



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:33 PM UTC

PDB ID : 7WI3 / pdb_00007wi3
EMDB ID : EMD-32520
Title : Cryo-EM structure of E.Coli FtsH-HflkC AAA protease complex
Authors : Qiao, Z.; Gao, Y.G.
Deposited on : 2022-01-02
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

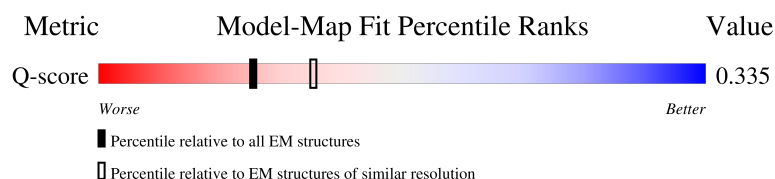
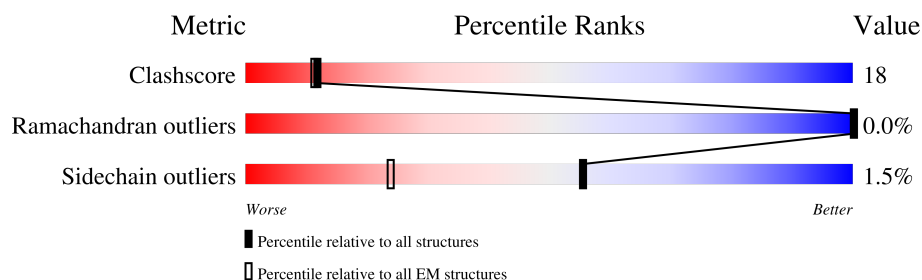
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 Å.

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



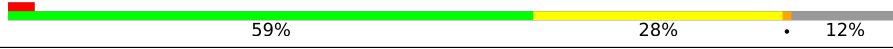
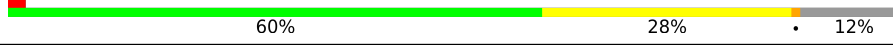
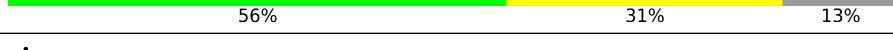
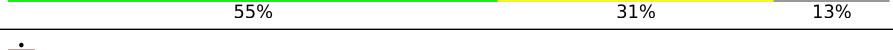
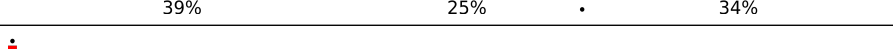
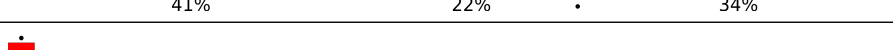
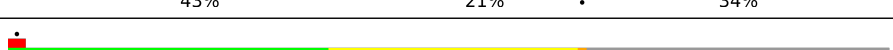
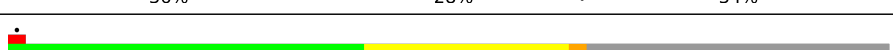
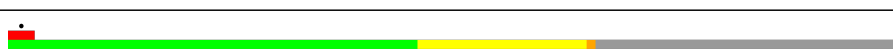
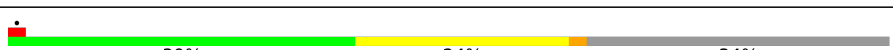
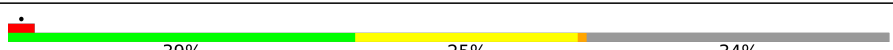
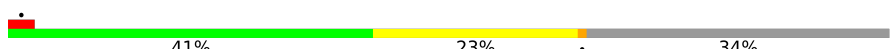
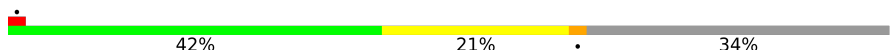
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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

Mol	Chain	Length	Quality of chain
1	A	334	 55% 32% 12%
1	C	334	 62% 23% 14%
1	D	334	 59% 27% 13%
1	M	334	 57% 30% 12%

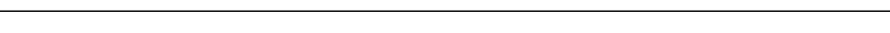
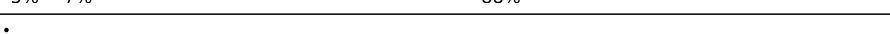
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Mol	Chain	Length	Quality of chain
1	O	334	
1	P	334	
1	Y	334	
1	Z	334	
1	c	334	
1	d	334	
1	e	334	
1	f	334	
2	B	419	
2	F	419	
2	G	419	
2	N	419	
2	R	419	
2	S	419	
2	a	419	
2	b	419	
2	i	419	
2	j	419	
2	k	419	
2	l	419	
3	E	644	
3	H	644	
3	I	644	
3	J	644	
3	K	644	

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Mol	Chain	Length	Quality of chain
3	L	644	 88%
3	Q	644	 87%
3	T	644	 87%
3	U	644	 88%
3	V	644	 88%
3	W	644	 88%
3	X	644	 88%
3	g	644	 87%
3	h	644	 87%
3	m	644	 87%
3	n	644	 87%
3	o	644	 88%
3	p	644	 88%
3	q	644	 88%
3	r	644	 88%
3	s	644	 88%
3	t	644	 88%
3	u	644	 88%
3	v	644	 88%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 69304 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 Modulator of FtsH protease HflC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	293	Total	C	N	O	S	0	0
			2338	1472	419	437	10		
1	C	287	Total	C	N	O	S	0	0
			2290	1444	411	426	9		
1	D	290	Total	C	N	O	S	0	0
			2311	1457	414	430	10		
1	Y	293	Total	C	N	O	S	0	0
			2338	1472	419	437	10		
1	c	287	Total	C	N	O	S	0	0
			2290	1444	411	426	9		
1	e	290	Total	C	N	O	S	0	0
			2311	1457	414	430	10		
1	Z	293	Total	C	N	O	S	0	0
			2338	1472	419	437	10		
1	d	287	Total	C	N	O	S	0	0
			2290	1444	411	426	9		
1	f	290	Total	C	N	O	S	0	0
			2311	1457	414	430	10		
1	M	293	Total	C	N	O	S	0	0
			2338	1472	419	437	10		
1	O	287	Total	C	N	O	S	0	0
			2290	1444	411	426	9		
1	P	290	Total	C	N	O	S	0	0
			2311	1457	414	430	10		

- Molecule 2 is a protein called Modulator of FtsH protease HflK.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	275	Total	C	N	O	S	0	0
			2169	1362	383	418	6		
2	F	275	Total	C	N	O	S	0	0
			2165	1360	383	416	6		
2	G	275	Total	C	N	O	S	0	0
			2173	1364	384	419	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	275	Total	C	N	O	S	0	0
			2169	1362	383	418	6		
2	i	275	Total	C	N	O	S	0	0
			2165	1360	383	416	6		
2	k	275	Total	C	N	O	S	0	0
			2173	1364	384	419	6		
2	b	275	Total	C	N	O	S	0	0
			2169	1362	383	418	6		
2	j	275	Total	C	N	O	S	0	0
			2165	1360	383	416	6		
2	l	275	Total	C	N	O	S	0	0
			2173	1364	384	419	6		
2	N	275	Total	C	N	O	S	0	0
			2169	1362	383	418	6		
2	R	275	Total	C	N	O	S	0	0
			2165	1360	383	416	6		
2	S	275	Total	C	N	O	S	0	0
			2173	1364	384	419	6		

- Molecule 3 is a protein called ATP-dependent zinc metalloprotease FtsH.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	81	Total	C	N	O	S	0	0
			658	418	113	126	1		
3	H	81	Total	C	N	O	S	0	0
			658	418	113	126	1		
3	I	79	Total	C	N	O		0	0
			643	408	111	124			
3	J	78	Total	C	N	O		0	0
			635	405	107	123			
3	K	79	Total	C	N	O		0	0
			643	408	111	124			
3	L	79	Total	C	N	O		0	0
			643	408	111	124			
3	g	81	Total	C	N	O	S	0	0
			658	418	113	126	1		
3	m	81	Total	C	N	O	S	0	0
			658	418	113	126	1		
3	o	79	Total	C	N	O		0	0
			643	408	111	124			
3	q	78	Total	C	N	O		0	0
			635	405	107	123			

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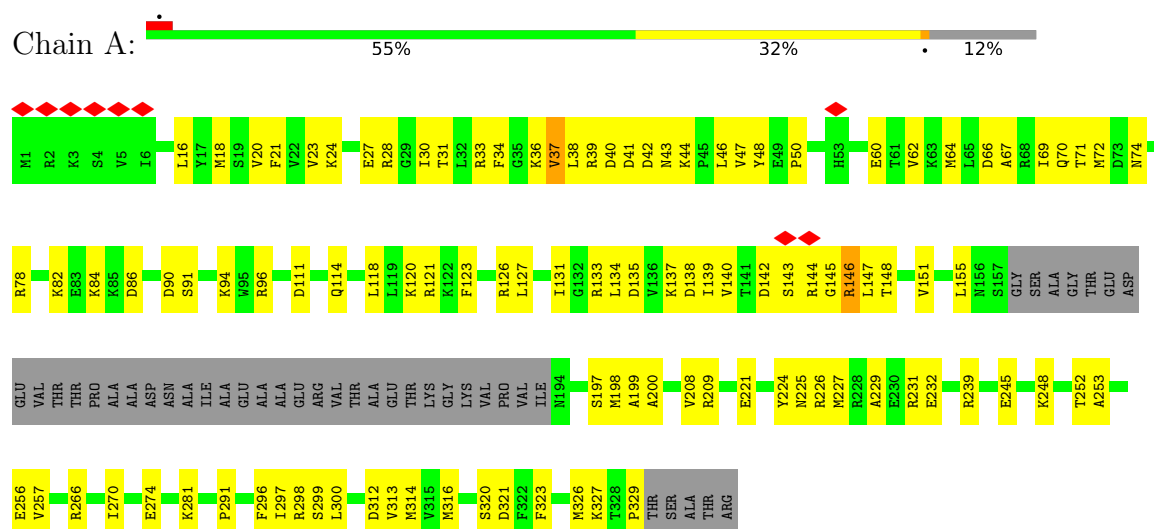
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Mol	Chain	Residues	Atoms				AltConf	Trace
3	s	79	Total 643	C 408	N 111	O 124	0	0
3	u	79	Total 643	C 408	N 111	O 124	0	0
3	h	81	Total 658	C 418	N 113	O 126 S 1	0	0
3	n	81	Total 658	C 418	N 113	O 126 S 1	0	0
3	p	79	Total 643	C 408	N 111	O 124	0	0
3	r	78	Total 635	C 405	N 107	O 123	0	0
3	t	79	Total 643	C 408	N 111	O 124	0	0
3	v	79	Total 643	C 408	N 111	O 124	0	0
3	Q	81	Total 658	C 418	N 113	O 126 S 1	0	0
3	T	81	Total 658	C 418	N 113	O 126 S 1	0	0
3	U	79	Total 643	C 408	N 111	O 124	0	0
3	V	78	Total 635	C 405	N 107	O 123	0	0
3	W	79	Total 643	C 408	N 111	O 124	0	0
3	X	79	Total 643	C 408	N 111	O 124	0	0

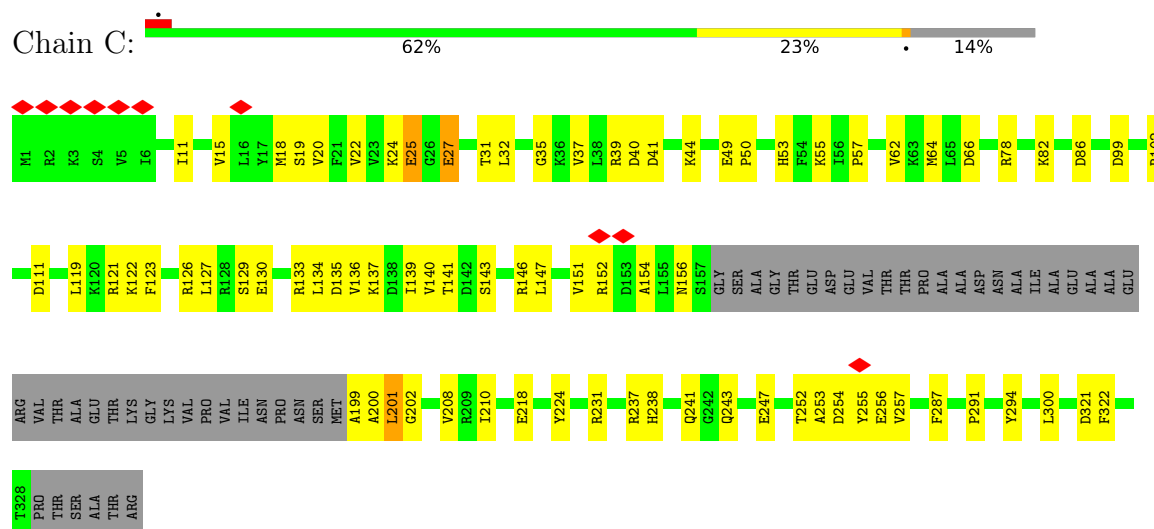
3 Residue-property plots

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.

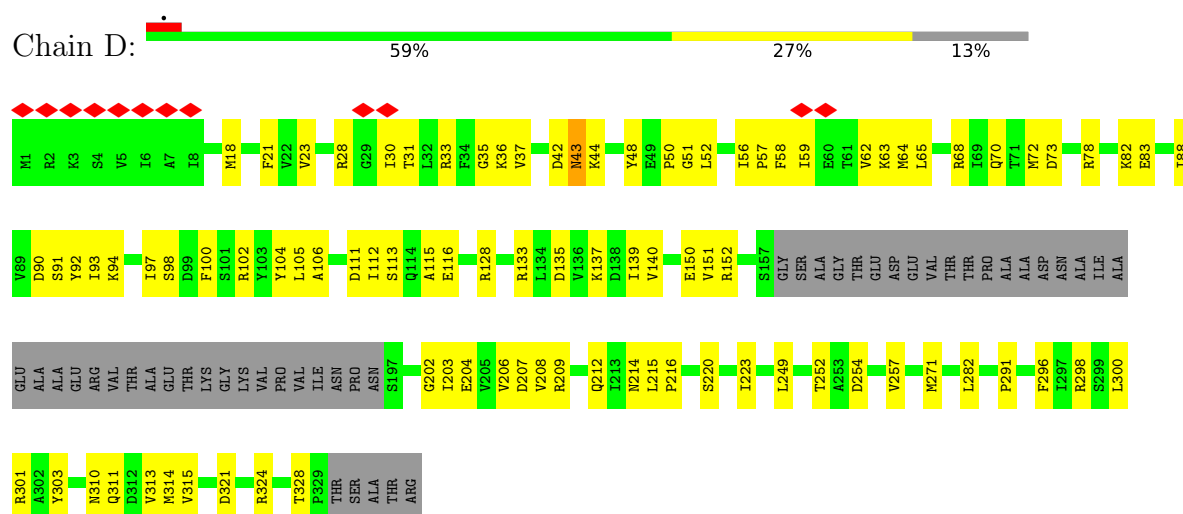
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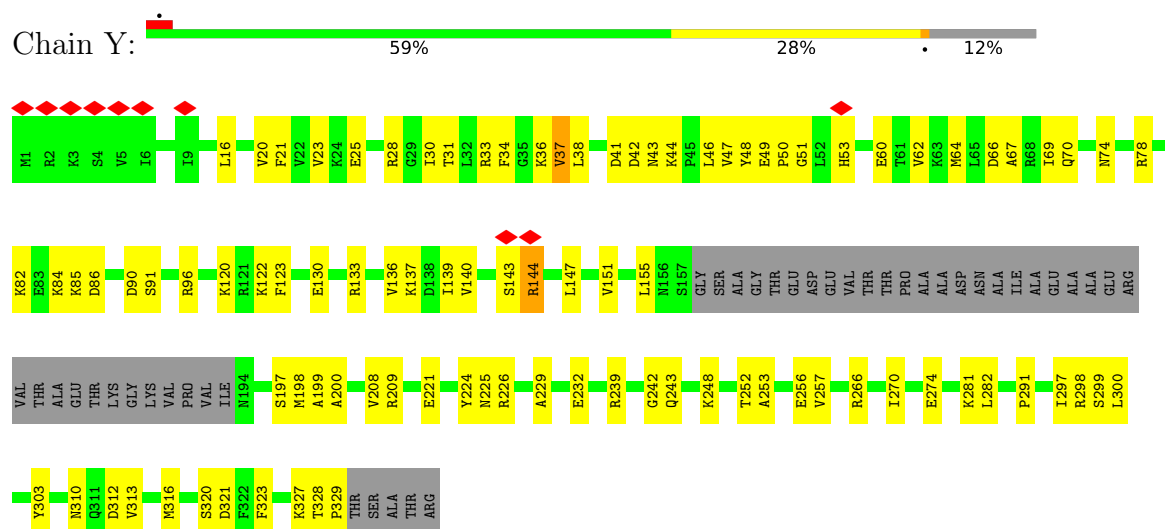
• Molecule 1: Modulator of FtsH protease HflC



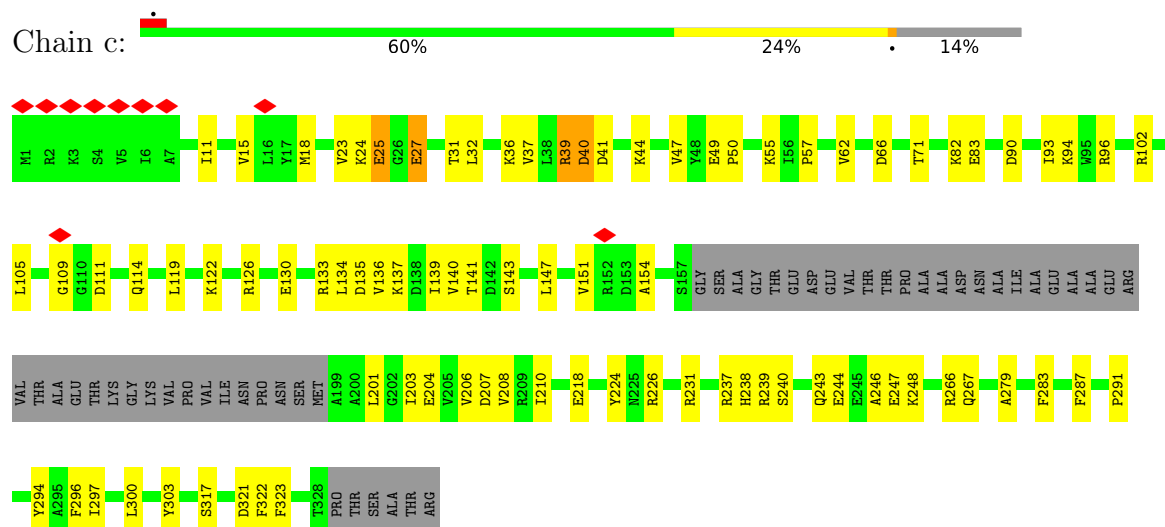
• Molecule 1: Modulator of FtsH protease HflC



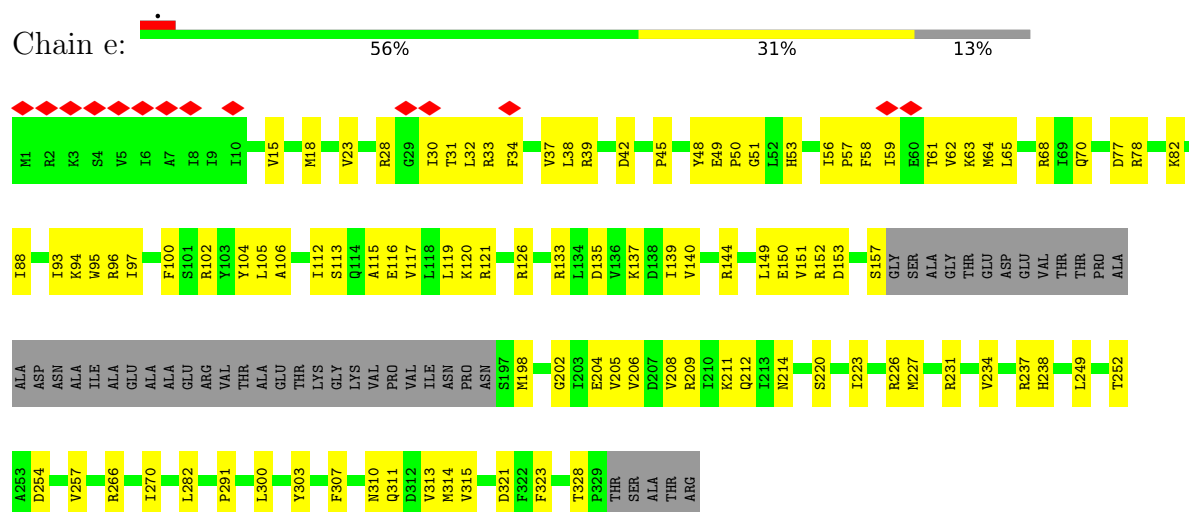
• Molecule 1: Modulator of FtsH protease HflC



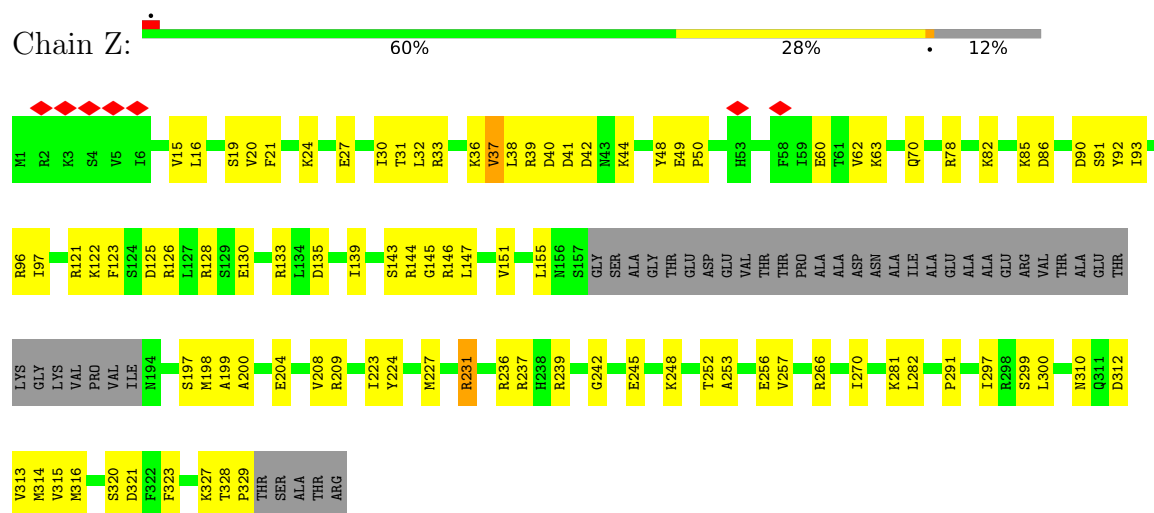
• Molecule 1: Modulator of FtsH protease HflC



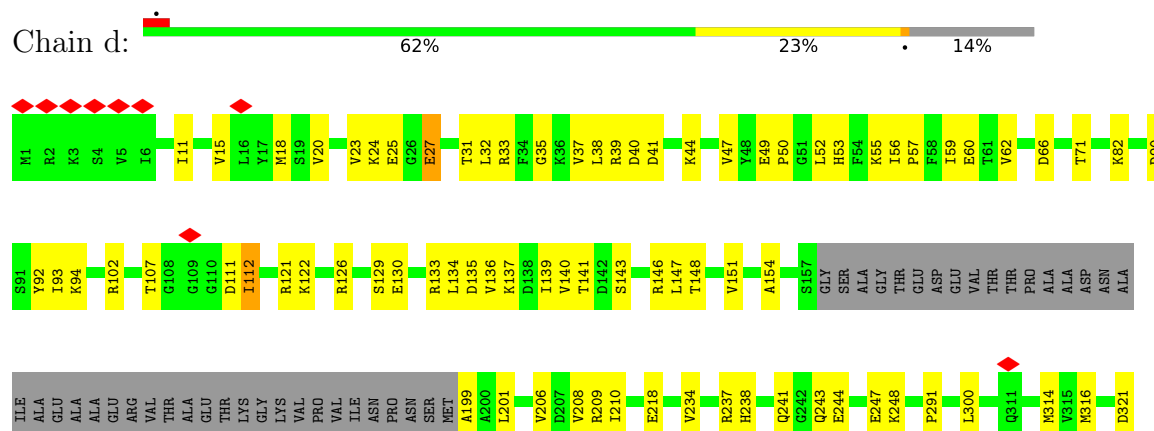
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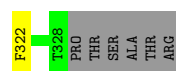


• Molecule 1: Modulator of FtsH protease HflC

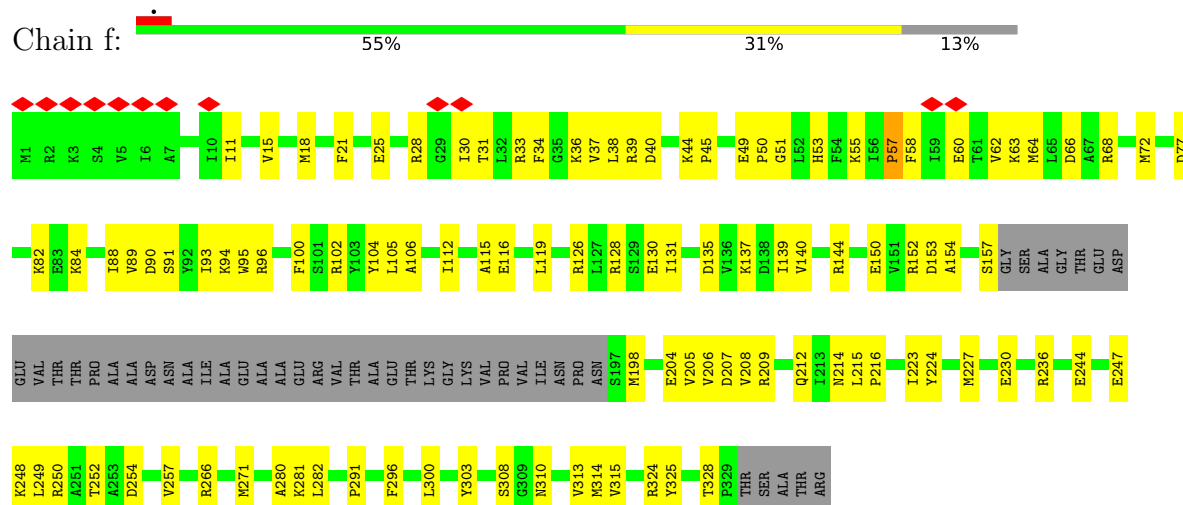


• Molecule 1: Modulator of FtsH protease HflC

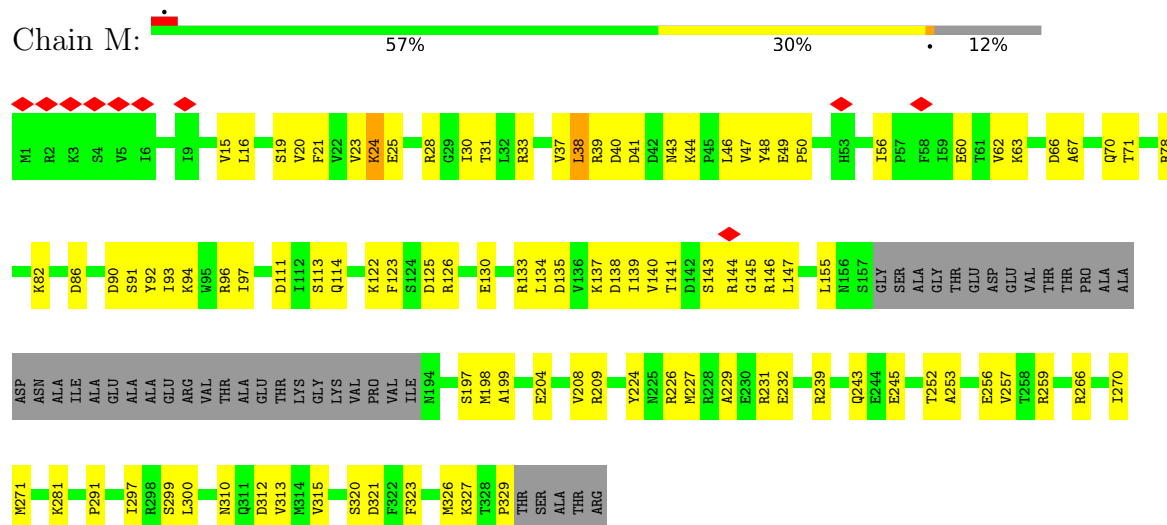




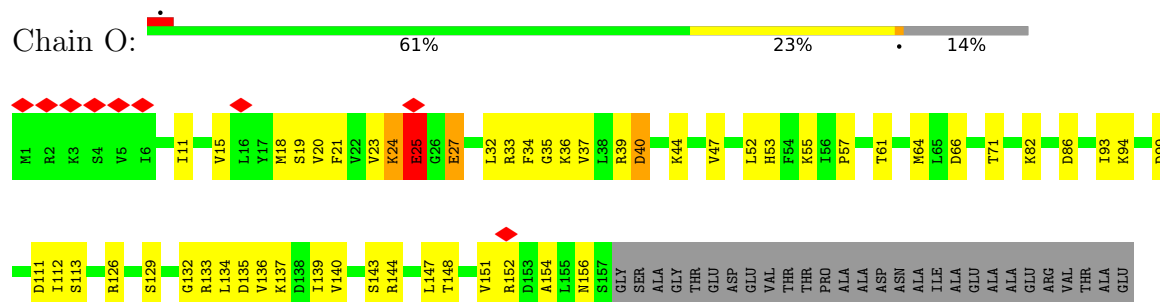
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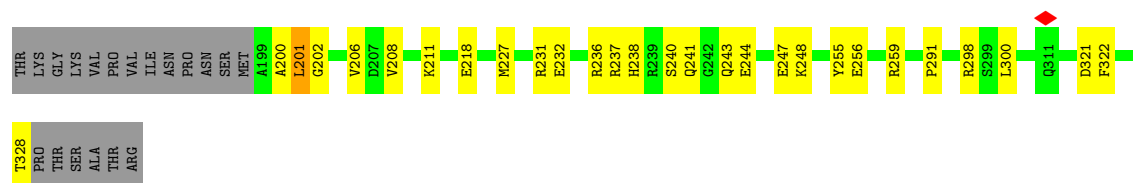


• Molecule 1: Modulator of FtsH protease HflC



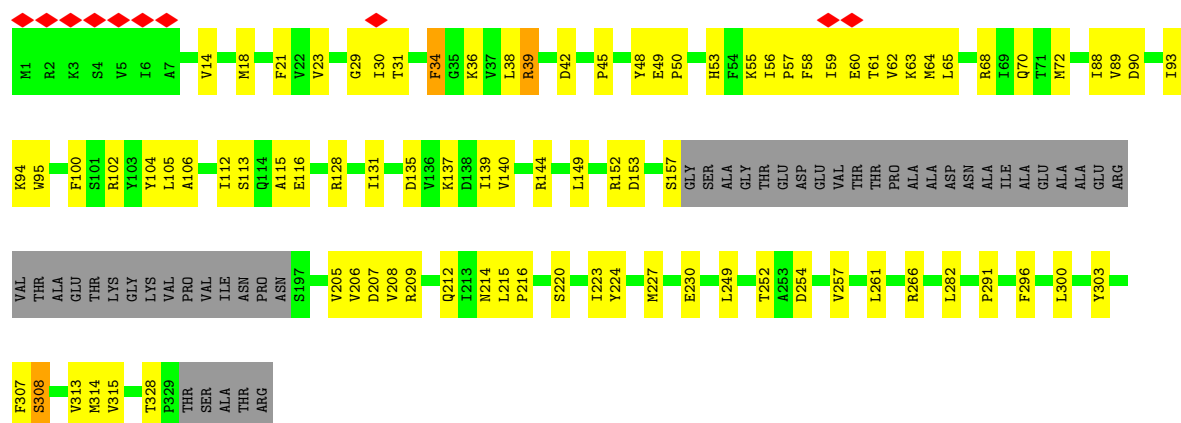
• Molecule 1: Modulator of FtsH protease HflC





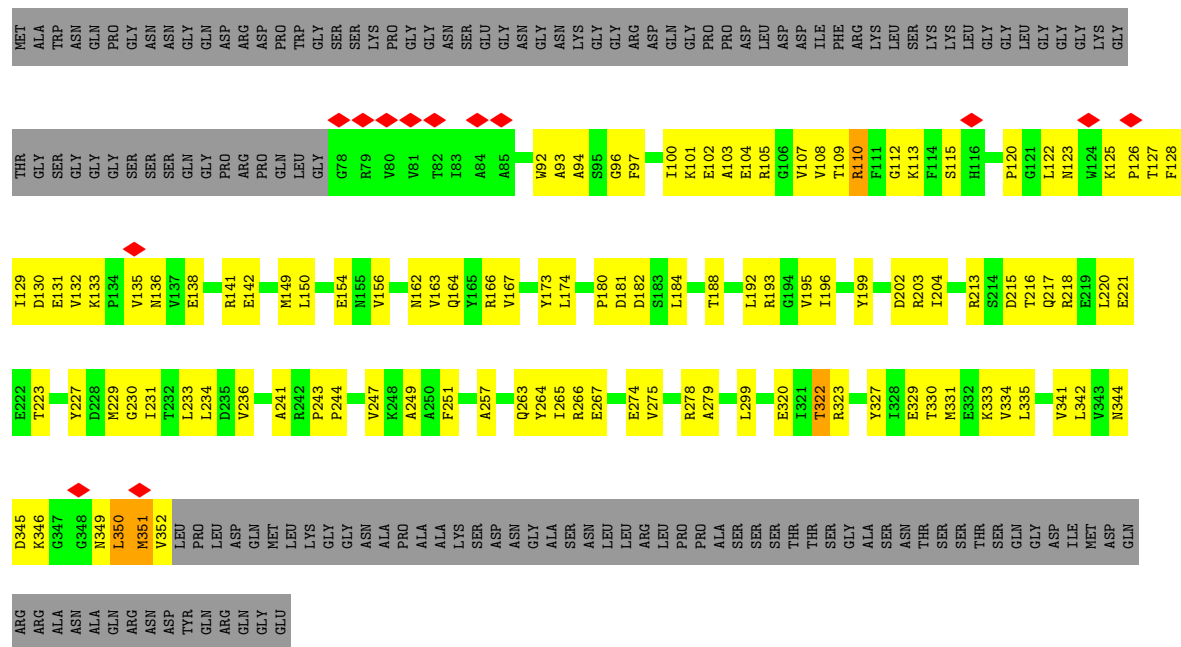
• Molecule 1: Modulator of FtsH protease HflC

Chain P: 60% 25% 13%



• Molecule 2: Modulator of FtsH protease HflK

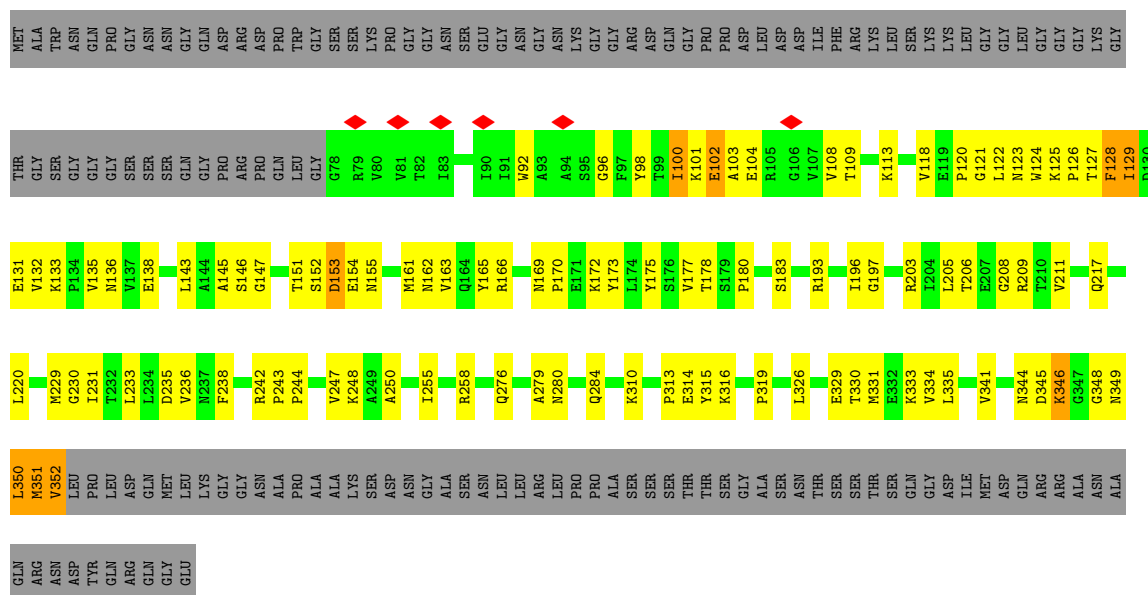
Chain B: 39% 25% 34%



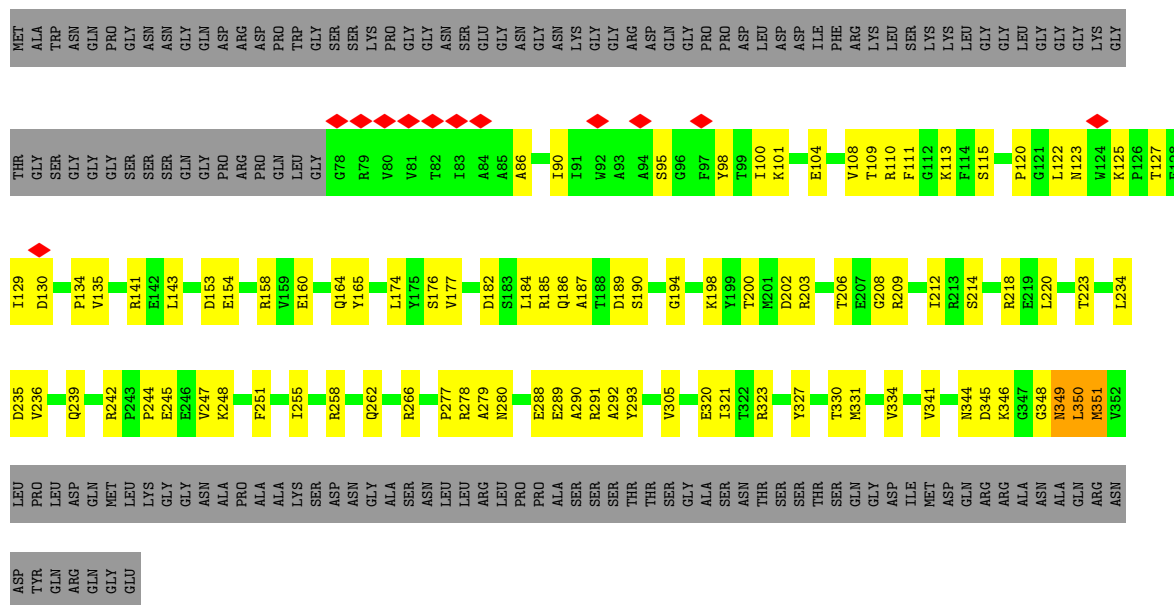
• Molecule 2: Modulator of FtsH protease HflK

Chain F: 41% 22% 34%

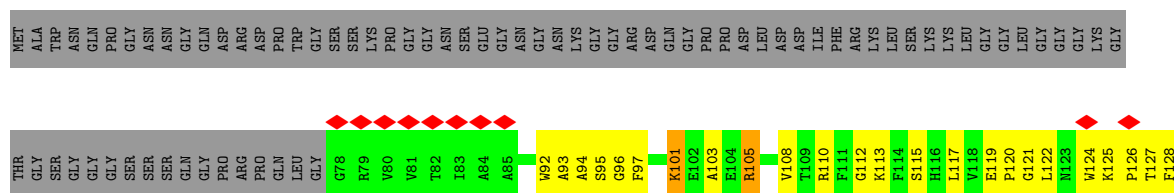




• Molecule 2: Modulator of FtsH protease HflK



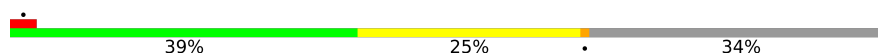
• Molecule 2: Modulator of FtsH protease HflK



GLY ASN ALA TRP PRO GLN ALA LYS SER ASP ASN GLN GLY ALA SER ASN LEU LEU ARG LEU PRO PRO ALA ALA SER SER GLY THR THR SER GLY ALA SER ASN THR THR SER GLY

• Molecule 2: Modulator of FtsH protease HflK

Chain b:



MET ALA TRP ASN GLN PRO GLY ASN ASN GLN ASP ARG ASP PRO TRP LEU GLY SER SER LYS PRO ALA GLY SER SER GLY ASN THR THR SER GLY

THR GLY SER GLY GLY SER SER SER GLY G78 R79 V80 V81 T82 T83 A84 A85 A86 A87 W92 A93 G96 F97 T100 K101 E102 A103 E104 R105 T108 V109 R110 F111 G112 K113 H116 P120 G121 L122 N123 W124 K125 P126 T127 F128 I129

D130 E131 V132 V135 N136 V137 E138 M149 E154 M155 V156 V157 R158 V163 R166 M169 P170 E171 K172 Y173 L174 A175 S176 V177 P180 D181 D182 S183 L184 R185 Q186 A187 T188 L189 R193 G194 V195 I196 G197 K198 Y199 D202 R203 T204 L205 R209 T210 V211 I212 R213

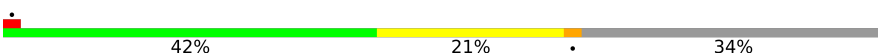
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K333 V334 L335 R339 K340 V341 L342 V343 N344 D345 K346 G347 G348 M349 L350 R351 V352 LEU PRO LEU LEU ASP GLN GLN GLN ARG ALA ARG ASN G348 M349 L350 R351 V352 LEU PRO LEU LEU ASP GLN GLN GLN ARG ALA ARG ASN

SER THR SER GLN ASP ILE MET ASP GLN ARG ALA ASN ALA LEU ARG ASN ASP TYR GLN GLN GLY GLU

• Molecule 2: Modulator of FtsH protease HflK

Chain j:



MET ALA TRP ASN GLN PRO GLY ASN ASN GLN GLY ASP ARG ASP PRO TRP LEU GLY SER SER LYS PRO PRO GLY SER SER GLY THR THR SER GLY

THR GLY SER GLY GLY SER SER SER GLY G78 R79 V80 V81 T82 T83 A84 A85 I90 A94 G96 F97 Y98 T99 I100 K101 E102 A103 E104 R105 G106 V107 V108 T109 R110 K113 F114 V118 E119 P120 M123 W124 K125 P126 T127 F128 I129

V132 V135 N136 V137 E138 A139 A145 S146 G147 H148 M149 S152 D153 E154 N155 V156 M161 N162 V163 R166 V167 T168 P169 P170 F171 K172 Y173 V177 T178 S179 P180 S183 L184 R185 T188 R193 G194 V195 I196 G197 K198 M201 D202 R203 T204 L205 T206 K125 P126 T127 F128 I129

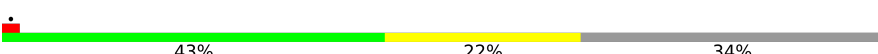
R209 L220 M229 L233 L234 D235 N237 R242 P243 P244 F251 L255 R258 Y271 E274 Q284 L312 P313 E314 Y315 K316 E324 I328 E329 M331 E332 K333 V334 L335 R339 K340 V341 L342 V343 N344 K346 L350 M351 V352 LEU PRO T206 K125 P126 T127 F128 I129

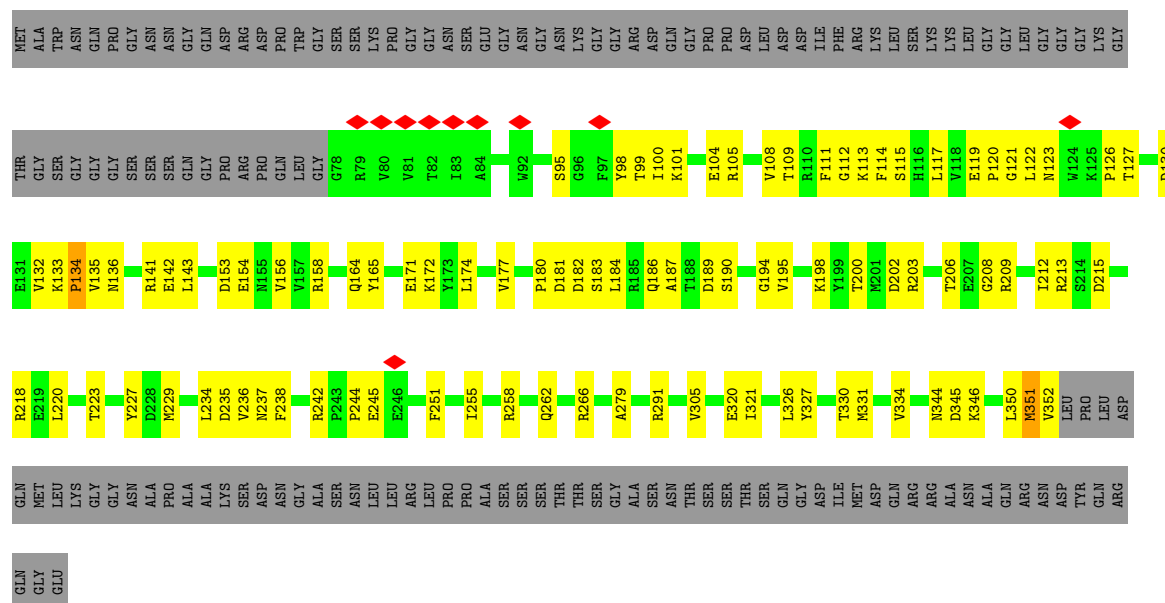
ASP GLN MET LEU LYS GLY ASN ALA PRO GLY ASP ALA SER ASN LEU LEU ARG LEU PRO PRO ALA ALA SER SER THR THR SER GLY SER ASN THR THR SER GLY

ARG GLN GLY GLU

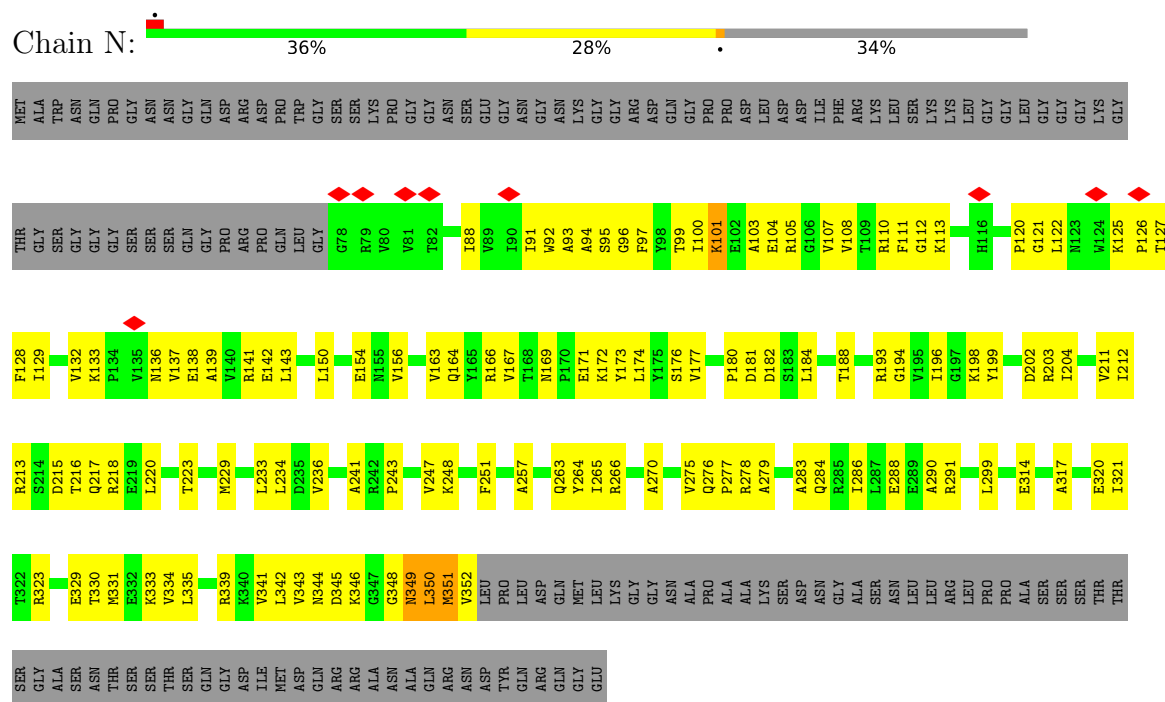
• Molecule 2: Modulator of FtsH protease HflK

Chain l:

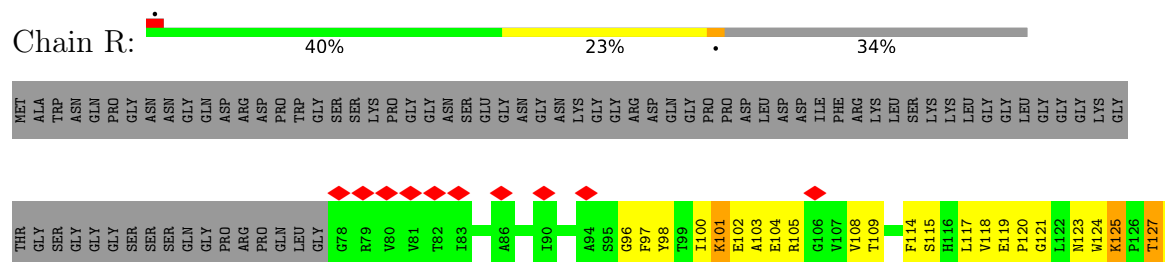




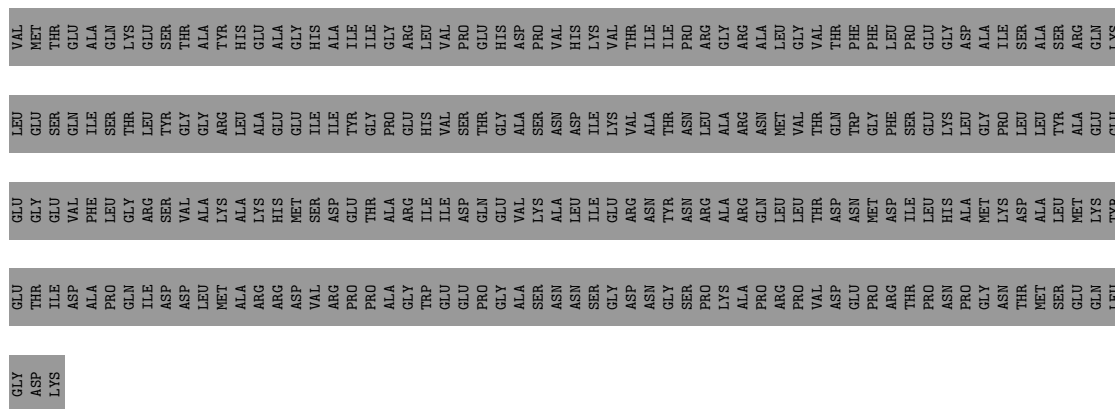
• Molecule 2: Modulator of FtsH protease HflK



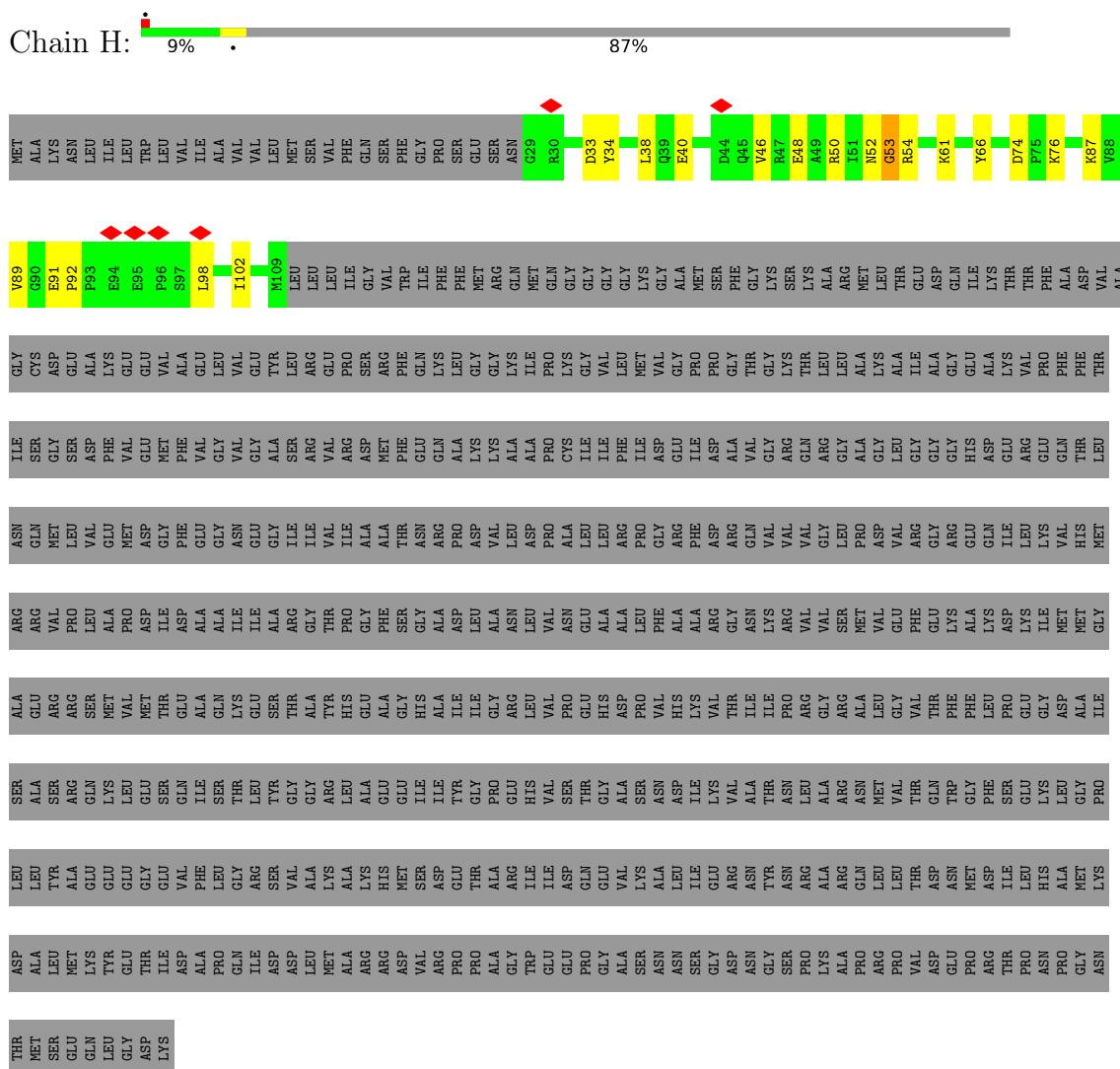
• Molecule 2: Modulator of FtsH protease HflK







- Molecule 3: ATP-dependent zinc metalloprotease FtsH



- Molecule 3: ATP-dependent zinc metalloprotease FtsH





[illegible]

- Molecule 3: ATP-dependent zinc metalloprotease FtsH



ALA	PRO	ARG	GLN	ARG	ARG	ARG	SER	LEU	LEU	GLY	LEU	MET	T67	MET
PRO	ARG	LEU	LEU	ALA	ALA	VAL	VAL	PRO	ASP	LYS	ALA	THR	T68	ALA
PRO	VAL	VAL	THR	GLY	VAL	PHE	GLU	VAL	ARG	ILE	ILE	GLU	Y69	ASN
ASP	ASP	THR	ASP	THR	PHE	THR	GLU	GLY	GLY	GLY	GLN	ASP	P71	LEU
GLU	GLU	ASN	TRP	GLY	PHE	THR	LYS	ARG	ARG	GLY	ILE	ILE	D74	LEU
PRO	PRO	MET	MET	GLY	PHE	ALA	ALA	GLU	THR	GLU	LYS	LYS		TRP
ARG	THR	ILE	PHE	GLY	LEU	ASP	LYS	GLN	ASP	GLU	THR	THR	L77	LEU
PRO	PRO	LEU	GLU	GLY	PRO	GLU	LEU	LEU	ARG	VAL	THR	THR	L78	VAL
ASN	ASN	HIS	HIS	LYS	GLY	ILE	ILE	LEU	ARG	PRO	ALA	PHE	L81	ILE
PRO	PRO	ALA	LEU	ASP	ASP	MET	MET	VAL	GLN	PHE	ASP	ALA		ALA
GLY	GLY	MET	GLY	ALA	ILE	GLY	GLY	PHE	THR	PHE	VAL	VAL	K84	VAL
ASN	THR	LYS	LYS	ILE	SER	ALA	ALA	ARG	ASN	THR	ALA	GLY	E91	LEU
THR	MET	ALA	LEU	ALA	GLU	GLU	ARG	ARG	GLN	ILE	CYS	THR		MET
SER	SER	LEU	LEU	SER	ARG	ARG	ARG	PRO	MET	GLY	ASP	ASP	E94	VAL
GLU	GLU	MET	ALA	GLN	GLY	SER	SER	LEU	VAL	ASP	ALA	ALA	E95	GLN
LEU	LEU	LYS	GLY	LYS	GLY	MET	MET	ALA	GLU	PHE	LYS	LYS	P96	SER
GLY	GLY	GLU	GLU	LEU	LEU	VAL	VAL	PRO	MET	VAL	GLU	GLU	S97	PHE
ASP	ASP	ILE	ILE	SER	SER	THR	THR	PRO	ASP	GLU	VAL	VAL	L98	GLY
LYS	LYS	PHE	PHE	ALA	ALA	GLU	GLU	ALA	PHE	ALA	ALA	ALA		PRO
		ALA	ALA	ALA	ILE	GLY	GLN	ILE	GLY	GLY	LEU	LEU	F103	SER
		GLN	GLY	THR	LEU	THR	LYS	ILE	ASN	VAL	VAL	VAL	W106	SER
		LEU	LEU	THR	LEU	GLY	GLY	ILE	GLU	GLY	GLU	GLU	F107	ASN
		SER	SER	TYR	TYR	THR	SER	ARG	GLY	ALA	THR	TYR	PRO	G29
		VAL	VAL	GLY	GLY	ALA	THR	ARG	ILE	SER	ILE	MET	V32	
		ALA	ALA	GLY	GLY	GLY	ALA	GLY	ILE	ARG	ARG	LEU	D33	
		ALA	ALA	ARG	ARG	TYR	TYR	VAL	VAL	VAL	GLU	LEU	Y34	
		ALA	ALA	LEU	LEU	HIS	HIS	ILE	ILE	ARG	PRO	ILE	S35	
		ARG	ARG	ALA	GLU	GLU	GLU	ALA	ALA	ASP	SER	GLY	T36	
		ARG	GLU	GLU	ALA	ALA	ALA	PHE	PHE	MET	ARG	VAL	F37	
		ASP	MET	GLU	GLU	GLY	GLY	THR	THR	PHE	GLN	TRP	L38	
		HIS	HIS	ILE	ILE	ILE	HIS	GLY	ASN	THR	Q39	Q39		
		MET	SER	ILE	ILE	ILE	ILE	GLY	ARG	GLU	LYS	ILE	E40	
		ASP	ASP	ILE	ILE	ILE	ALA	ASP	PRO	ALA	LEU	PHE	V41	
		THR	THR	GLY	GLY	ILE	ILE	LEU	ASP	LYS	GLY	GLY	N42	
		ALA	ALA	PRO	GLU	GLY	GLY	ALA	VAL	LYS	GLY	MET		
		ARG	GLY	GLU	GLU	ARG	ARG	ASN	VAL	ALA	LYS	ARG	R47	
		TRP	TRP	ILE	VAL	VAL	LEU	LEU	ASP	ALA	ILE	GLN		
		GLU	GLU	ILE	VAL	VAL	VAL	THR	PRO	ALA	ILE	MET	R50	
		GLU	GLU	ASP	SER	SER	PRO	ASN	ALA	CYS	LYS	GLY	I51	
		PRO	PRO	THR	THR	THR	GLU	GLU	LEU	ILE	GLY	GLY	N52	
		GLY	GLY	GLY	GLY	HIS	HIS	ILE	LEU	PHE	VAL	GLY	G53	
		ALA	ALA	VAL	ALA	ASP	ASP	ALA	ARG	THR	LEU	GLY	R54	
		SER	SER	LYS	SER	PRO	PRO	ALA	PRO	ILE	MET	GLY	E55	
		ASN	ALA	ASN	ASN	VAL	THR	PHE	GLY	ASP	LYS	LYS	I56	
		ASN	ASN	LEU	LEU	ASP	HIS	ALA	ARG	GLU	GLY	ALA	N57	
		SER	SER	ILE	ILE	VAL	LYS	ALA	PHE	ILE	PRO	ALA	V58	
		GLY	GLY	GLY	GLY	VAL	VAL	ARG	ASP	ASP	PRO	MET		
		ASN	ASN	ARG	VAL	THR	THR	GLY	ARG	ALA	GLY	SER	K61	
		ASN	ASN	ALA	ALA	ILE	ILE	GLY	ASN	VAL	THR	PHE	D62	
		TYR	TYR	THR	THR	ILE	ILE	LYS	LYS	GLY	GLY	GLY	S63	
		SER	SER	ASN	ASN	PRO	PRO	ARG	PRO	VAL	LYS	SER	R64	
		PRO	PRO	ARG	ARG	LEU	LEU	VAL	THR	GLN	THR	LYS	R65	
		LYS	LYS	ALA	ALA	GLY	GLY	VAL	GLY	ARG	LEU	ALA	Y66	

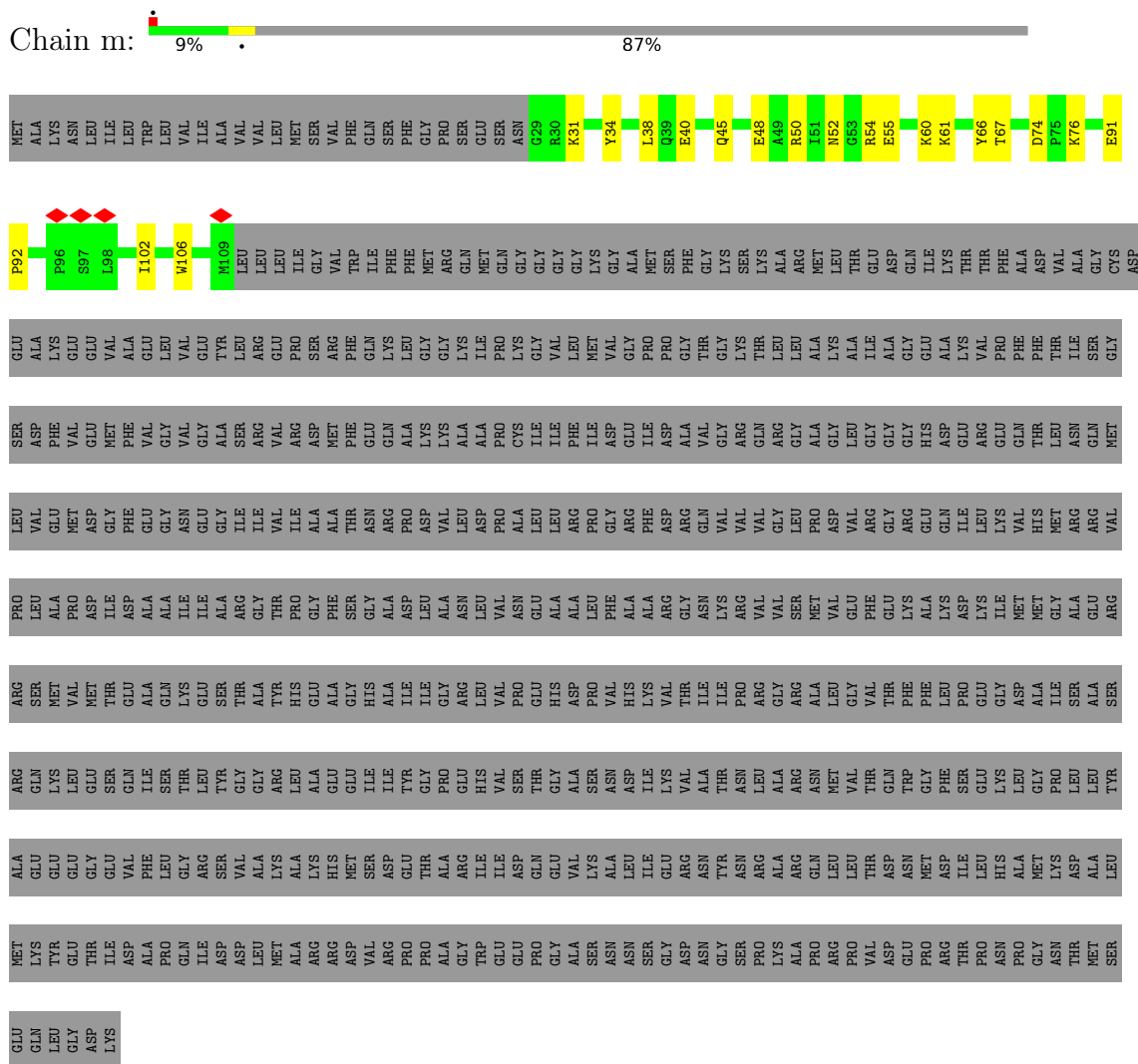
- Molecule 3: ATP-dependent zinc metalloprotease FtsH



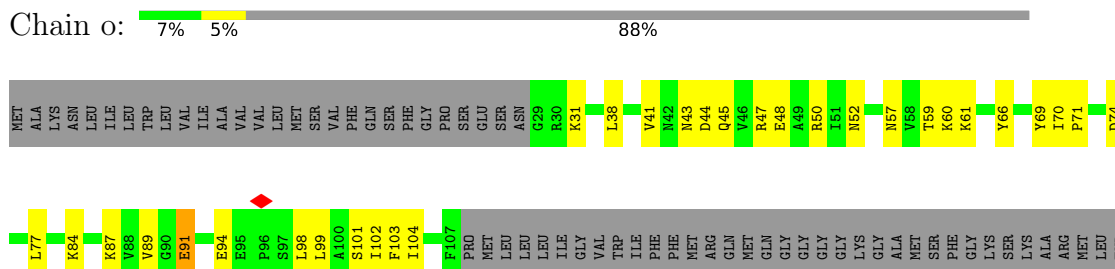
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-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



- Molecule 3: ATP-dependent zinc metalloprotease FtsH



- Molecule 3: ATP-dependent zinc metalloprotease FtsH

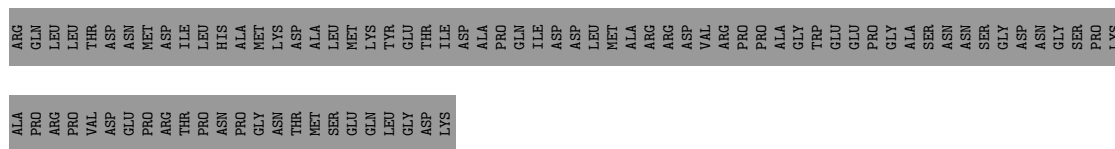


[illegible]

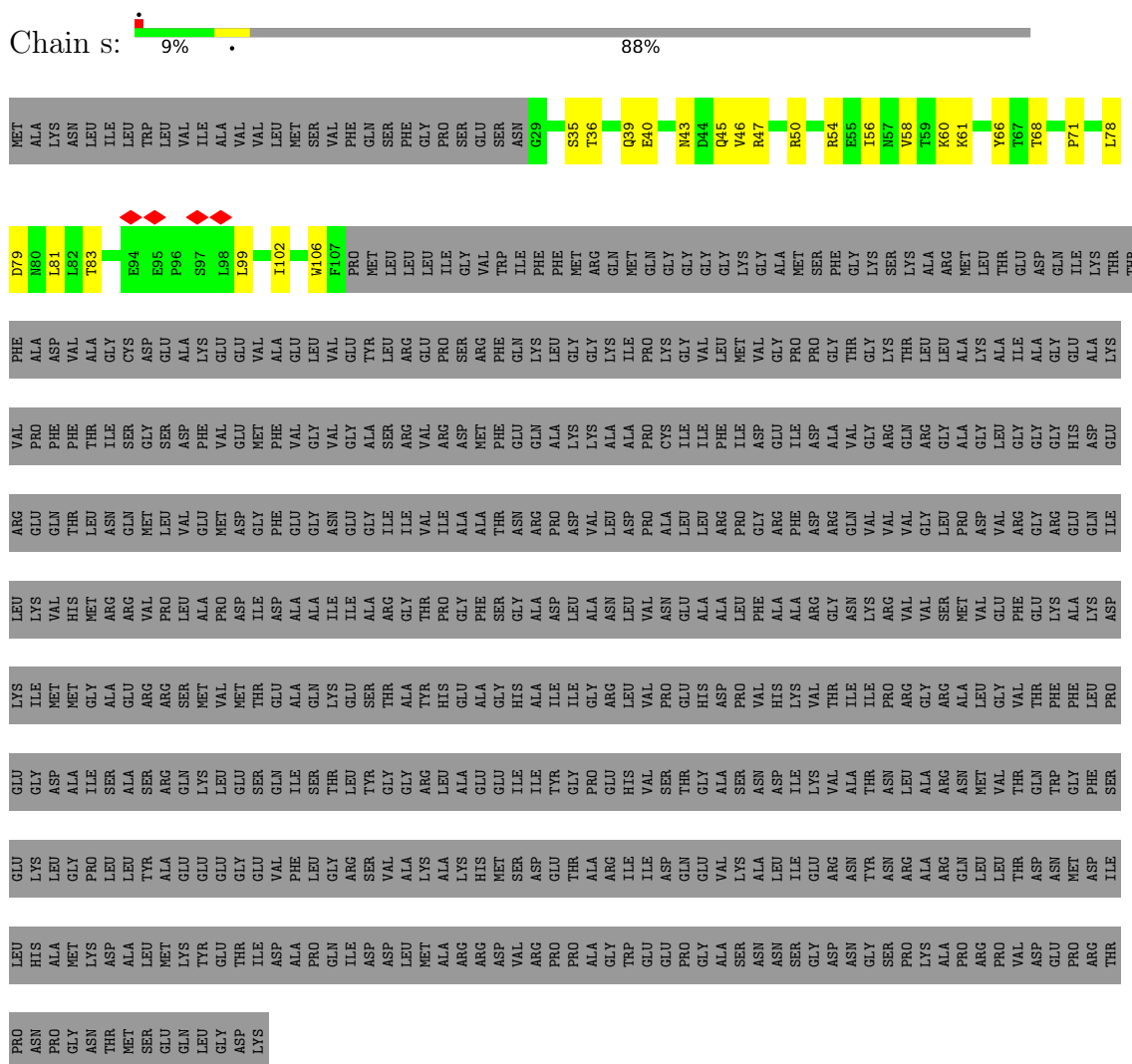
- Molecule 3: ATP-dependent zinc metalloprotease FtsH

Chain q:  6% 5% 88%

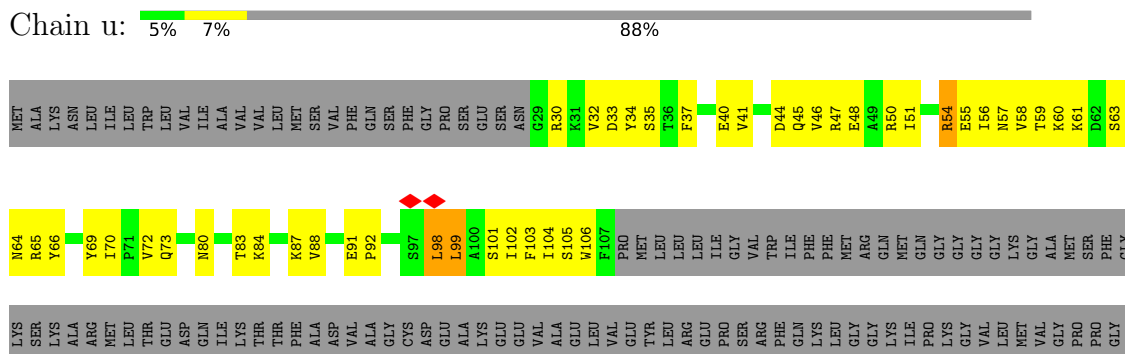
ARG	ASN	ALA	ARG	SER	LEU	GLY	LEU	GLY	LEU	MET	N64
ASN	MET	LEU	PHE	MET	PRO	GLY	ASP	GLY	LEU	THR	R65
VAL	VAL	GLY	VAL	PHE	VAL	GLY	ARG	ILE	GLU	ASP	Y66
THR	THR	VAL	THR	GLY	GLY	GLY	GLY	ILE	ASP		I70
GLN	THR	PHE	GLY	GLY	ARG	GLY	ARG	GLY	GLN	ILE	L78
GLY	PHE	PHE	GLY	ALA	GLY	HIS	GLY	GLY	LYS	LYS	D79
PHE	LEU	LEU	LEU	ASP	GLN	ALA	THR	ALA	THR	THR	N80
SER	SER	PRO	PRO	ASP	ILE	GLU	ILE	GLY	THR	THR	L81
GLY	GLY	GLU	GLU	LYS	LEU	VAL	LEU	VAL	PHE	PHE	L82
LYS	LYS	GLY	GLY	ILE	LYS	GLU	PRO	ALA	ALA	ALA	T83
LEU	LEU	ASP	VAL	MET	VAL	GLN	PHE	ASP	ASP		K87
GLY	GLY	ALA	ALA	MET	HIS	THR	PHE	THR	VAL	VAL	V88
PRO	PRO	ILE	ILE	GLY	MET	LEU	THR	ALA	ALA	ALA	V89
LEU	LEU	SER	ALA	ALA	ARG	ASN	ILE	GLY	GLY	GLY	G99
LEU	LEU	SER	ALA	GLU	ARG	GLN	SER	CYS	CYS		E91
TYR	TYR	SER	SER	ARG	VAL	MET	VAL	GLY	ASP	ASP	P92
ALA	ARG	ARG	ARG	ARG	PRO	LEU	SER	GLY	GLU	GLU	
GLU	GLU	GLN	GLN	SER	LEU	VAL	ASP	ASP	ALA	ALA	P96
GLY	GLY	LYS	LYS	MET	ALA	GLY	PHE	LYS	GLY	LYS	S97
GLU	GLU	LEU	LEU	VAL	PRO	MET	VAL	VAL	GLU	GLU	L98
GLY	GLY	GLU	GLU	MET	ILE	GLY	GLY	MET	VAL	VAL	L99
VAL	VAL	GLN	GLN	GLU	ASP	PHE	PHE	PHE	ALA	ALA	
PHE	PHE	ILE	ILE	ALA	ALA	GLY	VAL	VAL	GLY	LEU	F103
LEU	LEU	SER	THR	LYS	ILE	ASN	VAL	VAL	VAL	VAL	
GLY	GLY	THR	LEU	GLY	ILE	GLY	GLY	GLY	GLY	GLY	P108
ARG	SER	TYR	TYR	SER	ALA	GLY	ALA	ALA	TYR	TYR	MET
VAL	VAL	GLY	GLY	THR	ARG	ILE	SER	LEU	LEU	LEU	LEU
LYS	LYS	GLY	ALA	ALA	GLY	ILE	ARG	ARG	ARG	ARG	V32
ALA	ALA	LEU	LEU	HIS	PRO	TYR	VAL	GLU	GLU	GLU	D33
LYS	LYS	ALA	ALA	GLY	GLY	ILE	ARG	PRO	PRO	ILE	Y34
HIS	HIS	GLU	ALA	ALA	PHE	ALA	ASP	SER	SER	GLY	S35
MET	MET	GLU	GLU	GLY	SER	THR	THR	ARG	ARG	VAL	T36
SER	SER	ILE	ILE	HIS	GLY	HIS	PHE	PHE	PHE	TRP	F37
ASP	ASP	ILE	ALA	ALA	GLY	ASN	GLU	LYS	LYS	ILE	L38
GLY	GLY	TYR	ILE	ILE	ASP	PRO	ALA	LEU	PHE	PHE	Q39
THR	THR	GLY	GLY	ILE	LEU	ASP	LYS	GLY	GLY	MET	E40
ALA	ALA	PRO	PRO	GLY	ALA	VAL	LYS	GLY	GLY	ARG	V41
ARG	ARG	GLY	ASN	GLY	ALA	VAL	LYS	GLY	GLY	GLN	Q45
ILE	ILE	HIS	LEU	LEU	LEU	ASP	ALA	LYS	LYS	MET	V46
ILE	ILE	VAL	VAL	VAL	LEU	LEU	ILE	ILE	PRO	GLN	R47
ASP	ASP	SER	SER	PRO	ASN	ASN	CYS	LYS	LYS	GLY	E48
GLN	GLN	THR	THR	GLY	GLY	LEU	ILE	GLY	GLY	GLY	A49
VAL	VAL	GLY	GLY	HIS	ALA	LEU	ILE	VAL	LEU	GLY	R50
VAL	VAL	ALA	ALA	ASP	ALA	LEU	PHE	VAL	GLY	GLY	I51
ASN	ASN	SER	SER	PRO	LEU	LEU	ILE	MET	MET	LYS	
ALA	ALA	ASN	PHE	VAL	PHE	GLY	ASP	VAL	GLY	GLY	R54
ILE	ILE	ASP	ASP	HIS	ALA	ARG	ILE	PRO	PRO	MET	E55
GLU	GLU	ILE	ILE	LYS	VAL	PHE	ILE	ASP	ASP	SER	I56
ASN	ASN	VAL	LYS	VAL	ARG	GLY	ARG	ALA	GLY	SER	N57
TYR	TYR	ALA	THR	ILE	GLY	GLN	ALA	THR	PHE	PHE	V58
ASN	ASN	THR	THR	ILE	LYS	VAL	GLY	GLY	GLY	LYS	K60
ASN	ASN	ASN	THR	ILE	ARG	VAL	VAL	GLY	LYS	SER	R61
ARG	ARG	LEU	VAL	ARG	VAL	VAL	GLN	THR	THR	LYS	D62
ALA	ALA	ALA	ALA	GLY	VAL	GLY	ARG	ILE	ILE	ALA	F63



- Molecule 3: ATP-dependent zinc metalloprotease FtsH

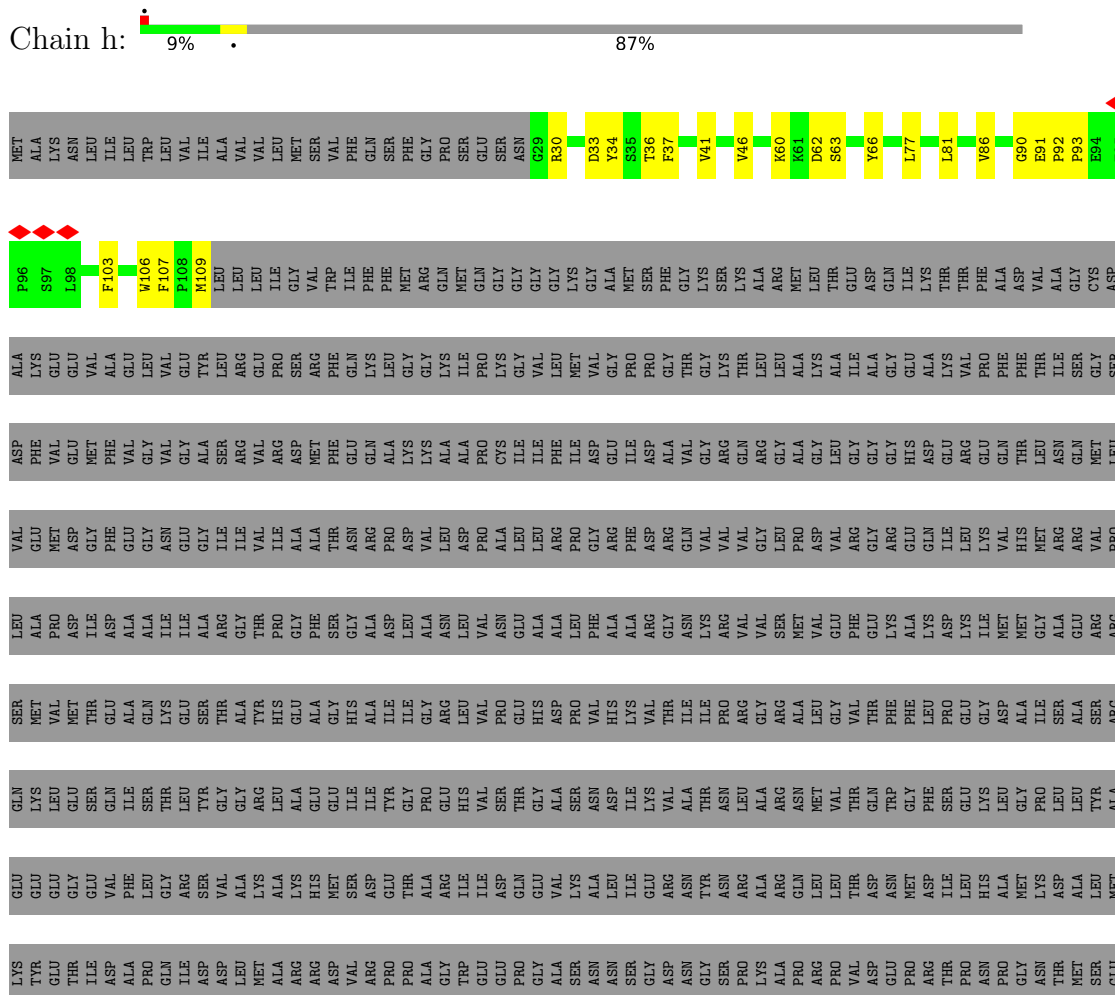


- Molecule 3: ATP-dependent zinc metalloprotease FtsH



[illegible]

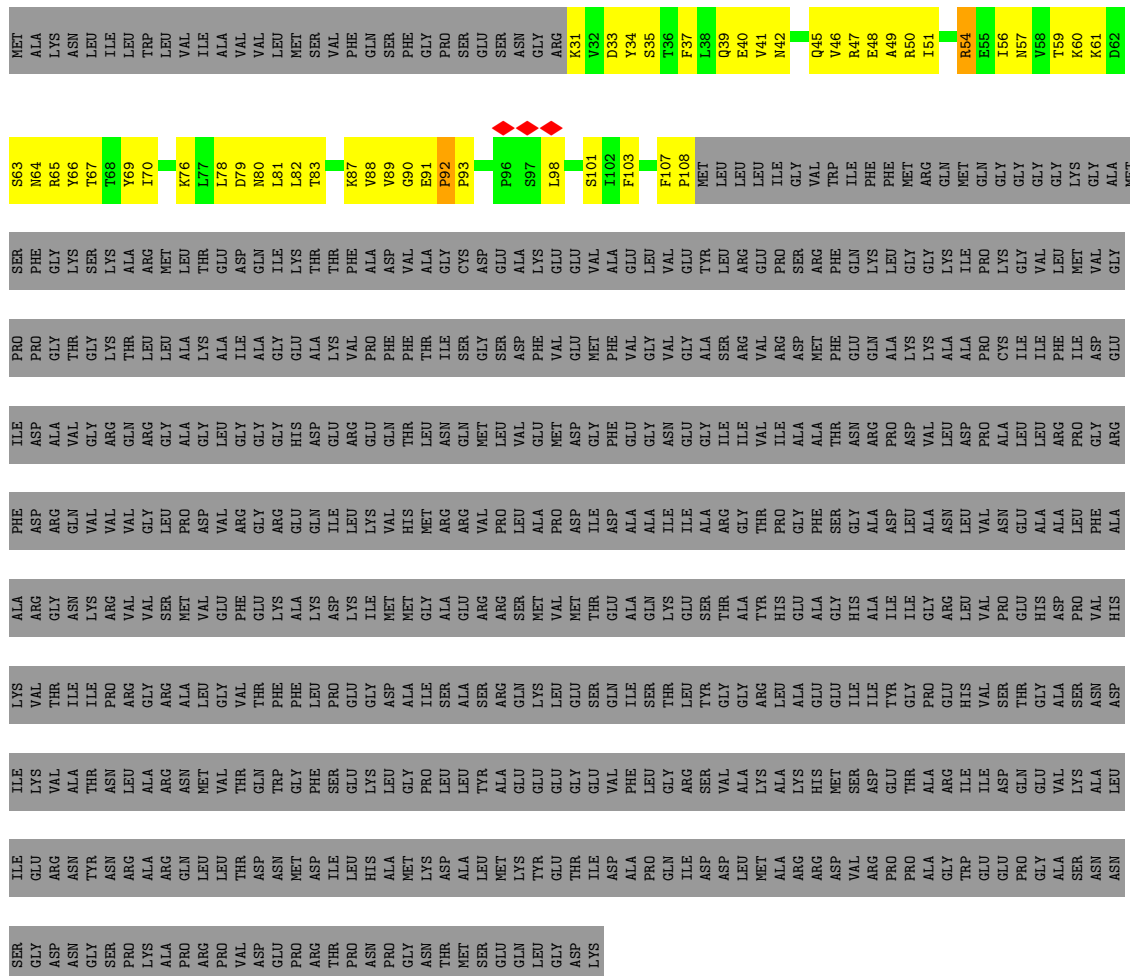
- Molecule 3: ATP-dependent zinc metalloprotease FtsH



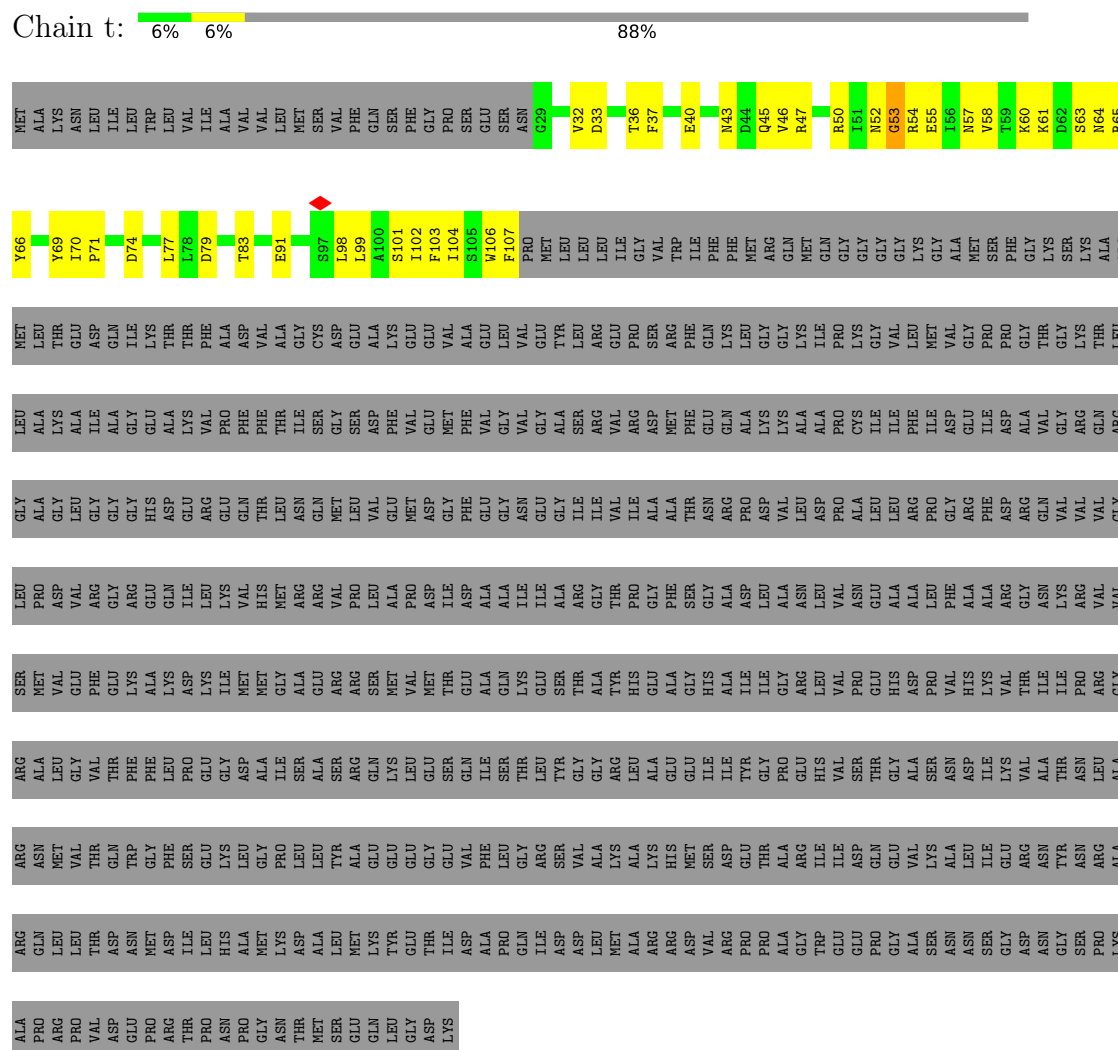
[illegible]

- Molecule 3: ATP-dependent zinc metalloprotease FtsH

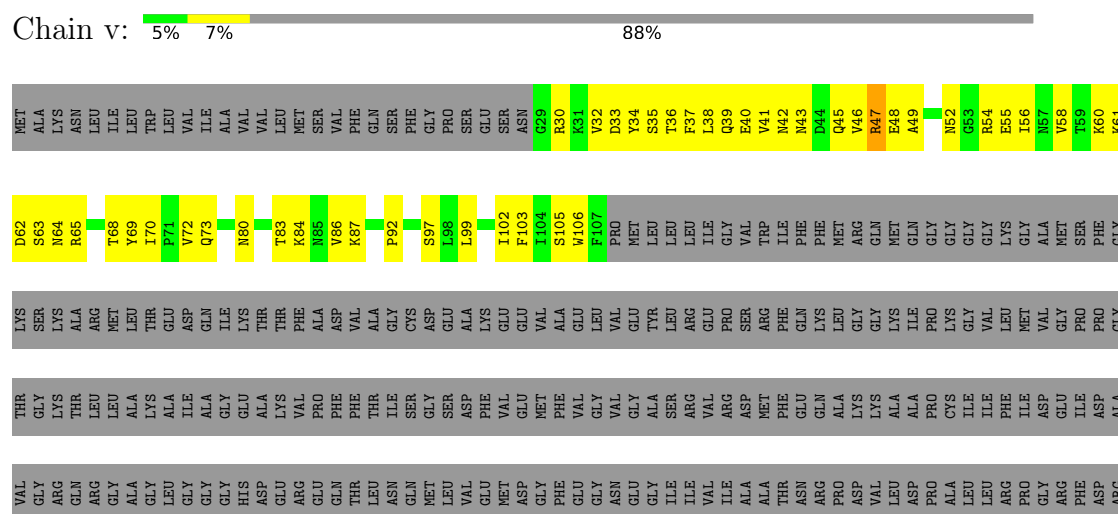
Chain r: 5% 7% 88%



● Molecule 3: ATP-dependent zinc metalloprotease FtsH



● Molecule 3: ATP-dependent zinc metalloprotease FtsH



LEU	GLY	ASP	LYS	TYR	GLU	GLY	LYS	MET	ALA	GLU	PHE	LYS	A100	MET
GLY	THR	GLU	GLU	GLU	GLU	GLY	LEU	VAL	PRO	ASP	VAL	GLU	S101	ALA
ASP	ILE	GLU	GLU	THR	THR	SER	THR	ILE	ASP	ILE	MET	VAL	I102	LYS
ALA	ASP	VAL	GLN	ILE	GLU	GLN	ALA	ALA	ASP	PHE	PHE	ALA	F103	ASN
PRO	PRO	PHE	LEU	SER	THR	THR	ALA	ALA	ALA	GLU	VAL	GLU	W106	ILE
GLN	ILE	GLY	THR	GLU	ILE	GLU	ILE	ILE	ILE	ASN	VAL	VAL	F107	TRP
ASP	ASP	ARG	LEU	THR	GLU	GLU	ALA	ALA	ALA	GLY	GLY	GLU	P108	LEU
LEU	ASP	VAL	GLY	THR	THR	GLY	ARG	ARG	ALA	ILE	SER	TYR	M109	VAL
MET	ALA	LYS	ARG	TYR	ALA	GLY	GLY	THR	THR	ILE	ARG	ARG	LEU	ILE
ALA	ARG	ALA	LEU	HIS	PRO	LEU	THR	PRO	VAL	VAL	VAL	GLU	LEU	ALA
ARG	ARG	LYS	ALA	GLU	GLY	ALA	GLY	GLY	ILE	ILE	ASP	PRO	GLY	VAL
ARG	ASP	HIS	GLU	ALA	PHE	ASN	ALA	ALA	ALA	ALA	PHE	PHE	LEU	LEU
ASP	ASP	ILE	GLU	GLY	GLY	GLY	HIS	ALA	ASP	ASN	GLU	GLN	PHE	PHE
PRO	PRO	TYR	TYR	ILE	ILE	ILE	ILE	ASP	PRO	PRO	ALA	LEU	MET	GLN
PRO	ALA	PRO	GLY	GLY	THR	GLY	GLY	LEU	LEU	GLY	LYS	GLY	ARG	SER
ALA	GLY	ALA	ALA	HIS	ALA	ALA	HIS	ALA	ALA	ARG	PHE	VAL	GLN	GLY
ASN	ASN	LYS	LYS	ASN	VAL	VAL	VAL	PHE	LEU	GLY	ASP	ILE	ALA	SER
ASN	ASN	LEU	ILE	LYS	ALA	ALA	ALA	ALA	ALA	ARG	ILE	GLY	ALA	GLY
SER	GLY	ILE	LYS	VAL	ARG	VAL	VAL	ARG	ARG	PHE	ILE	PRO	SER	GLY
ASP	ASN	ALA	ALA	THR	ASN	VAL	ALA	ILE	GLY	ARG	ALA	GLY	GLY	GLY
ASN	ASN	THR	THR	THR	THR	THR	THR	ILE	ASN	GLN	VAL	THR	LYS	ASN
PRO	GLY	ARG	ASN	ASN	ASN	ASN	ASN	ASN	VAL	VAL	GLN	LYS	ALA	ALA
LYS	ALA	ALA	ALA	GLY	ALA	GLY	ALA	VAL	VAL	GLY	ARG	LEU	ARG	R54
ALA	ARG	ARG	ARG	ARG	ARG	ARG	ARG	SER	SER	GLY	GLY	LEU	MET	GLY
PRO	GLN	ASN	ASN	ALA	ASN	ASN	ASN	MET	PRO	PRO	ALA	ALA	LEU	LYS
ARG	LEU	LEU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY	GLY	LYS	THR	THR
PRO	LEU	THR	THR	THR	THR	THR	THR	PHE	GLU	ARG	ILE	ASP	GLU	D62
ASP	ASP	THR	GLN	PHE	THR	THR	THR	GLY	GLY	GLY	GLY	GLN	GLN	R65
GLU	ASN	MET	TRP	ASN	ASN	ASN	ASN	LYS	ALA	ARG	ILE	LYS	ILE	GLY
PRO	THR	ASP	PHE	PHE	PHE	PHE	PHE	ALA	GLU	GLU	HIS	GLU	THR	GLY
ARG	ARG	ILE	SER	SER	SER	SER	SER	ASN	ASN	ILE	GLU	LYS	THR	THR
PRO	PRO	LEU	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	VAL	PHE	K76
ASN	HIS	HIS	LYS	LYS	LYS	LYS	ILE	ILE	ILE	LYS	GLU	PRO	ALA	ALA
PRO	ALA	ALA	LEU	ASP	MET	MET	ASP	MET	MET	VAL	GLN	ASP	ASP	K87
GLY	MET	GLY	PRO	ILE	GLY	GLY	ALA	GLY	GLY	GLY	THR	PHE	VAL	GLY
ASN	LYS	LYS	LYS	ILE	PRO	ILE	ILE	GLY	GLY	THR	THR	PHE	ALA	P92
THR	ASP	ASP	ASP	THR	ASP	ASP	ALA	GLY	ALA	ASN	ILE	THR	ALA	GLY
MET	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ARG	ALA	ARG	GLN	SER	CYS	P96
SER	LEU	LEU	TYR	SER	ARG	ARG	SER	ARG	ARG	VAL	MET	GLY	ASP	S97
GLU	MET	MET	ALA	ALA	ARG	ARG	ASN	ASN	ASN	PRO	LEU	SER	GLU	L98
GLN	LYS	LYS	GLU	GLN	SER	SER	GLN	SER	SER	LEU	VAL	ASP	ALA	L99

Chain U: 7% 5% 88%

[illegible]

[illegible]

- Molecule 3: ATP-dependent zinc metalloprotease FtsH



- Molecule 3: ATP-dependent zinc metalloprotease FtsH



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26863	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.032	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	384.384, 384.384, 384.384	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3728, 1.3728, 1.3728	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.23	0/2371	0.80	6/3187 (0.2%)
1	C	0.31	0/2321	0.78	4/3118 (0.1%)
1	D	0.25	0/2343	0.58	1/3148 (0.0%)
1	M	0.29	0/2371	0.70	4/3187 (0.1%)
1	O	0.29	0/2321	0.74	7/3118 (0.2%)
1	P	1.40	8/2343 (0.3%)	0.79	10/3148 (0.3%)
1	Y	0.23	0/2371	0.89	5/3187 (0.2%)
1	Z	0.23	0/2371	0.76	5/3187 (0.2%)
1	c	0.28	0/2321	0.58	1/3118 (0.0%)
1	d	0.30	0/2321	0.61	1/3118 (0.0%)
1	e	0.25	0/2343	0.59	1/3148 (0.0%)
1	f	0.31	0/2343	0.68	4/3148 (0.1%)
2	B	0.31	0/2202	1.05	9/2984 (0.3%)
2	F	0.33	0/2198	0.84	8/2979 (0.3%)
2	G	0.28	0/2206	0.62	2/2989 (0.1%)
2	N	0.33	0/2202	0.73	3/2984 (0.1%)
2	R	0.32	0/2198	0.78	3/2979 (0.1%)
2	S	0.29	0/2206	0.58	2/2989 (0.1%)
2	a	0.35	0/2202	0.82	6/2984 (0.2%)
2	b	0.41	1/2202 (0.0%)	0.84	10/2984 (0.3%)
2	i	0.32	0/2198	0.98	12/2979 (0.4%)
2	j	0.33	0/2198	0.93	10/2979 (0.3%)
2	k	0.27	0/2206	0.70	3/2989 (0.1%)
2	l	0.29	0/2206	0.58	0/2989
3	E	0.26	0/671	0.52	0/911
3	H	0.25	0/671	0.60	2/911 (0.2%)
3	I	0.44	0/655	0.69	1/889 (0.1%)
3	J	0.21	0/648	0.56	0/882
3	K	0.24	0/655	0.68	0/889
3	L	0.22	0/655	0.58	0/889
3	Q	0.24	0/671	0.56	0/911
3	T	0.27	0/671	0.65	1/911 (0.1%)
3	U	0.38	0/655	0.67	1/889 (0.1%)
3	V	0.27	0/648	0.77	1/882 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	W	0.22	0/655	0.55	0/889
3	X	0.22	0/655	0.58	0/889
3	g	0.24	0/671	0.61	0/911
3	h	0.28	0/671	0.62	2/911 (0.2%)
3	m	0.29	0/671	0.55	0/911
3	n	0.26	0/671	0.63	2/911 (0.2%)
3	o	0.34	0/655	0.63	0/889
3	p	0.35	0/655	0.70	1/889 (0.1%)
3	q	0.32	0/648	0.68	2/882 (0.2%)
3	r	0.35	0/648	0.77	2/882 (0.2%)
3	s	0.27	0/655	0.60	0/889
3	t	0.21	0/655	0.52	1/889 (0.1%)
3	u	0.25	0/655	0.84	5/889 (0.6%)
3	v	0.26	0/655	0.74	1/889 (0.1%)
All	All	0.39	9/70384 (0.0%)	0.73	139/95104 (0.1%)

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	O	0	1
1	c	0	2
2	R	0	1
2	S	0	2
2	a	0	1
2	b	0	1
2	j	0	1
2	k	0	2
2	l	0	1
3	h	0	1
3	q	0	1
All	All	0	14

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	34	PHE	CE1-CZ	27.17	2.20	1.38
1	P	34	PHE	CD2-CE2	27.07	2.19	1.38
1	P	34	PHE	CD1-CE1	26.21	2.17	1.38
1	P	39	ARG	CD-NE	26.13	1.82	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	34	PHE	CE2-CZ	24.97	2.13	1.38
1	P	34	PHE	CG-CD2	18.68	1.78	1.38
1	P	34	PHE	CG-CD1	18.42	1.77	1.38
1	P	39	ARG	NE-CZ	16.07	1.50	1.33
2	b	320	GLU	C-N	-9.18	1.22	1.33

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	37	VAL	N-CA-C	-34.87	70.80	110.21
2	B	101	LYS	N-CA-C	34.30	148.66	111.28
1	A	37	VAL	N-CA-C	-28.11	72.42	109.80
1	C	201	LEU	N-CA-C	-26.93	74.98	110.53
1	Z	37	VAL	N-CA-C	-26.43	73.08	109.55
2	B	102	GLU	N-CA-C	-24.05	71.72	109.95
2	a	346	LYS	N-CA-C	-22.96	74.75	108.96
2	F	129	ILE	N-CA-C	-21.79	92.28	113.20
1	P	39	ARG	CD-NE-CZ	21.27	154.19	124.40
2	i	101	LYS	CB-CA-C	-20.96	75.36	110.16
1	O	24	LYS	N-CA-C	20.52	142.85	111.04
2	R	101	LYS	CB-CA-C	-20.40	76.29	110.16
2	b	321	ILE	N-CA-C	-19.70	95.95	111.90
2	j	101	LYS	CB-CA-C	-18.72	79.86	111.31
2	i	129	ILE	N-CA-C	-18.20	95.70	113.53
2	k	346	LYS	N-CA-C	18.16	130.50	111.07
2	j	101	LYS	N-CA-C	14.80	135.27	107.75
2	F	100	ILE	CB-CA-C	14.12	130.91	111.70
2	j	139	ALA	N-CA-C	-13.98	89.50	108.38
1	M	38	LEU	N-CA-C	-13.96	84.21	108.23
1	Y	38	LEU	N-CA-CB	-13.60	91.79	110.42
1	M	39	ARG	N-CA-C	-13.32	86.47	108.32
2	R	101	LYS	N-CA-C	13.18	129.89	108.41
2	i	126	PRO	CB-CA-C	-13.00	90.11	111.56
2	i	101	LYS	N-CA-C	12.27	128.41	108.41
1	A	38	LEU	N-CA-CB	-12.16	92.01	110.25
2	j	129	ILE	CB-CA-C	11.73	130.53	111.29
2	j	138	GLU	N-CA-C	-11.58	89.76	108.41
2	j	102	GLU	N-CA-C	11.32	126.86	111.24
2	j	139	ALA	N-CA-CB	10.76	128.25	111.24
2	k	346	LYS	CB-CA-C	-10.66	94.14	110.88
1	Z	38	LEU	N-CA-CB	-10.45	94.58	110.25
2	i	128	PHE	N-CA-C	-10.35	94.10	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	126	PRO	N-CA-C	10.17	133.42	112.47
3	u	99	LEU	N-CA-C	10.08	127.90	111.37
2	R	102	GLU	N-CA-C	9.98	125.17	111.39
1	P	308	SER	N-CA-CB	9.91	125.91	110.84
1	M	39	ARG	N-CA-CB	9.85	127.22	110.57
1	P	39	ARG	NE-CZ-NH1	9.65	131.15	121.50
2	a	346	LYS	CB-CA-C	9.49	132.62	111.09
3	r	92	PRO	CA-N-CD	-9.47	98.74	112.00
2	B	102	GLU	N-CA-CB	-8.92	96.58	110.85
2	G	348	GLY	N-CA-C	-8.87	92.17	113.18
2	b	250	ALA	N-CA-C	-8.79	97.50	109.54
1	P	308	SER	N-CA-C	-8.65	92.63	108.02
2	b	320	GLU	CB-CA-C	-8.45	95.95	109.13
2	a	317	ALA	N-CA-C	8.43	120.55	111.36
3	q	50	ARG	CA-CB-CG	8.40	130.91	114.10
1	Y	37	VAL	CB-CA-C	8.40	120.86	111.45
2	B	101	LYS	CB-CA-C	-8.39	96.87	110.79
2	i	346	LYS	N-CA-C	8.06	119.70	111.07
2	F	128	PHE	N-CA-C	-8.00	96.67	109.39
2	b	320	GLU	N-CA-C	7.90	124.60	114.56
2	b	209	ARG	N-CA-C	7.75	122.77	113.16
2	B	103	ALA	N-CA-C	-7.67	95.09	108.20
2	b	320	GLU	O-C-N	-7.63	114.01	122.10
2	i	128	PHE	CB-CA-C	-7.62	100.69	112.12
1	C	201	LEU	CB-CA-C	7.56	125.18	109.68
1	O	25	GLU	N-CA-CB	7.46	123.10	110.49
2	b	249	ALA	CB-CA-C	-7.40	100.09	112.00
1	Y	144	ARG	N-CA-C	7.37	118.95	111.07
2	N	349	ASN	N-CA-C	7.32	120.69	111.24
2	i	129	ILE	N-CA-CB	7.31	121.99	112.12
2	N	317	ALA	N-CA-C	7.20	119.03	111.03
2	B	103	ALA	N-CA-CB	7.16	122.19	110.37
3	I	92	PRO	N-CA-C	7.10	117.28	110.47
2	i	324	GLU	N-CA-C	-7.02	104.34	113.12
3	n	53	GLY	N-CA-C	-6.96	98.07	111.02
2	j	346	LYS	N-CA-C	-6.92	104.09	112.54
1	f	57	PRO	CA-N-CD	-6.82	102.45	112.00
2	k	347	GLY	N-CA-C	6.78	129.24	113.18
2	j	129	ILE	N-CA-C	-6.76	95.28	109.34
1	A	296	PHE	CB-CA-C	-6.74	100.25	110.90
2	F	102	GLU	N-CA-C	-6.65	97.99	108.63
1	P	39	ARG	CG-CD-NE	6.63	126.59	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	90	GLY	CA-C-N	-6.53	111.42	123.11
3	h	90	GLY	C-N-CA	-6.53	111.42	123.11
3	H	54	ARG	N-CA-C	6.50	120.46	111.55
2	S	346	LYS	CB-CA-C	-6.49	96.62	109.67
1	A	146	ARG	N-CA-C	-6.46	106.61	114.75
1	O	23	VAL	N-CA-C	-6.39	99.26	108.53
3	H	53	GLY	N-CA-C	-6.39	99.13	111.02
1	P	307	PHE	N-CA-C	-6.33	96.08	107.98
1	O	201	LEU	N-CA-C	-6.33	101.49	110.35
1	f	66	ASP	N-CA-C	6.31	119.64	110.42
1	O	23	VAL	CB-CA-C	6.30	120.39	110.81
1	O	24	LYS	CB-CA-C	-6.28	101.40	111.39
1	Z	38	LEU	N-CA-C	-6.25	102.81	111.81
3	p	47	ARG	CB-CG-CD	6.24	125.65	111.30
2	F	100	ILE	N-CA-C	-6.21	100.47	109.29
2	a	322	THR	CB-CA-C	-6.20	100.30	110.85
2	F	129	ILE	N-CA-CB	6.19	122.14	112.67
1	e	291	PRO	N-CA-CB	6.19	109.75	103.25
1	f	291	PRO	N-CA-CB	6.17	109.73	103.25
1	D	291	PRO	N-CA-CB	6.17	109.73	103.25
2	b	351	MET	CB-CA-C	-6.17	109.47	116.63
1	Y	291	PRO	N-CA-CB	6.16	110.10	103.33
2	G	349	ASN	N-CA-C	-6.14	94.22	107.49
1	Z	291	PRO	N-CA-CB	6.14	110.09	103.33
1	M	291	PRO	N-CA-CB	6.14	110.08	103.33
1	P	291	PRO	N-CA-CB	6.14	109.70	103.25
3	v	47	ARG	CB-CG-CD	6.12	125.36	111.30
1	A	145	GLY	N-CA-C	6.11	120.28	112.83
3	u	54	ARG	CA-CB-CG	6.08	126.27	114.10
3	V	54	ARG	N-CA-C	-6.07	104.39	112.94
2	i	137	VAL	N-CA-C	6.05	116.53	110.23
1	A	291	PRO	N-CA-CB	6.05	109.99	103.33
2	B	322	THR	N-CA-C	-6.04	104.77	111.36
3	n	86	VAL	N-CA-C	6.01	117.33	109.58
3	U	92	PRO	N-CA-C	5.90	117.89	110.70
2	b	209	ARG	N-CA-CB	-5.87	101.45	110.44
2	i	323	ARG	CB-CA-C	-5.82	98.85	110.42
3	r	92	PRO	N-CD-CG	-5.82	94.48	103.20
3	T	53	GLY	N-CA-C	-5.80	100.24	111.02
2	j	201	MET	N-CA-C	5.77	117.26	110.97
1	f	308	SER	N-CA-CB	5.74	119.85	110.90
1	C	291	PRO	N-CA-CB	5.68	109.80	103.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	231	ARG	CB-CG-CD	-5.67	98.26	111.30
1	c	291	PRO	N-CA-CB	5.65	109.77	103.44
1	O	291	PRO	N-CA-CB	5.65	109.77	103.44
1	d	291	PRO	N-CA-CB	5.58	109.69	103.44
2	b	249	ALA	N-CA-C	-5.54	100.59	109.39
2	a	317	ALA	CB-CA-C	-5.42	101.63	110.85
1	P	39	ARG	CB-CG-CD	5.42	123.77	111.30
1	P	39	ARG	NH1-CZ-NH2	-5.41	112.26	119.30
1	C	111	ASP	N-CA-C	-5.38	100.94	109.76
3	q	50	ARG	CD-NE-CZ	5.35	131.89	124.40
3	u	98	LEU	N-CA-C	5.34	122.18	110.80
3	u	98	LEU	CB-CA-C	5.32	121.01	110.42
2	B	110	ARG	CB-CG-CD	-5.16	99.43	111.30
1	P	39	ARG	CA-CB-CG	5.15	124.40	114.10
2	F	128	PHE	CA-C-N	-5.13	116.41	122.36
2	F	128	PHE	C-N-CA	-5.13	116.41	122.36
2	a	319	PRO	N-CA-C	5.12	123.02	112.47
3	t	53	GLY	N-CA-C	-5.11	101.07	113.18
2	N	351	MET	CB-CA-C	-5.09	110.68	116.54
2	B	102	GLU	CB-CA-C	5.09	118.69	109.37
2	S	291	ARG	CA-CB-CG	5.06	124.23	114.10
3	u	54	ARG	CB-CG-CD	5.04	122.89	111.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	40	ASP	Peptide
2	R	137	VAL	Peptide
2	S	134	PRO	Peptide
2	S	135	VAL	Peptide
2	a	240	ALA	Peptide
2	b	320	GLU	Mainchain
1	c	39	ARG	Peptide
1	c	40	ASP	Peptide
3	h	91	GLU	Peptide
2	j	243	PRO	Peptide
2	k	134	PRO	Peptide
2	k	135	VAL	Peptide
2	l	134	PRO	Peptide
3	q	57	ASN	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	A	2338	0	2354	93	0
1	C	2290	0	2310	75	0
1	D	2311	0	2331	77	0
1	M	2338	0	2354	88	0
1	O	2290	0	2310	71	0
1	P	2311	0	2331	106	0
1	Y	2338	0	2354	75	0
1	Z	2338	0	2354	81	0
1	c	2290	0	2310	75	0
1	d	2290	0	2310	61	0
1	e	2311	0	2331	94	0
1	f	2311	0	2331	99	0
2	B	2169	0	2180	92	0
2	F	2165	0	2176	91	0
2	G	2173	0	2186	82	0
2	N	2169	0	2180	110	0
2	R	2165	0	2176	83	0
2	S	2173	0	2186	75	0
2	a	2169	0	2180	91	0
2	b	2169	0	2180	89	0
2	i	2165	0	2176	84	0
2	j	2165	0	2176	88	0
2	k	2173	0	2186	73	0
2	l	2173	0	2186	94	0
3	E	658	0	662	13	0
3	H	658	0	662	17	0
3	I	643	0	646	34	0
3	J	635	0	637	46	0
3	K	643	0	646	37	0
3	L	643	0	646	38	0
3	Q	658	0	662	18	0
3	T	658	0	662	18	0
3	U	643	0	646	24	0
3	V	635	0	637	58	0
3	W	643	0	646	28	0
3	X	643	0	646	48	0
3	g	658	0	662	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	h	658	0	662	13	0
3	m	658	0	662	17	0
3	n	658	0	662	30	0
3	o	643	0	646	27	0
3	p	643	0	646	28	0
3	q	635	0	637	34	0
3	r	635	0	637	49	0
3	s	643	0	646	20	0
3	t	643	0	646	37	0
3	u	643	0	646	51	0
3	v	643	0	646	50	0
All	All	69304	0	69744	2436	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 18.

All (2436) 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:P:34:PHE:CD2	1:P:34:PHE:CG	1.78	1.68
1:P:34:PHE:CG	1:P:34:PHE:CD1	1.77	1.61
3:V:88:VAL:CG2	3:X:35:SER:HB3	1.09	1.51
1:P:39:ARG:CD	1:P:39:ARG:NE	1.82	1.42
3:V:88:VAL:HG22	3:X:35:SER:CB	1.51	1.39
2:b:351:MET:HE3	2:j:351:MET:SD	1.62	1.38
1:P:34:PHE:CZ	1:P:34:PHE:CE2	2.13	1.36
1:P:34:PHE:CD2	1:P:39:ARG:NE	1.92	1.33
1:P:34:PHE:CD1	1:P:34:PHE:CE1	2.17	1.31
1:P:34:PHE:CZ	1:P:34:PHE:CE1	2.20	1.29
1:P:34:PHE:CD2	1:P:34:PHE:CE2	2.19	1.29
1:P:34:PHE:CE2	1:P:39:ARG:NE	2.01	1.29
1:P:34:PHE:CG	1:P:39:ARG:NE	2.00	1.28
1:P:34:PHE:CD1	1:P:39:ARG:NE	2.03	1.26
3:V:88:VAL:CG2	3:X:35:SER:CB	2.05	1.25
1:P:34:PHE:CE1	1:P:39:ARG:NE	2.14	1.14
3:u:98:LEU:O	3:u:102:ILE:HD13	1.47	1.14
1:P:34:PHE:CZ	1:P:39:ARG:NE	2.17	1.12
3:u:98:LEU:O	3:u:102:ILE:CD1	1.99	1.10
2:b:351:MET:CE	2:j:351:MET:SD	2.40	1.09
3:V:88:VAL:HG23	3:X:35:SER:HB3	1.17	1.06
1:P:34:PHE:CZ	1:P:39:ARG:HD3	1.94	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:34:PHE:CE1	1:P:39:ARG:CD	2.42	1.01
2:F:127:THR:HB	2:F:129:ILE:HG23	1.39	1.01
1:O:227:MET:SD	2:R:248:LYS:NZ	2.33	1.00
1:P:34:PHE:CZ	1:P:39:ARG:CD	2.43	1.00
3:q:50:ARG:HH11	3:q:57:ASN:HB3	1.22	1.00
2:F:128:PHE:O	2:F:128:PHE:CD2	2.15	0.99
1:P:34:PHE:CZ	1:P:39:ARG:CZ	2.47	0.98
3:q:50:ARG:NH1	3:q:57:ASN:HB3	1.81	0.95
1:M:38:LEU:O	1:M:44:LYS:HB2	1.65	0.95
1:P:34:PHE:CE1	1:P:39:ARG:CZ	2.49	0.95
3:r:81:LEU:HD13	3:r:88:VAL:HG21	1.47	0.94
2:B:351:MET:HA	2:F:350:LEU:HA	1.48	0.94
2:N:88:ILE:O	2:N:92:TRP:HB2	1.67	0.93
2:F:128:PHE:O	2:F:128:PHE:HD2	1.53	0.91
1:c:210:ILE:HG23	2:i:193:ARG:HH22	1.33	0.91
1:P:34:PHE:CE1	1:P:39:ARG:HD2	2.05	0.90
1:c:27:GLU:HB3	1:c:66:ASP:HA	1.49	0.90
2:j:185:ARG:NH1	3:n:45:GLN:OE1	2.05	0.90
1:Y:36:LYS:C	1:Y:37:VAL:O	1.93	0.88
1:M:114:GLN:HG3	3:T:47:ARG:HH12	1.39	0.88
1:d:210:ILE:HG23	2:j:193:ARG:HH22	1.37	0.88
1:C:255:TYR:CE2	2:G:292:ALA:HB3	2.09	0.88
1:D:72:MET:HE2	1:D:116:GLU:HG3	1.56	0.88
3:v:45:GLN:O	3:v:47:ARG:NH2	2.08	0.87
3:H:52:ASN:HD21	3:H:91:GLU:HB2	1.40	0.86
2:S:172:LYS:NZ	2:S:228:ASP:O	2.06	0.86
1:P:34:PHE:CE2	1:P:39:ARG:CZ	2.57	0.86
1:A:248:LYS:HE2	2:F:284:GLN:HG3	1.58	0.85
1:Z:48:TYR:O	2:b:113:LYS:NZ	2.10	0.85
1:D:257:VAL:HG23	2:G:279:ALA:HB2	1.58	0.84
1:f:152:ARG:NH1	1:f:206:VAL:O	2.09	0.84
2:j:201:MET:O	2:j:205:LEU:HD23	1.78	0.84
1:D:36:LYS:HD2	2:a:121:GLY:HA2	1.58	0.83
2:i:101:LYS:O	2:i:104:GLU:HG2	1.76	0.83
3:V:88:VAL:HG22	3:X:35:SER:HB3	0.85	0.83
1:O:243:GLN:OE1	2:S:278:ARG:NH2	2.12	0.83
1:Z:82:LYS:NZ	1:Z:133:ARG:O	2.11	0.83
2:l:182:ASP:OD1	2:l:186:GLN:NE2	2.11	0.83
2:N:141:ARG:HH22	2:N:167:VAL:HG13	1.43	0.83
2:j:201:MET:HE3	2:j:205:LEU:HD21	1.60	0.83
3:n:93:PRO:HD3	3:p:54:ARG:HH12	1.45	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:GLU:OE2	2:G:291:ARG:NH2	2.12	0.82
3:V:47:ARG:NH1	3:V:60:LYS:O	2.11	0.82
1:O:82:LYS:NZ	1:O:132:GLY:O	2.13	0.81
3:V:31:LYS:N	3:V:67:THR:O	2.14	0.81
1:Y:74:ASN:HB3	1:Y:120:LYS:HZ2	1.45	0.81
1:P:34:PHE:CD1	1:P:39:ARG:CD	2.63	0.81
1:P:34:PHE:CE2	1:P:39:ARG:CD	2.62	0.81
2:B:141:ARG:HH22	2:B:167:VAL:HG13	1.44	0.81
3:m:92:PRO:HA	3:o:69:TYR:HE2	1.45	0.81
1:d:71:THR:HG22	1:d:94:LYS:HE3	1.63	0.81
3:u:45:GLN:HB3	3:u:60:LYS:HE2	1.60	0.81
3:q:81:LEU:HD13	3:q:88:VAL:HG21	1.62	0.81
1:P:257:VAL:HG23	2:S:279:ALA:HB2	1.63	0.81
1:O:32:LEU:HA	1:O:37:VAL:HA	1.62	0.81
3:J:81:LEU:HD13	3:J:88:VAL:HG21	1.63	0.81
1:f:38:LEU:HB3	1:f:44:LYS:HZ1	1.44	0.81
3:n:87:LYS:NZ	3:p:33:ASP:OD2	2.14	0.81
1:A:274:GLU:OE2	2:F:310:LYS:NZ	2.14	0.80
3:u:98:LEU:O	3:u:102:ILE:HD12	1.80	0.80
2:G:182:ASP:OD1	2:G:186:GLN:NE2	2.15	0.80
2:a:141:ARG:HH22	2:a:167:VAL:HG13	1.46	0.80
3:T:92:PRO:HA	3:U:69:TYR:HE1	1.47	0.80
2:R:352:VAL:HG23	2:S:350:LEU:HD13	1.64	0.79
3:t:50:ARG:HB2	3:t:57:ASN:HB2	1.62	0.79
2:b:275:VAL:HA	2:b:278:ARG:HH12	1.47	0.79
3:H:92:PRO:HA	3:I:69:TYR:HE1	1.48	0.79
1:M:48:TYR:O	2:N:113:LYS:NZ	2.13	0.79
1:C:32:LEU:HA	1:C:37:VAL:HA	1.65	0.79
1:Z:239:ARG:HH12	2:b:257:ALA:HA	1.48	0.79
3:J:47:ARG:H	3:J:60:LYS:HA	1.47	0.79
3:r:47:ARG:NH1	3:r:60:LYS:O	2.15	0.78
1:P:34:PHE:CZ	1:P:39:ARG:NH1	2.51	0.78
1:D:128:ARG:HH22	2:a:213:ARG:HH12	1.32	0.78
1:A:48:TYR:O	2:B:113:LYS:NZ	2.13	0.78
3:V:88:VAL:HG22	3:X:35:SER:HB2	1.66	0.78
1:c:37:VAL:O	1:c:39:ARG:NH1	2.17	0.78
2:R:205:LEU:HG	2:R:206:THR:HG23	1.65	0.78
3:u:30:ARG:HH21	3:u:65:ARG:HG3	1.49	0.77
1:P:34:PHE:CD1	1:P:39:ARG:CZ	2.67	0.77
1:D:310:ASN:OD1	1:D:311:GLN:N	2.17	0.77
3:K:103:PHE:HA	3:K:106:TRP:HD1	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:213:ARG:HH21	2:a:237:ASN:HA	1.49	0.77
2:i:155:ASN:ND2	2:i:201:MET:SD	2.57	0.76
2:k:235:ASP:OD1	2:k:236:VAL:N	2.18	0.76
2:k:133:LYS:HE2	2:k:174:LEU:HD22	1.67	0.76
3:p:45:GLN:HA	3:p:61:LYS:NZ	2.01	0.76
1:A:82:LYS:NZ	1:A:133:ARG:O	2.18	0.76
3:V:45:GLN:O	3:V:61:LYS:N	2.14	0.76
3:J:54:ARG:NH1	3:J:55:GLU:OE2	2.18	0.76
3:V:88:VAL:HG23	3:X:35:SER:CB	1.95	0.76
2:i:162:ASN:HB3	2:i:237:ASN:HB2	1.66	0.76
2:b:110:ARG:HH11	2:b:111:PHE:H	1.30	0.76
2:l:101:LYS:HE2	2:l:104:GLU:HG3	1.66	0.76
2:j:155:ASN:ND2	2:j:201:MET:SD	2.59	0.76
2:l:184:LEU:HD12	2:l:187:ALA:HB3	1.66	0.76
1:f:212:GLN:HE22	1:f:214:ASN:HB3	1.49	0.76
2:G:245:GLU:HG2	2:G:247:VAL:H	1.49	0.75
1:e:310:ASN:OD1	1:e:311:GLN:N	2.16	0.75
2:R:205:LEU:HD13	2:R:243:PRO:HG2	1.67	0.75
1:C:200:ALA:C	1:C:201:LEU:O	2.13	0.75
3:r:46:VAL:HA	3:r:60:LYS:HA	1.67	0.75
1:P:212:GLN:HE22	1:P:214:ASN:HB3	1.51	0.75
1:f:126:ARG:NH2	1:f:150:GLU:OE1	2.18	0.75
2:j:242:ARG:HG2	2:j:244:PRO:HD3	1.68	0.75
3:V:59:THR:HA	3:V:65:ARG:HH21	1.51	0.75
3:J:54:ARG:NH2	3:J:70:ILE:O	2.19	0.75
1:M:38:LEU:O	1:M:44:LYS:CB	2.35	0.75
3:v:103:PHE:HA	3:v:106:TRP:HE3	1.52	0.75
3:u:103:PHE:HA	3:u:106:TRP:HD1	1.51	0.75
3:I:48:GLU:HB2	3:I:59:THR:HB	1.68	0.74
2:j:101:LYS:HG3	2:j:101:LYS:O	1.88	0.74
1:P:30:ILE:HD11	1:P:100:PHE:HB3	1.69	0.74
2:k:133:LYS:NZ	2:k:135:VAL:O	2.18	0.74
1:f:128:ARG:HH12	2:N:213:ARG:HE	1.34	0.74
2:j:101:LYS:O	2:j:104:GLU:OE2	2.05	0.74
2:N:125:LYS:HE3	2:N:126:PRO:HD2	1.70	0.74
2:S:182:ASP:OD1	2:S:186:GLN:NE2	2.19	0.74
3:p:47:ARG:HD3	3:p:61:LYS:HG2	1.68	0.74
1:O:137:LYS:NZ	2:R:152:SER:O	2.20	0.74
1:O:55:LYS:NZ	1:O:57:PRO:O	2.20	0.74
3:q:50:ARG:O	3:q:57:ASN:HB2	1.88	0.73
3:v:30:ARG:NH2	3:v:64:ASN:OD1	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:v:47:ARG:HH11	3:v:61:LYS:HG2	1.54	0.73
3:W:50:ARG:NH2	3:W:91:GLU:OE1	2.21	0.73
1:C:243:GLN:OE1	2:G:278:ARG:NH2	2.22	0.73
1:e:257:VAL:HG23	2:k:279:ALA:HB2	1.69	0.73
2:i:205:LEU:HD13	2:i:243:PRO:HG2	1.68	0.73
3:V:93:PRO:HB3	3:X:54:ARG:NH2	2.04	0.73
1:D:314:MET:HE3	2:a:342:LEU:HD23	1.69	0.73
1:f:94:LYS:HG3	1:f:206:VAL:HB	1.70	0.73
1:e:212:GLN:HE22	1:e:214:ASN:HB3	1.55	0.72
2:b:188:THR:HG22	2:b:220:LEU:HD11	1.71	0.72
2:l:165:TYR:CE1	2:l:184:LEU:HD23	2.24	0.72
2:R:329:GLU:OE2	2:R:333:LYS:NZ	2.16	0.72
3:V:50:ARG:HH12	3:V:57:ASN:HB2	1.53	0.72
1:c:40:ASP:HB3	1:c:44:LYS:HD3	1.70	0.72
2:S:245:GLU:HG3	2:S:247:VAL:H	1.54	0.72
3:o:50:ARG:HB2	3:o:57:ASN:HB2	1.70	0.72
1:Z:39:ARG:NH1	1:Z:42:ASP:O	2.23	0.72
3:K:56:ILE:HD11	3:K:70:ILE:HG13	1.70	0.72
2:B:104:GLU:HG3	2:B:138:GLU:HG2	1.70	0.72
1:D:300:LEU:HD22	2:G:330:THR:HG21	1.71	0.71
1:Y:274:GLU:OE1	2:i:310:LYS:NZ	2.24	0.71
3:p:47:ARG:NH1	3:p:61:LYS:HB3	2.05	0.71
1:C:40:ASP:HB3	1:C:44:LYS:HD3	1.71	0.71
3:h:103:PHE:O	3:h:107:PHE:N	2.22	0.71
1:A:74:ASN:HB3	1:A:120:LYS:HZ1	1.55	0.71
1:C:55:LYS:NZ	1:C:57:PRO:O	2.23	0.71
2:j:194:GLY:O	2:j:198:LYS:NZ	2.21	0.71
1:A:111:ASP:OD1	1:A:114:GLN:NE2	2.22	0.71
2:k:105:ARG:HH12	2:k:117:LEU:HD13	1.54	0.71
1:D:30:ILE:HD11	1:D:100:PHE:HB3	1.71	0.71
1:f:300:LEU:HD22	2:l:330:THR:HG21	1.72	0.71
3:v:47:ARG:HH11	3:v:61:LYS:H	1.38	0.71
3:u:47:ARG:HH22	3:u:63:SER:H	1.39	0.71
2:j:104:GLU:HG2	2:j:136:ASN:HA	1.71	0.71
1:O:256:GLU:OE1	1:O:259:ARG:NH2	2.24	0.71
1:Z:300:LEU:HG	2:b:330:THR:HG21	1.71	0.71
2:a:213:ARG:NH2	2:a:236:VAL:O	2.23	0.71
1:c:55:LYS:NZ	1:c:57:PRO:O	2.24	0.71
1:e:300:LEU:HD12	2:k:330:THR:HG21	1.71	0.71
3:W:74:ASP:OD2	3:W:77:LEU:N	2.13	0.71
1:Y:239:ARG:HH12	2:a:257:ALA:HA	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:138:GLU:OE1	2:b:166:ARG:NH1	2.24	0.71
2:B:110:ARG:HD3	2:B:130:ASP:HA	1.72	0.71
2:a:93:ALA:HA	2:a:126:PRO:HA	1.72	0.71
3:u:44:ASP:O	3:u:61:LYS:NZ	2.24	0.71
2:b:331:MET:HA	2:b:334:VAL:HG12	1.73	0.71
1:f:244:GLU:OE2	2:N:278:ARG:NH2	2.24	0.71
1:P:34:PHE:CE1	1:P:39:ARG:NH1	2.57	0.71
2:B:213:ARG:NH2	2:B:236:VAL:O	2.23	0.70
3:m:40:GLU:OE1	3:m:66:TYR:OH	2.08	0.70
1:d:40:ASP:HB3	1:d:44:LYS:HD3	1.72	0.70
3:t:74:ASP:OD2	3:t:77:LEU:N	2.24	0.70
1:M:82:LYS:NZ	1:M:133:ARG:O	2.21	0.70
1:A:74:ASN:HB3	1:A:120:LYS:NZ	2.06	0.70
1:A:221:GLU:OE2	1:A:225:ASN:ND2	2.24	0.70
1:A:300:LEU:HG	2:B:330:THR:HG21	1.73	0.70
3:v:49:ALA:HB2	3:v:58:VAL:HG23	1.73	0.70
3:t:43:ASN:HB3	3:t:45:GLN:HE22	1.56	0.70
1:d:102:ARG:NH1	1:d:201:LEU:O	2.24	0.70
1:P:300:LEU:HD22	2:S:330:THR:HG21	1.73	0.70
3:V:46:VAL:HA	3:V:60:LYS:HA	1.73	0.70
1:A:134:LEU:HD13	1:A:138:ASP:HB3	1.74	0.70
1:C:37:VAL:O	1:C:39:ARG:NH1	2.24	0.70
1:f:30:ILE:HD11	1:f:100:PHE:HB3	1.74	0.70
1:M:300:LEU:HG	2:N:330:THR:HG21	1.74	0.70
3:U:34:TYR:HE1	3:U:70:ILE:HG12	1.56	0.70
1:Z:231:ARG:CZ	2:b:251:PHE:HB3	2.21	0.70
1:e:102:ARG:O	1:e:106:ALA:HB2	1.91	0.70
3:t:47:ARG:HB3	3:t:61:LYS:HG2	1.74	0.70
1:O:126:ARG:HG2	1:O:154:ALA:HB1	1.74	0.70
1:c:94:LYS:HB2	1:c:207:ASP:H	1.57	0.69
2:b:105:ARG:O	2:b:136:ASN:ND2	2.24	0.69
1:e:121:ARG:NH1	2:b:235:ASP:OD2	2.24	0.69
3:o:101:SER:HA	3:o:104:ILE:HG22	1.73	0.69
1:d:37:VAL:O	1:d:39:ARG:NH1	2.26	0.69
3:r:50:ARG:NH2	3:r:51:ILE:O	2.19	0.69
1:M:96:ARG:HD3	1:M:97:ILE:H	1.56	0.69
3:W:52:ASN:ND2	3:W:91:GLU:OE2	2.23	0.69
1:f:128:ARG:HA	1:f:131:ILE:HG22	1.75	0.69
3:V:47:ARG:HD3	3:V:61:LYS:HA	1.73	0.69
1:f:281:LYS:N	2:N:314:GLU:OE2	2.25	0.69
3:t:55:GLU:HG2	3:t:69:TYR:HE1	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:91:GLU:HB2	3:U:92:PRO:HD2	1.75	0.69
2:G:245:GLU:OE2	2:G:248:LYS:NZ	2.20	0.69
1:Y:197:SER:HG	1:Y:200:ALA:H	1.37	0.69
2:l:114:PHE:HE1	2:l:171:GLU:HG3	1.57	0.69
3:v:47:ARG:NH1	3:v:61:LYS:H	1.90	0.69
3:v:47:ARG:NH1	3:v:61:LYS:HG2	2.06	0.69
1:O:71:THR:HG22	1:O:94:LYS:HE3	1.75	0.69
2:R:217:GLN:HB2	2:R:236:VAL:HG21	1.73	0.69
2:S:110:ARG:HH21	2:S:130:ASP:H	1.39	0.69
1:D:128:ARG:HH22	2:a:213:ARG:NH1	1.91	0.69
2:F:153:ASP:HB3	2:F:155:ASN:HD22	1.57	0.69
2:G:165:TYR:HE1	2:G:184:LEU:HD23	1.57	0.69
3:s:46:VAL:HG22	3:s:60:LYS:HG2	1.74	0.69
2:G:98:TYR:OH	2:G:125:LYS:NZ	2.23	0.69
2:a:331:MET:HA	2:a:334:VAL:HG12	1.73	0.69
3:I:50:ARG:HH22	3:I:91:GLU:HB2	1.58	0.68
1:Z:327:LYS:HG3	1:Z:329:PRO:HD2	1.74	0.68
1:f:257:VAL:HG23	2:l:279:ALA:HB2	1.75	0.68
1:M:78:ARG:NH2	1:M:86:ASP:OD2	2.27	0.68
2:N:173:TYR:HD2	2:N:174:LEU:HD22	1.57	0.68
1:D:298:ARG:HH21	1:D:301:ARG:HH21	1.40	0.68
2:a:188:THR:HG22	2:a:220:LEU:HD11	1.74	0.68
1:M:253:ALA:HB1	2:N:275:VAL:HG11	1.75	0.68
1:D:43:ASN:O	1:D:43:ASN:ND2	2.26	0.68
3:K:56:ILE:HD13	3:K:68:THR:HG23	1.76	0.68
3:t:102:ILE:HG23	3:t:106:TRP:CZ3	2.28	0.68
2:B:331:MET:HA	2:B:334:VAL:HG12	1.75	0.68
3:q:47:ARG:HH22	3:q:61:LYS:HA	1.57	0.68
3:r:78:LEU:HD12	3:r:81:LEU:HD11	1.75	0.68
3:X:49:ALA:HB2	3:X:58:VAL:HG23	1.76	0.68
1:O:300:LEU:HD22	2:R:330:THR:HG21	1.76	0.68
2:F:102:GLU:O	2:F:104:GLU:OE2	2.10	0.68
2:B:110:ARG:NH1	2:B:129:ILE:O	2.27	0.68
3:L:49:ALA:HB2	3:L:58:VAL:HG23	1.76	0.68
3:v:47:ARG:HH12	3:v:60:LYS:HE2	1.58	0.68
1:P:34:PHE:CD2	1:P:39:ARG:CZ	2.76	0.68
1:Y:221:GLU:OE2	1:Y:225:ASN:ND2	2.27	0.68
1:e:23:VAL:HB	1:e:51:GLY:HA2	1.75	0.68
3:r:60:LYS:HD2	3:r:64:ASN:HB3	1.76	0.68
1:D:102:ARG:O	1:D:106:ALA:HB2	1.94	0.67
3:q:49:ALA:N	3:q:87:LYS:O	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:94:LYS:HE3	2:l:227:TYR:CE1	2.29	0.67
2:S:235:ASP:OD1	2:S:236:VAL:N	2.26	0.67
1:Y:327:LYS:HG3	1:Y:329:PRO:HD2	1.75	0.67
3:W:33:ASP:CG	3:X:87:LYS:HZ1	2.03	0.67
2:B:163:VAL:HG12	2:B:236:VAL:HG12	1.77	0.67
1:C:135:ASP:OD2	1:C:136:VAL:N	2.28	0.67
3:u:47:ARG:HH11	3:u:59:THR:HG22	1.60	0.67
1:Z:78:ARG:NH1	1:Z:86:ASP:OD2	2.27	0.67
2:j:169:ASN:HD22	2:j:172:LYS:NZ	1.92	0.67
3:V:32:VAL:HB	3:V:66:TYR:CE2	2.30	0.67
1:Y:78:ARG:NH2	1:Y:86:ASP:OD2	2.27	0.67
1:Y:82:LYS:NZ	1:Y:133:ARG:O	2.21	0.67
1:f:55:LYS:HD3	1:f:60:GLU:HB3	1.77	0.67
2:N:188:THR:HG22	2:N:220:LEU:HD11	1.77	0.67
1:P:102:ARG:O	1:P:106:ALA:HB2	1.94	0.67
2:F:217:GLN:HB2	2:F:236:VAL:HG21	1.75	0.67
2:N:331:MET:HA	2:N:334:VAL:HG12	1.77	0.67
1:Y:74:ASN:HB3	1:Y:120:LYS:NZ	2.09	0.67
1:e:68:ARG:NH2	2:k:174:LEU:O	2.27	0.67
3:s:43:ASN:HB3	3:s:45:GLN:HE22	1.60	0.67
2:l:351:MET:CE	2:N:351:MET:HB2	2.25	0.67
1:O:40:ASP:HB3	1:O:44:LYS:HD3	1.75	0.67
2:B:350:LEU:HA	2:S:351:MET:HG2	1.75	0.67
1:M:327:LYS:HG3	1:M:329:PRO:HD2	1.77	0.67
3:J:47:ARG:NH1	3:J:60:LYS:O	2.28	0.66
1:A:69:ILE:HG13	1:A:96:ARG:HH11	1.59	0.66
2:i:220:LEU:HD22	2:i:233:LEU:HD21	1.77	0.66
1:f:57:PRO:HD2	1:f:58:PHE:H	1.60	0.66
2:l:262:GLN:HB3	2:l:266:ARG:HH21	1.61	0.66
1:O:135:ASP:OD2	1:O:136:VAL:N	2.27	0.66
1:A:78:ARG:NH2	1:A:86:ASP:OD2	2.28	0.66
2:a:163:VAL:HG12	2:a:236:VAL:HG12	1.78	0.66
1:c:226:ARG:NH2	2:i:154:GLU:O	2.29	0.66
1:f:31:THR:HG21	1:f:63:LYS:HG2	1.76	0.66
2:l:235:ASP:OD1	2:l:236:VAL:N	2.29	0.66
1:c:94:LYS:HA	1:c:94:LYS:HE3	1.76	0.66
1:c:151:VAL:HB	1:c:208:VAL:HG22	1.78	0.66
3:q:54:ARG:NH2	3:q:70:ILE:O	2.28	0.66
1:d:151:VAL:HB	1:d:208:VAL:HG22	1.78	0.66
1:f:96:ARG:NH1	1:f:204:GLU:OE2	2.28	0.66
2:R:331:MET:HA	2:R:334:VAL:HG12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:173:TYR:HD2	2:b:174:LEU:HD22	1.61	0.66
3:t:103:PHE:O	3:t:107:PHE:N	2.28	0.66
1:Z:96:ARG:HD3	1:Z:97:ILE:H	1.59	0.65
2:l:242:ARG:NH1	2:l:244:PRO:O	2.30	0.65
2:R:100:ILE:HB	2:R:121:GLY:H	1.62	0.65
2:a:173:TYR:HD2	2:a:174:LEU:HD22	1.62	0.65
1:d:126:ARG:HG2	1:d:154:ALA:HB1	1.78	0.65
3:T:100:ALA:HA	3:T:103:PHE:CE1	2.32	0.65
3:V:88:VAL:HG21	3:X:35:SER:HB3	1.59	0.65
2:a:125:LYS:HB3	2:a:127:THR:HG22	1.79	0.65
1:c:32:LEU:HA	1:c:37:VAL:HA	1.78	0.65
2:b:163:VAL:HG12	2:b:236:VAL:HG12	1.79	0.65
2:B:173:TYR:HD2	2:B:174:LEU:HD22	1.62	0.65
1:e:30:ILE:HD11	1:e:100:PHE:HB3	1.77	0.65
2:b:108:VAL:HG22	2:b:132:VAL:HG12	1.77	0.65
2:l:165:TYR:HE1	2:l:184:LEU:HD23	1.61	0.65
1:M:28:ARG:HH21	1:M:46:LEU:HD13	1.61	0.65
2:R:351:MET:HA	2:S:350:LEU:HB2	1.79	0.65
1:C:255:TYR:CE2	2:G:289:GLU:HA	2.31	0.65
1:D:82:LYS:HD3	1:D:133:ARG:HH12	1.61	0.65
1:c:210:ILE:HG23	2:i:193:ARG:NH2	2.08	0.65
1:P:34:PHE:CD2	1:P:39:ARG:CD	2.80	0.65
1:C:151:VAL:HB	1:C:208:VAL:HG22	1.79	0.65
1:Y:253:ALA:HB1	2:a:275:VAL:HG11	1.77	0.65
3:Q:106:TRP:HA	3:Q:109:MET:HB2	1.79	0.65
2:S:100:ILE:HD11	2:S:120:PRO:HA	1.78	0.65
1:Y:49:GLU:HB3	2:a:113:LYS:HE2	1.79	0.65
3:o:31:LYS:HA	3:o:31:LYS:HE3	1.80	0.64
2:R:145:ALA:HB3	2:R:161:MET:HB3	1.79	0.64
2:b:93:ALA:HA	2:b:126:PRO:HA	1.79	0.64
2:S:262:GLN:HB3	2:S:266:ARG:HH21	1.62	0.64
2:G:109:THR:OG1	2:G:113:LYS:N	2.31	0.64
3:L:47:ARG:HH11	3:L:59:THR:HG22	1.63	0.64
2:k:242:ARG:NH1	2:k:244:PRO:O	2.30	0.64
1:d:20:VAL:HG13	1:d:53:HIS:HB3	1.78	0.64
1:d:32:LEU:HA	1:d:37:VAL:HA	1.79	0.64
3:r:33:ASP:OD2	3:r:35:SER:OG	2.12	0.64
3:v:33:ASP:OD1	3:v:34:TYR:N	2.31	0.64
3:X:40:GLU:OE2	3:X:66:TYR:OH	2.08	0.64
3:K:47:ARG:HG3	3:K:61:LYS:HG2	1.78	0.64
3:V:48:GLU:O	3:V:59:THR:OG1	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ARG:HG2	1:C:154:ALA:HB1	1.80	0.64
1:f:15:VAL:HA	1:f:18:MET:HG2	1.78	0.64
2:B:108:VAL:HG22	2:B:132:VAL:HG12	1.79	0.64
2:l:331:MET:HA	2:l:334:VAL:HG12	1.78	0.64
3:q:63:SER:HB3	3:q:65:ARG:HH12	1.63	0.64
1:f:102:ARG:O	1:f:106:ALA:HB2	1.98	0.64
2:N:105:ARG:O	2:N:136:ASN:ND2	2.22	0.64
2:j:235:ASP:OD2	2:j:237:ASN:ND2	2.31	0.64
3:t:52:ASN:ND2	3:t:91:GLU:OE2	2.29	0.64
2:N:100:ILE:HB	2:N:120:PRO:HA	1.80	0.64
1:D:44:LYS:H	1:D:44:LYS:HD2	1.63	0.64
1:e:314:MET:HE3	2:b:342:LEU:HD13	1.79	0.64
2:k:262:GLN:HB3	2:k:266:ARG:HH21	1.63	0.64
2:l:351:MET:HE2	2:N:351:MET:HB2	1.77	0.63
3:r:103:PHE:O	3:r:107:PHE:N	2.27	0.63
1:O:232:GLU:OE2	1:O:236:ARG:NH2	2.31	0.63
1:P:34:PHE:CD1	1:P:39:ARG:HD2	2.33	0.63
3:J:54:ARG:HH12	3:J:69:TYR:HD1	1.44	0.63
1:c:126:ARG:HG2	1:c:154:ALA:HB1	1.80	0.63
3:n:48:GLU:OE1	3:n:50:ARG:NH1	2.31	0.63
3:r:93:PRO:HG3	3:v:54:ARG:HD3	1.80	0.63
1:O:151:VAL:HB	1:O:208:VAL:HG22	1.80	0.63
1:c:36:LYS:HD2	1:c:39:ARG:HH22	1.63	0.63
2:G:262:GLN:HB3	2:G:266:ARG:HH21	1.63	0.63
2:R:103:ALA:HA	2:R:120:PRO:HG3	1.81	0.63
2:S:172:LYS:HZ3	2:S:176:SER:HB2	1.64	0.63
2:i:98:TYR:OH	2:i:123:ASN:ND2	2.31	0.63
1:f:50:PRO:HA	2:l:113:LYS:HE3	1.81	0.63
2:l:95:SER:HB3	2:l:127:THR:N	2.14	0.63
2:l:141:ARG:HD2	2:l:165:TYR:HB2	1.78	0.63
3:E:103:PHE:O	3:E:107:PHE:N	2.31	0.63
3:I:50:ARG:HB3	3:I:57:ASN:HB2	1.81	0.63
2:a:105:ARG:HB3	2:a:117:LEU:HD12	1.80	0.63
2:l:184:LEU:HD11	2:l:220:LEU:HD11	1.80	0.63
1:C:231:ARG:NH2	2:F:248:LYS:O	2.30	0.63
1:D:152:ARG:NH1	1:D:206:VAL:O	2.26	0.63
2:N:108:VAL:HG22	2:N:132:VAL:HG12	1.81	0.63
3:I:102:ILE:O	3:I:106:TRP:HB2	1.99	0.62
1:Z:31:THR:H	1:Z:44:LYS:HZ1	1.47	0.62
3:X:47:ARG:HH11	3:X:59:THR:HG22	1.63	0.62
2:B:202:ASP:OD2	2:B:203:ARG:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:48:GLU:O	3:J:59:THR:OG1	2.16	0.62
2:b:180:PRO:HA	2:b:229:MET:HE1	1.81	0.62
2:B:110:ARG:NH2	2:B:129:ILE:HD12	2.14	0.62
1:Y:66:ASP:OD2	1:Y:67:ALA:N	2.33	0.62
2:l:109:THR:OG1	2:l:113:LYS:N	2.31	0.62
3:L:33:ASP:OD1	3:L:34:TYR:N	2.33	0.62
2:b:125:LYS:HA	2:b:125:LYS:HE3	1.82	0.62
1:P:34:PHE:CG	1:P:39:ARG:CD	2.83	0.62
3:J:31:LYS:N	3:J:67:THR:O	2.33	0.62
1:f:68:ARG:NH1	2:l:177:VAL:O	2.33	0.62
3:r:40:GLU:OE1	3:r:66:TYR:OH	2.18	0.62
1:M:310:ASN:O	2:N:339:ARG:NH1	2.32	0.62
1:d:300:LEU:HD22	2:j:330:THR:HG21	1.80	0.62
3:r:60:LYS:NZ	3:r:64:ASN:O	2.33	0.62
2:a:125:LYS:HA	2:a:125:LYS:HE3	1.82	0.62
1:c:137:LYS:NZ	2:i:152:SER:O	2.32	0.62
1:c:210:ILE:O	2:i:193:ARG:NH2	2.32	0.62
1:e:56:ILE:HG13	1:e:57:PRO:HD2	1.82	0.62
1:Z:310:ASN:O	2:b:339:ARG:NH1	2.32	0.62
3:X:33:ASP:OD1	3:X:34:TYR:N	2.33	0.62
3:L:40:GLU:OE2	3:L:66:TYR:OH	2.08	0.62
3:o:48:GLU:HB3	3:o:50:ARG:HH12	1.63	0.62
2:S:143:LEU:HD12	2:S:165:TYR:HE2	1.65	0.62
3:q:51:ILE:HG23	3:q:55:GLU:O	2.00	0.62
3:r:50:ARG:NH1	3:r:91:GLU:HB3	2.15	0.62
2:B:274:GLU:OE2	2:B:278:ARG:NH1	2.33	0.62
1:Y:33:ARG:HB3	1:Y:36:LYS:HG3	1.81	0.62
1:P:34:PHE:CG	1:P:39:ARG:CZ	2.83	0.62
3:K:32:VAL:HG11	3:K:66:TYR:CD2	2.35	0.61
2:l:95:SER:HB3	2:l:127:THR:H	1.64	0.61
1:A:94:LYS:HG3	2:B:227:TYR:HE1	1.65	0.61
2:G:242:ARG:NH1	2:G:244:PRO:O	2.33	0.61
1:f:207:ASP:OD1	1:f:208:VAL:N	2.32	0.61
2:j:202:ASP:OD1	2:j:203:ARG:N	2.33	0.61
1:P:53:HIS:CE1	1:P:55:LYS:HG3	2.35	0.61
3:X:30:ARG:NH2	3:X:64:ASN:HB3	2.15	0.61
2:F:127:THR:CB	2:F:129:ILE:HG23	2.22	0.61
3:o:48:GLU:HB2	3:o:59:THR:HB	1.82	0.61
3:T:99:LEU:HA	3:T:102:ILE:HD12	1.81	0.61
3:H:92:PRO:HA	3:I:69:TYR:CE1	2.32	0.61
1:f:249:LEU:HA	1:f:252:THR:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:r:31:LYS:N	3:r:67:THR:O	2.33	0.61
3:t:63:SER:O	3:t:65:ARG:NH1	2.33	0.61
1:C:300:LEU:HD22	2:F:330:THR:HG21	1.82	0.61
1:e:28:ARG:HG3	1:e:100:PHE:CZ	2.35	0.61
3:q:47:ARG:HH12	3:q:61:LYS:HG2	1.65	0.61
1:d:137:LYS:NZ	2:j:152:SER:O	2.33	0.61
1:e:234:VAL:HG22	1:e:238:HIS:CE1	2.35	0.61
1:d:33:ARG:HG2	1:d:38:LEU:HB2	1.81	0.61
2:B:213:ARG:NH1	1:P:128:ARG:HH12	1.98	0.61
3:T:103:PHE:HA	3:T:106:TRP:HB2	1.82	0.61
1:e:223:ILE:HD12	1:e:226:ARG:HE	1.65	0.61
2:i:136:ASN:OD1	2:i:136:ASN:O	2.18	0.61
1:f:93:ILE:HA	1:f:208:VAL:HG12	1.82	0.61
1:f:128:ARG:NH1	2:N:213:ARG:HE	1.97	0.61
3:t:46:VAL:HA	3:t:60:LYS:HA	1.81	0.61
1:M:140:VAL:HG11	2:N:150:LEU:HD23	1.83	0.61
1:A:66:ASP:OD2	1:A:67:ALA:N	2.34	0.61
1:C:218:GLU:HG2	2:G:255:ILE:HG21	1.83	0.61
3:I:50:ARG:NH2	3:I:91:GLU:HB2	2.14	0.61
3:L:30:ARG:NH2	3:L:64:ASN:HB3	2.15	0.61
1:c:321:ASP:OD1	1:c:322:PHE:N	2.34	0.61
2:i:103:ALA:HA	2:i:120:PRO:HG3	1.83	0.61
1:Z:130:GLU:HG3	1:Z:151:VAL:HG22	1.83	0.61
3:v:46:VAL:HG11	3:v:58:VAL:HG22	1.83	0.61
1:O:321:ASP:OD2	1:O:322:PHE:N	2.34	0.61
2:R:98:TYR:OH	2:R:123:ASN:ND2	2.33	0.61
1:Y:303:TYR:HE1	1:c:323:PHE:HD2	1.49	0.60
1:e:39:ARG:HH11	1:e:39:ARG:HG3	1.65	0.60
3:g:108:PRO:HG3	3:s:106:TRP:CZ3	2.36	0.60
3:h:60:LYS:HZ2	3:h:66:TYR:HE1	1.49	0.60
3:v:80:ASN:O	3:v:83:THR:OG1	2.19	0.60
1:C:27:GLU:HB3	1:C:66:ASP:HA	1.82	0.60
1:C:257:VAL:HG13	2:F:279:ALA:HB2	1.83	0.60
1:d:93:ILE:HD12	1:d:208:VAL:HG12	1.82	0.60
1:M:66:ASP:OD2	1:M:67:ALA:N	2.34	0.60
1:P:34:PHE:CE2	1:P:39:ARG:HA	2.35	0.60
2:G:100:ILE:HD11	2:G:120:PRO:HA	1.82	0.60
1:c:244:GLU:HG2	1:c:248:LYS:HE2	1.81	0.60
2:b:202:ASP:OD2	2:b:203:ARG:N	2.34	0.60
1:f:94:LYS:NZ	1:f:207:ASP:HB3	2.16	0.60
1:P:49:GLU:HG3	1:P:50:PRO:HD3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:50:ARG:NH1	3:V:57:ASN:O	2.35	0.60
1:c:23:VAL:HB	1:c:50:PRO:HA	1.84	0.60
2:l:133:LYS:NZ	2:l:135:VAL:O	2.30	0.60
2:R:344:ASN:OD1	2:R:345:ASP:N	2.35	0.60
3:T:92:PRO:HA	3:U:69:TYR:CE1	2.33	0.60
1:A:33:ARG:HB3	1:A:36:LYS:HG3	1.83	0.60
1:A:126:ARG:HG3	1:A:155:LEU:HD13	1.82	0.60
3:L:47:ARG:HH12	3:L:63:SER:HA	1.65	0.60
1:c:266:ARG:NH2	1:c:267:GLN:OE1	2.34	0.60
1:Z:313:VAL:HG13	2:j:341:VAL:HG23	1.83	0.60
1:A:140:VAL:HG11	2:B:150:LEU:HD23	1.84	0.60
2:j:135:VAL:HG21	2:j:170:PRO:HB3	1.83	0.60
1:O:200:ALA:O	1:O:201:LEU:C	2.45	0.60
3:J:50:ARG:HH22	3:J:91:GLU:HG2	1.66	0.60
1:e:31:THR:HG21	1:e:63:LYS:HG2	1.82	0.60
3:o:47:ARG:HG3	3:o:48:GLU:HG2	1.83	0.60
1:Z:282:LEU:HG	2:b:305:VAL:HG21	1.84	0.60
2:j:331:MET:HA	2:j:334:VAL:HG22	1.83	0.60
1:A:144:ARG:HD3	1:A:209:ARG:HH22	1.67	0.60
1:A:224:TYR:HE1	2:B:156:VAL:HG21	1.67	0.60
1:c:300:LEU:HD22	2:i:330:THR:HG21	1.84	0.60
3:X:47:ARG:HH12	3:X:63:SER:HA	1.65	0.60
2:N:180:PRO:HA	2:N:229:MET:HE1	1.84	0.59
3:U:47:ARG:NH1	3:U:60:LYS:O	2.34	0.59
1:A:23:VAL:HG13	1:A:64:MET:HE1	1.84	0.59
1:A:36:LYS:C	1:A:37:VAL:O	2.24	0.59
1:Y:155:LEU:HG	1:Y:198:MET:HE2	1.83	0.59
3:g:79:ASP:O	3:g:83:THR:HG23	2.02	0.59
1:Z:82:LYS:NZ	1:Z:135:ASP:OD1	2.32	0.59
3:n:40:GLU:OE1	3:n:66:TYR:OH	2.19	0.59
1:M:16:LEU:O	1:M:20:VAL:HG13	2.02	0.59
1:P:53:HIS:CE1	1:P:55:LYS:CG	2.86	0.59
2:S:242:ARG:NH1	2:S:244:PRO:O	2.35	0.59
2:F:100:ILE:HB	2:F:121:GLY:H	1.66	0.59
2:a:329:GLU:OE2	2:a:333:LYS:NZ	2.34	0.59
1:A:312:ASP:OD1	1:A:313:VAL:N	2.34	0.59
2:b:184:LEU:O	2:b:188:THR:HG23	2.03	0.59
1:P:152:ARG:NH1	1:P:206:VAL:O	2.26	0.59
1:D:208:VAL:C	1:D:209:ARG:HD2	2.28	0.59
1:Z:49:GLU:HB3	2:b:113:LYS:HE2	1.85	0.59
1:M:96:ARG:HD3	1:M:97:ILE:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:126:ARG:HG3	1:M:155:LEU:HD13	1.82	0.59
2:G:95:SER:HB3	2:G:127:THR:N	2.18	0.59
1:M:224:TYR:CD1	2:N:247:VAL:HG11	2.37	0.59
1:A:30:ILE:HG13	1:A:44:LYS:HD2	1.85	0.59
3:V:51:ILE:HA	3:V:56:ILE:HG23	1.83	0.59
2:B:344:ASN:OD1	2:B:345:ASP:N	2.34	0.59
1:C:231:ARG:HH12	2:F:248:LYS:C	2.10	0.59
3:s:35:SER:HB3	3:u:88:VAL:HG12	1.84	0.59
1:f:90:ASP:OD1	1:f:91:SER:N	2.36	0.59
3:E:108:PRO:HA	3:K:106:TRP:CH2	2.38	0.59
2:F:205:LEU:HD13	2:F:243:PRO:HG2	1.84	0.59
1:Z:312:ASP:OD1	1:Z:313:VAL:N	2.35	0.59
2:N:202:ASP:OD2	2:N:203:ARG:N	2.35	0.59
1:Z:41:ASP:OD1	1:Z:42:ASP:N	2.36	0.58
1:Z:315:VAL:HG21	2:b:350:LEU:HD11	1.85	0.58
2:l:208:GLY:O	2:l:212:ILE:HG12	2.03	0.58
2:N:163:VAL:HG12	2:N:236:VAL:HG12	1.85	0.58
3:U:47:ARG:NH2	3:U:61:LYS:O	2.36	0.58
3:U:102:ILE:HG23	3:U:106:TRP:CE2	2.38	0.58
2:B:125:LYS:HB3	2:B:127:THR:HG22	1.85	0.58
2:i:177:VAL:HG22	2:i:178:THR:H	1.67	0.58
2:k:165:TYR:HE1	2:k:233:LEU:HD13	1.68	0.58
2:k:350:LEU:O	2:b:349:ASN:HB2	2.02	0.58
1:C:254:ASP:O	1:C:257:VAL:HB	2.03	0.58
1:c:130:GLU:HA	1:c:133:ARG:HH12	1.67	0.58
2:i:235:ASP:OD1	2:i:236:VAL:N	2.36	0.58
3:n:40:GLU:HA	3:n:45:GLN:HE21	1.67	0.58
1:C:82:LYS:NZ	1:C:133:ARG:O	2.33	0.58
1:Y:85:LYS:HD3	2:i:255:ILE:HD12	1.84	0.58
2:a:180:PRO:HA	2:a:229:MET:HE1	1.85	0.58
2:i:105:ARG:NH2	2:i:118:VAL:O	2.37	0.58
1:A:23:VAL:H	1:A:50:PRO:HG3	1.67	0.58
2:G:153:ASP:OD2	2:G:200:THR:OG1	2.20	0.58
3:s:54:ARG:HH21	3:s:71:PRO:HA	1.69	0.58
2:b:329:GLU:OE2	2:b:333:LYS:NZ	2.36	0.58
1:A:327:LYS:HG3	1:A:329:PRO:HD2	1.84	0.58
3:I:38:LEU:HA	3:I:41:VAL:HG22	1.85	0.58
1:e:68:ARG:NH1	2:k:177:VAL:O	2.37	0.58
2:a:202:ASP:OD2	2:a:203:ARG:N	2.36	0.58
3:u:80:ASN:O	3:u:83:THR:OG1	2.19	0.58
2:S:331:MET:HA	2:S:334:VAL:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:ARG:NH2	1:D:301:ARG:HH21	2.01	0.58
3:g:41:VAL:HG23	3:g:46:VAL:HG11	1.85	0.58
1:f:28:ARG:NE	1:f:49:GLU:HB3	2.19	0.58
1:M:155:LEU:HG	1:M:198:MET:HE2	1.84	0.58
3:W:43:ASN:O	3:W:45:GLN:NE2	2.37	0.58
2:G:184:LEU:HD12	2:G:187:ALA:HB3	1.85	0.58
3:J:41:VAL:HG12	3:J:46:VAL:HG21	1.86	0.58
1:f:282:LEU:HD23	2:l:305:VAL:HG21	1.85	0.58
2:R:220:LEU:HD22	2:R:233:LEU:HD11	1.86	0.58
2:G:349:ASN:HB3	2:a:349:ASN:HD21	1.69	0.58
3:q:78:LEU:HD12	3:q:81:LEU:HD11	1.86	0.58
1:f:18:MET:CB	1:f:57:PRO:HB3	2.33	0.58
3:V:46:VAL:O	3:V:61:LYS:NZ	2.37	0.58
2:B:329:GLU:OE2	2:B:333:LYS:NZ	2.36	0.57
3:K:58:VAL:HG11	3:K:66:TYR:CZ	2.38	0.57
1:O:231:ARG:NH2	2:R:248:LYS:O	2.38	0.57
3:W:32:VAL:HG22	3:W:33:ASP:H	1.67	0.57
1:D:28:ARG:HG3	1:D:100:PHE:CZ	2.39	0.57
2:F:92:TRP:CH2	2:F:127:THR:HG23	2.39	0.57
2:F:98:TYR:OH	2:F:123:ASN:ND2	2.37	0.57
3:K:103:PHE:HA	3:K:106:TRP:CD1	2.37	0.57
2:a:94:ALA:HA	2:a:97:PHE:HD2	1.68	0.57
1:C:255:TYR:CD2	2:G:292:ALA:HB3	2.39	0.57
1:Y:30:ILE:HG13	1:Y:44:LYS:HD2	1.85	0.57
3:u:30:ARG:NH2	3:u:65:ARG:HG3	2.16	0.57
3:u:50:ARG:HB3	3:u:57:ASN:HD21	1.68	0.57
1:d:244:GLU:HG2	1:d:248:LYS:HE2	1.85	0.57
2:l:98:TYR:OH	2:l:123:ASN:HB2	2.05	0.57
2:l:114:PHE:CE1	2:l:171:GLU:HG3	2.39	0.57
1:M:134:LEU:HD11	1:M:139:ILE:HG13	1.86	0.57
3:W:35:SER:OG	3:X:87:LYS:HD2	2.05	0.57
1:A:226:ARG:NH2	2:B:154:GLU:O	2.36	0.57
1:A:231:ARG:NH1	2:B:251:PHE:HB2	2.19	0.57
1:A:313:VAL:HG13	2:F:341:VAL:HG23	1.85	0.57
1:D:48:TYR:CD2	1:D:50:PRO:HD3	2.39	0.57
3:K:74:ASP:OD2	3:K:77:LEU:N	2.38	0.57
3:u:98:LEU:C	3:u:102:ILE:HD13	2.28	0.57
1:d:33:ARG:NH1	1:d:59:ILE:O	2.33	0.57
3:H:50:ARG:HH11	3:H:89:VAL:HG21	1.70	0.57
3:u:64:ASN:OD1	3:u:65:ARG:N	2.35	0.57
1:Z:36:LYS:C	1:Z:37:VAL:O	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:96:ARG:HD3	1:Z:97:ILE:N	2.19	0.57
1:f:57:PRO:HD2	1:f:58:PHE:N	2.18	0.57
3:t:58:VAL:HG11	3:t:66:TYR:CZ	2.40	0.57
3:m:52:ASN:ND2	3:m:91:GLU:OE2	2.35	0.57
2:l:180:PRO:O	2:l:183:SER:OG	2.20	0.57
3:T:47:ARG:HB2	3:T:61:LYS:HD3	1.87	0.57
1:A:72:MET:SD	1:A:120:LYS:NZ	2.74	0.57
1:Z:146:ARG:HG3	1:Z:147:LEU:HD22	1.86	0.57
1:M:226:ARG:NH2	2:N:154:GLU:O	2.37	0.57
1:M:239:ARG:HH12	2:N:257:ALA:HA	1.69	0.57
2:B:180:PRO:HA	2:B:229:MET:HE1	1.86	0.57
3:J:58:VAL:HG21	3:J:66:TYR:CE1	2.40	0.57
1:e:82:LYS:HD3	1:e:133:ARG:HH12	1.70	0.57
2:k:134:PRO:HB2	2:k:135:VAL:HG13	1.85	0.57
1:C:102:ARG:NH1	1:C:200:ALA:O	2.38	0.57
1:e:50:PRO:HB3	2:k:113:LYS:HD3	1.86	0.57
1:e:112:ILE:O	1:e:115:ALA:N	2.38	0.57
3:u:33:ASP:OD2	3:u:34:TYR:N	2.38	0.57
1:Z:155:LEU:HG	1:Z:198:MET:HE2	1.86	0.57
3:n:40:GLU:HG3	3:n:45:GLN:NE2	2.20	0.57
3:t:54:ARG:NH2	3:t:71:PRO:O	2.26	0.57
1:Y:312:ASP:OD1	1:Y:313:VAL:N	2.37	0.56
3:u:50:ARG:NH1	3:u:51:ILE:O	2.38	0.56
1:M:92:TYR:OH	1:M:209:ARG:HG3	2.05	0.56
2:N:92:TRP:HE1	2:N:128:PHE:H	1.52	0.56
3:W:79:ASP:O	3:W:83:THR:HG23	2.05	0.56
3:K:32:VAL:HG22	3:K:33:ASP:H	1.70	0.56
1:f:33:ARG:O	1:f:33:ARG:HD3	2.06	0.56
1:P:34:PHE:CD2	1:P:34:PHE:CB	2.79	0.56
3:I:60:LYS:HG3	3:I:62:ASP:H	1.68	0.56
2:a:184:LEU:O	2:a:188:THR:HG23	2.04	0.56
3:o:99:LEU:HA	3:o:102:ILE:HD12	1.87	0.56
3:q:79:ASP:O	3:q:83:THR:HG23	2.05	0.56
1:Z:253:ALA:HB1	2:b:275:VAL:HG11	1.86	0.56
2:b:100:ILE:HB	2:b:120:PRO:HA	1.87	0.56
2:l:112:GLY:C	2:l:113:LYS:HD2	2.30	0.56
1:D:90:ASP:OD2	1:D:91:SER:N	2.38	0.56
2:F:183:SER:HB2	2:F:229:MET:HE1	1.88	0.56
2:k:108:VAL:O	2:k:115:SER:HB2	2.04	0.56
2:k:245:GLU:HG3	2:k:247:VAL:H	1.70	0.56
3:p:60:LYS:HZ1	3:p:66:TYR:HE1	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:257:VAL:HG23	2:N:279:ALA:HB2	1.87	0.56
1:O:231:ARG:HH11	2:R:250:ALA:HB3	1.70	0.56
2:R:235:ASP:OD2	2:R:237:ASN:ND2	2.38	0.56
1:A:143:SER:HB3	2:B:193:ARG:HH22	1.71	0.56
1:A:144:ARG:HD3	1:A:209:ARG:NH2	2.20	0.56
3:L:54:ARG:HB2	3:L:70:ILE:HB	1.87	0.56
1:d:218:GLU:HG2	2:l:255:ILE:HG21	1.86	0.56
2:l:100:ILE:HD11	2:l:120:PRO:HA	1.88	0.56
1:M:122:LYS:HB3	1:M:155:LEU:HD11	1.87	0.56
1:A:18:MET:HA	1:A:18:MET:HE3	1.88	0.56
3:K:63:SER:O	3:K:65:ARG:NH1	2.38	0.56
2:j:152:SER:OG	2:j:153:ASP:OD1	2.21	0.56
1:Y:282:LEU:HG	2:a:305:VAL:HG21	1.86	0.56
1:e:93:ILE:HA	1:e:208:VAL:HG12	1.87	0.56
1:e:223:ILE:CD1	1:e:226:ARG:HE	2.18	0.56
2:i:161:MET:HA	2:i:161:MET:HE2	1.87	0.56
1:O:19:SER:HA	1:O:55:LYS:HG3	1.88	0.56
1:A:16:LEU:O	1:A:20:VAL:HG13	2.05	0.56
2:B:220:LEU:HA	2:B:223:THR:HG22	1.88	0.56
2:F:177:VAL:HG22	2:F:178:THR:H	1.70	0.56
1:e:282:LEU:HD23	2:k:305:VAL:HG21	1.87	0.56
1:Z:16:LEU:O	1:Z:20:VAL:HG13	2.06	0.56
1:Z:227:MET:HE1	2:b:156:VAL:H	1.71	0.56
1:O:238:HIS:CD2	2:R:258:ARG:HH12	2.24	0.56
1:A:23:VAL:HG21	1:A:47:VAL:HB	1.87	0.56
1:D:68:ARG:NH2	2:G:174:LEU:O	2.38	0.56
2:G:327:TYR:HE1	2:G:331:MET:HG3	1.71	0.56
1:D:31:THR:HG21	1:D:63:LYS:HG2	1.88	0.56
3:J:79:ASP:O	3:J:83:THR:HG23	2.06	0.56
2:a:185:ARG:HH11	2:a:185:ARG:HG3	1.71	0.56
3:u:40:GLU:OE2	3:u:66:TYR:OH	2.11	0.56
1:Z:257:VAL:HG23	2:b:279:ALA:HB2	1.88	0.56
2:N:351:MET:HA	2:R:350:LEU:HA	1.88	0.56
3:X:102:ILE:O	3:X:105:SER:OG	2.22	0.56
1:C:237:ARG:HH21	1:C:238:HIS:CD2	2.25	0.55
2:G:208:GLY:O	2:G:212:ILE:HG12	2.06	0.55
1:Y:313:VAL:HG13	2:i:341:VAL:HG23	1.86	0.55
1:c:135:ASP:OD2	1:c:136:VAL:N	2.39	0.55
3:o:47:ARG:HE	3:o:61:LYS:HA	1.71	0.55
1:O:255:TYR:CZ	2:S:291:ARG:NH1	2.73	0.55
3:Q:56:ILE:HD11	3:Q:70:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LEU:HG	1:A:198:MET:HE2	1.89	0.55
2:B:350:LEU:CA	2:S:351:MET:HG2	2.37	0.55
1:D:282:LEU:HD23	2:G:305:VAL:HG21	1.88	0.55
3:J:38:LEU:HA	3:J:41:VAL:HG22	1.88	0.55
3:J:50:ARG:HD2	3:J:57:ASN:HD21	1.71	0.55
3:K:33:ASP:HB2	3:K:36:THR:HG22	1.89	0.55
3:s:50:ARG:NH1	3:s:50:ARG:HB2	2.21	0.55
1:d:27:GLU:HB3	1:d:66:ASP:HA	1.87	0.55
1:d:133:ARG:HG3	1:d:133:ARG:HH11	1.71	0.55
3:h:81:LEU:HD12	3:h:86:VAL:HG21	1.88	0.55
3:v:30:ARG:H	3:v:65:ARG:HH22	1.54	0.55
1:M:31:THR:HA	1:M:62:VAL:HG12	1.87	0.55
2:N:184:LEU:O	2:N:188:THR:HG23	2.05	0.55
3:Q:33:ASP:HB2	3:Q:36:THR:HG22	1.88	0.55
3:Q:59:THR:HG22	3:Q:65:ARG:HG2	1.87	0.55
3:U:50:ARG:HB2	3:U:57:ASN:HB2	1.88	0.55
3:V:37:PHE:HE1	3:V:58:VAL:HG22	1.71	0.55
3:X:50:ARG:HH11	3:X:91:GLU:HB2	1.71	0.55
1:Y:23:VAL:H	1:Y:50:PRO:HG3	1.71	0.55
1:e:94:LYS:O	1:e:206:VAL:N	2.40	0.55
1:f:33:ARG:HH22	1:f:36:LYS:NZ	2.03	0.55
1:f:38:LEU:HB3	1:f:44:LYS:NZ	2.19	0.55
1:f:51:GLY:H	2:l:113:LYS:NZ	2.04	0.55
1:f:135:ASP:O	1:f:139:ILE:HD12	2.06	0.55
1:A:138:ASP:OD2	1:A:146:ARG:NH2	2.39	0.55
2:R:242:ARG:C	2:R:244:PRO:HD3	2.32	0.55
3:V:36:THR:HA	3:V:39:GLN:OE1	2.07	0.55
1:e:30:ILE:HD12	1:e:65:LEU:HG	1.88	0.55
1:M:15:VAL:O	1:M:19:SER:CB	2.54	0.55
1:O:218:GLU:HG2	2:S:255:ILE:HG21	1.88	0.55
3:V:79:ASP:O	3:V:83:THR:HG23	2.06	0.55
1:C:49:GLU:OE2	2:F:113:LYS:HA	2.07	0.55
2:G:108:VAL:O	2:G:115:SER:HB2	2.07	0.55
1:Y:16:LEU:O	1:Y:20:VAL:HG13	2.07	0.55
1:c:237:ARG:HH22	1:c:238:HIS:CE1	2.25	0.55
1:e:28:ARG:O	1:e:64:MET:O	2.25	0.55
1:Z:236:ARG:HD2	2:j:274:GLU:OE1	2.06	0.55
3:r:79:ASP:O	3:r:83:THR:HG23	2.06	0.55
1:P:153:ASP:O	1:P:157:SER:OG	2.18	0.55
2:R:242:ARG:NH1	2:R:246:GLU:OE2	2.37	0.55
3:X:54:ARG:HB2	3:X:70:ILE:HB	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:342:LEU:HD23	1:P:314:MET:HE3	1.88	0.55
1:D:137:LYS:HA	1:D:140:VAL:HG22	1.89	0.55
3:J:49:ALA:HB3	3:J:88:VAL:HG22	1.89	0.55
1:Y:320:SER:OG	1:Y:321:ASP:N	2.39	0.55
1:e:223:ILE:HD13	2:k:154:GLU:OE2	2.06	0.55
1:Z:30:ILE:HG22	1:Z:63:LYS:H	1.72	0.55
1:d:55:LYS:NZ	1:d:57:PRO:O	2.40	0.55
2:j:220:LEU:HD22	2:j:233:LEU:HD11	1.88	0.55
3:E:79:ASP:O	3:E:83:THR:HG23	2.05	0.55
3:o:43:ASN:CG	3:o:45:GLN:HE22	2.14	0.55
3:q:47:ARG:NH2	3:q:61:LYS:HA	2.21	0.55
1:Z:231:ARG:NH1	2:b:251:PHE:HB3	2.22	0.55
1:P:56:ILE:HD13	1:P:58:PHE:HE1	1.70	0.55
2:S:108:VAL:O	2:S:115:SER:HB2	2.06	0.55
3:U:43:ASN:CG	3:U:45:GLN:HE22	2.14	0.55
3:V:63:SER:O	3:V:65:ARG:NH1	2.40	0.55
1:c:71:THR:HG22	1:c:94:LYS:NZ	2.22	0.55
1:e:313:VAL:HG22	2:b:341:VAL:HG22	1.88	0.55
2:i:96:GLY:O	2:i:125:LYS:N	2.39	0.55
2:N:351:MET:HG3	2:R:349:ASN:O	2.07	0.55
3:Q:109:MET:HB3	3:T:108:PRO:HG3	1.88	0.55
1:D:21:PHE:HE2	1:D:52:LEU:HA	1.72	0.55
1:D:82:LYS:NZ	1:D:133:ARG:O	2.26	0.55
3:J:59:THR:HA	3:J:65:ARG:NH2	2.21	0.55
2:N:110:ARG:HE	2:N:129:ILE:HD12	1.72	0.55
1:Y:224:TYR:HE1	2:a:156:VAL:HG21	1.72	0.54
1:c:36:LYS:HG3	1:c:39:ARG:HH12	1.72	0.54
3:o:50:ARG:HH21	3:o:89:VAL:H	1.54	0.54
2:b:334:VAL:HG13	2:b:335:LEU:HD12	1.88	0.54
1:M:312:ASP:OD1	1:M:313:VAL:N	2.39	0.54
1:D:23:VAL:H	1:D:51:GLY:HA2	1.72	0.54
2:F:169:ASN:HD22	2:F:172:LYS:HZ2	1.56	0.54
1:Z:39:ARG:NH1	1:Z:40:ASP:O	2.41	0.54
1:Z:252:THR:O	1:Z:256:GLU:HG2	2.07	0.54
3:v:47:ARG:HH11	3:v:61:LYS:CG	2.19	0.54
2:F:131:GLU:OE1	2:F:133:LYS:HE3	2.06	0.54
3:J:33:ASP:HB3	3:J:36:THR:OG1	2.08	0.54
1:Y:23:VAL:HG21	1:Y:47:VAL:HB	1.88	0.54
1:f:33:ARG:HH22	1:f:36:LYS:HZ2	1.53	0.54
3:p:59:THR:HG22	3:p:65:ARG:HG2	1.88	0.54
1:O:111:ASP:OD2	1:O:112:ILE:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:TYR:HD2	1:D:50:PRO:HD3	1.72	0.54
2:F:220:LEU:HD22	2:F:233:LEU:HD11	1.88	0.54
1:d:314:MET:HE2	1:d:316:MET:HE3	1.88	0.54
3:n:52:ASN:ND2	3:n:91:GLU:OE2	2.30	0.54
3:r:45:GLN:HE22	3:r:60:LYS:HD3	1.72	0.54
1:C:252:THR:O	1:C:256:GLU:HG2	2.07	0.54
2:F:235:ASP:OD1	2:F:236:VAL:N	2.41	0.54
3:J:78:LEU:HD12	3:J:81:LEU:HD11	1.88	0.54
3:L:50:ARG:HH11	3:L:91:GLU:HB2	1.71	0.54
2:a:97:PHE:HE1	2:a:124:TRP:HD1	1.54	0.54
2:i:111:PHE:N	2:i:129:ILE:O	2.35	0.54
2:i:326:LEU:O	2:i:330:THR:HG22	2.08	0.54
2:b:102:GLU:O	2:b:104:GLU:HG2	2.06	0.54
3:t:60:LYS:HZ1	3:t:66:TYR:HD1	1.53	0.54
3:v:48:GLU:HA	3:v:86:VAL:HG13	1.90	0.54
2:F:124:TRP:CH2	2:F:126:PRO:HA	2.43	0.54
2:F:315:TYR:HE2	2:F:319:PRO:HA	1.72	0.54
3:H:48:GLU:OE1	3:H:50:ARG:NH1	2.34	0.54
3:I:98:LEU:O	3:I:102:ILE:HG12	2.07	0.54
3:p:63:SER:O	3:p:63:SER:OG	2.24	0.54
1:O:231:ARG:HH22	2:R:248:LYS:HG3	1.72	0.54
2:R:351:MET:HA	2:S:350:LEU:CB	2.37	0.54
1:D:93:ILE:HA	1:D:208:VAL:HG12	1.88	0.54
3:I:91:GLU:HB3	3:I:92:PRO:HD2	1.90	0.54
1:Y:123:PHE:HE1	1:Y:208:VAL:HG21	1.72	0.54
2:R:265:ILE:HG23	2:R:266:ARG:HD2	1.89	0.54
2:B:334:VAL:HG13	2:B:335:LEU:HD12	1.89	0.54
2:F:329:GLU:OE2	2:F:333:LYS:HE2	2.08	0.54
3:I:88:VAL:HG11	3:J:34:TYR:HB3	1.90	0.54
3:L:102:ILE:O	3:L:105:SER:OG	2.22	0.54
1:c:49:GLU:OE2	2:i:113:LYS:HA	2.07	0.54
3:q:92:PRO:HB3	3:u:69:TYR:CE1	2.43	0.54
2:j:145:ALA:HB3	2:j:161:MET:HB3	1.90	0.54
3:r:50:ARG:O	3:r:57:ASN:N	2.37	0.54
1:M:143:SER:O	1:M:147:LEU:HB2	2.08	0.54
1:A:41:ASP:OD1	1:A:42:ASP:N	2.41	0.54
1:D:102:ARG:O	1:D:106:ALA:CB	2.56	0.54
2:G:331:MET:HA	2:G:334:VAL:HG12	1.88	0.54
2:b:110:ARG:HH21	2:b:129:ILE:HD12	1.71	0.54
2:N:334:VAL:HG13	2:N:335:LEU:HD12	1.90	0.54
1:A:224:TYR:CD2	2:B:247:VAL:HG21	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:GLN:OE1	2:B:236:VAL:HG22	2.08	0.53
1:D:112:ILE:O	1:D:115:ALA:N	2.41	0.53
2:F:349:ASN:OD1	2:G:349:ASN:N	2.34	0.53
1:e:120:LYS:HD2	1:e:121:ARG:HE	1.72	0.53
3:u:50:ARG:HH22	3:u:91:GLU:HB3	1.72	0.53
2:b:125:LYS:HE3	2:b:126:PRO:HD2	1.89	0.53
1:f:137:LYS:HA	1:f:140:VAL:HG22	1.90	0.53
2:l:108:VAL:HA	2:l:132:VAL:HA	1.90	0.53
3:r:49:ALA:N	3:r:87:LYS:O	2.41	0.53
1:P:223:ILE:HD11	2:S:154:GLU:HB3	1.90	0.53
1:A:227:MET:HE1	2:B:156:VAL:HG22	1.90	0.53
2:B:349:ASN:HA	2:F:348:GLY:HA2	1.89	0.53
1:C:49:GLU:CD	1:C:50:PRO:HD2	2.33	0.53
2:G:109:THR:HG1	2:G:113:LYS:H	1.55	0.53
2:G:220:LEU:HA	2:G:223:THR:HG22	1.90	0.53
1:Y:41:ASP:OD1	1:Y:42:ASP:N	2.40	0.53
2:a:181:ASP:OD1	2:a:182:ASP:N	2.42	0.53
2:j:98:TYR:CZ	2:j:123:ASN:HB3	2.43	0.53
3:v:54:ARG:NH1	3:v:70:ILE:O	2.42	0.53
3:v:56:ILE:HD13	3:v:68:THR:HG23	1.91	0.53
1:P:137:LYS:HA	1:P:140:VAL:HG22	1.90	0.53
2:F:344:ASN:OD1	2:F:345:ASP:N	2.40	0.53
3:I:48:GLU:HA	3:I:87:LYS:HE3	1.90	0.53
1:e:70:GLN:O	1:e:94:LYS:HG2	2.09	0.53
3:m:48:GLU:OE1	3:m:50:ARG:NH1	2.40	0.53
3:p:45:GLN:HA	3:p:61:LYS:HZ3	1.72	0.53
3:r:50:ARG:HB3	3:r:57:ASN:HB3	1.90	0.53
3:t:45:GLN:C	3:t:61:LYS:HZ3	2.17	0.53
2:N:110:ARG:NH1	2:N:111:PHE:H	2.05	0.53
1:D:68:ARG:NH1	2:G:177:VAL:O	2.41	0.53
1:e:152:ARG:NH1	1:e:206:VAL:O	2.29	0.53
2:k:225:ARG:HG2	2:k:225:ARG:HH11	1.73	0.53
2:b:149:MET:HE2	2:b:196:ILE:HG21	1.91	0.53
2:l:242:ARG:HG2	2:l:244:PRO:HD2	1.90	0.53
3:n:99:LEU:HA	3:n:102:ILE:HD12	1.91	0.53
3:p:74:ASP:OD2	3:p:77:LEU:N	2.42	0.53
3:r:49:ALA:HB3	3:r:88:VAL:HG22	1.91	0.53
3:t:107:PHE:CZ	3:v:106:TRP:HA	2.44	0.53
1:M:313:VAL:HG13	2:R:341:VAL:HG23	1.90	0.53
2:N:92:TRP:NE1	2:N:128:PHE:H	2.05	0.53
2:N:288:GLU:OE2	2:N:291:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:111:PHE:HE1	2:G:129:ILE:HB	1.73	0.53
3:K:52:ASN:O	3:K:55:GLU:HG3	2.08	0.53
3:s:58:VAL:HG11	3:s:66:TYR:CZ	2.44	0.53
3:u:32:VAL:HB	3:u:66:TYR:CE2	2.43	0.53
1:M:49:GLU:HB3	2:N:113:LYS:HE3	1.90	0.53
1:M:227:MET:HB3	2:N:248:LYS:NZ	2.23	0.53
3:W:63:SER:O	3:W:65:ARG:NH1	2.42	0.53
1:A:143:SER:O	1:A:147:LEU:HB2	2.08	0.53
2:G:141:ARG:HB2	2:G:165:TYR:HB2	1.88	0.53
2:G:143:LEU:HD22	2:G:185:ARG:NH2	2.24	0.53
1:Y:257:VAL:HG23	2:a:279:ALA:HB2	1.91	0.53
1:e:49:GLU:HG3	1:e:50:PRO:HD3	1.91	0.53
1:Z:144:ARG:HH11	1:Z:209:ARG:HH22	1.56	0.53
2:b:213:ARG:O	2:b:216:THR:HG22	2.09	0.53
3:V:46:VAL:C	3:V:61:LYS:HZ2	2.16	0.53
2:i:155:ASN:OD1	2:i:156:VAL:N	2.40	0.53
3:p:48:GLU:O	3:p:59:THR:OG1	2.26	0.53
3:W:33:ASP:HB3	3:X:87:LYS:NZ	2.24	0.53
2:B:96:GLY:HA3	2:B:125:LYS:O	2.09	0.53
2:B:100:ILE:HB	2:B:120:PRO:HA	1.90	0.53
1:C:210:ILE:HG23	2:F:193:ARG:HH22	1.73	0.53
1:e:33:ARG:O	1:e:33:ARG:HG3	2.08	0.53
1:f:94:LYS:HG2	1:f:207:ASP:O	2.08	0.53
3:r:60:LYS:H	3:r:65:ARG:NH2	2.06	0.53
2:N:93:ALA:O	2:N:97:PHE:N	2.41	0.53
1:O:152:ARG:O	1:O:156:ASN:ND2	2.34	0.53
1:P:135:ASP:O	1:P:139:ILE:HD12	2.08	0.53
1:d:94:LYS:HB2	1:d:206:VAL:HB	1.91	0.53
1:f:49:GLU:HG3	1:f:50:PRO:HD3	1.91	0.53
2:j:344:ASN:OD1	2:j:345:ASP:N	2.42	0.53
2:B:213:ARG:NH1	1:P:128:ARG:HH22	2.07	0.53
2:F:118:VAL:HG21	2:F:123:ASN:HD22	1.74	0.53
3:L:47:ARG:NH2	3:L:61:LYS:O	2.42	0.53
2:j:162:ASN:OD1	2:j:163:VAL:N	2.42	0.53
2:R:177:VAL:HG22	2:R:178:THR:H	1.74	0.53
3:V:33:ASP:OD2	3:V:35:SER:OG	2.11	0.53
3:X:47:ARG:NH2	3:X:61:LYS:O	2.42	0.53
1:A:143:SER:HB3	2:B:193:ARG:NH2	2.24	0.52
2:F:127:THR:HG22	2:F:128:PHE:N	2.24	0.52
2:F:138:GLU:HA	2:F:166:ARG:HD2	1.89	0.52
2:F:161:MET:HA	2:F:161:MET:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:106:TRP:CD1	3:J:108:PRO:HB3	2.44	0.52
1:Y:34:PHE:HE2	2:i:122:LEU:H	1.57	0.52
2:i:162:ASN:OD1	2:i:163:VAL:N	2.42	0.52
1:f:247:GLU:O	1:f:250:ARG:HB2	2.09	0.52
3:v:33:ASP:OD2	3:v:35:SER:OG	2.26	0.52
2:B:184:LEU:O	2:B:188:THR:HG23	2.08	0.52
1:D:28:ARG:O	1:D:64:MET:O	2.27	0.52
2:G:98:TYR:HH	2:G:125:LYS:HZ2	1.51	0.52
1:e:234:VAL:HG23	1:e:237:ARG:HE	1.73	0.52
2:k:182:ASP:O	2:k:186:GLN:HG2	2.09	0.52
1:d:122:LYS:HZ3	1:d:199:ALA:N	2.07	0.52
3:t:98:LEU:O	3:t:101:SER:OG	2.18	0.52
1:O:94:LYS:HB2	1:O:206:VAL:HB	1.90	0.52
2:R:315:TYR:HE2	2:R:319:PRO:HA	1.73	0.52
2:F:326:LEU:O	2:F:330:THR:HG22	2.09	0.52
3:I:43:ASN:CG	3:I:45:GLN:HE22	2.18	0.52
3:I:50:ARG:NH1	3:I:51:ILE:O	2.42	0.52
2:a:176:SER:OG	2:a:177:VAL:N	2.42	0.52
2:k:327:TYR:HE1	2:k:331:MET:HG3	1.74	0.52
3:u:47:ARG:HH22	3:u:63:SER:N	2.06	0.52
1:d:234:VAL:O	1:d:237:ARG:HG3	2.09	0.52
1:f:11:ILE:O	1:f:15:VAL:HG23	2.09	0.52
3:n:34:TYR:HE1	3:n:70:ILE:HG12	1.75	0.52
1:O:134:LEU:HD23	1:O:139:ILE:HD13	1.90	0.52
2:S:326:LEU:O	2:S:330:THR:HG22	2.09	0.52
1:A:231:ARG:CZ	2:B:251:PHE:HB2	2.40	0.52
2:F:331:MET:HA	2:F:334:VAL:HG22	1.90	0.52
2:G:288:GLU:OE1	2:G:291:ARG:NH2	2.37	0.52
2:a:334:VAL:HG13	2:a:335:LEU:HD12	1.90	0.52
2:b:217:GLN:OE1	2:b:236:VAL:HG22	2.10	0.52
3:t:79:ASP:O	3:t:83:THR:HG23	2.10	0.52
2:N:94:ALA:HA	2:N:97:PHE:HB2	1.92	0.52
1:P:53:HIS:CE1	1:P:55:LYS:HE3	2.44	0.52
2:R:135:VAL:HG21	2:R:170:PRO:HB3	1.90	0.52
2:k:208:GLY:O	2:k:212:ILE:HG12	2.09	0.52
1:f:313:VAL:HG22	2:N:341:VAL:HG22	1.92	0.52
2:l:327:TYR:CE1	2:l:331:MET:HG3	2.45	0.52
2:N:169:ASN:ND2	2:N:172:LYS:HG2	2.24	0.52
2:R:118:VAL:HG21	2:R:123:ASN:HD22	1.75	0.52
1:D:135:ASP:O	1:D:139:ILE:HD12	2.10	0.52
1:Y:28:ARG:HH21	1:Y:46:LEU:HD13	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:36:LYS:O	1:Y:37:VAL:C	2.42	0.52
3:h:62:ASP:O	3:h:63:SER:OG	2.26	0.52
3:n:40:GLU:HG3	3:n:45:GLN:HE21	1.74	0.52
1:P:48:TYR:CD2	1:P:50:PRO:HD2	2.45	0.52
2:S:111:PHE:HB2	2:S:113:LYS:NZ	2.24	0.52
3:J:60:LYS:H	3:J:65:ARG:HH21	1.57	0.52
2:a:263:GLN:HA	2:a:266:ARG:NH1	2.25	0.52
2:B:93:ALA:HA	2:B:126:PRO:HA	1.91	0.52
2:B:199:TYR:HB2	2:B:204:ILE:HD11	1.92	0.52
1:M:113:SER:OG	3:T:87:LYS:NZ	2.43	0.52
1:M:315:VAL:HB	2:R:343:VAL:HG22	1.91	0.52
2:N:93:ALA:HA	2:N:125:LYS:O	2.10	0.52
2:N:220:LEU:HD22	2:N:233:LEU:HD11	1.90	0.52
2:G:143:LEU:HD22	2:G:185:ARG:HH21	1.75	0.52
2:G:349:ASN:HB3	2:a:349:ASN:ND2	2.24	0.52
1:c:147:LEU:HD12	1:c:208:VAL:HG23	1.92	0.52
2:k:331:MET:HA	2:k:334:VAL:HG12	1.91	0.52
2:b:180:PRO:O	2:b:184:LEU:HG	2.10	0.52
1:f:236:ARG:HH22	2:N:270:ALA:HB1	1.75	0.52
1:M:71:THR:HG22	1:M:94:LYS:HE3	1.92	0.52
1:O:231:ARG:HH12	2:R:248:LYS:C	2.18	0.52
2:R:101:LYS:O	2:R:104:GLU:HG2	2.09	0.52
2:S:101:LYS:HE2	2:S:104:GLU:OE1	2.10	0.52
1:A:297:ILE:C	1:A:299:SER:H	2.18	0.52
2:B:181:ASP:OD1	2:B:182:ASP:N	2.43	0.52
1:D:70:GLN:O	1:D:94:LYS:HG2	2.09	0.52
3:I:47:ARG:CZ	3:I:61:LYS:HA	2.40	0.52
1:Y:226:ARG:NH2	2:a:154:GLU:O	2.39	0.52
1:Y:310:ASN:HB2	2:a:339:ARG:HH12	1.74	0.52
1:e:254:ASP:HA	1:e:257:VAL:HG12	1.92	0.52
2:k:109:THR:OG1	2:k:113:LYS:N	2.42	0.52
1:Z:33:ARG:HA	1:Z:60:GLU:HB3	1.91	0.52
1:O:129:SER:HB2	1:O:133:ARG:HH12	1.75	0.52
3:W:52:ASN:O	3:W:55:GLU:HG3	2.08	0.52
1:A:114:GLN:O	1:A:118:LEU:HD23	2.10	0.51
2:F:135:VAL:HG21	2:F:170:PRO:HB3	1.91	0.51
3:L:30:ARG:HH22	3:L:64:ASN:HB3	1.75	0.51
2:i:138:GLU:HA	2:i:166:ARG:HD2	1.92	0.51
2:b:199:TYR:HB2	2:b:204:ILE:HD11	1.93	0.51
1:d:18:MET:O	1:d:55:LYS:HE3	2.09	0.51
1:P:282:LEU:HD23	2:S:305:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:HIS:CG	2:F:258:ARG:HH12	2.28	0.51
3:K:54:ARG:HH21	3:K:71:PRO:HA	1.74	0.51
3:r:45:GLN:NE2	3:r:60:LYS:HB2	2.24	0.51
1:M:92:TYR:HE2	1:M:94:LYS:HZ2	1.58	0.51
2:B:351:MET:N	2:S:351:MET:SD	2.83	0.51
1:D:223:ILE:HD11	2:G:154:GLU:HB3	1.93	0.51
1:Y:47:VAL:HG21	1:Y:64:MET:HE1	1.93	0.51
2:i:105:ARG:HH22	2:i:118:VAL:C	2.18	0.51
2:j:161:MET:HE2	2:j:161:MET:HA	1.91	0.51
3:Q:54:ARG:NH2	3:Q:70:ILE:O	2.44	0.51
3:Q:102:ILE:HD11	3:Q:106:TRP:CH2	2.46	0.51
1:A:320:SER:OG	1:A:321:ASP:N	2.42	0.51
1:D:23:VAL:HB	1:D:50:PRO:O	2.11	0.51
3:E:81:LEU:HD12	3:E:86:VAL:HG11	1.93	0.51
3:I:48:GLU:HG3	3:I:87:LYS:HE3	1.92	0.51
1:Y:123:PHE:CE1	1:Y:208:VAL:HG21	2.46	0.51
2:b:97:PHE:HE1	2:b:124:TRP:HD1	1.58	0.51
2:l:326:LEU:O	2:l:330:THR:HG22	2.10	0.51
2:R:183:SER:HB2	2:R:229:MET:HE1	1.93	0.51
2:F:331:MET:HE3	2:F:335:LEU:HG	1.91	0.51
2:i:97:PHE:HA	2:i:124:TRP:HA	1.93	0.51
1:f:112:ILE:O	1:f:115:ALA:N	2.42	0.51
3:r:34:TYR:HE1	3:r:70:ILE:HD13	1.75	0.51
2:N:176:SER:OG	2:N:177:VAL:N	2.43	0.51
1:O:237:ARG:HH21	1:O:238:HIS:CD2	2.28	0.51
1:P:34:PHE:CD1	1:P:34:PHE:CB	2.80	0.51
3:K:56:ILE:HG22	3:K:58:VAL:HG22	1.90	0.51
1:d:147:LEU:HD12	1:d:208:VAL:HG23	1.93	0.51
1:f:271:MET:SD	2:l:291:ARG:HB2	2.51	0.51
1:C:231:ARG:NH1	2:F:250:ALA:H	2.09	0.51
3:K:65:ARG:HH11	3:K:65:ARG:HG3	1.76	0.51
3:L:48:GLU:HB3	3:L:87:LYS:HB3	1.93	0.51
1:c:218:GLU:HG2	2:k:255:ILE:HG21	1.91	0.51
3:u:33:ASP:OD1	3:u:35:SER:OG	2.28	0.51
2:b:220:LEU:HD22	2:b:233:LEU:HD11	1.92	0.51
2:l:220:LEU:HA	2:l:223:THR:HG22	1.91	0.51
3:t:43:ASN:O	3:t:45:GLN:NE2	2.43	0.51
3:t:52:ASN:O	3:t:53:GLY:C	2.53	0.51
1:A:31:THR:HA	1:A:62:VAL:HG12	1.92	0.51
1:D:313:VAL:HG22	2:a:341:VAL:HG22	1.92	0.51
1:Y:122:LYS:HB3	1:Y:155:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:251:PHE:O	2:k:255:ILE:HG12	2.11	0.51
1:Z:24:LYS:HG3	1:Z:27:GLU:OE1	2.11	0.51
1:M:224:TYR:CE1	2:N:247:VAL:HG11	2.46	0.51
1:M:227:MET:HE1	2:N:156:VAL:H	1.76	0.51
1:O:93:ILE:HD12	1:O:208:VAL:HG12	1.91	0.51
1:P:93:ILE:HA	1:P:208:VAL:HG12	1.93	0.51
2:S:172:LYS:NZ	2:S:176:SER:HB2	2.26	0.51
3:W:54:ARG:HH22	3:W:71:PRO:C	2.18	0.51
3:X:48:GLU:HB3	3:X:87:LYS:HB3	1.93	0.51
1:A:224:TYR:CE2	2:B:247:VAL:HG21	2.46	0.51
1:C:20:VAL:HA	1:C:53:HIS:O	2.11	0.51
2:G:251:PHE:O	2:G:255:ILE:HG12	2.11	0.51
3:I:101:SER:HA	3:I:104:ILE:HG22	1.91	0.51
1:e:37:VAL:HG22	1:e:38:LEU:H	1.76	0.51
2:i:341:VAL:HG22	2:i:343:VAL:HG23	1.92	0.51
3:T:48:GLU:OE1	3:T:50:ARG:NH1	2.39	0.51
3:V:50:ARG:HA	3:V:89:VAL:O	2.11	0.51
3:X:47:ARG:H	3:X:60:LYS:HA	1.76	0.51
2:B:138:GLU:C	2:B:166:ARG:HH12	2.18	0.51
1:C:126:ARG:HD3	1:C:130:GLU:HG3	1.92	0.51
1:D:303:TYR:OH	1:Y:323:PHE:HA	2.10	0.51
2:G:278:ARG:HG2	2:G:278:ARG:HH11	1.76	0.51
1:Y:48:TYR:O	2:a:113:LYS:NZ	2.31	0.51
1:c:31:THR:HA	1:c:62:VAL:HA	1.93	0.51
1:e:82:LYS:NZ	1:e:133:ARG:O	2.30	0.51
2:b:125:LYS:HB3	2:b:127:THR:HG22	1.93	0.51
1:f:37:VAL:HG22	1:f:38:LEU:H	1.75	0.51
1:M:224:TYR:HE2	2:N:156:VAL:HG21	1.76	0.51
1:M:320:SER:OG	1:M:321:ASP:N	2.42	0.51
3:X:30:ARG:HH22	3:X:64:ASN:HB3	1.75	0.51
3:H:52:ASN:ND2	3:H:91:GLU:HB2	2.19	0.50
1:Y:266:ARG:O	1:Y:270:ILE:HG12	2.11	0.50
2:a:158:ARG:HD3	2:a:245:GLU:HA	1.92	0.50
3:g:102:ILE:HG23	3:g:106:TRP:CE3	2.45	0.50
2:i:329:GLU:OE2	2:i:333:LYS:HE2	2.11	0.50
1:f:223:ILE:HD11	2:l:154:GLU:HB3	1.94	0.50
3:p:48:GLU:OE2	3:p:89:VAL:HG22	2.11	0.50
3:r:59:THR:HA	3:r:65:ARG:NH2	2.26	0.50
3:t:33:ASP:HB2	3:t:36:THR:HG23	1.92	0.50
3:t:102:ILE:HG23	3:t:106:TRP:HZ3	1.74	0.50
1:M:96:ARG:N	1:M:204:GLU:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:128:ARG:HA	1:P:131:ILE:HG22	1.92	0.50
3:Q:81:LEU:HD12	3:Q:86:VAL:HG21	1.92	0.50
3:Q:103:PHE:O	3:Q:107:PHE:N	2.45	0.50
2:R:276:GLN:NE2	2:R:280:ASN:OD1	2.44	0.50
2:S:208:GLY:O	2:S:212:ILE:HG12	2.10	0.50
2:B:213:ARG:HH12	1:P:128:ARG:HH12	1.59	0.50
1:D:18:MET:HG3	1:D:57:PRO:HB3	1.93	0.50
3:L:30:ARG:CZ	3:L:66:TYR:HB3	2.42	0.50
3:L:47:ARG:H	3:L:60:LYS:HA	1.76	0.50
1:Y:197:SER:OG	1:Y:200:ALA:N	2.36	0.50
2:a:110:ARG:CZ	2:a:129:ILE:HD12	2.42	0.50
2:a:112:GLY:O	2:a:113:LYS:HD3	2.11	0.50
1:e:102:ARG:O	1:e:106:ALA:CB	2.59	0.50
1:e:315:VAL:HG22	2:b:343:VAL:HA	1.94	0.50
2:k:98:TYR:HE1	2:k:125:LYS:HG3	1.77	0.50
3:X:30:ARG:CZ	3:X:66:TYR:HB3	2.42	0.50
1:D:62:VAL:HG12	1:D:64:MET:HE2	1.93	0.50
2:a:199:TYR:HB2	2:a:204:ILE:HD11	1.92	0.50
2:a:220:LEU:HD22	2:a:233:LEU:HD11	1.91	0.50
1:f:153:ASP:O	1:f:157:SER:OG	2.20	0.50
2:j:155:ASN:OD1	2:j:156:VAL:N	2.43	0.50
2:l:143:LEU:HD21	2:l:181:ASP:HB3	1.92	0.50
2:l:245:GLU:OE1	2:l:245:GLU:N	2.44	0.50
1:P:34:PHE:CE2	1:P:39:ARG:HD3	2.47	0.50
3:U:74:ASP:OD2	3:U:76:LYS:N	2.37	0.50
3:H:40:GLU:OE1	3:H:66:TYR:OH	2.29	0.50
3:J:49:ALA:HB1	3:J:51:ILE:HD11	1.93	0.50
1:c:109:GLY:HA3	1:c:114:GLN:HE22	1.76	0.50
1:e:95:TRP:HA	1:e:205:VAL:HA	1.94	0.50
1:e:137:LYS:HA	1:e:140:VAL:HG22	1.94	0.50
1:Z:15:VAL:O	1:Z:19:SER:CB	2.60	0.50
1:Z:82:LYS:HA	2:j:206:THR:HG21	1.92	0.50
1:Z:242:GLY:HA3	2:b:261:GLU:HG2	1.93	0.50
2:j:177:VAL:HG22	2:j:178:THR:H	1.76	0.50
2:l:109:THR:HG1	2:l:113:LYS:H	1.58	0.50
2:N:199:TYR:HB2	2:N:204:ILE:HD11	1.94	0.50
2:N:217:GLN:OE1	2:N:236:VAL:HG22	2.12	0.50
2:F:96:GLY:O	2:F:125:LYS:N	2.40	0.50
2:G:110:ARG:HG2	2:G:130:ASP:OD1	2.12	0.50
3:H:46:VAL:C	3:H:61:LYS:HZ2	2.18	0.50
1:e:62:VAL:HG12	1:e:64:MET:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:224:TYR:OH	2:b:245:GLU:OE2	2.23	0.50
1:f:227:MET:O	1:f:230:GLU:HG3	2.12	0.50
3:t:69:TYR:CE2	3:v:92:PRO:HD3	2.46	0.50
1:O:238:HIS:CG	2:R:258:ARG:HH12	2.29	0.50
2:S:133:LYS:HD3	2:S:135:VAL:HG22	1.94	0.50
2:F:103:ALA:HA	2:F:120:PRO:HG3	1.93	0.50
1:Y:243:GLN:O	1:Y:243:GLN:NE2	2.35	0.50
2:a:164:GLN:HB2	2:a:234:LEU:HB2	1.93	0.50
1:e:135:ASP:O	1:e:139:ILE:HD12	2.12	0.50
3:o:60:LYS:HZ2	3:o:66:TYR:HE1	1.59	0.50
1:d:143:SER:HB3	1:d:146:ARG:HH21	1.75	0.50
3:h:93:PRO:HD3	3:n:54:ARG:NH1	2.27	0.50
3:n:40:GLU:HA	3:n:45:GLN:NE2	2.26	0.50
2:N:92:TRP:O	2:N:95:SER:OG	2.20	0.50
2:N:194:GLY:O	2:N:198:LYS:NZ	2.45	0.50
1:O:32:LEU:HD13	1:O:35:GLY:H	1.77	0.50
2:R:243:PRO:N	2:R:244:PRO:HD3	2.27	0.50
2:S:164:GLN:NE2	2:S:235:ASP:HB3	2.26	0.50
3:U:38:LEU:HA	3:U:41:VAL:HG22	1.94	0.50
3:V:50:ARG:NH1	3:V:57:ASN:HB2	2.26	0.50
3:J:60:LYS:H	3:J:65:ARG:NH2	2.10	0.50
2:j:185:ARG:NH2	3:n:45:GLN:OE1	2.45	0.50
2:j:185:ARG:CZ	3:n:45:GLN:OE1	2.59	0.50
2:N:95:SER:HB3	2:N:128:PHE:HE1	1.77	0.50
2:S:189:ASP:OD1	2:S:190:SER:N	2.45	0.50
3:V:50:ARG:HH22	3:V:57:ASN:HB2	1.76	0.50
1:D:56:ILE:HD13	1:D:58:PHE:HE1	1.76	0.50
2:N:181:ASP:OD1	2:N:182:ASP:N	2.45	0.50
1:O:18:MET:HB3	1:O:55:LYS:HE3	1.94	0.50
2:B:149:MET:HE1	2:B:192:LEU:HG	1.93	0.50
1:C:126:ARG:O	1:C:129:SER:OG	2.26	0.50
3:K:42:ASN:HA	3:K:84:LYS:NZ	2.27	0.50
1:f:303:TYR:OH	1:M:323:PHE:HA	2.12	0.50
2:j:183:SER:HB2	2:j:229:MET:HE1	1.94	0.50
1:P:31:THR:HG21	1:P:63:LYS:HG2	1.94	0.50
1:P:102:ARG:O	1:P:106:ALA:CB	2.60	0.50
3:V:46:VAL:HG13	3:V:59:THR:O	2.12	0.50
1:A:314:MET:HE2	1:A:316:MET:SD	2.51	0.49
2:B:141:ARG:NH2	2:B:167:VAL:HG13	2.20	0.49
1:C:224:TYR:CE1	2:F:247:VAL:HG21	2.47	0.49
1:Y:242:GLY:HA3	2:a:261:GLU:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:92:TRP:HD1	2:a:128:PHE:HD1	1.60	0.49
1:e:94:LYS:HB3	1:e:206:VAL:HB	1.93	0.49
2:k:165:TYR:OH	2:k:184:LEU:HD21	2.11	0.49
2:k:327:TYR:CE1	2:k:331:MET:HG3	2.46	0.49
3:q:46:VAL:HG22	3:q:60:LYS:HD2	1.93	0.49
1:P:56:ILE:HG13	1:P:57:PRO:HD2	1.93	0.49
2:B:122:LEU:H	1:P:36:LYS:HD2	1.77	0.49
2:B:299:LEU:HD22	1:P:266:ARG:HD3	1.94	0.49
1:D:249:LEU:HA	1:D:252:THR:HG22	1.94	0.49
2:k:113:LYS:HA	2:k:113:LYS:HE2	1.94	0.49
2:j:105:ARG:HH11	2:j:118:VAL:C	2.20	0.49
1:O:82:LYS:HZ1	1:O:133:ARG:C	2.20	0.49
3:W:72:VAL:CG2	3:X:78:LEU:HD11	2.42	0.49
2:F:108:VAL:HG22	2:F:132:VAL:HG23	1.94	0.49
3:J:33:ASP:OD2	3:J:35:SER:OG	2.17	0.49
1:e:220:SER:O	1:e:223:ILE:HG22	2.11	0.49
1:Z:31:THR:HA	1:Z:62:VAL:HG12	1.94	0.49
2:b:351:MET:O	2:j:350:LEU:HA	2.12	0.49
1:P:249:LEU:HA	1:P:252:THR:HG22	1.94	0.49
3:T:54:ARG:HD2	3:T:54:ARG:O	2.12	0.49
1:A:39:ARG:HD3	1:A:40:ASP:O	2.12	0.49
1:A:142:ASP:N	1:A:142:ASP:OD1	2.45	0.49
3:K:50:ARG:HB2	3:K:57:ASN:HB2	1.94	0.49
1:c:36:LYS:HD2	1:c:39:ARG:NH2	2.27	0.49
1:f:314:MET:HE3	2:N:342:LEU:HD13	1.94	0.49
2:j:146:SER:OG	2:j:147:GLY:N	2.45	0.49
1:P:68:ARG:NH1	2:S:177:VAL:O	2.46	0.49
3:U:60:LYS:HZ1	3:U:64:ASN:HB3	1.76	0.49
2:B:352:VAL:C	2:F:351:MET:HG2	2.37	0.49
2:F:242:ARG:C	2:F:244:PRO:HD3	2.36	0.49
1:c:126:ARG:HD3	1:c:130:GLU:HG3	1.95	0.49
1:c:238:HIS:CE1	2:i:258:ARG:HH12	2.30	0.49
1:e:303:TYR:OH	1:Z:323:PHE:HA	2.11	0.49
2:i:135:VAL:HG21	2:i:170:PRO:HB3	1.94	0.49
3:q:33:ASP:OD2	3:q:36:THR:OG1	2.26	0.49
3:s:56:ILE:HD11	3:s:68:THR:HB	1.93	0.49
2:l:194:GLY:O	2:l:198:LYS:NZ	2.46	0.49
2:N:329:GLU:OE2	2:N:333:LYS:NZ	2.45	0.49
1:O:27:GLU:HB2	1:O:66:ASP:HA	1.93	0.49
3:V:60:LYS:HZ2	3:V:66:TYR:HD1	1.58	0.49
1:A:323:PHE:HA	1:P:303:TYR:OH	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:LEU:HD23	1:C:139:ILE:HD13	1.95	0.49
1:D:35:GLY:O	1:D:37:VAL:HG23	2.12	0.49
3:K:52:ASN:HB2	3:K:91:GLU:OE1	2.13	0.49
1:c:224:TYR:CE1	2:i:247:VAL:HG21	2.48	0.49
3:o:38:LEU:HA	3:o:41:VAL:HG22	1.94	0.49
1:f:40:ASP:HB3	1:f:45:PRO:HD3	1.94	0.49
1:f:68:ARG:NH2	2:l:174:LEU:O	2.46	0.49
2:N:95:SER:HB3	2:N:128:PHE:CE1	2.48	0.49
1:P:29:GLY:HA2	1:P:65:LEU:HB2	1.93	0.49
3:W:54:ARG:NH2	3:W:70:ILE:O	2.45	0.49
1:A:24:LYS:HG3	1:A:27:GLU:OE1	2.13	0.49
3:E:105:SER:O	3:E:108:PRO:HD2	2.13	0.49
3:J:45:GLN:O	3:J:61:LYS:HG2	2.13	0.49
1:Y:297:ILE:C	1:Y:299:SER:H	2.20	0.49
1:e:249:LEU:HA	1:e:252:THR:HG22	1.94	0.49
1:e:321:ASP:HB3	1:Z:328:THR:HG23	1.95	0.49
2:j:169:ASN:HD22	2:j:172:LYS:HZ2	1.58	0.49
2:l:143:LEU:HD13	2:l:165:TYR:CE2	2.48	0.49
1:P:34:PHE:CD2	1:P:39:ARG:NH2	2.80	0.49
1:C:19:SER:HA	1:C:55:LYS:HG3	1.93	0.49
3:H:98:LEU:HD13	3:I:100:ALA:HB2	1.95	0.49
3:K:52:ASN:O	3:K:53:GLY:C	2.54	0.49
1:c:119:LEU:HA	1:c:122:LYS:HG2	1.95	0.49
2:i:143:LEU:HD22	2:i:165:TYR:CE1	2.48	0.49
3:q:51:ILE:O	3:q:90:GLY:HA2	2.11	0.49
1:Z:135:ASP:O	1:Z:139:ILE:HD12	2.13	0.49
1:Z:320:SER:OG	1:Z:321:ASP:N	2.42	0.49
1:d:49:GLU:OE2	2:j:113:LYS:HA	2.13	0.49
1:P:38:LEU:HD23	1:P:38:LEU:H	1.76	0.49
2:S:327:TYR:CE1	2:S:331:MET:HG3	2.47	0.49
2:B:105:ARG:O	2:B:136:ASN:ND2	2.39	0.49
1:C:25:GLU:OE1	2:F:175:TYR:OH	2.23	0.49
2:G:111:PHE:CE1	2:G:129:ILE:HB	2.48	0.49
2:k:202:ASP:OD1	2:k:203:ARG:N	2.46	0.49
1:M:15:VAL:O	1:M:19:SER:HB2	2.12	0.49
1:P:254:ASP:HA	1:P:257:VAL:HG12	1.95	0.49
2:R:230:GLY:O	2:R:231:ILE:HD13	2.13	0.49
3:E:59:THR:HG22	3:E:65:ARG:HD3	1.95	0.49
2:G:182:ASP:O	2:G:186:GLN:HG2	2.13	0.49
3:I:43:ASN:O	3:I:45:GLN:NE2	2.46	0.49
3:L:44:ASP:OD1	3:L:84:LYS:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:49:GLU:CD	1:c:50:PRO:HD2	2.37	0.49
1:e:39:ARG:HG3	1:e:39:ARG:NH1	2.28	0.49
1:Z:143:SER:O	1:Z:147:LEU:HB2	2.11	0.49
1:Z:266:ARG:O	1:Z:270:ILE:HG12	2.13	0.49
3:r:89:VAL:HA	3:v:33:ASP:OD1	2.13	0.49
2:N:138:GLU:C	2:N:166:ARG:HH12	2.20	0.49
1:O:231:ARG:NH1	2:R:250:ALA:H	2.11	0.49
1:P:21:PHE:HD2	1:P:23:VAL:HG23	1.77	0.49
1:A:127:LEU:HD21	1:A:131:ILE:HD12	1.94	0.48
2:G:202:ASP:OD1	2:G:203:ARG:N	2.46	0.48
2:k:346:LYS:HE3	2:k:346:LYS:HB3	1.47	0.48
2:j:96:GLY:O	2:j:125:LYS:N	2.42	0.48
3:r:47:ARG:HH12	3:r:63:SER:HA	1.78	0.48
3:v:43:ASN:HB3	3:v:45:GLN:HE21	1.78	0.48
1:M:135:ASP:O	1:M:139:ILE:HD12	2.13	0.48
1:M:266:ARG:O	1:M:270:ILE:HG12	2.13	0.48
1:M:297:ILE:C	1:M:299:SER:H	2.20	0.48
2:N:99:THR:HG22	2:N:122:LEU:HD23	1.94	0.48
2:R:215:ASP:HA	2:R:218:ARG:NH1	2.28	0.48
2:S:251:PHE:O	2:S:255:ILE:HG12	2.12	0.48
3:E:40:GLU:OE2	3:E:60:LYS:HD3	2.13	0.48
1:Y:69:ILE:HG13	1:Y:96:ARG:HE	1.78	0.48
2:a:213:ARG:O	2:a:216:THR:HG22	2.13	0.48
3:o:47:ARG:NE	3:o:61:LYS:HA	2.28	0.48
3:s:36:THR:O	3:s:40:GLU:OE1	2.31	0.48
3:u:45:GLN:HA	3:u:61:LYS:HZ2	1.78	0.48
1:Z:144:ARG:NH1	1:Z:209:ARG:HH22	2.11	0.48
2:b:149:MET:HB2	2:b:196:ILE:HD13	1.95	0.48
1:d:134:LEU:HD23	1:d:139:ILE:HD13	1.93	0.48
2:l:251:PHE:O	2:l:255:ILE:HG12	2.13	0.48
3:r:50:ARG:NH1	3:r:89:VAL:HG13	2.28	0.48
2:N:91:ILE:HG22	2:N:128:PHE:HZ	1.78	0.48
2:N:96:GLY:HA3	2:N:125:LYS:H	1.78	0.48
1:O:64:MET:N	1:O:64:MET:SD	2.86	0.48
1:C:238:HIS:CD2	2:F:258:ARG:HH12	2.30	0.48
1:Y:140:VAL:HG11	2:a:150:LEU:HD23	1.95	0.48
2:a:346:LYS:HD3	2:a:346:LYS:HA	1.32	0.48
1:f:18:MET:HB3	1:f:57:PRO:HB3	1.95	0.48
3:p:106:TRP:HE1	3:r:108:PRO:HB3	1.77	0.48
3:t:65:ARG:HH11	3:t:65:ARG:HG3	1.79	0.48
1:P:70:GLN:O	1:P:94:LYS:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:THR:HG22	1:A:94:LYS:HE3	1.93	0.48
1:C:119:LEU:HA	1:C:122:LYS:HG2	1.94	0.48
2:F:162:ASN:OD1	2:F:163:VAL:N	2.45	0.48
2:a:195:VAL:HG12	2:a:215:ASP:OD2	2.14	0.48
1:e:28:ARG:HH22	1:e:48:TYR:HD1	1.61	0.48
3:o:98:LEU:O	3:o:102:ILE:HG13	2.13	0.48
1:d:11:ILE:O	1:d:15:VAL:HG23	2.14	0.48
2:l:344:ASN:OD1	2:l:345:ASP:N	2.46	0.48
1:O:135:ASP:O	1:O:139:ILE:HG12	2.12	0.48
1:O:147:LEU:HD12	1:O:208:VAL:HG23	1.94	0.48
3:V:48:GLU:OE1	3:V:50:ARG:HD2	2.13	0.48
2:a:108:VAL:HA	2:a:132:VAL:HG12	1.93	0.48
1:e:56:ILE:HD13	1:e:58:PHE:HE1	1.78	0.48
2:i:183:SER:HB2	2:i:229:MET:HE1	1.95	0.48
3:u:48:GLU:HG3	3:u:59:THR:HB	1.94	0.48
1:f:280:ALA:HB3	2:N:314:GLU:CD	2.38	0.48
1:f:315:VAL:HG22	2:N:343:VAL:HA	1.96	0.48
2:j:137:VAL:HG13	2:j:167:VAL:HG23	1.94	0.48
3:v:102:ILE:O	3:v:105:SER:HB3	2.14	0.48
2:N:141:ARG:NH2	2:N:167:VAL:HG13	2.22	0.48
1:O:321:ASP:OD1	1:P:328:THR:N	2.47	0.48
3:I:34:TYR:HE1	3:I:70:ILE:HG12	1.78	0.48
3:I:74:ASP:OD2	3:I:76:LYS:N	2.37	0.48
3:J:92:PRO:HD3	3:L:69:TYR:CD2	2.49	0.48
1:c:133:ARG:HH11	1:c:133:ARG:HG3	1.79	0.48
2:j:169:ASN:HD22	2:j:172:LYS:HZ3	1.59	0.48
2:l:119:GLU:HB3	2:l:120:PRO:HD2	1.94	0.48
2:l:255:ILE:HG23	2:l:258:ARG:NH1	2.29	0.48
3:v:47:ARG:NH1	3:v:60:LYS:HG2	2.29	0.48
2:N:164:GLN:HB2	2:N:234:LEU:HB2	1.95	0.48
1:O:243:GLN:HE22	2:S:277:PRO:HB2	1.79	0.48
2:R:109:THR:HG22	2:R:115:SER:H	1.78	0.48
2:R:123:ASN:OD1	2:R:124:TRP:N	2.47	0.48
2:R:137:VAL:HG13	2:R:167:VAL:HG23	1.96	0.48
2:R:146:SER:OG	2:R:147:GLY:N	2.47	0.48
2:R:262:GLN:HA	2:R:265:ILE:HG22	1.96	0.48
2:S:220:LEU:HA	2:S:223:THR:HG22	1.96	0.48
3:X:44:ASP:OD1	3:X:84:LYS:HD2	2.13	0.48
1:C:152:ARG:O	1:C:156:ASN:ND2	2.34	0.48
1:C:231:ARG:HH11	2:F:250:ALA:HB3	1.78	0.48
1:D:97:ILE:HA	1:D:203:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:205:LEU:HG	2:F:206:THR:HG23	1.96	0.48
1:Y:84:LYS:NZ	2:i:205:LEU:HD23	2.28	0.48
1:c:207:ASP:OD1	1:c:208:VAL:N	2.46	0.48
3:g:81:LEU:HD12	3:g:86:VAL:HG21	1.95	0.48
3:q:48:GLU:O	3:q:59:THR:HB	2.13	0.48
1:f:18:MET:HB2	1:f:57:PRO:HB3	1.95	0.48
2:N:276:GLN:HB3	2:N:277:PRO:HD3	1.96	0.48
1:P:296:PHE:CZ	1:P:300:LEU:HD11	2.48	0.48
1:A:197:SER:OG	1:A:200:ALA:N	2.41	0.48
1:C:31:THR:HA	1:C:62:VAL:HA	1.94	0.48
1:C:321:ASP:HB2	1:D:328:THR:HB	1.96	0.48
2:G:327:TYR:CE1	2:G:331:MET:HG3	2.48	0.48
3:H:46:VAL:O	3:H:61:LYS:NZ	2.43	0.48
3:K:41:VAL:O	3:K:84:LYS:NZ	2.29	0.48
1:e:153:ASP:O	1:e:157:SER:OG	2.18	0.48
3:g:98:LEU:O	3:g:101:SER:N	2.47	0.48
2:i:243:PRO:N	2:i:244:PRO:HD3	2.29	0.48
2:k:220:LEU:HA	2:k:223:THR:HG22	1.96	0.48
1:M:271:MET:SD	2:N:291:ARG:HB3	2.54	0.48
3:Q:37:PHE:CD2	3:Q:38:LEU:HD22	2.49	0.48
2:R:161:MET:HE2	2:R:161:MET:HA	1.96	0.48
2:B:133:LYS:HG3	2:B:135:VAL:HG22	1.95	0.48
1:D:321:ASP:O	1:D:324:ARG:HD2	2.14	0.48
2:G:214:SER:O	2:G:218:ARG:HG3	2.13	0.48
1:O:40:ASP:OD2	1:O:40:ASP:N	2.45	0.48
1:O:244:GLU:HG2	1:O:248:LYS:HE2	1.95	0.48
1:P:53:HIS:HE1	1:P:55:LYS:CG	2.27	0.48
3:W:74:ASP:OD2	3:W:76:LYS:N	2.47	0.48
1:c:25:GLU:OE1	2:i:109:THR:OG1	2.31	0.48
1:e:254:ASP:O	1:e:257:VAL:HG12	2.14	0.48
2:i:118:VAL:HG21	2:i:123:ASN:HD22	1.79	0.48
2:k:344:ASN:OD1	2:k:345:ASP:N	2.47	0.48
2:b:110:ARG:HD3	2:b:130:ASP:HA	1.96	0.48
2:N:348:GLY:O	2:R:347:GLY:O	2.31	0.48
1:P:144:ARG:HH12	1:P:209:ARG:HB3	1.78	0.48
3:E:48:GLU:HB3	3:E:59:THR:OG1	2.14	0.47
3:J:47:ARG:N	3:J:60:LYS:HA	2.22	0.47
2:a:125:LYS:HE3	2:a:126:PRO:HD2	1.96	0.47
2:k:164:GLN:HG2	2:k:234:LEU:HB2	1.95	0.47
1:Z:27:GLU:OE1	1:Z:27:GLU:N	2.47	0.47
1:Z:125:ASP:OD2	2:j:237:ASN:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:181:ASP:OD1	2:b:182:ASP:N	2.47	0.47
2:l:234:LEU:HD12	2:l:234:LEU:H	1.79	0.47
3:p:99:LEU:HA	3:p:102:ILE:HG22	1.95	0.47
3:t:32:VAL:HG22	3:t:33:ASP:H	1.78	0.47
3:t:47:ARG:NE	3:t:61:LYS:HA	2.29	0.47
3:v:32:VAL:O	3:v:68:THR:HB	2.13	0.47
2:N:343:VAL:HG12	2:N:344:ASN:O	2.14	0.47
1:O:33:ARG:HG3	1:O:34:PHE:CD2	2.49	0.47
1:P:21:PHE:CD2	1:P:23:VAL:HG23	2.48	0.47
2:R:162:ASN:OD1	2:R:163:VAL:N	2.47	0.47
2:R:169:ASN:HD22	2:R:172:LYS:NZ	2.11	0.47
2:i:108:VAL:HG22	2:i:132:VAL:HG23	1.96	0.47
2:i:146:SER:OG	2:i:147:GLY:N	2.47	0.47
3:s:43:ASN:O	3:s:45:GLN:NE2	2.47	0.47
3:u:46:VAL:HA	3:u:60:LYS:HA	1.95	0.47
1:Z:96:ARG:N	1:Z:204:GLU:O	2.31	0.47
1:f:21:PHE:HA	1:f:53:HIS:ND1	2.29	0.47
2:l:109:THR:HG1	2:l:113:LYS:N	2.10	0.47
2:S:105:ARG:O	2:S:136:ASN:HB2	2.13	0.47
3:V:37:PHE:O	3:V:41:VAL:HG23	2.14	0.47
3:V:39:GLN:HA	3:V:42:ASN:OD1	2.14	0.47
1:D:50:PRO:HG3	2:G:113:LYS:NZ	2.29	0.47
1:D:98:SER:OG	1:D:204:GLU:HG2	2.15	0.47
1:D:254:ASP:HA	1:D:257:VAL:HG12	1.96	0.47
2:G:235:ASP:OD1	2:G:236:VAL:N	2.43	0.47
2:b:110:ARG:HE	2:b:129:ILE:CG1	2.27	0.47
2:b:154:GLU:O	2:b:155:ASN:CG	2.58	0.47
1:f:82:LYS:NZ	1:f:135:ASP:HB2	2.28	0.47
1:f:94:LYS:HZ3	1:f:207:ASP:HB3	1.78	0.47
3:n:37:PHE:O	3:n:40:GLU:HB3	2.14	0.47
2:N:110:ARG:HH11	2:N:111:PHE:H	1.62	0.47
1:P:224:TYR:HE2	2:S:156:VAL:HG21	1.79	0.47
2:R:142:GLU:OE2	3:T:61:LYS:HG2	2.14	0.47
2:S:133:LYS:NZ	2:S:135:VAL:O	2.42	0.47
1:e:32:LEU:HD22	1:e:53:HIS:NE2	2.29	0.47
3:t:45:GLN:CA	3:t:61:LYS:HZ3	2.27	0.47
1:M:123:PHE:HE1	1:M:208:VAL:HG21	1.79	0.47
1:P:21:PHE:HA	1:P:55:LYS:HD2	1.96	0.47
1:P:39:ARG:HB2	1:P:45:PRO:HG3	1.94	0.47
1:P:227:MET:O	1:P:230:GLU:HG3	2.13	0.47
3:Q:79:ASP:O	3:Q:83:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:109:THR:CG2	2:R:114:PHE:HA	2.45	0.47
1:A:197:SER:C	1:A:199:ALA:H	2.22	0.47
1:D:28:ARG:NH2	1:D:48:TYR:HA	2.29	0.47
2:F:102:GLU:O	2:F:104:GLU:HG2	2.14	0.47
2:G:165:TYR:CE1	2:G:184:LEU:HD23	2.45	0.47
3:I:48:GLU:HG3	3:I:87:LYS:CE	2.44	0.47
2:a:264:TYR:O	2:a:267:GLU:HG3	2.14	0.47
1:c:119:LEU:HD12	1:c:122:LYS:HD2	1.95	0.47
1:c:240:SER:O	1:c:243:GLN:HG3	2.15	0.47
1:c:243:GLN:O	1:c:247:GLU:OE1	2.33	0.47
1:Z:297:ILE:C	1:Z:299:SER:H	2.22	0.47
1:d:56:ILE:H	1:d:56:ILE:HD12	1.79	0.47
1:d:135:ASP:O	1:d:139:ILE:HG12	2.15	0.47
1:d:321:ASP:HB2	1:f:328:THR:HB	1.97	0.47
1:f:126:ARG:NH1	1:f:130:GLU:HB2	2.29	0.47
3:t:45:GLN:O	3:t:60:LYS:HB2	2.15	0.47
1:M:30:ILE:HG22	1:M:63:LYS:H	1.80	0.47
1:M:259:ARG:HG2	1:M:259:ARG:HH11	1.79	0.47
2:N:95:SER:OG	2:N:127:THR:O	2.32	0.47
2:S:202:ASP:OD1	2:S:203:ARG:N	2.47	0.47
3:V:45:GLN:C	3:V:61:LYS:HG2	2.39	0.47
3:V:93:PRO:CB	3:X:54:ARG:NH2	2.74	0.47
1:A:28:ARG:HH21	1:A:46:LEU:HD13	1.79	0.47
2:B:92:TRP:HD1	2:B:128:PHE:HD1	1.61	0.47
1:C:321:ASP:OD1	1:C:322:PHE:N	2.47	0.47
2:F:243:PRO:N	2:F:244:PRO:HD3	2.29	0.47
1:Y:31:THR:HA	1:Y:62:VAL:HG12	1.96	0.47
3:g:30:ARG:HD2	3:g:30:ARG:O	2.15	0.47
2:i:230:GLY:O	2:i:231:ILE:HD13	2.13	0.47
3:u:102:ILE:HG22	3:u:106:TRP:NE1	2.30	0.47
1:Z:21:PHE:CZ	1:Z:50:PRO:HA	2.49	0.47
2:j:329:GLU:OE2	2:j:333:LYS:HE2	2.14	0.47
2:l:108:VAL:O	2:l:115:SER:HB2	2.14	0.47
3:r:45:GLN:HA	3:r:61:LYS:NZ	2.30	0.47
3:v:103:PHE:HA	3:v:106:TRP:CE3	2.41	0.47
2:N:94:ALA:HA	2:N:97:PHE:HD2	1.79	0.47
3:V:51:ILE:HG23	3:V:56:ILE:HG12	1.96	0.47
3:W:47:ARG:NE	3:W:61:LYS:HA	2.29	0.47
1:A:135:ASP:O	1:A:139:ILE:HD12	2.15	0.47
2:B:350:LEU:C	2:S:351:MET:HG2	2.39	0.47
2:G:98:TYR:CE2	2:G:123:ASN:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:217:GLN:OE1	2:a:236:VAL:N	2.48	0.47
1:e:231:ARG:O	1:e:234:VAL:HG12	2.15	0.47
1:e:234:VAL:HG22	1:e:238:HIS:HE1	1.79	0.47
3:g:98:LEU:O	3:g:102:ILE:HD12	2.14	0.47
3:o:70:ILE:HD12	3:o:71:PRO:HD2	1.97	0.47
3:q:36:THR:HA	3:q:39:GLN:HG3	1.96	0.47
3:q:58:VAL:HG11	3:q:66:TYR:CE1	2.49	0.47
1:d:40:ASP:CG	1:d:41:ASP:H	2.23	0.47
2:j:109:THR:CG2	2:j:114:PHE:HA	2.45	0.47
2:j:124:TRP:CH2	2:j:126:PRO:HG3	2.50	0.47
2:j:138:GLU:HA	2:j:166:ARG:HD2	1.95	0.47
2:j:271:TYR:O	2:j:274:GLU:HG2	2.14	0.47
2:l:164:GLN:HE22	2:l:235:ASP:HB3	1.78	0.47
3:r:80:ASN:O	3:r:83:THR:OG1	2.25	0.47
1:M:33:ARG:HA	1:M:60:GLU:CB	2.44	0.47
1:M:143:SER:HB3	2:N:193:ARG:NH2	2.30	0.47
2:N:241:ALA:C	2:N:243:PRO:HD3	2.39	0.47
1:O:237:ARG:HD2	1:O:241:GLN:HE22	1.79	0.47
1:P:55:LYS:HD3	1:P:60:GLU:OE1	2.15	0.47
1:P:112:ILE:O	1:P:115:ALA:N	2.47	0.47
3:Q:107:PHE:HB3	3:Q:108:PRO:HD3	1.96	0.47
2:S:346:LYS:H	2:S:346:LYS:HG3	1.39	0.47
2:S:350:LEU:C	2:S:351:MET:HG3	2.40	0.47
3:V:64:ASN:OD1	3:V:65:ARG:N	2.47	0.47
1:A:266:ARG:O	1:A:270:ILE:HG12	2.14	0.47
2:G:189:ASP:OD1	2:G:190:SER:N	2.47	0.47
1:Y:300:LEU:HB3	2:a:330:THR:HG21	1.97	0.47
2:a:241:ALA:C	2:a:243:PRO:HD3	2.39	0.47
3:g:54:ARG:NE	3:g:54:ARG:HA	2.29	0.47
3:t:33:ASP:OD1	3:v:87:LYS:HE2	2.15	0.47
1:M:125:ASP:OD2	2:R:237:ASN:HB3	2.15	0.47
2:N:211:VAL:HG13	2:N:212:ILE:HG23	1.96	0.47
1:O:47:VAL:HG21	1:O:52:LEU:HB2	1.96	0.47
3:T:59:THR:HG22	3:T:65:ARG:HG2	1.96	0.47
1:A:257:VAL:HG23	2:B:279:ALA:HB2	1.97	0.47
1:C:64:MET:SD	1:C:64:MET:N	2.88	0.47
2:F:153:ASP:HB3	2:F:155:ASN:ND2	2.27	0.47
2:G:194:GLY:O	2:G:198:LYS:NZ	2.48	0.47
2:j:351:MET:O	2:j:352:VAL:C	2.58	0.47
3:V:93:PRO:CA	3:X:54:ARG:HH22	2.28	0.47
2:B:217:GLN:OE1	2:B:236:VAL:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:152:SER:HB3	2:F:197:GLY:O	2.14	0.47
3:J:92:PRO:HA	3:L:54:ARG:HH12	1.79	0.47
3:K:35:SER:HB3	3:L:88:VAL:HG12	1.97	0.47
1:Y:144:ARG:HD2	1:Y:209:ARG:NH1	2.30	0.47
1:e:34:PHE:HB3	1:e:39:ARG:CZ	2.45	0.47
2:i:101:LYS:O	2:i:104:GLU:CG	2.58	0.47
3:s:56:ILE:HG12	3:s:68:THR:O	2.15	0.47
2:b:176:SER:OG	2:b:177:VAL:N	2.46	0.47
1:f:88:ILE:HB	1:f:214:ASN:OD1	2.15	0.47
2:l:142:GLU:C	2:l:143:LEU:HD12	2.40	0.47
3:n:106:TRP:NE1	3:p:107:PHE:O	2.48	0.47
3:r:47:ARG:HD3	3:r:59:THR:O	2.15	0.47
2:R:319:PRO:HD2	2:R:320:GLU:OE1	2.14	0.47
3:V:33:ASP:O	3:V:36:THR:OG1	2.31	0.47
2:F:203:ARG:HG2	2:F:203:ARG:HH11	1.79	0.46
2:F:242:ARG:HB3	2:F:244:PRO:HD3	1.97	0.46
2:a:122:LEU:HD12	2:a:124:TRP:CZ2	2.50	0.46
3:g:41:VAL:HG23	3:g:46:VAL:CG1	2.44	0.46
3:u:30:ARG:NE	3:u:66:TYR:HA	2.31	0.46
1:d:238:HIS:CD2	2:j:258:ARG:HH12	2.32	0.46
1:d:243:GLN:O	1:d:247:GLU:OE1	2.33	0.46
2:j:97:PHE:HD1	2:j:124:TRP:HB2	1.80	0.46
2:l:237:ASN:OD1	2:l:238:PHE:N	2.48	0.46
3:v:47:ARG:HH11	3:v:61:LYS:CB	2.28	0.46
1:M:243:GLN:HE22	2:N:264:TYR:HE1	1.62	0.46
1:P:144:ARG:O	1:P:149:LEU:HD23	2.15	0.46
3:Q:48:GLU:HB3	3:Q:59:THR:OG1	2.15	0.46
2:S:96:GLY:HA2	2:S:125:LYS:C	2.40	0.46
2:S:255:ILE:HG23	2:S:258:ARG:HH12	1.80	0.46
3:U:58:VAL:N	3:U:66:TYR:O	2.39	0.46
3:o:44:ASP:HB2	3:o:84:LYS:HE2	1.96	0.46
1:Z:144:ARG:HD3	1:Z:209:ARG:HH22	1.79	0.46
1:d:126:ARG:HD3	1:d:130:GLU:HG3	1.97	0.46
3:p:45:GLN:HA	3:p:61:LYS:HZ2	1.80	0.46
3:v:62:ASP:OD1	3:v:64:ASN:HB2	2.15	0.46
1:M:231:ARG:NH2	2:N:251:PHE:CD2	2.82	0.46
2:S:184:LEU:O	2:S:188:THR:HG23	2.15	0.46
3:U:92:PRO:HA	3:V:54:ARG:NH2	2.30	0.46
3:X:54:ARG:HA	3:X:70:ILE:HD12	1.97	0.46
1:c:130:GLU:HA	1:c:133:ARG:NH1	2.30	0.46
3:s:99:LEU:O	3:s:102:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:u:103:PHE:HA	3:u:106:TRP:CD1	2.41	0.46
1:Z:123:PHE:HE1	1:Z:208:VAL:HG21	1.80	0.46
1:d:321:ASP:OD1	1:d:322:PHE:N	2.48	0.46
1:f:34:PHE:CD1	1:f:39:ARG:HD2	2.50	0.46
1:f:36:LYS:CD	2:N:121:GLY:HA2	2.45	0.46
3:p:32:VAL:HG11	3:p:66:TYR:CE2	2.50	0.46
3:W:46:VAL:HG13	3:W:60:LYS:HA	1.96	0.46
2:B:241:ALA:C	2:B:243:PRO:HD3	2.40	0.46
1:D:212:GLN:HE22	1:D:214:ASN:HB3	1.81	0.46
2:F:123:ASN:OD1	2:F:124:TRP:N	2.47	0.46
2:F:173:TYR:CE1	2:F:180:PRO:HG2	2.51	0.46
2:i:92:TRP:CZ2	2:i:127:THR:HB	2.51	0.46
3:m:52:ASN:ND2	3:m:55:GLU:OE2	2.46	0.46
1:d:31:THR:HA	1:d:62:VAL:HA	1.96	0.46
1:d:47:VAL:HG21	1:d:52:LEU:HB2	1.97	0.46
1:M:21:PHE:CE2	1:M:50:PRO:HA	2.50	0.46
1:M:23:VAL:HG21	1:M:47:VAL:HB	1.97	0.46
1:O:99:ASP:OD1	1:O:202:GLY:HA3	2.15	0.46
3:I:50:ARG:HA	3:I:89:VAL:HG13	1.98	0.46
1:e:78:ARG:HG3	1:e:88:ILE:HD13	1.97	0.46
3:g:48:GLU:HB3	3:g:59:THR:OG1	2.15	0.46
3:q:58:VAL:HG21	3:q:66:TYR:OH	2.16	0.46
3:s:46:VAL:HA	3:s:60:LYS:HA	1.97	0.46
1:f:62:VAL:HG12	1:f:64:MET:HE2	1.97	0.46
2:j:312:LEU:HB3	2:j:313:PRO:HD3	1.98	0.46
1:O:36:LYS:HG3	1:O:39:ARG:NH1	2.30	0.46
3:X:89:VAL:HG12	3:X:90:GLY:O	2.16	0.46
1:D:78:ARG:HG3	1:D:88:ILE:HD13	1.98	0.46
2:i:208:GLY:O	2:i:211:VAL:HG12	2.16	0.46
3:h:41:VAL:HG22	3:h:46:VAL:HG21	1.98	0.46
2:l:127:THR:HG22	2:l:130:ASP:H	1.79	0.46
1:M:111:ASP:OD1	1:M:114:GLN:NE2	2.45	0.46
2:N:215:ASP:HA	2:N:218:ARG:NH1	2.30	0.46
1:A:134:LEU:HD21	1:A:147:LEU:HD21	1.98	0.46
1:C:40:ASP:CG	1:C:41:ASP:H	2.24	0.46
1:D:254:ASP:O	1:D:257:VAL:HG12	2.16	0.46
2:F:276:GLN:NE2	2:F:280:ASN:OD1	2.48	0.46
3:o:89:VAL:HG22	3:q:33:ASP:HB3	1.97	0.46
1:f:119:LEU:HA	1:f:198:MET:HE1	1.98	0.46
2:j:103:ALA:HA	2:j:120:PRO:HG3	1.97	0.46
2:j:149:MET:HE1	2:j:193:ARG:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:315:TYR:CG	2:j:316:LYS:N	2.83	0.46
3:n:59:THR:HG22	3:n:65:ARG:HG2	1.97	0.46
3:n:98:LEU:O	3:n:101:SER:OG	2.34	0.46
3:r:76:LYS:HB3	3:r:80:ASN:OD1	2.16	0.46
1:O:94:LYS:HA	1:O:94:LYS:HE2	1.97	0.46
1:A:33:ARG:HA	1:A:60:GLU:CB	2.45	0.46
2:B:164:GLN:HB2	2:B:234:LEU:HB2	1.98	0.46
3:E:60:LYS:HE2	3:E:66:TYR:HE1	1.80	0.46
2:G:109:THR:HG1	2:G:113:LYS:N	2.13	0.46
2:G:278:ARG:HA	2:G:278:ARG:CZ	2.46	0.46
3:K:65:ARG:NH1	3:K:65:ARG:HG3	2.30	0.46
2:a:96:GLY:HA3	2:a:125:LYS:O	2.15	0.46
3:s:78:LEU:HD13	3:s:81:LEU:HD12	1.98	0.46
2:b:92:TRP:HD1	2:b:128:PHE:HD1	1.63	0.46
2:l:141:ARG:HD3	2:l:165:TYR:HD2	1.81	0.46
1:M:197:SER:C	1:M:199:ALA:H	2.23	0.46
3:W:56:ILE:N	3:W:68:THR:O	2.46	0.46
1:A:253:ALA:HB1	2:B:275:VAL:HG11	1.97	0.46
1:C:99:ASP:OD1	1:C:202:GLY:HA3	2.16	0.46
3:K:32:VAL:HG12	3:K:67:THR:O	2.16	0.46
3:K:36:THR:O	3:K:40:GLU:OE1	2.34	0.46
3:L:54:ARG:HA	3:L:70:ILE:HD12	1.97	0.46
1:Y:281:LYS:HB2	2:i:314:GLU:OE1	2.16	0.46
1:c:40:ASP:CG	1:c:41:ASP:H	2.23	0.46
3:q:64:ASN:OD1	3:q:65:ARG:N	2.49	0.46
3:u:102:ILE:O	3:u:106:TRP:CD1	2.68	0.46
2:j:119:GLU:HB3	2:j:120:PRO:HD2	1.98	0.46
2:j:243:PRO:N	2:j:244:PRO:HD3	2.31	0.46
2:l:164:GLN:NE2	2:l:235:ASP:HB3	2.30	0.46
1:A:70:GLN:OE1	1:A:70:GLN:HA	2.16	0.46
2:B:213:ARG:O	2:B:216:THR:HG22	2.16	0.46
2:B:220:LEU:HD23	2:B:233:LEU:HD11	1.98	0.46
2:F:146:SER:OG	2:F:147:GLY:N	2.49	0.46
2:G:101:LYS:HE2	2:G:104:GLU:OE1	2.15	0.46
3:J:48:GLU:HG2	3:J:87:LYS:HB3	1.98	0.46
3:q:37:PHE:O	3:q:41:VAL:HG23	2.16	0.46
3:u:32:VAL:HB	3:u:66:TYR:CD2	2.51	0.46
1:d:49:GLU:CD	1:d:50:PRO:HD2	2.41	0.46
2:l:202:ASP:OD1	2:l:203:ARG:N	2.49	0.46
3:v:97:SER:O	3:v:99:LEU:N	2.47	0.46
1:M:245:GLU:OE1	2:N:265:ILE:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:20:VAL:HG13	1:O:53:HIS:HB3	1.97	0.46
2:R:138:GLU:HG3	2:R:138:GLU:O	2.16	0.46
1:C:200:ALA:O	1:C:201:LEU:C	2.49	0.45
1:D:315:VAL:HG12	2:G:341:VAL:HG13	1.98	0.45
2:G:277:PRO:HA	2:G:280:ASN:HB2	1.98	0.45
3:L:89:VAL:HG12	3:L:90:GLY:O	2.16	0.45
2:a:92:TRP:CD1	2:a:128:PHE:HD1	2.35	0.45
1:c:279:ALA:O	1:c:283:PHE:HD1	1.99	0.45
1:e:266:ARG:HD3	2:b:299:LEU:HD22	1.98	0.45
3:g:62:ASP:O	3:g:63:SER:OG	2.32	0.45
2:k:149:MET:HE1	2:k:159:VAL:HB	1.96	0.45
2:k:186:GLN:HA	2:k:189:ASP:OD2	2.16	0.45
2:k:349:ASN:HB3	2:b:347:GLY:O	2.16	0.45
3:q:63:SER:O	3:q:65:ARG:NH1	2.49	0.45
2:b:110:ARG:NH2	2:b:129:ILE:HD12	2.31	0.45
1:f:296:PHE:CZ	1:f:300:LEU:HD11	2.51	0.45
2:l:351:MET:HE2	2:N:351:MET:CB	2.46	0.45
3:t:98:LEU:O	3:t:102:ILE:HD12	2.16	0.45
2:N:213:ARG:O	2:N:216:THR:HG22	2.17	0.45
2:N:351:MET:O	2:N:352:VAL:C	2.59	0.45
1:A:33:ARG:HA	1:A:60:GLU:HB3	1.99	0.45
1:A:84:LYS:HB2	2:F:255:ILE:HD11	1.99	0.45
1:D:296:PHE:CZ	1:D:300:LEU:HD11	2.51	0.45
3:J:72:VAL:HG22	3:J:73:GLN:H	1.81	0.45
1:Y:20:VAL:HG12	1:Y:53:HIS:CD2	2.51	0.45
2:a:245:GLU:OE2	2:a:247:VAL:HB	2.17	0.45
1:c:94:LYS:HB3	1:c:206:VAL:HB	1.97	0.45
2:k:172:LYS:NZ	2:k:228:ASP:HB3	2.30	0.45
3:o:74:ASP:OD2	3:o:77:LEU:N	2.50	0.45
3:u:50:ARG:NH2	3:u:91:GLU:HB3	2.30	0.45
3:u:102:ILE:O	3:u:105:SER:HB3	2.17	0.45
1:Z:70:GLN:OE1	1:Z:70:GLN:HA	2.15	0.45
2:b:213:ARG:NE	2:b:236:VAL:O	2.37	0.45
2:j:108:VAL:HG22	2:j:132:VAL:HG23	1.98	0.45
3:E:30:ARG:HE	3:E:32:VAL:HG12	1.81	0.45
3:K:36:THR:HA	3:K:39:GLN:OE1	2.17	0.45
2:a:217:GLN:OE1	2:a:236:VAL:HG22	2.16	0.45
2:a:263:GLN:HA	2:a:266:ARG:HH11	1.80	0.45
1:c:294:TYR:HA	1:c:297:ILE:HG22	1.98	0.45
2:i:315:TYR:CG	2:i:316:LYS:N	2.85	0.45
2:k:326:LEU:O	2:k:330:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:33:ARG:HA	1:Z:60:GLU:CB	2.46	0.45
1:Z:197:SER:C	1:Z:199:ALA:H	2.24	0.45
2:b:205:LEU:CD2	2:b:243:PRO:HB2	2.47	0.45
3:h:106:TRP:HA	3:h:109:MET:HG2	1.97	0.45
2:l:189:ASP:OD1	2:l:190:SER:N	2.49	0.45
3:p:49:ALA:O	3:p:88:VAL:HG13	2.16	0.45
2:N:101:LYS:H	2:N:101:LYS:HG3	1.53	0.45
1:P:50:PRO:HB3	2:S:113:LYS:HD2	1.98	0.45
2:R:97:PHE:HA	2:R:124:TRP:HA	1.98	0.45
2:R:105:ARG:HH11	2:R:117:LEU:HD23	1.81	0.45
1:A:21:PHE:CE2	1:A:50:PRO:HA	2.51	0.45
3:g:104:ILE:HG12	3:s:102:ILE:HD11	1.97	0.45
2:i:341:VAL:O	2:i:341:VAL:HG13	2.17	0.45
3:m:40:GLU:HA	3:m:45:GLN:NE2	2.32	0.45
3:s:47:ARG:HB3	3:s:61:LYS:HG2	1.99	0.45
1:f:28:ARG:HE	1:f:49:GLU:HB3	1.80	0.45
1:f:282:LEU:CD2	2:l:305:VAL:HG21	2.47	0.45
2:j:173:TYR:CE1	2:j:180:PRO:HG2	2.52	0.45
3:v:54:ARG:HA	3:v:70:ILE:HD12	1.96	0.45
3:X:47:ARG:HB3	3:X:61:LYS:HG2	1.98	0.45
2:F:169:ASN:HD22	2:F:172:LYS:NZ	2.15	0.45
2:G:134:PRO:HD2	2:G:135:VAL:H	1.81	0.45
2:G:202:ASP:O	2:G:206:THR:HG23	2.17	0.45
3:g:38:LEU:HA	3:g:41:VAL:HG12	1.99	0.45
2:b:264:TYR:O	2:b:267:GLU:HG3	2.17	0.45
1:f:95:TRP:HA	1:f:205:VAL:HA	1.99	0.45
1:f:104:TYR:O	1:f:105:LEU:HB2	2.16	0.45
2:j:100:ILE:HB	2:j:120:PRO:HA	1.98	0.45
2:j:341:VAL:HG22	2:j:343:VAL:HG23	1.98	0.45
3:v:47:ARG:CZ	3:v:60:LYS:HG2	2.46	0.45
1:C:237:ARG:HD2	1:C:241:GLN:HE22	1.81	0.45
1:D:113:SER:HA	1:D:116:GLU:CD	2.42	0.45
2:F:128:PHE:O	2:F:128:PHE:CG	2.59	0.45
2:F:230:GLY:O	2:F:231:ILE:HD13	2.15	0.45
3:K:32:VAL:HG13	3:K:68:THR:HB	1.98	0.45
2:i:169:ASN:HD22	2:i:172:LYS:NZ	2.15	0.45
2:k:189:ASP:OD1	2:k:190:SER:N	2.50	0.45
3:u:54:ARG:O	3:u:54:ARG:HD3	2.16	0.45
3:u:54:ARG:HH11	3:u:69:TYR:HB3	1.82	0.45
1:f:51:GLY:N	2:l:113:LYS:HZ1	2.15	0.45
3:n:34:TYR:HE2	3:n:38:LEU:HD11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:t:40:GLU:OE1	3:t:46:VAL:HG23	2.16	0.45
3:t:54:ARG:NH2	3:t:70:ILE:O	2.50	0.45
1:O:11:ILE:O	1:O:15:VAL:HG23	2.17	0.45
2:R:97:PHE:CD1	2:R:124:TRP:HB2	2.52	0.45
2:R:105:ARG:HH22	2:R:119:GLU:CD	2.25	0.45
3:X:60:LYS:HG3	3:X:62:ASP:OD1	2.17	0.45
1:A:144:ARG:HH11	1:A:209:ARG:HH22	1.64	0.45
1:C:134:LEU:HG	1:C:135:ASP:H	1.82	0.45
1:D:73:ASP:HA	1:D:92:TYR:HA	1.99	0.45
1:Y:197:SER:C	1:Y:199:ALA:H	2.24	0.45
1:Y:310:ASN:HB2	2:a:339:ARG:NH1	2.32	0.45
2:a:113:LYS:HD3	2:a:113:LYS:HA	1.68	0.45
1:Z:122:LYS:HB3	1:Z:155:LEU:HD11	1.99	0.45
1:f:72:MET:SD	1:f:116:GLU:HG3	2.56	0.45
2:j:101:LYS:O	2:j:101:LYS:CG	2.31	0.45
2:j:110:ARG:HG2	2:j:129:ILE:HD12	1.98	0.45
2:j:341:VAL:O	2:j:341:VAL:HG13	2.16	0.45
1:M:25:GLU:HG2	1:M:48:TYR:OH	2.16	0.45
2:S:202:ASP:O	2:S:206:THR:HG23	2.17	0.45
3:X:46:VAL:HA	3:X:60:LYS:HA	1.99	0.45
1:A:239:ARG:HH12	2:B:257:ALA:HA	1.81	0.45
3:J:86:VAL:O	3:J:88:VAL:HG23	2.16	0.45
3:K:78:LEU:HD13	3:K:81:LEU:HD12	1.99	0.45
3:L:47:ARG:HB3	3:L:61:LYS:HG2	1.98	0.45
3:L:60:LYS:HG3	3:L:62:ASP:OD1	2.17	0.45
1:e:150:GLU:OE2	1:e:151:VAL:HG23	2.17	0.45
1:e:300:LEU:HD12	2:k:330:THR:CG2	2.44	0.45
3:m:102:ILE:HG23	3:m:106:TRP:CE2	2.52	0.45
1:Z:130:GLU:HA	1:Z:133:ARG:NH2	2.32	0.45
1:d:210:ILE:CG2	2:j:193:ARG:HH22	2.19	0.45
2:l:327:TYR:HE1	2:l:331:MET:HG3	1.82	0.45
1:M:82:LYS:NZ	1:M:135:ASP:OD1	2.46	0.45
1:M:90:ASP:OD1	1:M:91:SER:N	2.48	0.45
1:M:134:LEU:HD12	1:M:138:ASP:HB3	1.99	0.45
1:P:207:ASP:OD2	1:P:208:VAL:N	2.50	0.45
3:W:52:ASN:O	3:W:53:GLY:C	2.58	0.45
3:X:44:ASP:C	3:X:61:LYS:HZ1	2.25	0.45
1:A:69:ILE:HG12	1:A:96:ARG:HE	1.82	0.45
2:B:264:TYR:O	2:B:267:GLU:HG3	2.17	0.45
3:H:48:GLU:HG3	3:H:87:LYS:HG2	1.98	0.45
3:I:102:ILE:HG23	3:I:106:TRP:CE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:123:ASN:OD1	2:i:124:TRP:N	2.48	0.45
2:k:202:ASP:O	2:k:206:THR:HG23	2.17	0.45
3:s:102:ILE:HG13	3:s:106:TRP:CD1	2.52	0.45
2:b:100:ILE:O	2:b:120:PRO:HB3	2.17	0.45
2:j:271:TYR:HA	2:j:274:GLU:CD	2.42	0.45
1:O:71:THR:HG22	1:O:94:LYS:CE	2.46	0.45
2:R:129:ILE:H	2:R:129:ILE:HG13	1.44	0.45
2:R:138:GLU:HA	2:R:166:ARG:HD2	1.98	0.45
3:U:60:LYS:NZ	3:U:64:ASN:HB3	2.31	0.45
3:U:92:PRO:HA	3:V:54:ARG:HH22	1.81	0.45
2:B:142:GLU:OE2	2:B:162:ASN:HB2	2.17	0.45
2:F:341:VAL:O	2:F:341:VAL:HG13	2.17	0.45
1:Y:70:GLN:OE1	1:Y:70:GLN:HA	2.17	0.45
3:m:34:TYR:CZ	3:m:38:LEU:HD21	2.52	0.45
3:m:92:PRO:HA	3:o:69:TYR:CE2	2.37	0.45
3:o:84:LYS:HG3	3:o:84:LYS:O	2.17	0.45
1:d:112:ILE:H	1:d:112:ILE:HG13	1.49	0.45
2:l:209:ARG:HG2	2:l:238:PHE:CD2	2.52	0.45
2:l:351:MET:HE1	2:N:351:MET:HB2	1.96	0.45
3:v:36:THR:HA	3:v:39:GLN:NE2	2.32	0.45
2:S:92:TRP:NE1	2:S:126:PRO:HG3	2.32	0.45
2:S:95:SER:HB3	2:S:127:THR:N	2.32	0.45
2:B:195:VAL:HG12	2:B:215:ASP:OD2	2.18	0.44
3:I:36:THR:O	3:I:40:GLU:HG3	2.17	0.44
1:c:82:LYS:HB2	1:c:83:GLU:OE1	2.17	0.44
1:c:231:ARG:HD3	2:i:251:PHE:HD1	1.82	0.44
2:i:193:ARG:HA	2:i:196:ILE:HG22	1.98	0.44
3:v:35:SER:O	3:v:39:GLN:OE1	2.35	0.44
2:N:112:GLY:O	2:N:113:LYS:HD3	2.17	0.44
2:N:213:ARG:HD2	2:N:236:VAL:O	2.17	0.44
3:Q:91:GLU:O	3:T:54:ARG:NH1	2.50	0.44
1:D:315:VAL:HG22	2:a:343:VAL:HA	1.98	0.44
3:E:108:PRO:HA	3:K:106:TRP:CZ3	2.52	0.44
3:J:46:VAL:HA	3:J:60:LYS:HA	1.98	0.44
3:J:49:ALA:O	3:J:88:VAL:HA	2.18	0.44
1:Y:316:MET:HB3	1:Y:316:MET:HE3	1.72	0.44
1:c:90:ASP:O	1:c:210:ILE:HG13	2.16	0.44
1:e:117:VAL:O	1:e:120:LYS:HG3	2.17	0.44
1:e:144:ARG:O	1:e:149:LEU:HD23	2.17	0.44
2:k:98:TYR:CE1	2:k:125:LYS:HG3	2.51	0.44
2:k:269:GLU:OE2	2:k:273:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:50:ARG:HH21	3:o:89:VAL:N	2.16	0.44
1:d:130:GLU:HA	1:d:133:ARG:NH2	2.32	0.44
2:N:351:MET:HG2	2:R:351:MET:HB2	1.99	0.44
1:O:243:GLN:O	1:O:247:GLU:OE1	2.33	0.44
1:P:95:TRP:HA	1:P:205:VAL:HA	1.99	0.44
2:R:208:GLY:O	2:R:211:VAL:HG12	2.17	0.44
2:S:110:ARG:HB2	2:S:130:ASP:OD1	2.18	0.44
2:S:255:ILE:HG23	2:S:258:ARG:NH1	2.32	0.44
3:X:48:GLU:HA	3:X:87:LYS:O	2.18	0.44
1:C:243:GLN:O	1:C:247:GLU:OE1	2.35	0.44
3:L:46:VAL:N	3:L:61:LYS:HZ3	2.15	0.44
1:Y:85:LYS:HD3	2:i:255:ILE:HG23	2.00	0.44
2:a:321:ILE:H	2:a:321:ILE:HG12	1.69	0.44
1:Z:197:SER:OG	1:Z:200:ALA:N	2.39	0.44
3:n:100:ALA:O	3:n:104:ILE:HG12	2.18	0.44
3:v:35:SER:O	3:v:38:LEU:HB2	2.17	0.44
3:v:36:THR:HA	3:v:39:GLN:CD	2.42	0.44
1:C:143:SER:HB3	1:C:146:ARG:HH21	1.82	0.44
1:C:257:VAL:HG13	2:F:279:ALA:CB	2.48	0.44
1:D:58:PHE:CG	1:D:59:ILE:N	2.85	0.44
3:J:43:ASN:HB3	3:J:45:GLN:HE22	1.83	0.44
3:L:48:GLU:HA	3:L:87:LYS:O	2.18	0.44
2:a:185:ARG:HG3	2:a:185:ARG:NH1	2.33	0.44
1:e:77:ASP:OD1	1:e:77:ASP:N	2.50	0.44
3:u:54:ARG:NH1	3:u:69:TYR:HB3	2.32	0.44
1:d:82:LYS:HZ3	1:d:134:LEU:C	2.26	0.44
1:d:126:ARG:NE	1:d:126:ARG:HA	2.32	0.44
1:f:128:ARG:HH12	2:N:213:ARG:NE	2.10	0.44
3:h:92:PRO:HB3	3:n:69:TYR:CZ	2.53	0.44
1:M:70:GLN:HA	1:M:70:GLN:OE1	2.18	0.44
1:M:321:ASP:OD2	1:O:328:THR:OG1	2.35	0.44
1:P:104:TYR:O	1:P:105:LEU:HB2	2.17	0.44
2:R:173:TYR:CE1	2:R:180:PRO:HG2	2.53	0.44
2:B:193:ARG:HA	2:B:196:ILE:HG22	1.98	0.44
1:C:253:ALA:O	1:C:257:VAL:HG23	2.17	0.44
1:D:64:MET:O	1:D:65:LEU:C	2.61	0.44
3:I:62:ASP:C	3:I:64:ASN:H	2.24	0.44
3:J:45:GLN:O	3:J:60:LYS:HB2	2.18	0.44
2:a:311:LEU:O	2:a:314:GLU:HG3	2.18	0.44
1:e:39:ARG:HB2	1:e:45:PRO:HD2	2.00	0.44
2:i:173:TYR:CE1	2:i:180:PRO:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:126:ARG:O	1:d:129:SER:OG	2.27	0.44
2:l:195:VAL:HG23	2:l:215:ASP:OD2	2.17	0.44
3:r:51:ILE:HG12	3:r:56:ILE:HG23	2.00	0.44
3:r:92:PRO:HD3	3:v:69:TYR:CD2	2.52	0.44
3:v:37:PHE:HA	3:v:40:GLU:HG2	1.98	0.44
3:v:54:ARG:NH2	3:v:70:ILE:O	2.49	0.44
1:M:252:THR:O	1:M:256:GLU:HG2	2.18	0.44
2:N:112:GLY:C	2:N:113:LYS:HD3	2.42	0.44
1:O:25:GLU:HB3	2:R:175:TYR:OH	2.16	0.44
2:R:312:LEU:HB3	2:R:313:PRO:HD3	2.00	0.44
3:V:60:LYS:NZ	3:V:66:TYR:HD1	2.15	0.44
1:A:143:SER:HA	1:A:147:LEU:HD12	1.98	0.44
1:A:316:MET:HE2	1:A:323:PHE:HE1	1.82	0.44
2:B:221:GLU:OE1	2:B:233:LEU:HD12	2.18	0.44
1:C:86:ASP:OD1	1:C:86:ASP:N	2.45	0.44
3:J:51:ILE:HG13	3:J:56:ILE:HG12	2.00	0.44
1:Y:136:VAL:O	1:Y:139:ILE:HG22	2.18	0.44
1:e:144:ARG:HD2	1:e:209:ARG:NH1	2.33	0.44
3:o:50:ARG:NH2	3:o:89:VAL:HB	2.32	0.44
2:b:275:VAL:HA	2:b:278:ARG:NH1	2.24	0.44
3:h:37:PHE:O	3:h:41:VAL:HG23	2.17	0.44
3:p:93:PRO:HD3	3:r:69:TYR:CE1	2.53	0.44
1:M:33:ARG:HA	1:M:60:GLU:HB3	2.00	0.44
1:M:134:LEU:HD23	1:M:134:LEU:H	1.83	0.44
1:P:72:MET:SD	1:P:116:GLU:HG3	2.57	0.44
3:X:32:VAL:O	3:X:68:THR:HB	2.18	0.44
1:A:123:PHE:HE1	1:A:208:VAL:HG21	1.81	0.44
2:B:249:ALA:C	2:B:251:PHE:H	2.25	0.44
1:D:128:ARG:HH12	2:a:213:ARG:NH1	2.15	0.44
3:I:47:ARG:CD	3:I:61:LYS:HG3	2.48	0.44
1:Y:90:ASP:OD1	1:Y:91:SER:N	2.49	0.44
2:i:105:ARG:HB2	2:i:137:VAL:HG21	2.00	0.44
2:i:242:ARG:C	2:i:244:PRO:HD3	2.42	0.44
2:b:96:GLY:HA2	2:b:127:THR:O	2.18	0.44
2:b:169:ASN:OD1	2:b:171:GLU:HG3	2.18	0.44
1:d:92:TYR:CE2	1:d:209:ARG:HB2	2.53	0.44
1:f:102:ARG:O	1:f:106:ALA:CB	2.64	0.44
2:j:185:ARG:O	2:j:188:THR:HG22	2.18	0.44
2:l:213:ARG:HG2	2:l:213:ARG:HH11	1.83	0.44
3:X:46:VAL:N	3:X:61:LYS:HZ3	2.16	0.44
2:B:113:LYS:HA	2:B:113:LYS:HD3	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:80:ASN:O	3:J:83:THR:OG1	2.25	0.44
1:Y:33:ARG:HA	1:Y:60:GLU:HB3	2.00	0.44
1:c:18:MET:C	1:c:55:LYS:HE3	2.43	0.44
2:i:152:SER:OG	2:i:153:ASP:N	2.51	0.44
3:q:37:PHE:HA	3:q:40:GLU:CD	2.42	0.44
3:n:52:ASN:O	3:n:53:GLY:C	2.58	0.44
3:p:42:ASN:OD1	3:p:43:ASN:N	2.51	0.44
3:V:72:VAL:HG22	3:V:73:GLN:H	1.83	0.44
1:A:90:ASP:OD1	1:A:91:SER:N	2.51	0.44
1:A:245:GLU:OE1	2:B:265:ILE:HD12	2.17	0.44
1:A:316:MET:HE3	1:A:316:MET:HB3	1.74	0.44
2:F:310:LYS:HE3	2:F:310:LYS:HB2	1.52	0.44
2:G:255:ILE:HG23	2:G:258:ARG:NH1	2.33	0.44
3:L:44:ASP:C	3:L:61:LYS:HZ1	2.26	0.44
2:a:194:GLY:O	2:a:198:LYS:NZ	2.50	0.44
1:e:266:ARG:O	1:e:270:ILE:HG12	2.18	0.44
2:i:185:ARG:NH2	3:m:45:GLN:OE1	2.51	0.44
2:k:200:THR:HG23	2:k:203:ARG:HB3	2.00	0.44
3:m:74:ASP:OD2	3:m:76:LYS:N	2.51	0.44
3:u:91:GLU:HG2	3:u:92:PRO:HD2	2.00	0.44
1:d:136:VAL:O	1:d:140:VAL:HG23	2.17	0.44
1:f:224:TYR:HE2	2:l:156:VAL:HG21	1.82	0.44
2:j:271:TYR:HA	2:j:274:GLU:OE2	2.18	0.44
2:j:343:VAL:HG12	2:j:344:ASN:O	2.18	0.44
3:t:47:ARG:HE	3:t:61:LYS:HA	1.83	0.44
1:P:254:ASP:O	1:P:257:VAL:HG12	2.18	0.44
2:R:343:VAL:HG12	2:R:344:ASN:O	2.18	0.44
3:U:51:ILE:HB	3:U:90:GLY:HA3	2.00	0.44
1:A:34:PHE:CE2	2:F:122:LEU:HG	2.53	0.43
1:A:84:LYS:NZ	2:F:205:LEU:HD23	2.33	0.43
1:C:199:ALA:O	1:C:201:LEU:O	2.35	0.43
1:Y:252:THR:O	1:Y:256:GLU:HG2	2.18	0.43
1:c:126:ARG:NE	1:c:126:ARG:HA	2.32	0.43
1:e:18:MET:HG3	1:e:57:PRO:HB3	2.00	0.43
1:e:28:ARG:NH2	1:e:48:TYR:HA	2.34	0.43
1:Z:15:VAL:O	1:Z:19:SER:HB2	2.17	0.43
1:Z:85:LYS:HD3	2:j:255:ILE:HD12	1.98	0.43
2:b:230:GLY:C	2:b:231:ILE:HD12	2.43	0.43
2:j:109:THR:HG22	2:j:114:PHE:HA	1.99	0.43
3:n:74:ASP:OD1	3:n:76:LYS:N	2.51	0.43
2:S:327:TYR:HE1	2:S:331:MET:HG3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:GLU:CG	1:C:50:PRO:HD2	2.48	0.43
1:D:98:SER:N	1:D:202:GLY:O	2.37	0.43
1:D:220:SER:O	1:D:223:ILE:HG22	2.18	0.43
2:F:209:ARG:HD2	2:F:238:PHE:HE2	1.83	0.43
1:c:11:ILE:O	1:c:15:VAL:HG23	2.18	0.43
2:k:101:LYS:NZ	2:k:102:GLU:HG2	2.33	0.43
2:k:271:TYR:O	2:k:274:GLU:HG3	2.18	0.43
3:u:48:GLU:CB	3:u:87:LYS:HB3	2.48	0.43
1:Z:128:ARG:HG2	2:j:209:ARG:NH2	2.33	0.43
1:f:93:ILE:HG21	1:f:119:LEU:HD21	2.00	0.43
2:l:331:MET:SD	1:M:326:MET:HE2	2.58	0.43
1:M:15:VAL:O	1:M:19:SER:HB3	2.18	0.43
1:M:43:ASN:OD1	1:M:44:LYS:N	2.51	0.43
3:Q:62:ASP:HB3	2:S:143:LEU:HD21	2.01	0.43
2:R:149:MET:HE2	2:R:196:ILE:HG21	2.00	0.43
3:V:43:ASN:HB3	3:V:45:GLN:HE22	1.83	0.43
1:D:104:TYR:O	1:D:105:LEU:HB2	2.18	0.43
2:F:316:LYS:HD2	2:F:316:LYS:HA	1.81	0.43
2:F:346:LYS:H	2:F:346:LYS:HG3	1.46	0.43
2:G:165:TYR:HE1	2:G:184:LEU:CD2	2.25	0.43
2:G:278:ARG:HA	2:G:278:ARG:NE	2.34	0.43
2:a:101:LYS:HB2	2:a:101:LYS:HE2	1.83	0.43
2:a:149:MET:HE1	2:a:192:LEU:HG	2.00	0.43
2:a:169:ASN:ND2	2:a:172:LYS:HG2	2.33	0.43
1:e:31:THR:O	1:e:62:VAL:HG13	2.17	0.43
2:k:195:VAL:HG23	2:k:215:ASP:OD2	2.18	0.43
2:b:209:ARG:NH1	2:b:209:ARG:HB2	2.34	0.43
3:r:50:ARG:HH22	3:r:90:GLY:HA2	1.83	0.43
1:O:111:ASP:OD2	1:O:113:SER:N	2.46	0.43
1:P:88:ILE:HB	1:P:214:ASN:OD1	2.18	0.43
2:S:109:THR:OG1	2:S:113:LYS:N	2.51	0.43
1:D:68:ARG:HE	2:G:176:SER:C	2.26	0.43
2:k:158:ARG:HD3	2:k:242:ARG:CZ	2.48	0.43
2:k:200:THR:CG2	2:k:203:ARG:HB3	2.48	0.43
2:b:195:VAL:HG11	2:b:216:THR:CA	2.48	0.43
2:b:215:ASP:HA	2:b:218:ARG:HG2	2.00	0.43
3:h:30:ARG:O	3:h:30:ARG:HD2	2.18	0.43
2:j:105:ARG:NE	2:j:105:ARG:HA	2.33	0.43
2:j:152:SER:OG	2:j:153:ASP:N	2.51	0.43
2:N:283:ALA:O	2:N:286:ILE:HG22	2.18	0.43
3:T:52:ASN:O	3:T:53:GLY:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:ILE:O	1:C:15:VAL:HG23	2.18	0.43
3:H:34:TYR:CZ	3:H:38:LEU:HD11	2.54	0.43
3:K:32:VAL:HG22	3:K:33:ASP:N	2.33	0.43
3:K:37:PHE:HA	3:K:40:GLU:CD	2.43	0.43
2:i:100:ILE:HB	2:i:120:PRO:HA	2.00	0.43
2:i:205:LEU:HG	2:i:206:THR:HG23	1.99	0.43
3:u:72:VAL:HG12	3:u:73:GLN:N	2.33	0.43
1:Z:281:LYS:HB2	2:j:314:GLU:OE1	2.17	0.43
2:b:172:LYS:HE2	2:b:172:LYS:HB3	1.85	0.43
1:f:51:GLY:H	2:l:113:LYS:CE	2.31	0.43
1:f:254:ASP:O	1:f:257:VAL:HG12	2.18	0.43
2:j:201:MET:O	2:j:205:LEU:CD2	2.56	0.43
3:p:46:VAL:HG13	3:p:60:LYS:HA	2.00	0.43
2:N:92:TRP:HD1	2:N:128:PHE:CD1	2.37	0.43
1:O:298:ARG:HD2	1:O:298:ARG:HA	1.88	0.43
2:R:96:GLY:O	2:R:125:LYS:N	2.49	0.43
3:V:47:ARG:HH12	3:V:63:SER:H	1.67	0.43
3:X:72:VAL:HG22	3:X:73:GLN:H	1.83	0.43
2:B:94:ALA:HA	2:B:97:PHE:CD2	2.53	0.43
2:B:244:PRO:HG2	2:B:251:PHE:CZ	2.54	0.43
2:F:104:GLU:OE1	2:F:136:ASN:HA	2.19	0.43
2:b:110:ARG:HE	2:b:129:ILE:HG13	1.84	0.43
2:N:103:ALA:HA	2:N:120:PRO:HG2	2.01	0.43
2:R:127:THR:HB	2:R:129:ILE:HG13	2.01	0.43
3:V:37:PHE:O	3:V:40:GLU:HG3	2.18	0.43
3:W:34:TYR:HA	3:W:68:THR:HG21	2.01	0.43
1:A:43:ASN:OD1	1:A:44:LYS:N	2.50	0.43
1:A:252:THR:O	1:A:256:GLU:HG2	2.18	0.43
1:D:321:ASP:HB3	1:Y:328:THR:HG23	2.01	0.43
3:L:32:VAL:O	3:L:68:THR:HB	2.18	0.43
3:L:46:VAL:HA	3:L:60:LYS:HA	1.99	0.43
2:a:149:MET:HB2	2:a:196:ILE:HD13	2.01	0.43
1:e:64:MET:O	1:e:65:LEU:C	2.61	0.43
1:e:68:ARG:HH11	2:k:177:VAL:N	2.16	0.43
3:u:101:SER:O	3:u:104:ILE:HG22	2.18	0.43
2:j:243:PRO:HB2	2:j:251:PHE:HE2	1.84	0.43
3:p:46:VAL:HG13	3:p:59:THR:O	2.19	0.43
3:r:50:ARG:CZ	3:r:89:VAL:HG13	2.49	0.43
3:v:37:PHE:O	3:v:41:VAL:HG23	2.19	0.43
1:P:68:ARG:HE	2:S:176:SER:C	2.27	0.43
2:S:111:PHE:CE2	2:S:129:ILE:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:174:LEU:HD23	2:S:175:TYR:CE2	2.53	0.43
3:V:74:ASP:OD2	3:V:77:LEU:N	2.52	0.43
1:A:121:ARG:HD3	1:A:121:ARG:HA	1.83	0.43
1:A:297:ILE:O	1:A:298:ARG:HB3	2.19	0.43
3:L:72:VAL:HG22	3:L:73:GLN:H	1.83	0.43
1:c:102:ARG:HH12	1:c:201:LEU:C	2.26	0.43
1:e:15:VAL:O	1:e:18:MET:HB3	2.19	0.43
2:k:214:SER:O	2:k:218:ARG:HG3	2.19	0.43
2:k:320:GLU:HG2	2:k:321:ILE:N	2.34	0.43
1:Z:93:ILE:HD11	1:Z:123:PHE:CD1	2.53	0.43
1:Z:237:ARG:HD2	1:Z:237:ARG:C	2.43	0.43
1:d:40:ASP:H	1:d:44:LYS:HB2	1.83	0.43
1:f:266:ARG:HD3	2:N:299:LEU:HD22	2.01	0.43
1:f:324:ARG:NH1	1:f:325:TYR:CE1	2.87	0.43
3:v:39:GLN:HA	3:v:42:ASN:OD1	2.19	0.43
1:M:24:LYS:H	1:M:24:LYS:HG2	1.62	0.43
1:O:18:MET:C	1:O:55:LYS:HE3	2.43	0.43
1:P:89:VAL:HG12	1:P:90:ASP:N	2.34	0.43
3:U:55:GLU:HG3	3:U:69:TYR:HE2	1.82	0.43
3:V:49:ALA:O	3:V:88:VAL:HA	2.18	0.43
3:W:47:ARG:HE	3:W:61:LYS:HA	1.84	0.43
1:A:229:ALA:O	1:A:232:GLU:HG3	2.18	0.43
1:C:40:ASP:N	1:C:40:ASP:OD2	2.49	0.43
1:C:210:ILE:CG2	2:F:193:ARG:HH22	2.32	0.43
2:a:160:GLU:OE2	2:a:240:ALA:N	2.52	0.43
2:a:323:ARG:O	2:a:326:LEU:N	2.52	0.43
1:e:234:VAL:O	1:e:237:ARG:HG3	2.19	0.43
3:g:60:LYS:HE2	3:g:66:TYR:HE1	1.83	0.43
1:Z:123:PHE:CE1	1:Z:208:VAL:HG21	2.53	0.43
2:l:111:PHE:O	2:l:113:LYS:NZ	2.37	0.43
3:r:37:PHE:O	3:r:41:VAL:HG23	2.18	0.43
3:r:39:GLN:HA	3:r:42:ASN:OD1	2.18	0.43
1:M:137:LYS:O	1:M:141:THR:HG23	2.19	0.43
1:M:229:ALA:O	1:M:232:GLU:HG3	2.19	0.43
2:N:110:ARG:HA	2:N:110:ARG:HD2	1.72	0.43
3:W:63:SER:O	3:W:63:SER:OG	2.36	0.43
1:D:50:PRO:C	1:D:52:LEU:H	2.27	0.43
2:G:98:TYR:OH	2:G:125:LYS:HG2	2.19	0.43
3:I:59:THR:OG1	3:I:65:ARG:HG2	2.19	0.43
2:a:350:LEU:H	2:a:350:LEU:HG	1.69	0.43
1:e:211:LYS:HE3	2:k:189:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:136:ASN:O	2:i:136:ASN:CG	2.62	0.43
2:k:95:SER:HB2	2:k:127:THR:C	2.43	0.43
2:k:255:ILE:CD1	2:k:258:ARG:HH12	2.32	0.43
3:q:80:ASN:O	3:q:83:THR:OG1	2.30	0.43
1:d:90:ASP:O	1:d:210:ILE:HG13	2.18	0.43
3:h:34:TYR:OH	3:h:77:LEU:HD13	2.19	0.43
2:j:271:TYR:HA	2:j:274:GLU:HG2	2.00	0.43
2:l:108:VAL:HG23	2:l:132:VAL:HB	2.00	0.43
2:l:134:PRO:HG2	2:l:135:VAL:HG22	2.01	0.43
3:n:47:ARG:HB2	3:n:61:LYS:HE2	2.01	0.43
3:p:93:PRO:N	3:r:54:ARG:HH21	2.16	0.43
3:r:50:ARG:HH12	3:r:90:GLY:C	2.27	0.43
3:t:37:PHE:O	3:t:40:GLU:HG3	2.19	0.43
1:P:42:ASP:N	1:P:42:ASP:OD1	2.50	0.43
1:P:53:HIS:HE1	1:P:55:LYS:HG2	1.84	0.43
1:P:212:GLN:NE2	1:P:214:ASN:HB3	2.27	0.43
2:R:209:ARG:HA	2:R:212:ILE:HG22	2.01	0.43
1:D:150:GLU:OE2	1:D:151:VAL:HG23	2.19	0.42
2:F:127:THR:HG22	2:F:128:PHE:H	1.84	0.42
1:Y:137:LYS:NZ	2:a:154:GLU:OE2	2.38	0.42
2:a:276:GLN:HB3	2:a:277:PRO:HD3	2.01	0.42
1:e:59:ILE:HG22	1:e:61:THR:HG23	1.99	0.42
1:e:96:ARG:NH2	1:e:204:GLU:OE2	2.41	0.42
1:e:104:TYR:O	1:e:105:LEU:HB2	2.18	0.42
3:g:63:SER:HB2	2:k:137:VAL:HG11	2.00	0.42
3:g:88:VAL:HG23	3:m:34:TYR:HB3	2.01	0.42
2:i:92:TRP:HZ2	2:i:127:THR:HB	1.83	0.42
2:k:350:LEU:H	2:k:350:LEU:HG	1.53	0.42
1:Z:144:ARG:HG3	1:Z:145:GLY:N	2.34	0.42
1:Z:245:GLU:HA	1:Z:248:LYS:HB3	2.01	0.42
1:f:89:VAL:HG12	1:f:90:ASP:N	2.34	0.42
2:l:158:ARG:HD3	2:l:242:ARG:CZ	2.49	0.42
3:n:93:PRO:HB3	3:p:54:ARG:HH22	1.84	0.42
2:N:193:ARG:HA	2:N:196:ILE:HG22	2.00	0.42
1:O:32:LEU:HD11	1:O:61:THR:HG22	2.01	0.42
1:O:211:LYS:HB3	1:O:211:LYS:HE2	1.93	0.42
1:P:59:ILE:HG22	1:P:61:THR:HG23	2.01	0.42
1:P:315:VAL:HG12	2:S:341:VAL:HG13	2.01	0.42
2:S:195:VAL:HG23	2:S:215:ASP:OD2	2.19	0.42
1:A:82:LYS:NZ	1:A:135:ASP:OD1	2.46	0.42
2:F:143:LEU:HD22	2:F:165:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:145:ALA:HB3	2:F:161:MET:HB3	2.01	0.42
1:e:126:ARG:NE	1:e:126:ARG:HA	2.34	0.42
1:e:307:PHE:CD2	2:b:340:LYS:HE2	2.54	0.42
2:i:138:GLU:HG3	2:i:138:GLU:O	2.19	0.42
2:i:331:MET:HA	2:i:334:VAL:HG22	2.01	0.42
2:k:165:TYR:CE1	2:k:233:LEU:HD13	2.51	0.42
2:S:158:ARG:HD3	2:S:242:ARG:CZ	2.49	0.42
3:E:98:LEU:O	3:E:102:ILE:HG12	2.19	0.42
2:F:109:THR:HB	2:F:113:LYS:O	2.19	0.42
3:H:102:ILE:HA	3:I:104:ILE:HD13	2.01	0.42
1:e:226:ARG:NH2	2:k:155:ASN:OD1	2.52	0.42
2:i:142:GLU:OE1	3:m:61:LYS:NZ	2.26	0.42
2:k:184:LEU:HD23	2:k:184:LEU:C	2.44	0.42
3:u:30:ARG:O	3:u:30:ARG:HG2	2.19	0.42
1:Z:121:ARG:HD3	1:Z:121:ARG:HA	1.77	0.42
1:Z:208:VAL:O	1:Z:209:ARG:HD2	2.19	0.42
2:b:311:LEU:O	2:b:314:GLU:HG3	2.18	0.42
1:f:144:ARG:HH12	1:f:209:ARG:HB3	1.83	0.42
1:O:144:ARG:O	1:O:148:THR:HG22	2.20	0.42
3:Q:60:LYS:NZ	3:Q:66:TYR:HE1	2.17	0.42
3:T:74:ASP:OD2	3:T:76:LYS:N	2.52	0.42
2:B:107:VAL:O	2:B:133:LYS:N	2.36	0.42
2:B:215:ASP:OD1	2:B:218:ARG:NH1	2.52	0.42
1:C:130:GLU:O	1:C:133:ARG:HG2	2.20	0.42
1:C:147:LEU:HD12	1:C:208:VAL:HG23	2.00	0.42
1:D:207:ASP:OD2	1:D:208:VAL:N	2.53	0.42
2:G:320:GLU:HG2	2:G:321:ILE:N	2.34	0.42
3:J:52:ASN:ND2	3:J:91:GLU:OE2	2.52	0.42
1:Y:300:LEU:HD23	2:a:330:THR:HG21	2.00	0.42
2:a:103:ALA:HB1	2:a:120:PRO:HG2	1.99	0.42
2:a:193:ARG:HA	2:a:196:ILE:HG22	2.01	0.42
1:c:136:VAL:O	1:c:140:VAL:HG23	2.20	0.42
1:c:231:ARG:HD3	2:i:251:PHE:CD1	2.54	0.42
1:e:226:ARG:HD2	1:e:227:MET:N	2.34	0.42
3:s:36:THR:O	3:s:39:GLN:HB3	2.20	0.42
3:u:41:VAL:HG12	3:u:84:LYS:HE3	2.01	0.42
2:N:169:ASN:OD1	2:N:171:GLU:HG3	2.19	0.42
2:S:110:ARG:HH21	2:S:130:ASP:N	2.14	0.42
1:A:36:LYS:O	1:A:37:VAL:C	2.55	0.42
2:F:177:VAL:HG22	2:F:178:THR:N	2.33	0.42
2:F:351:MET:HG3	2:F:352:VAL:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:52:ASN:O	3:H:53:GLY:C	2.60	0.42
3:J:92:PRO:HD3	3:L:69:TYR:CE2	2.54	0.42
1:Y:34:PHE:HZ	2:i:122:LEU:HG	1.84	0.42
1:c:137:LYS:O	1:c:141:THR:HG23	2.20	0.42
3:g:59:THR:HG22	3:g:65:ARG:HD3	2.01	0.42
2:i:119:GLU:HB3	2:i:120:PRO:HD2	2.02	0.42
3:u:47:ARG:NH2	3:u:63:SER:H	2.13	0.42
1:Z:314:MET:HE2	1:Z:316:MET:SD	2.60	0.42
2:b:193:ARG:HA	2:b:196:ILE:HG22	2.01	0.42
1:d:23:VAL:HB	1:d:50:PRO:HA	2.01	0.42
3:Q:102:ILE:O	3:Q:106:TRP:HB2	2.19	0.42
3:V:48:GLU:HG2	3:V:87:LYS:O	2.19	0.42
3:X:50:ARG:NH1	3:X:91:GLU:HB2	2.34	0.42
2:F:208:GLY:O	2:F:211:VAL:HG12	2.20	0.42
3:J:54:ARG:HB2	3:J:70:ILE:HG22	2.02	0.42
3:K:32:VAL:HG11	3:K:66:TYR:HD2	1.81	0.42
1:Y:43:ASN:OD1	1:Y:44:LYS:N	2.51	0.42
2:k:108:VAL:HA	2:k:132:VAL:HA	2.02	0.42
3:o:89:VAL:HG22	3:q:33:ASP:CB	2.49	0.42
3:u:45:GLN:O	3:u:60:LYS:HG2	2.19	0.42
3:u:58:VAL:N	3:u:66:TYR:O	2.52	0.42
1:Z:90:ASP:OD1	1:Z:91:SER:N	2.51	0.42
1:d:102:ARG:HH12	1:d:201:LEU:C	2.24	0.42
1:d:314:MET:CE	1:d:316:MET:HE3	2.49	0.42
2:l:153:ASP:OD2	2:l:200:THR:OG1	2.22	0.42
1:M:92:TYR:CE1	1:M:209:ARG:HB2	2.54	0.42
1:M:125:ASP:OD2	2:R:237:ASN:ND2	2.53	0.42
1:M:130:GLU:OE2	1:M:146:ARG:NH1	2.53	0.42
3:V:60:LYS:HE2	3:V:60:LYS:HB2	1.87	0.42
2:B:341:VAL:HG22	1:P:313:VAL:HG22	2.01	0.42
1:D:215:LEU:HB3	1:D:216:PRO:HD2	2.02	0.42
2:G:122:LEU:HD23	2:G:122:LEU:H	1.85	0.42
1:e:34:PHE:HB3	1:e:39:ARG:NE	2.35	0.42
2:i:97:PHE:CD1	2:i:124:TRP:HB2	2.54	0.42
2:k:109:THR:HG1	2:k:113:LYS:H	1.68	0.42
2:k:119:GLU:HB3	2:k:120:PRO:HD2	2.02	0.42
3:m:60:LYS:HE2	3:m:66:TYR:HE1	1.84	0.42
2:b:122:LEU:HD12	2:b:124:TRP:CZ2	2.54	0.42
2:b:211:VAL:HG13	2:b:212:ILE:HG23	2.02	0.42
1:f:44:LYS:HA	1:f:44:LYS:HD3	1.66	0.42
3:t:101:SER:HA	3:t:104:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:45:GLN:O	3:T:60:LYS:HB2	2.20	0.42
3:U:64:ASN:OD1	3:U:65:ARG:N	2.52	0.42
2:B:110:ARG:HD3	2:B:130:ASP:CA	2.46	0.42
1:C:123:PHE:CZ	1:C:127:LEU:HD12	2.55	0.42
1:D:33:ARG:HG3	1:D:33:ARG:O	2.19	0.42
2:F:101:LYS:O	2:F:103:ALA:N	2.53	0.42
1:Y:21:PHE:HZ	1:Y:51:GLY:O	2.02	0.42
2:a:108:VAL:O	2:a:115:SER:HB3	2.20	0.42
1:c:243:GLN:O	1:c:246:ALA:HB3	2.20	0.42
1:e:119:LEU:HD12	1:e:120:LYS:N	2.35	0.42
2:k:164:GLN:N	2:k:164:GLN:OE1	2.53	0.42
1:d:201:LEU:O	1:d:201:LEU:HD23	2.19	0.42
2:j:316:LYS:HA	2:j:316:LYS:HD2	1.81	0.42
3:n:29:GLY:O	3:n:31:LYS:HD2	2.20	0.42
3:r:98:LEU:O	3:r:101:SER:OG	2.25	0.42
3:t:99:LEU:HA	3:t:102:ILE:HD13	2.01	0.42
1:M:56:ILE:H	1:M:56:ILE:HD12	1.85	0.42
2:N:263:GLN:HA	2:N:266:ARG:NH1	2.34	0.42
2:R:177:VAL:HG22	2:R:178:THR:N	2.34	0.42
2:R:203:ARG:HG2	2:R:203:ARG:HH11	1.85	0.42
2:R:341:VAL:HG13	2:R:341:VAL:O	2.19	0.42
3:V:34:TYR:O	3:V:37:PHE:HB3	2.19	0.42
3:W:54:ARG:NH2	3:W:70:ILE:HG13	2.35	0.42
1:D:83:GLU:HG3	1:D:83:GLU:O	2.20	0.42
2:F:310:LYS:C	2:F:313:PRO:HD2	2.45	0.42
2:G:160:GLU:HG2	2:G:239:GLN:HE21	1.85	0.42
1:e:30:ILE:CD1	1:e:100:PHE:HB3	2.49	0.42
1:e:113:SER:HA	1:e:116:GLU:CD	2.45	0.42
2:k:126:PRO:O	2:k:127:THR:OG1	2.32	0.42
2:k:255:ILE:HG23	2:k:258:ARG:NH1	2.35	0.42
3:o:52:ASN:HB3	3:o:91:GLU:HB2	2.02	0.42
1:Z:32:LEU:HD13	1:Z:37:VAL:HG12	2.01	0.42
3:t:65:ARG:NH1	3:t:65:ARG:HG3	2.35	0.42
1:M:123:PHE:CE1	1:M:208:VAL:HG21	2.55	0.42
1:O:255:TYR:HE1	2:S:292:ALA:HA	1.85	0.42
2:R:108:VAL:HG22	2:R:132:VAL:HG23	2.01	0.42
2:S:164:GLN:HE22	2:S:235:ASP:HB3	1.85	0.42
2:S:209:ARG:HG2	2:S:238:PHE:CD2	2.55	0.42
1:C:49:GLU:HG3	1:C:50:PRO:HD2	2.02	0.42
1:C:237:ARG:HD2	1:C:241:GLN:OE1	2.20	0.42
1:D:111:ASP:OD2	1:D:113:SER:OG	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:138:GLU:HG3	2:F:138:GLU:O	2.20	0.42
3:L:103:PHE:O	3:L:107:PHE:N	2.53	0.42
1:c:105:LEU:HD23	1:c:105:LEU:HA	1.88	0.42
1:Z:40:ASP:CG	1:Z:41:ASP:H	2.28	0.42
1:f:37:VAL:HG22	1:f:38:LEU:N	2.35	0.42
3:h:33:ASP:O	3:h:36:THR:OG1	2.34	0.42
3:p:93:PRO:CD	3:r:54:ARG:HH21	2.33	0.42
2:N:92:TRP:CD2	2:N:126:PRO:O	2.73	0.42
1:O:21:PHE:CZ	1:O:52:LEU:HG	2.55	0.42
2:R:158:ARG:NE	2:R:246:GLU:OE2	2.53	0.42
2:B:230:GLY:C	2:B:231:ILE:HD12	2.44	0.41
1:D:271:MET:SD	2:G:291:ARG:HB2	2.60	0.41
3:K:34:TYR:O	3:K:37:PHE:HB3	2.19	0.41
1:c:317:SER:HB3	2:i:345:ASP:HB3	2.01	0.41
3:u:37:PHE:O	3:u:41:VAL:HG23	2.19	0.41
1:Z:144:ARG:HD3	1:Z:209:ARG:NH2	2.35	0.41
2:b:158:ARG:HB2	2:b:242:ARG:O	2.19	0.41
2:l:99:THR:HG22	2:l:122:LEU:HB3	2.01	0.41
2:N:137:VAL:HG12	2:N:139:ALA:H	1.84	0.41
1:P:68:ARG:HH11	2:S:177:VAL:N	2.18	0.41
1:C:32:LEU:HD13	1:C:35:GLY:H	1.85	0.41
3:H:74:ASP:OD1	3:H:76:LYS:N	2.54	0.41
3:K:42:ASN:HA	3:K:84:LYS:HZ3	1.86	0.41
1:Y:33:ARG:HA	1:Y:60:GLU:CB	2.49	0.41
1:c:135:ASP:O	1:c:139:ILE:HG12	2.20	0.41
2:i:145:ALA:HB3	2:i:161:MET:HB3	2.03	0.41
3:o:99:LEU:HD23	3:o:103:PHE:CE1	2.56	0.41
3:q:48:GLU:HA	3:q:87:LYS:HB3	2.01	0.41
1:d:137:LYS:O	1:d:141:THR:HG23	2.21	0.41
1:f:126:ARG:HE	1:f:154:ALA:HB3	1.83	0.41
2:j:203:ARG:HG2	2:j:203:ARG:HH11	1.85	0.41
2:j:203:ARG:NH1	2:j:207:GLU:OE1	2.36	0.41
2:l:164:GLN:OE1	2:l:164:GLN:N	2.53	0.41
2:l:187:ALA:O	2:l:190:SER:OG	2.31	0.41
2:l:215:ASP:O	2:l:218:ARG:HG2	2.20	0.41
3:r:48:GLU:HG3	3:r:59:THR:HG21	2.02	0.41
3:v:41:VAL:HG12	3:v:84:LYS:HE3	2.01	0.41
2:N:217:GLN:OE1	2:N:236:VAL:N	2.53	0.41
1:O:259:ARG:HG2	1:O:259:ARG:HH11	1.85	0.41
3:X:32:VAL:HB	3:X:66:TYR:CE2	2.55	0.41
2:B:112:GLY:C	2:B:113:LYS:HD3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:113:LYS:HA	2:G:113:LYS:HD3	1.87	0.41
3:J:50:ARG:HD2	3:J:57:ASN:ND2	2.33	0.41
3:L:50:ARG:NH1	3:L:91:GLU:HB2	2.34	0.41
1:Y:229:ALA:O	1:Y:232:GLU:HG3	2.20	0.41
1:c:239:ARG:NH1	2:i:260:ASN:HD22	2.17	0.41
1:c:296:PHE:CG	2:i:323:ARG:NH1	2.89	0.41
2:b:238:PHE:CE2	2:b:241:ALA:HB2	2.55	0.41
3:p:106:TRP:NE1	3:r:108:PRO:HB3	2.35	0.41
3:r:34:TYR:CE1	3:r:70:ILE:HD13	2.55	0.41
3:v:47:ARG:HH11	3:v:61:LYS:N	2.10	0.41
1:M:93:ILE:HD11	1:M:123:PHE:CD1	2.55	0.41
2:N:198:LYS:HB2	2:N:198:LYS:HE2	1.70	0.41
1:O:240:SER:O	1:O:243:GLN:HG3	2.21	0.41
3:T:60:LYS:HG3	3:T:62:ASP:OD1	2.19	0.41
3:X:37:PHE:O	3:X:41:VAL:HG23	2.20	0.41
3:L:32:VAL:HB	3:L:66:TYR:CE2	2.55	0.41
3:L:45:GLN:C	3:L:61:LYS:HZ3	2.29	0.41
1:c:25:GLU:H	1:c:25:GLU:HG2	1.30	0.41
1:c:93:ILE:HD12	1:c:208:VAL:HG12	2.02	0.41
1:c:303:TYR:OH	1:e:323:PHE:HA	2.20	0.41
3:g:93:PRO:N	3:m:54:ARG:HH22	2.18	0.41
1:d:33:ARG:NH1	1:d:60:GLU:HB2	2.35	0.41
3:h:60:LYS:HB2	3:h:62:ASP:OD1	2.20	0.41
2:l:105:ARG:HH21	2:l:117:LEU:HD11	1.84	0.41
2:l:209:ARG:HG2	2:l:238:PHE:CE2	2.55	0.41
3:v:52:ASN:OD1	3:v:55:GLU:HB3	2.20	0.41
1:O:243:GLN:NE2	2:S:277:PRO:HB2	2.35	0.41
2:S:186:GLN:HA	2:S:189:ASP:OD2	2.20	0.41
2:S:255:ILE:HA	2:S:258:ARG:HH22	1.86	0.41
3:U:82:LEU:O	3:U:85:ASN:ND2	2.52	0.41
3:V:72:VAL:HG22	3:V:73:GLN:N	2.36	0.41
3:V:93:PRO:HB3	3:X:54:ARG:HH21	1.83	0.41
1:A:120:LYS:HA	1:A:120:LYS:HD3	1.91	0.41
1:A:281:LYS:HB2	2:F:314:GLU:OE1	2.21	0.41
1:A:326:MET:HE3	1:A:326:MET:HB2	1.84	0.41
2:B:108:VAL:HB	2:B:115:SER:HB3	2.01	0.41
2:B:123:ASN:O	2:B:125:LYS:HG2	2.20	0.41
2:B:162:ASN:OD1	2:B:162:ASN:N	2.54	0.41
1:C:18:MET:C	1:C:55:LYS:HE3	2.45	0.41
3:L:46:VAL:C	3:L:61:LYS:HG3	2.46	0.41
3:L:50:ARG:HH21	3:L:57:ASN:ND2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:47:VAL:HG12	1:c:49:GLU:H	1.86	0.41
1:e:144:ARG:HH12	1:e:209:ARG:HB3	1.85	0.41
3:q:35:SER:O	3:q:39:GLN:HG2	2.21	0.41
3:q:45:GLN:HB3	3:q:61:LYS:HG3	2.03	0.41
1:Z:197:SER:HG	1:Z:200:ALA:H	1.63	0.41
2:b:195:VAL:HG11	2:b:216:THR:HA	2.01	0.41
1:f:248:LYS:HD3	2:N:284:GLN:HG2	2.02	0.41
1:f:257:VAL:HG23	2:l:279:ALA:CB	2.49	0.41
3:r:48:GLU:O	3:r:59:THR:HB	2.20	0.41
3:W:40:GLU:OE2	3:W:45:GLN:HB2	2.20	0.41
3:X:46:VAL:C	3:X:61:LYS:HG3	2.46	0.41
2:B:233:LEU:HD23	2:B:233:LEU:HA	1.90	0.41
2:B:327:TYR:O	2:B:330:THR:HG22	2.20	0.41
1:D:42:ASP:OD1	1:D:42:ASP:N	2.53	0.41
3:H:38:LEU:HD23	3:H:38:LEU:HA	1.87	0.41
3:I:47:ARG:HD2	3:I:61:LYS:HG3	2.02	0.41
3:J:50:ARG:NH1	3:J:52:ASN:HB2	2.36	0.41
1:Y:82:LYS:C	1:Y:84:LYS:H	2.27	0.41
1:Y:143:SER:O	1:Y:147:LEU:HB2	2.19	0.41
1:Y:248:LYS:CD	2:i:284:GLN:HG2	2.50	0.41
1:c:82:LYS:HG3	1:c:134:LEU:O	2.20	0.41
1:c:96:ARG:HB3	1:c:204:GLU:HG3	2.02	0.41
2:i:109:THR:HB	2:i:113:LYS:O	2.21	0.41
2:k:164:GLN:NE2	2:k:235:ASP:HB3	2.36	0.41
1:Z:248:LYS:CD	2:j:284:GLN:HG2	2.50	0.41
3:n:84:LYS:HG3	3:n:84:LYS:O	2.20	0.41
1:M:281:LYS:HB2	2:R:314:GLU:OE1	2.20	0.41
2:N:107:VAL:HB	2:N:133:LYS:HB3	2.02	0.41
1:P:113:SER:HA	1:P:116:GLU:CD	2.46	0.41
3:W:81:LEU:O	3:W:86:VAL:HG22	2.20	0.41
1:A:144:ARG:HA	1:A:148:THR:HG23	2.02	0.41
1:C:121:ARG:NH1	2:G:235:ASP:OD1	2.53	0.41
1:D:296:PHE:CE2	2:G:323:ARG:HG3	2.55	0.41
2:G:351:MET:H	2:G:351:MET:HG3	1.81	0.41
3:J:63:SER:HA	3:J:65:ARG:HH12	1.85	0.41
1:Y:139:ILE:HG23	1:Y:140:VAL:HG13	2.02	0.41
1:c:321:ASP:OD2	1:e:328:THR:N	2.53	0.41
2:i:136:ASN:OD1	2:i:136:ASN:C	2.63	0.41
2:k:153:ASP:OD2	2:k:200:THR:OG1	2.24	0.41
3:u:30:ARG:HE	3:u:66:TYR:HA	1.86	0.41
3:u:56:ILE:HD11	3:u:70:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:166:ARG:HB2	2:b:234:LEU:HD21	2.02	0.41
1:d:148:THR:HA	1:d:151:VAL:HG12	2.01	0.41
1:f:18:MET:HA	1:f:55:LYS:HZ2	1.85	0.41
1:f:77:ASP:OD1	1:f:77:ASP:N	2.54	0.41
2:l:133:LYS:HG2	2:l:134:PRO:HD2	2.02	0.41
2:l:351:MET:HE2	2:N:350:LEU:O	2.21	0.41
1:C:287:PHE:CE2	1:C:294:TYR:CE1	3.08	0.41
3:I:106:TRP:CD1	3:I:106:TRP:N	2.88	0.41
3:J:40:GLU:OE2	3:J:45:GLN:HB2	2.21	0.41
2:a:136:ASN:N	2:a:136:ASN:OD1	2.54	0.41
2:i:331:MET:HE3	2:i:335:LEU:HD23	2.03	0.41
2:k:95:SER:HB2	2:k:127:THR:O	2.20	0.41
2:k:165:TYR:HE2	2:k:184:LEU:HD22	1.84	0.41
3:u:55:GLU:HA	3:u:69:TYR:HA	2.03	0.41
1:Z:92:TYR:CD1	2:b:186:GLN:NE2	2.89	0.41
2:b:149:MET:HE1	2:b:192:LEU:HG	2.02	0.41
2:b:205:LEU:HD23	2:b:243:PRO:HB2	2.03	0.41
1:d:40:ASP:OD2	1:d:40:ASP:N	2.53	0.41
1:f:39:ARG:HE	1:f:40:ASP:N	2.18	0.41
1:f:254:ASP:HA	1:f:257:VAL:HG12	2.03	0.41
2:l:320:GLU:HG2	2:l:321:ILE:N	2.36	0.41
3:n:54:ARG:H	3:n:54:ARG:HG3	1.74	0.41
1:P:215:LEU:HB3	1:P:216:PRO:HD2	2.02	0.41
2:R:213:ARG:HD3	2:R:236:VAL:HG23	2.03	0.41
3:U:44:ASP:HB2	3:U:84:LYS:HD2	2.03	0.41
3:X:103:PHE:O	3:X:107:PHE:N	2.53	0.41
1:A:231:ARG:HH12	2:B:251:PHE:HD2	1.69	0.41
2:B:104:GLU:H	2:B:120:PRO:HG3	1.86	0.41
1:C:19:SER:HA	1:C:55:LYS:HE3	2.03	0.41
1:C:136:VAL:O	1:C:140:VAL:HG23	2.21	0.41
3:E:89:VAL:HG22	3:H:33:ASP:OD1	2.20	0.41
2:G:344:ASN:OD1	2:G:345:ASP:N	2.54	0.41
3:K:55:GLU:HA	3:K:69:TYR:CD1	2.56	0.41
2:a:198:LYS:HE2	2:a:198:LYS:HB2	1.71	0.41
2:a:213:ARG:NH2	2:a:237:ASN:HA	2.25	0.41
1:c:143:SER:HB3	1:c:147:LEU:HD23	2.03	0.41
1:e:48:TYR:CD2	1:e:50:PRO:HD2	2.56	0.41
2:i:174:LEU:HD23	2:i:174:LEU:HA	1.86	0.41
3:m:52:ASN:HD21	3:m:91:GLU:CD	2.26	0.41
3:s:79:ASP:O	3:s:83:THR:HG23	2.21	0.41
2:j:97:PHE:CD1	2:j:124:TRP:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:324:GLU:O	2:j:328:ILE:HG12	2.20	0.41
2:j:335:LEU:HD12	2:j:340:LYS:HE2	2.03	0.41
2:l:172:LYS:HZ3	2:l:229:MET:C	2.28	0.41
3:n:60:LYS:HE2	3:n:66:TYR:HE1	1.86	0.41
3:t:60:LYS:HG2	3:t:64:ASN:O	2.21	0.41
3:v:33:ASP:HB3	3:v:36:THR:OG1	2.21	0.41
3:v:46:VAL:CG1	3:v:58:VAL:HG22	2.50	0.41
1:M:271:MET:HE3	2:N:290:ALA:HB3	2.03	0.41
1:O:136:VAL:O	1:O:140:VAL:HG23	2.21	0.41
1:O:227:MET:HE1	2:R:156:VAL:H	1.85	0.41
1:P:14:VAL:O	1:P:18:MET:HB2	2.21	0.41
3:Q:69:TYR:CZ	3:W:92:PRO:HB3	2.56	0.41
2:S:111:PHE:HB2	2:S:113:LYS:HZ1	1.86	0.41
3:U:34:TYR:CE1	3:U:70:ILE:HG12	2.46	0.41
3:W:34:TYR:CG	3:W:71:PRO:HD3	2.56	0.41
3:X:30:ARG:HD2	3:X:30:ARG:O	2.21	0.41
2:B:263:GLN:HA	2:B:266:ARG:NH1	2.36	0.41
3:K:54:ARG:O	3:K:70:ILE:N	2.28	0.41
3:K:56:ILE:HG22	3:K:58:VAL:CG2	2.51	0.41
2:a:310:LYS:HD2	2:a:310:LYS:HA	1.92	0.41
2:i:110:ARG:HA	2:i:130:ASP:HA	2.02	0.41
2:l:126:PRO:O	2:l:127:THR:OG1	2.29	0.41
3:p:37:PHE:O	3:p:40:GLU:HG2	2.21	0.41
2:N:142:GLU:O	2:N:143:LEU:HD23	2.21	0.41
1:A:248:LYS:HB2	1:A:248:LYS:HE3	1.89	0.40
1:C:218:GLU:HG2	2:G:255:ILE:CG2	2.50	0.40
3:I:32:VAL:HG22	3:I:36:THR:OG1	2.21	0.40
3:L:46:VAL:HA	3:L:60:LYS:HB2	2.04	0.40
1:Y:130:GLU:HG3	1:Y:151:VAL:HG22	2.03	0.40
2:a:119:GLU:HG2	2:a:120:PRO:HD2	2.03	0.40
1:c:40:ASP:N	1:c:40:ASP:OD2	2.54	0.40
1:c:119:LEU:HD13	1:c:203:ILE:HD12	2.03	0.40
2:i:100:ILE:HB	2:i:121:GLY:H	1.86	0.40
2:l:105:ARG:O	2:l:136:ASN:HB2	2.21	0.40
2:l:202:ASP:O	2:l:206:THR:HG23	2.21	0.40
1:M:30:ILE:HG13	1:M:31:THR:H	1.86	0.40
1:P:257:VAL:O	1:P:261:LEU:HD23	2.21	0.40
2:S:320:GLU:HG2	2:S:321:ILE:N	2.36	0.40
3:U:52:ASN:O	3:U:53:GLY:C	2.64	0.40
3:U:89:VAL:HB	3:V:33:ASP:OD1	2.20	0.40
3:X:50:ARG:HH21	3:X:57:ASN:ND2	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:MET:HE3	2:B:351:MET:HB3	1.85	0.40
1:C:32:LEU:HD13	1:C:35:GLY:HA2	2.04	0.40
1:C:78:ARG:HB3	2:G:209:ARG:HH22	1.86	0.40
2:F:350:LEU:O	2:G:350:LEU:HB2	2.22	0.40
2:G:290:ALA:O	2:G:293:TYR:HB3	2.22	0.40
3:L:37:PHE:O	3:L:41:VAL:HG23	2.20	0.40
1:Y:298:ARG:O	1:Y:298:ARG:HG3	2.21	0.40
2:a:162:ASN:OD1	2:a:237:ASN:HB2	2.21	0.40
1:e:95:TRP:HA	1:e:206:VAL:H	1.86	0.40
3:m:31:LYS:HG3	3:m:67:THR:HG23	2.03	0.40
3:o:87:LYS:HE2	3:q:33:ASP:OD1	2.21	0.40
2:j:193:ARG:HA	2:j:196:ILE:HG22	2.03	0.40
2:j:339:ARG:HE	2:j:339:ARG:HB3	1.68	0.40
3:r:49:ALA:O	3:r:89:VAL:HG12	2.22	0.40
3:r:56:ILE:HD11	3:r:70:ILE:HD11	2.02	0.40
1:M:21:PHE:CZ	1:M:50:PRO:HA	2.57	0.40
2:N:220:LEU:HA	2:N:223:THR:HG22	2.02	0.40
1:P:220:SER:O	1:P:223:ILE:HG22	2.21	0.40
1:P:296:PHE:CE2	2:S:323:ARG:HG3	2.56	0.40
3:V:33:ASP:HB3	3:V:36:THR:CG2	2.52	0.40
1:C:137:LYS:O	1:C:141:THR:HG23	2.21	0.40
2:G:158:ARG:HD3	2:G:242:ARG:CZ	2.51	0.40
2:G:234:LEU:H	2:G:234:LEU:HD12	1.85	0.40
2:a:95:SER:OG	2:a:128:PHE:HB3	2.21	0.40
1:c:283:PHE:HD2	1:c:287:PHE:CE2	2.39	0.40
1:e:42:ASP:N	1:e:42:ASP:OD2	2.53	0.40
1:e:97:ILE:HD12	1:e:202:GLY:O	2.22	0.40
1:e:119:LEU:HB3	1:e:198:MET:HE1	2.02	0.40
3:q:99:LEU:O	3:q:103:PHE:HB2	2.21	0.40
1:Z:126:ARG:HG3	1:Z:155:LEU:HD13	2.03	0.40
2:b:123:ASN:C	2:b:123:ASN:HD22	2.28	0.40
1:d:237:ARG:O	1:d:241:GLN:OE1	2.40	0.40
1:f:215:LEU:HB3	1:f:216:PRO:HD2	2.01	0.40
2:l:100:ILE:HG13	2:l:121:GLY:H	1.86	0.40
3:p:40:GLU:OE1	3:p:66:TYR:OH	2.38	0.40
3:r:81:LEU:HD12	3:r:82:LEU:N	2.36	0.40
3:v:56:ILE:HD11	3:v:70:ILE:HG13	2.03	0.40
3:v:72:VAL:HG22	3:v:73:GLN:H	1.86	0.40
1:M:227:MET:HB3	2:N:248:LYS:HZ2	1.84	0.40
1:O:86:ASP:OD1	1:O:86:ASP:N	2.44	0.40
1:A:147:LEU:O	1:A:151:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:THR:HG22	2:B:131:GLU:O	2.22	0.40
2:F:193:ARG:HA	2:F:196:ILE:HG22	2.03	0.40
2:G:86:ALA:O	2:G:90:ILE:HG13	2.21	0.40
2:G:164:GLN:N	2:G:164:GLN:OE1	2.55	0.40
2:a:287:LEU:HD23	2:a:287:LEU:HA	1.92	0.40
3:g:54:ARG:HA	3:g:54:ARG:HE	1.86	0.40
2:k:112:GLY:O	2:k:113:LYS:HD2	2.22	0.40
3:q:33:ASP:OD2	3:q:33:ASP:C	2.65	0.40
3:u:50:ARG:HB3	3:u:57:ASN:ND2	2.34	0.40
1:Z:223:ILE:HD11	2:b:154:GLU:HB3	2.03	0.40
2:b:195:VAL:O	2:b:198:LYS:NZ	2.51	0.40
2:b:245:GLU:HG2	2:b:247:VAL:H	1.87	0.40
1:d:32:LEU:HD12	1:d:35:GLY:C	2.47	0.40
1:d:121:ARG:NH1	2:l:235:ASP:OD1	2.54	0.40
1:f:25:GLU:OE1	2:l:114:PHE:N	2.54	0.40
1:f:84:LYS:HE2	1:f:84:LYS:HB2	1.88	0.40
1:M:114:GLN:H	1:M:114:GLN:CD	2.29	0.40
1:P:62:VAL:HG12	1:P:64:MET:HE2	2.04	0.40
2:R:294:LYS:O	2:R:298:ILE:HG22	2.21	0.40
2:S:133:LYS:HE2	2:S:174:LEU:HD13	2.03	0.40
3:V:52:ASN:OD1	3:V:53:GLY:N	2.54	0.40
1:A:137:LYS:NZ	2:B:154:GLU:OE2	2.36	0.40
1:C:25:GLU:H	1:C:25:GLU:HG3	1.54	0.40
3:J:59:THR:HA	3:J:65:ARG:HH21	1.85	0.40
3:J:88:VAL:HB	3:L:35:SER:HB3	2.04	0.40
2:i:118:VAL:HG21	2:i:123:ASN:ND2	2.36	0.40
3:s:102:ILE:O	3:s:106:TRP:HD1	2.04	0.40
3:u:30:ARG:HG2	3:u:66:TYR:HB2	2.04	0.40
1:f:212:GLN:HE22	1:f:214:ASN:CB	2.28	0.40
1:f:224:TYR:CE2	2:l:156:VAL:HG21	2.55	0.40
2:j:242:ARG:C	2:j:244:PRO:HD3	2.47	0.40
3:v:61:LYS:C	3:v:63:SER:H	2.30	0.40
1:M:144:ARG:HG3	1:M:145:GLY:N	2.37	0.40
1:O:143:SER:HB3	1:O:147:LEU:HD23	2.03	0.40
2:R:215:ASP:OD1	2:R:218:ARG:NH2	2.54	0.40
3:W:54:ARG:O	3:W:70:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	289/334 (86%)	260 (90%)	29 (10%)	0	100	100
1	C	283/334 (85%)	264 (93%)	19 (7%)	0	100	100
1	D	286/334 (86%)	263 (92%)	23 (8%)	0	100	100
1	M	289/334 (86%)	262 (91%)	27 (9%)	0	100	100
1	O	283/334 (85%)	259 (92%)	24 (8%)	0	100	100
1	P	286/334 (86%)	263 (92%)	23 (8%)	0	100	100
1	Y	289/334 (86%)	266 (92%)	23 (8%)	0	100	100
1	Z	289/334 (86%)	262 (91%)	27 (9%)	0	100	100
1	c	283/334 (85%)	266 (94%)	17 (6%)	0	100	100
1	d	283/334 (85%)	268 (95%)	15 (5%)	0	100	100
1	e	286/334 (86%)	263 (92%)	23 (8%)	0	100	100
1	f	286/334 (86%)	259 (91%)	27 (9%)	0	100	100
2	B	273/419 (65%)	251 (92%)	22 (8%)	0	100	100
2	F	273/419 (65%)	246 (90%)	27 (10%)	0	100	100
2	G	273/419 (65%)	257 (94%)	16 (6%)	0	100	100
2	N	273/419 (65%)	254 (93%)	19 (7%)	0	100	100
2	R	273/419 (65%)	245 (90%)	28 (10%)	0	100	100
2	S	273/419 (65%)	252 (92%)	21 (8%)	0	100	100
2	a	273/419 (65%)	254 (93%)	18 (7%)	1 (0%)	30	65
2	b	273/419 (65%)	256 (94%)	17 (6%)	0	100	100
2	i	273/419 (65%)	243 (89%)	30 (11%)	0	100	100
2	j	273/419 (65%)	245 (90%)	28 (10%)	0	100	100
2	k	273/419 (65%)	254 (93%)	19 (7%)	0	100	100
2	l	273/419 (65%)	256 (94%)	17 (6%)	0	100	100
3	E	79/644 (12%)	72 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	79/644 (12%)	71 (90%)	8 (10%)	0	100	100
3	I	77/644 (12%)	72 (94%)	5 (6%)	0	100	100
3	J	76/644 (12%)	69 (91%)	7 (9%)	0	100	100
3	K	77/644 (12%)	70 (91%)	7 (9%)	0	100	100
3	L	77/644 (12%)	73 (95%)	4 (5%)	0	100	100
3	Q	79/644 (12%)	74 (94%)	5 (6%)	0	100	100
3	T	79/644 (12%)	73 (92%)	6 (8%)	0	100	100
3	U	77/644 (12%)	72 (94%)	5 (6%)	0	100	100
3	V	76/644 (12%)	69 (91%)	7 (9%)	0	100	100
3	W	77/644 (12%)	70 (91%)	7 (9%)	0	100	100
3	X	77/644 (12%)	73 (95%)	4 (5%)	0	100	100
3	g	79/644 (12%)	73 (92%)	6 (8%)	0	100	100
3	h	79/644 (12%)	72 (91%)	7 (9%)	0	100	100
3	m	79/644 (12%)	72 (91%)	7 (9%)	0	100	100
3	n	79/644 (12%)	71 (90%)	8 (10%)	0	100	100
3	o	77/644 (12%)	70 (91%)	7 (9%)	0	100	100
3	p	77/644 (12%)	72 (94%)	5 (6%)	0	100	100
3	q	76/644 (12%)	70 (92%)	6 (8%)	0	100	100
3	r	76/644 (12%)	70 (92%)	6 (8%)	0	100	100
3	s	77/644 (12%)	70 (91%)	7 (9%)	0	100	100
3	t	77/644 (12%)	70 (91%)	7 (9%)	0	100	100
3	u	77/644 (12%)	71 (92%)	6 (8%)	0	100	100
3	v	77/644 (12%)	69 (90%)	8 (10%)	0	100	100
All	All	8568/24492 (35%)	7876 (92%)	691 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	a	319	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	A	248/283 (88%)	248 (100%)	0	100	100
1	C	241/283 (85%)	237 (98%)	4 (2%)	53	68
1	D	244/283 (86%)	243 (100%)	1 (0%)	84	84
1	M	248/283 (88%)	244 (98%)	4 (2%)	55	70
1	O	241/283 (85%)	238 (99%)	3 (1%)	63	73
1	P	244/283 (86%)	243 (100%)	1 (0%)	84	84
1	Y	248/283 (88%)	247 (100%)	1 (0%)	84	84
1	Z	248/283 (88%)	248 (100%)	0	100	100
1	c	241/283 (85%)	237 (98%)	4 (2%)	53	68
1	d	241/283 (85%)	235 (98%)	6 (2%)	42	62
1	e	244/283 (86%)	244 (100%)	0	100	100
1	f	244/283 (86%)	243 (100%)	1 (0%)	84	84
2	B	228/336 (68%)	222 (97%)	6 (3%)	40	61
2	F	227/336 (68%)	220 (97%)	7 (3%)	35	56
2	G	229/336 (68%)	226 (99%)	3 (1%)	61	72
2	N	228/336 (68%)	219 (96%)	9 (4%)	28	51
2	R	227/336 (68%)	217 (96%)	10 (4%)	25	48
2	S	229/336 (68%)	223 (97%)	6 (3%)	40	61
2	a	228/336 (68%)	219 (96%)	9 (4%)	28	51
2	b	228/336 (68%)	221 (97%)	7 (3%)	35	56
2	i	227/336 (68%)	221 (97%)	6 (3%)	40	61
2	j	227/336 (68%)	220 (97%)	7 (3%)	35	56
2	k	229/336 (68%)	225 (98%)	4 (2%)	53	68
2	l	229/336 (68%)	225 (98%)	4 (2%)	53	68
3	E	76/527 (14%)	76 (100%)	0	100	100
3	H	76/527 (14%)	76 (100%)	0	100	100
3	I	74/527 (14%)	73 (99%)	1 (1%)	59	71
3	J	74/527 (14%)	74 (100%)	0	100	100
3	K	74/527 (14%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	74/527 (14%)	74 (100%)	0	100	100
3	Q	76/527 (14%)	76 (100%)	0	100	100
3	T	76/527 (14%)	76 (100%)	0	100	100
3	U	74/527 (14%)	72 (97%)	2 (3%)	39	60
3	V	74/527 (14%)	74 (100%)	0	100	100
3	W	74/527 (14%)	74 (100%)	0	100	100
3	X	74/527 (14%)	74 (100%)	0	100	100
3	g	76/527 (14%)	76 (100%)	0	100	100
3	h	76/527 (14%)	76 (100%)	0	100	100
3	m	76/527 (14%)	76 (100%)	0	100	100
3	n	76/527 (14%)	76 (100%)	0	100	100
3	o	74/527 (14%)	72 (97%)	2 (3%)	39	60
3	p	74/527 (14%)	74 (100%)	0	100	100
3	q	74/527 (14%)	74 (100%)	0	100	100
3	r	74/527 (14%)	73 (99%)	1 (1%)	59	71
3	s	74/527 (14%)	74 (100%)	0	100	100
3	t	74/527 (14%)	74 (100%)	0	100	100
3	u	74/527 (14%)	73 (99%)	1 (1%)	59	71
3	v	74/527 (14%)	74 (100%)	0	100	100
All	All	7460/20076 (37%)	7350 (98%)	110 (2%)	55	70

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	320	GLU
2	B	322	THR
2	B	323	ARG
2	B	346	LYS
2	B	350	LEU
2	B	351	MET
1	C	22	VAL
1	C	24	LYS
1	C	25	GLU
1	C	27	GLU
1	D	43	ASN

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Mol	Chain	Res	Type
2	F	151	THR
2	F	153	ASP
2	F	154	GLU
2	F	346	LYS
2	F	350	LEU
2	F	351	MET
2	F	352	VAL
2	G	346	LYS
2	G	350	LEU
2	G	351	MET
3	I	61	LYS
1	Y	25	GLU
2	a	101	LYS
2	a	105	ARG
2	a	320	GLU
2	a	321	ILE
2	a	322	THR
2	a	346	LYS
2	a	349	ASN
2	a	350	LEU
2	a	352	VAL
1	c	24	LYS
1	c	25	GLU
1	c	27	GLU
1	c	111	ASP
2	i	102	GLU
2	i	127	THR
2	i	346	LYS
2	i	349	ASN
2	i	350	LEU
2	i	351	MET
2	k	346	LYS
2	k	350	LEU
2	k	351	MET
2	k	352	VAL
3	o	91	GLU
3	o	94	GLU
3	u	99	LEU
2	b	237	ASN
2	b	242	ARG
2	b	321	ILE
2	b	345	ASP

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Mol	Chain	Res	Type
2	b	346	LYS
2	b	350	LEU
2	b	351	MET
1	d	24	LYS
1	d	25	GLU
1	d	27	GLU
1	d	107	THR
1	d	111	ASP
1	d	112	ILE
1	f	310	ASN
2	j	102	GLU
2	j	125	LYS
2	j	127	THR
2	j	129	ILE
2	j	346	LYS
2	j	350	LEU
2	j	352	VAL
2	l	346	LYS
2	l	350	LEU
2	l	351	MET
2	l	352	VAL
3	r	54	ARG
1	M	24	LYS
1	M	37	VAL
1	M	40	ASP
1	M	41	ASP
2	N	101	LYS
2	N	104	GLU
2	N	320	GLU
2	N	321	ILE
2	N	323	ARG
2	N	345	ASP
2	N	346	LYS
2	N	349	ASN
2	N	350	LEU
1	O	24	LYS
1	O	25	GLU
1	O	27	GLU
1	P	308	SER
2	R	125	LYS
2	R	127	THR
2	R	128	PHE

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Mol	Chain	Res	Type
2	R	129	ILE
2	R	130	ASP
2	R	346	LYS
2	R	349	ASN
2	R	350	LEU
2	R	351	MET
2	R	352	VAL
2	S	345	ASP
2	S	346	LYS
2	S	349	ASN
2	S	350	LEU
2	S	351	MET
2	S	352	VAL
3	U	91	GLU
3	U	94	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
2	B	164	GLN
2	B	284	GLN
1	C	43	ASN
1	C	70	GLN
1	C	225	ASN
1	C	238	HIS
1	D	43	ASN
2	F	155	ASN
2	F	169	ASN
2	F	260	ASN
2	F	262	GLN
2	F	276	GLN
2	G	162	ASN
2	G	349	ASN
3	I	43	ASN
3	I	45	GLN
3	L	45	GLN
3	L	52	ASN
3	L	57	ASN
2	a	164	GLN
2	a	262	GLN
2	a	302	GLN

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Mol	Chain	Res	Type
2	a	349	ASN
1	c	70	GLN
1	c	114	GLN
1	c	225	ASN
1	e	212	GLN
1	e	243	GLN
2	i	123	ASN
2	i	260	ASN
2	k	162	ASN
3	m	64	ASN
3	o	45	GLN
3	o	80	ASN
3	q	45	GLN
3	s	45	GLN
1	Z	241	GLN
1	Z	243	GLN
2	b	262	GLN
1	d	238	HIS
1	f	212	GLN
2	j	169	ASN
2	j	237	ASN
2	j	260	ASN
2	l	162	ASN
2	l	349	ASN
3	p	52	ASN
3	r	45	GLN
3	t	39	GLN
3	t	45	GLN
3	v	52	ASN
2	N	262	GLN
1	O	43	ASN
1	O	70	GLN
1	O	238	HIS
1	P	53	HIS
1	P	212	GLN
2	R	123	ASN
2	R	260	ASN
2	R	276	GLN
2	S	123	ASN
2	S	162	ASN
2	S	186	GLN
2	S	282	GLN

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Mol	Chain	Res	Type
2	S	284	GLN
3	U	85	ASN
3	V	45	GLN
3	V	73	GLN
3	X	45	GLN
3	X	52	ASN
3	X	57	ASN
3	X	64	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

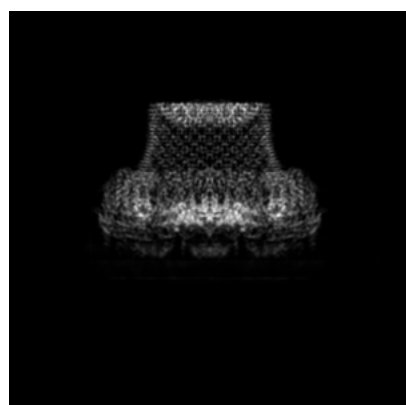
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32520. These allow visual inspection of the internal detail of the map and identification of artifacts.

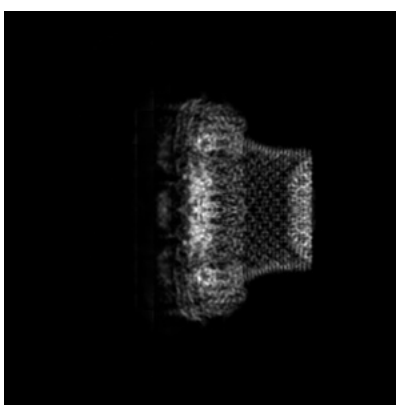
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

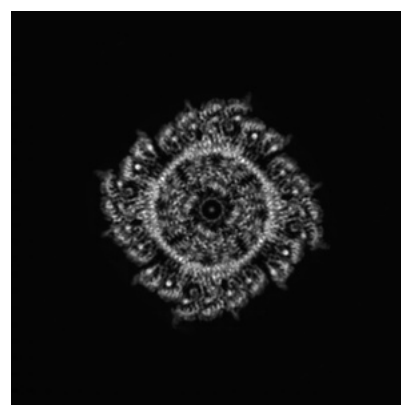
6.1.1 Primary map



X



Y

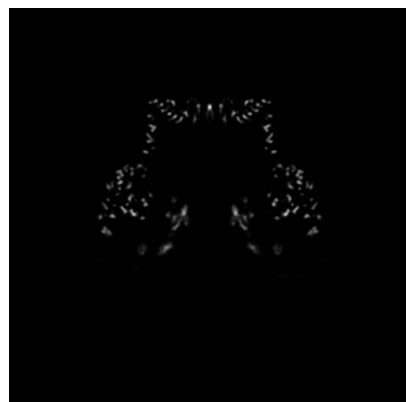


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 140



Y Index: 140

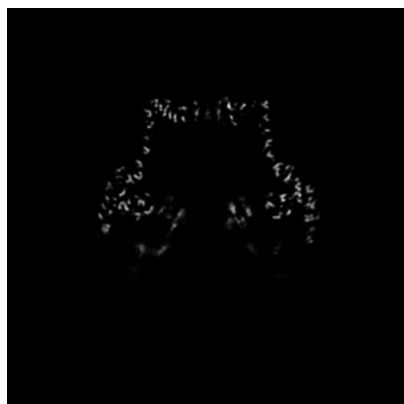


Z Index: 140

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 142



Y Index: 142

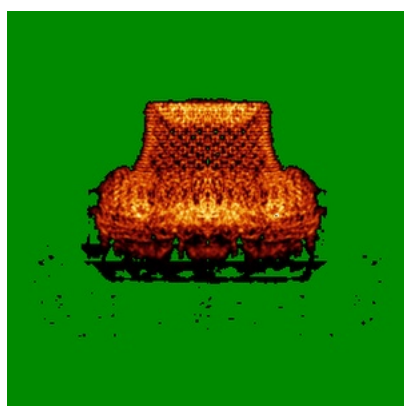


Z Index: 139

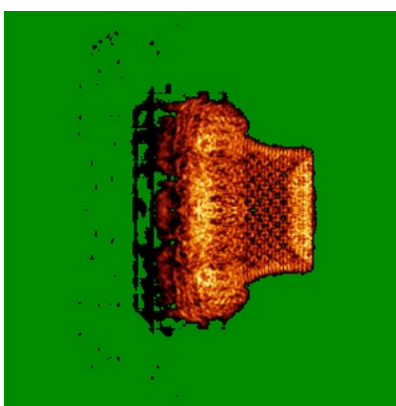
The images above show the largest variance slices of the map in three orthogonal directions.

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

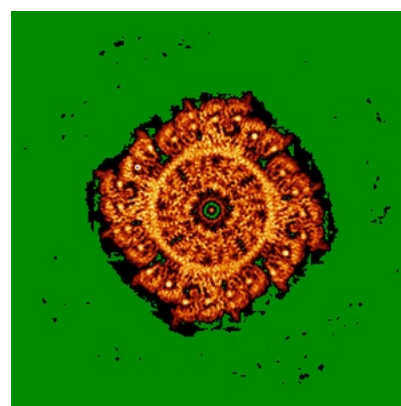
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

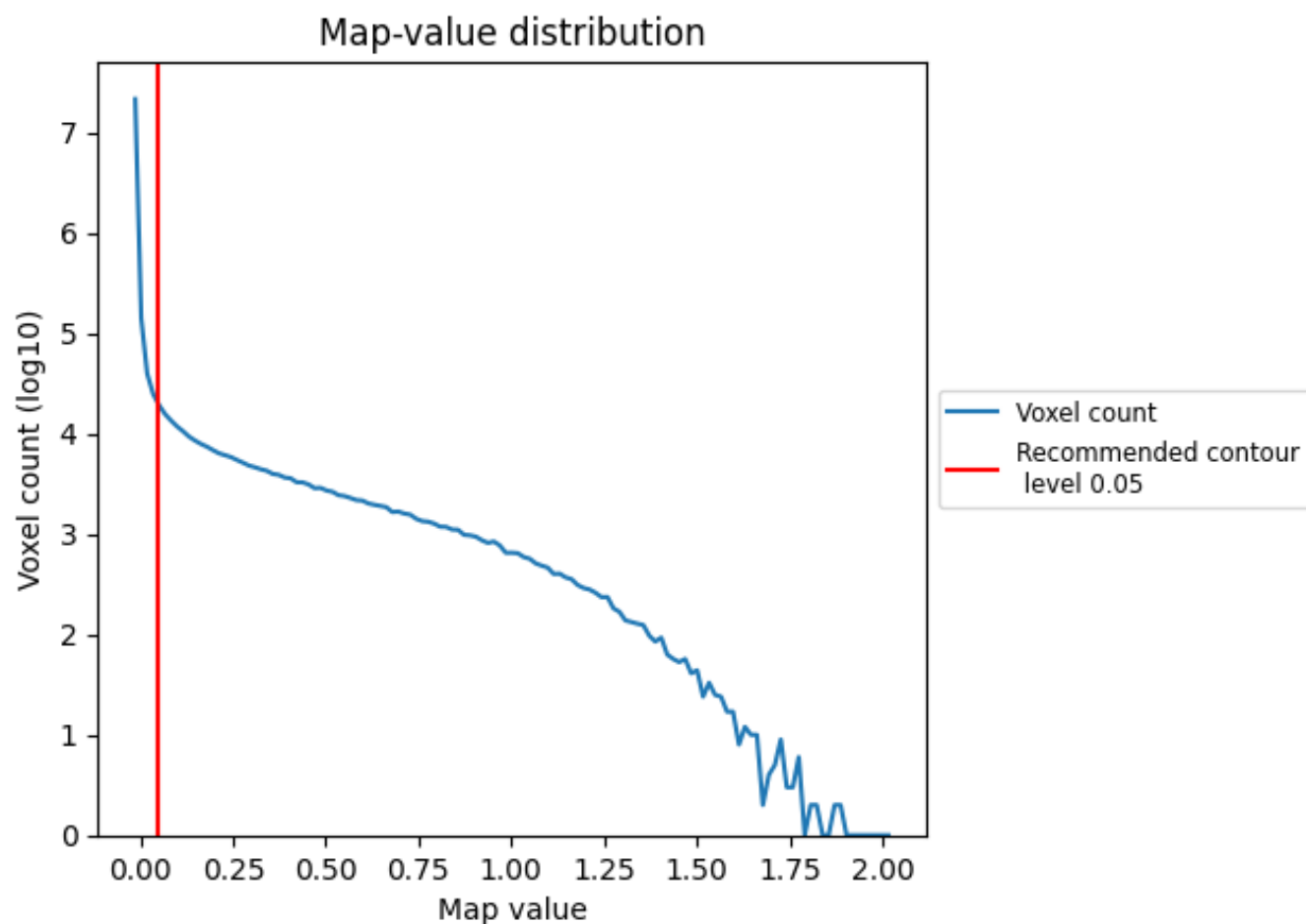
6.6 Mask visualisation

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

7 Map analysis [i](#)

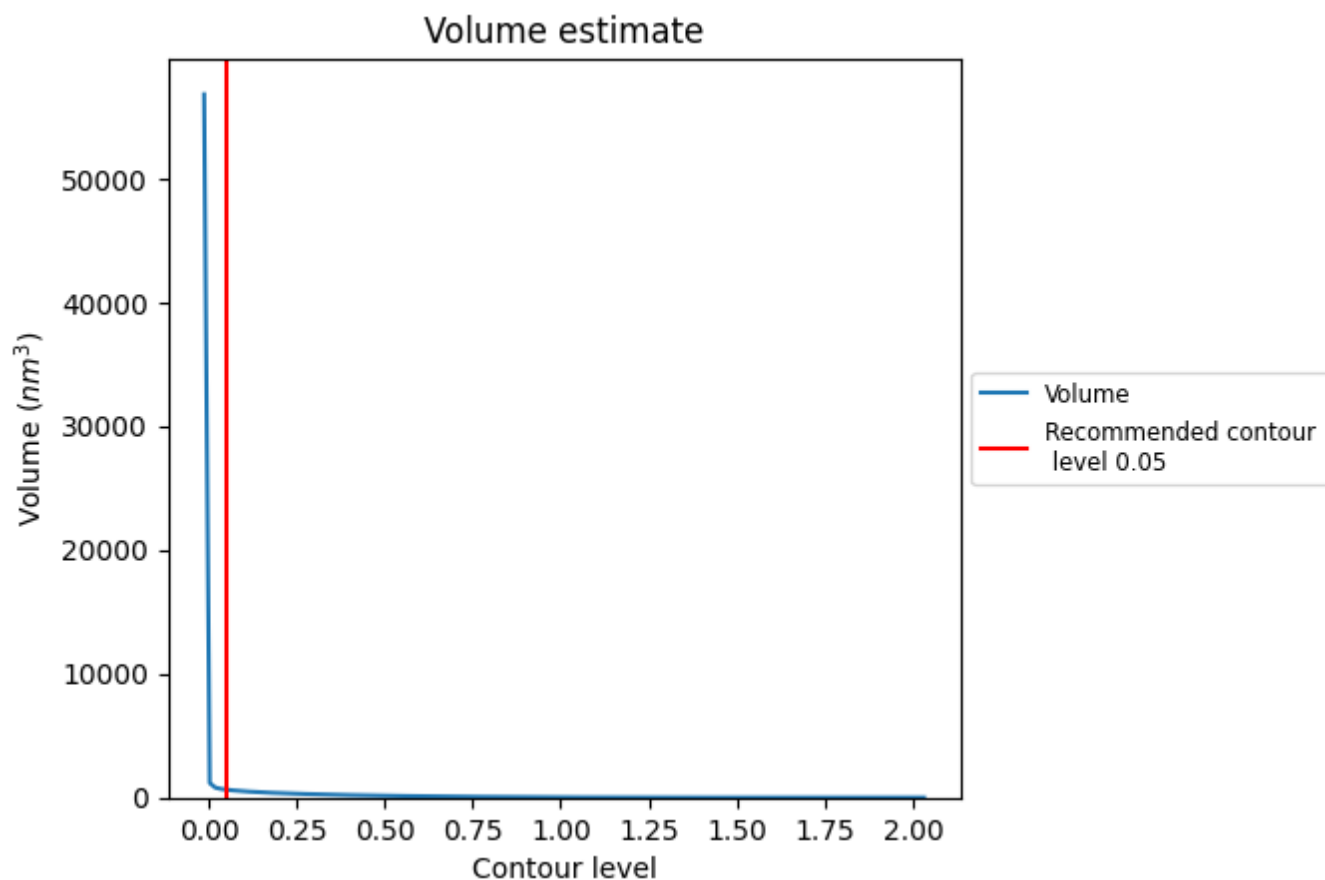
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

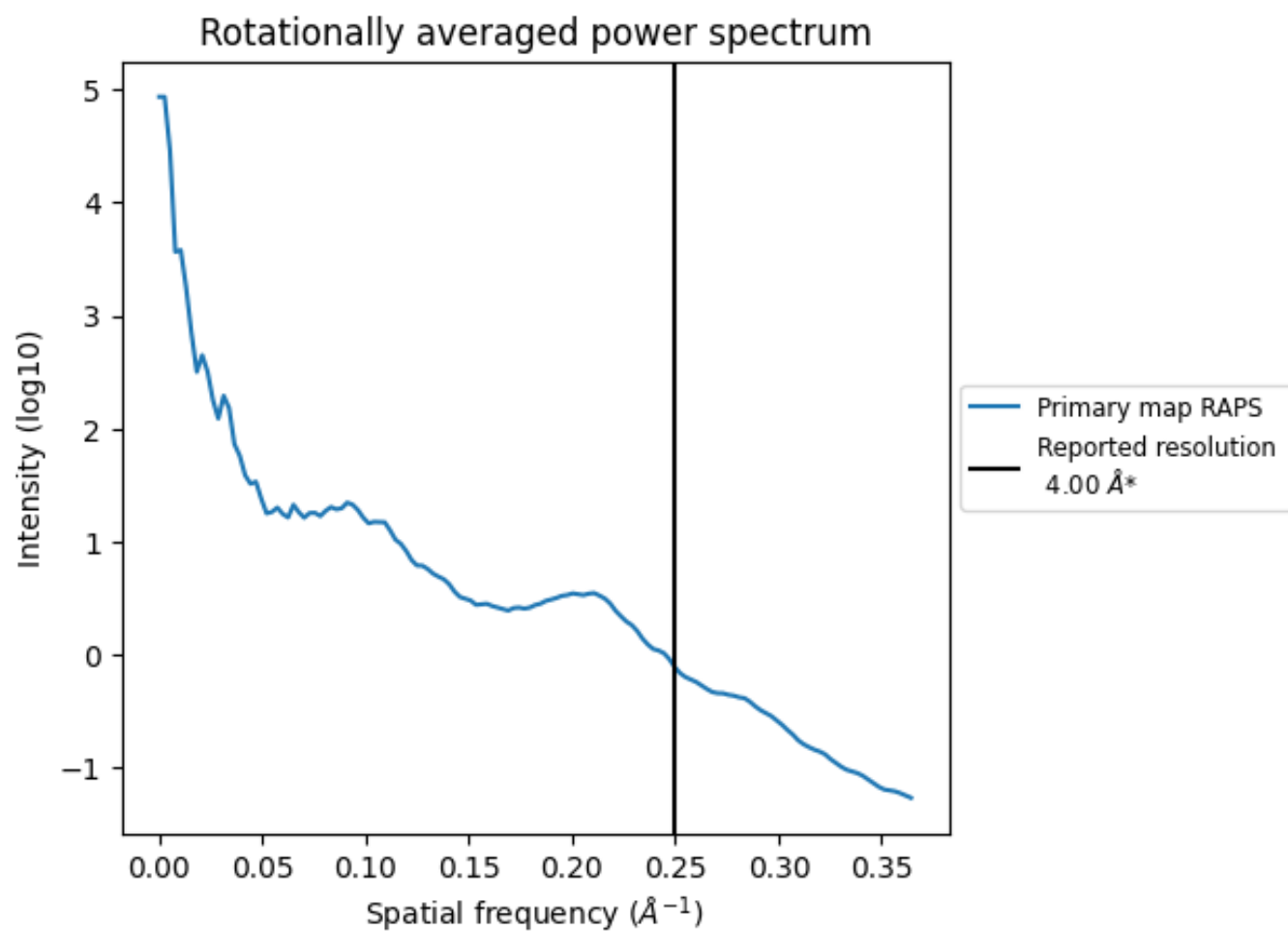
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 638 nm^3 ; this corresponds to an approximate mass of 577 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

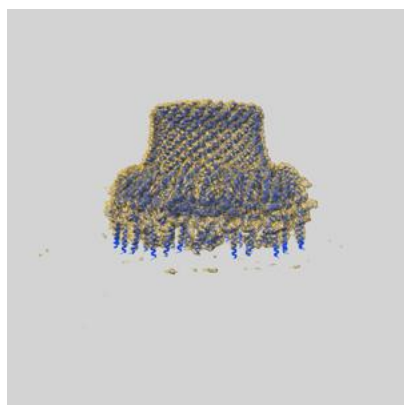
8 Fourier-Shell correlation

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

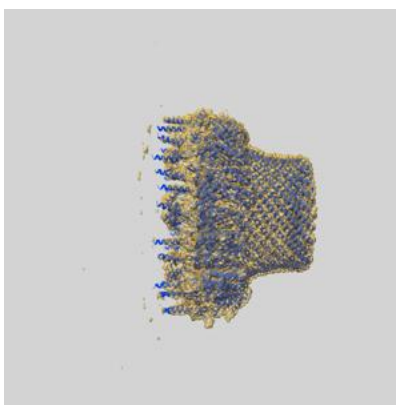
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32520 and PDB model 7WI3. Per-residue inclusion information can be found in section [3](#) on page [8](#).

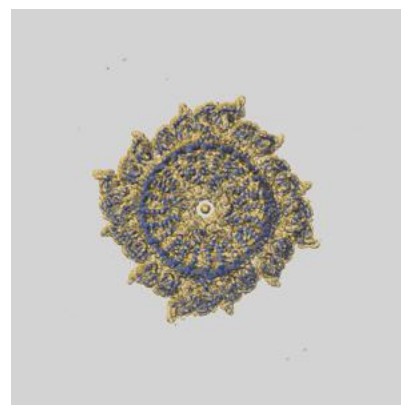
9.1 Map-model overlay [i](#)



X



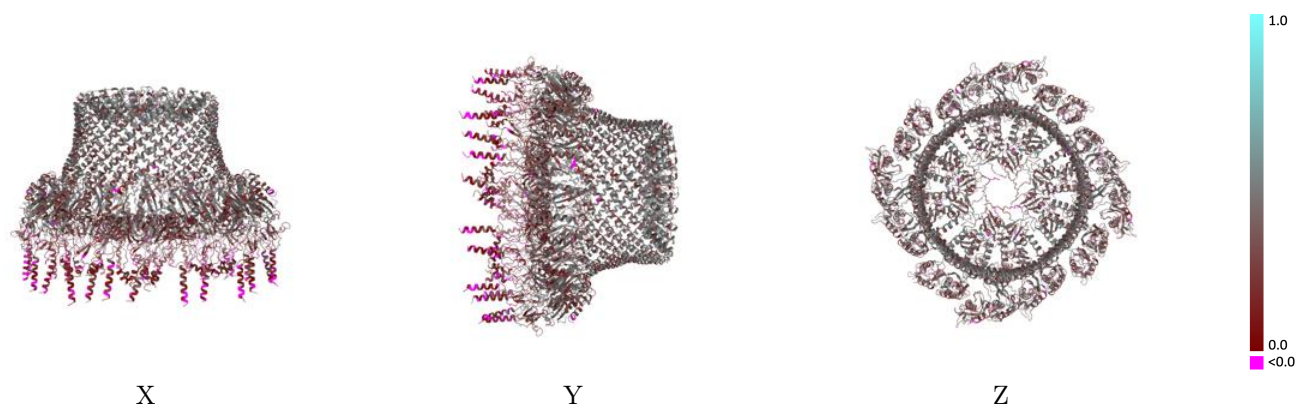
Y



Z

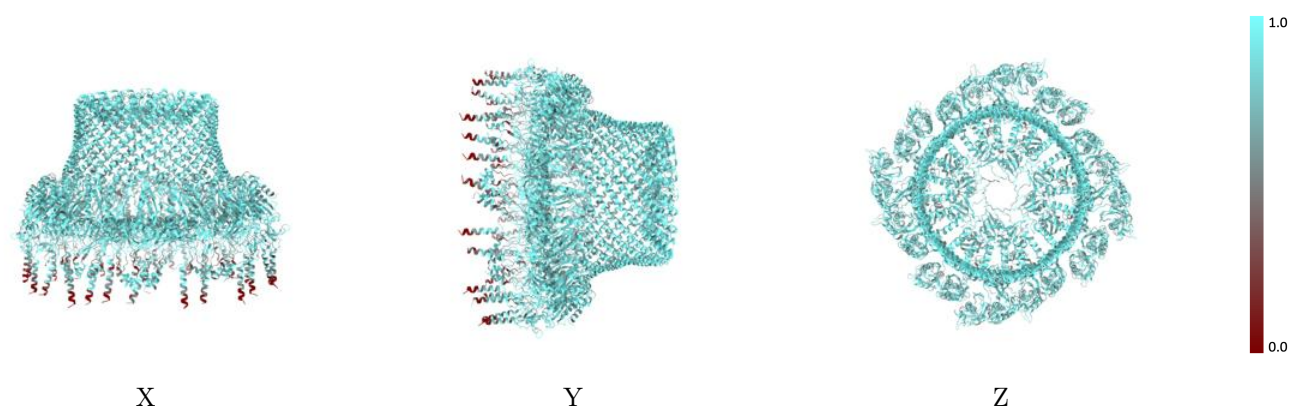
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



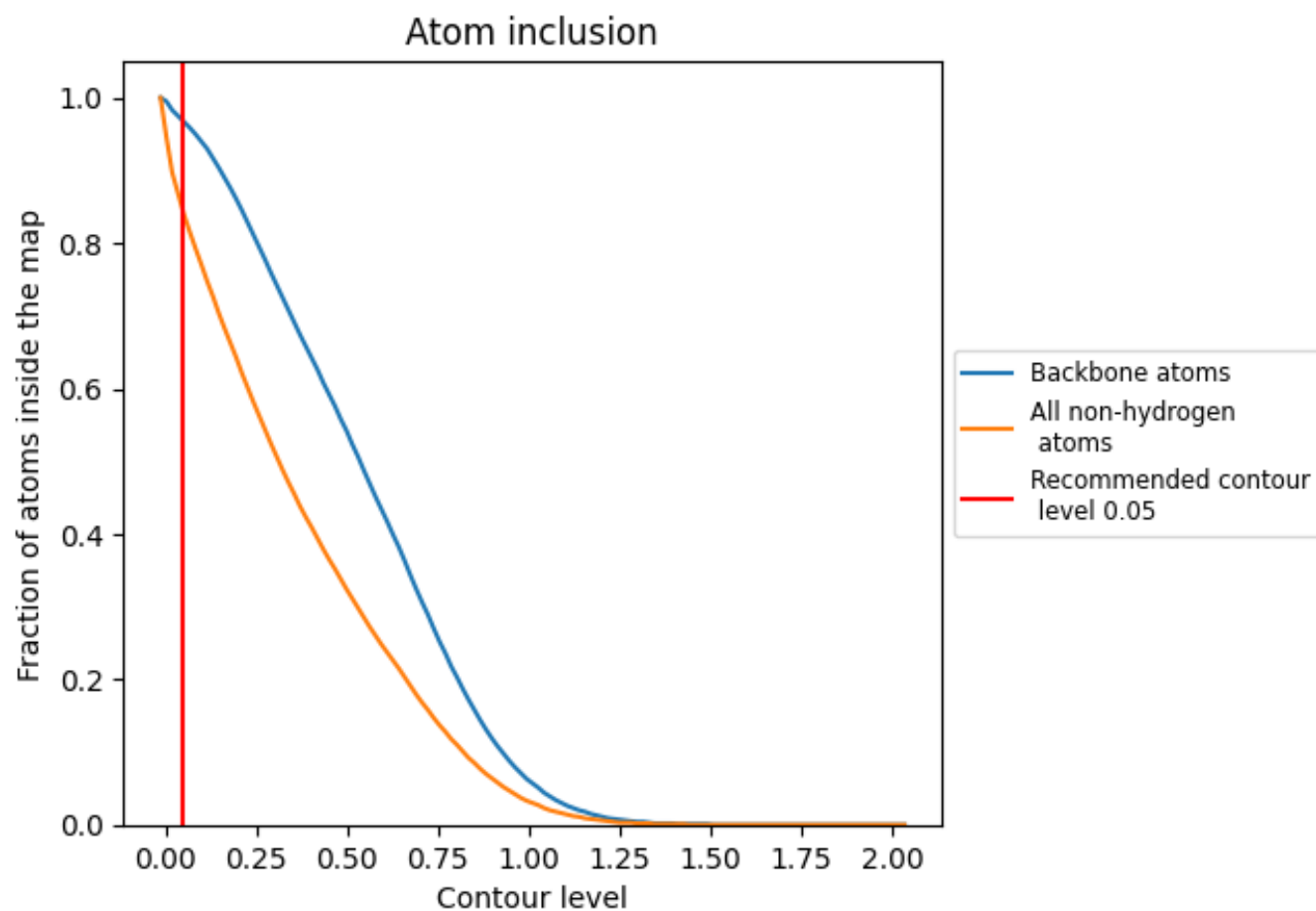
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 84% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.3350
A	 0.8590	 0.3640
B	 0.8360	 0.3420
C	 0.8300	 0.3410
D	 0.8280	 0.3310
E	 0.8250	 0.3270
F	 0.8700	 0.3760
G	 0.8430	 0.3500
H	 0.8370	 0.3540
I	 0.7900	 0.2600
J	 0.8520	 0.2250
K	 0.8300	 0.2860
L	 0.8630	 0.2260
M	 0.8580	 0.3600
N	 0.8540	 0.3470
O	 0.8360	 0.3410
P	 0.8270	 0.3310
Q	 0.8350	 0.3350
R	 0.8630	 0.3740
S	 0.8430	 0.3550
T	 0.8560	 0.3560
U	 0.7810	 0.2560
V	 0.8280	 0.2120
W	 0.8090	 0.2850
X	 0.8460	 0.2160
Y	 0.8540	 0.3620
Z	 0.8650	 0.3670
a	 0.8470	 0.3500
b	 0.8340	 0.3440
c	 0.8290	 0.3410
d	 0.8450	 0.3430
e	 0.8260	 0.3330
f	 0.8340	 0.3270
g	 0.8060	 0.3250
h	 0.8400	 0.3340



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Chain	Atom inclusion	Q-score
i	 0.8490	 0.3630
j	 0.8720	 0.3760
k	 0.8340	 0.3530
l	 0.8590	 0.3560
m	 0.8340	 0.3520
n	 0.8350	 0.3520
o	 0.8030	 0.2460
p	 0.7650	 0.2430
q	 0.8590	 0.2260
r	 0.8460	 0.2320
s	 0.8120	 0.2820
t	 0.8410	 0.2750
u	 0.8430	 0.2150
v	 0.8570	 0.2320