	CK	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	CO	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	CP	103/103 (100%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CQ	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	CU	103/103 (100%)	103 (100%)	0	100	100
1	CV	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	CW	103/103 (100%)	103 (100%)	0	100	100
1	DA	103/103 (100%)	103 (100%)	0	100	100
1	DB	103/103 (100%)	103 (100%)	0	100	100
1	DC	103/103 (100%)	103 (100%)	0	100	100
1	DG	103/103 (100%)	103 (100%)	0	100	100
1	DH	103/103 (100%)	103 (100%)	0	100	100
1	DI	103/103 (100%)	103 (100%)	0	100	100
1	DM	103/103 (100%)	103 (100%)	0	100	100
1	DN	103/103 (100%)	103 (100%)	0	100	100
1	DO	103/103 (100%)	103 (100%)	0	100	100
1	DS	103/103 (100%)	103 (100%)	0	100	100
1	DT	103/103 (100%)	103 (100%)	0	100	100
1	DU	103/103 (100%)	103 (100%)	0	100	100
1	DY	103/103 (100%)	103 (100%)	0	100	100
1	DZ	103/103 (100%)	103 (100%)	0	100	100
1	EA	103/103 (100%)	103 (100%)	0	100	100
1	EE	103/103 (100%)	103 (100%)	0	100	100
1	EF	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	EG	103/103 (100%)	103 (100%)	0	100	100
1	EK	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	EL	103/103 (100%)	103 (100%)	0	100	100
1	EM	103/103 (100%)	103 (100%)	0	100	100
1	EQ	103/103 (100%)	103 (100%)	0	100	100
1	ER	103/103 (100%)	103 (100%)	0	100	100
1	ES	103/103 (100%)	103 (100%)	0	100	100
1	EW	103/103 (100%)	103 (100%)	0	100	100
1	EX	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	EY	103/103 (100%)	102 (99%)	1 (1%)	76	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FC	103/103 (100%)	103 (100%)	0	100	100
1	FD	103/103 (100%)	103 (100%)	0	100	100
1	FE	103/103 (100%)	103 (100%)	0	100	100
1	FI	103/103 (100%)	103 (100%)	0	100	100
1	FJ	103/103 (100%)	103 (100%)	0	100	100
1	FK	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	FO	103/103 (100%)	103 (100%)	0	100	100
1	FP	103/103 (100%)	103 (100%)	0	100	100
1	FQ	103/103 (100%)	103 (100%)	0	100	100
1	FU	103/103 (100%)	103 (100%)	0	100	100
1	FV	103/103 (100%)	103 (100%)	0	100	100
1	FW	103/103 (100%)	103 (100%)	0	100	100
1	GA	103/103 (100%)	103 (100%)	0	100	100
1	GB	103/103 (100%)	103 (100%)	0	100	100
1	GC	103/103 (100%)	103 (100%)	0	100	100
1	GG	103/103 (100%)	103 (100%)	0	100	100
1	GH	103/103 (100%)	103 (100%)	0	100	100
1	GI	103/103 (100%)	103 (100%)	0	100	100
1	GM	103/103 (100%)	103 (100%)	0	100	100
1	GN	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	GO	103/103 (100%)	103 (100%)	0	100	100
1	GS	103/103 (100%)	103 (100%)	0	100	100
1	GT	103/103 (100%)	103 (100%)	0	100	100
1	GU	103/103 (100%)	103 (100%)	0	100	100
1	GY	103/103 (100%)	103 (100%)	0	100	100
1	GZ	103/103 (100%)	103 (100%)	0	100	100
1	HC	103/103 (100%)	103 (100%)	0	100	100
1	HD	103/103 (100%)	103 (100%)	0	100	100
1	HE	103/103 (100%)	103 (100%)	0	100	100
1	HI	103/103 (100%)	103 (100%)	0	100	100
1	HJ	103/103 (100%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	HK	103/103 (100%)	103 (100%)	0	100	100
1	HO	103/103 (100%)	103 (100%)	0	100	100
1	HP	103/103 (100%)	103 (100%)	0	100	100
1	HQ	103/103 (100%)	103 (100%)	0	100	100
1	HU	103/103 (100%)	103 (100%)	0	100	100
1	HV	103/103 (100%)	103 (100%)	0	100	100
1	HW	103/103 (100%)	103 (100%)	0	100	100
1	IA	103/103 (100%)	103 (100%)	0	100	100
1	IB	103/103 (100%)	103 (100%)	0	100	100
1	IC	103/103 (100%)	103 (100%)	0	100	100
1	IG	103/103 (100%)	103 (100%)	0	100	100
1	IH	103/103 (100%)	103 (100%)	0	100	100
1	II	103/103 (100%)	103 (100%)	0	100	100
1	IM	103/103 (100%)	103 (100%)	0	100	100
1	IN	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	IO	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	IS	103/103 (100%)	103 (100%)	0	100	100
1	IT	103/103 (100%)	103 (100%)	0	100	100
1	IU	103/103 (100%)	103 (100%)	0	100	100
1	IY	103/103 (100%)	103 (100%)	0	100	100
1	IZ	103/103 (100%)	103 (100%)	0	100	100
1	JA	103/103 (100%)	103 (100%)	0	100	100
1	JE	103/103 (100%)	103 (100%)	0	100	100
1	JF	103/103 (100%)	103 (100%)	0	100	100
1	JG	103/103 (100%)	103 (100%)	0	100	100
1	JK	103/103 (100%)	103 (100%)	0	100	100
1	JL	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	JM	103/103 (100%)	103 (100%)	0	100	100
1	JQ	103/103 (100%)	103 (100%)	0	100	100
1	JR	103/103 (100%)	103 (100%)	0	100	100
1	JS	103/103 (100%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	JW	103/103 (100%)	103 (100%)	0	100	100
1	JX	103/103 (100%)	103 (100%)	0	100	100
1	JY	103/103 (100%)	103 (100%)	0	100	100
1	KC	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	KD	103/103 (100%)	103 (100%)	0	100	100
1	KE	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	KI	103/103 (100%)	103 (100%)	0	100	100
1	KJ	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	KK	103/103 (100%)	103 (100%)	0	100	100
1	KO	103/103 (100%)	103 (100%)	0	100	100
1	KP	103/103 (100%)	103 (100%)	0	100	100
1	KQ	103/103 (100%)	103 (100%)	0	100	100
1	KU	103/103 (100%)	103 (100%)	0	100	100
1	KV	103/103 (100%)	103 (100%)	0	100	100
1	KW	103/103 (100%)	103 (100%)	0	100	100
1	LA	103/103 (100%)	103 (100%)	0	100	100
1	LB	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	LC	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	LG	103/103 (100%)	103 (100%)	0	100	100
1	LH	103/103 (100%)	103 (100%)	0	100	100
1	LI	103/103 (100%)	103 (100%)	0	100	100
1	LM	103/103 (100%)	103 (100%)	0	100	100
1	LN	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	LO	103/103 (100%)	103 (100%)	0	100	100
1	LS	103/103 (100%)	103 (100%)	0	100	100
1	LT	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	LU	103/103 (100%)	103 (100%)	0	100	100
1	LY	103/103 (100%)	103 (100%)	0	100	100
1	LZ	103/103 (100%)	103 (100%)	0	100	100
1	MA	103/103 (100%)	103 (100%)	0	100	100
1	ME	103/103 (100%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	MF	103/103 (100%)	103 (100%)	0	100	100
1	MG	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	MK	103/103 (100%)	103 (100%)	0	100	100
1	ML	103/103 (100%)	103 (100%)	0	100	100
1	MM	103/103 (100%)	103 (100%)	0	100	100
1	MQ	103/103 (100%)	103 (100%)	0	100	100
1	MR	103/103 (100%)	103 (100%)	0	100	100
1	MS	103/103 (100%)	103 (100%)	0	100	100
1	MW	103/103 (100%)	103 (100%)	0	100	100
1	MX	103/103 (100%)	103 (100%)	0	100	100
1	NA	103/103 (100%)	103 (100%)	0	100	100
1	NB	103/103 (100%)	103 (100%)	0	100	100
1	NC	103/103 (100%)	103 (100%)	0	100	100
1	NG	103/103 (100%)	103 (100%)	0	100	100
1	NH	103/103 (100%)	103 (100%)	0	100	100
1	NI	103/103 (100%)	103 (100%)	0	100	100
1	NM	103/103 (100%)	103 (100%)	0	100	100
1	NN	103/103 (100%)	102 (99%)	1 (1%)	76	91
1	NO	103/103 (100%)	103 (100%)	0	100	100
2	M	313/313 (100%)	313 (100%)	0	100	100
All	All	18647/18647 (100%)	18619 (100%)	28 (0%)	93	98

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	46	ARG
1	AO	90	LYS
1	BF	81	ARG
1	BL	88	ARG
1	BM	53	LYS
1	BX	88	ARG
1	CK	53	LYS
1	CO	53	LYS
1	CQ	46	ARG
1	CV	61	ARG

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Mol	Chain	Res	Type
1	EF	53	LYS
1	EK	81	ARG
1	EX	46	ARG
1	EY	21	ARG
1	FK	53	LYS
1	GN	46	ARG
1	IN	53	LYS
1	IO	21	ARG
1	JL	53	LYS
1	KC	21	ARG
1	KE	61	ARG
1	KJ	46	ARG
1	LB	81	ARG
1	LC	21	ARG
1	LN	46	ARG
1	LT	21	ARG
1	MG	90	LYS
1	NN	53	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	62	HIS
1	AC	62	HIS
1	AM	62	HIS
1	AS	56	GLN
1	BM	58	GLN
1	BQ	58	GLN
1	BY	62	HIS
1	CE	62	HIS
1	CJ	56	GLN
1	CW	62	HIS
1	DI	62	HIS
1	EG	62	HIS
1	EQ	47	HIS
1	EQ	62	HIS
1	EX	56	GLN
1	GC	56	GLN
1	GH	62	HIS
1	GH	82	GLN
1	GS	62	HIS
1	GT	58	GLN

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Mol	Chain	Res	Type
1	HE	58	GLN
1	HE	89	HIS
1	IC	56	GLN
1	IC	62	HIS
1	II	58	GLN
1	IN	56	GLN
1	IS	58	GLN
1	JK	55	ASN
1	KW	62	HIS
1	LI	62	HIS
1	MA	56	GLN
1	NA	89	HIS
2	M	177	HIS
2	M	209	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 236 ligands modelled in this entry, 236 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

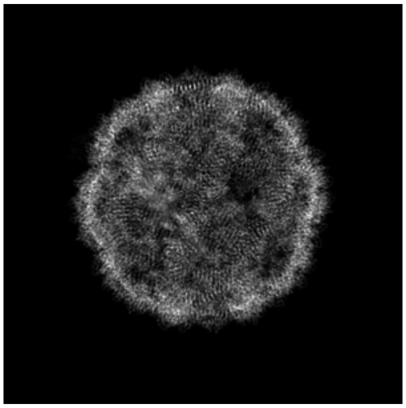
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-42163. These allow visual inspection of the internal detail of the map and identification of artifacts.

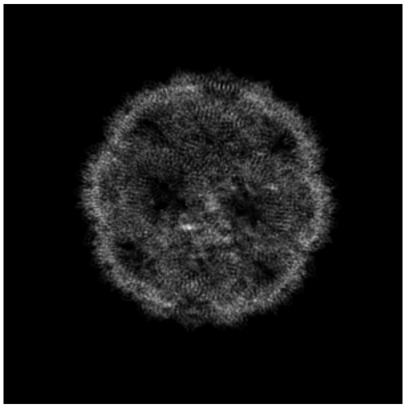
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

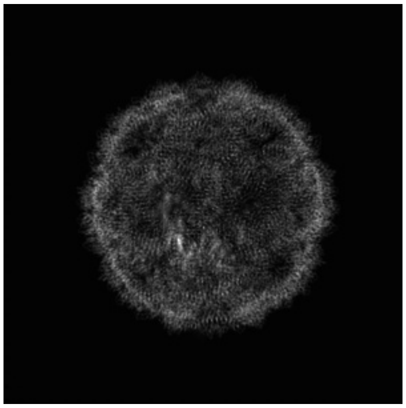
6.1.1 Primary map



X

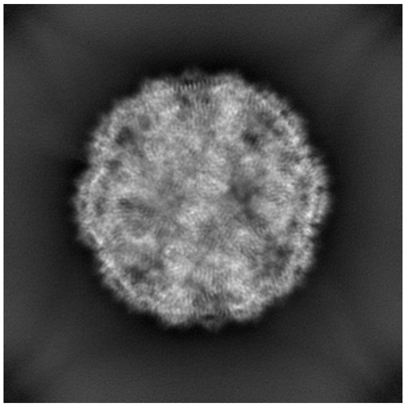


Y

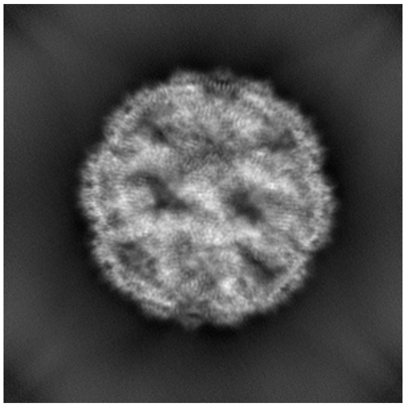


Z

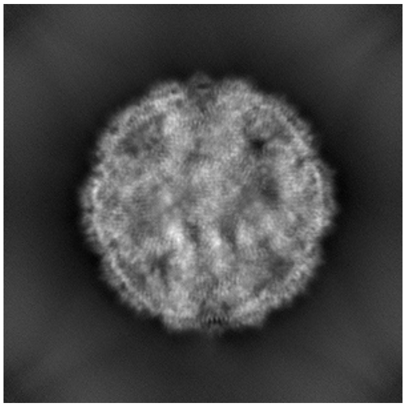
6.1.2 Raw map



X



Y

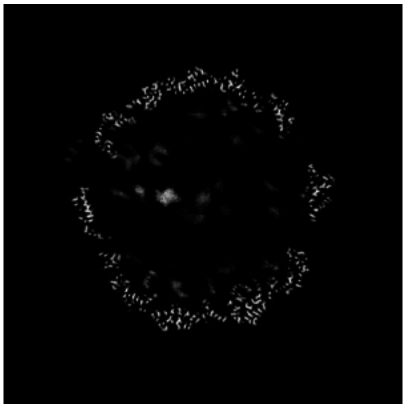


Z

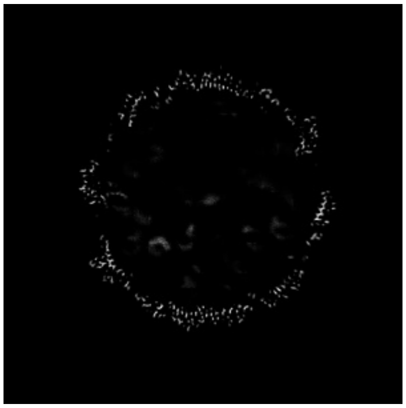
The images above show the map projected in three orthogonal directions.

6.2 Central slices

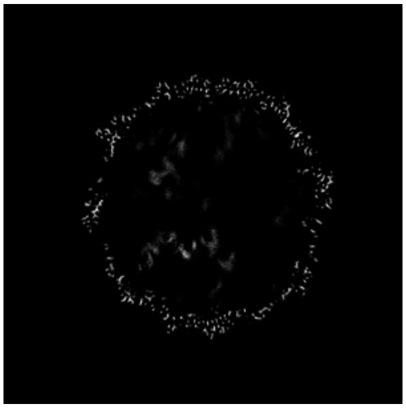
6.2.1 Primary map



X Index: 256

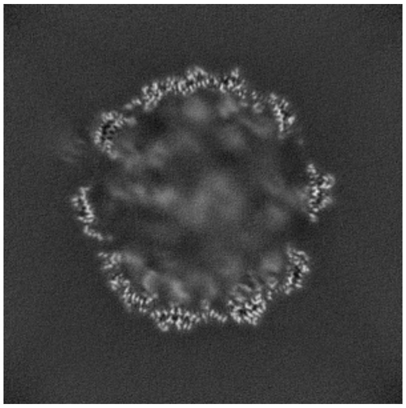


Y Index: 256

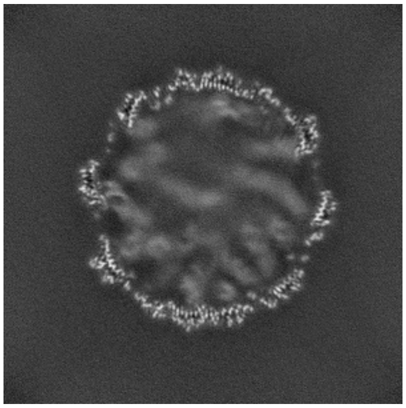


Z Index: 256

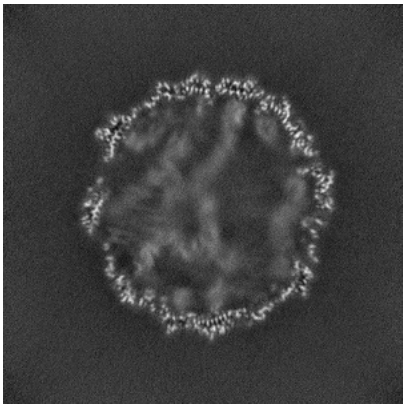
6.2.2 Raw map



X Index: 256



Y Index: 256

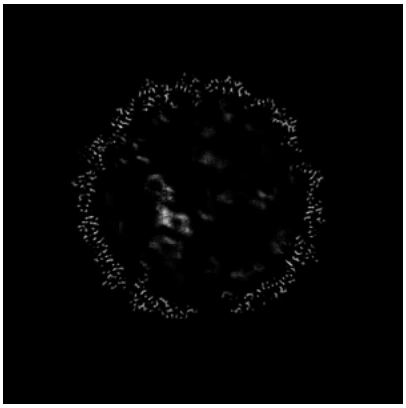


Z Index: 256

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

6.3 Largest variance slices

6.3.1 Primary map

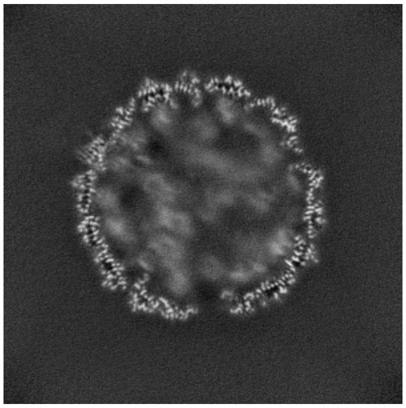


X Index: 224

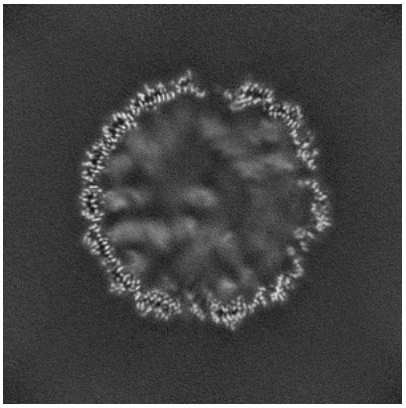
Y Index: 210

Z Index: 284

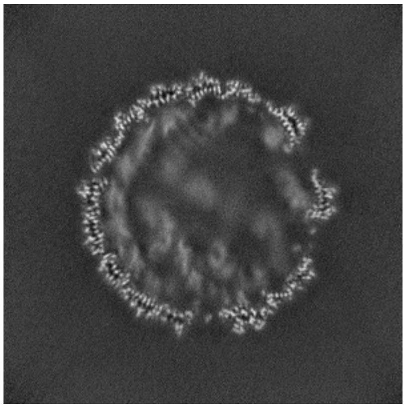
6.3.2 Raw map



X Index: 224



Y Index: 221

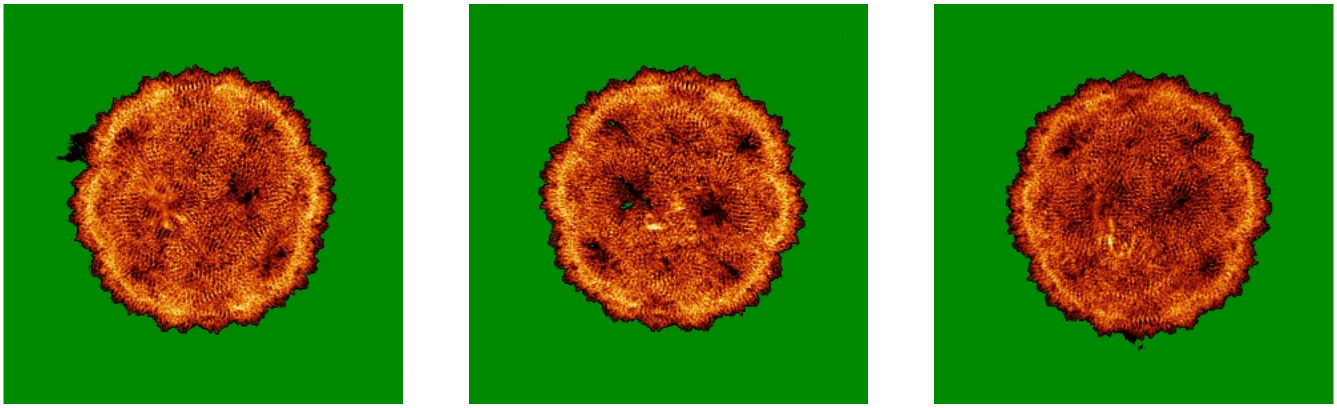


Z Index: 284

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

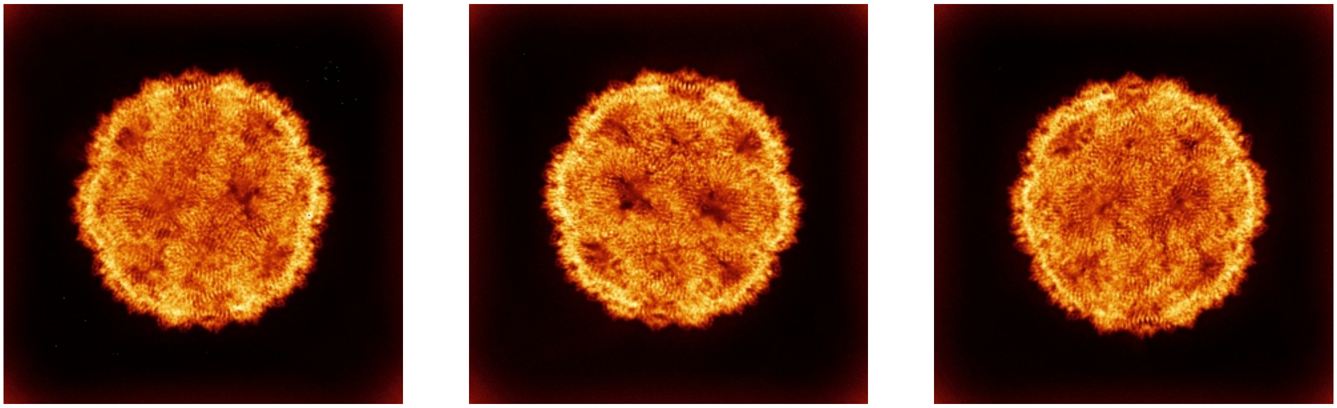
6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

The images above show the 3D surface view of the map at the recommended contour level 0.0334. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

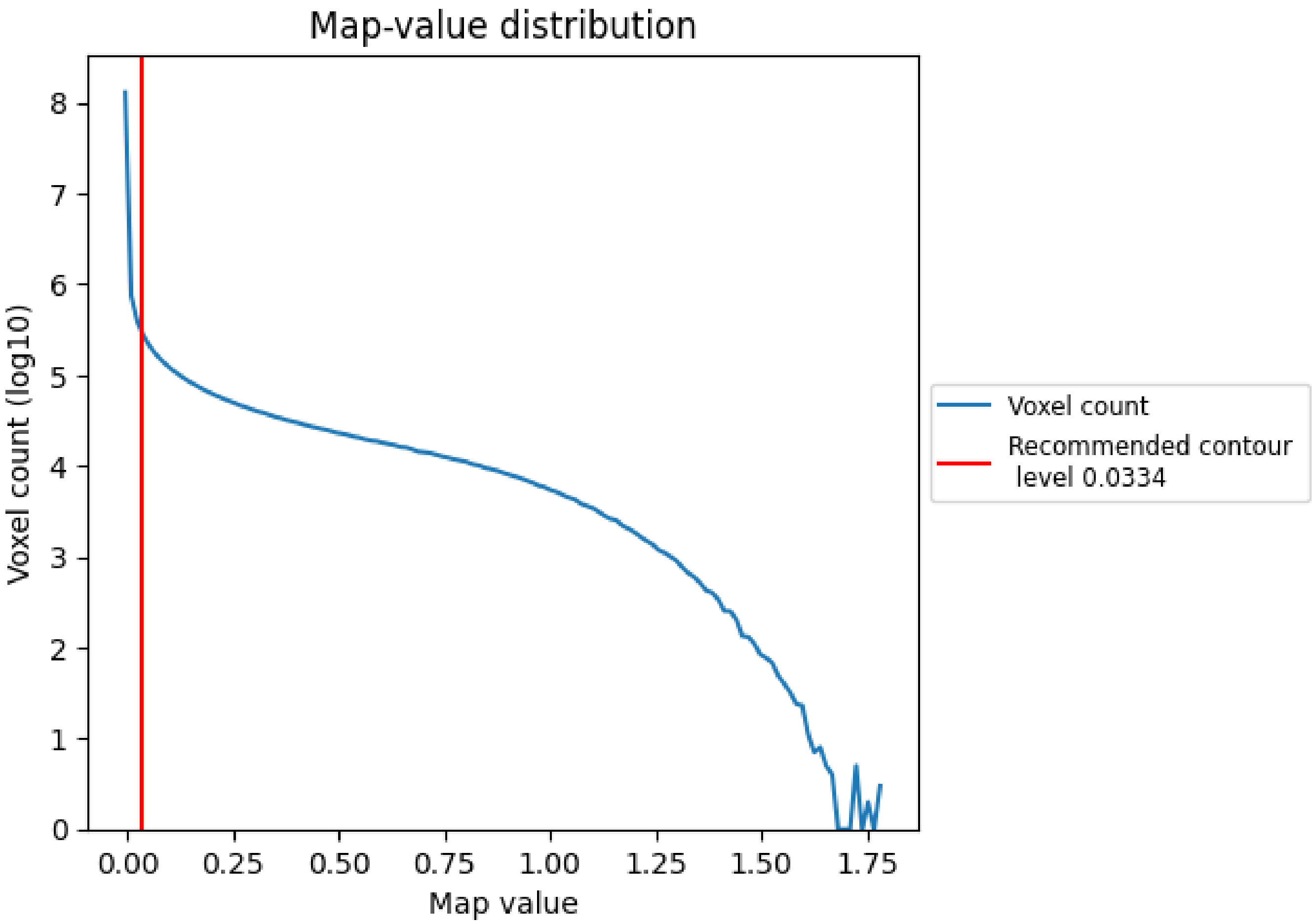
6.6 Mask visualisation (i)

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

7 Map analysis ⓘ

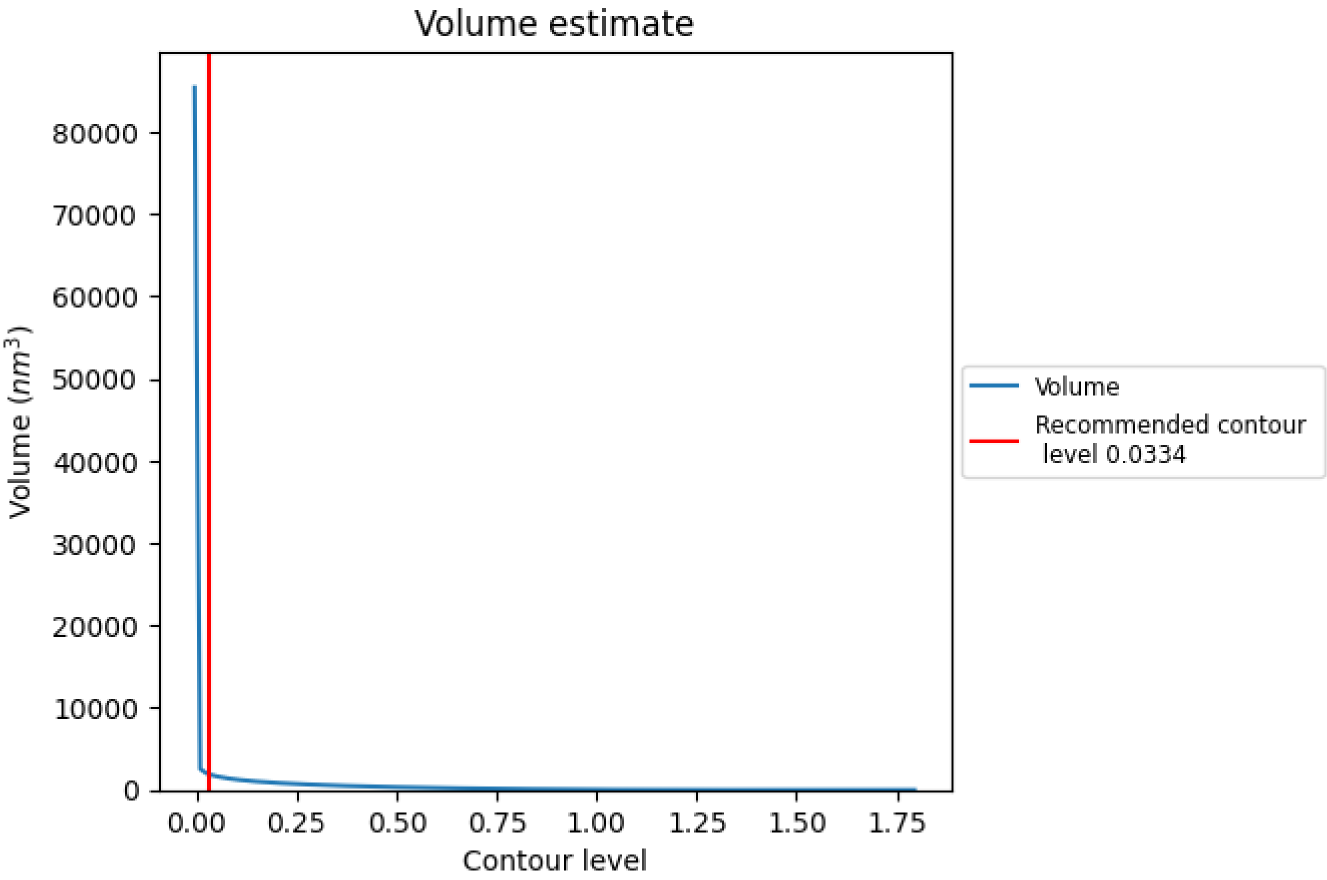
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

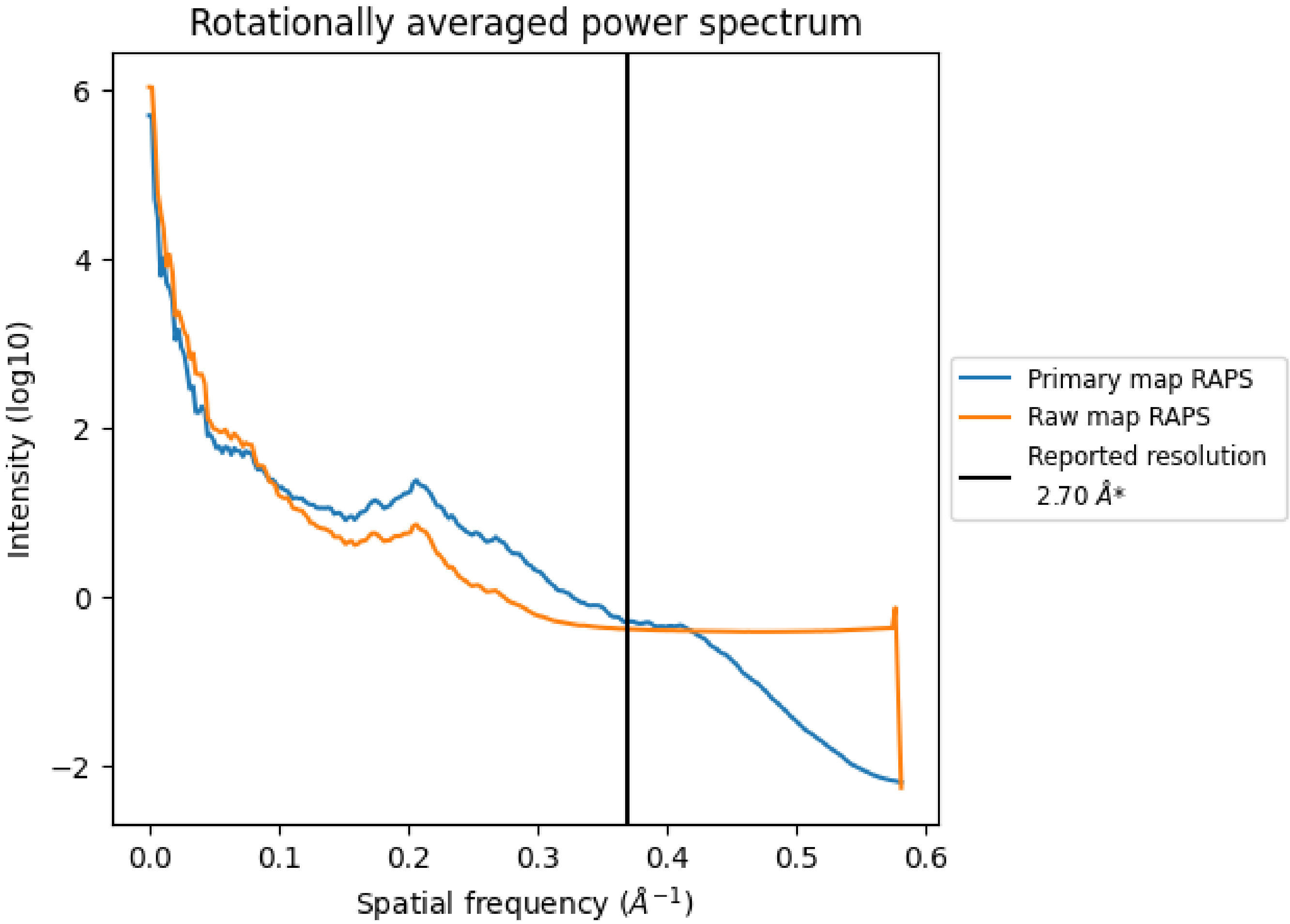
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1886 nm^3; this corresponds to an approximate mass of 1704 kDa.

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

7.3 Rotationally averaged power spectrum (i)

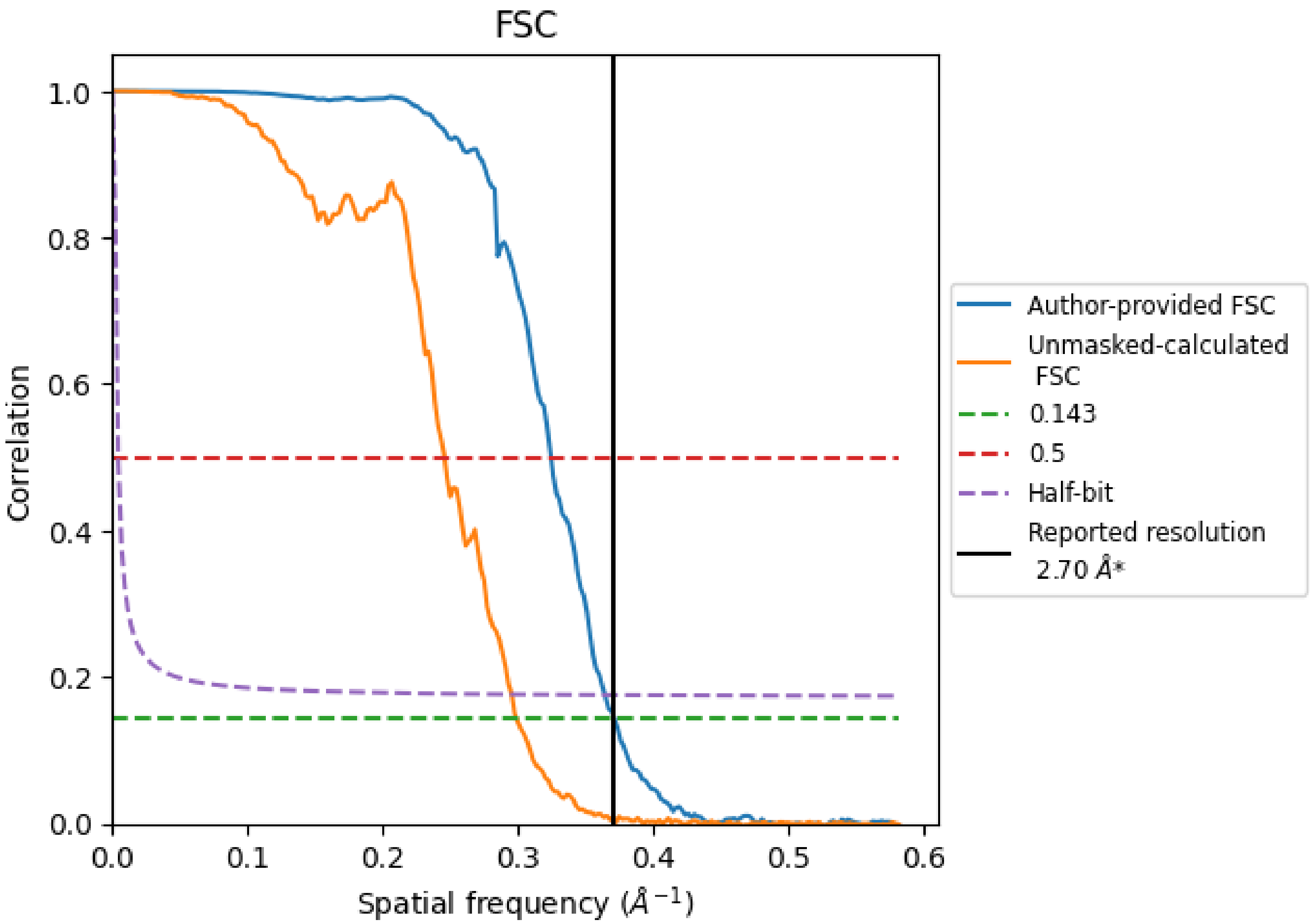


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates

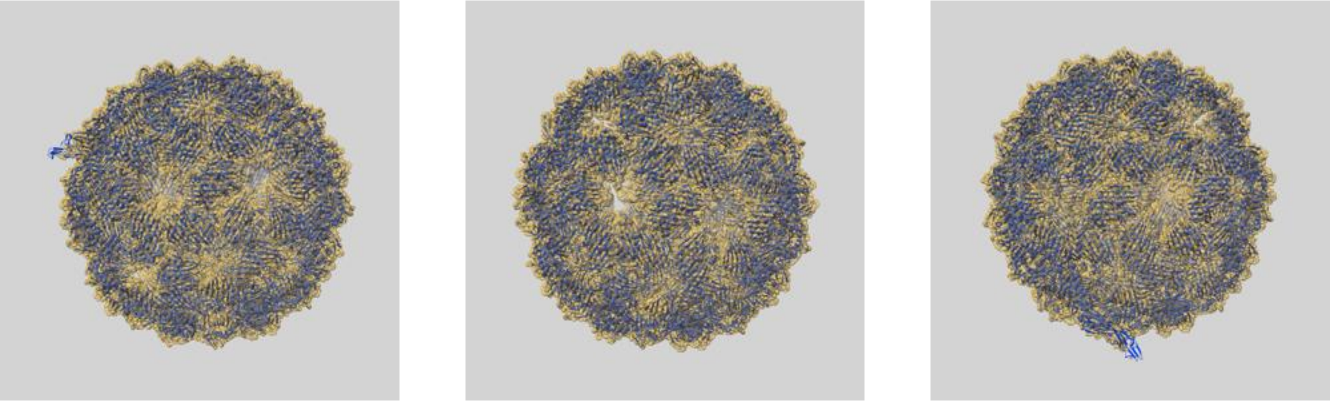
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.69	3.08	2.75
Unmasked-calculated*	3.35	4.07	3.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.35 differs from the reported value 2.7 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-42163 and PDB model 8UEJ. Per-residue inclusion information can be found in section 3 on page 26.

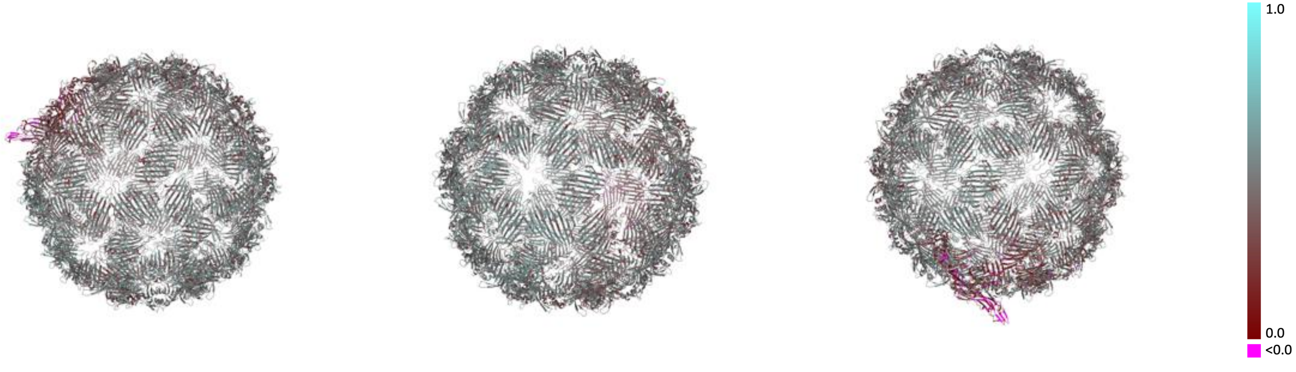
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0334 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.

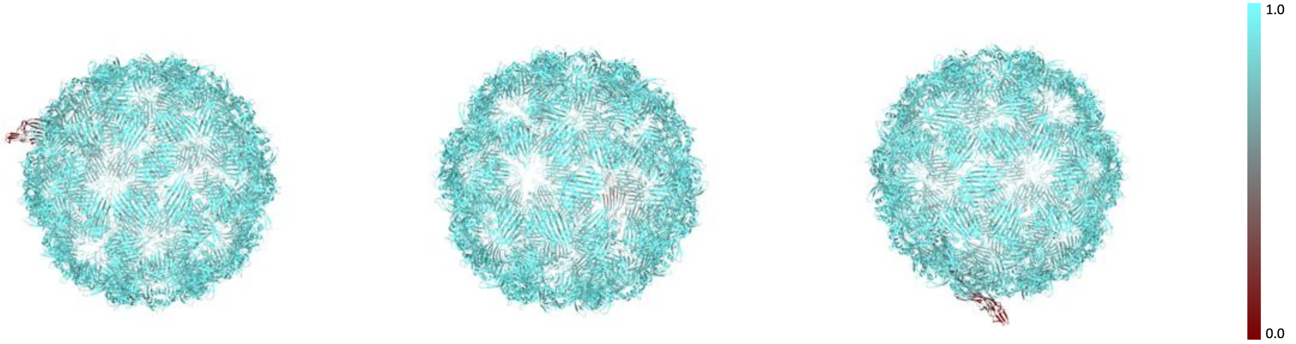
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

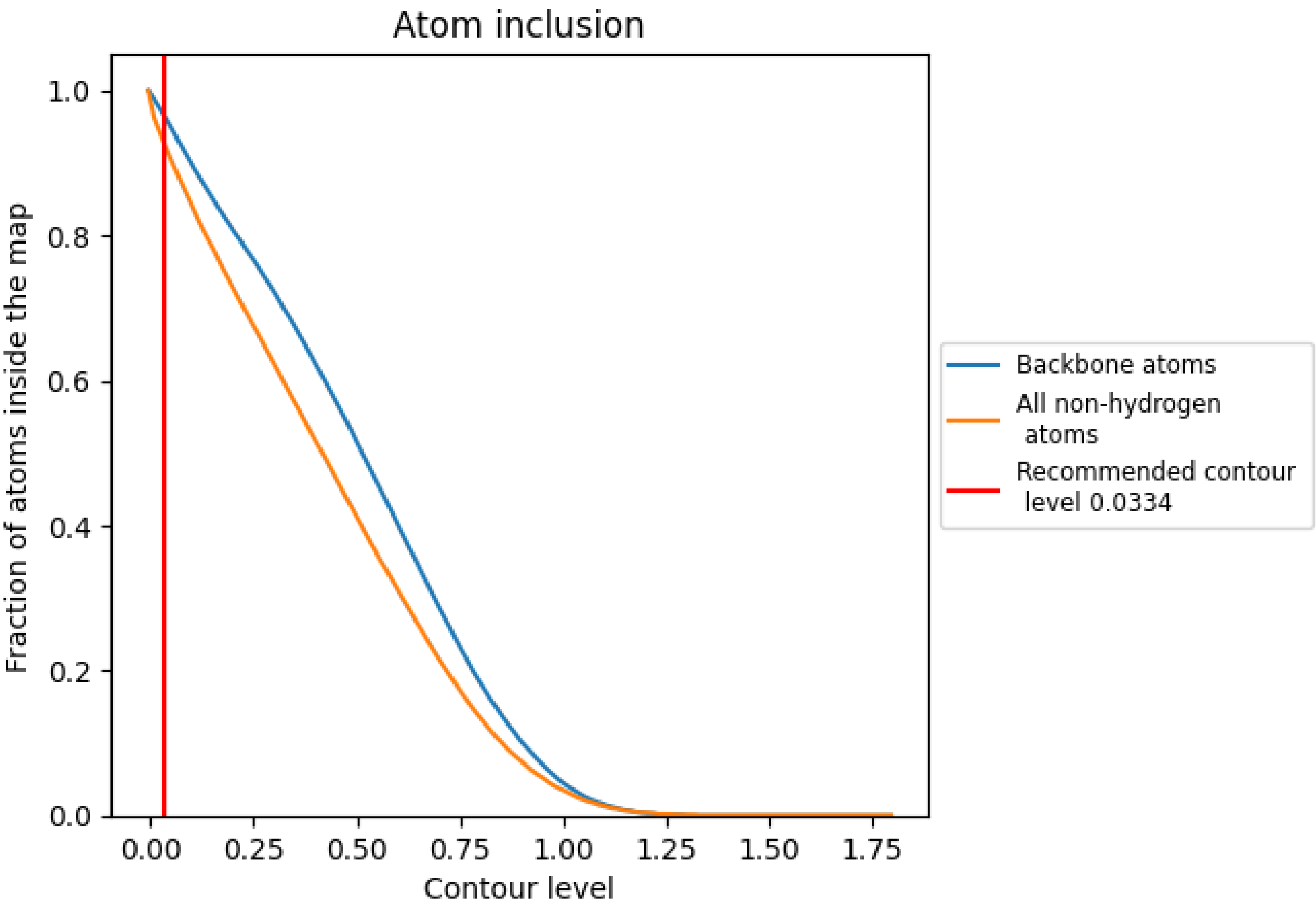
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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 (0.0334).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.0334) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9270	0.4490
AA	0.9500	0.4710
AB	0.9540	0.4970
AC	0.9460	0.4970
AG	0.9440	0.4940
AH	0.9570	0.4910
AI	0.9380	0.4810
AM	0.9420	0.4880
AN	0.9350	0.4560
AO	0.9390	0.4770
AS	0.9390	0.4470
AT	0.9190	0.4410
AU	0.9200	0.4040
AY	0.9320	0.4380
AZ	0.8900	0.3810
BA	0.9000	0.4050
BE	0.9130	0.3870
BF	0.9390	0.4610
BG	0.9150	0.4280
BK	0.9550	0.4970
BL	0.9450	0.4650
BM	0.9440	0.4670
BQ	0.9500	0.4860
BR	0.9280	0.4620
BS	0.9450	0.4760
BW	0.9240	0.4420
BX	0.9120	0.4400
BY	0.9140	0.4170
CC	0.9390	0.4780
CD	0.9410	0.4760
CE	0.9410	0.4650
CI	0.9360	0.4660
CJ	0.9420	0.4800
CK	0.9290	0.4410
CO	0.9380	0.4710

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Chain	Atom inclusion	Q-score
CP	0.9410	0.4830
CQ	0.9410	0.4650
CU	0.9310	0.4650
CV	0.9430	0.4770
CW	0.9290	0.4680
DA	0.9250	0.4580
DB	0.9450	0.4810
DC	0.9350	0.4730
DG	0.9380	0.4370
DH	0.9200	0.4460
DI	0.9300	0.4510
DM	0.9270	0.4540
DN	0.9240	0.4300
DO	0.9360	0.4430
DS	0.9270	0.4400
DT	0.9300	0.4340
DU	0.9230	0.4350
DY	0.9280	0.4200
DZ	0.9340	0.4390
EA	0.9280	0.4270
EE	0.9340	0.4330
EF	0.9360	0.4430
EG	0.9120	0.4270
EK	0.9370	0.4360
EL	0.9400	0.4940
EM	0.9400	0.4720
EQ	0.9550	0.5070
ER	0.9490	0.5010
ES	0.9500	0.5040
EW	0.9540	0.5060
EX	0.9480	0.4850
EY	0.9550	0.4910
FC	0.9360	0.4640
FD	0.9300	0.4550
FE	0.9260	0.4300
FI	0.9230	0.4380
FJ	0.9260	0.4430
FK	0.9180	0.4150
FO	0.9490	0.4920
FP	0.9290	0.4740
FQ	0.9480	0.4860
FU	0.9280	0.4630

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Chain	Atom inclusion	Q-score
FV	0.9360	0.4460
FW	0.9310	0.4340
GA	0.9350	0.4460
GB	0.9390	0.4750
GC	0.9330	0.4500
GG	0.9460	0.4840
GH	0.9380	0.4700
GI	0.9230	0.4630
GM	0.9370	0.4630
GN	0.9400	0.4800
GO	0.9390	0.4790
GS	0.9410	0.4980
GT	0.9300	0.4380
GU	0.9400	0.4900
GY	0.8880	0.3900
GZ	0.9230	0.4560
HC	0.9440	0.4750
HD	0.9320	0.4570
HE	0.9250	0.4290
HI	0.9320	0.4420
HJ	0.9310	0.4670
HK	0.9340	0.4270
HO	0.9550	0.4910
HP	0.9570	0.5150
HQ	0.9500	0.4980
HU	0.9400	0.4530
HV	0.9290	0.4920
HW	0.9460	0.4950
IA	0.9520	0.5130
IB	0.9420	0.4800
IC	0.9530	0.5110
IG	0.9240	0.4660
IH	0.9310	0.4480
II	0.9380	0.4520
IM	0.9400	0.4450
IN	0.9240	0.3960
IO	0.9100	0.3990
IS	0.9120	0.3920
IT	0.9300	0.4410
IU	0.8930	0.3380
IY	0.9410	0.4820
IZ	0.9440	0.4910

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Chain	Atom inclusion	Q-score
JA	0.9380	0.4650
JE	0.9530	0.4980
JF	0.9540	0.5020
JG	0.9420	0.4760
JK	0.9410	0.4850
JL	0.9450	0.4870
JM	0.9320	0.4670
JQ	0.9560	0.5060
JR	0.9460	0.4770
JS	0.9400	0.4610
JW	0.9420	0.4750
JX	0.9410	0.4830
JY	0.9350	0.4480
KC	0.9490	0.4690
KD	0.9210	0.4480
KE	0.9250	0.4520
KI	0.9370	0.4630
KJ	0.9300	0.4530
KK	0.9300	0.4500
KO	0.9380	0.4640
KP	0.9400	0.4950
KQ	0.9470	0.4910
KU	0.9380	0.4870
KV	0.9430	0.4600
KW	0.9370	0.4830
LA	0.9410	0.4720
LB	0.9340	0.4750
LC	0.9500	0.4790
LG	0.9380	0.4810
LH	0.9420	0.4860
LI	0.9510	0.4820
LM	0.9360	0.4610
LN	0.9500	0.4760
LO	0.9320	0.4330
LS	0.9360	0.4490
LT	0.9400	0.4490
LU	0.9200	0.4370
LY	0.9260	0.4490
LZ	0.9380	0.4510
M	0.5890	0.1940
MA	0.9240	0.4390
ME	0.9220	0.4390

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Chain	Atom inclusion	Q-score
MF	0.9550	0.4740
MG	0.9480	0.4700
MK	0.9320	0.4310
ML	0.9510	0.4940
MM	0.9490	0.4730
MQ	0.9390	0.4890
MR	0.8760	0.3330
MS	0.9420	0.4510
MW	0.8310	0.2490
MX	0.8530	0.2430
NA	0.8740	0.2710
NB	0.8610	0.2730
NC	0.8900	0.3050
NG	0.9060	0.3040
NH	0.9220	0.4030
NI	0.9230	0.4130
NM	0.9260	0.4390
NN	0.9380	0.4490
NO	0.9240	0.4210