



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:45 PM UTC

PDB ID : 8JOV / pdb_00008jov
EMDB ID : EMD-36463
Title : Portal-tail complex of phage GP4
Authors : Liu, H.; Chen, W.
Deposited on : 2023-06-08
Resolution : 3.80 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

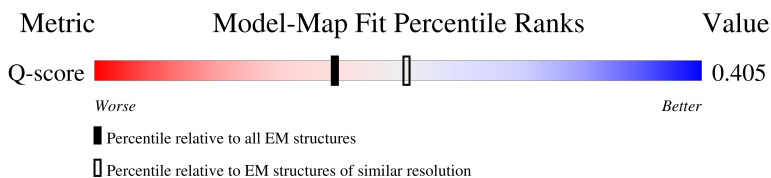
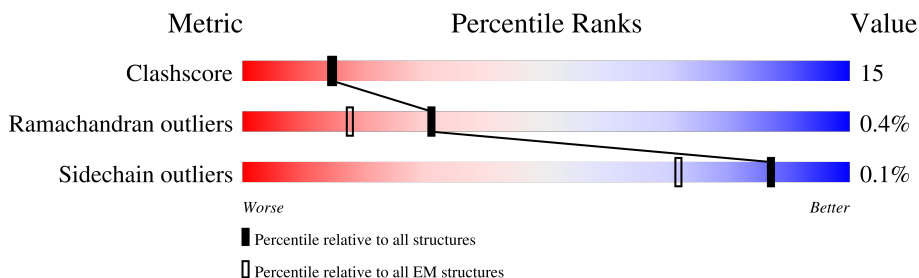
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.



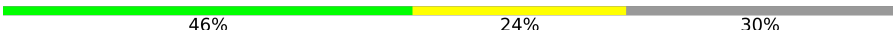
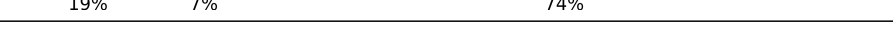
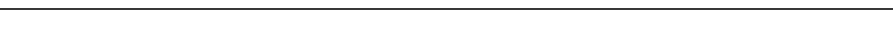
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	0	781	46% 23% 30%
1	3	781	48% 22% 30%
1	6	781	48% 22% 30%
1	U	781	48% 21% 30%

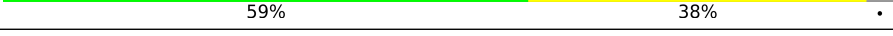
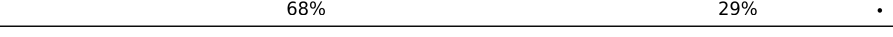
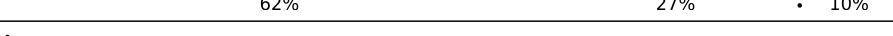
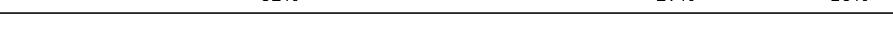
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Mol	Chain	Length	Quality of chain
1	Y	781	 46%24%30%
1	c	781	 49%21%30%
1	g	781	 47%22%30%
1	k	781	 50%20%30%
1	o	781	 49%21%30%
1	r	781	 49%21%30%
1	u	781	 48%22%30%
1	x	781	 50%20%30%
2	1	439	 17%10%74%
2	4	439	 18%8%74%
2	7	439	 18%8%74%
2	M	439	 16%10%74%
2	N	439	 19%7%74%
2	O	439	 19%7%74%
2	P	439	 18%9%74%
2	Q	439	 18%8%74%
2	R	439	 20%6%74%
2	V	439	 17%9%74%
2	Z	439	 17%9%74%
2	d	439	 18%8%74%
2	h	439	 18%8%74%
2	l	439	 19%7%74%
2	p	439	 19%7%74%
2	s	439	 18%8%74%
2	v	439	 17%9%74%

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Mol	Chain	Length	Quality of chain
2	y	439	
3	2	220	
3	5	220	
3	T	220	
3	X	220	
3	b	220	
3	f	220	
3	j	220	
3	n	220	
3	q	220	
3	t	220	
3	w	220	
3	z	220	
4	A	577	
4	B	577	
4	C	577	
4	D	577	
4	E	577	
4	F	577	
5	G	206	
5	H	206	
5	I	206	
5	J	206	
5	K	206	
5	L	206	

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Mol	Chain	Length	Quality of chain
5	S	206	66%33%
5	W	206	63%36%
5	a	206	65%34%
5	e	206	62%37%
5	i	206	63%36%
5	m	206	63%36%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 128070 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 Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	547	Total	C	N	O	S	0	0
			4297	2681	780	816	20		
1	3	547	Total	C	N	O	S	0	0
			4297	2681	780	816	20		
1	6	547	Total	C	N	O	S	0	0
			4297	2681	780	816	20		
1	U	547	Total	C	N	O	S	0	0
			4297	2681	780	816	20		
1	Y	547	Total	C	N	O	S	0	0
			4297	2681	780	816	20		
1	c	547	Total	C	N	O	S	0	0
			4297	2681	780	816	20		
1	g	547	Total	C	N	O	S	0	0
			4297	2681	780	816	20		
1	k	547	Total	C	N	O	S	0	0
			4297	2681	780	816	20		
1	o	547	Total	C	N	O	S	0	0
			4297	2681	780	816	20		
1	r	547	Total	C	N	O	S	0	0
			4297	2681	780	816	20		
1	u	547	Total	C	N	O	S	0	0
			4297	2681	780	816	20		
1	x	547	Total	C	N	O	S	0	0
			4297	2681	780	816	20		

- Molecule 2 is a protein called Putative tail fiber protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	4	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	7	116	Total	C	N	O	S	0	0
			829	507	150	170	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	N	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	O	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	P	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	Q	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	R	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	V	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	Z	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	d	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	h	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	l	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	p	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	s	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	v	116	Total	C	N	O	S	0	0
			829	507	150	170	2		
2	y	116	Total	C	N	O	S	0	0
			829	507	150	170	2		

- Molecule 3 is a protein called Virion associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	5	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	T	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	X	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	f	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	j	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	n	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	q	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	t	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	w	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		
3	z	213	Total	C	N	O	S	0	0
			1615	1013	281	316	5		

- Molecule 4 is a protein called Virion-associated phage protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	518	Total	C	N	O	S	0	0
			3812	2413	656	725	18		
4	B	518	Total	C	N	O	S	0	0
			3812	2413	656	725	18		
4	C	518	Total	C	N	O	S	0	0
			3812	2413	656	725	18		
4	D	518	Total	C	N	O	S	0	0
			3812	2413	656	725	18		
4	E	518	Total	C	N	O	S	0	0
			3812	2413	656	725	18		
4	F	518	Total	C	N	O	S	0	0
			3812	2413	656	725	18		

- Molecule 5 is a protein called gp81 of phage GP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	204	Total	C	N	O	S	0	0
			1611	1021	279	303	8		
5	H	204	Total	C	N	O	S	0	0
			1611	1021	279	303	8		
5	I	204	Total	C	N	O	S	0	0
			1611	1021	279	303	8		

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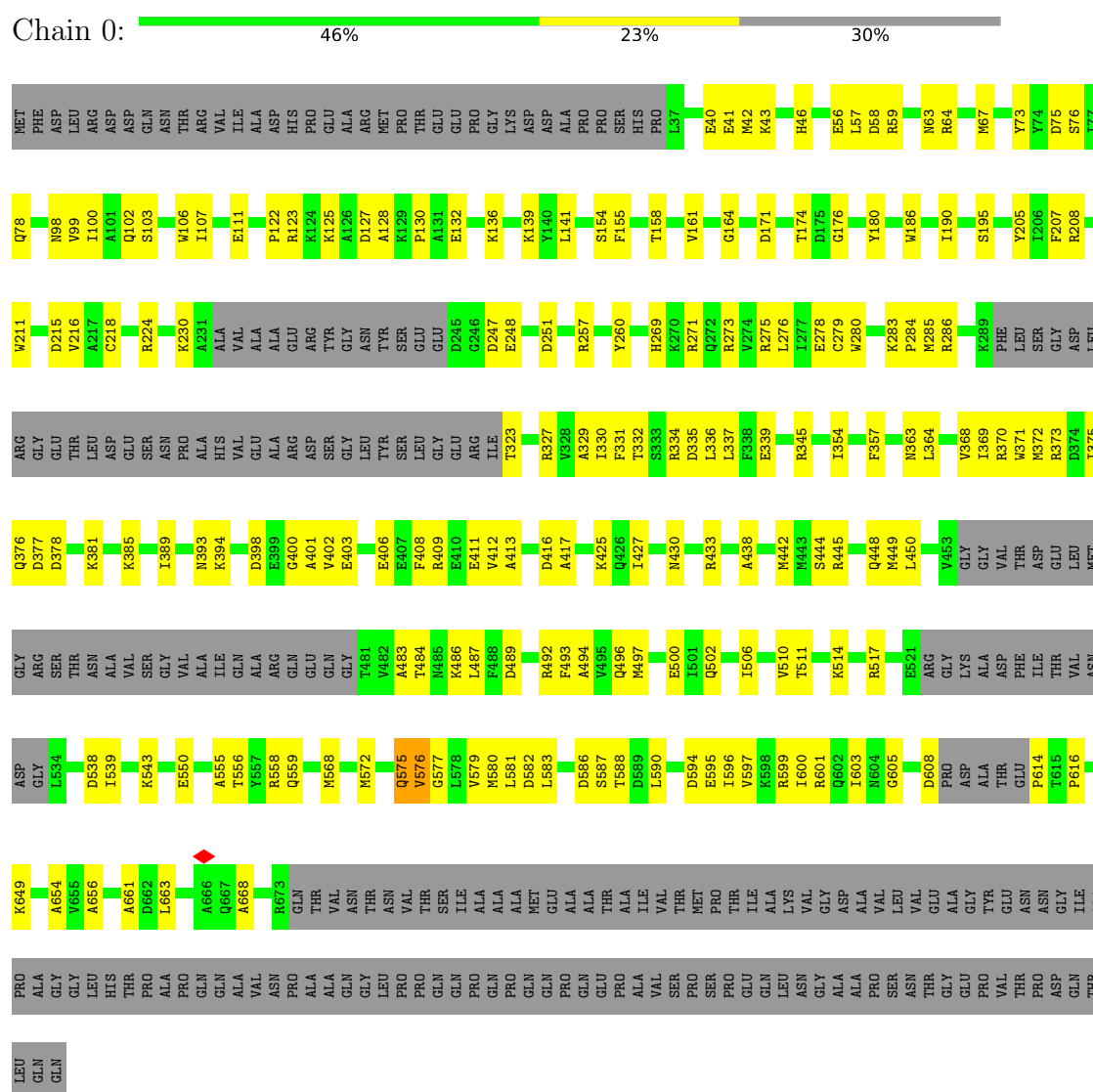
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	204	Total 1611	C 1021	N 279	O 303	S 8	0	0
5	K	204	Total 1611	C 1021	N 279	O 303	S 8	0	0
5	L	204	Total 1611	C 1021	N 279	O 303	S 8	0	0
5	S	204	Total 1611	C 1021	N 279	O 303	S 8	0	0
5	W	204	Total 1611	C 1021	N 279	O 303	S 8	0	0
5	a	204	Total 1611	C 1021	N 279	O 303	S 8	0	0
5	e	204	Total 1611	C 1021	N 279	O 303	S 8	0	0
5	i	204	Total 1611	C 1021	N 279	O 303	S 8	0	0
5	m	204	Total 1611	C 1021	N 279	O 303	S 8	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.

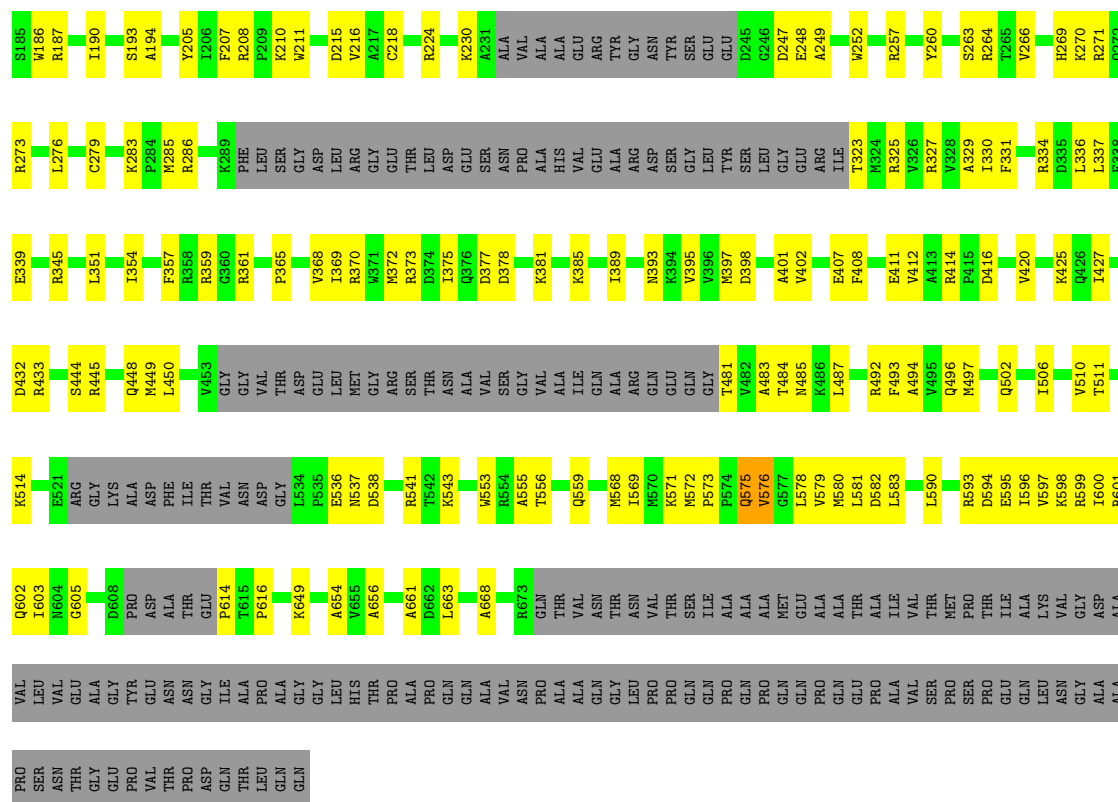
• Molecule 1: Portal protein



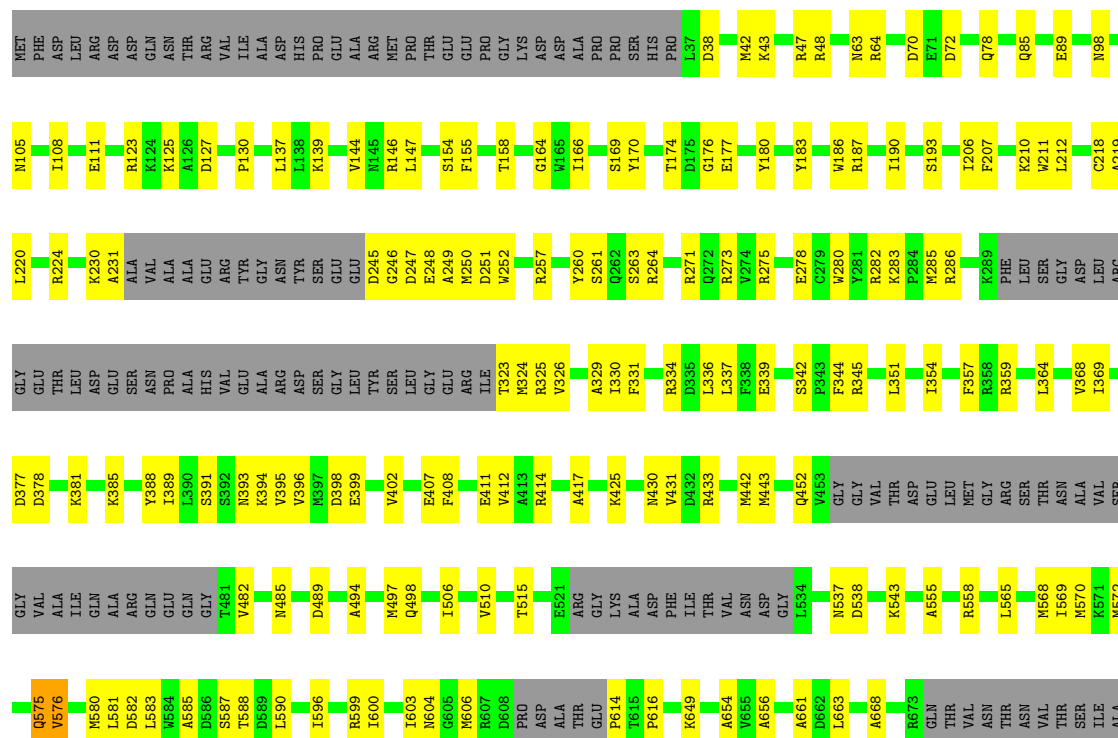
• Molecule 1: Portal protein



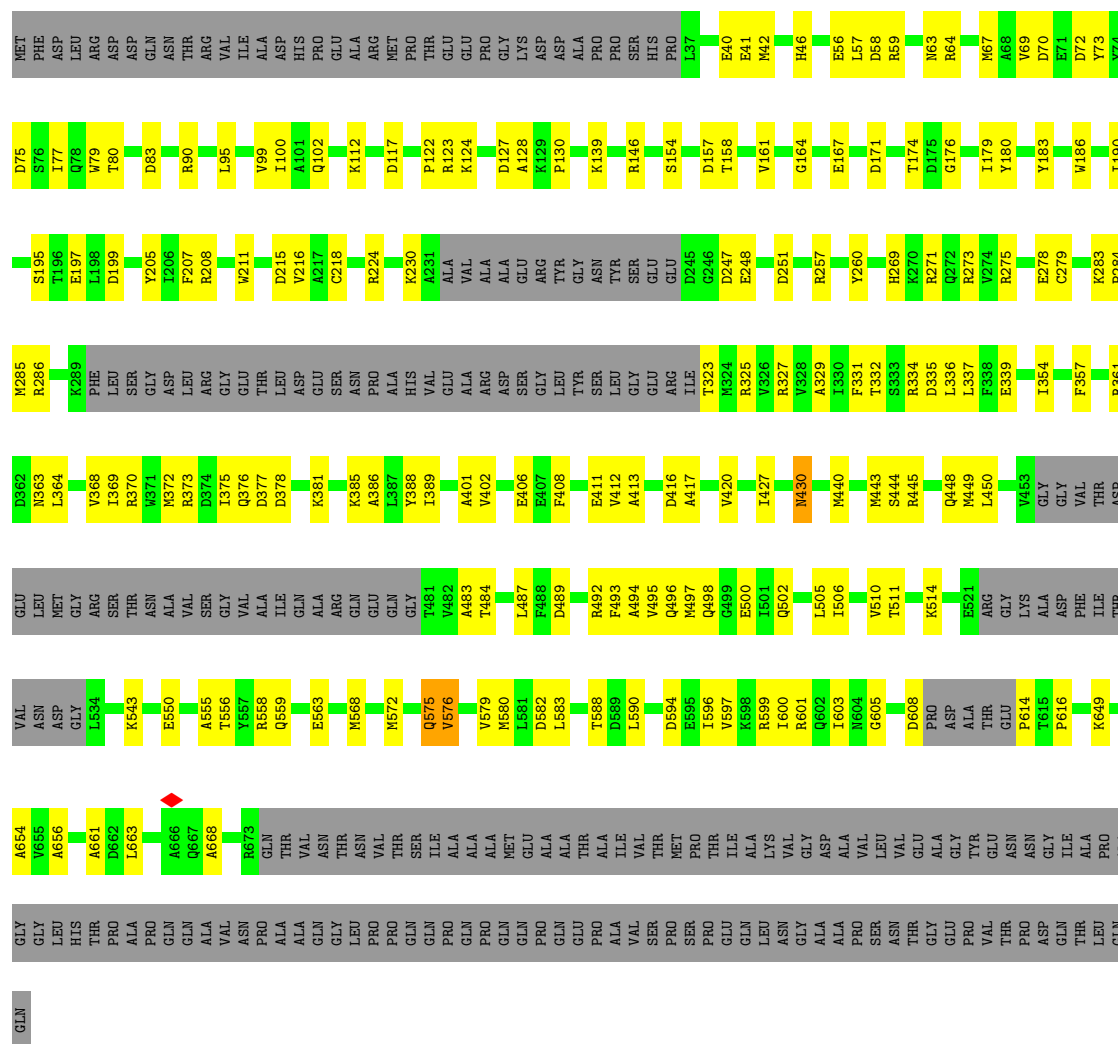




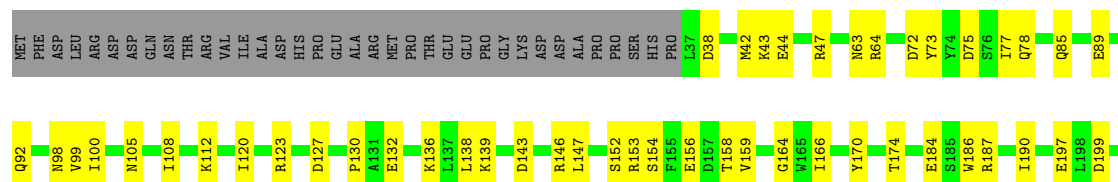
● Molecule 1: Portal protein

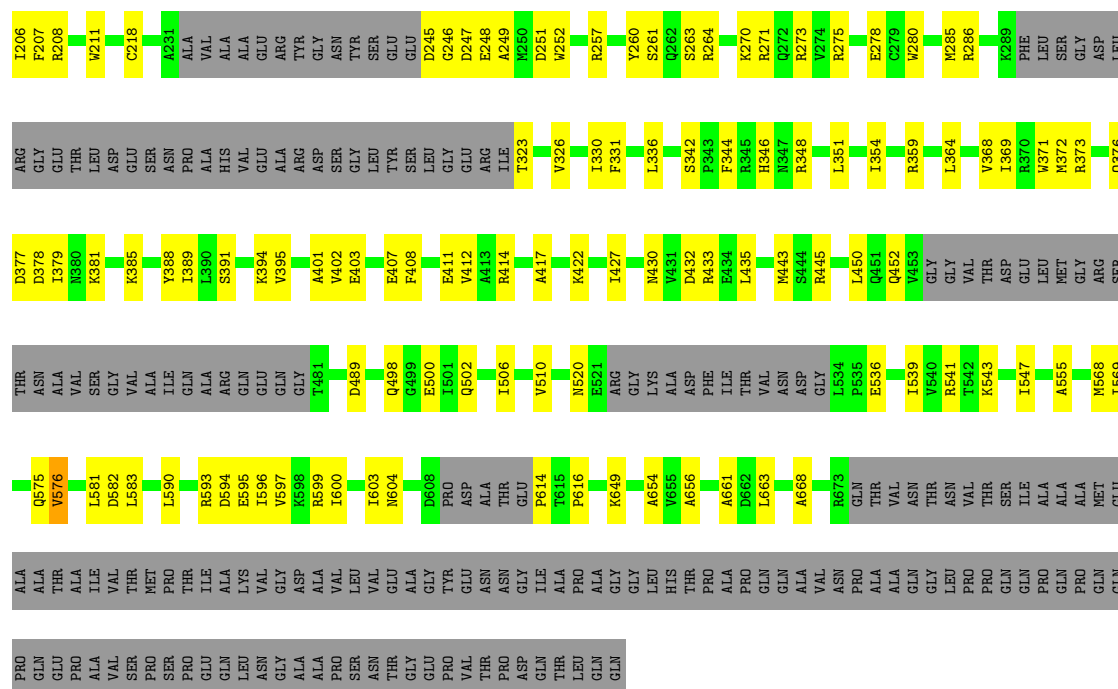


- Molecule 1: Portal protein



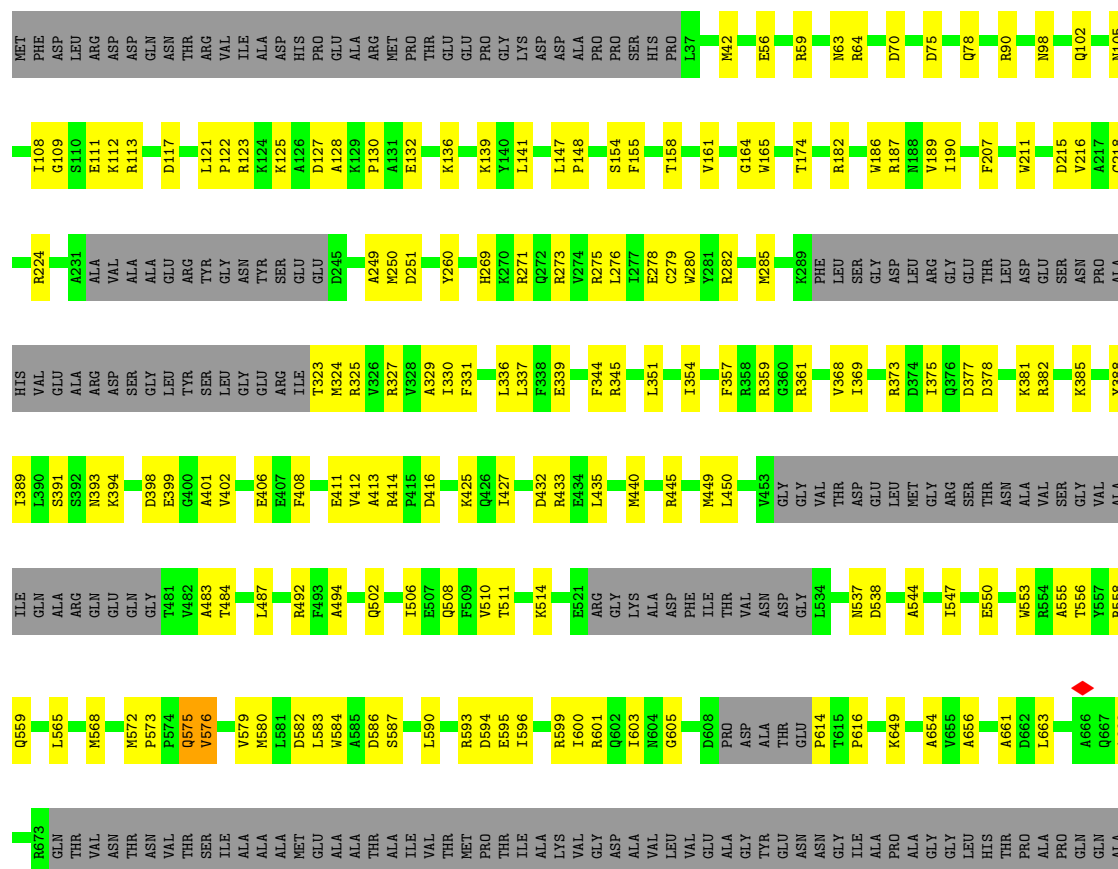
- Molecule 1: Portal protein

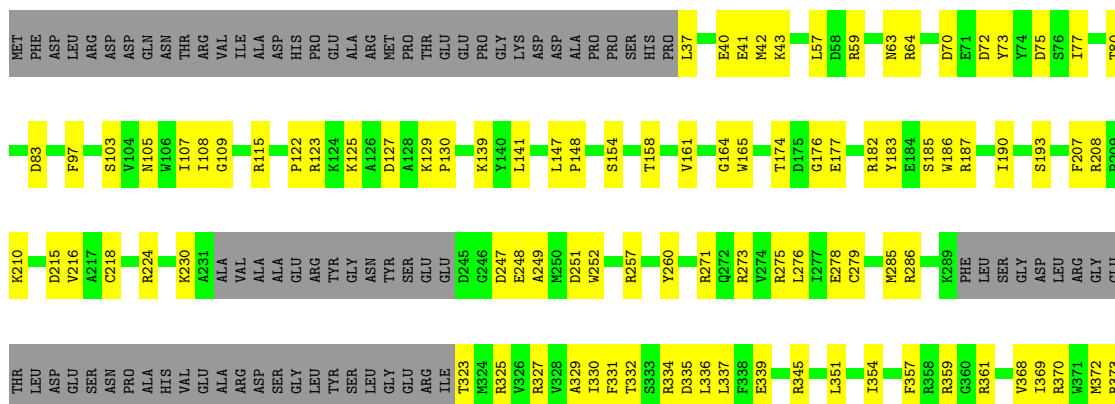
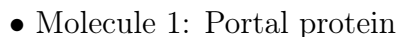
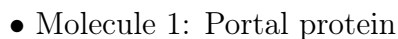




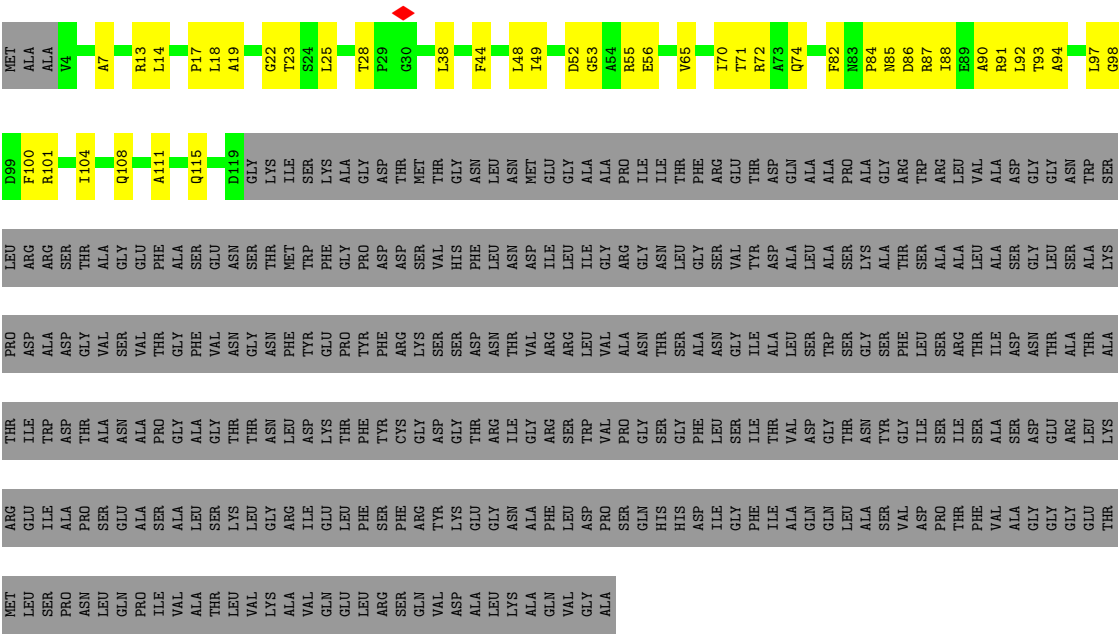
• Molecule 1: Portal protein

Chain o:

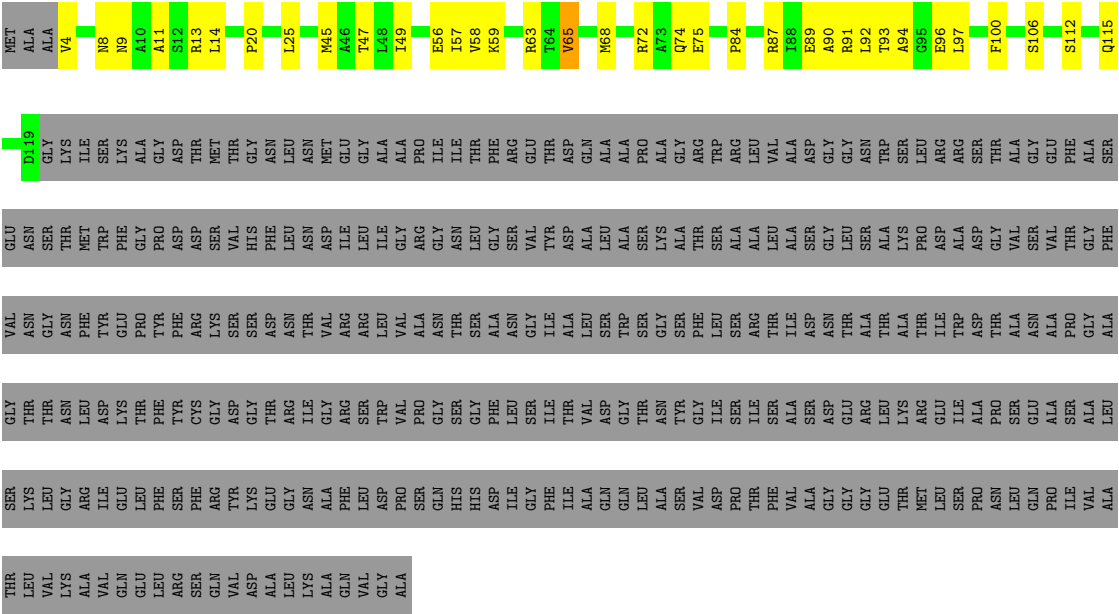




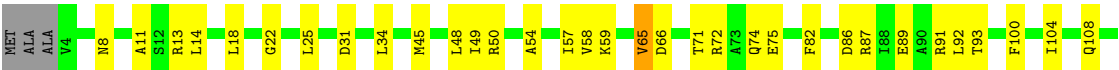




● Molecule 2: Putative tail fiber protein

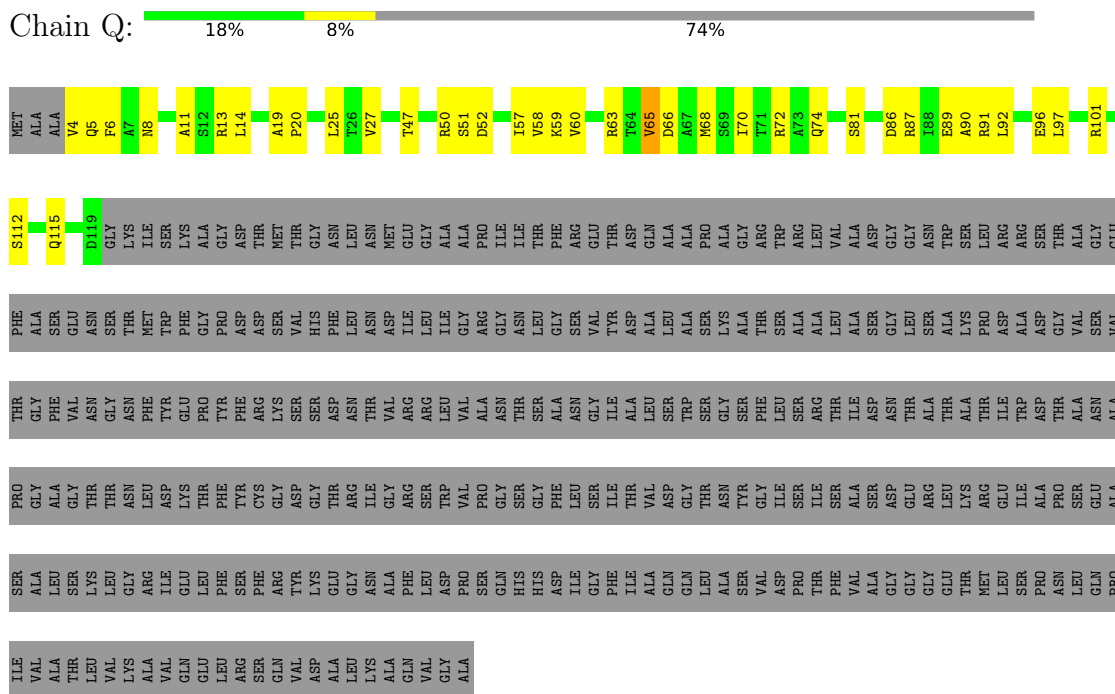


● Molecule 2: Putative tail fiber protein

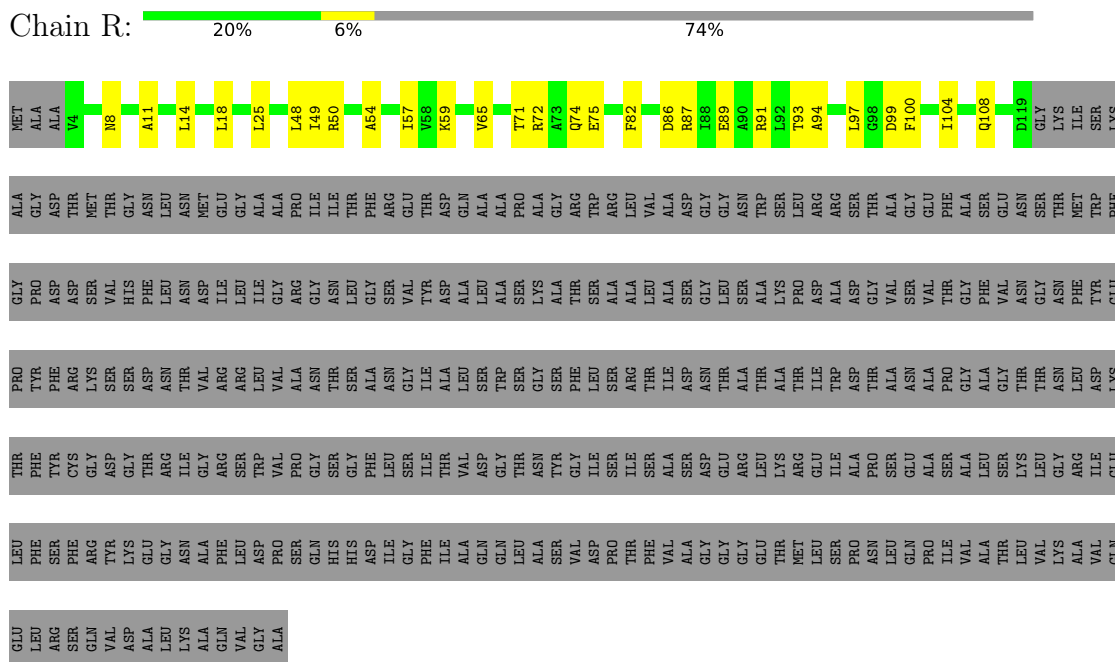




- Molecule 2: Putative tail fiber protein



- Molecule 2: Putative tail fiber protein



- Molecule 2: Putative tail fiber protein

MET	GLU	ILE	ARG	THR	PRO	LEU	T93
LEU	ILE	TRP	ASP	ALA	ASP	ARG	A94
SER	ALA	ASP	ASP	GLY	GLY	SER	L97
PRO	ASN	THR	VAL	VAL	THR	ALA	F100
LEU	SER	ALA	GLU	SER	THR	GLY	R101
GLN	ALA	ALA	VAL	VAL	THR	PHE	A111
PRO	SER	ALA	VAL	GLY	GLY	ALA	Q115
ILE	VAL	GLY	PHE	PHE	ASP	SER	D119
VAL	ALA	ALA	VAL	VAL	ASN	GLU	S24
THR	SER	GLY	THR	THR	ASN	ASN	LYS
LEU	LEU	THR	GLY	GLY	THR	SER	L25
LEU	LEU	THR	THR	ASN	THR	ILE	T28
VAL	VAL	ASP	THR	THR	THR	SER	F29
GLN	GLN	LYS	GLU	GLU	THR	LYS	G30
ASP	LEU	PHE	PRO	PRO	GLY	GLY	P36
LEU	LEU	TYR	PHE	PHE	ASP	THR	M45
ARG	ARG	CYS	ARG	ARG	ASP	THR	L48
GLN	GLN	GLY	LYS	LYS	SER	MET	I49
VAL	ALA	ASP	SER	SER	VAL	THR	D52
ASP	ALA	GLY	SER	SER	HIS	GLY	G53
LEU	GLU	THR	ASP	ASN	PHE	ASN	A54
LYS	LYS	ILE	THR	THR	ASN	ASN	R55
ALA	ALA	GLY	VAL	VAL	ASP	ILE	E56
GLN	PHE	ARG	ARG	ARG	ILE	GLU	I57
VAL	ASP	LEU	THR	LEU	GLY	GLY	N58
ALA	ASP	TRP	VAL	VAL	ASN	ILE	K59
GLN	HIS	GLY	THR	THR	ASN	THR	R63
VAL	HIS	SER	GLY	SER	LEU	ILE	T64
GLY	ASP	PHE	GLY	ASN	GLY	PHE	V65
VAL	ILE	ILE	LEU	ASN	SER	ARG	M68
ALA	ASP	GLY	GLY	GLY	VAL	THR	S69
GLN	PHE	ILE	ALA	ILE	ASP	ASP	I70
GLU	GLN	VAL	LEU	LEU	ALA	GLN	T71
LEU	GLN	GLY	SER	TRP	ASP	ALA	R72
LEU	LEU	THR	SER	SER	SER	ALA	A73
ALA	ALA	ASN	GLY	GLY	LYS	ALA	Q74
SER	SER	TYR	SER	SER	ALA	GLY	L80
VAL	VAL	GLY	PHE	PHE	THR	ARG	S81
ASP	ASP	ILE	LEU	LEU	ALA	TRP	F82
PRO	PRO	ILE	SER	SER	ALA	LEU	N85
THR	THR	ILE	ARG	THR	ALA	VAL	D86
PHE	PHE	SER	THR	THR	LEU	LEU	R87
VAL	VAL	ALA	ILE	ILE	ALA	ALA	I88
GLY	GLY	SER	ASP	ASN	SER	ASP	E89
ALA	GLY	ASP	GLY	THR	GLY	GLY	A90
GLY	GLY	GLY	ARG	ALA	SER	ASN	R91
THR	THR	LEU	THR	ALA	THR	SER	T92
ILE	LYS	LYS	LYS	ALA	LYS	THR	S93

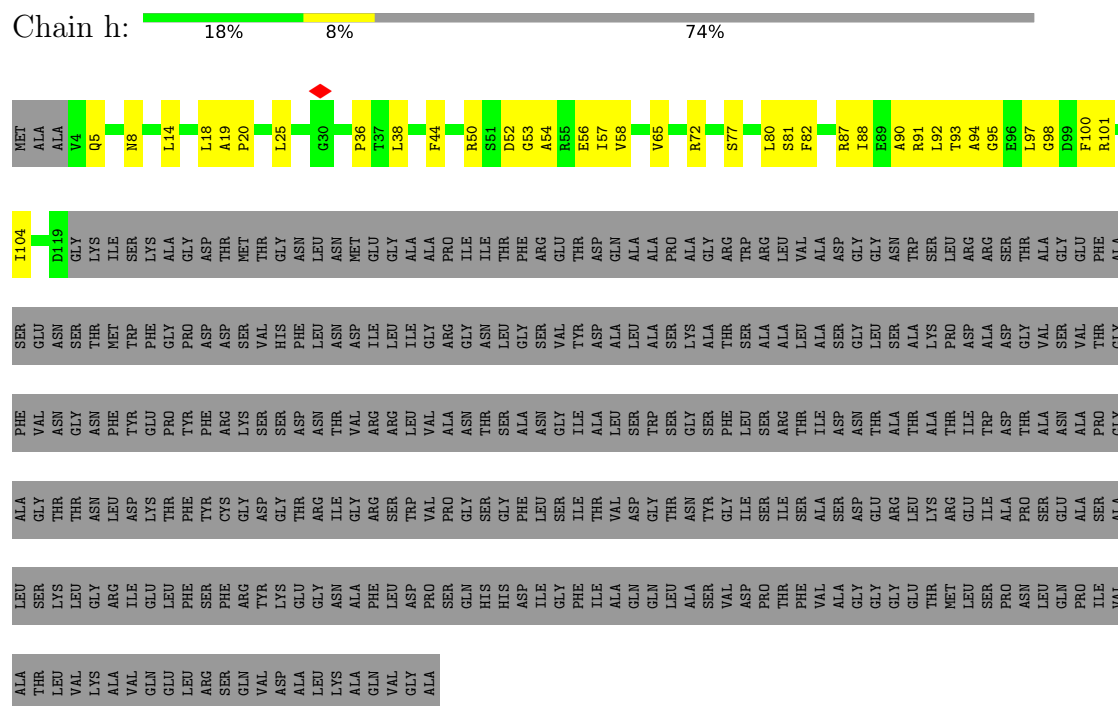
Chain Z: 17% 9% 74%

GLN	GLU	ASN	SER	GLY	R101	MET
PRO	ALA	ALA	VAL	GLU	ALA	ALA
ILE	SER	PRO	THR	PHE	S112	ALA
VAL	ALA	GLY	GLY	ALA	GLY	V4
ALA	LEU	ALA	PHE	SER	Q115	Q5
THR	SER	GLY	VAL	GLU	GLY	F6
LYS	LYS	THR	ASN	ASN	D119	A7
VAL	LEU	THR	GLY	SER	GLY	N8
ALA	GLY	LEU	ASN	THR	LYS	N9
ALA	ALA	LEU	PHE	MET	ILE	A10
VAL	ILE	ASP	TYR	TRP	SER	A11
GLN	GLU	LYS	GLU	PHE	LYS	S12
GLU	GLU	THR	PRO	GLY	ALA	R13
LEU	PHE	TYR	TYR	PRO	GLY	L14
ARG	SER	TYR	PHE	ASP	ASP	L14
GLN	PHE	CYS	ARG	ASP	THR	P20
GLN	ARG	GLY	LYS	SER	MET	THR
VAL	TYR	ASP	SER	VAL	THR	L25
ASP	ASP	GLY	SER	HIS	GLY	LYS
ALA	GLU	THR	ASP	PHE	ASN	W43
LEU	GLY	ARG	ASN	LEU	LEU	THR
LYS	ASN	ILE	THR	ASN	ASN	I49
ALA	ALA	GLY	VAL	ASP	MET	B50
GLN	PHE	ARG	ARG	ILE	GLU	THR
VAL	LEU	SER	ARG	LEU	GLY	R55
GLY	ASP	TRP	LEU	ILE	ALA	E56
PRO	PRO	VAL	VAL	GLY	ALA	I57
SER	SER	PRO	ALA	ARG	PRO	V58
GLN	GLN	GLY	ASN	GLY	ILE	K59
HIS	HIS	SER	THR	ASN	ILE	THR
ASP	ASP	PHE	SER	LEU	THR	S62
ILE	ILE	LEU	ASN	GLY	PHE	R63
PHE	PHE	ILE	GLY	VAL	ARG	T64
ILE	ILE	ILE	ILE	TYR	THR	V65
ALA	ALA	THR	ALA	ASP	ASP	THR
GLN	GLN	VAL	LEU	ALA	GLN	M68
LEU	GLN	ASP	SER	LEU	ALA	S69
LEU	GLN	GLY	TRP	ALA	ALA	I70
LEU	LEU	THR	SER	GLY	ALA	T71
ALA	ALA	ASN	GLY	SER	PRO	R72
SER	SER	LYS	LYS	ALA	ALA	A73
VAL	VAL	SER	SER	ALA	GLY	Q74
ASP	ASP	GLY	PHE	THR	ARG	E75
PRO	PRO	ILE	LEU	SER	TRP	THR
PHE	PHE	ILE	SER	ALA	LEU	S81
ALA	ALA	ILE	ARG	ALA	ALA	F82
VAL	VAL	SER	THR	LEU	VAL	N83
ALA	ALA	SER	ILE	SER	ALA	P84
GLY	GLY	SER	ASP	SER	ASP	R85
GLY	GLY	ASP	ASN	GLY	GLY	D86
GLY	GLY	ARG	ALA	SER	ASN	R87
GLU	GLU	LEU	THR	ALA	LYS	I88
THR	THR	LYS	ALA	LYS	TRP	E89
MET	MET	ARG	THR	PRO	SER	A90
LEU	LEU	GLU	ILE	ASP	LEU	R91
SER	SER	ILE	TRP	ALA	ARG	L92
PRO	PRO	ALA	ASP	ASP	SER	L97
ASN	ASN	PRO	THR	GLY	THR	G98
LEU	LEU	SER	VAL	VAL	ALA	ALA

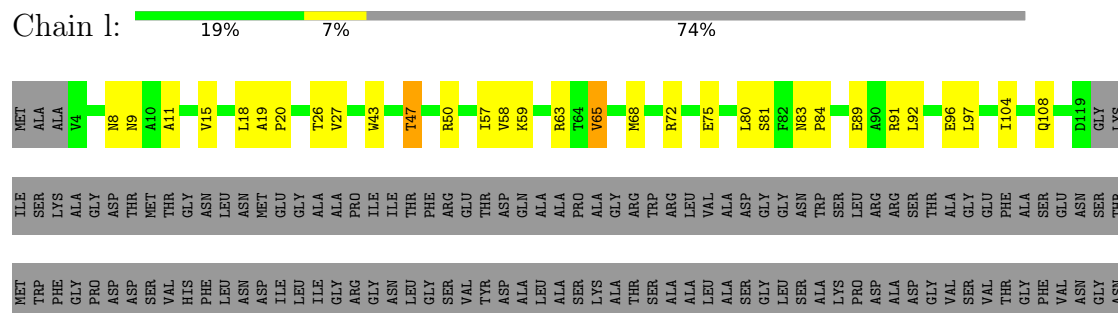
Chain d: 18% 8% 74%

MET	ALA	ALA	V4	Q5	F6	A7	N8	N9	A10	A11	S12	R13	L14	L18	A19	P20	D31	L34	T37	L38	W43	R63	T64	V65	D66	I70	Q74	E76	S81	F82	D86	R87	L88	E89	R91	L92	T93	L97	F100
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- Molecule 2: Putative tail fiber protein



- Molecule 2: Putative tail fiber protein





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

● Molecule 2: Putative tail fiber protein



MET	ALA	ALA	V4	Q5	P6	A7	N8	N9	A10	A11	L18	A19	P20	L25	T26	V27	L34	L38	V43	F44	T47	L48	L49	R50	S51	D52	I57	V58	K59	R63	T64	V65	D66	A67	M68	S69	T70	T71	R72	A73	Q74	F82	N83	P84	R87	I88	E89	L92		
T93	A94	G95	E96	L97	G98	A7	R101	N9	D119	GLY	LYS	ILE	SER	LYS	ALA	GLY	PRO	ASP	ASP	THR	MET	THR	GLY	ASN	LEU	ASN	ILE	GLY	PHE	ARG	GLY	ASP	GLN	ALA	ALA	PRO	LYS	ALA	GLY	THR	THR	ALA	ASP	GLY	GLY	ASN	TRP	SER	LEU	ARG
SER	THR	ALA	GLY	GLU	PHE	ALA	SER	GLU	ASN	SER	THR	MET	PHE	GLY	ASP	THR	VAL	HIS	PHE	ASN	VAL	ILE	GLY	LEU	ASN	ASP	GLY	LEU	GLY	TYR	ASP	ALA	ALA	ALA	LYS	ALA	ALA	THR	THR	ALA	ALA	SER	GLY	LEU	ASN	LYS	PRO	ASP	ALA	
ASP	GLY	VAL	SER	VAL	THR	GLY	PHE	ASN	THR	GLY	ASP	GLU	PRO	THR	PHE	TYR	ARG	SER	SER	VAL	SER	ARG	THR	ILE	GLY	ASN	THR	SER	ALA	ALA	THR	VAL	LEU	ALA	ASN	GLY	ILE	SER	GLY	PHE	THR	THR	ASN	THR	THR	ILE	THR	TRP		
ASP	THR	ALA	ASN	ALA	PRO	GLY	ALA	THR	ASN	ASP	LYS	THR	GLY	PHE	TYR	CYS	GLY	ASP	GLY	THR	GLY	THR	ARG	THR	VAL	GLY	THR	TRP	VAL	GLY	ASN	GLY	VAL	ILE	THR	ASN	TYR	GLY	PHE	THR	THR	ASN	THR	THR	ALA	LYS	ARG	GLU	ILE	
ALA	PRO	SER	GLU	ALA	SER	ILE	LEU	VAL	GLY	ARG	ILE	GLU	PHE	LEU	SER	PHE	ASN	ALA	ALA	ALA	PHE	LEU	ASP	PRO	GLN	HIS	ASP	ILE	PHE	GLY	ASN	GLY	PHE	ILE	THR	SER	VAL	ALA	GLY	GLY	THR	MET	THR	SER	LEU	SER				
PRO	ASN	LEU	GLN	PRO	PRO	ILE	VAL	ALA	THR	VAL	LYS	ALA	VAL	GLU	GLU	ARG	VAL	VAL	VAL	VAL	ILE	ALA	ALA	LYS	ALA	GLN	VAL	GLY	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA		

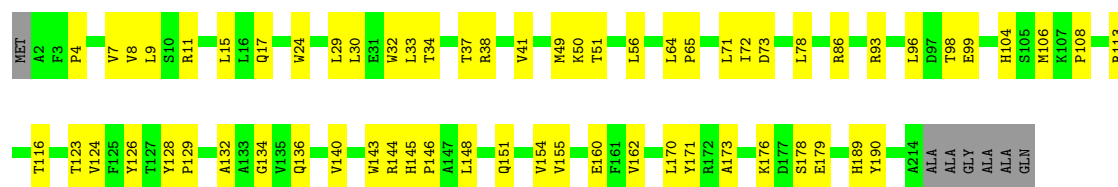
● Molecule 2: Putative tail fiber protein



ALA	VAL	ARG	LEU	ILE	ASP	PHE	TYR	MET	ILE	MET	ALA	VAL	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY	ASP	THR	ASN	GLY</
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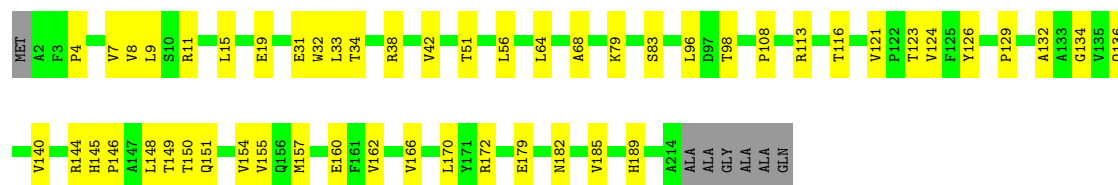
● Molecule 3: Virion associated protein

Chain 2:  68% 29% .



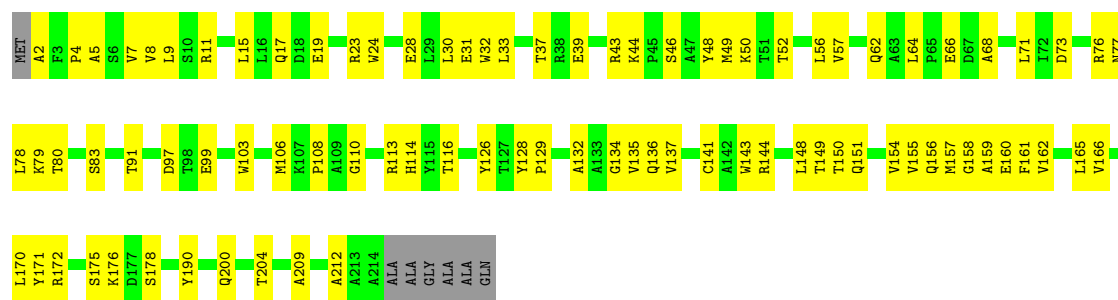
• Molecule 3: Virion associated protein

Chain 5:  73% 24% .



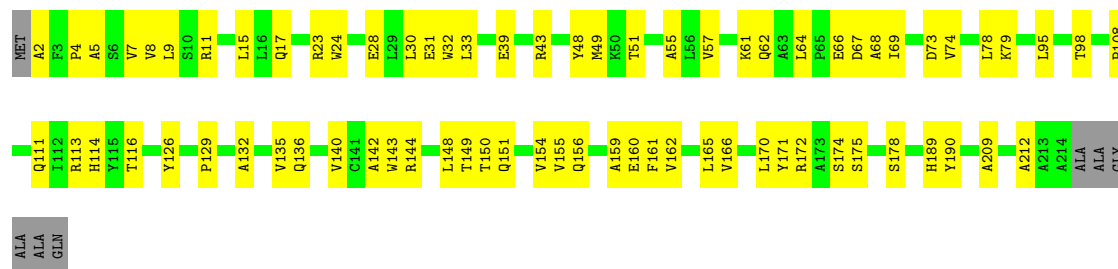
• Molecule 3: Virion associated protein

Chain T:  57% 40% .



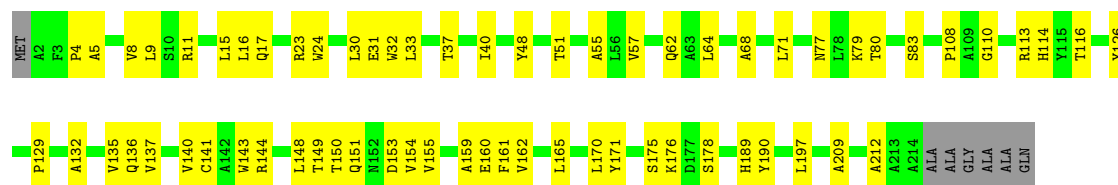
• Molecule 3: Virion associated protein

Chain X:  64% 33% .



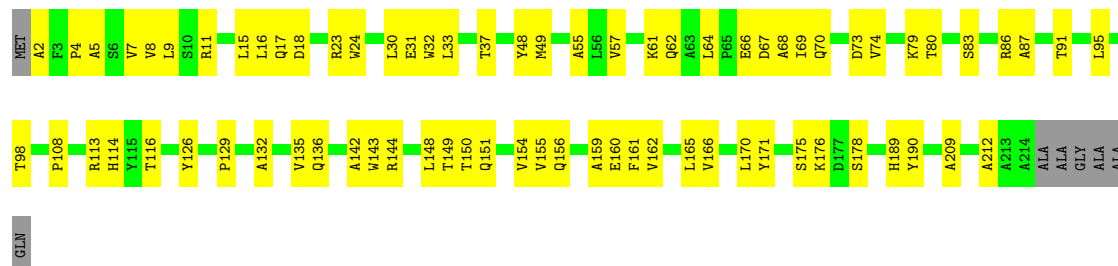
• Molecule 3: Virion associated protein

Chain b:  67% 30% .



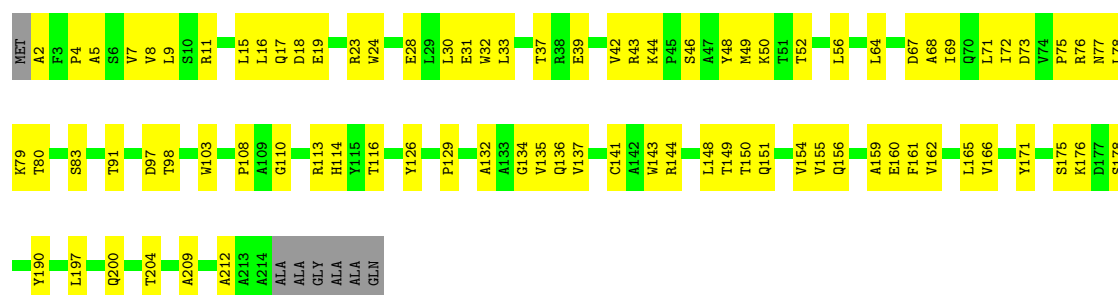
• Molecule 3: Virion associated protein

Chain f: 63% 34% .



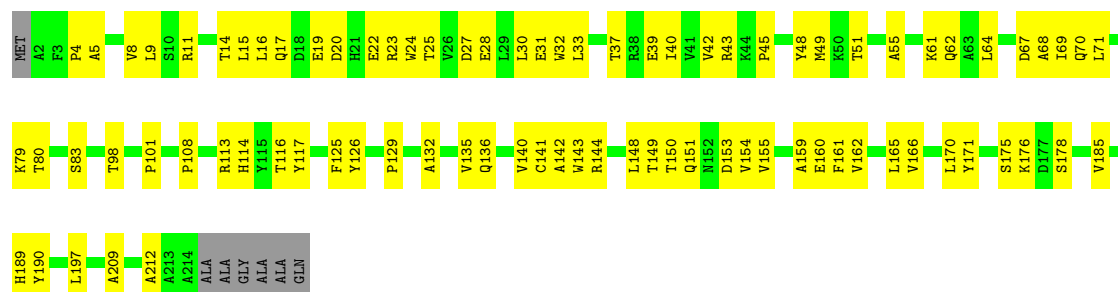
• Molecule 3: Virion associated protein

Chain j: 58% 39% .



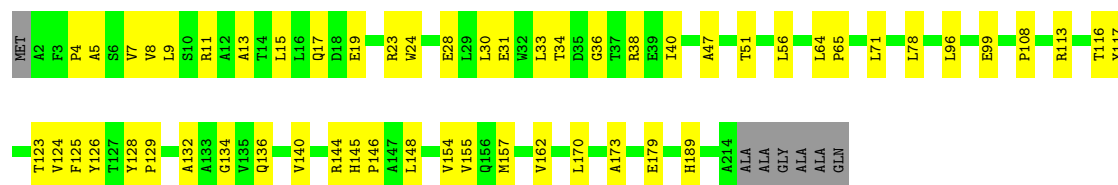
• Molecule 3: Virion associated protein

Chain n: 59% 38% .



• Molecule 3: Virion associated protein

Chain q: 72% 25% .



• Molecule 3: Virion associated protein



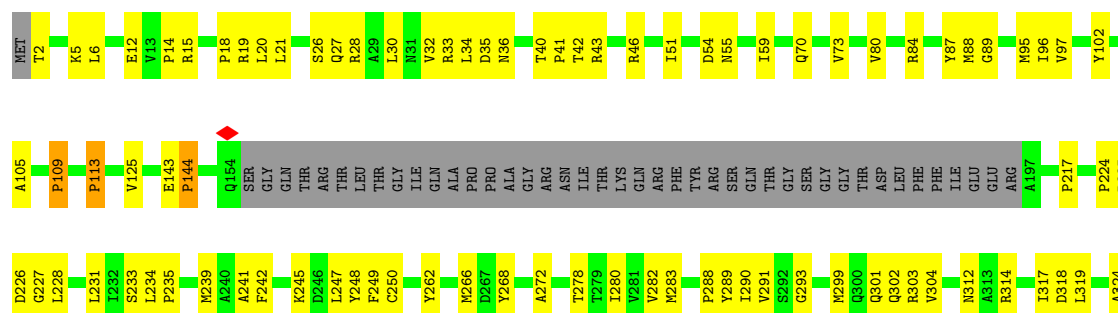
• Molecule 3: Virion associated protein



• Molecule 3: Virion associated protein

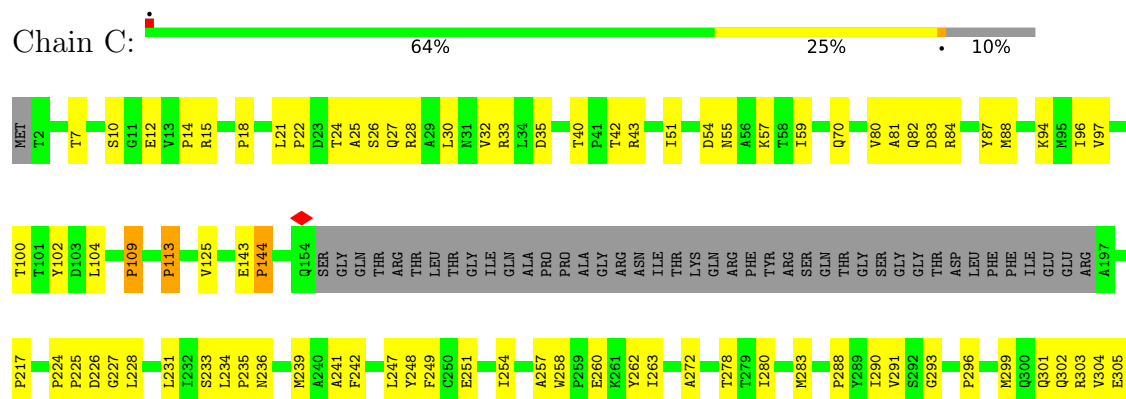


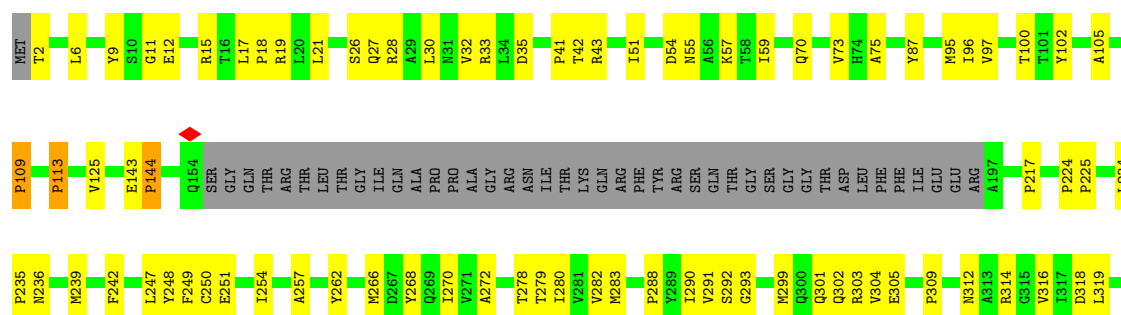
• Molecule 4: Virion-associated phage protein

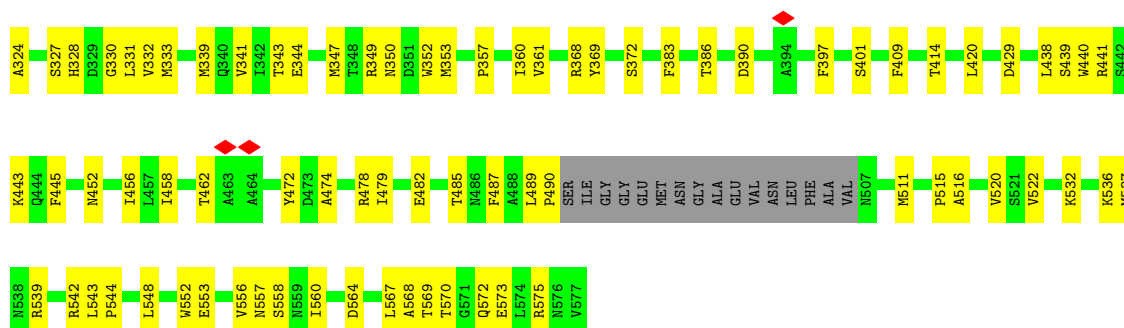


- Molecule 4: Virion-associated phage protein

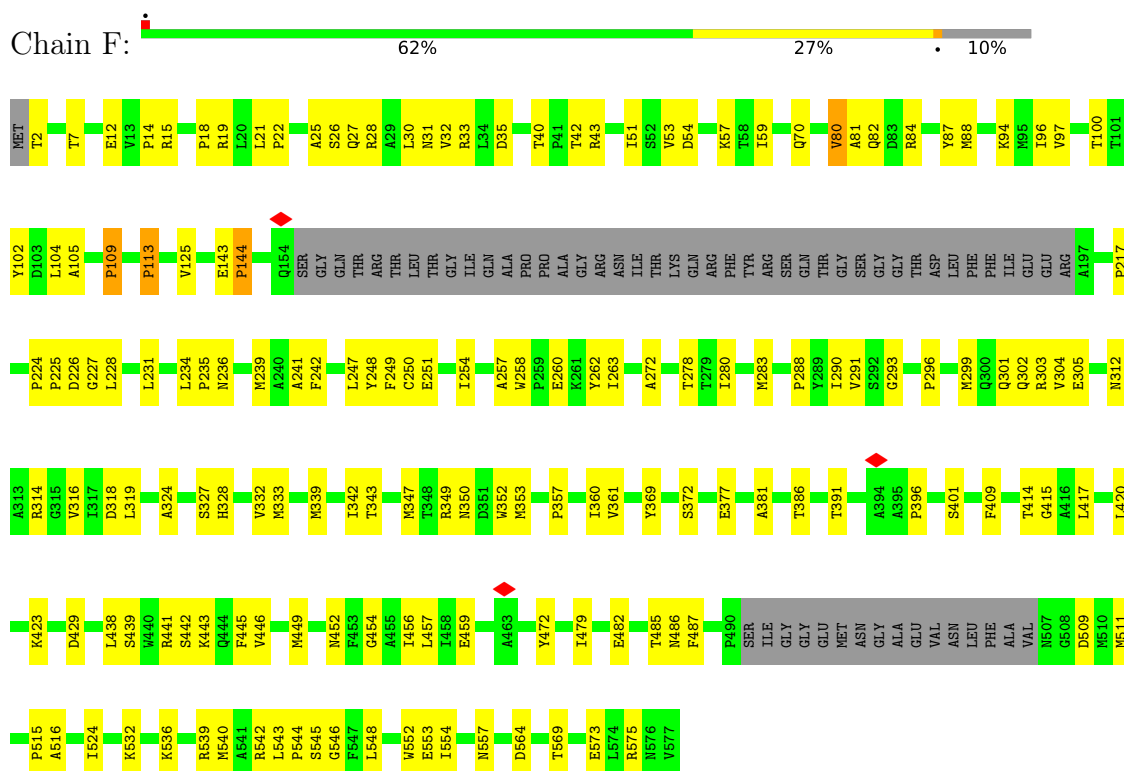
- Molecule 4: Virion-associated phage protein



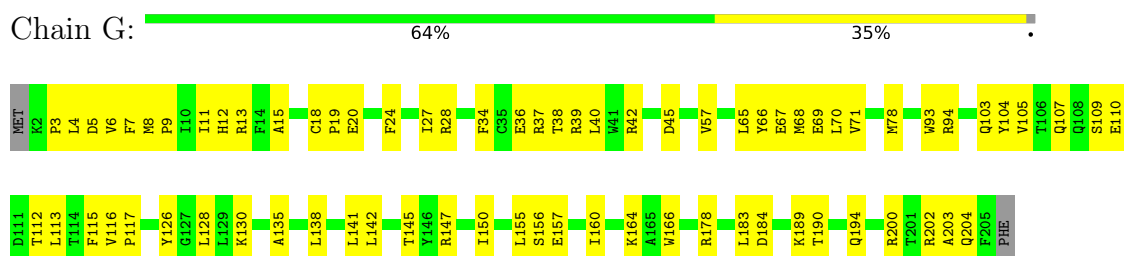




• Molecule 4: Virion-associated phage protein

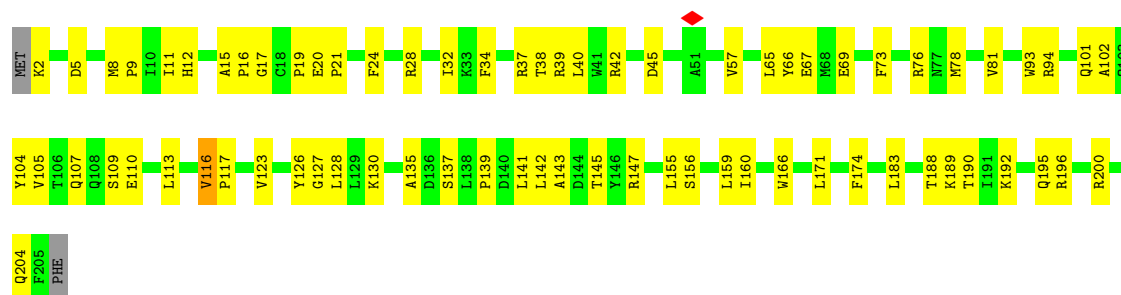


• Molecule 5: gp81 of phage GP4



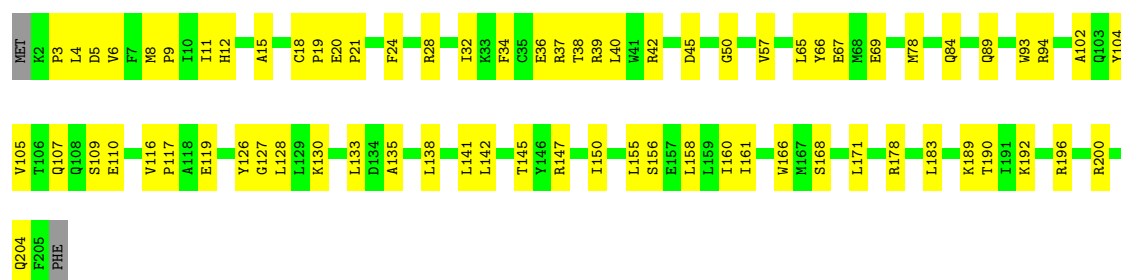
• Molecule 5: gp81 of phage GP4





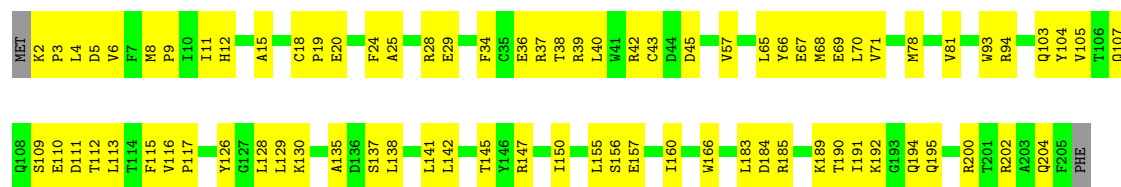
- Molecule 5: gp81 of phage GP4

Chain I: 64% 35% .



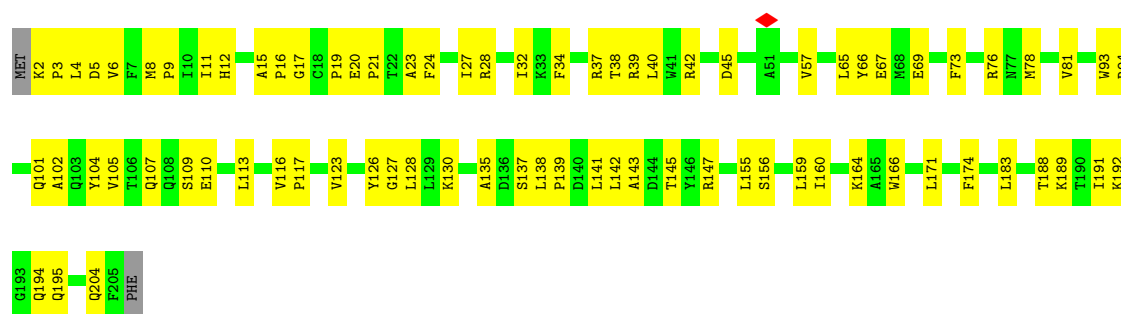
- Molecule 5: gp81 of phage GP4

Chain J: 61% 38% .



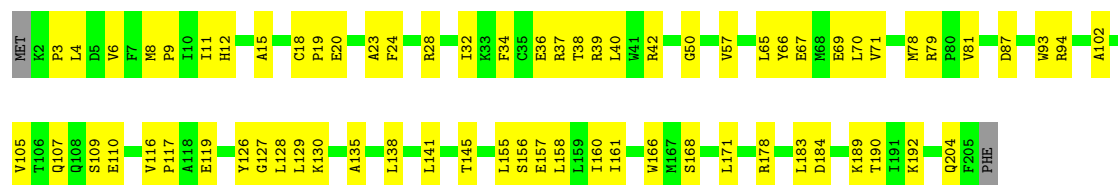
- Molecule 5: gp81 of phage GP4

Chain K: 61% 38% .

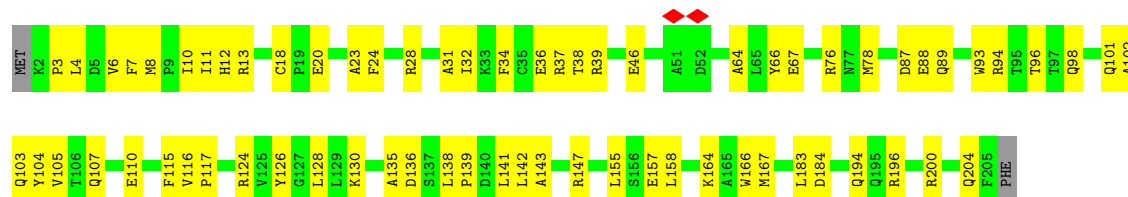


- Molecule 5: gp81 of phage GP4

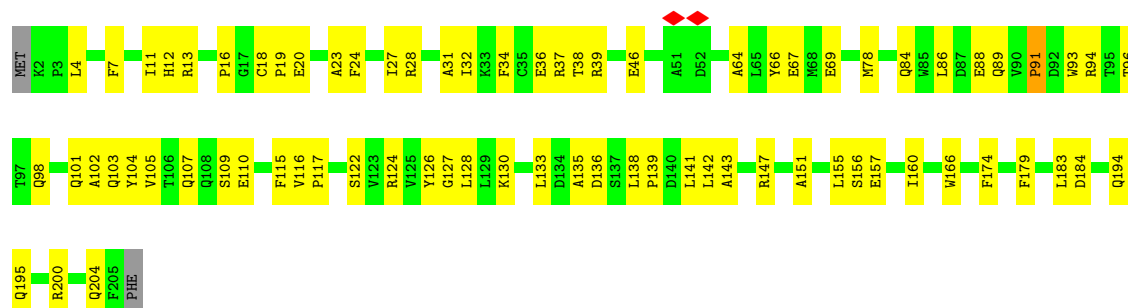
Chain L: 66% 33% .



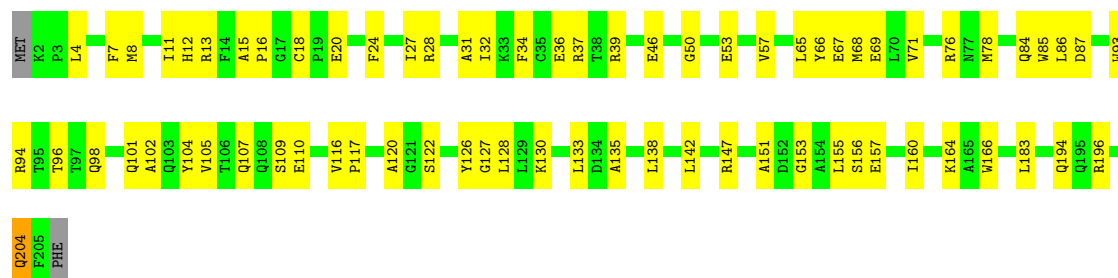
- Molecule 5: gp81 of phage GP4



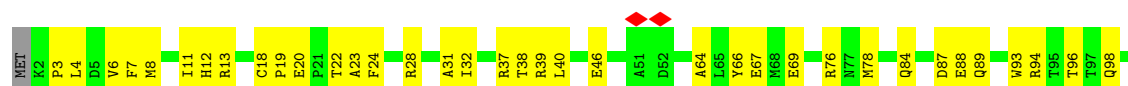
- Molecule 5: gp81 of phage GP4

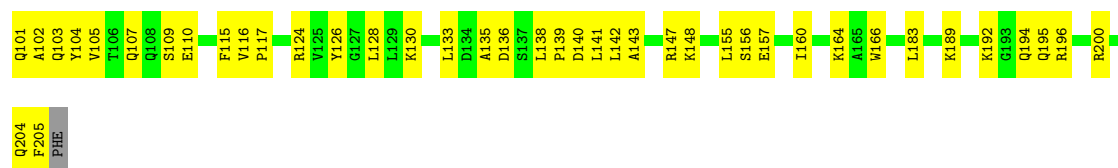


- Molecule 5: gp81 of phage GP4



- Molecule 5: gp81 of phage GP4





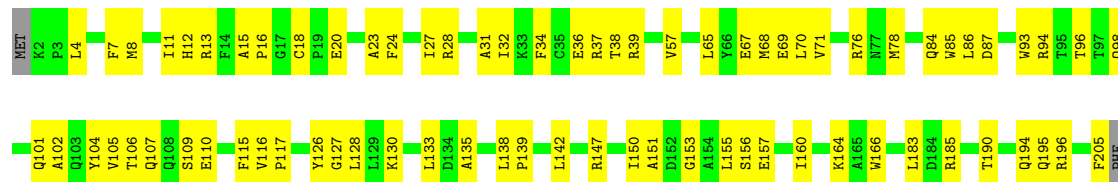
- Molecule 5: gp81 of phage GP4

Chain i:



- Molecule 5: gp81 of phage GP4

Chain m:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39883	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	100	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	31.901	Depositor
Minimum map value	-13.810	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.650	Depositor
Recommended contour level	3	Depositor
Map size (Å)	508.0, 508.0, 508.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.27, 1.27, 1.27	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.16	0/4368	0.41	4/5900 (0.1%)
1	3	0.14	0/4368	0.39	4/5900 (0.1%)
1	6	0.16	0/4368	0.40	4/5900 (0.1%)
1	U	0.14	0/4368	0.38	4/5900 (0.1%)
1	Y	0.17	0/4368	0.41	4/5900 (0.1%)
1	c	0.15	0/4368	0.39	4/5900 (0.1%)
1	g	0.15	0/4368	0.41	4/5900 (0.1%)
1	k	0.14	0/4368	0.37	2/5900 (0.0%)
1	o	0.16	0/4368	0.40	4/5900 (0.1%)
1	r	0.15	0/4368	0.40	4/5900 (0.1%)
1	u	0.17	0/4368	0.42	4/5900 (0.1%)
1	x	0.15	0/4368	0.39	4/5900 (0.1%)
2	1	0.16	0/840	0.41	0/1141
2	4	0.20	0/840	0.52	1/1141 (0.1%)
2	7	0.20	0/840	0.51	0/1141
2	M	0.19	0/840	0.46	0/1141
2	N	0.17	0/840	0.47	0/1141
2	O	0.17	0/840	0.49	0/1141
2	P	0.15	0/840	0.41	0/1141
2	Q	0.15	0/840	0.42	0/1141
2	R	0.17	0/840	0.48	0/1141
2	V	0.16	0/840	0.43	0/1141
2	Z	0.18	0/840	0.51	1/1141 (0.1%)
2	d	0.18	0/840	0.51	0/1141
2	h	0.19	0/840	0.45	0/1141
2	l	0.18	0/840	0.47	0/1141
2	p	0.16	0/840	0.43	0/1141
2	s	0.14	0/840	0.41	0/1141
2	v	0.19	0/840	0.54	1/1141 (0.1%)
2	y	0.16	0/840	0.44	0/1141
3	2	0.17	0/1653	0.38	0/2265
3	5	0.17	0/1653	0.38	0/2265
3	T	0.18	0/1653	0.44	0/2265
3	X	0.18	0/1653	0.41	0/2265

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	b	0.18	0/1653	0.43	0/2265
3	f	0.19	0/1653	0.43	0/2265
3	j	0.19	0/1653	0.43	0/2265
3	n	0.19	0/1653	0.44	0/2265
3	q	0.17	0/1653	0.37	0/2265
3	t	0.17	0/1653	0.39	0/2265
3	w	0.16	0/1653	0.37	0/2265
3	z	0.16	0/1653	0.37	0/2265
4	A	0.17	0/3893	0.46	4/5306 (0.1%)
4	B	0.16	0/3893	0.45	4/5306 (0.1%)
4	C	0.17	0/3893	0.46	4/5306 (0.1%)
4	D	0.17	0/3893	0.46	4/5306 (0.1%)
4	E	0.17	0/3893	0.46	4/5306 (0.1%)
4	F	0.17	0/3893	0.46	4/5306 (0.1%)
5	G	0.18	0/1648	0.40	0/2241
5	H	0.19	0/1648	0.41	0/2241
5	I	0.19	0/1648	0.42	0/2241
5	J	0.18	0/1648	0.40	0/2241
5	K	0.19	0/1648	0.42	0/2241
5	L	0.19	0/1648	0.41	0/2241
5	S	0.19	0/1648	0.39	0/2241
5	W	0.20	0/1648	0.43	1/2241 (0.0%)
5	a	0.18	0/1648	0.38	0/2241
5	e	0.18	0/1648	0.39	0/2241
5	i	0.20	0/1648	0.41	1/2241 (0.0%)
5	m	0.18	0/1648	0.38	0/2241
All	All	0.17	0/130506	0.42	75/177246 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	r	0	1
4	F	0	1
5	H	0	1
All	All	0	3

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	113	PRO	N-CA-CB	7.96	111.60	103.25
4	E	113	PRO	N-CA-CB	7.93	111.58	103.25
4	B	113	PRO	N-CA-CB	7.91	111.55	103.25
4	C	113	PRO	N-CA-CB	7.89	111.53	103.25
4	D	113	PRO	N-CA-CB	7.88	111.52	103.25
4	F	113	PRO	N-CA-CB	7.87	111.52	103.25
4	C	217	PRO	N-CA-CB	7.80	110.22	103.36
4	D	217	PRO	N-CA-CB	7.80	110.22	103.36
4	F	217	PRO	N-CA-CB	7.80	110.22	103.36
4	A	217	PRO	N-CA-CB	7.79	110.22	103.36
4	D	109	PRO	N-CA-CB	7.79	111.43	103.25
4	B	109	PRO	N-CA-CB	7.79	111.42	103.25
4	F	109	PRO	N-CA-CB	7.77	111.41	103.25
4	A	109	PRO	N-CA-CB	7.76	111.40	103.25
4	E	109	PRO	N-CA-CB	7.75	111.39	103.25
4	B	217	PRO	N-CA-CB	7.72	110.16	103.36
4	C	109	PRO	N-CA-CB	7.72	111.36	103.25
4	E	217	PRO	N-CA-CB	7.71	110.14	103.36
2	4	84	PRO	CA-N-CD	-7.70	101.22	112.00
2	Z	84	PRO	CA-N-CD	-7.50	101.50	112.00
4	B	144	PRO	N-CA-CB	7.12	110.72	103.25
4	A	144	PRO	N-CA-CB	7.10	110.70	103.25
4	D	144	PRO	N-CA-CB	7.09	110.69	103.25
4	F	144	PRO	N-CA-CB	7.08	110.69	103.25
4	E	144	PRO	N-CA-CB	7.07	110.68	103.25
4	C	144	PRO	N-CA-CB	7.07	110.67	103.25
1	c	614	PRO	N-CA-CB	6.77	110.44	103.00
1	o	614	PRO	N-CA-CB	6.76	110.44	103.00
1	6	614	PRO	N-CA-CB	6.76	110.44	103.00
1	g	614	PRO	N-CA-CB	6.76	110.44	103.00
1	3	614	PRO	N-CA-CB	6.75	110.43	103.00
1	0	614	PRO	N-CA-CB	6.75	110.42	103.00
1	U	614	PRO	N-CA-CB	6.75	110.42	103.00
1	x	614	PRO	N-CA-CB	6.74	110.41	103.00
1	u	614	PRO	N-CA-CB	6.74	110.41	103.00
1	Y	614	PRO	N-CA-CB	6.74	110.41	103.00
1	r	614	PRO	N-CA-CB	6.73	110.41	103.00
1	k	614	PRO	N-CA-CB	6.72	110.39	103.00
2	v	84	PRO	CA-N-CD	-6.71	102.60	112.00
5	W	91	PRO	CA-N-CD	-6.24	103.26	112.00
5	i	91	PRO	CA-N-CD	-6.21	103.31	112.00
1	r	616	PRO	N-CA-CB	6.15	110.09	103.33
1	3	616	PRO	N-CA-CB	6.13	110.07	103.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	616	PRO	N-CA-CB	6.13	110.07	103.33
1	U	616	PRO	N-CA-CB	6.10	110.04	103.33
1	k	616	PRO	N-CA-CB	6.09	110.03	103.33
1	x	616	PRO	N-CA-CB	6.07	110.01	103.33
1	g	616	PRO	N-CA-CB	5.95	110.10	103.44
1	Y	616	PRO	N-CA-CB	5.93	110.08	103.44
1	u	616	PRO	N-CA-CB	5.93	110.08	103.44
1	0	616	PRO	N-CA-CB	5.91	110.06	103.44
1	6	616	PRO	N-CA-CB	5.91	110.06	103.44
1	o	616	PRO	N-CA-CB	5.91	110.06	103.44
1	0	575	GLN	CA-C-N	5.80	132.41	121.97
1	0	575	GLN	C-N-CA	5.80	132.41	121.97
1	g	575	GLN	CA-C-N	5.77	132.35	121.97
1	g	575	GLN	C-N-CA	5.77	132.35	121.97
1	U	575	GLN	CA-C-N	5.70	132.23	121.97
1	U	575	GLN	C-N-CA	5.70	132.23	121.97
1	Y	575	GLN	CA-C-N	5.60	132.06	121.97
1	Y	575	GLN	C-N-CA	5.60	132.06	121.97
1	u	575	GLN	CA-C-N	5.60	132.05	121.97
1	u	575	GLN	C-N-CA	5.60	132.05	121.97
1	6	575	GLN	CA-C-N	5.58	132.00	121.97
1	6	575	GLN	C-N-CA	5.58	132.00	121.97
1	r	575	GLN	CA-C-N	5.55	131.96	121.97
1	r	575	GLN	C-N-CA	5.55	131.96	121.97
1	o	575	GLN	CA-C-N	5.49	131.85	121.97
1	o	575	GLN	C-N-CA	5.49	131.85	121.97
1	c	575	GLN	CA-C-N	5.15	131.24	121.97
1	c	575	GLN	C-N-CA	5.15	131.24	121.97
1	x	575	GLN	CA-C-N	5.08	131.11	121.97
1	x	575	GLN	C-N-CA	5.08	131.11	121.97
1	3	575	GLN	CA-C-N	5.05	131.06	121.97
1	3	575	GLN	C-N-CA	5.05	131.06	121.97

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	80	VAL	Peptide
5	H	116	VAL	Peptide
1	r	558	ARG	Sidechain

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	0	4297	0	4103	148	0
1	3	4297	0	4103	141	0
1	6	4297	0	4103	138	0
1	U	4297	0	4103	148	0
1	Y	4297	0	4103	160	0
1	c	4297	0	4103	142	0
1	g	4297	0	4103	140	0
1	k	4297	0	4103	123	0
1	o	4297	0	4103	138	0
1	r	4297	0	4103	131	0
1	u	4297	0	4103	137	0
1	x	4297	0	4103	134	0
2	1	829	0	810	35	0
2	4	829	0	810	29	0
2	7	829	0	810	27	0
2	M	829	0	810	33	0
2	N	829	0	810	26	0
2	O	829	0	810	26	0
2	P	829	0	810	35	0
2	Q	829	0	810	35	0
2	R	829	0	810	22	0
2	V	829	0	810	33	0
2	Z	829	0	810	34	0
2	d	829	0	810	26	0
2	h	829	0	810	28	0
2	l	829	0	810	23	0
2	p	829	0	810	24	0
2	s	829	0	810	34	0
2	v	829	0	810	35	0
2	y	829	0	810	22	0
3	2	1615	0	1565	56	0
3	5	1615	0	1565	47	0
3	T	1615	0	1565	69	0
3	X	1615	0	1565	61	0
3	b	1615	0	1565	55	0
3	f	1615	0	1565	66	0
3	j	1615	0	1565	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	n	1615	0	1565	73	0
3	q	1615	0	1565	48	0
3	t	1615	0	1565	57	0
3	w	1615	0	1565	56	0
3	z	1615	0	1565	52	0
4	A	3812	0	3582	122	0
4	B	3812	0	3582	120	0
4	C	3812	0	3582	117	0
4	D	3812	0	3582	120	0
4	E	3812	0	3582	122	0
4	F	3812	0	3582	137	0
5	G	1611	0	1583	64	0
5	H	1611	0	1583	61	0
5	I	1611	0	1583	65	0
5	J	1611	0	1583	71	0
5	K	1611	0	1583	71	0
5	L	1611	0	1583	61	0
5	S	1611	0	1583	59	0
5	W	1611	0	1583	68	0
5	a	1611	0	1583	65	0
5	e	1611	0	1583	71	0
5	i	1611	0	1583	67	0
5	m	1611	0	1583	71	0
All	All	128070	0	123084	3798	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 15.

All (3798) 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:r:323:THR:N	1:u:174:THR:HG1	1.41	1.17
1:g:323:THR:N	1:k:174:THR:HG1	1.46	1.12
1:6:323:THR:N	1:U:174:THR:HG1	1.48	1.10
1:U:323:THR:N	1:Y:174:THR:HG1	1.51	1.07
1:c:323:THR:N	1:g:174:THR:HG1	1.52	1.07
1:0:174:THR:HG1	1:x:323:THR:N	1.54	1.05
1:0:323:THR:N	1:3:174:THR:HG1	1.56	1.02
1:k:323:THR:N	1:o:174:THR:HG1	1.56	1.01
1:o:323:THR:N	1:r:174:THR:HG1	1.61	0.97
5:m:116:VAL:HG13	5:m:117:PRO:HD3	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:323:THR:N	1:c:174:THR:HG1	1.64	0.94
1:u:323:THR:N	1:x:174:THR:HG1	1.66	0.93
1:3:323:THR:N	1:6:174:THR:HG1	1.67	0.93
5:H:116:VAL:HG13	5:H:117:PRO:HD3	1.53	0.91
5:m:78:MET:HG2	5:m:105:VAL:HG23	1.54	0.90
5:e:139:PRO:HG2	5:e:142:LEU:HD13	1.53	0.88
5:i:116:VAL:HG13	5:i:117:PRO:HD3	1.54	0.86
4:B:542:ARG:HB3	3:X:23:ARG:HG3	1.56	0.86
5:S:139:PRO:HG2	5:S:142:LEU:HD13	1.58	0.85
4:D:456:ILE:HD11	4:D:543:LEU:HG	1.58	0.84
4:A:88:MET:HE3	4:A:228:LEU:HB3	1.58	0.84
1:o:122:PRO:HG2	1:o:125:LYS:HG2	1.60	0.84
5:J:78:MET:HG2	5:J:105:VAL:HG23	1.58	0.84
5:e:78:MET:HG2	5:e:105:VAL:HG23	1.58	0.83
1:c:569:ILE:HD13	1:c:581:LEU:HD23	1.60	0.83
2:d:18:LEU:HB3	2:d:82:PHE:HB2	1.61	0.83
5:S:39:ARG:HB3	5:S:128:LEU:HD13	1.60	0.83
5:G:78:MET:HG2	5:G:105:VAL:HG23	1.59	0.82
4:E:542:ARG:HB3	3:f:23:ARG:HG3	1.59	0.82
2:7:18:LEU:HB3	2:7:82:PHE:HB2	1.61	0.82
1:r:42:MET:HB3	1:r:336:LEU:HD11	1.61	0.82
5:L:78:MET:HG2	5:L:105:VAL:HG23	1.62	0.82
4:A:456:ILE:HD11	4:A:543:LEU:HG	1.61	0.81
5:H:139:PRO:HG2	5:H:142:LEU:HD13	1.63	0.81
1:u:148:PRO:HG3	1:u:553:TRP:HE1	1.45	0.81
5:I:78:MET:HG2	5:I:105:VAL:HG23	1.62	0.80
1:x:569:ILE:HD13	1:x:581:LEU:HD23	1.62	0.80
5:e:39:ARG:HB3	5:e:128:LEU:HD13	1.62	0.80
4:F:80:VAL:HG13	4:F:84:ARG:HH22	1.47	0.80
1:Y:148:PRO:HG3	1:Y:553:TRP:HE1	1.46	0.80
4:C:456:ILE:HD11	4:C:543:LEU:HG	1.63	0.80
5:K:139:PRO:HG2	5:K:142:LEU:HD13	1.64	0.80
1:0:286:ARG:NH2	1:3:218:CYS:SG	2.55	0.79
4:C:542:ARG:HB3	3:T:23:ARG:HG3	1.65	0.79
3:2:9:LEU:HD12	3:2:151:GLN:HG3	1.65	0.79
1:c:42:MET:HB3	1:c:336:LEU:HD11	1.65	0.79
1:Y:286:ARG:NH2	1:c:218:CYS:SG	2.55	0.79
2:y:104:ILE:HG22	2:y:108:GLN:HE22	1.47	0.79
4:F:456:ILE:HD11	4:F:543:LEU:HG	1.63	0.79
3:n:108:PRO:HB2	3:n:132:ALA:HB2	1.65	0.79
3:n:49:MET:HE1	3:n:142:ALA:HA	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:t:9:LEU:HD12	3:t:151:GLN:HG3	1.66	0.78
5:S:93:TRP:HD1	5:S:116:VAL:HG23	1.49	0.78
4:F:542:ARG:HB3	3:j:23:ARG:HG3	1.66	0.77
1:c:606:MET:HE1	1:g:599:ARG:HG2	1.65	0.77
4:F:349:ARG:HH12	4:F:353:MET:HE3	1.49	0.77
5:e:93:TRP:HD1	5:e:116:VAL:HG23	1.48	0.77
2:1:18:LEU:HD22	2:1:25:LEU:HD21	1.67	0.76
2:P:18:LEU:HD22	2:P:25:LEU:HD21	1.66	0.76
4:A:30:LEU:HB3	4:A:439:SER:HB3	1.66	0.76
3:b:108:PRO:HB2	3:b:132:ALA:HB2	1.68	0.76
4:D:30:LEU:HB3	4:D:439:SER:HB3	1.66	0.76
3:T:108:PRO:HB2	3:T:132:ALA:HB2	1.68	0.76
2:V:18:LEU:HD22	2:V:25:LEU:HD21	1.67	0.75
5:m:102:ALA:HA	5:m:117:PRO:HD2	1.68	0.75
1:3:432:ASP:HB2	1:3:435:LEU:HD13	1.67	0.75
4:A:542:ARG:HB3	3:n:23:ARG:HG3	1.68	0.75
5:K:93:TRP:HD1	5:K:116:VAL:HG23	1.50	0.75
1:U:576:VAL:HG23	1:Y:603:ILE:HD12	1.68	0.75
1:k:576:VAL:HG23	1:o:603:ILE:HD12	1.69	0.75
2:h:14:LEU:HB2	2:h:88:ILE:HD11	1.69	0.75
1:g:286:ARG:NH2	1:k:218:CYS:SG	2.59	0.75
3:j:108:PRO:HB2	3:j:132:ALA:HB2	1.69	0.75
1:r:575:GLN:O	1:r:576:VAL:HG12	1.86	0.75
5:m:39:ARG:HB3	5:m:128:LEU:HD13	1.68	0.75
1:U:575:GLN:O	1:U:576:VAL:HG12	1.87	0.74
4:A:327:SER:O	4:A:352:TRP:NE1	2.20	0.74
1:c:580:MET:HE1	1:g:596:ILE:HG23	1.68	0.74
2:y:18:LEU:HB3	2:y:82:PHE:HB2	1.68	0.74
5:K:116:VAL:HG13	5:K:117:PRO:HD3	1.68	0.74
5:S:37:ARG:HB3	5:S:183:LEU:HD11	1.69	0.74
3:f:108:PRO:HB2	3:f:132:ALA:HB2	1.69	0.74
5:m:93:TRP:CD1	5:m:116:VAL:HG23	2.22	0.74
1:3:575:GLN:O	1:3:576:VAL:HG12	1.87	0.74
1:0:603:ILE:HD12	1:x:576:VAL:HG23	1.69	0.74
3:X:67:ASP:HA	3:X:144:ARG:HH11	1.51	0.74
1:o:148:PRO:HG3	1:o:553:TRP:HE1	1.52	0.74
1:0:583:LEU:HD21	1:3:599:ARG:HH12	1.50	0.74
5:i:39:ARG:HB3	5:i:128:LEU:HD13	1.70	0.74
3:j:30:LEU:HD22	3:j:148:LEU:HB3	1.70	0.74
3:b:8:VAL:HG11	3:b:33:LEU:HD13	1.70	0.73
5:a:39:ARG:HB3	5:a:128:LEU:HD13	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:575:GLN:O	1:c:576:VAL:HG12	1.87	0.73
3:n:30:LEU:HD22	3:n:148:LEU:HB3	1.71	0.73
1:x:575:GLN:O	1:x:576:VAL:HG12	1.88	0.73
1:r:576:VAL:HG23	1:u:603:ILE:HD12	1.70	0.73
3:t:64:LEU:HD12	3:t:65:PRO:HD2	1.70	0.73
5:I:116:VAL:HG13	5:I:117:PRO:HD3	1.69	0.73
5:J:34:PHE:HA	5:J:183:LEU:HD21	1.70	0.73
5:L:39:ARG:HB3	5:L:128:LEU:HD13	1.71	0.73
3:2:64:LEU:HD12	3:2:65:PRO:HD2	1.71	0.73
4:A:303:ARG:HG3	4:F:235:PRO:HG3	1.71	0.73
3:2:38:ARG:NH2	3:2:146:PRO:O	2.21	0.72
3:w:51:THR:HG22	3:w:140:VAL:HG22	1.71	0.72
1:0:393:ASN:OD1	1:0:433:ARG:NH2	2.23	0.72
1:3:579:VAL:HG23	1:3:580:MET:HE3	1.71	0.72
4:D:235:PRO:HG3	4:E:303:ARG:HG3	1.71	0.72
5:L:38:THR:HB	5:L:40:LEU:HD23	1.71	0.72
2:d:31:ASP:HA	2:d:34:LEU:HD13	1.69	0.72
5:L:57:VAL:HG21	5:L:65:LEU:HD22	1.71	0.72
5:W:93:TRP:HD1	5:W:116:VAL:HG23	1.54	0.72
1:c:452:GLN:NE2	1:g:102:GLN:OE1	2.22	0.72
5:G:34:PHE:HA	5:G:183:LEU:HD21	1.72	0.72
1:r:57:LEU:HD11	1:r:247:ASP:HB2	1.72	0.72
4:D:327:SER:O	4:D:352:TRP:NE1	2.22	0.72
2:O:57:ILE:HG12	2:O:92:LEU:HD13	1.70	0.72
5:m:11:ILE:HA	5:m:155:LEU:HD21	1.72	0.72
5:m:34:PHE:HA	5:m:183:LEU:HD21	1.71	0.72
2:4:14:LEU:HD11	2:4:25:LEU:HB2	1.72	0.72
3:X:108:PRO:HB2	3:X:132:ALA:HB2	1.71	0.72
2:Z:14:LEU:HD11	2:Z:25:LEU:HB2	1.72	0.72
2:h:38:LEU:HD21	2:h:44:PHE:HD1	1.55	0.72
2:y:58:VAL:HA	2:y:74:GLN:HE22	1.55	0.72
1:r:379:ILE:HG23	1:r:443:MET:HG3	1.72	0.72
5:m:139:PRO:HD2	5:m:142:LEU:HD12	1.71	0.72
2:4:63:ARG:HB2	2:4:68:MET:HG2	1.71	0.71
2:N:63:ARG:NH2	2:N:65:VAL:O	2.23	0.71
3:f:67:ASP:HA	3:f:144:ARG:HH11	1.55	0.71
5:m:39:ARG:NH1	5:m:67:GLU:OE2	2.23	0.71
1:r:323:THR:N	1:u:174:THR:OG1	2.20	0.71
4:B:235:PRO:HG2	4:B:278:THR:HA	1.73	0.71
4:C:235:PRO:HG3	4:D:303:ARG:HG3	1.71	0.71
5:K:66:TYR:HB2	5:K:130:LYS:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:160:GLU:HG3	3:w:38:ARG:HB3	1.70	0.71
5:L:116:VAL:HG13	5:L:117:PRO:HD3	1.71	0.71
2:Q:96:GLU:HG3	2:Q:97:LEU:HD12	1.72	0.71
1:3:452:GLN:NE2	1:6:102:GLN:OE1	2.23	0.71
5:S:78:MET:HG2	5:S:105:VAL:HG23	1.71	0.71
4:E:30:LEU:HB3	4:E:439:SER:HB3	1.70	0.71
5:a:11:ILE:HA	5:a:155:LEU:HD21	1.73	0.71
3:n:160:GLU:HG3	3:q:38:ARG:HB3	1.71	0.71
3:q:51:THR:HG22	3:q:140:VAL:HG22	1.71	0.71
3:X:78:LEU:HD23	3:X:136:GLN:HG3	1.73	0.71
3:b:30:LEU:HD22	3:b:148:LEU:HB3	1.72	0.71
3:f:8:VAL:HG11	3:f:33:LEU:HD13	1.71	0.71
3:n:8:VAL:HG11	3:n:33:LEU:HD13	1.71	0.71
2:7:31:ASP:HA	2:7:34:LEU:HD13	1.70	0.71
5:J:93:TRP:CD1	5:J:116:VAL:HG23	2.26	0.71
2:v:96:GLU:HG3	2:v:97:LEU:HD12	1.72	0.71
1:k:452:GLN:NE2	1:o:102:GLN:OE1	2.23	0.71
2:s:18:LEU:HD11	2:s:22:GLY:HA3	1.72	0.71
5:G:69:GLU:OE2	5:W:84:GLN:NE2	2.24	0.71
5:I:57:VAL:HG21	5:I:65:LEU:HD22	1.73	0.71
1:U:57:LEU:HD11	1:U:247:ASP:HB2	1.73	0.71
4:A:235:PRO:HG3	4:B:303:ARG:HG3	1.71	0.70
1:U:568:MET:HE1	1:U:580:MET:HB3	1.73	0.70
2:l:63:ARG:NH2	2:l:65:VAL:O	2.24	0.70
1:x:385:LYS:HE3	1:x:389:ILE:HD11	1.73	0.70
1:3:576:VAL:HG23	1:6:603:ILE:HD12	1.73	0.70
5:G:38:THR:HB	5:G:40:LEU:HD23	1.73	0.70
5:H:39:ARG:HB3	5:H:128:LEU:HD13	1.72	0.70
2:O:18:LEU:HB3	2:O:82:PHE:HB2	1.72	0.70
1:k:286:ARG:NH2	1:o:218:CYS:O	2.24	0.70
2:O:57:ILE:HG21	2:O:92:LEU:HD22	1.73	0.70
3:2:160:GLU:OE1	3:n:144:ARG:NH2	2.23	0.70
1:3:286:ARG:NH2	1:6:218:CYS:O	2.24	0.70
4:E:235:PRO:HG3	4:F:303:ARG:HG3	1.72	0.70
3:t:51:THR:HG22	3:t:140:VAL:HG22	1.73	0.70
4:B:235:PRO:HG3	4:C:303:ARG:HG3	1.72	0.70
1:r:197:GLU:OE1	1:u:182:ARG:NH1	2.22	0.70
3:t:4:PRO:HA	3:t:154:VAL:HA	1.73	0.70
3:n:71:LEU:HA	3:n:141:CYS:HA	1.72	0.70
1:o:558:ARG:NH2	1:o:586:ASP:O	2.24	0.70
2:y:8:ASN:HA	2:y:91:ARG:HH21	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:107:GLN:NE2	5:S:110:GLU:O	2.25	0.70
2:Z:63:ARG:HB2	2:Z:68:MET:HG2	1.73	0.70
1:c:576:VAL:HG23	1:g:603:ILE:HD12	1.73	0.70
5:i:164:LYS:HB3	5:i:166:TRP:HE3	1.57	0.70
2:s:14:LEU:HB3	2:s:86:ASP:HB3	1.74	0.70
4:F:28:ARG:HH21	4:F:441:ARG:HD2	1.57	0.70
5:H:28:ARG:HD3	5:H:135:ALA:H	1.57	0.70
1:g:247:ASP:OD1	1:g:248:GLU:N	2.23	0.70
1:0:102:GLN:OE1	1:x:452:GLN:NE2	2.24	0.70
4:B:231:LEU:HD11	4:B:239:MET:HB3	1.73	0.70
5:K:39:ARG:HB3	5:K:128:LEU:HD13	1.72	0.70
1:Y:123:ARG:NH1	1:Y:543:LYS:O	2.24	0.70
5:a:57:VAL:HG11	5:a:65:LEU:HD22	1.74	0.70
1:r:568:MET:HE1	1:r:580:MET:HB3	1.72	0.70
2:s:18:LEU:HD22	2:s:25:LEU:HD21	1.74	0.70
5:G:28:ARG:HD3	5:G:135:ALA:H	1.57	0.69
1:6:393:ASN:OD1	1:6:433:ARG:NH2	2.25	0.69
5:J:28:ARG:HD3	5:J:135:ALA:H	1.56	0.69
5:J:39:ARG:NH1	5:J:67:GLU:OE1	2.24	0.69
3:X:15:LEU:HG	3:X:170:LEU:HD11	1.73	0.69
4:B:30:LEU:HB3	4:B:439:SER:HB3	1.74	0.69
5:K:39:ARG:NH1	5:K:67:GLU:OE1	2.25	0.69
3:X:30:LEU:HD22	3:X:148:LEU:HB3	1.74	0.69
1:r:348:ARG:NH2	1:r:500:GLU:OE1	2.25	0.69
5:H:39:ARG:NH1	5:H:67:GLU:OE2	2.25	0.69
5:I:39:ARG:NH1	5:I:67:GLU:OE1	2.25	0.69
5:J:38:THR:HB	5:J:40:LEU:HD23	1.73	0.69
5:L:93:TRP:HD1	5:L:116:VAL:HG23	1.56	0.69
3:T:39:GLU:OE2	3:T:43:ARG:NH1	2.26	0.69
3:X:8:VAL:HG11	3:X:33:LEU:HD13	1.73	0.69
3:w:4:PRO:HA	3:w:154:VAL:HA	1.75	0.69
5:L:40:LEU:HD21	5:L:189:LYS:HB3	1.74	0.69
1:U:190:ILE:HB	1:U:207:PHE:HB2	1.75	0.69
5:i:116:VAL:CG1	5:i:117:PRO:HD3	2.23	0.69
3:t:38:ARG:NH2	3:t:146:PRO:O	2.25	0.69
5:J:8:MET:HG3	5:J:12:HIS:HD2	1.57	0.69
1:U:379:ILE:HG23	1:U:443:MET:HG3	1.74	0.69
5:i:39:ARG:NH1	5:i:67:GLU:OE2	2.26	0.69
1:k:385:LYS:HE3	1:k:389:ILE:HD11	1.75	0.69
1:k:575:GLN:O	1:k:576:VAL:HG12	1.93	0.69
1:r:190:ILE:HB	1:r:207:PHE:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:51:THR:HG22	3:5:140:VAL:HG22	1.75	0.69
5:W:11:ILE:HD13	5:W:23:ALA:HB1	1.74	0.69
1:c:385:LYS:HE3	1:c:389:ILE:HD11	1.74	0.69
5:m:107:GLN:NE2	5:m:110:GLU:O	2.25	0.69
1:3:569:ILE:HD13	1:3:581:LEU:HD23	1.75	0.69
5:K:93:TRP:CD1	5:K:116:VAL:HG23	2.28	0.69
5:G:8:MET:HG3	5:G:12:HIS:HD2	1.56	0.68
2:R:14:LEU:HB3	2:R:86:ASP:HB2	1.74	0.68
2:l:91:ARG:NH1	2:l:96:GLU:OE2	2.26	0.68
4:C:532:LYS:HB2	4:C:544:PRO:HD3	1.76	0.68
3:T:30:LEU:HD22	3:T:148:LEU:HB3	1.75	0.68
3:f:30:LEU:HD22	3:f:148:LEU:HB3	1.74	0.68
5:m:116:VAL:CG1	5:m:117:PRO:HD3	2.20	0.68
5:I:28:ARG:HD3	5:I:135:ALA:H	1.58	0.68
5:J:70:LEU:HD23	5:i:94:ARG:HH12	1.58	0.68
2:V:48:LEU:HD13	2:V:88:ILE:HG13	1.74	0.68
5:W:39:ARG:HB3	5:W:128:LEU:HD13	1.74	0.68
1:c:187:ARG:HD3	1:c:249:ALA:HB1	1.75	0.68
2:1:48:LEU:HD13	2:1:88:ILE:HG13	1.73	0.68
5:J:116:VAL:HG13	5:J:117:PRO:HD3	1.75	0.68
2:V:18:LEU:HD11	2:V:22:GLY:HA3	1.75	0.68
2:V:94:ALA:HB2	2:Z:8:ASN:HB2	1.75	0.68
3:z:7:VAL:HB	3:z:11:ARG:HH21	1.59	0.68
4:D:84:ARG:HG2	4:D:97:VAL:HG22	1.75	0.68
5:W:116:VAL:HG13	5:W:117:PRO:HD3	1.75	0.68
2:p:57:ILE:HG21	2:p:92:LEU:HD22	1.74	0.68
1:r:385:LYS:HE3	1:r:389:ILE:HD11	1.75	0.68
5:I:69:GLU:H	5:I:127:GLY:HA2	1.57	0.68
3:j:71:LEU:HA	3:j:141:CYS:HA	1.75	0.68
3:q:64:LEU:HD12	3:q:65:PRO:HD2	1.76	0.68
3:2:4:PRO:HA	3:2:154:VAL:HA	1.76	0.68
4:B:327:SER:O	4:B:352:TRP:NE1	2.24	0.68
5:K:28:ARG:HD3	5:K:135:ALA:H	1.58	0.68
5:K:116:VAL:CG1	5:K:117:PRO:HD3	2.23	0.68
3:w:64:LEU:HD12	3:w:65:PRO:HD2	1.76	0.68
4:E:235:PRO:HG2	4:E:278:THR:HA	1.74	0.68
5:H:66:TYR:HB2	5:H:130:LYS:HB2	1.74	0.68
5:L:116:VAL:CG1	5:L:117:PRO:HD3	2.24	0.68
3:j:8:VAL:HG11	3:j:33:LEU:HD13	1.74	0.68
3:5:160:GLU:OE2	3:T:144:ARG:NH2	2.23	0.68
5:G:66:TYR:HB2	5:G:130:LYS:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:57:VAL:HG21	5:H:65:LEU:HD22	1.76	0.68
5:L:28:ARG:HD3	5:L:135:ALA:H	1.59	0.68
2:d:93:THR:HG23	2:d:97:LEU:HD12	1.75	0.68
5:m:37:ARG:HB3	5:m:183:LEU:HD22	1.75	0.68
3:5:4:PRO:HA	3:5:154:VAL:HA	1.76	0.67
1:U:606:MET:HE1	1:Y:599:ARG:HG2	1.75	0.67
1:k:190:ILE:HB	1:k:207:PHE:HB2	1.76	0.67
1:x:187:ARG:HD3	1:x:249:ALA:HB1	1.76	0.67
5:G:93:TRP:CD1	5:G:116:VAL:HG23	2.28	0.67
5:I:93:TRP:HD1	5:I:116:VAL:HG23	1.58	0.67
1:c:286:ARG:NH2	1:g:218:CYS:O	2.28	0.67
1:k:187:ARG:HD3	1:k:249:ALA:HB1	1.76	0.67
2:l:19:ALA:O	2:l:72:ARG:NH2	2.27	0.67
1:0:331:PHE:HA	1:0:336:LEU:HA	1.77	0.67
1:U:248:GLU:O	1:U:252:TRP:HB2	1.94	0.67
3:t:108:PRO:HB2	3:t:132:ALA:HB2	1.76	0.67
4:C:347:MET:HE1	4:C:352:TRP:HE3	1.59	0.67
1:u:247:ASP:OD1	1:u:248:GLU:N	2.28	0.67
1:0:123:ARG:NH1	1:0:543:LYS:O	2.26	0.67
1:3:408:PHE:O	1:3:412:VAL:HG23	1.94	0.67
4:C:54:ASP:HA	4:C:423:LYS:HD3	1.77	0.67
5:I:116:VAL:CG1	5:I:117:PRO:HD3	2.24	0.67
3:b:9:LEU:HD12	3:b:151:GLN:HG3	1.77	0.67
2:s:7:ALA:HB3	2:s:91:ARG:HD2	1.75	0.67
4:C:377:GLU:HB3	4:C:381:ALA:HB3	1.77	0.67
5:L:11:ILE:HA	5:L:155:LEU:HD21	1.75	0.67
1:g:331:PHE:HA	1:g:336:LEU:HA	1.76	0.67
4:A:346:LEU:HD12	4:A:347:MET:HG3	1.77	0.67
4:F:80:VAL:HG13	4:F:84:ARG:NH2	2.09	0.67
3:z:38:ARG:NH2	3:z:146:PRO:O	2.27	0.67
4:D:346:LEU:HD12	4:D:347:MET:HG3	1.77	0.67
1:U:385:LYS:HE3	1:U:389:ILE:HD11	1.77	0.67
2:p:59:LYS:HZ3	2:p:61:THR:HG22	1.59	0.67
1:u:123:ARG:NH1	1:u:543:LYS:O	2.27	0.67
1:3:190:ILE:HB	1:3:207:PHE:HB2	1.76	0.67
1:u:484:THR:HG23	1:u:487:LEU:HD12	1.77	0.67
1:x:379:ILE:HG23	1:x:443:MET:HG3	1.77	0.67
2:y:104:ILE:O	2:y:108:GLN:NE2	2.29	0.67
3:5:7:VAL:HB	3:5:11:ARG:HH21	1.60	0.66
4:F:532:LYS:HB2	4:F:544:PRO:HD3	1.76	0.66
5:J:69:GLU:OE1	5:i:84:GLN:NE2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:279:CYS:HB3	1:Y:329:ALA:HB3	1.76	0.66
5:J:116:VAL:CG1	5:J:117:PRO:HD3	2.25	0.66
5:W:28:ARG:HD3	5:W:135:ALA:H	1.61	0.66
5:W:107:GLN:NE2	5:W:110:GLU:O	2.28	0.66
3:w:7:VAL:HB	3:w:11:ARG:HH21	1.61	0.66
3:2:108:PRO:HB2	3:2:132:ALA:HB2	1.77	0.66
1:3:385:LYS:HE3	1:3:389:ILE:HD11	1.77	0.66
3:5:38:ARG:NH2	3:5:146:PRO:O	2.28	0.66
3:T:160:GLU:HG3	3:t:42:VAL:HG21	1.77	0.66
3:X:4:PRO:HA	3:X:154:VAL:HA	1.77	0.66
5:a:93:TRP:CD1	5:a:116:VAL:HG23	2.31	0.66
3:q:7:VAL:HB	3:q:11:ARG:HH21	1.60	0.66
1:r:569:ILE:HD13	1:r:581:LEU:HD23	1.77	0.66
1:6:596:ILE:O	1:6:600:ILE:HG12	1.94	0.66
5:G:200:ARG:HD2	1:U:414:ARG:HH21	1.60	0.66
5:H:93:TRP:CD1	5:H:116:VAL:HG23	2.30	0.66
2:Q:63:ARG:HG3	2:Q:68:MET:HG3	1.77	0.66
1:U:286:ARG:NH2	1:Y:218:CYS:O	2.28	0.66
1:0:247:ASP:OD1	1:0:248:GLU:N	2.23	0.66
2:1:18:LEU:HD11	2:1:22:GLY:HA3	1.75	0.66
5:J:11:ILE:HA	5:J:155:LEU:HD21	1.77	0.66
5:L:69:GLU:H	5:L:127:GLY:HA2	1.60	0.66
1:u:286:ARG:HE	1:x:219:ALA:HA	1.60	0.66
2:4:20:PRO:HA	2:4:72:ARG:HH22	1.60	0.66
1:6:182:ARG:NH2	1:6:184:GLU:OE2	2.29	0.66
4:E:349:ARG:HH12	4:E:353:MET:HE3	1.61	0.66
3:T:4:PRO:HA	3:T:154:VAL:HA	1.77	0.66
1:U:117:ASP:OD2	1:U:139:LYS:NZ	2.28	0.66
5:e:156:SER:O	5:e:160:ILE:HG12	1.96	0.66
2:p:57:ILE:HG12	2:p:92:LEU:HD13	1.78	0.66
3:z:4:PRO:HA	3:z:154:VAL:HA	1.76	0.66
3:z:51:THR:HG22	3:z:140:VAL:HG22	1.76	0.66
1:3:554:ARG:NH2	1:3:563:GLU:OE2	2.28	0.66
4:C:377:GLU:N	4:C:381:ALA:O	2.28	0.66
1:Y:247:ASP:OD1	1:Y:248:GLU:N	2.27	0.66
5:a:34:PHE:HA	5:a:183:LEU:HD21	1.76	0.66
1:c:190:ILE:HB	1:c:207:PHE:HB2	1.78	0.66
3:j:4:PRO:HA	3:j:154:VAL:HA	1.78	0.66
2:s:92:LEU:HD11	2:v:8:ASN:HD21	1.61	0.66
2:v:94:ALA:H	2:y:8:ASN:HD21	1.40	0.66
3:2:51:THR:HG22	3:2:140:VAL:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:378:ASP:OD1	1:6:382:ARG:NH1	2.29	0.66
4:B:239:MET:N	4:B:250:CYS:SG	2.66	0.66
2:M:14:LEU:HB2	2:M:88:ILE:HD11	1.77	0.66
2:R:14:LEU:HD21	2:R:18:LEU:HD23	1.78	0.66
1:u:59:ARG:HD2	1:x:257:ARG:HE	1.61	0.66
1:0:218:CYS:O	1:x:286:ARG:NH2	2.28	0.66
2:1:94:ALA:HB2	2:4:8:ASN:HB2	1.77	0.66
1:6:331:PHE:HA	1:6:336:LEU:HA	1.78	0.66
5:G:116:VAL:CG1	5:G:117:PRO:HD3	2.26	0.66
5:L:34:PHE:HA	5:L:183:LEU:HD21	1.78	0.66
5:e:107:GLN:NE2	5:e:110:GLU:O	2.28	0.66
1:r:606:MET:HE1	1:u:599:ARG:HG2	1.78	0.66
5:G:116:VAL:HG13	5:G:117:PRO:HD3	1.77	0.66
2:v:5:GLN:NE2	2:v:6:PHE:O	2.29	0.66
3:2:38:ARG:HB3	3:j:160:GLU:HG3	1.76	0.65
4:D:324:ALA:HB1	4:D:331:LEU:HD11	1.78	0.65
1:U:543:LYS:HD3	1:Y:144:VAL:HA	1.78	0.65
1:o:331:PHE:HA	1:o:336:LEU:HA	1.77	0.65
3:q:145:HIS:HE1	3:q:155:VAL:HA	1.61	0.65
1:u:331:PHE:HA	1:u:336:LEU:HA	1.78	0.65
3:z:108:PRO:HB2	3:z:132:ALA:HB2	1.78	0.65
5:I:93:TRP:CD1	5:I:116:VAL:HG23	2.30	0.65
5:J:66:TYR:HB2	5:J:130:LYS:HB2	1.77	0.65
5:L:93:TRP:CD1	5:L:116:VAL:HG23	2.31	0.65
2:P:14:LEU:HB3	2:P:86:ASP:HB3	1.78	0.65
5:W:116:VAL:CG1	5:W:117:PRO:HD3	2.25	0.65
5:a:28:ARG:HD3	5:a:135:ALA:H	1.61	0.65
5:m:87:ASP:OD1	5:m:94:ARG:NH1	2.27	0.65
1:r:248:GLU:O	1:r:252:TRP:HB2	1.95	0.65
1:u:558:ARG:NH2	1:u:586:ASP:O	2.26	0.65
3:w:145:HIS:HE1	3:w:155:VAL:HA	1.61	0.65
3:5:108:PRO:HB2	3:5:132:ALA:HB2	1.77	0.65
4:D:57:LYS:NZ	4:D:70:GLN:O	2.27	0.65
5:L:18:CYS:HA	5:L:166:TRP:CH2	2.32	0.65
2:Q:57:ILE:HG21	2:Q:92:LEU:HD22	1.77	0.65
4:A:386:THR:HB	4:A:401:SER:HB3	1.79	0.65
4:C:332:VAL:HG22	4:C:339:MET:HE3	1.78	0.65
3:X:7:VAL:O	3:X:11:ARG:HG2	1.97	0.65
3:f:4:PRO:HA	3:f:154:VAL:HA	1.79	0.65
2:1:108:GLN:NE2	2:4:106:SER:OG	2.27	0.65
1:3:123:ARG:NH1	1:3:543:LYS:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:187:ARG:HD3	1:3:249:ALA:HB1	1.76	0.65
1:6:64:ARG:NH2	1:6:186:TRP:O	2.30	0.65
4:F:57:LYS:NZ	4:F:70:GLN:O	2.30	0.65
5:H:78:MET:HG2	5:H:105:VAL:HG23	1.78	0.65
5:K:57:VAL:HG21	5:K:65:LEU:HD22	1.77	0.65
2:Q:19:ALA:O	2:Q:72:ARG:NH1	2.30	0.65
2:V:93:THR:HB	2:V:97:LEU:HD12	1.79	0.65
1:Y:385:LYS:HE3	1:Y:389:ILE:HD11	1.79	0.65
5:e:40:LEU:HD21	5:e:189:LYS:HB3	1.78	0.65
1:r:286:ARG:NH2	1:u:218:CYS:O	2.29	0.65
1:3:211:TRP:HB3	1:3:273:ARG:HH21	1.61	0.65
3:5:19:GLU:HG2	4:C:546:GLY:HA3	1.77	0.65
1:6:184:GLU:OE2	1:6:208:ARG:NH1	2.29	0.65
4:F:377:GLU:N	4:F:381:ALA:O	2.30	0.65
5:G:39:ARG:HB3	5:G:128:LEU:HD13	1.77	0.65
5:i:11:ILE:HD13	5:i:23:ALA:HB1	1.77	0.65
5:i:93:TRP:HD1	5:i:116:VAL:HG23	1.62	0.65
3:q:108:PRO:HB2	3:q:132:ALA:HB2	1.78	0.65
5:K:78:MET:HG2	5:K:105:VAL:HG23	1.79	0.65
5:W:93:TRP:CD1	5:W:116:VAL:HG23	2.31	0.65
5:a:39:ARG:NH1	5:a:67:GLU:OE2	2.30	0.65
5:J:39:ARG:HB3	5:J:128:LEU:HD13	1.77	0.65
1:g:402:VAL:HG21	1:g:408:PHE:HB2	1.77	0.65
3:w:38:ARG:NH2	3:w:146:PRO:O	2.30	0.65
1:3:99:VAL:H	1:3:376:GLN:NE2	1.95	0.65
5:K:126:TYR:CZ	5:m:94:ARG:HD3	2.32	0.65
1:Y:579:VAL:HG23	1:Y:580:MET:HE2	1.78	0.65
5:a:107:GLN:NE2	5:a:110:GLU:O	2.30	0.65
1:c:63:ASN:HD22	1:c:364:LEU:HD12	1.60	0.65
2:d:8:ASN:HA	2:d:91:ARG:HH21	1.62	0.65
3:f:11:ARG:NH2	3:z:31:GLU:OE2	2.30	0.65
1:g:100:ILE:HD12	1:g:372:MET:HB3	1.78	0.65
1:k:430:ASN:OD1	1:k:433:ARG:NE	2.29	0.65
3:q:33:LEU:HD22	3:q:148:LEU:HG	1.79	0.65
2:4:49:ILE:HB	2:4:87:ARG:HB2	1.80	0.64
3:5:42:VAL:HG21	3:X:160:GLU:HG3	1.78	0.64
1:6:123:ARG:NH1	1:6:543:LYS:O	2.30	0.64
5:I:11:ILE:HA	5:I:155:LEU:HD21	1.79	0.64
1:x:190:ILE:HB	1:x:207:PHE:HB2	1.79	0.64
1:0:558:ARG:NH2	1:0:586:ASP:O	2.30	0.64
1:Y:286:ARG:HE	1:c:219:ALA:HA	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:385:LYS:HE2	1:o:389:ILE:HD11	1.78	0.64
3:q:4:PRO:HA	3:q:154:VAL:HA	1.79	0.64
1:x:42:MET:HB3	1:x:336:LEU:HD11	1.79	0.64
5:G:11:ILE:HA	5:G:155:LEU:HD21	1.79	0.64
1:0:63:ASN:ND2	1:0:364:LEU:HB3	2.12	0.64
4:F:332:VAL:HG22	4:F:339:MET:HE3	1.78	0.64
1:r:375:ILE:HB	1:r:450:LEU:HD21	1.78	0.64
3:t:7:VAL:HB	3:t:11:ARG:HH21	1.63	0.64
3:2:7:VAL:HB	3:2:11:ARG:HH21	1.63	0.64
1:Y:331:PHE:HA	1:Y:336:LEU:HA	1.79	0.64
5:i:28:ARG:HD3	5:i:135:ALA:H	1.61	0.64
3:w:33:LEU:HD22	3:w:148:LEU:HG	1.79	0.64
1:U:569:ILE:HD13	1:U:581:LEU:HD23	1.80	0.64
1:6:430:ASN:ND2	1:6:430:ASN:O	2.30	0.64
2:p:59:LYS:HB2	2:p:74:GLN:HG2	1.80	0.64
2:v:18:LEU:HD13	2:v:25:LEU:HB3	1.80	0.64
1:3:44:GLU:OE2	1:6:269:HIS:NE2	2.30	0.64
4:A:2:THR:N	4:A:573:GLU:OE2	2.30	0.64
4:A:5:LYS:HG3	4:A:566:VAL:HG12	1.78	0.64
4:E:332:VAL:HG22	4:E:339:MET:HE3	1.78	0.64
5:J:200:ARG:HD2	1:r:414:ARG:HH21	1.62	0.64
5:L:126:TYR:CZ	5:S:94:ARG:HD3	2.32	0.64
1:u:276:LEU:HD23	1:u:330:ILE:HD11	1.79	0.64
4:D:455:ALA:HB1	4:D:574:LEU:HD22	1.78	0.64
5:G:126:TYR:CE2	5:W:94:ARG:HD2	2.33	0.64
3:T:7:VAL:O	3:T:11:ARG:HG2	1.98	0.64
2:Z:20:PRO:HA	2:Z:72:ARG:HH22	1.62	0.64
1:x:63:ASN:HD22	1:x:364:LEU:HD12	1.62	0.64
5:G:57:VAL:HG21	5:G:65:LEU:HD22	1.78	0.64
5:W:102:ALA:HA	5:W:117:PRO:HD2	1.80	0.64
3:b:4:PRO:HA	3:b:154:VAL:HA	1.79	0.64
1:o:583:LEU:HD21	1:r:599:ARG:HH12	1.63	0.64
4:D:43:ARG:NH1	4:D:429:ASP:O	2.31	0.63
5:J:18:CYS:HA	5:J:166:TRP:CH2	2.34	0.63
3:f:69:ILE:N	3:f:142:ALA:O	2.28	0.63
1:x:147:LEU:HD11	1:x:498:GLN:HE22	1.64	0.63
4:F:54:ASP:HA	4:F:423:LYS:HD3	1.80	0.63
5:H:126:TYR:CZ	5:a:94:ARG:HD3	2.33	0.63
2:P:101:ARG:HD2	2:Q:6:PHE:HE2	1.61	0.63
1:U:435:LEU:HD21	1:Y:433:ARG:HH11	1.64	0.63
5:a:196:ARG:HH12	1:g:406:GLU:HG3	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:149:THR:HG23	3:f:150:THR:HG23	1.80	0.63
3:j:7:VAL:O	3:j:11:ARG:HG2	1.98	0.63
1:k:569:ILE:HD13	1:k:581:LEU:HD23	1.80	0.63
1:r:64:ARG:HD3	1:r:186:TRP:HZ3	1.62	0.63
1:u:208:ARG:NH2	1:u:278:GLU:OE1	2.32	0.63
1:6:132:GLU:OE2	1:6:136:LYS:HE3	1.98	0.63
2:P:19:ALA:O	2:P:72:ARG:NH2	2.32	0.63
1:U:100:ILE:HG12	1:U:372:MET:HE2	1.80	0.63
2:V:14:LEU:HB3	2:V:86:ASP:HB3	1.81	0.63
3:X:149:THR:HG23	3:X:150:THR:HG23	1.80	0.63
5:i:102:ALA:HA	5:i:117:PRO:HD2	1.80	0.63
1:g:430:ASN:O	1:g:430:ASN:ND2	2.31	0.63
1:u:502:GLN:O	1:u:506:ILE:HD12	1.98	0.63
1:0:357:PHE:HE2	1:0:368:VAL:HG22	1.64	0.63
5:I:126:TYR:CZ	5:e:94:ARG:HD3	2.34	0.63
5:e:39:ARG:NH1	5:e:67:GLU:OE1	2.31	0.63
3:j:149:THR:HG23	3:j:150:THR:HG23	1.81	0.63
3:z:93:ARG:NH1	3:z:97:ASP:OD2	2.32	0.63
1:6:502:GLN:O	1:6:506:ILE:HD12	1.98	0.63
5:S:39:ARG:NH1	5:S:67:GLU:OE1	2.31	0.63
4:A:249:PHE:HB2	4:A:262:TYR:HB3	1.80	0.63
1:Y:502:GLN:O	1:Y:506:ILE:HD12	1.98	0.63
5:e:116:VAL:CG1	5:e:117:PRO:HD3	2.29	0.63
3:n:11:ARG:NE	3:q:31:GLU:OE2	2.32	0.63
1:0:276:LEU:HD23	1:0:330:ILE:HD11	1.80	0.63
1:6:385:LYS:HE2	1:6:389:ILE:HD11	1.81	0.63
4:A:43:ARG:NH2	4:B:350:ASN:OD1	2.32	0.63
5:G:18:CYS:HA	5:G:166:TRP:CH2	2.34	0.63
1:r:445:ARG:HD3	1:u:440:MET:HE3	1.80	0.63
5:S:28:ARG:HD3	5:S:135:ALA:H	1.63	0.63
1:Y:345:ARG:HD2	1:Y:538:ASP:HB2	1.80	0.63
1:o:502:GLN:O	1:o:506:ILE:HD12	1.98	0.63
1:0:190:ILE:HB	1:0:207:PHE:HB2	1.81	0.62
1:6:357:PHE:HE2	1:6:368:VAL:HG22	1.64	0.62
4:D:247:LEU:HB2	4:D:266:MET:HE1	1.81	0.62
2:N:14:LEU:HB2	2:N:86:ASP:HB2	1.80	0.62
1:g:123:ARG:NH1	1:g:543:LYS:O	2.32	0.62
1:k:248:GLU:O	1:k:252:TRP:HB2	1.98	0.62
1:o:276:LEU:HD23	1:o:330:ILE:HD11	1.79	0.62
3:q:38:ARG:NH2	3:q:146:PRO:O	2.30	0.62
5:G:19:PRO:HD3	5:G:166:TRP:HH2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:116:VAL:CG1	5:S:117:PRO:HD3	2.29	0.62
1:6:42:MET:HB3	1:6:336:LEU:HD21	1.80	0.62
4:D:2:THR:N	4:D:573:GLU:OE2	2.32	0.62
5:i:40:LEU:HD21	5:i:189:LYS:HB3	1.81	0.62
4:F:2:THR:N	4:F:573:GLU:OE2	2.31	0.62
5:J:57:VAL:HG21	5:J:65:LEU:HD22	1.80	0.62
5:a:93:TRP:HD1	5:a:116:VAL:HG23	1.64	0.62
3:b:149:THR:HG23	3:b:150:THR:HG23	1.82	0.62
3:b:171:TYR:CD1	3:b:190:TYR:HB2	2.35	0.62
3:n:4:PRO:HA	3:n:154:VAL:HA	1.82	0.62
3:n:9:LEU:HD12	3:n:151:GLN:HG3	1.81	0.62
3:n:149:THR:HG23	3:n:150:THR:HG23	1.80	0.62
1:3:248:GLU:O	1:3:252:TRP:HB2	1.99	0.62
1:r:100:ILE:HG12	1:r:372:MET:HE2	1.80	0.62
2:v:63:ARG:HG3	2:v:68:MET:HG3	1.81	0.62
4:B:2:THR:N	4:B:573:GLU:OE2	2.31	0.62
2:Q:50:ARG:NH1	2:Q:81:SER:O	2.32	0.62
2:Z:50:ARG:NH1	2:Z:81:SER:O	2.33	0.62
3:b:71:LEU:HA	3:b:141:CYS:HA	1.81	0.62
1:g:502:GLN:O	1:g:506:ILE:HD12	2.00	0.62
4:E:57:LYS:NZ	4:E:70:GLN:O	2.32	0.62
5:K:8:MET:HG3	5:K:12:HIS:HD2	1.64	0.62
1:o:402:VAL:HG21	1:o:408:PHE:HB2	1.81	0.62
1:u:385:LYS:HE3	1:u:389:ILE:HD11	1.81	0.62
1:x:377:ASP:OD1	1:x:378:ASP:N	2.33	0.62
4:B:105:ALA:HA	4:B:224:PRO:HD2	1.82	0.62
5:J:202:ARG:NH2	5:i:88:GLU:OE1	2.27	0.62
1:U:42:MET:HB3	1:U:336:LEU:HD11	1.81	0.62
5:m:28:ARG:HD3	5:m:135:ALA:H	1.63	0.62
4:A:43:ARG:NH1	4:A:429:ASP:O	2.31	0.62
1:c:408:PHE:O	1:c:412:VAL:HG23	2.00	0.62
1:r:408:PHE:O	1:r:412:VAL:HG23	2.00	0.62
2:M:18:LEU:HD22	2:M:25:LEU:HD21	1.82	0.62
1:o:42:MET:HB3	1:o:336:LEU:HD21	1.81	0.62
1:o:132:GLU:OE2	1:o:136:LYS:HE3	1.99	0.62
1:u:125:LYS:NZ	1:x:587:SER:O	2.32	0.62
1:O:42:MET:HB3	1:O:336:LEU:HD21	1.82	0.61
1:6:276:LEU:HD23	1:6:330:ILE:HD11	1.82	0.61
1:6:323:THR:N	1:U:174:THR:OG1	2.27	0.61
4:E:105:ALA:HA	4:E:224:PRO:HD2	1.82	0.61
2:P:18:LEU:HD11	2:P:22:GLY:HA3	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:211:TRP:HB3	1:k:273:ARG:HH21	1.65	0.61
5:S:11:ILE:HA	5:S:155:LEU:HD21	1.82	0.61
1:g:42:MET:HB3	1:g:336:LEU:HD21	1.82	0.61
1:g:357:PHE:HE2	1:g:368:VAL:HG22	1.64	0.61
5:L:37:ARG:HB3	5:L:183:LEU:HD22	1.82	0.61
1:U:408:PHE:O	1:U:412:VAL:HG23	2.00	0.61
5:a:116:VAL:CG1	5:a:117:PRO:HD3	2.30	0.61
1:c:377:ASP:OD1	1:c:378:ASP:N	2.33	0.61
5:e:28:ARG:HD3	5:e:135:ALA:H	1.65	0.61
5:e:196:ARG:HH22	1:o:406:GLU:HB2	1.64	0.61
2:y:25:LEU:HB3	2:y:70:ILE:HD11	1.82	0.61
3:2:93:ARG:NH2	3:j:73:ASP:OD2	2.34	0.61
4:A:532:LYS:HB2	4:A:544:PRO:HD3	1.83	0.61
5:J:67:GLU:OE2	5:e:196:ARG:NE	2.34	0.61
2:V:19:ALA:O	2:V:72:ARG:NH2	2.33	0.61
5:W:39:ARG:NH1	5:W:67:GLU:OE1	2.33	0.61
2:Z:58:VAL:HG11	2:Z:72:ARG:HD2	1.83	0.61
1:r:63:ASN:HD22	1:r:364:LEU:HD22	1.66	0.61
1:u:408:PHE:O	1:u:412:VAL:HG23	2.00	0.61
3:w:108:PRO:HB2	3:w:132:ALA:HB2	1.80	0.61
1:6:484:THR:HG23	1:6:487:LEU:HD12	1.82	0.61
4:A:324:ALA:HB1	4:A:331:LEU:HD11	1.82	0.61
5:i:18:CYS:SG	5:i:22:THR:OG1	2.57	0.61
1:u:401:ALA:HB1	1:u:427:ILE:HG12	1.82	0.61
3:w:34:THR:O	3:w:38:ARG:HG2	2.00	0.61
1:0:502:GLN:O	1:0:506:ILE:HD12	2.00	0.61
2:4:59:LYS:HD2	2:4:74:GLN:HG2	1.83	0.61
4:C:43:ARG:NH2	4:D:350:ASN:OD1	2.33	0.61
1:Y:276:LEU:HD23	1:Y:330:ILE:HD11	1.83	0.61
5:i:11:ILE:HA	5:i:155:LEU:HD21	1.81	0.61
1:x:408:PHE:O	1:x:412:VAL:HG23	2.00	0.61
3:f:9:LEU:HD12	3:f:151:GLN:HG3	1.83	0.61
3:z:34:THR:O	3:z:38:ARG:HG2	2.01	0.61
4:D:532:LYS:HB2	4:D:544:PRO:HD3	1.83	0.61
2:R:18:LEU:HB2	2:R:82:PHE:HB2	1.81	0.61
1:g:323:THR:N	1:k:174:THR:OG1	2.26	0.61
5:K:12:HIS:ND1	5:K:16:PRO:O	2.28	0.61
1:Y:377:ASP:OD1	1:Y:378:ASP:N	2.34	0.61
2:l:43:TRP:CD1	2:l:59:LYS:HD2	2.35	0.61
1:u:345:ARG:HD2	1:u:538:ASP:HB2	1.81	0.61
1:6:134:LYS:NZ	1:6:507:GLU:OE2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:92:LEU:HD11	2:Q:8:ASN:HD21	1.64	0.61
2:Q:14:LEU:HD21	2:Q:25:LEU:HD13	1.83	0.61
3:T:149:THR:HG23	3:T:150:THR:HG23	1.83	0.61
3:n:171:TYR:CD1	3:n:190:TYR:HB2	2.36	0.61
2:M:93:THR:HB	2:M:97:LEU:HD12	1.82	0.60
3:z:170:LEU:HB3	3:z:189:HIS:CD2	2.36	0.60
1:3:374:ASP:OD1	1:3:375:ILE:N	2.34	0.60
4:E:95:MET:HE1	4:E:97:VAL:HG23	1.83	0.60
5:H:69:GLU:OE2	5:a:84:GLN:NE2	2.35	0.60
5:K:69:GLU:OE2	5:m:84:GLN:NE2	2.35	0.60
1:U:375:ILE:HB	1:U:450:LEU:HD21	1.83	0.60
2:V:49:ILE:HG23	2:V:55:ARG:HG2	1.82	0.60
3:q:34:THR:O	3:q:38:ARG:HG2	2.00	0.60
1:r:579:VAL:HG23	1:r:580:MET:HE2	1.83	0.60
2:v:57:ILE:HG21	2:v:92:LEU:HB2	1.83	0.60
1:x:374:ASP:OD1	1:x:375:ILE:N	2.34	0.60
1:0:375:ILE:HB	1:0:450:LEU:HD21	1.83	0.60
2:7:14:LEU:HB3	2:7:86:ASP:HB2	1.82	0.60
4:B:6:LEU:HB3	4:B:9:TYR:HE2	1.66	0.60
4:D:249:PHE:HB2	4:D:262:TYR:HB3	1.83	0.60
1:U:568:MET:HG3	1:Y:590:LEU:HD11	1.83	0.60
2:Z:59:LYS:HD2	2:Z:74:GLN:HG2	1.82	0.60
2:d:14:LEU:HB3	2:d:86:ASP:HB2	1.83	0.60
1:o:596:ILE:O	1:o:600:ILE:HG12	2.02	0.60
1:0:556:THR:HG22	1:0:559:GLN:HG3	1.83	0.60
1:0:575:GLN:O	1:0:576:VAL:HG12	2.00	0.60
2:1:49:ILE:HG23	2:1:55:ARG:HG2	1.83	0.60
4:C:57:LYS:NZ	4:C:70:GLN:O	2.27	0.60
5:L:178:ARG:NH1	5:S:157:GLU:OE2	2.33	0.60
5:S:46:GLU:HG2	5:S:124:ARG:HG2	1.81	0.60
5:e:196:ARG:HH12	1:o:406:GLU:HG3	1.66	0.60
1:0:286:ARG:HE	1:3:219:ALA:HA	1.65	0.60
3:f:175:SER:O	3:f:178:SER:OG	2.20	0.60
1:g:375:ILE:HB	1:g:450:LEU:HD21	1.84	0.60
2:y:14:LEU:HB3	2:y:86:ASP:HB2	1.82	0.60
4:A:350:ASN:OD1	4:F:43:ARG:NH2	2.35	0.60
4:B:57:LYS:NZ	4:B:70:GLN:O	2.34	0.60
4:E:6:LEU:HB3	4:E:9:TYR:HE2	1.66	0.60
2:M:45:MET:HE1	2:M:74:GLN:HE21	1.65	0.60
2:P:49:ILE:HG23	2:P:55:ARG:HG2	1.81	0.60
3:T:71:LEU:HA	3:T:141:CYS:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:147:LEU:HD11	1:k:498:GLN:HE22	1.67	0.60
2:1:19:ALA:O	2:1:72:ARG:NH2	2.34	0.60
1:3:145:ASN:ND2	1:3:179:ILE:O	2.32	0.60
2:7:57:ILE:HG21	2:7:75:GLU:HG3	1.83	0.60
4:D:487:PHE:O	2:M:87:ARG:NH2	2.35	0.60
4:F:234:LEU:HD11	4:F:280:ILE:HG12	1.83	0.60
1:g:575:GLN:O	1:g:576:VAL:HG12	2.02	0.60
3:n:51:THR:HG22	3:n:140:VAL:HG22	1.84	0.60
1:u:583:LEU:HD21	1:x:599:ARG:HH12	1.67	0.60
1:0:100:ILE:HD12	1:0:372:MET:HB3	1.83	0.60
4:D:489:LEU:HD12	4:D:511:MET:HE1	1.83	0.60
5:a:69:GLU:H	5:a:127:GLY:HA2	1.67	0.60
3:b:51:THR:HG22	3:b:140:VAL:HG22	1.84	0.60
4:A:28:ARG:HE	4:A:441:ARG:HD3	1.67	0.60
4:F:386:THR:HB	4:F:401:SER:HB3	1.84	0.60
5:S:11:ILE:HD13	5:S:23:ALA:HB1	1.83	0.60
3:j:144:ARG:NH2	3:z:160:GLU:OE2	2.26	0.60
1:k:271:ARG:HH21	1:k:273:ARG:HH11	1.49	0.60
2:v:63:ARG:NH1	2:v:65:VAL:O	2.31	0.60
2:4:93:THR:HA	2:4:96:GLU:HG2	1.82	0.60
4:A:247:LEU:HB2	4:A:266:MET:HE1	1.84	0.60
4:C:234:LEU:HD11	4:C:280:ILE:HG12	1.82	0.60
5:G:39:ARG:NH1	5:G:67:GLU:OE2	2.34	0.60
5:I:40:LEU:HD21	5:I:189:LYS:HB3	1.82	0.60
2:Q:47:THR:OG1	2:Q:89:GLU:O	2.20	0.60
3:X:69:ILE:N	3:X:142:ALA:O	2.27	0.60
5:a:66:TYR:HB2	5:a:130:LYS:HB2	1.83	0.60
5:a:76:ARG:HH12	5:a:101:GLN:HB2	1.66	0.60
5:e:11:ILE:HD13	5:e:23:ALA:HB1	1.84	0.60
1:o:190:ILE:HB	1:o:207:PHE:HB2	1.84	0.60
5:I:18:CYS:HA	5:I:166:TRP:CH2	2.37	0.59
1:U:170:TYR:H	1:U:344:PHE:HZ	1.49	0.59
1:c:442:MET:HE1	1:g:440:MET:SD	2.41	0.59
2:v:27:VAL:HG13	2:v:68:MET:HE1	1.84	0.59
3:5:34:THR:O	3:5:38:ARG:HG2	2.02	0.59
5:S:87:ASP:OD1	5:S:94:ARG:NH1	2.34	0.59
1:U:391:SER:OG	5:W:204:GLN:O	2.20	0.59
3:f:171:TYR:CD1	3:f:190:TYR:HB2	2.37	0.59
1:g:190:ILE:HB	1:g:207:PHE:HB2	1.83	0.59
1:g:440:MET:HE2	1:g:440:MET:HA	1.84	0.59
1:g:582:ASP:OD1	1:g:583:LEU:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:100:PHE:HD2	2:y:104:ILE:HD12	1.66	0.59
3:w:145:HIS:HD2	3:w:146:PRO:HD2	1.67	0.59
2:V:45:MET:HE1	2:V:74:GLN:HG2	1.84	0.59
3:X:79:LYS:HD3	3:X:111:GLN:HE21	1.67	0.59
3:n:185:VAL:HG22	3:n:189:HIS:CE1	2.37	0.59
1:u:190:ILE:HB	1:u:207:PHE:HB2	1.85	0.59
1:6:565:LEU:HD21	1:6:583:LEU:HB3	1.84	0.59
4:C:21:LEU:HB2	4:C:443:LYS:HG3	1.84	0.59
5:H:8:MET:HG3	5:H:12:HIS:HD2	1.66	0.59
1:o:123:ARG:NH1	1:o:544:ALA:O	2.31	0.59
4:D:386:THR:HB	4:D:401:SER:HB3	1.83	0.59
4:F:314:ARG:HH21	4:F:361:VAL:HG22	1.67	0.59
1:g:408:PHE:O	1:g:412:VAL:HG23	2.02	0.59
2:N:19:ALA:O	2:N:72:ARG:NH1	2.31	0.59
1:U:187:ARG:HD3	1:U:249:ALA:HB1	1.83	0.59
2:d:13:ARG:HD3	2:d:86:ASP:H	1.68	0.59
5:i:93:TRP:CD1	5:i:116:VAL:HG23	2.37	0.59
2:M:98:GLY:HA2	2:M:101:ARG:HD3	1.85	0.59
5:W:88:GLU:HG3	5:W:89:GLN:OE1	2.03	0.59
1:c:569:ILE:HG12	1:c:580:MET:HB3	1.85	0.59
5:i:8:MET:HG3	5:i:12:HIS:CD2	2.37	0.59
3:j:8:VAL:HG22	3:j:162:VAL:HG23	1.84	0.59
1:o:579:VAL:HG23	1:o:580:MET:HE3	1.84	0.59
1:r:184:GLU:HG3	1:r:208:ARG:HH12	1.68	0.59
2:s:8:ASN:HB2	2:y:94:ALA:HB2	1.84	0.59
5:J:141:LEU:O	5:J:145:THR:OG1	2.21	0.59
3:j:175:SER:O	3:j:178:SER:OG	2.20	0.59
1:o:408:PHE:O	1:o:412:VAL:HG23	2.03	0.59
1:r:117:ASP:OD2	1:r:139:LYS:NZ	2.34	0.59
1:0:497:MET:HE1	1:3:146:ARG:NE	2.18	0.59
5:G:202:ARG:HH21	5:W:88:GLU:CD	2.11	0.59
1:U:348:ARG:HH21	1:U:539:ILE:HD12	1.66	0.59
5:e:88:GLU:HG3	5:e:89:GLN:OE1	2.02	0.59
1:g:385:LYS:HE3	1:g:389:ILE:HD11	1.84	0.59
3:q:15:LEU:HG	3:q:170:LEU:HD21	1.84	0.59
1:0:211:TRP:HB3	1:0:273:ARG:HH21	1.68	0.58
4:A:33:ARG:O	4:A:40:THR:OG1	2.20	0.58
4:C:80:VAL:HG13	4:C:84:ARG:NH2	2.18	0.58
5:S:88:GLU:HG3	5:S:89:GLN:OE1	2.03	0.58
1:g:211:TRP:HB3	1:g:273:ARG:HH21	1.68	0.58
3:t:34:THR:O	3:t:38:ARG:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:w:170:LEU:HB3	3:w:189:HIS:CD2	2.38	0.58
1:x:78:GLN:HE22	1:x:98:ASN:HA	1.68	0.58
2:1:91:ARG:HE	2:7:93:THR:HG21	1.68	0.58
3:2:34:THR:O	3:2:38:ARG:HG2	2.03	0.58
1:3:42:MET:HB3	1:3:336:LEU:HD11	1.86	0.58
1:c:271:ARG:HH21	1:c:273:ARG:HH11	1.51	0.58
3:t:160:GLU:OE1	3:t:160:GLU:N	2.28	0.58
1:x:211:TRP:HB3	1:x:273:ARG:HH21	1.67	0.58
1:x:401:ALA:HB1	1:x:427:ILE:HD11	1.85	0.58
3:2:144:ARG:NH2	3:j:159:ALA:H	2.00	0.58
4:E:2:THR:N	4:E:573:GLU:OE2	2.35	0.58
5:H:69:GLU:H	5:H:127:GLY:HA2	1.67	0.58
2:d:49:ILE:HB	2:d:87:ARG:HB2	1.85	0.58
3:q:145:HIS:HD2	3:q:146:PRO:HD2	1.69	0.58
1:u:122:PRO:HB2	1:u:125:LYS:HA	1.86	0.58
1:u:377:ASP:OD1	1:u:378:ASP:N	2.35	0.58
1:0:323:THR:N	1:3:174:THR:OG1	2.31	0.58
1:6:145:ASN:ND2	1:6:179:ILE:O	2.28	0.58
4:A:235:PRO:HG2	4:A:278:THR:HA	1.85	0.58
4:D:43:ARG:NH2	4:E:350:ASN:OD1	2.36	0.58
4:F:14:PRO:HG2	4:F:347:MET:HG3	1.85	0.58
5:G:157:GLU:OE2	5:S:13:ARG:NH1	2.36	0.58
1:U:64:ARG:HD3	1:U:186:TRP:HZ3	1.69	0.58
3:X:73:ASP:OD1	3:X:74:VAL:N	2.36	0.58
1:g:377:ASP:OD1	1:g:378:ASP:N	2.37	0.58
1:g:445:ARG:HG3	1:g:449:MET:HE2	1.84	0.58
5:m:69:GLU:H	5:m:127:GLY:HA2	1.69	0.58
2:v:59:LYS:HD3	2:v:74:GLN:HG3	1.85	0.58
1:0:445:ARG:HG3	1:0:449:MET:HE2	1.84	0.58
4:A:19:ARG:NH2	4:F:564:ASP:OD2	2.36	0.58
4:B:312:ASN:ND2	4:B:360:ILE:O	2.36	0.58
5:i:34:PHE:O	5:i:38:THR:OG1	2.22	0.58
1:r:388:TYR:OH	1:u:416:ASP:OD2	2.22	0.58
4:D:234:LEU:HD11	4:D:280:ILE:HG12	1.85	0.58
4:F:235:PRO:HG2	4:F:278:THR:HA	1.85	0.58
5:e:116:VAL:HG13	5:e:117:PRO:HD3	1.85	0.58
5:i:32:ILE:HG23	5:i:130:LYS:HD2	1.86	0.58
1:k:369:ILE:HA	1:k:372:MET:HE2	1.85	0.58
3:n:27:ASP:OD1	3:n:28:GLU:N	2.37	0.58
1:o:661:ALA:HB2	1:r:656:ALA:HA	1.86	0.58
3:5:170:LEU:HB3	3:5:189:HIS:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:406:GLU:HB2	5:S:196:ARG:HH22	1.69	0.58
4:C:386:THR:HB	4:C:401:SER:HB3	1.86	0.58
5:G:40:LEU:HD21	5:G:189:LYS:HB3	1.84	0.58
5:I:37:ARG:HB3	5:I:183:LEU:HD22	1.86	0.58
2:d:14:LEU:HB2	2:d:88:ILE:HD11	1.85	0.58
3:n:48:TYR:O	3:n:49:MET:HE2	2.03	0.58
1:o:484:THR:HG23	1:o:487:LEU:HD12	1.84	0.58
1:u:668:ALA:HB2	1:x:663:LEU:HA	1.85	0.58
2:y:63:ARG:HG3	2:y:68:MET:HE2	1.85	0.58
4:A:234:LEU:HD11	4:A:280:ILE:HG12	1.85	0.58
5:H:11:ILE:HA	5:H:155:LEU:HD21	1.85	0.58
5:J:109:SER:OG	5:J:110:GLU:N	2.36	0.58
5:K:69:GLU:H	5:K:127:GLY:HA2	1.69	0.58
2:Q:14:LEU:HB2	2:Q:86:ASP:HB2	1.85	0.58
1:U:248:GLU:O	1:U:252:TRP:CB	2.51	0.58
1:Y:279:CYS:N	1:Y:329:ALA:O	2.32	0.58
5:a:204:GLN:HE21	5:a:204:GLN:HA	1.69	0.58
1:c:393:ASN:ND2	1:c:430:ASN:OD1	2.36	0.58
5:i:107:GLN:NE2	5:i:110:GLU:O	2.35	0.58
1:r:568:MET:HG3	1:u:590:LEU:HD11	1.85	0.58
3:2:33:LEU:HD22	3:2:148:LEU:HG	1.86	0.58
1:3:493:PHE:HE1	1:6:146:ARG:HD3	1.69	0.58
4:F:30:LEU:HD23	4:F:31:ASN:HB2	1.85	0.58
1:k:445:ARG:HH21	1:o:440:MET:HG3	1.69	0.58
3:n:48:TYR:HE2	3:n:143:TRP:HD1	1.52	0.58
1:0:224:ARG:NH1	1:0:337:LEU:O	2.37	0.58
1:0:408:PHE:O	1:0:412:VAL:HG23	2.04	0.58
4:E:324:ALA:HB1	4:E:331:LEU:HD11	1.84	0.58
1:U:393:ASN:ND2	1:U:430:ASN:OD1	2.37	0.58
1:g:661:ALA:HB2	1:k:656:ALA:HA	1.86	0.58
4:E:441:ARG:NH2	4:E:553:GLU:OE2	2.37	0.57
4:F:28:ARG:NH1	4:F:439:SER:OG	2.37	0.57
2:Q:5:GLN:NE2	2:Q:6:PHE:O	2.36	0.57
1:g:440:MET:HE1	1:g:443:MET:HE3	1.85	0.57
1:o:432:ASP:OD1	1:r:430:ASN:ND2	2.28	0.57
1:r:401:ALA:HB1	1:r:427:ILE:HD11	1.85	0.57
1:3:489:ASP:OD1	1:6:115:ARG:NH2	2.37	0.57
4:C:235:PRO:HG2	4:C:278:THR:HA	1.86	0.57
5:H:37:ARG:HB3	5:H:183:LEU:HD22	1.87	0.57
5:W:11:ILE:HA	5:W:155:LEU:HD21	1.84	0.57
1:c:329:ALA:HA	1:c:339:GLU:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:583:LEU:HD23	1:k:599:ARG:HH12	1.69	0.57
1:o:117:ASP:OD2	1:o:139:LYS:NZ	2.36	0.57
1:r:433:ARG:HB2	1:r:433:ARG:HH11	1.69	0.57
1:0:579:VAL:HG23	1:0:580:MET:HE3	1.86	0.57
2:1:87:ARG:NH2	4:C:487:PHE:O	2.37	0.57
4:A:487:PHE:O	2:h:87:ARG:NH2	2.36	0.57
4:B:249:PHE:HB2	4:B:262:TYR:HB3	1.86	0.57
4:F:487:PHE:O	2:V:87:ARG:NH2	2.37	0.57
5:J:25:ALA:O	5:J:29:GLU:HG3	2.04	0.57
1:c:78:GLN:HE22	1:c:98:ASN:HA	1.69	0.57
1:c:402:VAL:HG21	1:c:408:PHE:HB2	1.86	0.57
3:f:160:GLU:HG3	3:z:42:VAL:HG21	1.85	0.57
1:g:583:LEU:CD2	1:k:599:ARG:HH12	2.17	0.57
5:m:93:TRP:HE1	5:m:116:VAL:HA	1.70	0.57
1:o:445:ARG:HG3	1:o:449:MET:HE2	1.86	0.57
1:3:596:ILE:O	1:3:600:ILE:HG13	2.04	0.57
3:5:33:LEU:HD22	3:5:148:LEU:HG	1.86	0.57
4:C:33:ARG:HG3	4:C:42:THR:HG22	1.87	0.57
4:D:235:PRO:HG2	4:D:278:THR:HA	1.85	0.57
3:X:171:TYR:CD1	3:X:190:TYR:HB2	2.39	0.57
5:m:93:TRP:HD1	5:m:116:VAL:HG23	1.67	0.57
2:4:97:LEU:HD22	2:7:100:PHE:HE2	1.69	0.57
1:6:583:LEU:HD21	1:U:599:ARG:HH12	1.68	0.57
4:A:14:PRO:HG2	4:A:347:MET:HG2	1.86	0.57
4:C:30:LEU:HB3	4:C:439:SER:HB3	1.86	0.57
4:F:543:LEU:O	3:j:23:ARG:HG2	2.03	0.57
5:L:158:LEU:O	5:L:161:ILE:HG12	2.05	0.57
5:S:116:VAL:HG13	5:S:117:PRO:HD3	1.86	0.57
1:Y:481:THR:O	1:Y:485:ASN:ND2	2.37	0.57
1:Y:511:THR:HG23	1:Y:514:LYS:H	1.68	0.57
1:0:539:ILE:O	1:0:543:LYS:HG2	2.05	0.57
1:3:369:ILE:HA	1:3:372:MET:HE2	1.86	0.57
1:6:575:GLN:O	1:6:576:VAL:HG12	2.05	0.57
4:B:361:VAL:HB	4:B:372:SER:HB3	1.86	0.57
4:F:312:ASN:ND2	4:F:360:ILE:O	2.38	0.57
5:K:164:LYS:HZ1	5:K:166:TRP:HZ3	1.51	0.57
3:T:73:ASP:OD2	3:t:93:ARG:NH2	2.37	0.57
1:k:408:PHE:O	1:k:412:VAL:HG23	2.05	0.57
1:k:596:ILE:O	1:k:600:ILE:HG13	2.05	0.57
1:o:388:TYR:OH	1:r:416:ASP:OD2	2.21	0.57
3:q:170:LEU:HB3	3:q:189:HIS:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:r:64:ARG:HH22	1:r:190:ILE:HD13	1.69	0.57
1:r:433:ARG:HB2	1:r:433:ARG:NH1	2.20	0.57
1:u:575:GLN:O	1:u:576:VAL:HG12	2.03	0.57
3:z:33:LEU:HD22	3:z:148:LEU:HG	1.86	0.57
4:B:441:ARG:NH2	4:B:553:GLU:OE2	2.37	0.57
4:C:43:ARG:NH1	4:C:429:ASP:O	2.37	0.57
4:C:54:ASP:OD1	4:C:55:ASN:N	2.38	0.57
4:C:543:LEU:O	3:T:23:ARG:HG2	2.05	0.57
4:D:14:PRO:HG2	4:D:347:MET:HG2	1.86	0.57
3:T:8:VAL:HG22	3:T:162:VAL:HG23	1.87	0.57
1:Y:154:SER:O	1:Y:158:THR:HG23	2.05	0.57
5:e:11:ILE:HA	5:e:155:LEU:HD21	1.87	0.57
1:0:377:ASP:OD1	1:0:378:ASP:N	2.38	0.57
2:4:45:MET:HE1	2:4:59:LYS:HG2	1.85	0.57
4:C:97:VAL:O	4:C:100:THR:OG1	2.23	0.57
4:C:283:MET:HE1	4:C:316:VAL:HG11	1.86	0.57
4:F:33:ARG:O	4:F:40:THR:OG1	2.22	0.57
3:T:171:TYR:CD1	3:T:190:TYR:HB2	2.40	0.57
1:c:211:TRP:HB3	1:c:273:ARG:HH21	1.68	0.57
3:n:25:THR:N	3:n:28:GLU:OE2	2.29	0.57
1:r:285:MET:N	1:r:323:THR:O	2.37	0.57
1:r:534:LEU:HD12	1:r:535:PRO:HD2	1.86	0.57
1:0:154:SER:O	1:0:158:THR:HG23	2.04	0.57
3:5:32:TRP:HH2	3:X:15:LEU:HD21	1.69	0.57
4:E:487:PHE:O	2:P:87:ARG:NH2	2.37	0.57
4:F:30:LEU:HB3	4:F:439:SER:HB3	1.87	0.57
1:Y:569:ILE:HD13	1:Y:581:LEU:HD23	1.86	0.57
5:e:46:GLU:HG2	5:e:124:ARG:HG2	1.87	0.57
1:r:248:GLU:O	1:r:252:TRP:CB	2.52	0.57
2:1:93:THR:HB	2:1:97:LEU:HD12	1.86	0.57
1:6:661:ALA:HB2	1:U:656:ALA:HA	1.87	0.57
4:F:21:LEU:HB2	4:F:443:LYS:HG3	1.86	0.57
1:Y:575:GLN:O	1:Y:576:VAL:HG12	2.04	0.57
5:a:116:VAL:HG13	5:a:117:PRO:HD3	1.87	0.57
1:g:154:SER:O	1:g:158:THR:HG23	2.04	0.57
1:g:511:THR:HG23	1:g:514:LYS:H	1.68	0.57
5:m:57:VAL:HG11	5:m:65:LEU:HD22	1.86	0.57
3:q:145:HIS:CE1	3:q:155:VAL:HA	2.40	0.57
3:t:30:LEU:HD22	3:t:148:LEU:HB3	1.85	0.57
2:v:47:THR:OG1	2:v:89:GLU:O	2.21	0.57
1:0:73:TYR:HD1	1:0:78:GLN:HG2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:401:ALA:HB1	1:3:427:ILE:HD11	1.86	0.56
1:Y:668:ALA:HB2	1:c:663:LEU:HA	1.86	0.56
2:h:97:LEU:HA	2:h:100:PHE:HD1	1.70	0.56
4:A:35:ASP:OD1	4:A:36:ASN:N	2.38	0.56
5:G:141:LEU:O	5:G:145:THR:OG1	2.22	0.56
5:H:12:HIS:ND1	5:H:16:PRO:O	2.28	0.56
2:s:19:ALA:O	2:s:72:ARG:NH2	2.38	0.56
1:0:385:LYS:HE3	1:0:389:ILE:HD11	1.88	0.56
1:3:379:ILE:HG23	1:3:443:MET:HG3	1.88	0.56
4:B:33:ARG:O	4:B:40:THR:OG1	2.22	0.56
4:C:14:PRO:HG2	4:C:347:MET:HG3	1.87	0.56
4:D:542:ARG:HB3	3:b:23:ARG:HG3	1.86	0.56
5:K:37:ARG:HB3	5:K:183:LEU:HD22	1.87	0.56
2:M:47:THR:HA	2:M:57:ILE:HD12	1.88	0.56
2:P:98:GLY:HA2	2:P:101:ARG:HD3	1.86	0.56
1:Y:661:ALA:HB2	1:c:656:ALA:HA	1.86	0.56
2:Z:49:ILE:HB	2:Z:87:ARG:HB2	1.86	0.56
1:c:64:ARG:HD3	1:c:186:TRP:HZ3	1.69	0.56
1:c:154:SER:O	1:c:158:THR:HG23	2.06	0.56
3:f:73:ASP:OD2	3:f:74:VAL:N	2.38	0.56
5:i:156:SER:O	5:i:160:ILE:HG12	2.05	0.56
1:k:348:ARG:NH2	1:k:500:GLU:OE1	2.37	0.56
1:o:565:LEU:HD21	1:o:583:LEU:HB3	1.86	0.56
2:s:52:ASP:OD1	2:s:53:GLY:N	2.34	0.56
1:x:263:SER:O	1:x:264:ARG:NE	2.37	0.56
3:2:24:TRP:CD1	3:2:176:LYS:HZ2	2.24	0.56
1:3:206:ILE:HD12	1:3:351:LEU:HD12	1.88	0.56
4:A:543:LEU:O	3:n:23:ARG:HG2	2.05	0.56
4:E:312:ASN:ND2	4:E:360:ILE:O	2.38	0.56
4:F:33:ARG:HG3	4:F:42:THR:HG22	1.86	0.56
4:F:479:ILE:HD13	4:F:515:PRO:HA	1.88	0.56
5:J:20:GLU:OE1	3:z:113:ARG:NH2	2.36	0.56
5:K:11:ILE:HA	5:K:155:LEU:HD21	1.87	0.56
5:K:32:ILE:HG23	5:K:130:LYS:HD2	1.86	0.56
5:W:69:GLU:H	5:W:127:GLY:HA2	1.70	0.56
5:m:32:ILE:O	5:m:36:GLU:HG2	2.06	0.56
1:o:377:ASP:OD1	1:o:378:ASP:N	2.39	0.56
1:0:668:ALA:HB2	1:3:663:LEU:HA	1.87	0.56
1:3:442:MET:HE1	1:6:387:LEU:HB2	1.87	0.56
5:K:12:HIS:HB3	3:n:98:THR:HB	1.87	0.56
1:U:251:ASP:OD1	1:U:275:ARG:NH2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:78:MET:HE1	5:W:103:GLN:C	2.29	0.56
1:Y:372:MET:HA	1:Y:450:LEU:HD11	1.88	0.56
5:a:87:ASP:OD1	5:a:94:ARG:NH1	2.29	0.56
1:o:668:ALA:HB2	1:r:663:LEU:HA	1.87	0.56
1:0:174:THR:OG1	1:x:323:THR:N	2.33	0.56
1:6:408:PHE:O	1:6:412:VAL:HG23	2.06	0.56
4:A:105:ALA:HA	4:A:224:PRO:HD2	1.86	0.56
4:F:43:ARG:NH1	4:F:429:ASP:O	2.37	0.56
2:O:58:VAL:HB	2:O:70:ILE:HD11	1.86	0.56
1:U:184:GLU:HG3	1:U:208:ARG:HH12	1.70	0.56
1:U:224:ARG:HH11	1:U:337:LEU:HD13	1.69	0.56
1:c:154:SER:HB3	1:c:354:ILE:HD12	1.87	0.56
1:c:357:PHE:HE2	1:c:368:VAL:HG22	1.70	0.56
1:o:435:LEU:HD21	1:r:433:ARG:HE	1.69	0.56
2:s:98:GLY:HA2	2:s:101:ARG:HD3	1.86	0.56
3:t:33:LEU:HD22	3:t:148:LEU:HG	1.86	0.56
1:0:661:ALA:HB2	1:3:656:ALA:HA	1.87	0.56
4:E:43:ARG:NH1	4:E:429:ASP:O	2.37	0.56
5:K:195:GLN:HE22	5:m:106:THR:HA	1.71	0.56
5:W:12:HIS:HB3	3:t:98:THR:HB	1.87	0.56
3:b:15:LEU:HG	3:b:170:LEU:HD21	1.87	0.56
1:c:489:ASP:OD2	1:g:112:LYS:HD3	2.06	0.56
2:d:57:ILE:HG13	2:d:75:GLU:HB2	1.88	0.56
1:k:42:MET:HB3	1:k:336:LEU:HD11	1.87	0.56
1:k:379:ILE:HG23	1:k:443:MET:HG3	1.87	0.56
5:m:164:LYS:HB3	5:m:166:TRP:HE3	1.71	0.56
1:o:187:ARG:HD3	1:o:249:ALA:HB1	1.87	0.56
1:u:511:THR:HG23	1:u:514:LYS:H	1.69	0.56
4:A:242:PHE:HA	4:A:247:LEU:HA	1.88	0.56
4:E:97:VAL:O	4:E:100:THR:OG1	2.22	0.56
1:c:558:ARG:HH22	1:c:587:SER:HA	1.71	0.56
1:u:147:LEU:HD21	1:u:498:GLN:HE22	1.71	0.56
1:x:271:ARG:HH21	1:x:273:ARG:HH11	1.54	0.56
2:7:45:MET:HB3	2:7:92:LEU:HD12	1.88	0.56
4:B:43:ARG:NH1	4:B:429:ASP:O	2.37	0.56
4:B:247:LEU:HB2	4:B:266:MET:HE1	1.88	0.56
4:D:21:LEU:HB2	4:D:443:LYS:HG3	1.87	0.56
4:D:383:PHE:HE1	2:N:20:PRO:HG2	1.70	0.56
4:D:479:ILE:HD13	4:D:515:PRO:HA	1.88	0.56
1:Y:42:MET:HB3	1:Y:336:LEU:HD21	1.88	0.56
1:g:492:ARG:HD2	1:g:550:GLU:OE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:559:GLN:O	1:g:563:GLU:HG2	2.06	0.56
1:k:600:ILE:HA	1:k:603:ILE:HG22	1.88	0.56
1:u:661:ALA:HB2	1:x:656:ALA:HA	1.86	0.56
2:1:13:ARG:HD2	2:1:87:ARG:HD3	1.87	0.56
2:7:50:ARG:HB3	2:7:54:ALA:HB3	1.87	0.56
2:7:50:ARG:HD3	2:7:82:PHE:CD1	2.41	0.56
4:E:234:LEU:HD11	4:E:280:ILE:HG12	1.87	0.56
5:I:34:PHE:HA	5:I:183:LEU:HD21	1.86	0.56
1:U:285:MET:HG3	1:U:325:ARG:HE	1.71	0.56
5:W:66:TYR:HB2	5:W:130:LYS:HB2	1.88	0.56
2:l:92:LEU:HD11	2:p:8:ASN:HB2	1.87	0.56
2:p:14:LEU:HB3	2:p:86:ASP:HB2	1.87	0.56
3:w:38:ARG:NE	3:w:145:HIS:O	2.39	0.56
1:O:511:THR:HG23	1:O:514:LYS:H	1.69	0.55
1:6:668:ALA:HB2	1:U:663:LEU:HA	1.88	0.55
4:F:349:ARG:NH1	4:F:353:MET:HE3	2.20	0.55
5:H:141:LEU:O	5:H:145:THR:OG1	2.24	0.55
5:I:158:LEU:O	5:I:161:ILE:HG12	2.06	0.55
2:R:50:ARG:HB2	2:R:54:ALA:HB3	1.87	0.55
5:S:93:TRP:CD1	5:S:116:VAL:HG23	2.38	0.55
3:X:9:LEU:HD12	3:X:151:GLN:HG3	1.88	0.55
3:X:66:GLU:O	3:X:144:ARG:NH1	2.39	0.55
1:k:206:ILE:HD12	1:k:351:LEU:HD12	1.88	0.55
1:o:154:SER:O	1:o:158:THR:HG23	2.05	0.55
2:s:71:THR:OG1	2:s:74:GLN:NE2	2.39	0.55
1:O:56:GLU:HG3	1:O:205:TYR:HE1	1.70	0.55
3:2:170:LEU:HD23	3:2:189:HIS:NE2	2.22	0.55
3:5:79:LYS:HB3	3:5:83:SER:HB3	1.89	0.55
1:6:154:SER:O	1:6:158:THR:HG23	2.05	0.55
1:6:377:ASP:OD1	1:6:378:ASP:N	2.38	0.55
1:6:511:THR:HG23	1:6:514:LYS:H	1.72	0.55
4:A:80:VAL:HG11	4:A:84:ARG:HD3	1.88	0.55
5:G:11:ILE:O	5:G:15:ALA:N	2.37	0.55
5:S:66:TYR:HB2	5:S:130:LYS:HB2	1.88	0.55
1:U:64:ARG:HH22	1:U:190:ILE:HD13	1.70	0.55
3:f:79:LYS:HD2	3:f:83:SER:HB3	1.88	0.55
1:g:224:ARG:NH1	1:g:337:LEU:O	2.39	0.55
3:j:97:ASP:OD2	3:j:103:TRP:NE1	2.36	0.55
2:v:19:ALA:O	2:v:72:ARG:NH1	2.38	0.55
1:x:64:ARG:HD3	1:x:186:TRP:HZ3	1.70	0.55
1:x:377:ASP:O	1:x:381:LYS:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:33:ARG:O	4:C:40:THR:OG1	2.23	0.55
4:F:283:MET:HE1	4:F:316:VAL:HG11	1.88	0.55
5:J:37:ARG:HB3	5:J:183:LEU:HD22	1.87	0.55
3:n:79:LYS:HD2	3:n:83:SER:HB3	1.88	0.55
4:E:361:VAL:HB	4:E:372:SER:HB3	1.88	0.55
5:W:156:SER:O	5:W:160:ILE:HG12	2.06	0.55
2:Z:97:LEU:HD22	2:d:100:PHE:HE2	1.71	0.55
5:a:37:ARG:HB3	5:a:183:LEU:HD22	1.87	0.55
3:b:144:ARG:NH2	3:t:160:GLU:OE1	2.39	0.55
1:c:285:MET:N	1:c:323:THR:O	2.37	0.55
2:h:19:ALA:O	2:h:72:ARG:NH2	2.39	0.55
3:j:171:TYR:CD1	3:j:190:TYR:HB2	2.42	0.55
3:q:38:ARG:NE	3:q:145:HIS:O	2.39	0.55
1:r:329:ALA:HA	1:r:339:GLU:HG3	1.89	0.55
2:4:56:GLU:OE2	2:4:72:ARG:NE	2.31	0.55
5:L:66:TYR:HB2	5:L:130:LYS:HB2	1.88	0.55
5:L:141:LEU:O	5:L:145:THR:OG1	2.24	0.55
2:O:13:ARG:HH21	2:O:87:ARG:HA	1.72	0.55
1:Y:285:MET:HG3	1:Y:325:ARG:HE	1.72	0.55
5:e:66:TYR:HB2	5:e:130:LYS:HB2	1.88	0.55
3:f:161:PHE:O	3:f:165:LEU:HD23	2.06	0.55
1:0:583:LEU:HD21	1:3:599:ARG:NH1	2.20	0.55
4:A:542:ARG:HH11	3:n:23:ARG:HD3	1.72	0.55
4:C:575:ARG:NH1	4:D:449:MET:SD	2.79	0.55
2:s:6:PHE:CE2	2:y:97:LEU:HG	2.41	0.55
1:u:154:SER:O	1:u:158:THR:HG23	2.05	0.55
1:0:599:ARG:HG2	1:x:606:MET:HE1	1.89	0.55
3:2:30:LEU:HD22	3:2:148:LEU:HB3	1.88	0.55
1:3:63:ASN:ND2	1:3:364:LEU:HB3	2.21	0.55
1:6:398:ASP:HB3	1:6:425:LYS:HB3	1.89	0.55
3:b:11:ARG:NE	3:w:31:GLU:OE2	2.40	0.55
1:r:187:ARG:HD3	1:r:249:ALA:HB1	1.88	0.55
1:6:401:ALA:HB1	1:6:427:ILE:HG12	1.88	0.55
4:A:21:LEU:HB2	4:A:443:LYS:HG3	1.88	0.55
5:H:11:ILE:O	5:H:15:ALA:N	2.36	0.55
5:L:157:GLU:HA	5:L:160:ILE:HD12	1.89	0.55
3:X:162:VAL:O	3:X:166:VAL:HG23	2.07	0.55
1:k:248:GLU:O	1:k:252:TRP:CB	2.55	0.55
1:k:368:VAL:HG22	1:k:372:MET:HE1	1.88	0.55
1:r:73:TYR:HD1	1:r:78:GLN:HG2	1.72	0.55
1:u:393:ASN:HD21	1:u:429:LEU:HB3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:326:VAL:HG23	1:x:342:SER:HB3	1.88	0.55
3:z:79:LYS:HB3	3:z:83:SER:HB3	1.89	0.55
1:6:108:ILE:O	1:6:111:GLU:HG3	2.07	0.55
4:C:291:VAL:HG22	4:C:301:GLN:HB3	1.89	0.55
2:R:11:ALA:HA	2:R:89:GLU:HB3	1.89	0.55
1:Y:190:ILE:HB	1:Y:207:PHE:HB2	1.87	0.55
2:l:96:GLU:HG2	2:l:97:LEU:N	2.21	0.55
3:n:45:PRO:O	3:n:49:MET:HE3	2.06	0.55
2:v:49:ILE:N	2:v:87:ARG:O	2.36	0.55
1:x:248:GLU:O	1:x:252:TRP:HB2	2.07	0.55
2:4:47:THR:HG22	2:4:57:ILE:HD13	1.89	0.55
1:6:402:VAL:HG21	1:6:408:PHE:HB2	1.88	0.55
4:B:334:ALA:HB2	4:B:339:MET:HE1	1.89	0.55
2:R:8:ASN:HA	2:R:91:ARG:HH21	1.71	0.55
2:V:86:ASP:OD1	2:V:87:ARG:N	2.37	0.55
5:W:32:ILE:HG23	5:W:130:LYS:HD2	1.88	0.55
2:d:5:GLN:HE22	2:d:38:LEU:HA	1.72	0.55
5:e:204:GLN:O	1:k:391:SER:OG	2.25	0.55
3:n:5:ALA:HB2	3:n:148:LEU:HD12	1.89	0.55
1:o:492:ARG:HD2	1:o:550:GLU:OE2	2.07	0.55
1:u:402:VAL:HG21	1:u:408:PHE:HB2	1.88	0.55
4:A:570:THR:HG22	4:A:572:GLN:H	1.72	0.54
4:B:234:LEU:HD11	4:B:280:ILE:HG12	1.88	0.54
4:B:314:ARG:HH21	4:B:361:VAL:HG22	1.73	0.54
4:E:28:ARG:HH12	4:E:441:ARG:HH11	1.55	0.54
5:I:141:LEU:O	5:I:145:THR:OG1	2.25	0.54
5:K:81:VAL:O	5:i:195:GLN:NE2	2.40	0.54
1:U:596:ILE:O	1:U:600:ILE:HG13	2.07	0.54
3:b:5:ALA:HB2	3:b:148:LEU:HD12	1.88	0.54
1:o:122:PRO:HG3	1:o:128:ALA:HA	1.89	0.54
2:1:86:ASP:OD1	2:1:87:ARG:N	2.37	0.54
3:5:8:VAL:HG22	3:5:162:VAL:HG23	1.88	0.54
4:B:97:VAL:O	4:B:100:THR:OG1	2.26	0.54
4:E:32:VAL:HG23	4:E:438:LEU:HD11	1.90	0.54
5:L:156:SER:O	5:L:160:ILE:HG13	2.06	0.54
2:O:59:LYS:HB2	2:O:74:GLN:HG2	1.87	0.54
1:U:154:SER:O	1:U:158:THR:HG23	2.07	0.54
1:U:285:MET:N	1:U:323:THR:O	2.40	0.54
5:W:16:PRO:O	5:W:166:TRP:NE1	2.34	0.54
1:c:323:THR:N	1:g:174:THR:OG1	2.30	0.54
1:g:668:ALA:HB2	1:k:663:LEU:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:154:SER:O	1:x:158:THR:HG23	2.06	0.54
1:x:154:SER:HB3	1:x:354:ILE:HD12	1.90	0.54
1:0:416:ASP:OD2	1:x:388:TYR:OH	2.23	0.54
1:6:221:VAL:HG21	1:6:337:LEU:HD13	1.88	0.54
4:A:479:ILE:HD13	4:A:515:PRO:HA	1.88	0.54
4:E:482:GLU:HA	4:E:485:THR:HG22	1.89	0.54
5:H:81:VAL:O	5:W:195:GLN:NE2	2.39	0.54
5:J:8:MET:HG3	5:J:12:HIS:CD2	2.40	0.54
5:S:31:ALA:HB1	5:S:142:LEU:HD23	1.89	0.54
1:U:208:ARG:HB3	1:U:278:GLU:HB2	1.90	0.54
1:U:388:TYR:OH	1:Y:416:ASP:OD2	2.24	0.54
3:X:8:VAL:HG22	3:X:162:VAL:HG23	1.89	0.54
5:a:8:MET:HG3	5:a:12:HIS:CD2	2.42	0.54
5:a:20:GLU:HG3	3:b:114:HIS:CD2	2.42	0.54
3:f:32:TRP:HH2	3:w:15:LEU:HD21	1.72	0.54
1:x:357:PHE:HE2	1:x:368:VAL:HG22	1.71	0.54
1:0:596:ILE:O	1:0:600:ILE:HG12	2.06	0.54
2:1:14:LEU:HB3	2:1:86:ASP:HB3	1.88	0.54
2:7:13:ARG:HD3	2:7:86:ASP:H	1.72	0.54
4:C:242:PHE:HA	4:C:247:LEU:HA	1.89	0.54
5:I:24:PHE:O	5:I:28:ARG:HG3	2.08	0.54
2:O:14:LEU:HB3	2:O:86:ASP:HB2	1.90	0.54
5:W:34:PHE:O	5:W:38:THR:OG1	2.23	0.54
3:b:64:LEU:HD13	3:b:68:ALA:HB3	1.88	0.54
1:c:388:TYR:OH	1:g:416:ASP:OD2	2.24	0.54
3:f:24:TRP:CD1	3:f:176:LYS:HZ2	2.26	0.54
1:o:575:GLN:O	1:o:576:VAL:HG12	2.06	0.54
3:q:36:GLY:O	3:q:40:ILE:HG13	2.08	0.54
1:r:153:ARG:NH2	1:r:183:TYR:OH	2.40	0.54
1:r:489:ASP:OD2	1:u:115:ARG:NH2	2.41	0.54
1:u:558:ARG:NH1	1:u:589:ASP:OD1	2.40	0.54
3:w:145:HIS:CE1	3:w:155:VAL:HA	2.40	0.54
1:x:345:ARG:NH1	1:x:508:GLN:HG3	2.21	0.54
1:0:394:LYS:NZ	1:3:412:VAL:O	2.34	0.54
4:B:35:ASP:O	4:C:15:ARG:NH1	2.40	0.54
5:H:34:PHE:HA	5:H:183:LEU:HD21	1.89	0.54
2:M:19:ALA:O	2:M:72:ARG:NH2	2.41	0.54
5:a:164:LYS:HB3	5:a:166:TRP:HE3	1.73	0.54
5:m:8:MET:HG3	5:m:12:HIS:CD2	2.42	0.54
1:o:511:THR:HG23	1:o:514:LYS:H	1.71	0.54
1:0:656:ALA:HA	1:x:661:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:324:ALA:HB1	4:B:331:LEU:HD11	1.89	0.54
4:E:314:ARG:HH21	4:E:361:VAL:HG22	1.71	0.54
1:U:112:LYS:HG2	1:U:152:SER:HB2	1.90	0.54
1:Y:357:PHE:HE2	1:Y:368:VAL:HG22	1.73	0.54
5:e:31:ALA:HB1	5:e:142:LEU:HD23	1.89	0.54
1:g:224:ARG:HD2	1:g:337:LEU:HA	1.89	0.54
1:g:568:MET:HG2	1:k:590:LEU:HD11	1.90	0.54
3:n:161:PHE:O	3:n:165:LEU:HD23	2.08	0.54
1:r:357:PHE:HE2	1:r:368:VAL:HG22	1.71	0.54
1:x:402:VAL:HG21	1:x:408:PHE:HB2	1.90	0.54
5:G:178:ARG:NH1	5:W:157:GLU:OE2	2.36	0.54
1:U:534:LEU:HD12	1:U:535:PRO:HD2	1.89	0.54
3:X:69:ILE:HB	3:X:142:ALA:HB3	1.90	0.54
1:c:596:ILE:O	1:c:600:ILE:HG13	2.07	0.54
1:x:123:ARG:NH1	1:x:543:LYS:O	2.40	0.54
4:C:318:ASP:OD2	4:D:303:ARG:NH2	2.41	0.54
4:C:479:ILE:HD13	4:C:515:PRO:HA	1.88	0.54
4:F:291:VAL:HG22	4:F:301:GLN:HB3	1.90	0.54
3:T:11:ARG:NH1	3:t:31:GLU:OE2	2.40	0.54
1:g:500:GLU:OE1	1:k:146:ARG:NH2	2.34	0.54
5:i:46:GLU:HG2	5:i:124:ARG:HG2	1.90	0.54
1:k:208:ARG:HD3	1:k:351:LEU:HD11	1.89	0.54
1:r:596:ILE:O	1:r:600:ILE:HG13	2.08	0.54
3:t:170:LEU:HD23	3:t:189:HIS:NE2	2.22	0.54
3:z:149:THR:HG23	3:z:150:THR:HG23	1.90	0.54
4:C:241:ALA:O	4:C:248:TYR:N	2.27	0.54
4:C:290:ILE:O	4:C:302:GLN:N	2.41	0.54
4:D:84:ARG:NH2	4:D:95:MET:SD	2.72	0.54
5:H:32:ILE:HG23	5:H:130:LYS:HD2	1.90	0.54
2:N:57:ILE:HG13	2:N:92:LEU:HD22	1.88	0.54
1:U:402:VAL:HG21	1:U:408:PHE:HB2	1.88	0.54
1:c:583:LEU:HD21	1:g:599:ARG:NH2	2.22	0.54
3:j:79:LYS:HD2	3:j:83:SER:HB3	1.90	0.54
1:o:568:MET:HG3	1:r:590:LEU:HD11	1.90	0.54
1:u:582:ASP:OD1	1:u:583:LEU:N	2.41	0.54
1:x:562:SER:HG	1:x:584:TRP:CD1	2.25	0.54
1:x:596:ILE:O	1:x:600:ILE:HG13	2.08	0.54
3:2:38:ARG:NE	3:2:145:HIS:O	2.40	0.54
1:3:64:ARG:HD3	1:3:186:TRP:HZ3	1.72	0.54
1:6:64:ARG:HH22	1:6:187:ARG:HA	1.73	0.54
1:6:215:ASP:OD1	1:6:216:VAL:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:482:GLU:HA	4:B:485:THR:HG22	1.89	0.54
4:F:97:VAL:O	4:F:100:THR:OG1	2.24	0.54
1:c:206:ILE:HD12	1:c:351:LEU:HD12	1.90	0.54
1:k:44:GLU:OE1	1:o:269:HIS:NE2	2.41	0.54
1:r:600:ILE:HA	1:r:603:ILE:HG22	1.89	0.54
4:A:303:ARG:NH2	4:F:318:ASP:OD2	2.41	0.53
4:D:35:ASP:OD1	4:D:36:ASN:N	2.41	0.53
4:D:332:VAL:HG22	4:D:339:MET:HE3	1.89	0.53
2:M:72:ARG:HH12	2:M:80:LEU:H	1.54	0.53
1:U:263:SER:O	1:U:264:ARG:NE	2.37	0.53
5:W:46:GLU:HG2	5:W:124:ARG:HG2	1.90	0.53
1:r:285:MET:HG3	1:r:325:ARG:HE	1.72	0.53
3:t:64:LEU:HD13	3:t:71:LEU:HD23	1.91	0.53
4:A:87:TYR:HE1	4:A:96:ILE:HG13	1.74	0.53
4:B:28:ARG:HH12	4:B:441:ARG:HH11	1.56	0.53
4:C:35:ASP:O	4:D:15:ARG:NH1	2.41	0.53
4:C:575:ARG:HG2	4:D:449:MET:HG3	1.91	0.53
5:G:8:MET:HG3	5:G:12:HIS:CD2	2.41	0.53
5:I:109:SER:OG	5:I:110:GLU:N	2.41	0.53
5:K:34:PHE:HA	5:K:183:LEU:HD21	1.89	0.53
2:P:47:THR:HB	2:P:90:ALA:HB3	1.90	0.53
1:Y:578:LEU:HA	1:Y:581:LEU:HD12	1.89	0.53
1:Y:583:LEU:HD21	1:c:599:ARG:HH12	1.72	0.53
3:b:113:ARG:HB2	3:b:129:PRO:HD3	1.91	0.53
5:i:139:PRO:HD2	5:i:142:LEU:HD12	1.90	0.53
5:i:164:LYS:HB3	5:i:166:TRP:CE3	2.41	0.53
3:j:77:ASN:HA	3:j:137:VAL:HG13	1.89	0.53
1:x:208:ARG:HD3	1:x:351:LEU:HD11	1.89	0.53
1:x:285:MET:N	1:x:323:THR:O	2.40	0.53
4:E:548:LEU:O	3:w:23:ARG:NH2	2.41	0.53
5:J:94:ARG:HD3	5:e:126:TYR:CZ	2.44	0.53
3:b:79:LYS:HD2	3:b:83:SER:HB3	1.90	0.53
1:c:359:ARG:HG3	1:g:75:ASP:OD2	2.08	0.53
1:c:661:ALA:HB2	1:g:656:ALA:HA	1.91	0.53
5:i:15:ALA:HB1	5:i:166:TRP:HD1	1.74	0.53
5:i:200:ARG:HH12	1:u:414:ARG:HG3	1.73	0.53
1:k:63:ASN:ND2	1:k:364:LEU:HB3	2.23	0.53
1:r:403:GLU:HG3	1:r:422:LYS:HE3	1.91	0.53
3:2:8:VAL:HG22	3:2:162:VAL:HG23	1.89	0.53
1:6:392:SER:HB3	5:G:203:ALA:HB2	1.91	0.53
4:B:239:MET:HA	4:B:239:MET:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:28:ARG:NH1	4:C:439:SER:OG	2.42	0.53
4:E:55:ASN:HB3	4:E:70:GLN:HE22	1.73	0.53
4:F:242:PHE:HA	4:F:247:LEU:HA	1.89	0.53
4:F:524:ILE:HG13	4:F:543:LEU:HD21	1.88	0.53
4:F:536:LYS:HG2	4:F:539:ARG:HH21	1.72	0.53
5:I:156:SER:O	5:I:160:ILE:HG13	2.08	0.53
5:J:40:LEU:HD21	5:J:189:LYS:HB3	1.90	0.53
1:Y:64:ARG:HD3	1:Y:186:TRP:HZ3	1.73	0.53
1:k:184:GLU:OE2	1:k:208:ARG:NH1	2.41	0.53
3:n:153:ASP:OD1	3:n:154:VAL:N	2.40	0.53
1:0:568:MET:O	1:0:572:MET:HG2	2.08	0.53
1:0:588:THR:HG23	1:0:590:LEU:HG	1.90	0.53
2:1:38:LEU:HD21	2:1:44:PHE:HD2	1.74	0.53
1:3:248:GLU:O	1:3:252:TRP:CB	2.56	0.53
1:6:582:ASP:OD1	1:6:583:LEU:N	2.41	0.53
5:a:204:GLN:O	1:c:391:SER:OG	2.26	0.53
1:g:117:ASP:OD2	1:g:139:LYS:NZ	2.38	0.53
1:o:568:MET:HE1	1:o:580:MET:HB3	1.90	0.53
1:r:99:VAL:N	1:r:376:GLN:OE1	2.28	0.53
1:r:224:ARG:HH11	1:r:337:LEU:HD13	1.74	0.53
2:v:49:ILE:HB	2:v:87:ARG:HB3	1.91	0.53
2:y:49:ILE:HB	2:y:87:ARG:HB2	1.90	0.53
1:0:75:ASP:OD2	1:x:359:ARG:HG3	2.08	0.53
1:3:661:ALA:HB2	1:6:656:ALA:HA	1.90	0.53
4:A:455:ALA:HB1	4:A:574:LEU:HD22	1.91	0.53
4:E:242:PHE:HA	4:E:247:LEU:HA	1.90	0.53
5:I:66:TYR:HB2	5:I:130:LYS:HB2	1.89	0.53
5:K:94:ARG:HD3	5:i:126:TYR:CZ	2.44	0.53
1:U:55:GLN:O	1:U:59:ARG:HB2	2.08	0.53
1:U:543:LYS:NZ	1:Y:144:VAL:O	2.41	0.53
1:U:600:ILE:HA	1:U:603:ILE:HG22	1.89	0.53
5:W:200:ARG:HH12	1:Y:414:ARG:HG3	1.74	0.53
1:g:568:MET:O	1:g:572:MET:HG2	2.08	0.53
2:l:11:ALA:HA	2:l:89:GLU:HB3	1.89	0.53
5:m:20:GLU:HG3	3:n:114:HIS:CD2	2.44	0.53
1:r:359:ARG:HG3	1:u:75:ASP:OD2	2.08	0.53
1:6:375:ILE:HB	1:6:450:LEU:HD21	1.91	0.53
4:A:15:ARG:NH1	4:F:35:ASP:O	2.42	0.53
4:E:569:THR:HG22	4:E:573:GLU:OE1	2.09	0.53
5:I:67:GLU:OE2	5:a:196:ARG:HG2	2.08	0.53
2:P:71:THR:OG1	2:P:74:GLN:NE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:79:LYS:HD3	3:f:80:THR:N	2.24	0.53
3:n:79:LYS:HD3	3:n:80:THR:N	2.23	0.53
1:r:208:ARG:HB3	1:r:278:GLU:HB2	1.89	0.53
1:r:348:ARG:HH21	1:r:539:ILE:HD12	1.74	0.53
1:u:42:MET:HB3	1:u:336:LEU:HD21	1.90	0.53
1:u:70:ASP:HB3	1:u:369:ILE:HD12	1.89	0.53
1:x:600:ILE:HA	1:x:603:ILE:HG22	1.91	0.53
1:3:154:SER:O	1:3:158:THR:HG23	2.08	0.53
1:3:377:ASP:O	1:3:381:LYS:HG2	2.08	0.53
4:A:241:ALA:O	4:A:248:TYR:N	2.26	0.53
4:B:283:MET:HE1	4:B:316:VAL:HG11	1.90	0.53
4:B:479:ILE:HD13	4:B:515:PRO:HA	1.91	0.53
5:G:109:SER:OG	5:G:110:GLU:N	2.42	0.53
5:I:196:ARG:HH22	5:e:69:GLU:HG3	1.74	0.53
2:N:27:VAL:HG13	2:N:68:MET:HE1	1.91	0.53
3:T:15:LEU:HD21	3:t:32:TRP:HH2	1.73	0.53
1:U:430:ASN:OD1	1:U:433:ARG:NH2	2.27	0.53
1:U:500:GLU:OE2	1:Y:146:ARG:NH2	2.40	0.53
1:Y:263:SER:O	1:Y:264:ARG:NE	2.36	0.53
5:a:102:ALA:HA	5:a:117:PRO:HG2	1.91	0.53
5:e:87:ASP:OD1	5:e:94:ARG:NH1	2.42	0.53
1:g:401:ALA:HB1	1:g:427:ILE:HG12	1.91	0.53
1:o:211:TRP:HB3	1:o:273:ARG:HH21	1.74	0.53
1:o:215:ASP:OD1	1:o:216:VAL:N	2.41	0.53
1:o:547:ILE:HD11	1:r:556:THR:HB	1.89	0.53
1:u:64:ARG:HD3	1:u:186:TRP:HZ3	1.72	0.53
3:2:106:MET:HE3	3:2:129:PRO:HB3	1.90	0.53
1:3:562:SER:OG	1:3:588:THR:OG1	2.22	0.53
1:3:668:ALA:HB2	1:6:663:LEU:HA	1.91	0.53
1:6:60:GLN:HE22	1:6:364:LEU:HD22	1.74	0.53
4:B:306:LEU:HB2	4:B:339:MET:HG2	1.91	0.53
4:E:35:ASP:O	4:F:15:ARG:NH1	2.42	0.53
4:F:290:ILE:O	4:F:302:GLN:N	2.42	0.53
5:G:19:PRO:HD3	5:G:166:TRP:CH2	2.44	0.53
5:J:24:PHE:O	5:J:28:ARG:HG3	2.09	0.53
1:U:64:ARG:HD3	1:U:186:TRP:CZ3	2.43	0.53
3:b:175:SER:O	3:b:178:SER:OG	2.23	0.53
3:n:64:LEU:HD13	3:n:68:ALA:HB3	1.91	0.53
1:r:263:SER:O	1:r:264:ARG:NE	2.36	0.53
1:r:554:ARG:NH2	1:r:563:GLU:OE2	2.42	0.53
3:t:123:THR:HG23	3:t:124:VAL:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:64:ARG:HD3	1:0:186:TRP:HZ3	1.74	0.53
1:3:600:ILE:HA	1:3:603:ILE:HG22	1.91	0.53
1:6:105:ASN:HA	1:6:108:ILE:HG12	1.90	0.53
4:D:570:THR:HG22	4:D:572:GLN:H	1.74	0.53
5:L:11:ILE:O	5:L:15:ALA:N	2.39	0.53
5:W:101:GLN:O	5:W:117:PRO:HG2	2.08	0.53
3:f:69:ILE:HB	3:f:142:ALA:HB3	1.91	0.53
1:o:601:ARG:O	1:o:605:GLY:N	2.32	0.53
1:r:154:SER:O	1:r:158:THR:HG23	2.08	0.53
1:r:170:TYR:H	1:r:344:PHE:HZ	1.55	0.53
1:r:251:ASP:OD1	1:r:275:ARG:NH2	2.36	0.53
3:z:182:ASN:HB3	3:z:185:VAL:HG12	1.91	0.53
1:3:125:LYS:NZ	1:6:589:ASP:OD2	2.42	0.52
1:6:211:TRP:HB3	1:6:273:ARG:HH21	1.74	0.52
4:A:225:PRO:HG2	4:A:248:TYR:HE2	1.74	0.52
4:B:225:PRO:HG2	4:B:248:TYR:HE2	1.74	0.52
4:C:472:TYR:OH	4:C:516:ALA:O	2.27	0.52
1:c:399:GLU:HA	1:g:420:VAL:HG13	1.90	0.52
1:c:600:ILE:HA	1:c:603:ILE:HG22	1.92	0.52
1:r:231:ALA:HA	1:r:334:ARG:HH12	1.75	0.52
3:z:8:VAL:HG22	3:z:162:VAL:HG23	1.90	0.52
1:3:278:GLU:HG2	1:3:330:ILE:HG12	1.90	0.52
1:6:568:MET:O	1:6:572:MET:HG2	2.09	0.52
4:C:324:ALA:HB2	4:C:333:MET:HG2	1.90	0.52
4:F:324:ALA:HB2	4:F:333:MET:HG2	1.92	0.52
5:L:24:PHE:O	5:L:28:ARG:HG3	2.08	0.52
2:M:92:LEU:HD13	2:M:95:GLY:H	1.75	0.52
2:O:58:VAL:HG12	2:O:72:ARG:HD3	1.90	0.52
2:P:52:ASP:OD1	2:P:53:GLY:N	2.35	0.52
3:T:162:VAL:O	3:T:166:VAL:HG23	2.09	0.52
3:b:17:GLN:OE1	3:w:176:LYS:NZ	2.40	0.52
2:h:98:GLY:O	2:h:101:ARG:HG2	2.09	0.52
3:n:175:SER:O	3:n:178:SER:OG	2.23	0.52
3:2:8:VAL:HA	3:2:11:ARG:HG2	1.92	0.52
1:3:414:ARG:HB2	1:3:417:ALA:HB2	1.91	0.52
4:B:487:PHE:O	2:s:87:ARG:NH2	2.42	0.52
5:G:24:PHE:O	5:G:28:ARG:HG3	2.10	0.52
5:J:195:GLN:NE2	5:i:105:VAL:HG12	2.25	0.52
5:a:78:MET:HE1	5:a:102:ALA:HB1	1.91	0.52
3:j:78:LEU:HD23	3:j:136:GLN:HG3	1.91	0.52
1:k:402:VAL:HG21	1:k:408:PHE:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:154:SER:OG	1:u:354:ILE:HD12	2.09	0.52
3:2:170:LEU:HB3	3:2:189:HIS:CD2	2.45	0.52
3:5:166:VAL:O	3:5:170:LEU:HD23	2.10	0.52
4:A:95:MET:HE2	4:A:95:MET:HA	1.91	0.52
5:H:109:SER:OG	5:H:110:GLU:N	2.43	0.52
5:J:36:GLU:HG2	5:J:66:TYR:CE1	2.44	0.52
2:M:56:GLU:HB3	2:M:82:PHE:HZ	1.75	0.52
2:N:90:ALA:C	2:N:91:ARG:HD3	2.35	0.52
1:c:224:ARG:HH11	1:c:337:LEU:HD13	1.74	0.52
1:g:100:ILE:HD11	1:g:376:GLN:HB2	1.89	0.52
1:o:401:ALA:HB1	1:o:427:ILE:HG12	1.91	0.52
1:o:572:MET:HE3	1:o:573:PRO:HD2	1.91	0.52
1:r:661:ALA:HB2	1:u:656:ALA:HA	1.91	0.52
1:6:70:ASP:HB3	1:6:369:ILE:HD12	1.91	0.52
4:A:291:VAL:HG22	4:A:301:GLN:HB3	1.92	0.52
4:E:347:MET:HE1	4:E:352:TRP:CE3	2.44	0.52
3:T:97:ASP:OD2	3:T:103:TRP:NE1	2.40	0.52
1:U:414:ARG:HB2	1:U:417:ALA:HB2	1.91	0.52
1:U:661:ALA:HB2	1:Y:656:ALA:HA	1.91	0.52
1:k:377:ASP:O	1:k:381:LYS:HG2	2.09	0.52
1:r:64:ARG:HD3	1:r:186:TRP:CZ3	2.45	0.52
2:s:38:LEU:HD21	2:s:44:PHE:HD1	1.75	0.52
2:s:86:ASP:OD1	2:s:87:ARG:N	2.39	0.52
2:s:101:ARG:NE	2:v:4:VAL:O	2.43	0.52
1:0:208:ARG:NH2	1:0:278:GLU:OE1	2.32	0.52
1:0:558:ARG:NH1	1:0:587:SER:O	2.42	0.52
3:2:32:TRP:HH2	3:j:15:LEU:HD21	1.74	0.52
3:2:93:ARG:HH12	3:j:75:PRO:HB3	1.75	0.52
1:6:154:SER:OG	1:6:354:ILE:HD12	2.10	0.52
5:J:11:ILE:O	5:J:15:ALA:N	2.36	0.52
1:c:137:LEU:HD11	1:c:515:THR:HG22	1.90	0.52
1:k:154:SER:O	1:k:158:THR:HG23	2.09	0.52
1:k:385:LYS:O	1:k:389:ILE:HG13	2.09	0.52
1:o:375:ILE:HB	1:o:450:LEU:HD21	1.92	0.52
1:o:553:TRP:CZ3	1:o:555:ALA:HA	2.44	0.52
1:r:377:ASP:O	1:r:381:LYS:HG2	2.10	0.52
1:3:543:LYS:HD3	1:6:144:VAL:HA	1.91	0.52
4:A:301:GLN:HG3	4:F:236:ASN:HA	1.91	0.52
4:A:482:GLU:HA	4:A:485:THR:HG22	1.91	0.52
4:F:32:VAL:HG23	4:F:438:LEU:HD11	1.91	0.52
4:F:231:LEU:HD11	4:F:239:MET:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:361:VAL:HB	4:F:372:SER:HB3	1.92	0.52
5:K:11:ILE:O	5:K:15:ALA:N	2.37	0.52
3:T:159:ALA:H	3:t:144:ARG:NH2	2.08	0.52
1:U:123:ARG:NH1	1:U:543:LYS:O	2.43	0.52
1:U:359:ARG:HG3	1:Y:75:ASP:OD2	2.08	0.52
5:W:78:MET:HE2	5:W:105:VAL:HG23	1.91	0.52
3:X:175:SER:O	3:X:178:SER:OG	2.22	0.52
5:e:205:PHE:CZ	1:k:92:GLN:HB2	2.45	0.52
1:g:556:THR:HG22	1:g:559:GLN:HG3	1.92	0.52
5:i:66:TYR:HB2	5:i:130:LYS:HB2	1.89	0.52
3:j:161:PHE:O	3:j:165:LEU:HD23	2.10	0.52
1:u:569:ILE:HD13	1:u:581:LEU:HD23	1.92	0.52
1:3:537:ASN:OD1	1:6:176:GLY:N	2.35	0.52
4:A:88:MET:SD	4:A:231:LEU:HB2	2.50	0.52
4:B:291:VAL:HG22	4:B:301:GLN:HB3	1.92	0.52
5:G:37:ARG:HB3	5:G:183:LEU:HD22	1.91	0.52
5:J:12:HIS:HB3	3:j:98:THR:HB	1.92	0.52
2:M:90:ALA:C	2:M:91:ARG:HD3	2.35	0.52
3:T:11:ARG:NH1	3:t:35:ASP:OD1	2.43	0.52
3:X:33:LEU:HD12	3:X:165:LEU:HD12	1.91	0.52
1:c:248:GLU:O	1:c:252:TRP:HB2	2.09	0.52
2:d:58:VAL:HB	2:d:70:ILE:HD11	1.92	0.52
5:i:20:GLU:HG3	3:j:114:HIS:CD2	2.45	0.52
1:k:64:ARG:HD3	1:k:186:TRP:HZ3	1.74	0.52
1:k:326:VAL:HG23	1:k:342:SER:OG	2.10	0.52
1:r:430:ASN:OD1	1:r:433:ARG:NH1	2.43	0.52
1:0:154:SER:OG	1:0:354:ILE:HD12	2.09	0.52
3:2:123:THR:HG23	3:2:124:VAL:HG23	1.91	0.52
1:6:345:ARG:HE	1:6:538:ASP:HB2	1.75	0.52
1:6:399:GLU:HG3	5:G:184:ASP:OD2	2.10	0.52
4:A:59:ILE:HG13	4:A:409:PHE:HB2	1.92	0.52
4:A:458:ILE:HG21	4:A:520:VAL:HG11	1.92	0.52
4:B:84:ARG:NH2	4:B:95:MET:SD	2.72	0.52
4:E:266:MET:HE3	4:E:282:VAL:HG11	1.92	0.52
4:E:479:ILE:HD13	4:E:515:PRO:HA	1.91	0.52
5:L:161:ILE:HD11	5:L:166:TRP:CE3	2.45	0.52
1:U:105:ASN:HA	1:U:108:ILE:HG12	1.92	0.52
5:W:67:GLU:O	5:W:128:LEU:N	2.43	0.52
3:j:9:LEU:HD12	3:j:151:GLN:HG3	1.91	0.52
3:j:162:VAL:O	3:j:166:VAL:HG23	2.10	0.52
2:p:14:LEU:HB2	2:p:88:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:q:8:VAL:HA	3:q:11:ARG:HG2	1.92	0.52
1:u:398:ASP:HB3	1:u:425:LYS:HB3	1.91	0.52
2:v:43:TRP:CD1	2:v:59:LYS:HZ2	2.28	0.52
1:x:147:LEU:HD11	1:x:498:GLN:NE2	2.25	0.52
2:y:48:LEU:HB3	2:y:82:PHE:CE1	2.44	0.52
1:0:269:HIS:HB3	1:x:48:ARG:HD3	1.92	0.52
1:3:198:LEU:HD21	1:6:153:ARG:HH11	1.75	0.52
1:3:562:SER:HG	1:3:584:TRP:CD1	2.28	0.52
3:5:182:ASN:HB3	3:5:185:VAL:HG12	1.91	0.52
1:6:572:MET:HE1	1:U:581:LEU:HB3	1.91	0.52
4:B:266:MET:HE2	4:B:270:ILE:HD11	1.92	0.52
4:D:525:TYR:HB2	4:D:553:GLU:HG3	1.92	0.52
4:F:327:SER:O	4:F:352:TRP:NE1	2.43	0.52
2:P:86:ASP:OD1	2:P:87:ARG:N	2.38	0.52
2:Q:112:SER:O	2:Q:115:GLN:HG3	2.10	0.52
2:R:93:THR:HA	2:R:97:LEU:HD13	1.92	0.52
1:Y:154:SER:OG	1:Y:354:ILE:HD12	2.10	0.52
3:b:79:LYS:HD3	3:b:80:THR:N	2.25	0.52
3:b:161:PHE:O	3:b:165:LEU:HD23	2.08	0.52
1:g:63:ASN:ND2	1:g:364:LEU:HB3	2.24	0.52
1:g:70:ASP:HB3	1:g:369:ILE:HD12	1.92	0.52
2:h:91:ARG:NH2	2:p:93:THR:OG1	2.43	0.52
1:o:154:SER:OG	1:o:354:ILE:HD12	2.10	0.52
1:u:369:ILE:HG22	1:u:373:ARG:HB2	1.92	0.52
3:z:8:VAL:HA	3:z:11:ARG:HG2	1.92	0.52
1:6:445:ARG:HG3	1:6:449:MET:HE2	1.91	0.51
4:A:278:THR:HG23	4:B:302:GLN:HG3	1.91	0.51
4:B:569:THR:HG22	4:B:573:GLU:OE1	2.10	0.51
4:C:319:LEU:HD11	4:C:369:TYR:HD1	1.75	0.51
4:D:59:ILE:HG13	4:D:409:PHE:HB2	1.92	0.51
4:D:319:LEU:HD11	4:D:369:TYR:HD1	1.75	0.51
4:E:570:THR:HG22	4:E:572:GLN:H	1.75	0.51
4:F:18:PRO:HB3	4:F:27:GLN:NE2	2.25	0.51
4:F:472:TYR:OH	4:F:516:ALA:O	2.28	0.51
4:F:482:GLU:HA	4:F:485:THR:HG22	1.92	0.51
5:I:69:GLU:OE1	5:e:84:GLN:NE2	2.43	0.51
1:U:399:GLU:HG3	1:Y:420:VAL:HG12	1.92	0.51
5:e:93:TRP:CD1	5:e:116:VAL:HG23	2.36	0.51
1:k:278:GLU:HG2	1:k:330:ILE:HG12	1.90	0.51
1:k:661:ALA:HB2	1:o:656:ALA:HA	1.92	0.51
1:o:108:ILE:O	1:o:111:GLU:HG3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:193:SER:OG	1:x:257:ARG:NH1	2.42	0.51
2:v:58:VAL:HG11	2:v:72:ARG:HG2	1.92	0.51
4:D:290:ILE:O	4:D:302:GLN:N	2.43	0.51
5:I:161:ILE:HD11	5:I:166:TRP:CE3	2.45	0.51
5:W:23:ALA:O	5:W:27:ILE:HG12	2.10	0.51
1:Y:117:ASP:OD2	1:Y:139:LYS:NZ	2.33	0.51
2:d:59:LYS:HB2	2:d:74:GLN:HG2	1.91	0.51
1:k:331:PHE:HA	1:k:336:LEU:HA	1.91	0.51
5:m:104:TYR:HD2	5:m:116:VAL:HG11	1.76	0.51
3:t:106:MET:HE3	3:t:129:PRO:HB3	1.90	0.51
3:w:36:GLY:O	3:w:40:ILE:HG13	2.09	0.51
1:x:210:LYS:HD2	1:x:212:LEU:HD11	1.91	0.51
3:z:64:LEU:HD13	3:z:68:ALA:HB3	1.92	0.51
1:3:403:GLU:HG3	1:3:422:LYS:HE3	1.91	0.51
4:A:290:ILE:O	4:A:302:GLN:N	2.40	0.51
4:A:319:LEU:HD11	4:A:369:TYR:HD1	1.74	0.51
4:B:55:ASN:HB3	4:B:70:GLN:HE22	1.75	0.51
4:B:458:ILE:HG21	4:B:520:VAL:HG11	1.93	0.51
4:E:291:VAL:HG22	4:E:301:GLN:HB3	1.93	0.51
2:P:71:THR:C	2:P:74:GLN:HE22	2.18	0.51
1:U:377:ASP:OD1	1:U:378:ASP:N	2.44	0.51
5:a:76:ARG:NH1	5:a:101:GLN:HB2	2.25	0.51
1:c:393:ASN:HA	1:c:433:ARG:HH22	1.75	0.51
5:e:200:ARG:NH2	1:o:411:GLU:OE2	2.43	0.51
1:g:64:ARG:HD3	1:g:186:TRP:HZ3	1.76	0.51
1:g:594:ASP:OD1	1:g:594:ASP:N	2.44	0.51
2:s:18:LEU:HB3	2:s:82:PHE:HD2	1.75	0.51
1:0:283:LYS:HE2	1:0:285:MET:HE1	1.90	0.51
1:0:402:VAL:HG21	1:0:408:PHE:HB2	1.91	0.51
1:6:369:ILE:HG22	1:6:373:ARG:HB2	1.91	0.51
4:B:349:ARG:HH12	4:B:353:MET:HE3	1.74	0.51
4:C:87:TYR:HE1	4:C:96:ILE:HG13	1.75	0.51
4:D:454:GLY:H	4:D:569:THR:HA	1.75	0.51
4:D:459:GLU:OE1	4:E:19:ARG:NH1	2.44	0.51
4:F:352:TRP:NE1	4:F:357:PRO:HB3	2.26	0.51
5:J:19:PRO:HB3	3:z:96:LEU:HG	1.93	0.51
5:L:109:SER:OG	5:L:110:GLU:N	2.43	0.51
2:P:8:ASN:HB2	2:R:94:ALA:HB2	1.91	0.51
3:X:24:TRP:HA	3:X:28:GLU:OE2	2.10	0.51
1:c:377:ASP:O	1:c:381:LYS:HG2	2.09	0.51
5:m:101:GLN:O	5:m:117:PRO:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:n:113:ARG:HB2	3:n:129:PRO:HD3	1.92	0.51
4:D:33:ARG:O	4:D:40:THR:OG1	2.24	0.51
4:F:87:TYR:HE1	4:F:96:ILE:HG13	1.74	0.51
4:F:319:LEU:HD11	4:F:369:TYR:HD1	1.76	0.51
5:J:157:GLU:OE2	5:e:13:ARG:NH1	2.43	0.51
5:L:36:GLU:HA	5:L:66:TYR:CE2	2.46	0.51
2:N:63:ARG:CB	2:N:68:MET:HG3	2.41	0.51
2:O:20:PRO:HD3	2:O:81:SER:HB2	1.93	0.51
3:b:48:TYR:HE2	3:b:143:TRP:HD1	1.59	0.51
1:g:208:ARG:NH2	1:g:278:GLU:OE1	2.33	0.51
5:i:69:GLU:H	5:i:127:GLY:HA2	1.75	0.51
2:l:20:PRO:HD3	2:l:81:SER:HA	1.93	0.51
3:n:16:LEU:HD23	3:n:24:TRP:CZ3	2.46	0.51
1:6:556:THR:HG22	1:6:559:GLN:HG3	1.92	0.51
2:7:11:ALA:HA	2:7:89:GLU:HB3	1.92	0.51
4:B:278:THR:HG23	4:C:302:GLN:HG3	1.93	0.51
4:B:343:THR:O	4:B:347:MET:N	2.35	0.51
4:C:32:VAL:HG23	4:C:438:LEU:HD11	1.92	0.51
4:D:97:VAL:O	4:D:100:THR:OG1	2.25	0.51
4:D:312:ASN:ND2	4:D:360:ILE:O	2.44	0.51
4:D:482:GLU:HA	4:D:485:THR:HG22	1.91	0.51
4:F:352:TRP:HE1	4:F:357:PRO:HB3	1.75	0.51
2:M:36:PRO:HG2	2:M:44:PHE:CD1	2.46	0.51
2:M:97:LEU:HA	2:M:100:PHE:HD1	1.76	0.51
1:U:48:ARG:HD3	1:Y:269:HIS:HB3	1.93	0.51
3:X:48:TYR:CE2	3:X:143:TRP:HB3	2.46	0.51
3:f:32:TRP:CH2	3:w:15:LEU:HD21	2.45	0.51
3:j:5:ALA:HB2	3:j:148:LEU:HD12	1.92	0.51
5:m:23:ALA:O	5:m:27:ILE:HG12	2.11	0.51
1:o:398:ASP:HB3	1:o:425:LYS:HB3	1.92	0.51
1:u:285:MET:HA	1:u:285:MET:HE3	1.93	0.51
1:0:224:ARG:HD2	1:0:337:LEU:HA	1.92	0.51
1:0:279:CYS:N	1:0:329:ALA:O	2.33	0.51
2:1:17:PRO:HG3	2:1:84:PRO:HB3	1.92	0.51
4:B:87:TYR:HE1	4:B:96:ILE:HG13	1.75	0.51
4:C:524:ILE:HG13	4:C:543:LEU:HD21	1.93	0.51
4:E:291:VAL:HA	4:E:301:GLN:HA	1.93	0.51
3:X:5:ALA:HB2	3:X:148:LEU:HD12	1.93	0.51
2:Z:49:ILE:N	2:Z:87:ARG:O	2.43	0.51
3:f:32:TRP:HA	3:f:32:TRP:CE3	2.46	0.51
3:f:48:TYR:CE2	3:f:143:TRP:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:63:ASN:OD1	1:u:359:ARG:NH2	2.43	0.51
2:7:59:LYS:HB2	2:7:74:GLN:HG2	1.93	0.51
4:D:242:PHE:HA	4:D:247:LEU:HA	1.93	0.51
4:E:59:ILE:HG13	4:E:409:PHE:HB2	1.93	0.51
5:I:94:ARG:HD3	5:a:126:TYR:CZ	2.46	0.51
5:L:94:ARG:HD3	5:m:126:TYR:CZ	2.46	0.51
5:S:102:ALA:HA	5:S:117:PRO:HD2	1.93	0.51
3:T:79:LYS:HD2	3:T:83:SER:HB3	1.92	0.51
1:Y:402:VAL:HG21	1:Y:408:PHE:HB2	1.92	0.51
5:e:196:ARG:NH2	1:o:406:GLU:HB2	2.25	0.51
2:l:27:VAL:HG13	2:l:68:MET:HE1	1.93	0.51
2:l:63:ARG:CB	2:l:68:MET:HG3	2.41	0.51
1:o:582:ASP:OD1	1:o:583:LEU:N	2.44	0.51
2:s:56:GLU:OE2	2:s:72:ARG:NH1	2.44	0.51
1:u:594:ASP:OD2	1:u:594:ASP:N	2.44	0.51
4:B:291:VAL:HA	4:B:301:GLN:HA	1.92	0.51
4:C:445:PHE:N	4:C:552:TRP:O	2.39	0.51
4:E:225:PRO:HG2	4:E:248:TYR:HE2	1.74	0.51
4:E:479:ILE:O	4:E:482:GLU:HG3	2.11	0.51
4:E:522:VAL:HG22	4:E:556:VAL:HG13	1.92	0.51
5:G:13:ARG:NE	3:T:99:GLU:OE2	2.37	0.51
1:Y:63:ASN:OD1	1:Y:359:ARG:NH2	2.44	0.51
2:l:50:ARG:CZ	2:l:80:LEU:HD13	2.41	0.51
1:r:506:ILE:O	1:r:510:VAL:HG22	2.10	0.51
1:u:215:ASP:OD1	1:u:216:VAL:N	2.44	0.51
1:3:331:PHE:HA	1:3:336:LEU:HA	1.93	0.51
3:5:123:THR:HG23	3:5:124:VAL:HG23	1.93	0.51
3:5:149:THR:HG23	3:5:150:THR:HG23	1.91	0.51
4:D:87:TYR:HE1	4:D:96:ILE:HG13	1.75	0.51
4:E:249:PHE:HB2	4:E:262:TYR:HB3	1.92	0.51
5:I:19:PRO:HB3	3:w:96:LEU:HG	1.93	0.51
5:J:184:ASP:OD2	1:o:399:GLU:HG3	2.09	0.51
3:T:78:LEU:HD23	3:T:136:GLN:HG3	1.92	0.51
2:V:71:THR:OG1	2:V:74:GLN:NE2	2.44	0.51
1:Y:194:ALA:HA	1:c:257:ARG:CZ	2.41	0.51
2:d:11:ALA:HA	2:d:89:GLU:HB3	1.93	0.51
3:f:66:GLU:O	3:f:144:ARG:NH1	2.43	0.51
1:g:596:ILE:O	1:g:600:ILE:HG12	2.10	0.51
2:h:72:ARG:HH12	2:h:80:LEU:H	1.58	0.51
3:j:33:LEU:HD12	3:j:165:LEU:HD12	1.92	0.51
5:m:76:ARG:NH1	5:m:101:GLN:HB2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:t:69:ILE:HD11	3:t:144:ARG:HB3	1.93	0.51
1:0:100:ILE:HD11	1:0:376:GLN:HB2	1.91	0.50
1:0:492:ARG:HD2	1:0:550:GLU:OE2	2.10	0.50
3:2:145:HIS:HD2	3:2:146:PRO:HD2	1.77	0.50
1:3:368:VAL:HG22	1:3:372:MET:HE1	1.91	0.50
1:6:224:ARG:HD2	1:6:337:LEU:HA	1.93	0.50
4:A:18:PRO:HB3	4:A:27:GLN:NE2	2.26	0.50
4:B:251:GLU:HB3	4:B:254:ILE:HB	1.92	0.50
4:C:231:LEU:HD11	4:C:239:MET:HB3	1.91	0.50
4:C:249:PHE:HB2	4:C:262:TYR:HB3	1.93	0.50
4:D:18:PRO:HB3	4:D:27:GLN:NE2	2.26	0.50
5:H:24:PHE:O	5:H:28:ARG:HG3	2.11	0.50
5:I:11:ILE:O	5:I:15:ALA:N	2.38	0.50
2:O:43:TRP:HZ3	2:O:45:MET:HB3	1.77	0.50
1:Y:70:ASP:HB3	1:Y:369:ILE:HD12	1.93	0.50
1:c:48:ARG:HD3	1:g:269:HIS:HB3	1.92	0.50
2:h:8:ASN:HB2	2:p:94:ALA:HB2	1.92	0.50
5:i:15:ALA:HB1	5:i:166:TRP:CD1	2.47	0.50
1:o:224:ARG:HD2	1:o:337:LEU:HA	1.93	0.50
3:q:123:THR:HG23	3:q:124:VAL:HG23	1.93	0.50
1:0:599:ARG:NH2	1:x:583:LEU:HD21	2.26	0.50
4:B:479:ILE:O	4:B:482:GLU:HG3	2.11	0.50
4:B:522:VAL:HG22	4:B:556:VAL:HG13	1.92	0.50
4:E:283:MET:HE1	4:E:316:VAL:HG11	1.93	0.50
4:F:225:PRO:HG2	4:F:248:TYR:HE2	1.76	0.50
5:K:143:ALA:O	5:K:147:ARG:HB3	2.11	0.50
3:T:49:MET:HG2	3:t:121:VAL:HG22	1.93	0.50
3:X:31:GLU:OE2	3:q:11:ARG:NH1	2.45	0.50
5:a:50:GLY:HA2	5:a:120:ALA:HA	1.92	0.50
5:a:96:THR:HG22	5:a:98:GLN:H	1.75	0.50
3:n:61:LYS:HA	3:n:126:TYR:CD2	2.47	0.50
3:q:8:VAL:HG22	3:q:162:VAL:HG23	1.93	0.50
3:w:8:VAL:HA	3:w:11:ARG:HG2	1.93	0.50
3:w:123:THR:HG23	3:w:124:VAL:HG23	1.92	0.50
3:z:38:ARG:NE	3:z:145:HIS:O	2.43	0.50
4:A:226:ASP:OD1	4:A:227:GLY:N	2.44	0.50
4:C:352:TRP:HE1	4:C:357:PRO:HB3	1.75	0.50
4:E:266:MET:HE2	4:E:270:ILE:HD11	1.93	0.50
2:M:57:ILE:HG22	2:M:77:SER:OG	2.11	0.50
2:R:14:LEU:HD11	2:R:25:LEU:HB2	1.93	0.50
3:T:79:LYS:HD3	3:T:80:THR:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:215:ASP:OD1	1:Y:216:VAL:N	2.44	0.50
2:Z:57:ILE:HD13	2:Z:92:LEU:HD13	1.94	0.50
5:e:102:ALA:HA	5:e:117:PRO:HD2	1.93	0.50
3:f:16:LEU:HD23	3:f:24:TRP:CH2	2.47	0.50
3:j:44:LYS:HE3	3:j:200:GLN:HG3	1.94	0.50
1:o:378:ASP:OD1	1:o:382:ARG:NH1	2.44	0.50
1:r:154:SER:HB3	1:r:354:ILE:HD12	1.93	0.50
1:r:398:ASP:OD2	1:r:426:GLN:HG2	2.12	0.50
2:s:45:MET:HE3	2:s:46:ALA:H	1.75	0.50
1:x:285:MET:HG3	1:x:325:ARG:HE	1.77	0.50
3:2:96:LEU:HG	5:K:19:PRO:HB3	1.93	0.50
4:C:84:ARG:HG3	4:C:97:VAL:HG22	1.94	0.50
4:E:278:THR:HG23	4:F:302:GLN:HG3	1.93	0.50
4:F:97:VAL:HB	4:F:102:TYR:HE2	1.76	0.50
4:F:251:GLU:HB2	4:F:257:ALA:HB3	1.93	0.50
5:J:191:ILE:HG12	1:o:406:GLU:OE2	2.12	0.50
5:K:24:PHE:O	5:K:28:ARG:HG3	2.11	0.50
1:Y:597:VAL:O	1:Y:601:ARG:HG3	2.11	0.50
3:f:15:LEU:HD21	3:z:32:TRP:HH2	1.76	0.50
1:g:279:CYS:N	1:g:329:ALA:O	2.33	0.50
3:j:42:VAL:HG21	3:z:160:GLU:HB2	1.93	0.50
1:o:63:ASN:OD1	1:o:359:ARG:NH2	2.45	0.50
3:t:145:HIS:HD2	3:t:146:PRO:HD2	1.76	0.50
1:0:594:ASP:N	1:0:594:ASP:OD1	2.44	0.50
1:3:359:ARG:HG3	1:6:75:ASP:OD2	2.11	0.50
1:6:357:PHE:CE1	1:6:486:LYS:HD3	2.47	0.50
1:6:413:ALA:HB3	5:G:204:GLN:HG2	1.94	0.50
4:A:569:THR:HG22	4:A:573:GLU:OE1	2.12	0.50
4:B:21:LEU:HB2	4:B:443:LYS:HG3	1.92	0.50
4:C:18:PRO:HB3	4:C:27:GLN:NE2	2.27	0.50
4:F:441:ARG:NH2	4:F:553:GLU:OE2	2.39	0.50
5:H:8:MET:HG3	5:H:12:HIS:CD2	2.47	0.50
5:I:178:ARG:NH1	5:e:157:GLU:OE1	2.43	0.50
2:P:18:LEU:HB3	2:P:82:PHE:HD2	1.76	0.50
1:g:572:MET:HE1	1:k:581:LEU:HB3	1.92	0.50
3:t:8:VAL:HG22	3:t:162:VAL:HG23	1.93	0.50
1:u:597:VAL:O	1:u:601:ARG:HG3	2.12	0.50
2:7:59:LYS:HB3	2:7:71:THR:OG1	2.11	0.50
4:D:452:ASN:HB3	3:t:17:GLN:OE1	2.11	0.50
5:J:110:GLU:OE2	5:e:140:ASP:HB3	2.12	0.50
3:T:2:ALA:HA	3:T:156:GLN:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:a:15:ALA:HB1	5:a:166:TRP:CD1	2.47	0.50
3:b:32:TRP:CH2	3:t:15:LEU:HD21	2.46	0.50
1:c:568:MET:HE1	1:c:580:MET:HE3	1.93	0.50
5:e:32:ILE:HG23	5:e:130:LYS:HD2	1.93	0.50
1:g:56:GLU:HG3	1:g:205:TYR:HE1	1.76	0.50
1:k:73:TYR:CD1	1:k:373:ARG:HG2	2.46	0.50
5:m:164:LYS:HB3	5:m:166:TRP:CE3	2.46	0.50
3:z:97:ASP:OD1	3:z:103:TRP:NE1	2.42	0.50
1:0:215:ASP:OD1	1:0:216:VAL:N	2.45	0.50
3:2:64:LEU:HD13	3:2:71:LEU:HD23	1.94	0.50
5:G:94:ARG:HD3	5:S:126:TYR:CZ	2.46	0.50
5:H:192:LYS:NZ	1:c:407:GLU:OE1	2.37	0.50
5:J:185:ARG:HH22	5:i:36:GLU:HB3	1.77	0.50
5:K:109:SER:OG	5:K:110:GLU:N	2.42	0.50
5:W:139:PRO:HD2	5:W:142:LEU:HD12	1.93	0.50
1:c:263:SER:O	1:c:264:ARG:NE	2.38	0.50
1:g:154:SER:OG	1:g:354:ILE:HD12	2.11	0.50
5:i:101:GLN:O	5:i:117:PRO:HG2	2.11	0.50
3:q:64:LEU:HD13	3:q:71:LEU:HD23	1.92	0.50
1:r:414:ARG:HB2	1:r:417:ALA:HB2	1.93	0.50
1:x:206:ILE:HD12	1:x:351:LEU:HD12	1.94	0.50
3:z:9:LEU:HD13	3:z:151:GLN:HG3	1.94	0.50
3:z:113:ARG:HB2	3:z:129:PRO:HD3	1.93	0.50
3:5:8:VAL:HA	3:5:11:ARG:HG2	1.93	0.50
1:6:506:ILE:O	1:6:510:VAL:HG22	2.12	0.50
4:A:34:LEU:HD12	4:A:399:ILE:HD11	1.93	0.50
4:C:251:GLU:HB3	4:C:254:ILE:HB	1.94	0.50
4:D:278:THR:HG23	4:E:302:GLN:HG3	1.93	0.50
5:I:20:GLU:OE1	3:w:113:ARG:NH2	2.40	0.50
5:S:67:GLU:O	5:S:128:LEU:N	2.45	0.50
3:T:157:MET:HG2	3:T:158:GLY:N	2.26	0.50
1:U:506:ILE:O	1:U:510:VAL:HG22	2.11	0.50
3:b:8:VAL:HG22	3:b:162:VAL:HG23	1.93	0.50
5:m:96:THR:HG22	5:m:98:GLN:H	1.75	0.50
2:1:98:GLY:HA2	2:1:101:ARG:HD3	1.94	0.50
1:3:326:VAL:HG23	1:3:342:SER:OG	2.12	0.50
4:B:34:LEU:HD12	4:B:399:ILE:HD11	1.93	0.50
4:B:445:PHE:N	4:B:552:TRP:O	2.38	0.50
4:C:97:VAL:HB	4:C:102:TYR:HE2	1.76	0.50
5:H:94:ARG:HD3	5:W:126:TYR:CZ	2.46	0.50
5:K:141:LEU:HD12	5:K:142:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:87:ASP:OD1	5:L:94:ARG:NH1	2.25	0.50
1:U:377:ASP:O	1:U:381:LYS:HG2	2.11	0.50
1:Y:397:MET:HG3	1:Y:398:ASP:O	2.12	0.50
2:Z:112:SER:O	2:Z:115:GLN:HG3	2.12	0.50
5:a:93:TRP:HE1	5:a:116:VAL:HA	1.77	0.50
1:c:210:LYS:HD2	1:c:212:LEU:HD11	1.94	0.50
2:d:37:THR:HA	2:d:63:ARG:HH21	1.76	0.50
3:j:2:ALA:HA	3:j:156:GLN:HA	1.94	0.50
1:k:197:GLU:HG3	1:k:199:ASP:H	1.77	0.50
1:o:111:GLU:HG2	1:o:155:PHE:CD2	2.47	0.50
1:u:271:ARG:HH21	1:u:273:ARG:HH11	1.60	0.50
1:u:568:MET:HG3	1:x:590:LEU:HD11	1.92	0.50
4:A:558:SER:OG	4:A:560:ILE:O	2.28	0.49
4:B:242:PHE:HA	4:B:247:LEU:HA	1.94	0.49
4:C:482:GLU:HA	4:C:485:THR:HG22	1.93	0.49
4:E:251:GLU:HB2	4:E:257:ALA:HB3	1.94	0.49
3:T:33:LEU:HD12	3:T:165:LEU:HD12	1.94	0.49
1:U:569:ILE:HG12	1:U:580:MET:HB2	1.93	0.49
5:i:67:GLU:O	5:i:128:LEU:N	2.45	0.49
3:j:79:LYS:HD3	3:j:80:THR:N	2.27	0.49
1:o:56:GLU:OE2	1:o:59:ARG:NH2	2.44	0.49
1:r:576:VAL:HG21	1:u:600:ILE:HD13	1.94	0.49
1:6:411:GLU:OE2	5:S:200:ARG:NH2	2.45	0.49
4:F:84:ARG:HG3	4:F:97:VAL:HG22	1.92	0.49
2:O:36:PRO:O	2:O:63:ARG:NH1	2.44	0.49
5:S:76:ARG:HH22	5:S:103:GLN:HG2	1.76	0.49
3:T:8:VAL:HG11	3:T:33:LEU:HD13	1.94	0.49
3:T:91:THR:HB	5:W:19:PRO:HG3	1.93	0.49
2:Z:20:PRO:HA	2:Z:72:ARG:NH2	2.27	0.49
5:a:85:TRP:HE3	5:a:86:LEU:HD23	1.76	0.49
5:e:12:HIS:HE1	3:f:114:HIS:HE1	1.59	0.49
3:n:40:ILE:HD11	3:n:197:LEU:HD21	1.94	0.49
2:p:18:LEU:HD12	2:p:25:LEU:HB3	1.94	0.49
2:s:91:ARG:HE	2:y:93:THR:HG21	1.77	0.49
3:t:170:LEU:HB3	3:t:189:HIS:CD2	2.46	0.49
3:w:78:LEU:HD23	3:w:136:GLN:HG3	1.95	0.49
2:7:49:ILE:HB	2:7:87:ARG:HB2	1.94	0.49
4:D:34:LEU:HD12	4:D:399:ILE:HD11	1.93	0.49
5:J:204:GLN:O	1:o:391:SER:OG	2.31	0.49
5:K:40:LEU:HD21	5:K:189:LYS:HB3	1.94	0.49
1:U:595:GLU:O	1:U:598:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:78:MET:HE1	5:W:104:TYR:N	2.27	0.49
1:Y:506:ILE:O	1:Y:510:VAL:HG22	2.13	0.49
3:b:16:LEU:HD23	3:b:24:TRP:CH2	2.47	0.49
2:h:56:GLU:HB3	2:h:82:PHE:HZ	1.77	0.49
1:o:59:ARG:HD2	1:r:257:ARG:HA	1.95	0.49
1:u:125:LYS:HD2	1:x:558:ARG:NH1	2.27	0.49
1:3:568:MET:HG3	1:6:590:LEU:HD11	1.94	0.49
4:E:456:ILE:HG12	4:E:567:LEU:HD22	1.95	0.49
4:F:26:SER:HB3	4:F:441:ARG:O	2.13	0.49
4:F:249:PHE:HB2	4:F:262:TYR:HB3	1.94	0.49
5:G:166:TRP:CD1	5:G:166:TRP:N	2.80	0.49
5:S:12:HIS:HE1	3:X:114:HIS:HE1	1.61	0.49
1:Y:594:ASP:OD2	1:Y:594:ASP:N	2.44	0.49
1:k:78:GLN:HE22	1:k:98:ASN:HA	1.76	0.49
1:o:393:ASN:HA	1:o:433:ARG:HH22	1.77	0.49
4:A:55:ASN:HB3	4:A:70:GLN:HE22	1.78	0.49
4:A:282:VAL:HB	4:A:289:TYR:HB2	1.93	0.49
4:A:522:VAL:HG22	4:A:556:VAL:HG13	1.93	0.49
5:G:147:ARG:HH21	5:W:133:LEU:HB2	1.76	0.49
5:I:32:ILE:HG23	5:I:130:LYS:HD2	1.94	0.49
2:M:8:ASN:HB2	2:O:94:ALA:HB2	1.93	0.49
2:M:52:ASP:OD2	2:M:53:GLY:N	2.45	0.49
2:R:97:LEU:HA	2:R:100:PHE:HD2	1.77	0.49
3:T:24:TRP:HA	3:T:28:GLU:OE2	2.12	0.49
1:U:489:ASP:OD2	1:Y:112:LYS:HD3	2.11	0.49
2:V:13:ARG:HD2	2:V:87:ARG:HD3	1.95	0.49
1:g:601:ARG:O	1:g:605:GLY:N	2.28	0.49
3:z:15:LEU:HB3	3:z:170:LEU:HD11	1.95	0.49
2:4:112:SER:O	2:4:115:GLN:HG3	2.12	0.49
4:B:414:THR:HG22	4:C:328:HIS:HE1	1.77	0.49
4:E:368:ARG:HG2	4:E:390:ASP:HB3	1.94	0.49
4:F:319:LEU:HD21	4:F:369:TYR:HB2	1.94	0.49
5:S:96:THR:HG22	5:S:98:GLN:H	1.77	0.49
1:U:668:ALA:HB2	1:Y:663:LEU:HA	1.94	0.49
1:Y:184:GLU:CD	1:Y:208:ARG:HD2	2.38	0.49
3:b:32:TRP:HA	3:b:32:TRP:CE3	2.48	0.49
1:c:170:TYR:HB3	1:c:344:PHE:HE1	1.78	0.49
1:g:59:ARG:HD3	1:k:257:ARG:HG3	1.94	0.49
1:g:497:MET:HE1	1:k:146:ARG:HD2	1.93	0.49
1:k:112:LYS:HG2	1:k:152:SER:HB2	1.94	0.49
1:r:562:SER:HG	1:r:584:TRP:CD1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:165:TRP:HB3	1:u:351:LEU:HD22	1.94	0.49
3:w:15:LEU:HG	3:w:170:LEU:HD21	1.93	0.49
3:w:64:LEU:HD13	3:w:71:LEU:HD23	1.94	0.49
1:x:331:PHE:HA	1:x:336:LEU:HA	1.93	0.49
1:0:59:ARG:HD3	1:3:257:ARG:HG3	1.95	0.49
4:A:288:PRO:HB2	4:A:304:VAL:HG11	1.94	0.49
4:C:225:PRO:HG2	4:C:248:TYR:HE2	1.77	0.49
4:C:327:SER:O	4:C:352:TRP:NE1	2.45	0.49
4:C:352:TRP:NE1	4:C:357:PRO:HB3	2.28	0.49
4:F:82:GLN:HG2	4:F:84:ARG:NE	2.28	0.49
5:J:110:GLU:OE2	5:e:141:LEU:N	2.46	0.49
3:X:113:ARG:HB2	3:X:129:PRO:HD3	1.93	0.49
1:c:414:ARG:HB2	1:c:417:ALA:HB2	1.92	0.49
3:f:2:ALA:HA	3:f:156:GLN:HA	1.95	0.49
2:p:50:ARG:HB2	2:p:54:ALA:HB3	1.94	0.49
1:u:40:GLU:HG2	1:u:41:GLU:N	2.28	0.49
2:v:10:ALA:HA	2:v:34:LEU:HD21	1.95	0.49
1:0:568:MET:HG2	1:3:590:LEU:HD11	1.95	0.49
2:1:13:ARG:HH21	2:1:85:ASN:HA	1.77	0.49
3:2:56:LEU:O	3:2:134:GLY:HA2	2.13	0.49
3:5:136:GLN:H	3:5:136:GLN:CD	2.20	0.49
4:D:414:THR:HA	4:E:328:HIS:ND1	2.28	0.49
4:E:332:VAL:CG2	4:E:339:MET:HE3	2.43	0.49
5:G:142:LEU:HD22	5:G:150:ILE:HD11	1.93	0.49
2:M:18:LEU:HD11	2:M:22:GLY:HA3	1.94	0.49
3:b:40:ILE:HG13	3:b:197:LEU:HD11	1.94	0.49
3:f:5:ALA:HB2	3:f:148:LEU:HD12	1.95	0.49
1:g:215:ASP:OD1	1:g:216:VAL:N	2.45	0.49
1:g:483:ALA:HA	1:k:105:ASN:HB3	1.94	0.49
2:s:31:ASP:HA	2:s:34:LEU:HD23	1.95	0.49
3:t:72:ILE:HG22	3:t:73:ASP:OD1	2.13	0.49
1:x:105:ASN:HA	1:x:108:ILE:HG12	1.95	0.49
3:5:38:ARG:NE	3:5:145:HIS:O	2.42	0.49
3:5:64:LEU:HD13	3:5:68:ALA:HB3	1.94	0.49
4:F:569:THR:HG22	4:F:573:GLU:OE1	2.13	0.49
5:L:19:PRO:HB3	3:q:96:LEU:HG	1.94	0.49
3:T:77:ASN:HA	3:T:137:VAL:HG13	1.94	0.49
1:U:145:ASN:ND2	1:U:179:ILE:O	2.38	0.49
1:U:583:LEU:HD21	1:Y:599:ARG:NH2	2.28	0.49
1:c:38:ASP:HA	1:c:42:MET:HB2	1.95	0.49
1:g:568:MET:HE3	1:k:596:ILE:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:i:46:GLU:OE2	5:i:122:SER:OG	2.25	0.49
3:j:24:TRP:HA	3:j:28:GLU:OE2	2.12	0.49
1:k:668:ALA:HB2	1:o:663:LEU:HA	1.95	0.49
5:m:15:ALA:HB1	5:m:166:TRP:CD1	2.48	0.49
3:t:8:VAL:HA	3:t:11:ARG:HG2	1.94	0.49
1:u:57:LEU:HD22	1:u:247:ASP:HB2	1.94	0.49
1:x:169:SER:HB2	1:x:180:TYR:CE1	2.47	0.49
2:y:50:ARG:HB2	2:y:54:ALA:HB3	1.94	0.49
2:1:92:LEU:HD11	2:4:8:ASN:HD21	1.76	0.49
1:3:127:ASP:OD1	1:3:127:ASP:N	2.46	0.49
3:5:113:ARG:HE	5:G:20:GLU:CD	2.21	0.49
4:A:245:LYS:HD3	4:F:81:ALA:O	2.13	0.49
4:B:266:MET:HE3	4:B:282:VAL:HG11	1.95	0.49
4:D:266:MET:HG3	4:D:301:GLN:OE1	2.12	0.49
4:D:319:LEU:O	4:D:364:GLN:NE2	2.45	0.49
4:D:542:ARG:HH11	3:b:23:ARG:HD3	1.76	0.49
5:J:142:LEU:HD22	5:J:150:ILE:HD11	1.94	0.49
2:d:20:PRO:HD3	2:d:81:SER:HB2	1.95	0.49
1:g:588:THR:HG23	1:g:590:LEU:HG	1.94	0.49
3:n:55:ALA:HA	3:n:136:GLN:HA	1.94	0.49
1:r:568:MET:HE2	1:u:596:ILE:HD12	1.94	0.49
1:x:248:GLU:O	1:x:252:TRP:CB	2.61	0.49
3:z:32:TRP:HA	3:z:32:TRP:CE3	2.48	0.49
1:0:139:LYS:HE2	1:0:555:ALA:O	2.13	0.48
1:0:582:ASP:OD1	1:0:583:LEU:N	2.45	0.48
1:3:208:ARG:HD3	1:3:351:LEU:HD11	1.94	0.48
1:6:389:ILE:O	1:6:433:ARG:NH1	2.46	0.48
4:B:472:TYR:OH	4:B:516:ALA:O	2.26	0.48
4:C:442:SER:N	4:C:554:ILE:O	2.27	0.48
4:D:458:ILE:HG21	4:D:520:VAL:HG11	1.94	0.48
4:E:266:MET:HG3	4:E:301:GLN:OE1	2.13	0.48
4:F:442:SER:OG	4:F:554:ILE:N	2.36	0.48
3:T:50:LYS:NZ	3:T:52:THR:OG1	2.42	0.48
3:T:175:SER:O	3:T:178:SER:OG	2.27	0.48
1:U:331:PHE:HA	1:U:336:LEU:HA	1.95	0.48
1:U:403:GLU:HG3	1:U:422:LYS:HE3	1.95	0.48
1:U:537:ASN:OD1	1:Y:176:GLY:N	2.40	0.48
1:Y:395:VAL:HG11	1:Y:408:PHE:HZ	1.78	0.48
5:a:164:LYS:HB3	5:a:166:TRP:CE3	2.47	0.48
5:e:67:GLU:O	5:e:128:LEU:N	2.44	0.48
1:r:123:ARG:NH1	1:r:543:LYS:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:263:SER:O	1:3:264:ARG:NE	2.40	0.48
4:A:454:GLY:N	4:A:568:ALA:O	2.45	0.48
4:B:266:MET:HG3	4:B:301:GLN:OE1	2.12	0.48
4:D:225:PRO:HG2	4:D:248:TYR:HE2	1.77	0.48
2:v:57:ILE:HG12	2:v:92:LEU:HD13	1.95	0.48
1:3:105:ASN:HA	1:3:108:ILE:HG12	1.95	0.48
1:6:432:ASP:OD1	1:U:430:ASN:ND2	2.46	0.48
4:B:456:ILE:HG12	4:B:567:LEU:HD22	1.95	0.48
4:B:532:LYS:HB2	4:B:544:PRO:HD3	1.95	0.48
4:E:247:LEU:HB2	4:E:266:MET:HE1	1.93	0.48
5:L:157:GLU:OE2	5:m:13:ARG:NH1	2.45	0.48
1:c:326:VAL:HG23	1:c:342:SER:OG	2.12	0.48
1:c:394:LYS:HD2	1:c:431:VAL:HB	1.94	0.48
3:n:14:THR:HG21	3:q:28:GLU:HG3	1.95	0.48
1:o:111:GLU:HG2	1:o:155:PHE:HD2	1.78	0.48
3:t:56:LEU:O	3:t:134:GLY:HA2	2.14	0.48
1:x:393:ASN:ND2	1:x:430:ASN:OD1	2.40	0.48
1:0:438:ALA:O	1:0:442:MET:HG2	2.13	0.48
3:2:32:TRP:CE3	3:2:32:TRP:HA	2.46	0.48
1:6:583:LEU:CD2	1:U:599:ARG:HH12	2.26	0.48
4:A:95:MET:HB3	4:A:102:TYR:HB2	1.95	0.48
4:A:266:MET:HG3	4:A:301:GLN:OE1	2.13	0.48
4:B:548:LEU:O	3:q:23:ARG:NH2	2.46	0.48
5:I:4:LEU:HD11	5:I:138:LEU:HG	1.96	0.48
2:N:50:ARG:CZ	2:N:80:LEU:HD13	2.42	0.48
2:O:50:ARG:HB3	2:O:54:ALA:HB3	1.96	0.48
2:P:31:ASP:HA	2:P:34:LEU:HD23	1.95	0.48
3:X:2:ALA:HA	3:X:156:GLN:HA	1.95	0.48
1:Y:56:GLU:OE2	1:Y:205:TYR:OH	2.31	0.48
1:Y:398:ASP:HB3	1:Y:425:LYS:HB3	1.95	0.48
3:f:16:LEU:HD23	3:f:24:TRP:CZ3	2.48	0.48
2:h:90:ALA:C	2:h:91:ARG:HD3	2.39	0.48
1:k:506:ILE:O	1:k:510:VAL:HG22	2.13	0.48
3:n:39:GLU:OE2	3:n:43:ARG:NH2	2.39	0.48
2:p:5:GLN:OE1	2:p:38:LEU:HA	2.13	0.48
1:x:506:ILE:O	1:x:510:VAL:HG22	2.13	0.48
3:z:145:HIS:CE1	3:z:155:VAL:HA	2.48	0.48
3:2:15:LEU:HD21	3:n:32:TRP:CH2	2.48	0.48
1:3:112:LYS:HG2	1:3:152:SER:HB2	1.94	0.48
2:4:94:ALA:H	2:7:8:ASN:HD21	1.61	0.48
5:H:143:ALA:O	5:H:147:ARG:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:116:THR:OG1	3:b:126:TYR:HB2	2.13	0.48
1:c:105:ASN:HA	1:c:108:ILE:HG12	1.95	0.48
1:c:158:THR:HG22	1:c:164:GLY:N	2.28	0.48
1:k:346:HIS:HB2	1:k:539:ILE:HD11	1.94	0.48
1:o:565:LEU:HD23	1:o:584:TRP:HA	1.94	0.48
1:r:230:LYS:HE2	1:r:334:ARG:HD2	1.96	0.48
2:v:98:GLY:HA2	2:v:101:ARG:NH1	2.28	0.48
3:w:106:MET:HE1	3:w:128:TYR:CE1	2.49	0.48
1:x:569:ILE:HG21	1:x:581:LEU:HD21	1.95	0.48
3:z:7:VAL:O	3:z:11:ARG:HG2	2.14	0.48
3:z:166:VAL:O	3:z:170:LEU:HD23	2.13	0.48
1:0:132:GLU:OE2	1:0:136:LYS:HE3	2.13	0.48
2:1:52:ASP:OD1	2:1:53:GLY:N	2.44	0.48
1:3:323:THR:N	1:6:174:THR:OG1	2.42	0.48
1:6:139:LYS:HE2	1:6:555:ALA:O	2.14	0.48
4:B:272:ALA:HB3	4:B:316:VAL:HG21	1.96	0.48
4:D:33:ARG:HG3	4:D:42:THR:HG22	1.95	0.48
4:E:458:ILE:HG21	4:E:520:VAL:HG11	1.94	0.48
5:H:141:LEU:HD12	5:H:142:LEU:HD12	1.95	0.48
2:M:25:LEU:HB2	2:M:68:MET:SD	2.53	0.48
2:Q:59:LYS:HD3	2:Q:74:GLN:HG3	1.96	0.48
5:S:32:ILE:HG23	5:S:130:LYS:HD2	1.94	0.48
1:Y:568:MET:HE2	1:c:596:ILE:HD13	1.96	0.48
1:c:282:ARG:HG2	1:c:326:VAL:HG12	1.94	0.48
1:k:123:ARG:NH1	1:k:543:LYS:O	2.47	0.48
1:o:90:ARG:HD3	1:o:388:TYR:CZ	2.49	0.48
3:q:128:TYR:HD2	3:q:129:PRO:HA	1.79	0.48
1:x:38:ASP:HA	1:x:42:MET:HB2	1.95	0.48
1:3:654:ALA:HB2	1:6:649:LYS:HA	1.95	0.48
4:E:414:THR:HA	4:F:328:HIS:ND1	2.28	0.48
4:F:241:ALA:O	4:F:248:TYR:N	2.25	0.48
5:H:45:ASP:OD2	5:H:45:ASP:N	2.47	0.48
1:U:592:ASN:O	1:U:596:ILE:HD12	2.13	0.48
2:Z:90:ALA:C	2:Z:91:ARG:HD3	2.39	0.48
5:e:18:CYS:HA	5:e:166:TRP:CZ2	2.48	0.48
1:g:444:SER:O	1:g:448:GLN:HG2	2.13	0.48
2:h:92:LEU:HD13	2:h:95:GLY:H	1.78	0.48
1:k:263:SER:O	1:k:264:ARG:NE	2.41	0.48
1:k:394:LYS:NZ	1:o:412:VAL:O	2.38	0.48
1:k:536:GLU:O	1:k:541:ARG:NH1	2.47	0.48
3:n:23:ARG:HB2	3:n:24:TRP:CE3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:71:THR:C	2:s:74:GLN:HE22	2.21	0.48
1:u:493:PHE:HE2	1:x:146:ARG:HD3	1.79	0.48
1:x:224:ARG:HH11	1:x:337:LEU:HD13	1.79	0.48
1:0:63:ASN:O	1:0:67:MET:HG3	2.14	0.48
1:0:558:ARG:CZ	1:0:587:SER:HA	2.44	0.48
3:5:32:TRP:CE3	3:5:32:TRP:HA	2.49	0.48
4:B:59:ILE:HG13	4:B:409:PHE:HB2	1.94	0.48
4:B:290:ILE:O	4:B:302:GLN:N	2.46	0.48
4:D:55:ASN:HB3	4:D:70:GLN:HE22	1.79	0.48
4:E:272:ALA:HB3	4:E:316:VAL:HG21	1.94	0.48
5:H:2:LYS:HB3	5:H:137:SER:HB2	1.96	0.48
5:H:40:LEU:HD21	5:H:189:LYS:HB3	1.95	0.48
2:O:50:ARG:NH1	2:O:81:SER:O	2.47	0.48
3:T:161:PHE:O	3:T:165:LEU:HD23	2.12	0.48
2:Z:75:GLU:HG3	2:Z:92:LEU:HD23	1.96	0.48
3:b:24:TRP:CD1	3:b:176:LYS:HZ2	2.31	0.48
1:g:377:ASP:O	1:g:381:LYS:HG2	2.14	0.48
1:g:495:VAL:HA	1:g:498:GLN:HG2	1.95	0.48
5:m:109:SER:OG	5:m:110:GLU:N	2.46	0.48
3:n:8:VAL:HG22	3:n:162:VAL:HG23	1.95	0.48
3:q:78:LEU:HD23	3:q:136:GLN:HG3	1.95	0.48
3:z:56:LEU:O	3:z:134:GLY:HA2	2.13	0.48
3:5:7:VAL:O	3:5:11:ARG:HG2	2.14	0.48
3:5:96:LEU:HG	5:G:19:PRO:HB3	1.96	0.48
4:A:35:ASP:O	4:B:15:ARG:NH1	2.46	0.48
4:A:542:ARG:HH21	3:n:17:GLN:HB3	1.79	0.48
4:E:319:LEU:HD11	4:E:369:TYR:HD1	1.79	0.48
5:H:17:GLY:H	5:H:166:TRP:HE1	1.62	0.48
2:M:100:PHE:O	2:M:104:ILE:HG12	2.14	0.48
5:S:7:PHE:CD1	5:S:147:ARG:HG3	2.48	0.48
5:S:18:CYS:HA	5:S:166:TRP:CZ2	2.49	0.48
1:U:179:ILE:HD12	1:U:505:LEU:HB3	1.95	0.48
1:U:376:GLN:CA	1:U:376:GLN:HE21	2.27	0.48
2:V:13:ARG:HB2	2:V:28:THR:HG23	1.94	0.48
5:W:18:CYS:HA	5:W:166:TRP:CZ2	2.49	0.48
3:X:170:LEU:O	3:X:174:SER:OG	2.32	0.48
5:a:32:ILE:HG23	5:a:130:LYS:HD2	1.95	0.48
1:c:569:ILE:HG21	1:c:581:LEU:HD21	1.96	0.48
2:l:63:ARG:HB2	2:l:68:MET:HG3	1.95	0.48
3:w:7:VAL:O	3:w:11:ARG:HG2	2.14	0.48
1:x:346:HIS:HB2	1:x:539:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:663:LEU:HA	1:x:668:ALA:HB2	1.95	0.48
2:1:71:THR:C	2:1:74:GLN:HE22	2.21	0.48
2:1:97:LEU:HD22	2:4:100:PHE:HE1	1.78	0.48
4:A:312:ASN:ND2	4:A:360:ILE:O	2.47	0.48
4:B:18:PRO:HB3	4:B:27:GLN:NE2	2.28	0.48
4:E:349:ARG:NH1	4:E:353:MET:HE3	2.28	0.48
5:I:39:ARG:HB3	5:I:128:LEU:HD13	1.96	0.48
3:T:114:HIS:CD2	5:W:20:GLU:HG3	2.49	0.48
2:Z:25:LEU:HD11	2:Z:68:MET:HE3	1.95	0.48
2:Z:63:ARG:CB	2:Z:68:MET:HG2	2.43	0.48
5:a:109:SER:OG	5:a:110:GLU:N	2.47	0.48
1:c:193:SER:O	1:g:257:ARG:NH2	2.47	0.48
1:c:668:ALA:HB2	1:g:663:LEU:HA	1.95	0.48
1:g:123:ARG:NH2	1:k:143:ASP:OD2	2.46	0.48
2:p:43:TRP:CG	2:p:59:LYS:HE2	2.49	0.48
1:x:482:VAL:HA	1:x:485:ASN:OD1	2.14	0.48
3:z:123:THR:HG23	3:z:124:VAL:HG23	1.94	0.48
1:3:154:SER:HB3	1:3:354:ILE:HD12	1.95	0.47
3:5:56:LEU:O	3:5:134:GLY:HA2	2.14	0.47
3:5:98:THR:HB	5:S:12:HIS:HB3	1.97	0.47
4:A:459:GLU:OE1	4:B:19:ARG:NH1	2.46	0.47
4:F:51:ILE:HG13	4:F:420:LEU:HD12	1.96	0.47
5:G:42:ARG:HG2	5:G:128:LEU:HD23	1.96	0.47
5:G:45:ASP:OD2	5:G:45:ASP:N	2.46	0.47
5:H:19:PRO:HB3	3:t:96:LEU:HG	1.95	0.47
2:N:11:ALA:HA	2:N:89:GLU:HB3	1.96	0.47
2:P:101:ARG:HD2	2:Q:6:PHE:CE2	2.45	0.47
1:U:654:ALA:HB2	1:Y:649:LYS:HA	1.95	0.47
1:o:105:ASN:HA	1:o:108:ILE:HG12	1.95	0.47
2:s:25:LEU:HB2	2:s:68:MET:SD	2.54	0.47
1:u:105:ASN:HA	1:u:108:ILE:HG12	1.95	0.47
1:u:596:ILE:O	1:u:600:ILE:HG12	2.14	0.47
3:w:106:MET:HE1	3:w:128:TYR:HE1	1.79	0.47
1:x:64:ARG:HD3	1:x:186:TRP:CZ3	2.49	0.47
2:1:97:LEU:HA	2:1:100:PHE:HD2	1.79	0.47
1:3:285:MET:N	1:3:323:THR:O	2.46	0.47
4:B:17:LEU:HD12	4:B:18:PRO:HD2	1.96	0.47
4:C:251:GLU:HB2	4:C:257:ALA:HB3	1.94	0.47
4:E:290:ILE:O	4:E:302:GLN:N	2.44	0.47
4:E:472:TYR:OH	4:E:516:ALA:O	2.27	0.47
4:F:59:ILE:HG13	4:F:409:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:8:MET:HE1	5:L:23:ALA:HB3	1.96	0.47
5:L:102:ALA:HA	5:L:117:PRO:HG2	1.95	0.47
5:L:107:GLN:HG2	5:L:109:SER:O	2.13	0.47
2:N:104:ILE:O	2:N:108:GLN:HG2	2.13	0.47
2:R:49:ILE:HB	2:R:87:ARG:HB2	1.96	0.47
3:T:113:ARG:HB2	3:T:129:PRO:HD3	1.96	0.47
1:U:554:ARG:NH2	1:U:563:GLU:OE2	2.48	0.47
3:f:113:ARG:HB2	3:f:129:PRO:HD3	1.95	0.47
3:f:116:THR:OG1	3:f:126:TYR:HB2	2.14	0.47
1:g:161:VAL:HG21	1:g:186:TRP:CG	2.49	0.47
1:k:43:LYS:O	1:k:47:ARG:HG3	2.14	0.47
3:n:32:TRP:HA	3:n:32:TRP:CE3	2.48	0.47
3:t:9:LEU:HD22	3:t:29:LEU:HB3	1.95	0.47
1:O:40:GLU:HG2	1:O:41:GLU:N	2.29	0.47
1:O:649:LYS:HA	1:x:654:ALA:HB2	1.97	0.47
4:E:445:PHE:N	4:E:552:TRP:O	2.37	0.47
5:H:156:SER:O	5:H:160:ILE:HG13	2.14	0.47
5:a:46:GLU:OE2	5:a:122:SER:OG	2.29	0.47
1:g:139:LYS:HE2	1:g:555:ALA:O	2.14	0.47
1:k:105:ASN:HA	1:k:108:ILE:HG12	1.95	0.47
1:u:556:THR:HG23	1:u:559:GLN:H	1.80	0.47
3:2:7:VAL:O	3:2:11:ARG:HG2	2.15	0.47
2:7:58:VAL:HG12	2:7:72:ARG:HD3	1.95	0.47
4:A:33:ARG:HG3	4:A:42:THR:HG22	1.95	0.47
4:B:33:ARG:HG3	4:B:42:THR:HG22	1.95	0.47
4:B:542:ARG:HH11	3:X:23:ARG:HD3	1.79	0.47
4:C:26:SER:HB3	4:C:441:ARG:O	2.13	0.47
4:C:361:VAL:HB	4:C:372:SER:HB3	1.95	0.47
4:C:453:PHE:HA	4:C:569:THR:HA	1.97	0.47
4:D:483:ASN:O	4:D:487:PHE:HB2	2.14	0.47
4:D:542:ARG:HH21	3:b:17:GLN:HB3	1.77	0.47
4:E:33:ARG:HG3	4:E:42:THR:HG22	1.95	0.47
4:E:489:LEU:HD12	4:E:511:MET:HE1	1.96	0.47
4:F:333:MET:HE2	4:F:342:ILE:HB	1.96	0.47
5:G:107:GLN:OE1	5:S:194:GLN:HB2	2.15	0.47
5:I:192:LYS:HZ3	1:k:407:GLU:CD	2.23	0.47
5:K:45:ASP:OD2	5:K:45:ASP:N	2.47	0.47
1:U:158:THR:HG22	1:U:164:GLY:N	2.29	0.47
3:X:116:THR:OG1	3:X:126:TYR:HB2	2.14	0.47
5:i:24:PHE:O	5:i:28:ARG:HG3	2.14	0.47
3:j:113:ARG:HB2	3:j:129:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:161:VAL:HG21	1:o:186:TRP:CD1	2.49	0.47
1:r:595:GLU:O	1:r:598:LYS:HG3	2.13	0.47
1:6:414:ARG:HG3	5:S:200:ARG:HH12	1.80	0.47
4:A:247:LEU:CB	4:A:266:MET:HE1	2.43	0.47
4:B:79:PRO:HD2	4:B:255:PRO:HG3	1.97	0.47
4:B:542:ARG:HH21	3:X:17:GLN:HB3	1.80	0.47
4:C:81:ALA:O	4:D:245:LYS:HD3	2.15	0.47
4:F:249:PHE:CE2	4:F:299:MET:HG3	2.50	0.47
5:H:104:TYR:HD1	5:H:116:VAL:HG11	1.79	0.47
5:I:168:SER:OG	5:I:171:LEU:HB2	2.14	0.47
5:J:147:ARG:HH21	5:i:133:LEU:HB2	1.78	0.47
5:a:31:ALA:HB1	5:a:142:LEU:HD13	1.95	0.47
1:c:125:LYS:HG3	1:g:558:ARG:CZ	2.44	0.47
1:c:285:MET:HG3	1:c:325:ARG:HE	1.80	0.47
3:f:31:GLU:OE2	3:w:11:ARG:NH1	2.47	0.47
1:g:514:LYS:HA	1:g:514:LYS:HD3	1.81	0.47
3:n:159:ALA:HB3	3:q:144:ARG:NE	2.29	0.47
1:r:37:LEU:O	1:r:42:MET:HG2	2.14	0.47
3:t:7:VAL:O	3:t:11:ARG:HG2	2.14	0.47
1:u:279:CYS:N	1:u:329:ALA:O	2.39	0.47
3:w:8:VAL:HG22	3:w:162:VAL:HG23	1.96	0.47
1:x:158:THR:HG22	1:x:164:GLY:N	2.29	0.47
1:6:40:GLU:HG2	1:6:41:GLU:N	2.29	0.47
1:6:125:LYS:HG3	1:U:558:ARG:NE	2.29	0.47
4:A:330:GLY:HA2	4:A:352:TRP:CD1	2.50	0.47
4:C:319:LEU:HD21	4:C:369:TYR:HB2	1.96	0.47
4:C:333:MET:HE2	4:C:342:ILE:HB	1.96	0.47
4:D:438:LEU:O	4:D:557:ASN:HA	2.14	0.47
4:D:472:TYR:OH	4:D:516:ALA:O	2.28	0.47
4:D:558:SER:OG	4:D:560:ILE:O	2.28	0.47
4:E:452:ASN:HB3	3:w:17:GLN:OE1	2.15	0.47
5:G:4:LEU:HD11	5:G:138:LEU:HG	1.95	0.47
5:I:45:ASP:OD2	5:I:45:ASP:N	2.47	0.47
3:T:5:ALA:HB2	3:T:148:LEU:HD12	1.96	0.47
3:T:64:LEU:HD13	3:T:68:ALA:HB3	1.97	0.47
1:Y:132:GLU:OE2	1:Y:136:LYS:HE3	2.15	0.47
2:Z:43:TRP:CD1	2:Z:59:LYS:HZ1	2.32	0.47
3:b:153:ASP:OD1	3:b:154:VAL:N	2.48	0.47
1:c:169:SER:HB2	1:c:180:TYR:CE1	2.49	0.47
1:c:248:GLU:O	1:c:252:TRP:CB	2.63	0.47
1:c:452:GLN:HE22	1:g:99:VAL:HG13	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:200:ARG:HH12	1:o:414:ARG:HG3	1.80	0.47
5:i:205:PHE:CZ	1:r:92:GLN:HB2	2.50	0.47
3:n:116:THR:OG1	3:n:126:TYR:HB2	2.14	0.47
1:r:78:GLN:HE22	1:r:98:ASN:HA	1.80	0.47
1:r:346:HIS:HB2	1:r:539:ILE:HD11	1.96	0.47
1:u:483:ALA:HA	1:x:105:ASN:HB3	1.95	0.47
1:0:271:ARG:HH21	1:0:273:ARG:HH11	1.63	0.47
1:0:483:ALA:HA	1:3:105:ASN:HB3	1.97	0.47
1:3:506:ILE:O	1:3:510:VAL:HG22	2.15	0.47
2:4:63:ARG:CB	2:4:68:MET:HG2	2.42	0.47
2:4:93:THR:HB	2:4:97:LEU:HD12	1.96	0.47
3:5:15:LEU:HB3	3:5:170:LEU:HD11	1.96	0.47
3:5:145:HIS:CE1	3:5:155:VAL:HA	2.49	0.47
3:5:145:HIS:CE1	3:5:155:VAL:HG13	2.49	0.47
4:A:97:VAL:HB	4:A:102:TYR:HE2	1.79	0.47
4:B:306:LEU:HD23	4:B:339:MET:HB3	1.96	0.47
4:C:59:ILE:HG13	4:C:409:PHE:HB2	1.97	0.47
4:C:82:GLN:HG2	4:C:84:ARG:NE	2.29	0.47
4:E:17:LEU:HD12	4:E:18:PRO:HD2	1.95	0.47
4:F:88:MET:HE3	4:F:228:LEU:HB3	1.96	0.47
5:J:192:LYS:NZ	1:r:407:GLU:OE2	2.40	0.47
5:K:156:SER:O	5:K:160:ILE:HG13	2.13	0.47
2:Q:101:ARG:NH2	2:R:99:ASP:HB3	2.29	0.47
3:T:9:LEU:HD22	3:T:151:GLN:HG3	1.95	0.47
3:T:44:LYS:HE3	3:T:200:GLN:HG3	1.95	0.47
1:Y:553:TRP:CZ3	1:Y:555:ALA:HA	2.50	0.47
5:e:24:PHE:O	5:e:28:ARG:HG3	2.15	0.47
5:e:38:THR:HG23	5:e:183:LEU:HD12	1.95	0.47
1:g:40:GLU:HG2	1:g:41:GLU:N	2.30	0.47
1:g:385:LYS:O	1:g:389:ILE:HG13	2.14	0.47
3:n:20:ASP:OD2	3:n:22:GLU:HG2	2.14	0.47
1:o:78:GLN:HE22	1:o:98:ASN:HA	1.78	0.47
1:o:141:LEU:HD12	1:o:506:ILE:HD11	1.97	0.47
3:q:7:VAL:O	3:q:11:ARG:HG2	2.14	0.47
1:r:421:LYS:HD2	1:r:427:ILE:HG12	1.96	0.47
1:r:583:LEU:HD21	1:u:599:ARG:NH2	2.29	0.47
1:r:668:ALA:HB2	1:u:663:LEU:HA	1.95	0.47
1:u:506:ILE:O	1:u:510:VAL:HG22	2.15	0.47
3:z:145:HIS:CE1	3:z:155:VAL:HG13	2.49	0.47
1:0:413:ALA:HB3	5:L:204:GLN:HG2	1.97	0.47
1:0:572:MET:HE1	1:3:581:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:13:ARG:HB2	2:1:28:THR:HG23	1.97	0.47
1:3:401:ALA:HB1	1:3:427:ILE:CD1	2.44	0.47
1:3:493:PHE:CE1	1:6:146:ARG:HD3	2.48	0.47
1:6:394:LYS:NZ	1:U:412:VAL:O	2.46	0.47
4:B:319:LEU:HD11	4:B:369:TYR:HD1	1.80	0.47
4:B:391:THR:HA	4:B:396:PRO:HB3	1.97	0.47
4:C:542:ARG:HH21	3:T:17:GLN:HB3	1.79	0.47
4:D:26:SER:HB3	4:D:441:ARG:O	2.14	0.47
4:D:550:ARG:HG3	4:D:551:ILE:HD12	1.96	0.47
5:I:34:PHE:O	5:I:38:THR:OG1	2.23	0.47
5:I:200:ARG:HD2	1:k:414:ARG:HH21	1.80	0.47
5:K:101:GLN:O	5:K:117:PRO:HG2	2.15	0.47
5:L:94:ARG:HD3	5:m:126:TYR:CE2	2.50	0.47
5:L:126:TYR:CE2	5:S:94:ARG:HD3	2.50	0.47
2:M:13:ARG:NE	2:M:86:ASP:O	2.35	0.47
2:N:57:ILE:HG21	2:N:92:LEU:HD22	1.96	0.47
2:P:57:ILE:HG12	2:P:92:LEU:HD13	1.97	0.47
2:Q:58:VAL:HG12	2:Q:72:ARG:HA	1.96	0.47
1:U:376:GLN:HE21	1:U:376:GLN:C	2.23	0.47
2:V:52:ASP:OD2	2:V:53:GLY:N	2.45	0.47
5:a:15:ALA:HB1	5:a:166:TRP:HD1	1.80	0.47
5:m:71:VAL:HG11	5:m:105:VAL:HG21	1.96	0.47
1:o:594:ASP:OD1	1:o:594:ASP:N	2.48	0.47
1:r:105:ASN:HA	1:r:108:ILE:HG12	1.96	0.47
1:u:372:MET:HA	1:u:450:LEU:HD11	1.95	0.47
1:x:414:ARG:HB2	1:x:417:ALA:HB2	1.95	0.47
1:0:76:SER:HB3	1:0:98:ASN:HD22	1.79	0.47
1:3:224:ARG:HH11	1:3:337:LEU:HD13	1.80	0.47
1:6:483:ALA:HA	1:U:105:ASN:HB3	1.97	0.47
4:C:88:MET:HE3	4:C:228:LEU:HB3	1.97	0.47
4:C:314:ARG:HH21	4:C:361:VAL:HG22	1.78	0.47
4:E:386:THR:HB	4:E:401:SER:HB3	1.97	0.47
4:F:542:ARG:HH11	3:j:23:ARG:HD3	1.80	0.47
4:F:542:ARG:HH21	3:j:17:GLN:HB3	1.80	0.47
1:Y:211:TRP:HB3	1:Y:273:ARG:HH21	1.80	0.47
1:Y:596:ILE:O	1:Y:600:ILE:HG12	2.14	0.47
5:e:8:MET:HG3	5:e:12:HIS:CD2	2.50	0.47
2:h:58:VAL:HG12	2:h:72:ARG:HA	1.97	0.47
1:k:154:SER:HB3	1:k:354:ILE:HD12	1.97	0.47
1:k:371:TRP:NE1	1:k:372:MET:SD	2.88	0.47
1:o:506:ILE:O	1:o:510:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:q:56:LEU:O	3:q:134:GLY:HA2	2.15	0.47
1:r:55:GLN:O	1:r:59:ARG:HB2	2.15	0.47
1:r:654:ALA:HB2	1:u:649:LYS:HA	1.97	0.47
1:u:361:ARG:HD3	1:x:72:ASP:OD2	2.14	0.47
1:x:401:ALA:HB1	1:x:427:ILE:CD1	2.45	0.47
2:1:7:ALA:HB3	2:1:91:ARG:HD2	1.96	0.47
1:3:371:TRP:NE1	1:3:372:MET:SD	2.88	0.47
4:C:7:THR:HG22	4:D:20:LEU:HD11	1.97	0.47
4:E:21:LEU:HB2	4:E:443:LYS:HG3	1.96	0.47
4:F:296:PRO:HA	4:F:299:MET:HE2	1.97	0.47
1:Y:105:ASN:HA	1:Y:108:ILE:HG12	1.96	0.47
1:Y:327:ARG:HH12	1:Y:339:GLU:HG3	1.80	0.47
1:Y:432:ASP:OD1	1:c:430:ASN:ND2	2.48	0.47
5:a:71:VAL:HG11	5:a:105:VAL:HG21	1.97	0.47
1:c:506:ILE:O	1:c:510:VAL:HG22	2.15	0.47
1:g:506:ILE:O	1:g:510:VAL:HG22	2.15	0.47
1:o:377:ASP:O	1:o:381:LYS:HG2	2.15	0.47
3:t:32:TRP:HA	3:t:32:TRP:CE3	2.49	0.47
3:t:78:LEU:HB3	3:t:136:GLN:HG2	1.97	0.47
1:u:59:ARG:HG2	1:x:260:TYR:HA	1.96	0.47
1:0:484:THR:HG23	1:0:487:LEU:HD12	1.97	0.46
3:2:98:THR:HB	5:i:12:HIS:HB3	1.96	0.46
1:3:388:TYR:OH	1:6:416:ASP:OD2	2.30	0.46
4:A:483:ASN:O	4:A:487:PHE:HB2	2.13	0.46
4:E:97:VAL:HB	4:E:102:TYR:HE2	1.80	0.46
5:G:36:GLU:HA	5:G:66:TYR:CE2	2.51	0.46
5:H:159:LEU:HD23	5:H:171:LEU:HB3	1.98	0.46
5:J:57:VAL:HG22	5:J:111:ASP:HB3	1.96	0.46
5:K:188:THR:O	5:K:192:LYS:HG3	2.15	0.46
5:L:32:ILE:HG23	5:L:130:LYS:HD2	1.96	0.46
2:M:18:LEU:HG	2:M:72:ARG:HH21	1.80	0.46
2:M:50:ARG:HB3	2:M:82:PHE:CD2	2.50	0.46
1:Y:497:MET:HE1	1:c:146:ARG:NE	2.30	0.46
5:e:141:LEU:HD12	5:e:142:LEU:HD12	1.97	0.46
1:g:63:ASN:O	1:g:67:MET:HG3	2.15	0.46
1:0:284:PRO:O	1:0:285:MET:HE2	2.15	0.46
3:2:11:ARG:NH1	3:n:31:GLU:OE2	2.48	0.46
2:4:75:GLU:HG3	2:4:92:LEU:HD23	1.96	0.46
4:A:438:LEU:O	4:A:557:ASN:HA	2.16	0.46
4:C:486:ASN:ND2	4:C:511:MET:SD	2.89	0.46
4:E:279:THR:HG22	4:E:292:SER:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:532:LYS:HB2	4:E:544:PRO:HD3	1.97	0.46
2:M:14:LEU:HB3	2:M:86:ASP:HB3	1.97	0.46
5:S:24:PHE:O	5:S:28:ARG:HG3	2.14	0.46
3:T:116:THR:OG1	3:T:126:TYR:HB2	2.15	0.46
1:U:568:MET:HE2	1:Y:596:ILE:HD12	1.96	0.46
2:V:111:ALA:O	2:V:115:GLN:HG3	2.16	0.46
5:W:96:THR:HG22	5:W:98:GLN:H	1.80	0.46
3:f:159:ALA:HB3	3:z:144:ARG:NE	2.29	0.46
1:g:167:GLU:OE2	1:g:208:ARG:NH1	2.49	0.46
3:j:49:MET:HE3	3:j:72:ILE:HD12	1.96	0.46
2:l:58:VAL:HG11	2:l:72:ARG:HD3	1.98	0.46
1:r:399:GLU:HA	1:u:420:VAL:HG13	1.96	0.46
1:u:601:ARG:O	1:u:605:GLY:N	2.30	0.46
1:0:444:SER:O	1:0:448:GLN:HG2	2.16	0.46
1:6:78:GLN:HE22	1:6:98:ASN:HA	1.80	0.46
4:B:452:ASN:HB3	3:q:17:GLN:OE1	2.15	0.46
4:F:251:GLU:HB3	4:F:254:ILE:HB	1.98	0.46
5:J:5:ASP:O	5:J:9:PRO:HD3	2.15	0.46
2:O:65:VAL:HG12	2:O:66:ASP:N	2.31	0.46
2:Q:27:VAL:HG13	2:Q:68:MET:HE1	1.96	0.46
2:R:48:LEU:HB3	2:R:82:PHE:CE1	2.50	0.46
1:U:63:ASN:ND2	1:U:364:LEU:HB3	2.30	0.46
3:b:31:GLU:OE2	3:t:11:ARG:NH1	2.48	0.46
5:e:96:THR:HG22	5:e:98:GLN:H	1.79	0.46
3:f:16:LEU:O	3:f:18:ASP:N	2.41	0.46
3:j:69:ILE:HD12	3:j:69:ILE:H	1.80	0.46
5:m:104:TYR:CD2	5:m:116:VAL:HG11	2.50	0.46
1:o:279:CYS:O	1:o:329:ALA:N	2.48	0.46
2:p:65:VAL:HG12	2:p:66:ASP:N	2.30	0.46
2:v:63:ARG:HG2	2:v:63:ARG:HH11	1.79	0.46
1:0:251:ASP:OD1	1:0:275:ARG:NH2	2.49	0.46
3:2:99:GLU:OE1	5:i:13:ARG:HB2	2.15	0.46
4:C:414:THR:HG22	4:D:328:HIS:HE1	1.80	0.46
4:E:288:PRO:HB2	4:E:304:VAL:HG11	1.96	0.46
5:L:168:SER:OG	5:L:171:LEU:HB2	2.16	0.46
1:U:56:GLU:OE2	1:U:193:SER:N	2.45	0.46
1:U:438:ALA:O	1:U:442:MET:HG2	2.15	0.46
5:W:139:PRO:HB2	5:W:141:LEU:HD23	1.96	0.46
1:Y:127:ASP:C	1:Y:130:PRO:HD2	2.40	0.46
3:b:32:TRP:HH2	3:t:15:LEU:HD21	1.79	0.46
1:c:654:ALA:HB2	1:g:649:LYS:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:57:ILE:HG12	2:l:92:LEU:HD22	1.96	0.46
2:p:13:ARG:HD3	2:p:86:ASP:H	1.80	0.46
2:s:48:LEU:HD11	2:s:86:ASP:CG	2.40	0.46
3:w:9:LEU:HD11	3:w:30:LEU:HD21	1.96	0.46
1:0:279:CYS:O	1:0:329:ALA:N	2.48	0.46
3:5:32:TRP:CH2	3:X:15:LEU:HD21	2.50	0.46
4:A:46:ARG:NH2	4:A:433:GLN:OE1	2.48	0.46
4:B:386:THR:HB	4:B:401:SER:HB3	1.98	0.46
4:D:239:MET:N	4:D:250:CYS:SG	2.88	0.46
2:N:93:THR:OG1	2:O:8:ASN:OD1	2.30	0.46
1:U:67:MET:HB2	1:U:186:TRP:CZ3	2.51	0.46
1:U:125:LYS:HE2	1:Y:593:ARG:NH1	2.31	0.46
1:Y:167:GLU:OE2	1:Y:351:LEU:HD21	2.16	0.46
1:c:395:VAL:HG11	1:c:408:PHE:HE2	1.81	0.46
2:d:18:LEU:HD22	2:d:82:PHE:CD2	2.51	0.46
5:e:18:CYS:HG	5:e:22:THR:HG1	1.64	0.46
1:g:251:ASP:OD1	1:g:275:ARG:NH2	2.48	0.46
3:j:64:LEU:HD13	3:j:68:ALA:HB3	1.97	0.46
5:m:67:GLU:O	5:m:128:LEU:N	2.46	0.46
1:o:148:PRO:HG3	1:o:553:TRP:NE1	2.26	0.46
1:o:393:ASN:HA	1:o:433:ARG:NH2	2.31	0.46
3:q:9:LEU:HD11	3:q:30:LEU:HD21	1.98	0.46
1:u:553:TRP:CZ3	1:u:555:ALA:HA	2.51	0.46
3:w:56:LEU:O	3:w:134:GLY:HA2	2.15	0.46
1:x:282:ARG:HG2	1:x:326:VAL:HG12	1.96	0.46
1:3:377:ASP:OD1	1:3:378:ASP:N	2.48	0.46
1:3:398:ASP:OD2	1:3:426:GLN:HG2	2.16	0.46
1:3:594:ASP:OD1	1:3:595:GLU:N	2.49	0.46
4:A:328:HIS:HE1	4:F:414:THR:HG22	1.81	0.46
5:J:204:GLN:HG2	1:o:413:ALA:HB3	1.97	0.46
5:L:20:GLU:OE1	3:q:113:ARG:NH2	2.48	0.46
2:N:63:ARG:HB2	2:N:68:MET:HG3	1.98	0.46
2:O:59:LYS:HB3	2:O:71:THR:OG1	2.16	0.46
1:Y:361:ARG:HD3	1:c:72:ASP:OD2	2.15	0.46
1:Y:369:ILE:HG22	1:Y:373:ARG:HB2	1.97	0.46
2:Z:62:SER:OG	2:Z:69:SER:OG	2.23	0.46
5:e:7:PHE:CD1	5:e:147:ARG:HG3	2.51	0.46
5:i:107:GLN:HG2	5:i:109:SER:O	2.16	0.46
1:r:395:VAL:HG11	1:r:408:PHE:HE2	1.79	0.46
2:y:11:ALA:HA	2:y:89:GLU:HB3	1.97	0.46
1:0:57:LEU:HD22	1:0:247:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:176:GLY:N	1:x:537:ASN:OD1	2.43	0.46
3:2:72:ILE:HG22	3:2:73:ASP:OD1	2.15	0.46
1:6:63:ASN:OD1	1:6:359:ARG:NH2	2.48	0.46
4:D:224:PRO:HG3	4:D:258:TRP:HD1	1.81	0.46
4:E:18:PRO:HB3	4:E:27:GLN:NE2	2.31	0.46
5:G:109:SER:HB3	5:G:112:THR:OG1	2.16	0.46
5:I:107:GLN:OE1	5:a:194:GLN:HB2	2.14	0.46
2:O:50:ARG:HD3	2:O:86:ASP:OD2	2.15	0.46
2:Q:57:ILE:HD13	2:Q:92:LEU:HD13	1.98	0.46
1:U:326:VAL:HG23	1:U:342:SER:OG	2.16	0.46
1:c:147:LEU:HD11	1:c:498:GLN:HE22	1.80	0.46
3:f:55:ALA:HA	3:f:136:GLN:HA	1.97	0.46
1:g:195:SER:O	1:g:363:ASN:ND2	2.49	0.46
2:p:36:PRO:O	2:p:63:ARG:NH1	2.45	0.46
1:r:326:VAL:HG23	1:r:342:SER:OG	2.16	0.46
1:r:556:THR:HG23	1:r:559:GLN:H	1.81	0.46
1:r:569:ILE:HG12	1:r:580:MET:HB2	1.98	0.46
1:u:357:PHE:HE2	1:u:368:VAL:HG22	1.79	0.46
1:0:377:ASP:O	1:0:381:LYS:HG2	2.16	0.46
1:3:399:GLU:HA	1:6:420:VAL:HG13	1.96	0.46
1:6:59:ARG:HD2	1:U:257:ARG:HA	1.97	0.46
4:A:225:PRO:HG2	4:A:248:TYR:CE2	2.51	0.46
4:B:304:VAL:HG22	4:B:305:GLU:H	1.81	0.46
4:C:296:PRO:HA	4:C:299:MET:HE2	1.96	0.46
4:C:442:SER:OG	4:C:554:ILE:N	2.37	0.46
4:F:486:ASN:ND2	4:F:511:MET:SD	2.89	0.46
5:H:174:PHE:CE2	5:a:160:ILE:HD13	2.51	0.46
5:K:5:ASP:O	5:K:9:PRO:HD3	2.16	0.46
5:K:159:LEU:HD23	5:K:171:LEU:HB3	1.97	0.46
5:K:160:ILE:HD13	5:i:174:PHE:CE2	2.51	0.46
2:Q:92:LEU:O	2:Q:96:GLU:HG2	2.16	0.46
5:S:8:MET:HG3	5:S:12:HIS:CD2	2.51	0.46
5:S:64:ALA:N	5:S:130:LYS:O	2.46	0.46
1:U:576:VAL:HG21	1:Y:600:ILE:HD13	1.98	0.46
5:W:64:ALA:N	5:W:130:LYS:O	2.44	0.46
5:a:156:SER:O	5:a:160:ILE:HG13	2.16	0.46
5:e:136:ASP:OD1	5:e:136:ASP:N	2.47	0.46
2:h:5:GLN:OE1	2:h:38:LEU:HD23	2.15	0.46
1:k:414:ARG:HB2	1:k:417:ALA:HB2	1.96	0.46
1:o:654:ALA:HB2	1:r:649:LYS:HA	1.98	0.46
1:r:158:THR:HG22	1:r:164:GLY:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:45:MET:HB2	2:s:96:GLU:OE1	2.16	0.46
1:u:568:MET:HE2	1:x:596:ILE:HD13	1.97	0.46
1:0:430:ASN:OD1	1:0:433:ARG:HB2	2.16	0.46
3:2:78:LEU:HB3	3:2:136:GLN:HG2	1.97	0.46
1:3:75:ASP:O	1:3:77:ILE:HD12	2.15	0.46
4:A:20:LEU:HD11	4:F:7:THR:HG22	1.98	0.46
4:A:88:MET:HE1	4:A:241:ALA:HB1	1.98	0.46
4:A:377:GLU:HG2	4:A:378:PRO:HD2	1.98	0.46
4:D:35:ASP:O	4:E:15:ARG:NH1	2.49	0.46
5:H:102:ALA:HA	5:H:117:PRO:HB2	1.98	0.46
5:H:188:THR:O	5:H:192:LYS:HG3	2.16	0.46
5:J:12:HIS:HA	5:J:15:ALA:O	2.15	0.46
1:U:63:ASN:O	1:U:67:MET:HG3	2.16	0.46
1:U:435:LEU:HD21	1:Y:433:ARG:HD3	1.98	0.46
1:Y:108:ILE:HG13	1:Y:109:GLY:N	2.31	0.46
3:b:159:ALA:HB3	3:w:144:ARG:NE	2.31	0.46
1:c:231:ALA:HA	1:c:334:ARG:HH12	1.81	0.46
1:c:247:ASP:OD1	1:c:248:GLU:N	2.46	0.46
5:e:192:LYS:HE2	5:e:192:LYS:HB2	1.81	0.46
5:i:139:PRO:HB2	5:i:141:LEU:HD23	1.98	0.46
1:k:654:ALA:HB2	1:o:649:LYS:HA	1.97	0.46
1:o:90:ARG:HD3	1:o:388:TYR:CE2	2.50	0.46
1:o:121:LEU:HD21	1:r:559:GLN:NE2	2.31	0.46
1:r:63:ASN:HB2	1:r:364:LEU:HD13	1.97	0.46
4:F:332:VAL:CG2	4:F:339:MET:HE3	2.46	0.46
5:H:160:ILE:HD13	5:W:174:PHE:CE2	2.52	0.46
2:P:48:LEU:HD11	2:P:86:ASP:OD2	2.15	0.46
1:Y:56:GLU:OE1	1:Y:193:SER:N	2.47	0.46
2:Z:55:ARG:HH21	2:d:9:ASN:HD22	1.63	0.46
1:c:569:ILE:HG12	1:c:580:MET:CB	2.44	0.46
5:e:12:HIS:HB3	3:z:98:THR:HB	1.98	0.46
1:g:283:LYS:HE2	1:g:285:MET:HE1	1.97	0.46
1:g:493:PHE:O	1:g:497:MET:HG2	2.15	0.46
3:j:31:GLU:OE2	3:z:11:ARG:NH1	2.49	0.46
5:m:142:LEU:HD22	5:m:150:ILE:HD11	1.97	0.46
2:y:97:LEU:HA	2:y:100:PHE:HD1	1.80	0.46
1:3:78:GLN:HE22	1:3:98:ASN:HA	1.81	0.45
1:6:377:ASP:O	1:6:381:LYS:HG2	2.16	0.45
4:A:365:PHE:HB3	4:A:370:PHE:CE1	2.51	0.45
4:A:442:SER:N	4:A:554:ILE:O	2.28	0.45
4:C:391:THR:HA	4:C:396:PRO:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:43:ARG:NH2	4:F:350:ASN:OD1	2.49	0.45
4:E:225:PRO:HG2	4:E:248:TYR:CE2	2.51	0.45
4:E:251:GLU:HB3	4:E:254:ILE:HB	1.98	0.45
4:E:283:MET:HE1	4:E:316:VAL:CG1	2.46	0.45
5:L:107:GLN:OE1	5:m:194:GLN:HB2	2.17	0.45
1:Y:158:THR:HG22	1:Y:164:GLY:N	2.31	0.45
3:b:16:LEU:HD23	3:b:24:TRP:CZ3	2.50	0.45
1:g:197:GLU:HG3	1:g:199:ASP:H	1.81	0.45
1:g:361:ARG:HD3	1:k:72:ASP:OD1	2.16	0.45
1:k:38:ASP:HA	1:k:42:MET:HB2	1.98	0.45
1:0:354:ILE:HG12	1:0:494:ALA:HB3	1.98	0.45
1:0:506:ILE:O	1:0:510:VAL:HG22	2.16	0.45
1:6:158:THR:HG22	1:6:164:GLY:N	2.30	0.45
4:B:88:MET:HE1	4:B:231:LEU:HD13	1.97	0.45
4:C:347:MET:CE	4:C:352:TRP:HE3	2.28	0.45
4:F:288:PRO:HB2	4:F:304:VAL:HG11	1.99	0.45
4:F:377:GLU:HB3	4:F:381:ALA:HB3	1.99	0.45
4:F:454:GLY:HA2	3:j:23:ARG:HH11	1.81	0.45
5:H:147:ARG:HE	5:a:133:LEU:HG	1.81	0.45
5:J:19:PRO:HD3	5:J:166:TRP:HH2	1.82	0.45
5:K:174:PHE:CE2	5:m:160:ILE:HD13	2.51	0.45
5:L:4:LEU:HD11	5:L:138:LEU:HG	1.98	0.45
2:M:49:ILE:HG23	2:M:55:ARG:HG2	1.98	0.45
2:R:57:ILE:HG21	2:R:75:GLU:HG3	1.98	0.45
1:U:63:ASN:HD22	1:U:364:LEU:HD22	1.81	0.45
1:U:395:VAL:HG11	1:U:408:PHE:HE2	1.82	0.45
1:Y:271:ARG:HH21	1:Y:273:ARG:HH11	1.63	0.45
1:Y:393:ASN:HA	1:Y:433:ARG:HH22	1.80	0.45
3:b:160:GLU:OE1	3:w:144:ARG:NH2	2.41	0.45
1:c:247:ASP:CG	1:c:248:GLU:H	2.24	0.45
1:g:271:ARG:HH21	1:g:273:ARG:HH11	1.63	0.45
5:i:32:ILE:O	5:i:36:GLU:HG3	2.16	0.45
1:o:250:MET:SD	1:o:250:MET:N	2.88	0.45
1:x:247:ASP:CG	1:x:248:GLU:H	2.24	0.45
1:0:493:PHE:O	1:0:497:MET:HG2	2.16	0.45
1:3:132:GLU:HG2	1:3:136:LYS:HE3	1.98	0.45
1:6:122:PRO:HG3	1:6:128:ALA:HA	1.98	0.45
1:6:370:ARG:O	1:6:373:ARG:HB3	2.15	0.45
4:A:479:ILE:O	4:A:482:GLU:HG3	2.16	0.45
4:B:43:ARG:HB2	4:B:429:ASP:HA	1.98	0.45
4:C:22:PRO:HD2	4:C:25:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:236:ASN:HA	4:D:301:GLN:HG3	1.98	0.45
4:C:288:PRO:HB2	4:C:304:VAL:HG11	1.97	0.45
4:D:377:GLU:HG2	4:D:378:PRO:HD2	1.99	0.45
4:F:454:GLY:H	4:F:569:THR:HA	1.81	0.45
5:I:204:GLN:HG2	1:g:413:ALA:HB3	1.98	0.45
5:J:107:GLN:OE1	5:e:194:GLN:HB2	2.16	0.45
5:K:17:GLY:H	5:K:166:TRP:HE1	1.64	0.45
5:L:39:ARG:HB2	5:L:190:THR:HG21	1.99	0.45
2:P:100:PHE:O	2:P:104:ILE:HG12	2.16	0.45
1:Y:569:ILE:HG12	1:Y:580:MET:HB3	1.97	0.45
5:a:85:TRP:CE3	5:a:86:LEU:HD23	2.51	0.45
5:a:101:GLN:O	5:a:117:PRO:HG2	2.16	0.45
5:e:78:MET:HG2	5:e:105:VAL:CG2	2.38	0.45
5:e:101:GLN:O	5:e:117:PRO:HG2	2.16	0.45
3:f:170:LEU:HB3	3:f:189:HIS:CE1	2.51	0.45
1:g:285:MET:N	1:g:323:THR:O	2.47	0.45
1:g:354:ILE:HG12	1:g:494:ALA:HB3	1.98	0.45
2:h:92:LEU:CD1	2:h:95:GLY:H	2.29	0.45
1:k:489:ASP:OD1	1:o:112:LYS:HD3	2.16	0.45
1:r:167:GLU:OE1	1:r:208:ARG:NH2	2.49	0.45
1:r:401:ALA:HB1	1:r:427:ILE:CD1	2.45	0.45
3:z:34:THR:O	3:z:37:THR:OG1	2.30	0.45
1:0:411:GLU:HB3	1:0:417:ALA:HB1	1.99	0.45
4:A:324:ALA:HB2	4:A:333:MET:HG2	1.99	0.45
4:C:249:PHE:CE2	4:C:299:MET:HG3	2.51	0.45
4:C:278:THR:HG23	4:D:302:GLN:HG3	1.98	0.45
4:D:245:LYS:HE3	4:D:268:TYR:N	2.32	0.45
4:D:479:ILE:O	4:D:482:GLU:HG3	2.17	0.45
5:a:53:GLU:OE1	5:a:53:GLU:N	2.49	0.45
5:e:19:PRO:HG3	3:f:91:THR:HB	1.98	0.45
5:e:104:TYR:O	5:e:115:PHE:HA	2.16	0.45
2:h:57:ILE:HG22	2:h:77:SER:OG	2.17	0.45
3:j:67:ASP:HA	3:j:144:ARG:HH11	1.82	0.45
1:k:401:ALA:HB1	1:k:427:ILE:CD1	2.46	0.45
5:m:32:ILE:HG23	5:m:130:LYS:HD2	1.99	0.45
1:o:345:ARG:HE	1:o:538:ASP:HB2	1.82	0.45
3:q:5:ALA:O	3:q:9:LEU:HG	2.16	0.45
1:3:43:LYS:O	1:3:47:ARG:HG3	2.16	0.45
1:3:334:ARG:HG2	1:3:334:ARG:HH11	1.82	0.45
2:4:90:ALA:C	2:4:91:ARG:HD3	2.41	0.45
1:6:123:ARG:NH2	1:U:143:ASP:OD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:248:GLU:O	1:6:252:TRP:HB2	2.16	0.45
4:C:438:LEU:O	4:C:557:ASN:HA	2.17	0.45
4:D:288:PRO:HB2	4:D:304:VAL:HG11	1.97	0.45
4:D:291:VAL:HA	4:D:301:GLN:HA	1.99	0.45
4:E:324:ALA:HB2	4:E:333:MET:HG2	1.99	0.45
4:F:226:ASP:OD1	4:F:227:GLY:N	2.49	0.45
5:L:67:GLU:OE2	5:m:196:ARG:HG2	2.16	0.45
5:a:13:ARG:HB2	3:w:99:GLU:OE2	2.16	0.45
1:c:64:ARG:HD3	1:c:186:TRP:CZ3	2.49	0.45
3:j:48:TYR:CE2	3:j:143:TRP:HB3	2.52	0.45
1:o:64:ARG:HD3	1:o:186:TRP:HZ3	1.81	0.45
1:o:251:ASP:OD1	1:o:275:ARG:NH2	2.44	0.45
1:x:283:LYS:HE3	1:x:283:LYS:HB2	1.84	0.45
1:0:257:ARG:NH2	1:x:193:SER:O	2.49	0.45
1:3:158:THR:HG22	1:3:164:GLY:N	2.32	0.45
1:6:285:MET:HG3	1:6:325:ARG:HE	1.82	0.45
4:A:302:GLN:HG3	4:F:278:THR:HG23	1.98	0.45
4:B:26:SER:HB3	4:B:441:ARG:O	2.17	0.45
4:D:51:ILE:HG13	4:D:420:LEU:HD12	1.99	0.45
4:D:94:LYS:HA	4:D:104:LEU:H	1.82	0.45
4:F:479:ILE:O	4:F:482:GLU:HG3	2.17	0.45
4:F:539:ARG:HD2	4:F:540:MET:O	2.17	0.45
5:G:94:ARG:HD3	5:S:126:TYR:CE2	2.52	0.45
1:U:547:ILE:HD13	1:Y:556:THR:HB	1.98	0.45
3:X:51:THR:HG22	3:X:140:VAL:HG22	1.98	0.45
3:X:172:ARG:HD3	3:X:172:ARG:HA	1.77	0.45
1:Y:59:ARG:NH2	1:c:257:ARG:HE	2.14	0.45
2:Z:98:GLY:O	2:Z:101:ARG:HG2	2.17	0.45
5:e:64:ALA:N	5:e:130:LYS:O	2.46	0.45
1:g:411:GLU:HB3	1:g:417:ALA:HB1	1.98	0.45
1:g:484:THR:HG23	1:g:487:LEU:HD12	1.99	0.45
5:m:13:ARG:HB2	3:q:99:GLU:OE2	2.17	0.45
1:o:282:ARG:HB3	1:o:324:MET:SD	2.56	0.45
3:q:13:ALA:HB1	3:q:19:GLU:HA	1.98	0.45
1:r:218:CYS:SG	1:r:229:LYS:NZ	2.90	0.45
1:0:403:GLU:HB3	5:m:185:ARG:HH21	1.81	0.45
1:0:601:ARG:O	1:0:605:GLY:N	2.34	0.45
1:6:251:ASP:OD1	1:6:275:ARG:NH2	2.46	0.45
1:6:271:ARG:HH21	1:6:273:ARG:HH11	1.65	0.45
4:B:97:VAL:HB	4:B:102:TYR:HE2	1.82	0.45
4:B:283:MET:HE1	4:B:316:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:8:ALA:O	4:D:24:THR:OG1	2.30	0.45
5:G:113:LEU:HD23	5:G:113:LEU:H	1.80	0.45
5:L:28:ARG:O	5:L:32:ILE:HG13	2.17	0.45
1:Y:224:ARG:HD2	1:Y:337:LEU:HA	1.99	0.45
1:Y:370:ARG:O	1:Y:373:ARG:HB3	2.17	0.45
1:Y:377:ASP:O	1:Y:381:LYS:HG2	2.17	0.45
5:a:4:LEU:HD11	5:a:138:LEU:HG	1.98	0.45
3:b:170:LEU:HB3	3:b:189:HIS:ND1	2.32	0.45
1:g:80:THR:HG23	1:g:83:ASP:H	1.82	0.45
1:k:197:GLU:OE1	1:o:182:ARG:NH2	2.49	0.45
1:k:359:ARG:HG3	1:o:75:ASP:OD2	2.17	0.45
1:o:351:LEU:HD23	1:o:351:LEU:HA	1.81	0.45
1:0:125:LYS:HG3	1:3:558:ARG:HD3	1.98	0.45
1:0:345:ARG:HE	1:0:538:ASP:HB2	1.80	0.45
2:1:100:PHE:O	2:1:104:ILE:HG12	2.17	0.45
2:4:25:LEU:HD11	2:4:68:MET:HE3	1.97	0.45
2:4:57:ILE:HG12	2:4:92:LEU:HD22	1.99	0.45
3:5:9:LEU:CD1	3:5:151:GLN:HG3	2.47	0.45
4:B:293:GLY:HA3	4:B:299:MET:SD	2.56	0.45
4:C:312:ASN:ND2	4:C:360:ILE:O	2.50	0.45
5:G:5:ASP:O	5:G:9:PRO:HD3	2.17	0.45
5:L:3:PRO:O	5:L:6:VAL:HG22	2.17	0.45
5:L:42:ARG:HG2	5:L:128:LEU:HD23	1.98	0.45
2:O:43:TRP:CZ3	2:O:45:MET:HB3	2.52	0.45
2:V:71:THR:C	2:V:74:GLN:HE22	2.25	0.45
2:h:36:PRO:HG2	2:h:44:PHE:CD1	2.52	0.45
2:h:38:LEU:HD11	2:h:44:PHE:CE1	2.52	0.45
5:i:96:THR:HG22	5:i:98:GLN:H	1.81	0.45
1:k:99:VAL:HG22	1:k:376:GLN:OE1	2.16	0.45
1:o:70:ASP:HB3	1:o:369:ILE:HD12	1.99	0.45
2:p:48:LEU:N	2:p:56:GLU:O	2.42	0.45
1:r:56:GLU:OE2	1:r:193:SER:N	2.45	0.45
2:v:65:VAL:HG12	2:v:66:ASP:N	2.32	0.45
1:0:75:ASP:OD1	1:0:75:ASP:N	2.49	0.45
1:0:354:ILE:HG12	1:0:494:ALA:CB	2.46	0.45
1:0:398:ASP:HB3	1:0:425:LYS:HE2	1.98	0.45
1:0:445:ARG:O	1:0:449:MET:HG2	2.17	0.45
2:1:111:ALA:O	2:1:115:GLN:HG3	2.17	0.45
3:2:104:HIS:CE1	3:j:76:ARG:HD3	2.52	0.45
1:3:38:ASP:HA	1:3:42:MET:HB2	1.99	0.45
1:3:184:GLU:OE2	1:3:208:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:397:MET:HG3	1:3:398:ASP:O	2.17	0.45
1:3:430:ASN:OD1	1:3:433:ARG:NE	2.50	0.45
1:6:282:ARG:HB3	1:6:324:MET:SD	2.57	0.45
4:A:545:SER:OG	3:n:176:LYS:HD3	2.17	0.45
4:A:550:ARG:NH1	4:F:459:GLU:OE2	2.37	0.45
4:C:332:VAL:CG2	4:C:339:MET:HE3	2.45	0.45
2:R:59:LYS:HB3	2:R:71:THR:OG1	2.17	0.45
1:U:38:ASP:HA	1:U:42:MET:HB2	1.99	0.45
5:W:24:PHE:O	5:W:28:ARG:HG3	2.17	0.45
1:Y:165:TRP:HB3	1:Y:351:LEU:HD22	1.98	0.45
5:a:7:PHE:CD1	5:a:147:ARG:HG3	2.52	0.45
1:g:158:THR:HG22	1:g:164:GLY:N	2.31	0.45
5:i:19:PRO:HG3	3:j:91:THR:HB	1.98	0.45
3:n:61:LYS:HA	3:n:126:TYR:HD2	1.82	0.45
3:n:160:GLU:OE1	3:q:144:ARG:NH2	2.42	0.45
1:0:385:LYS:O	1:0:389:ILE:HG13	2.16	0.45
1:0:496:GLN:O	1:0:500:GLU:OE1	2.35	0.45
2:1:101:ARG:NE	2:4:4:VAL:O	2.49	0.45
1:6:127:ASP:C	1:6:130:PRO:HD2	2.42	0.45
2:7:65:VAL:HG12	2:7:66:ASP:N	2.32	0.45
4:A:32:VAL:HG23	4:A:438:LEU:HD11	1.98	0.45
4:C:283:MET:HE1	4:C:316:VAL:CG1	2.46	0.45
4:E:6:LEU:HD23	4:E:440:TRP:HZ3	1.82	0.45
4:E:575:ARG:O	4:F:449:MET:HB3	2.16	0.45
5:H:113:LEU:HD23	5:H:113:LEU:H	1.81	0.45
5:K:8:MET:HG3	5:K:12:HIS:CD2	2.48	0.45
5:L:12:HIS:HB3	3:X:98:THR:HB	1.99	0.45
5:L:50:GLY:HA2	5:L:119:GLU:O	2.17	0.45
5:S:78:MET:HG2	5:S:105:VAL:CG2	2.43	0.45
2:V:101:ARG:NE	2:Z:4:VAL:O	2.50	0.45
2:Z:56:GLU:OE2	2:Z:72:ARG:NE	2.34	0.45
5:a:104:TYR:CD1	5:a:116:VAL:HG11	2.51	0.45
3:b:209:ALA:HB3	3:b:212:ALA:HB2	1.99	0.45
5:i:4:LEU:HD11	5:i:138:LEU:HG	1.98	0.45
1:o:394:LYS:NZ	1:r:412:VAL:O	2.45	0.45
1:r:438:ALA:O	1:r:442:MET:HG2	2.16	0.45
1:x:394:LYS:HD2	1:x:431:VAL:HB	1.99	0.45
1:6:60:GLN:O	1:6:64:ARG:HG3	2.18	0.44
4:B:322:SER:HB3	4:B:333:MET:HB2	1.98	0.44
4:D:32:VAL:HG23	4:D:438:LEU:HD11	1.98	0.44
4:D:80:VAL:HG11	4:D:84:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:347:MET:CE	4:F:352:TRP:HE3	2.30	0.44
5:I:5:ASP:O	5:I:9:PRO:HD3	2.17	0.44
5:K:78:MET:HE2	5:K:78:MET:HB2	1.62	0.44
5:L:70:LEU:HD12	5:L:71:VAL:H	1.82	0.44
2:M:59:LYS:HB3	2:M:71:THR:OG1	2.17	0.44
3:T:166:VAL:O	3:T:170:LEU:HG	2.17	0.44
1:c:250:MET:SD	1:c:250:MET:N	2.89	0.44
5:e:37:ARG:HB3	5:e:183:LEU:HD11	1.99	0.44
1:g:445:ARG:O	1:g:449:MET:HG2	2.16	0.44
1:o:278:GLU:CD	1:o:280:TRP:HE1	2.25	0.44
1:u:430:ASN:OD1	1:u:433:ARG:HG3	2.17	0.44
1:0:158:THR:HG22	1:0:164:GLY:N	2.31	0.44
3:2:9:LEU:HD22	3:2:29:LEU:HB3	1.98	0.44
3:2:15:LEU:HD21	3:n:32:TRP:HH2	1.82	0.44
4:A:245:LYS:HE3	4:A:268:TYR:N	2.31	0.44
4:A:542:ARG:HB2	3:n:22:GLU:OE2	2.18	0.44
4:B:414:THR:HA	4:C:328:HIS:ND1	2.31	0.44
4:C:479:ILE:O	4:C:482:GLU:HG3	2.16	0.44
4:D:291:VAL:HG22	4:D:301:GLN:HB3	1.99	0.44
4:E:28:ARG:HH12	4:E:441:ARG:NH1	2.14	0.44
4:E:327:SER:O	4:E:352:TRP:NE1	2.49	0.44
4:F:438:LEU:O	4:F:557:ASN:HA	2.17	0.44
4:F:452:ASN:HB3	3:z:17:GLN:OE1	2.15	0.44
5:I:39:ARG:HB2	5:I:190:THR:HG21	1.99	0.44
5:L:6:VAL:O	5:L:9:PRO:HD2	2.17	0.44
2:Q:65:VAL:HG12	2:Q:66:ASP:N	2.33	0.44
2:R:59:LYS:HB2	2:R:74:GLN:CD	2.42	0.44
5:S:101:GLN:O	5:S:117:PRO:HG2	2.17	0.44
3:T:132:ALA:O	3:T:135:VAL:HG13	2.17	0.44
1:U:75:ASP:O	1:U:77:ILE:HD12	2.17	0.44
2:V:18:LEU:HD23	2:V:82:PHE:CE2	2.52	0.44
1:Y:40:GLU:HG2	1:Y:41:GLU:N	2.31	0.44
5:e:4:LEU:HD11	5:e:138:LEU:HG	1.99	0.44
1:g:57:LEU:HD22	1:g:247:ASP:HB2	1.99	0.44
2:h:100:PHE:O	2:h:104:ILE:HG12	2.17	0.44
5:i:136:ASP:OD2	5:i:136:ASP:N	2.50	0.44
1:k:75:ASP:O	1:k:77:ILE:HD12	2.18	0.44
5:m:7:PHE:CD1	5:m:147:ARG:HG3	2.52	0.44
1:o:483:ALA:HA	1:r:105:ASN:HB3	1.98	0.44
1:r:247:ASP:OD1	1:r:248:GLU:N	2.50	0.44
2:v:92:LEU:HG	2:y:8:ASN:ND2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:568:MET:HE2	1:6:596:ILE:HD12	1.99	0.44
1:6:111:GLU:HG2	1:6:155:PHE:HD2	1.81	0.44
4:B:32:VAL:HG23	4:B:438:LEU:HD11	1.98	0.44
4:D:365:PHE:HB3	4:D:370:PHE:CE1	2.52	0.44
4:E:43:ARG:HB2	4:E:429:ASP:HA	1.97	0.44
5:H:5:ASP:O	5:H:9:PRO:HD3	2.17	0.44
5:I:20:GLU:HG3	3:w:114:HIS:CD2	2.52	0.44
5:I:147:ARG:HH21	5:e:133:LEU:HB2	1.82	0.44
5:J:126:TYR:CZ	5:i:94:ARG:HD2	2.52	0.44
5:K:191:ILE:HD11	1:u:406:GLU:OE1	2.18	0.44
2:P:6:PHE:CD2	2:R:97:LEU:HB3	2.53	0.44
1:Y:279:CYS:O	1:Y:329:ALA:N	2.50	0.44
5:e:76:ARG:HH22	5:e:103:GLN:HG2	1.83	0.44
3:n:67:ASP:HA	3:n:144:ARG:HH11	1.82	0.44
2:p:59:LYS:HB3	2:p:71:THR:OG1	2.17	0.44
3:t:145:HIS:CE1	3:t:155:VAL:HG13	2.53	0.44
1:x:569:ILE:HG12	1:x:580:MET:HB3	1.99	0.44
1:0:161:VAL:HG21	1:0:186:TRP:CG	2.52	0.44
2:1:18:LEU:HD23	2:1:82:PHE:CE2	2.52	0.44
3:5:121:VAL:HG22	3:X:49:MET:HG2	1.97	0.44
1:6:654:ALA:HB2	1:U:649:LYS:HA	2.00	0.44
4:B:230:GLY:O	4:B:241:ALA:HA	2.18	0.44
4:D:249:PHE:CE2	4:D:299:MET:HG3	2.52	0.44
4:E:383:PHE:CE1	2:Q:20:PRO:HG2	2.53	0.44
4:F:291:VAL:HA	4:F:301:GLN:HA	2.00	0.44
5:J:42:ARG:HG2	5:J:128:LEU:HD23	1.99	0.44
5:J:45:ASP:OD2	5:J:45:ASP:N	2.46	0.44
5:J:204:GLN:OE1	5:J:204:GLN:HA	2.18	0.44
5:K:34:PHE:CZ	5:K:38:THR:HG21	2.52	0.44
5:S:23:ALA:HA	5:S:158:LEU:HD11	1.99	0.44
2:V:90:ALA:C	2:V:91:ARG:HD3	2.42	0.44
5:W:67:GLU:HB3	5:W:128:LEU:HD12	1.99	0.44
1:Y:568:MET:HG3	1:c:590:LEU:HD11	1.98	0.44
1:Y:579:VAL:O	1:Y:582:ASP:OD1	2.36	0.44
1:Y:582:ASP:HB3	1:Y:600:ILE:HG22	1.99	0.44
1:c:85:GLN:O	1:c:89:GLU:HG2	2.18	0.44
3:f:33:LEU:HD12	3:f:165:LEU:HD12	1.99	0.44
3:j:4:PRO:O	3:j:7:VAL:HG22	2.17	0.44
5:m:156:SER:O	5:m:160:ILE:HG13	2.17	0.44
1:o:139:LYS:HE2	1:o:555:ALA:O	2.18	0.44
1:r:449:MET:HG3	1:u:97:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:370:ARG:O	1:u:373:ARG:HB3	2.16	0.44
1:u:654:ALA:HB2	1:x:649:LYS:HA	1.99	0.44
1:0:654:ALA:HB2	1:3:649:LYS:HA	2.00	0.44
4:A:328:HIS:ND1	4:F:414:THR:HA	2.33	0.44
4:D:226:ASP:OD1	4:D:227:GLY:N	2.50	0.44
4:D:414:THR:HG22	4:E:328:HIS:HE1	1.82	0.44
4:F:22:PRO:HD2	4:F:25:ALA:HB3	1.99	0.44
5:H:34:PHE:CZ	5:H:38:THR:HG21	2.53	0.44
5:I:142:LEU:HD22	5:I:150:ILE:HD11	2.00	0.44
5:K:39:ARG:NH2	5:i:185:ARG:HH22	2.16	0.44
5:K:73:PHE:HD1	5:K:123:VAL:HG22	1.82	0.44
2:M:45:MET:HE3	2:M:57:ILE:HG13	1.99	0.44
2:N:68:MET:N	2:N:68:MET:SD	2.91	0.44
1:U:230:LYS:HE2	1:U:334:ARG:HD2	1.98	0.44
1:Y:165:TRP:CE3	1:Y:351:LEU:HB3	2.52	0.44
1:Y:354:ILE:HG12	1:Y:494:ALA:HB3	1.98	0.44
1:Y:654:ALA:HB2	1:c:649:LYS:HA	1.99	0.44
3:f:4:PRO:O	3:f:7:VAL:HG22	2.18	0.44
1:g:654:ALA:HB2	1:k:649:LYS:HA	1.99	0.44
1:k:388:TYR:OH	1:o:416:ASP:OD2	2.29	0.44
1:k:395:VAL:HG11	1:k:408:PHE:HE2	1.82	0.44
3:t:15:LEU:HB3	3:t:170:LEU:HD21	2.00	0.44
2:v:51:SER:O	2:v:52:ASP:HB2	2.17	0.44
1:0:247:ASP:OD1	1:0:248:GLU:HG2	2.17	0.44
4:A:12:GLU:CD	4:A:28:ARG:H	2.25	0.44
4:A:414:THR:HA	4:B:328:HIS:ND1	2.32	0.44
4:D:472:TYR:OH	4:D:476:ARG:NH2	2.51	0.44
4:E:347:MET:HE1	4:E:352:TRP:HE3	1.83	0.44
4:F:12:GLU:HG2	4:F:14:PRO:HD3	2.00	0.44
5:I:126:TYR:CE2	5:e:94:ARG:HD3	2.52	0.44
5:J:4:LEU:HD11	5:J:138:LEU:HG	1.98	0.44
2:P:28:THR:OG1	2:P:31:ASP:OD1	2.32	0.44
3:T:76:ARG:HD3	3:t:104:HIS:CE1	2.52	0.44
1:U:247:ASP:OD1	1:U:248:GLU:N	2.48	0.44
1:U:346:HIS:HB2	1:U:539:ILE:HD11	1.99	0.44
5:W:151:ALA:O	5:W:155:LEU:HG	2.17	0.44
3:X:4:PRO:O	3:X:7:VAL:HG22	2.17	0.44
3:X:160:GLU:OE1	3:X:160:GLU:N	2.51	0.44
1:Y:38:ASP:HA	1:Y:42:MET:HB2	1.99	0.44
1:Y:80:THR:HG23	1:Y:83:ASP:H	1.82	0.44
1:c:166:ILE:HG21	1:c:498:GLN:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:164:LYS:HZ3	3:f:95:LEU:HD11	1.83	0.44
3:f:57:VAL:HG12	3:f:62:GLN:OE1	2.18	0.44
1:g:279:CYS:O	1:g:329:ALA:N	2.49	0.44
1:k:285:MET:N	1:k:323:THR:O	2.48	0.44
5:m:76:ARG:HH12	5:m:101:GLN:HB2	1.81	0.44
5:m:85:TRP:HE3	5:m:86:LEU:HD23	1.83	0.44
3:t:3:PHE:CD2	3:t:159:ALA:HA	2.53	0.44
3:2:17:GLN:OE1	4:A:452:ASN:HB3	2.16	0.44
1:6:161:VAL:HG21	1:6:186:TRP:CD1	2.52	0.44
4:A:486:ASN:ND2	4:A:511:MET:SD	2.91	0.44
4:B:279:THR:HG22	4:B:292:SER:HA	1.99	0.44
4:B:462:THR:HG23	4:B:537:MET:HE1	1.99	0.44
4:C:15:ARG:HB2	4:C:347:MET:CA	2.48	0.44
4:C:568:ALA:HB1	4:C:573:GLU:HB2	2.00	0.44
4:E:318:ASP:OD2	4:F:303:ARG:NH2	2.51	0.44
5:G:105:VAL:HG22	5:G:115:PHE:CD1	2.52	0.44
5:G:164:LYS:HD2	5:G:166:TRP:CE3	2.53	0.44
5:I:94:ARG:HD3	5:a:126:TYR:CE2	2.52	0.44
5:I:104:TYR:HB2	5:I:116:VAL:HG12	2.00	0.44
5:J:113:LEU:HD23	5:J:113:LEU:H	1.82	0.44
2:N:96:GLU:OE1	2:N:96:GLU:N	2.45	0.44
2:Q:63:ARG:HG3	2:Q:68:MET:CG	2.45	0.44
3:T:209:ALA:HB3	3:T:212:ALA:HB2	2.00	0.44
1:Y:401:ALA:HB1	1:Y:427:ILE:HG12	2.00	0.44
1:Y:537:ASN:OD1	1:c:176:GLY:N	2.43	0.44
1:k:100:ILE:HG12	1:k:372:MET:HB3	1.98	0.44
1:k:450:LEU:HD23	1:k:450:LEU:HA	1.89	0.44
1:o:165:TRP:CE3	1:o:351:LEU:HB3	2.52	0.44
2:v:63:ARG:HH12	2:v:65:VAL:C	2.23	0.44
1:x:585:ALA:HA	1:x:588:THR:HG22	2.00	0.44
1:0:43:LYS:HD2	1:0:43:LYS:HA	1.75	0.44
1:3:71:GLU:OE1	1:3:186:TRP:NE1	2.48	0.44
1:3:127:ASP:C	1:3:130:PRO:HD2	2.42	0.44
1:3:385:LYS:O	1:3:389:ILE:HG13	2.17	0.44
1:6:537:ASN:OD1	1:U:176:GLY:N	2.46	0.44
4:A:51:ILE:HG13	4:A:420:LEU:HD12	2.00	0.44
4:A:489:LEU:HD12	4:A:511:MET:HE1	2.00	0.44
4:E:54:ASP:OD1	4:E:55:ASN:N	2.50	0.44
4:F:224:PRO:HG3	4:F:258:TRP:CD1	2.53	0.44
5:G:68:MET:HE1	5:G:113:LEU:HB3	1.99	0.44
5:K:147:ARG:HE	5:m:133:LEU:HG	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:580:MET:HE3	1:Y:600:ILE:HD11	2.00	0.44
2:V:92:LEU:HD23	2:V:92:LEU:H	1.82	0.44
1:c:127:ASP:OD1	1:c:127:ASP:N	2.48	0.44
5:e:78:MET:HE2	5:e:78:MET:HB2	1.86	0.44
1:g:69:VAL:HA	1:g:72:ASP:OD2	2.18	0.44
1:g:327:ARG:HH12	1:g:339:GLU:HG3	1.82	0.44
1:g:496:GLN:O	1:g:500:GLU:HG3	2.18	0.44
2:h:20:PRO:HG3	2:h:81:SER:HB2	1.99	0.44
3:j:116:THR:OG1	3:j:126:TYR:HB2	2.18	0.44
1:k:593:ARG:O	1:k:597:VAL:HG23	2.18	0.44
2:l:83:ASN:OD1	2:l:84:PRO:HD2	2.18	0.44
5:m:65:LEU:HD21	5:m:68:MET:HG2	2.00	0.44
3:n:33:LEU:HD12	3:n:165:LEU:HD12	1.99	0.44
1:o:271:ARG:HH21	1:o:273:ARG:HH11	1.65	0.44
2:s:101:ARG:HD2	2:v:6:PHE:HE2	1.82	0.44
1:u:127:ASP:C	1:u:130:PRO:HD2	2.43	0.44
1:u:224:ARG:HD2	1:u:337:LEU:HA	2.00	0.44
3:w:5:ALA:O	3:w:9:LEU:HG	2.17	0.44
2:1:18:LEU:HB3	2:1:82:PHE:HD2	1.82	0.44
1:6:245:ASP:HB3	1:6:246:GLY:H	1.61	0.44
1:6:582:ASP:HB3	1:6:604:ASN:HD22	1.83	0.44
4:A:548:LEU:HD12	4:A:548:LEU:HA	1.87	0.44
4:B:536:LYS:HD2	4:B:539:ARG:NE	2.32	0.44
4:C:226:ASP:OD1	4:C:227:GLY:N	2.50	0.44
4:D:97:VAL:HB	4:D:102:TYR:HE2	1.83	0.44
4:D:324:ALA:HB2	4:D:333:MET:HG3	2.00	0.44
4:E:564:ASP:OD2	4:F:19:ARG:NH2	2.51	0.44
4:F:94:LYS:HA	4:F:104:LEU:H	1.82	0.44
4:F:283:MET:HE1	4:F:316:VAL:CG1	2.47	0.44
5:I:89:GLN:HE22	1:c:89:GLU:HA	1.82	0.44
5:K:126:TYR:CE1	5:m:94:ARG:HD3	2.53	0.44
5:L:39:ARG:NH1	5:L:67:GLU:OE1	2.51	0.44
2:N:94:ALA:HB2	2:O:8:ASN:ND2	2.33	0.44
2:P:38:LEU:HD21	2:P:44:PHE:HD1	1.83	0.44
1:U:193:SER:O	1:Y:257:ARG:NH2	2.51	0.44
3:X:32:TRP:CE3	3:X:32:TRP:HA	2.52	0.44
1:Y:601:ARG:O	1:Y:605:GLY:N	2.32	0.44
5:a:24:PHE:O	5:a:28:ARG:HG3	2.17	0.44
3:b:77:ASN:HA	3:b:137:VAL:HG13	1.99	0.44
3:b:132:ALA:O	3:b:135:VAL:HG13	2.18	0.44
2:d:65:VAL:HG12	2:d:66:ASP:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:132:GLU:HG2	1:k:136:LYS:HE3	2.00	0.44
5:m:24:PHE:O	5:m:28:ARG:HG3	2.18	0.44
1:r:592:ASN:O	1:r:596:ILE:HD12	2.18	0.44
1:u:80:THR:HG23	1:u:83:ASP:H	1.83	0.44
1:u:497:MET:HE1	1:x:146:ARG:NE	2.32	0.44
2:v:63:ARG:NH1	2:v:63:ARG:HG2	2.33	0.44
1:0:171:ASP:HB2	1:0:180:TYR:CE1	2.53	0.43
1:3:393:ASN:HB2	1:3:412:VAL:HG12	2.00	0.43
1:6:594:ASP:OD2	1:6:594:ASP:N	2.48	0.43
4:A:249:PHE:CE2	4:A:299:MET:HG3	2.53	0.43
4:B:6:LEU:HD23	4:B:440:TRP:HZ3	1.82	0.43
4:F:445:PHE:N	4:F:552:TRP:O	2.42	0.43
4:F:509:ASP:OD1	4:F:509:ASP:N	2.51	0.43
5:J:67:GLU:O	5:J:128:LEU:N	2.51	0.43
2:Q:58:VAL:HG11	2:Q:72:ARG:HG2	1.99	0.43
2:Q:60:VAL:HG13	2:Q:68:MET:HB3	2.00	0.43
2:V:80:LEU:HB2	2:V:82:PHE:HE1	1.83	0.43
5:W:4:LEU:HD11	5:W:138:LEU:HG	2.00	0.43
3:X:49:MET:HE2	3:X:140:VAL:HG12	1.99	0.43
1:c:585:ALA:HA	1:c:588:THR:HG22	2.00	0.43
3:f:15:LEU:HD21	3:z:32:TRP:CH2	2.52	0.43
3:f:49:MET:HG2	3:z:121:VAL:HG22	1.98	0.43
3:n:70:GLN:O	3:n:142:ALA:N	2.32	0.43
3:n:148:LEU:HD11	3:n:155:VAL:HG22	2.00	0.43
2:p:58:VAL:HG12	2:p:72:ARG:HD3	1.99	0.43
2:s:28:THR:OG1	2:s:31:ASP:OD1	2.33	0.43
3:t:49:MET:HE3	3:t:72:ILE:HG13	2.00	0.43
1:u:158:THR:HG22	1:u:164:GLY:N	2.33	0.43
1:0:401:ALA:HB1	1:0:427:ILE:HG12	1.99	0.43
1:0:601:ARG:NH1	1:0:608:ASP:H	2.16	0.43
3:2:145:HIS:CE1	3:2:155:VAL:HA	2.53	0.43
3:2:171:TYR:CD1	3:2:190:TYR:HB2	2.53	0.43
4:B:12:GLU:CD	4:B:28:ARG:H	2.26	0.43
4:B:225:PRO:HG2	4:B:248:TYR:CE2	2.51	0.43
4:B:525:TYR:HB2	4:B:553:GLU:HG3	2.00	0.43
4:C:233:SER:C	4:C:234:LEU:HD22	2.42	0.43
4:D:54:ASP:O	4:D:70:GLN:NE2	2.51	0.43
4:D:543:LEU:O	3:b:23:ARG:HG2	2.18	0.43
4:D:545:SER:OG	3:b:176:LYS:HD3	2.18	0.43
4:F:28:ARG:NH2	4:F:441:ARG:HD2	2.28	0.43
5:H:42:ARG:HG2	5:H:128:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:42:ARG:HG2	5:I:128:LEU:HD23	2.00	0.43
5:K:104:TYR:HD2	5:K:116:VAL:HG11	1.83	0.43
1:U:449:MET:HG3	1:Y:97:PHE:CE2	2.53	0.43
5:W:31:ALA:HB1	5:W:142:LEU:HD13	2.01	0.43
5:W:109:SER:OG	5:W:110:GLU:N	2.51	0.43
1:Y:122:PRO:HG3	1:Y:128:ALA:HA	2.00	0.43
2:Z:101:ARG:NH1	2:d:5:GLN:HA	2.33	0.43
1:g:122:PRO:HG3	1:g:128:ALA:HA	1.99	0.43
3:j:16:LEU:H	3:j:16:LEU:HD12	1.83	0.43
3:j:32:TRP:HA	3:j:32:TRP:CE3	2.53	0.43
1:k:158:THR:HG22	1:k:164:GLY:N	2.33	0.43
1:k:245:ASP:HB3	1:k:246:GLY:H	1.60	0.43
3:n:15:LEU:HG	3:n:170:LEU:HD21	2.00	0.43
3:n:132:ALA:O	3:n:135:VAL:HG13	2.18	0.43
3:n:209:ALA:HB3	3:n:212:ALA:HB2	2.00	0.43
1:o:127:ASP:C	1:o:130:PRO:HD2	2.43	0.43
1:o:158:THR:HG22	1:o:164:GLY:N	2.32	0.43
2:p:71:THR:OG1	2:p:74:GLN:NE2	2.51	0.43
1:r:193:SER:O	1:u:257:ARG:NH2	2.51	0.43
1:r:361:ARG:HD3	1:u:72:ASP:OD2	2.18	0.43
1:u:73:TYR:HD1	1:u:77:ILE:O	2.00	0.43
1:x:122:PRO:HG2	1:x:125:LYS:HG2	2.00	0.43
1:x:166:ILE:HG21	1:x:498:GLN:CD	2.44	0.43
3:z:9:LEU:CD1	3:z:151:GLN:HG3	2.48	0.43
2:1:71:THR:OG1	2:1:74:GLN:NE2	2.50	0.43
1:3:261:SER:HB3	1:3:264:ARG:HG2	2.00	0.43
1:3:568:MET:HE1	1:3:580:MET:HB3	2.00	0.43
3:5:172:ARG:HA	3:5:172:ARG:HD2	1.89	0.43
1:6:445:ARG:O	1:6:449:MET:HG2	2.19	0.43
4:A:291:VAL:HA	4:A:301:GLN:HA	1.99	0.43
4:B:28:ARG:HH12	4:B:441:ARG:NH1	2.16	0.43
4:D:507:ASN:OD1	2:M:87:ARG:HD2	2.18	0.43
4:E:12:GLU:CD	4:E:28:ARG:H	2.26	0.43
4:F:545:SER:OG	3:j:176:LYS:HD2	2.18	0.43
5:G:194:GLN:CD	5:W:107:GLN:HE22	2.26	0.43
5:I:50:GLY:HA2	5:I:119:GLU:O	2.19	0.43
5:J:65:LEU:HD21	5:J:68:MET:HG2	2.01	0.43
2:O:59:LYS:O	2:O:70:ILE:HD12	2.18	0.43
2:P:18:LEU:HG	2:P:72:ARG:HH21	1.83	0.43
2:P:57:ILE:HG22	2:P:77:SER:OG	2.18	0.43
5:S:136:ASP:N	5:S:136:ASP:OD1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:7:PHE:CD1	5:W:147:ARG:HG3	2.54	0.43
5:W:32:ILE:O	5:W:36:GLU:HG3	2.18	0.43
3:X:57:VAL:HG12	3:X:62:GLN:OE1	2.18	0.43
1:c:278:GLU:HG2	1:c:330:ILE:HG12	1.99	0.43
3:f:166:VAL:O	3:f:170:LEU:HG	2.18	0.43
1:g:579:VAL:HG23	1:g:580:MET:HE2	1.99	0.43
5:i:31:ALA:HB1	5:i:142:LEU:HD13	2.00	0.43
3:j:39:GLU:OE2	3:j:43:ARG:NH2	2.51	0.43
1:k:247:ASP:OD1	1:k:248:GLU:N	2.48	0.43
1:k:583:LEU:HD21	1:o:599:ARG:HH22	1.83	0.43
2:s:48:LEU:HD11	2:s:86:ASP:OD2	2.17	0.43
1:u:161:VAL:HG21	1:u:186:TRP:CG	2.53	0.43
1:x:165:TRP:CE3	1:x:351:LEU:HB3	2.54	0.43
2:4:63:ARG:NH1	2:4:65:VAL:O	2.51	0.43
4:C:224:PRO:HG3	4:C:258:TRP:CD1	2.54	0.43
4:E:352:TRP:NE1	4:E:357:PRO:HB3	2.34	0.43
4:F:542:ARG:HB3	3:j:23:ARG:CG	2.43	0.43
5:I:8:MET:HG3	5:I:12:HIS:CD2	2.54	0.43
5:I:12:HIS:HB3	3:f:98:THR:HB	2.00	0.43
5:J:109:SER:HB3	5:J:112:THR:OG1	2.18	0.43
5:L:20:GLU:HB2	3:q:128:TYR:HE1	1.83	0.43
2:N:20:PRO:HA	2:N:72:ARG:NH2	2.34	0.43
5:W:7:PHE:CZ	5:W:143:ALA:HA	2.54	0.43
1:Y:59:ARG:NH1	1:Y:193:SER:HB3	2.32	0.43
5:a:32:ILE:O	5:a:36:GLU:HG3	2.17	0.43
3:b:37:THR:N	3:b:165:LEU:HD11	2.33	0.43
1:k:377:ASP:OD1	1:k:378:ASP:N	2.52	0.43
3:n:37:THR:N	3:n:165:LEU:HD11	2.33	0.43
1:o:161:VAL:HG21	1:o:186:TRP:CG	2.54	0.43
1:o:344:PHE:HA	1:o:508:GLN:HE22	1.83	0.43
1:o:558:ARG:HH22	1:o:593:ARG:HD2	1.83	0.43
2:p:7:ALA:HB3	2:p:91:ARG:CZ	2.48	0.43
1:x:251:ASP:OD1	1:x:275:ARG:NH2	2.27	0.43
1:0:58:ASP:OD1	1:0:59:ARG:N	2.52	0.43
1:0:67:MET:HB3	1:0:161:VAL:HB	2.01	0.43
1:6:278:GLU:CD	1:6:280:TRP:HE1	2.27	0.43
1:6:572:MET:HE3	1:6:573:PRO:HD2	2.01	0.43
2:7:57:ILE:HG23	2:7:92:LEU:HD13	1.99	0.43
4:B:570:THR:HG22	4:B:572:GLN:H	1.84	0.43
4:E:536:LYS:HD2	4:E:539:ARG:NE	2.34	0.43
5:I:3:PRO:O	5:I:6:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:113:LEU:HD23	5:K:113:LEU:H	1.82	0.43
2:Q:50:ARG:HG3	2:Q:51:SER:O	2.18	0.43
2:V:45:MET:HE1	2:V:59:LYS:HB2	2.00	0.43
5:W:13:ARG:HB2	3:t:99:GLU:OE1	2.18	0.43
2:Z:58:VAL:CG2	2:Z:70:ILE:HD11	2.49	0.43
5:a:104:TYR:HD1	5:a:116:VAL:HG11	1.81	0.43
5:a:153:GLY:O	5:a:157:GLU:HG2	2.18	0.43
3:f:160:GLU:OE1	3:f:160:GLU:N	2.51	0.43
1:o:165:TRP:CE2	1:o:189:VAL:HG11	2.53	0.43
1:o:558:ARG:NE	1:o:587:SER:O	2.52	0.43
1:u:327:ARG:HH12	1:u:339:GLU:HG3	1.84	0.43
1:x:127:ASP:OD1	1:x:127:ASP:N	2.44	0.43
1:x:230:LYS:HE2	1:x:334:ARG:HD2	2.00	0.43
2:4:20:PRO:HA	2:4:72:ARG:NH2	2.30	0.43
3:5:144:ARG:NE	3:X:159:ALA:HB3	2.34	0.43
1:6:56:GLU:OE2	1:6:59:ARG:NH2	2.52	0.43
1:6:111:GLU:HG2	1:6:155:PHE:CD2	2.53	0.43
4:A:365:PHE:HZ	4:B:349:ARG:HE	1.66	0.43
4:A:575:ARG:HA	3:q:179:GLU:HG2	2.01	0.43
4:B:288:PRO:HB2	4:B:304:VAL:HG11	2.01	0.43
4:C:12:GLU:HG2	4:C:14:PRO:HD3	1.99	0.43
4:C:291:VAL:HA	4:C:301:GLN:HA	2.01	0.43
4:D:509:ASP:N	4:D:509:ASP:OD1	2.51	0.43
4:E:26:SER:HB3	4:E:441:ARG:O	2.18	0.43
4:F:224:PRO:HG3	4:F:258:TRP:HD1	1.83	0.43
4:F:260:GLU:O	4:F:263:ILE:HG12	2.19	0.43
5:I:28:ARG:O	5:I:32:ILE:HG13	2.18	0.43
2:M:57:ILE:HG12	2:M:92:LEU:HD23	2.00	0.43
2:N:63:ARG:HB3	2:N:68:MET:HG3	2.01	0.43
3:T:114:HIS:HE1	5:W:12:HIS:HE1	1.66	0.43
5:W:46:GLU:OE2	5:W:122:SER:OG	2.24	0.43
3:X:67:ASP:HA	3:X:144:ARG:NH1	2.29	0.43
1:Y:283:LYS:HG3	1:Y:285:MET:HE2	2.00	0.43
2:Z:5:GLN:OE1	2:Z:6:PHE:N	2.51	0.43
1:c:139:LYS:HE2	1:c:555:ALA:O	2.18	0.43
1:c:230:LYS:HE2	1:c:334:ARG:HD2	2.01	0.43
1:c:497:MET:SD	1:g:146:ARG:NH2	2.87	0.43
1:g:127:ASP:C	1:g:130:PRO:HD2	2.44	0.43
2:h:18:LEU:HD22	2:h:25:LEU:HD21	2.01	0.43
2:l:57:ILE:HG23	2:l:75:GLU:HB2	1.99	0.43
5:m:102:ALA:HA	5:m:117:PRO:CD	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:n:159:ALA:HB1	3:q:38:ARG:NH1	2.33	0.43
1:o:147:LEU:N	1:o:148:PRO:HD2	2.34	0.43
1:0:558:ARG:HH11	1:x:125:LYS:NZ	2.16	0.43
2:1:23:THR:C	2:1:70:ILE:HG22	2.44	0.43
1:6:134:LYS:O	1:6:138:LEU:HD23	2.18	0.43
5:H:28:ARG:O	5:H:32:ILE:HG13	2.18	0.43
5:H:107:GLN:OE1	5:W:194:GLN:HB2	2.18	0.43
5:I:20:GLU:N	5:I:21:PRO:HD2	2.34	0.43
5:K:2:LYS:HB3	5:K:137:SER:HB2	2.00	0.43
5:K:28:ARG:O	5:K:32:ILE:HG13	2.18	0.43
5:K:104:TYR:CD2	5:K:116:VAL:HG11	2.54	0.43
2:Q:13:ARG:HA	2:Q:86:ASP:O	2.19	0.43
5:S:164:LYS:HZ3	3:X:95:LEU:HD11	1.83	0.43
3:X:55:ALA:HA	3:X:136:GLN:HA	2.01	0.43
1:Y:493:PHE:HE2	1:c:146:ARG:HD3	1.82	0.43
1:c:283:LYS:HE3	1:c:283:LYS:HB2	1.84	0.43
3:f:159:ALA:HB1	3:z:38:ARG:NH1	2.33	0.43
5:m:16:PRO:O	5:m:166:TRP:NE1	2.51	0.43
5:m:153:GLY:O	5:m:157:GLU:HG2	2.19	0.43
1:o:357:PHE:HE2	1:o:368:VAL:HG22	1.83	0.43
1:r:245:ASP:HB3	1:r:246:GLY:H	1.58	0.43
1:r:344:PHE:HB3	1:r:346:HIS:CD2	2.53	0.43
1:r:583:LEU:HD21	1:u:599:ARG:HH22	1.84	0.43
1:0:558:ARG:NH1	1:x:125:LYS:HD2	2.34	0.43
3:2:144:ARG:HH21	3:j:159:ALA:H	1.65	0.43
1:6:354:ILE:HG12	1:6:494:ALA:HB3	2.00	0.43
1:6:361:ARG:HD3	1:U:72:ASP:OD1	2.19	0.43
4:C:414:THR:HA	4:D:328:HIS:ND1	2.34	0.43
4:E:15:ARG:HB2	4:E:347:MET:CA	2.48	0.43
4:E:414:THR:HG22	4:F:328:HIS:HE1	1.83	0.43
5:I:6:VAL:O	5:I:9:PRO:HD2	2.18	0.43
5:J:34:PHE:CZ	5:J:38:THR:HG21	2.54	0.43
5:J:194:GLN:NE2	5:i:110:GLU:OE1	2.52	0.43
5:K:192:LYS:NZ	1:x:407:GLU:OE1	2.32	0.43
2:P:47:THR:HA	2:P:57:ILE:HD12	1.99	0.43
2:R:93:THR:HG23	2:R:97:LEU:HD22	1.99	0.43
5:S:167:MET:HE2	5:S:167:MET:HB3	1.93	0.43
3:T:172:ARG:HD3	3:T:172:ARG:HA	1.78	0.43
1:U:323:THR:N	1:Y:174:THR:OG1	2.31	0.43
5:W:179:PHE:CZ	5:W:183:LEU:HD11	2.54	0.43
1:Y:43:LYS:HA	1:Y:43:LYS:HD2	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:48:TYR:HE2	3:b:143:TRP:CD1	2.37	0.43
2:d:6:PHE:CZ	2:d:100:PHE:HZ	2.37	0.43
5:e:109:SER:OG	5:e:110:GLU:N	2.52	0.43
3:f:86:ARG:HG2	3:f:87:ALA:N	2.33	0.43
1:g:370:ARG:O	1:g:373:ARG:HB3	2.18	0.43
1:g:386:ALA:CB	1:g:440:MET:HE3	2.49	0.43
1:x:394:LYS:O	1:x:431:VAL:HG23	2.19	0.43
1:0:103:SER:O	1:0:107:ILE:HG13	2.19	0.43
1:0:127:ASP:C	1:0:130:PRO:HD2	2.43	0.43
1:0:195:SER:O	1:0:363:ASN:ND2	2.52	0.43
1:0:286:ARG:HH21	1:3:218:CYS:C	2.26	0.43
3:2:160:GLU:HB2	3:n:42:VAL:HG21	2.01	0.43
2:7:48:LEU:HD11	2:7:58:VAL:HG11	2.01	0.43
4:B:43:ARG:NH2	4:C:350:ASN:OD1	2.52	0.43
4:B:247:LEU:CB	4:B:266:MET:HE1	2.48	0.43
4:C:260:GLU:O	4:C:263:ILE:HG12	2.18	0.43
5:G:3:PRO:O	5:G:6:VAL:HG22	2.18	0.43
5:H:204:GLN:NE2	1:Y:414:ARG:HD3	2.33	0.43
5:K:204:GLN:NE2	1:u:414:ARG:HD3	2.34	0.43
2:Q:86:ASP:C	2:Q:87:ARG:HD2	2.43	0.43
2:Q:90:ALA:C	2:Q:91:ARG:HD3	2.44	0.43
3:T:15:LEU:HD21	3:t:32:TRP:CH2	2.54	0.43
1:U:147:LEU:HD11	1:U:498:GLN:HE22	1.84	0.43
1:U:399:GLU:HB3	5:W:184:ASP:OD2	2.18	0.43
3:X:161:PHE:O	3:X:165:LEU:HD23	2.18	0.43
3:f:37:THR:N	3:f:165:LEU:HD11	2.33	0.43
3:f:132:ALA:O	3:f:135:VAL:HG13	2.19	0.43
1:g:568:MET:HE1	1:g:580:MET:HG3	2.00	0.43
1:g:601:ARG:NH1	1:g:608:ASP:H	2.17	0.43
1:k:372:MET:HG3	1:k:450:LEU:HD22	2.00	0.43
2:p:13:ARG:NE	2:p:13:ARG:HA	2.34	0.43
2:y:58:VAL:HG12	2:y:72:ARG:HG2	2.01	0.43
1:3:197:GLU:HG3	1:3:199:ASP:H	1.83	0.43
1:6:161:VAL:HG21	1:6:186:TRP:CG	2.54	0.43
4:C:94:LYS:HA	4:C:104:LEU:H	1.84	0.43
4:D:236:ASN:ND2	4:D:294:THR:O	2.46	0.43
4:E:247:LEU:CB	4:E:266:MET:HE1	2.49	0.43
4:F:239:MET:N	4:F:250:CYS:SG	2.90	0.43
1:U:42:MET:HG3	1:U:339:GLU:OE2	2.19	0.43
1:Y:445:ARG:HD3	1:c:443:MET:HE1	2.01	0.43
1:Y:572:MET:HE3	1:Y:573:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:331:PHE:HA	1:c:336:LEU:HA	2.01	0.43
3:j:37:THR:N	3:j:165:LEU:HD11	2.34	0.43
1:k:120:ILE:HD11	1:k:138:LEU:HD12	1.99	0.43
1:k:594:ASP:OD1	1:k:595:GLU:N	2.51	0.43
2:l:47:THR:HG22	2:l:57:ILE:HD13	2.01	0.43
1:r:537:ASN:OD1	1:u:176:GLY:N	2.49	0.43
3:t:116:THR:OG1	3:t:126:TYR:HB2	2.19	0.43
1:u:377:ASP:O	1:u:381:LYS:HG2	2.19	0.43
1:x:348:ARG:NH2	1:x:539:ILE:HD12	2.34	0.43
1:0:403:GLU:HB3	5:m:185:ARG:NH2	2.34	0.42
1:3:407:GLU:O	1:3:411:GLU:HG2	2.19	0.42
1:6:279:CYS:O	1:6:329:ALA:N	2.49	0.42
1:6:386:ALA:O	1:6:390:LEU:HD23	2.19	0.42
2:7:14:LEU:HD13	2:7:25:LEU:HD23	2.01	0.42
4:C:293:GLY:HA3	4:C:299:MET:SD	2.59	0.42
4:D:224:PRO:HG3	4:D:258:TRP:CD1	2.54	0.42
4:D:293:GLY:HA3	4:D:299:MET:SD	2.60	0.42
5:G:39:ARG:HB2	5:G:190:THR:HG21	2.01	0.42
5:H:76:ARG:NH1	5:H:101:GLN:HB3	2.34	0.42
3:T:57:VAL:HG12	3:T:62:GLN:OE1	2.19	0.42
1:U:167:GLU:OE1	1:U:208:ARG:NH2	2.52	0.42
2:V:56:GLU:HG2	2:V:58:VAL:HG13	2.01	0.42
2:V:97:LEU:HA	2:V:100:PHE:HD2	1.84	0.42
1:Y:582:ASP:HB3	1:Y:600:ILE:CG2	2.49	0.42
1:c:127:ASP:C	1:c:130:PRO:HD2	2.44	0.42
1:c:245:ASP:HB3	1:c:246:GLY:H	1.59	0.42
1:c:569:ILE:HG21	1:c:581:LEU:CD2	2.49	0.42
1:g:157:ASP:OD2	1:g:183:TYR:OH	2.36	0.42
3:q:47:ALA:HB1	3:q:157:MET:HE3	2.01	0.42
1:r:156:GLU:O	1:r:160:LYS:HG3	2.18	0.42
3:t:31:GLU:O	3:t:34:THR:HG22	2.18	0.42
3:t:171:TYR:CD1	3:t:190:TYR:HB2	2.54	0.42
1:u:43:LYS:HD2	1:u:43:LYS:HA	1.75	0.42
1:0:141:LEU:HD12	1:0:506:ILE:HD11	2.01	0.42
3:2:24:TRP:CD1	3:2:173:ALA:HB1	2.54	0.42
3:2:179:GLU:O	4:F:575:ARG:NE	2.48	0.42
4:A:239:MET:N	4:A:250:CYS:SG	2.87	0.42
4:F:454:GLY:O	4:F:542:ARG:HA	2.19	0.42
5:I:102:ALA:HA	5:I:117:PRO:HG2	2.00	0.42
2:N:96:GLU:HG2	2:N:97:LEU:HD23	2.00	0.42
3:T:56:LEU:O	3:T:134:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:372:MET:HB2	1:U:450:LEU:HD22	2.01	0.42
1:Y:375:ILE:HB	1:Y:450:LEU:HD13	2.01	0.42
3:b:55:ALA:HA	3:b:136:GLN:HA	2.01	0.42
1:c:70:ASP:HB3	1:c:369:ILE:HD12	2.01	0.42
1:c:220:LEU:HD23	1:c:220:LEU:HA	1.87	0.42
3:f:159:ALA:H	3:z:144:ARG:NH2	2.17	0.42
5:i:151:ALA:O	5:i:155:LEU:HG	2.18	0.42
3:j:16:LEU:O	3:j:18:ASP:N	2.46	0.42
3:n:185:VAL:HG22	3:n:189:HIS:HE1	1.79	0.42
1:o:327:ARG:NH1	1:o:339:GLU:OE2	2.52	0.42
1:u:537:ASN:OD1	1:x:176:GLY:N	2.42	0.42
2:v:58:VAL:HG23	2:v:70:ILE:HD11	2.00	0.42
1:0:558:ARG:HD3	1:x:125:LYS:HD2	2.01	0.42
2:4:94:ALA:HB2	2:7:8:ASN:ND2	2.34	0.42
3:5:113:ARG:HB2	3:5:129:PRO:HD3	2.01	0.42
3:5:116:THR:OG1	3:5:126:TYR:HB2	2.19	0.42
1:6:43:LYS:HG3	1:6:47:ARG:HH12	1.85	0.42
1:6:391:SER:OG	5:G:204:GLN:O	2.37	0.42
4:A:84:ARG:HG2	4:A:97:VAL:HG22	2.00	0.42
4:A:88:MET:HE1	4:A:241:ALA:CB	2.49	0.42
4:A:233:SER:C	4:A:234:LEU:HD22	2.44	0.42
4:A:272:ALA:O	4:A:283:MET:HB2	2.18	0.42
4:B:318:ASP:OD2	4:C:303:ARG:NH2	2.52	0.42
4:E:293:GLY:HA3	4:E:299:MET:SD	2.59	0.42
5:S:4:LEU:HD11	5:S:138:LEU:HG	2.00	0.42
5:S:10:ILE:HG22	5:S:155:LEU:HD11	2.01	0.42
1:U:376:GLN:HE21	1:U:376:GLN:HA	1.83	0.42
1:U:585:ALA:HA	1:U:588:THR:HG22	2.02	0.42
1:Y:73:TYR:HD1	1:Y:77:ILE:O	2.02	0.42
1:c:280:TRP:HH2	1:c:344:PHE:HE2	1.66	0.42
1:c:537:ASN:OD1	1:g:176:GLY:N	2.39	0.42
1:k:568:MET:HG3	1:o:590:LEU:HD11	2.00	0.42
5:m:15:ALA:HB1	5:m:166:TRP:HD1	1.83	0.42
3:w:79:LYS:HB2	3:w:79:LYS:HE3	1.83	0.42
2:y:14:LEU:HD13	2:y:25:LEU:HB2	2.01	0.42
1:0:332:THR:N	1:0:335:ASP:O	2.52	0.42
2:1:56:GLU:OE2	2:1:72:ARG:NH1	2.53	0.42
1:3:361:ARG:HD3	1:6:72:ASP:OD2	2.20	0.42
1:6:385:LYS:O	1:6:389:ILE:HG13	2.19	0.42
1:6:534:LEU:HD12	1:6:535:PRO:HD2	2.02	0.42
4:F:19:ARG:NE	4:F:446:VAL:HG21	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:293:GLY:HA3	4:F:299:MET:SD	2.59	0.42
5:H:8:MET:HE3	5:H:24:PHE:CE1	2.55	0.42
5:J:81:VAL:O	5:e:195:GLN:NE2	2.52	0.42
5:J:105:VAL:HG22	5:J:115:PHE:CD1	2.55	0.42
5:L:102:ALA:HB2	5:L:119:GLU:OE1	2.19	0.42
5:S:7:PHE:CZ	5:S:143:ALA:HA	2.54	0.42
3:T:15:LEU:HG	3:T:170:LEU:HD21	2.00	0.42
1:Y:210:LYS:HG2	1:Y:276:LEU:O	2.19	0.42
1:Y:408:PHE:O	1:Y:412:VAL:HG23	2.19	0.42
1:Y:595:GLU:HG3	1:Y:599:ARG:NH1	2.34	0.42
5:i:39:ARG:HB2	5:i:190:THR:HG21	2.02	0.42
5:i:167:MET:HE2	5:i:167:MET:HB3	1.96	0.42
3:j:209:ALA:HB3	3:j:212:ALA:HB2	2.00	0.42
1:k:139:LYS:HE2	1:k:555:ALA:O	2.19	0.42
1:k:261:SER:HB3	1:k:264:ARG:HG2	2.00	0.42
5:m:34:PHE:CZ	5:m:38:THR:HG21	2.55	0.42
1:u:187:ARG:HD3	1:u:249:ALA:HB1	2.01	0.42
1:x:122:PRO:HB2	1:x:125:LYS:HA	2.02	0.42
3:z:79:LYS:HB2	3:z:79:LYS:HE3	1.71	0.42
1:3:402:VAL:HG21	1:3:408:PHE:HB2	2.00	0.42
2:4:11:ALA:HA	2:4:89:GLU:HB3	2.01	0.42
3:5:179:GLU:H	4:B:540:MET:HE1	1.84	0.42
4:A:293:GLY:HA3	4:A:299:MET:SD	2.60	0.42
4:A:318:ASP:OD2	4:B:303:ARG:NH2	2.52	0.42
4:B:383:PHE:CE1	2:v:20:PRO:HG2	2.54	0.42
4:C:542:ARG:HB3	3:T:23:ARG:CG	2.44	0.42
4:D:457:LEU:HD12	4:D:457:LEU:HA	1.88	0.42
4:E:341:VAL:HG12	4:E:344:GLU:H	1.85	0.42
4:F:53:VAL:HG13	4:F:70:GLN:NE2	2.34	0.42
4:F:343:THR:O	4:F:347:MET:N	2.43	0.42
5:G:70:LEU:HD12	5:G:71:VAL:H	1.84	0.42
5:S:104:TYR:O	5:S:115:PHE:HA	2.20	0.42
3:T:37:THR:N	3:T:165:LEU:HD11	2.35	0.42
1:U:579:VAL:HG23	1:U:580:MET:HE2	2.01	0.42
5:W:107:GLN:HG2	5:W:109:SER:O	2.20	0.42
3:X:209:ALA:HB3	3:X:212:ALA:HB2	2.02	0.42
1:Y:578:LEU:HD23	1:Y:581:LEU:HD12	2.01	0.42
5:a:16:PRO:O	5:a:166:TRP:NE1	2.52	0.42
3:f:64:LEU:HD13	3:f:68:ALA:HB3	2.00	0.42
5:i:16:PRO:O	5:i:166:TRP:NE1	2.52	0.42
5:i:64:ALA:N	5:i:130:LYS:O	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j:132:ALA:O	3:j:135:VAL:HG13	2.17	0.42
1:k:85:GLN:O	1:k:89:GLU:HG2	2.19	0.42
1:k:159:VAL:O	1:k:368:VAL:HG12	2.20	0.42
1:o:506:ILE:HG23	1:o:510:VAL:HG11	2.02	0.42
2:p:48:LEU:HB3	2:p:82:PHE:HE1	1.84	0.42
1:x:144:VAL:HG11	1:x:177:GLU:HB3	2.02	0.42
3:2:113:ARG:HB2	3:2:129:PRO:HD3	2.01	0.42
1:3:170:TYR:HB3	1:3:344:PHE:HE1	1.85	0.42
4:B:319:LEU:HD21	4:B:369:TYR:HB2	2.00	0.42
4:C:83:ASP:O	4:C:84:ARG:HD3	2.19	0.42
4:E:11:GLY:HA3	4:E:397:PHE:CD1	2.54	0.42
4:E:57:LYS:O	4:E:314:ARG:NH1	2.51	0.42
4:F:15:ARG:HB2	4:F:347:MET:CA	2.49	0.42
4:F:548:LEU:HD12	4:F:548:LEU:HA	1.85	0.42
5:H:126:TYR:CE2	5:a:94:ARG:HD3	2.53	0.42
5:H:195:GLN:HA	5:a:68:MET:HG2	2.01	0.42
5:I:84:GLN:NE2	5:a:69:GLU:OE1	2.52	0.42
5:J:70:LEU:HD12	5:J:71:VAL:H	1.84	0.42
5:K:8:MET:HE3	5:K:24:PHE:CE1	2.54	0.42
2:P:92:LEU:HD11	2:Q:8:ASN:ND2	2.32	0.42
1:U:247:ASP:CG	1:U:248:GLU:H	2.28	0.42
3:X:148:LEU:HD11	3:X:155:VAL:HG22	2.01	0.42
1:Y:351:LEU:HA	1:Y:351:LEU:HD23	1.70	0.42
3:f:170:LEU:HB3	3:f:189:HIS:ND1	2.34	0.42
1:g:285:MET:HG3	1:g:325:ARG:HE	1.85	0.42
2:h:18:LEU:HG	2:h:72:ARG:HH21	1.84	0.42
1:k:403:GLU:HG3	1:k:422:LYS:HE3	2.00	0.42
5:m:39:ARG:HB2	5:m:190:THR:HG21	2.02	0.42
1:o:445:ARG:O	1:o:449:MET:HG2	2.19	0.42
2:s:50:ARG:HA	2:s:86:ASP:OD1	2.19	0.42
1:0:430:ASN:CG	1:0:433:ARG:HE	2.28	0.42
1:0:568:MET:HE1	1:0:580:MET:SD	2.60	0.42
1:3:407:GLU:CD	5:L:192:LYS:HZ3	2.24	0.42
4:A:12:GLU:HG2	4:A:14:PRO:HD3	2.01	0.42
4:A:312:ASN:OD1	4:A:314:ARG:N	2.53	0.42
4:D:332:VAL:CG2	4:D:339:MET:HE3	2.49	0.42
4:E:438:LEU:O	4:E:557:ASN:HA	2.20	0.42
5:G:12:HIS:HA	5:G:15:ALA:O	2.20	0.42
5:H:73:PHE:HD1	5:H:123:VAL:HG22	1.83	0.42
1:U:231:ALA:HA	1:U:334:ARG:HH21	1.84	0.42
3:X:64:LEU:HD13	3:X:68:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:132:ALA:O	3:X:135:VAL:HG13	2.20	0.42
1:Y:579:VAL:HG23	1:Y:580:MET:CE	2.46	0.42
1:c:123:ARG:NH1	1:c:543:LYS:O	2.52	0.42
1:c:345:ARG:HG2	1:c:538:ASP:HB2	2.01	0.42
2:h:52:ASP:OD1	2:h:53:GLY:N	2.46	0.42
2:h:94:ALA:HB2	2:l:8:ASN:HB2	2.02	0.42
3:j:46:SER:HB3	3:j:204:THR:H	1.85	0.42
5:m:37:ARG:HD3	5:m:37:ARG:HA	1.81	0.42
1:r:282:ARG:HG2	1:r:326:VAL:HG12	2.02	0.42
1:u:37:LEU:O	1:u:42:MET:HG2	2.20	0.42
1:u:139:LYS:HE2	1:u:555:ALA:O	2.20	0.42
1:u:369:ILE:O	1:u:372:MET:N	2.52	0.42
2:v:11:ALA:HA	2:v:89:GLU:HB3	2.00	0.42
3:w:47:ALA:HB1	3:w:157:MET:HE3	2.01	0.42
1:x:147:LEU:HD22	1:x:502:GLN:HE22	1.85	0.42
1:3:398:ASP:OD2	1:3:426:GLN:N	2.50	0.42
2:4:13:ARG:HD2	2:4:13:ARG:N	2.35	0.42
4:B:548:LEU:HD12	4:B:548:LEU:HA	1.86	0.42
5:H:196:ARG:HD2	1:c:407:GLU:OE2	2.19	0.42
5:K:194:GLN:CD	5:m:107:GLN:HE22	2.28	0.42
2:P:101:ARG:NE	2:Q:4:VAL:O	2.52	0.42
5:S:3:PRO:O	5:S:6:VAL:HG22	2.20	0.42
2:V:13:ARG:HH21	2:V:85:ASN:HA	1.84	0.42
1:Y:134:LYS:O	1:Y:138:LEU:HD23	2.19	0.42
3:f:160:GLU:OE1	3:z:144:ARG:NH2	2.50	0.42
1:g:73:TYR:HD1	1:g:77:ILE:O	2.02	0.42
3:n:159:ALA:C	3:n:162:VAL:HG12	2.45	0.42
1:o:109:GLY:O	1:o:113:ARG:HG2	2.20	0.42
3:t:113:ARG:HB2	3:t:129:PRO:HD3	2.01	0.42
1:u:354:ILE:HG12	1:u:494:ALA:HB3	2.02	0.42
1:u:571:LYS:HE2	1:x:570:MET:HE3	2.00	0.42
1:u:598:LYS:HE2	1:u:602:GLN:NE2	2.35	0.42
1:x:43:LYS:O	1:x:47:ARG:HG3	2.19	0.42
1:x:247:ASP:OD1	1:x:248:GLU:N	2.46	0.42
3:2:49:MET:HE3	3:2:72:ILE:HG13	2.02	0.42
3:5:31:GLU:OE2	3:X:11:ARG:NE	2.52	0.42
2:7:113:ALA:O	2:7:117:THR:HG23	2.20	0.42
4:A:6:LEU:HD23	4:A:440:TRP:HZ3	1.85	0.42
4:B:54:ASP:OD2	4:B:55:ASN:N	2.53	0.42
4:B:509:ASP:OD1	4:B:509:ASP:N	2.53	0.42
4:C:51:ILE:HG13	4:C:420:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:236:ASN:HA	4:F:301:GLN:HG3	2.02	0.42
5:K:76:ARG:NH1	5:K:101:GLN:HB3	2.34	0.42
1:U:88:LYS:HD2	1:U:88:LYS:HA	1.91	0.42
1:U:283:LYS:HE3	1:U:283:LYS:HB2	1.82	0.42
3:X:61:LYS:HA	3:X:126:TYR:CD1	2.55	0.42
1:c:576:VAL:O	1:c:580:MET:HG2	2.20	0.42
1:k:64:ARG:HD3	1:k:186:TRP:CZ3	2.54	0.42
1:o:285:MET:HG3	1:o:325:ARG:HE	1.85	0.42
2:v:38:LEU:HD21	2:v:44:PHE:HD2	1.85	0.42
1:x:112:LYS:HG2	1:x:152:SER:HB2	2.01	0.42
1:x:177:GLU:HA	1:x:178:PRO:HD3	1.86	0.42
3:z:114:HIS:N	3:z:128:TYR:O	2.44	0.42
1:0:517:ARG:HA	1:0:517:ARG:HD3	1.96	0.42
3:2:32:TRP:CH2	3:j:15:LEU:HD21	2.54	0.42
1:6:109:GLY:O	1:6:113:ARG:HG2	2.20	0.42
1:6:224:ARG:NH1	1:6:224:ARG:HB2	2.35	0.42
4:A:54:ASP:O	4:A:70:GLN:NE2	2.52	0.42
4:A:343:THR:HA	4:A:346:LEU:HG	2.02	0.42
4:A:529:LYS:HE3	4:A:529:LYS:HB3	1.72	0.42
4:C:509:ASP:N	4:C:509:ASP:OD1	2.51	0.42
4:D:574:LEU:HG	3:w:179:GLU:OE2	2.20	0.42
4:F:105:ALA:HA	4:F:224:PRO:HD2	2.02	0.42
4:F:225:PRO:HG2	4:F:248:TYR:CE2	2.55	0.42
5:G:7:PHE:HB3	5:G:27:ILE:HD13	2.02	0.42
5:I:28:ARG:HD2	5:I:133:LEU:O	2.19	0.42
5:L:81:VAL:O	5:m:195:GLN:NE2	2.53	0.42
2:P:8:ASN:ND2	2:R:75:GLU:OE1	2.53	0.42
2:R:93:THR:O	2:R:97:LEU:HB2	2.20	0.42
5:S:38:THR:HG23	5:S:183:LEU:CD1	2.50	0.42
5:a:4:LEU:HG	5:a:27:ILE:HG21	2.01	0.42
1:c:396:VAL:HG12	1:c:431:VAL:HG22	2.02	0.42
1:c:582:ASP:HB2	1:c:604:ASN:ND2	2.35	0.42
1:g:492:ARG:HD3	1:g:492:ARG:HA	1.91	0.42
1:k:547:ILE:HD13	1:o:556:THR:HB	2.02	0.42
1:k:582:ASP:HB2	1:k:604:ASN:HD22	1.85	0.42
3:q:116:THR:OG1	3:q:126:TYR:HB2	2.20	0.42
1:x:85:GLN:O	1:x:89:GLU:HG2	2.19	0.42
1:0:111:GLU:HG3	1:0:155:PHE:CD2	2.55	0.41
1:3:391:SER:OG	5:S:204:GLN:O	2.38	0.41
1:6:43:LYS:HD2	1:6:43:LYS:HA	1.75	0.41
4:D:272:ALA:HB3	4:D:316:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:40:LEU:HD23	5:H:40:LEU:HA	1.91	0.41
5:J:3:PRO:O	5:J:6:VAL:HG22	2.19	0.41
5:K:102:ALA:HA	5:K:117:PRO:HD2	2.01	0.41
1:U:57:LEU:HD12	1:U:57:LEU:HA	1.91	0.41
1:U:127:ASP:C	1:U:130:PRO:HD2	2.45	0.41
1:U:376:GLN:HA	1:U:376:GLN:NE2	2.34	0.41
1:Y:57:LEU:HD22	1:Y:247:ASP:HB2	2.02	0.41
1:Y:598:LYS:HE2	1:Y:602:GLN:NE2	2.35	0.41
3:b:159:ALA:HB1	3:w:38:ARG:NH1	2.35	0.41
1:c:111:GLU:HG3	1:c:155:PHE:CD2	2.55	0.41
1:c:377:ASP:OD1	1:c:377:ASP:C	2.63	0.41
1:g:58:ASP:OD1	1:g:59:ARG:N	2.52	0.41
1:g:90:ARG:HD2	1:g:388:TYR:CE1	2.55	0.41
5:i:54:CYS:HB2	5:i:112:THR:HB	2.01	0.41
1:u:59:ARG:HB3	1:x:257:ARG:HH21	1.85	0.41
2:v:63:ARG:HG3	2:v:68:MET:CG	2.49	0.41
3:w:5:ALA:HB2	3:w:148:LEU:HD12	2.01	0.41
1:x:245:ASP:HB3	1:x:246:GLY:H	1.59	0.41
1:0:327:ARG:HH12	1:0:339:GLU:HG3	1.84	0.41
3:2:128:TYR:CZ	5:K:21:PRO:HD3	2.55	0.41
1:3:85:GLN:O	1:3:89:GLU:HG2	2.19	0.41
1:3:393:ASN:HA	1:3:433:ARG:HH22	1.84	0.41
1:6:248:GLU:O	1:6:252:TRP:CB	2.68	0.41
2:7:104:ILE:O	2:7:108:GLN:OE1	2.38	0.41
4:A:41:PRO:HA	4:A:438:LEU:HD12	2.02	0.41
4:B:489:LEU:HD12	4:B:511:MET:HE1	2.01	0.41
4:C:545:SER:OG	3:T:176:LYS:HD2	2.20	0.41
4:E:304:VAL:HG22	4:E:305:GLU:H	1.85	0.41
4:E:330:GLY:HA2	4:E:352:TRP:CD1	2.55	0.41
4:F:442:SER:N	4:F:554:ILE:O	2.28	0.41
5:H:183:LEU:HD23	5:H:183:LEU:HA	1.92	0.41
5:K:3:PRO:O	5:K:6:VAL:HG22	2.20	0.41
5:K:12:HIS:HA	5:K:15:ALA:O	2.19	0.41
3:T:32:TRP:HA	3:T:32:TRP:CE3	2.55	0.41
1:U:139:LYS:HE3	1:U:143:ASP:OD1	2.20	0.41
1:U:218:CYS:SG	1:U:229:LYS:NZ	2.93	0.41
1:U:282:ARG:HG2	1:U:326:VAL:HG12	2.02	0.41
2:V:59:LYS:HB3	2:V:59:LYS:HE2	1.74	0.41
2:V:91:ARG:HE	2:d:93:THR:HG21	1.85	0.41
3:X:39:GLU:HG3	3:X:43:ARG:HH12	1.85	0.41
1:Y:141:LEU:HD12	1:Y:506:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:63:ARG:NH1	2:Z:65:VAL:O	2.52	0.41
3:b:159:ALA:HB1	3:w:38:ARG:HH12	1.85	0.41
1:c:43:LYS:HA	1:c:43:LYS:HD2	1.87	0.41
1:c:43:LYS:O	1:c:47:ARG:HG3	2.19	0.41
1:g:257:ARG:NH1	1:g:257:ARG:HB2	2.35	0.41
1:g:284:PRO:O	1:g:285:MET:HE2	2.19	0.41
1:g:497:MET:HE1	1:k:146:ARG:CD	2.50	0.41
3:j:110:GLY:O	3:j:135:VAL:HG11	2.20	0.41
1:k:432:ASP:HB2	1:k:435:LEU:HD23	2.00	0.41
5:m:151:ALA:O	5:m:155:LEU:HG	2.20	0.41
1:o:279:CYS:N	1:o:329:ALA:O	2.39	0.41
3:q:170:LEU:HD23	3:q:189:HIS:NE2	2.35	0.41
1:r:211:TRP:HB3	1:r:273:ARG:HH21	1.85	0.41
1:u:285:MET:HG3	1:u:325:ARG:HD2	2.02	0.41
1:u:505:LEU:HD23	1:u:505:LEU:HA	1.95	0.41
2:v:18:LEU:HB3	2:v:82:PHE:HB2	2.00	0.41
3:w:170:LEU:HD23	3:w:189:HIS:NE2	2.35	0.41
1:0:99:VAL:HG13	1:x:452:GLN:HE22	1.84	0.41
1:0:122:PRO:HG3	1:0:128:ALA:HA	2.01	0.41
1:0:125:LYS:HZ1	1:3:589:ASP:HA	1.84	0.41
1:0:278:GLU:CD	1:0:280:TRP:HE1	2.28	0.41
3:2:113:ARG:HE	5:K:20:GLU:CD	2.28	0.41
3:2:178:SER:HA	4:F:540:MET:HE1	2.01	0.41
3:5:11:ARG:NH1	3:T:31:GLU:OE2	2.53	0.41
3:5:38:ARG:NH1	3:X:159:ALA:HB1	2.35	0.41
4:A:445:PHE:N	4:A:552:TRP:O	2.41	0.41
4:A:490:PRO:C	4:A:507:ASN:HA	2.46	0.41
4:D:318:ASP:OD2	4:E:303:ARG:NH2	2.53	0.41
4:D:377:GLU:N	4:D:381:ALA:O	2.51	0.41
4:D:545:SER:OG	4:D:546:GLY:N	2.54	0.41
4:E:543:LEU:O	3:f:23:ARG:HG2	2.20	0.41
5:G:70:LEU:HD23	5:W:94:ARG:HH12	1.84	0.41
5:G:78:MET:HE2	5:G:78:MET:HB2	1.83	0.41
5:K:4:LEU:HD11	5:K:138:LEU:HG	2.01	0.41
5:K:107:GLN:OE1	5:i:194:GLN:HB2	2.19	0.41
5:K:141:LEU:CD1	5:K:142:LEU:HD12	2.50	0.41
2:N:108:GLN:NE2	2:O:106:SER:OG	2.50	0.41
2:P:93:THR:HG21	2:Q:91:ARG:HH21	1.86	0.41
2:Q:11:ALA:HA	2:Q:89:GLU:HB3	2.02	0.41
1:U:227:GLU:HA	1:U:230:LYS:HG2	2.01	0.41
5:W:104:TYR:O	5:W:115:PHE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:407:GLU:HG2	1:Y:411:GLU:OE2	2.20	0.41
2:Z:11:ALA:HA	2:Z:89:GLU:HB3	2.02	0.41
3:b:110:GLY:O	3:b:135:VAL:HG11	2.21	0.41
1:c:568:MET:SD	1:c:572:MET:HE2	2.61	0.41
3:f:79:LYS:HB3	3:f:83:SER:HB3	2.03	0.41
1:g:79:TRP:NE1	1:g:95:LEU:O	2.53	0.41
5:i:109:SER:OG	5:i:110:GLU:N	2.52	0.41
3:j:43:ARG:HD2	3:j:197:LEU:HG	2.03	0.41
2:l:15:VAL:HG22	2:l:26:THR:O	2.19	0.41
2:l:18:LEU:HG	2:l:72:ARG:NH2	2.35	0.41
5:m:4:LEU:HD11	5:m:138:LEU:HG	2.01	0.41
5:m:18:CYS:HA	5:m:166:TRP:CZ2	2.55	0.41
5:m:31:ALA:HB1	5:m:142:LEU:HD13	2.02	0.41
1:o:139:LYS:HA	1:o:139:LYS:HD2	1.91	0.41
2:p:50:ARG:HA	2:p:86:ASP:OD2	2.21	0.41
3:q:5:ALA:HB2	3:q:148:LEU:HD12	2.03	0.41
1:u:108:ILE:HG13	1:u:109:GLY:N	2.35	0.41
2:1:90:ALA:C	2:1:91:ARG:HD3	2.46	0.41
1:3:245:ASP:HB3	1:3:246:GLY:H	1.59	0.41
4:A:73:VAL:HG13	4:A:89:GLY:H	1.84	0.41
4:B:11:GLY:HA3	4:B:397:PHE:CD1	2.55	0.41
4:B:57:LYS:O	4:B:314:ARG:NH1	2.52	0.41
4:D:19:ARG:HG2	4:D:446:VAL:HG21	2.02	0.41
4:D:548:LEU:HD12	4:D:548:LEU:HA	1.87	0.41
5:G:103:GLN:HG3	5:G:104:TYR:CD2	2.55	0.41
5:H:20:GLU:CD	3:t:113:ARG:HE	2.28	0.41
5:I:107:GLN:HG2	5:I:109:SER:O	2.20	0.41
3:T:4:PRO:O	3:T:7:VAL:HG22	2.20	0.41
5:W:86:LEU:HD13	5:W:93:TRP:NE1	2.35	0.41
1:Y:444:SER:O	1:Y:448:GLN:HG2	2.20	0.41
1:Y:571:LYS:HE2	1:c:570:MET:HE3	2.02	0.41
2:Z:90:ALA:HA	2:Z:91:ARG:NH1	2.36	0.41
3:b:57:VAL:HG12	3:b:62:GLN:OE1	2.20	0.41
1:c:137:LEU:HD23	1:c:137:LEU:HA	1.94	0.41
1:c:261:SER:HB3	1:c:264:ARG:HG2	2.01	0.41
2:d:5:GLN:NE2	2:d:38:LEU:HA	2.35	0.41
3:f:15:LEU:HG	3:f:170:LEU:HD21	2.03	0.41
1:g:171:ASP:HB2	1:g:180:TYR:CE1	2.56	0.41
3:q:24:TRP:CD1	3:q:173:ALA:HB1	2.55	0.41
1:r:100:ILE:HA	1:r:372:MET:HE1	2.03	0.41
1:r:227:GLU:HA	1:r:230:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:101:ARG:HD2	2:v:6:PHE:CE2	2.55	0.41
1:u:230:LYS:HG3	1:u:334:ARG:HH11	1.86	0.41
1:u:279:CYS:O	1:u:329:ALA:N	2.52	0.41
1:u:375:ILE:HB	1:u:450:LEU:HD13	2.02	0.41
3:2:116:THR:OG1	3:2:126:TYR:HB2	2.20	0.41
1:3:577:GLY:O	1:3:581:LEU:HG	2.21	0.41
1:6:449:MET:HG3	1:U:97:PHE:HE2	1.85	0.41
2:7:8:ASN:HA	2:7:91:ARG:NH2	2.35	0.41
4:B:80:VAL:HG11	4:B:84:ARG:NH1	2.35	0.41
4:C:57:LYS:O	4:C:314:ARG:NH1	2.47	0.41
4:E:239:MET:N	4:E:250:CYS:SG	2.93	0.41
4:E:489:LEU:HA	4:E:490:PRO:HD3	1.94	0.41
5:H:141:LEU:CD1	5:H:142:LEU:HD12	2.50	0.41
5:J:78:MET:HE2	5:J:78:MET:HB2	1.81	0.41
2:R:18:LEU:HB3	2:R:72:ARG:HH21	1.85	0.41
1:Y:161:VAL:HG21	1:Y:186:TRP:CG	2.56	0.41
5:a:151:ALA:O	5:a:155:LEU:HG	2.19	0.41
1:c:543:LYS:HD2	1:c:543:LYS:HA	1.78	0.41
3:f:162:VAL:O	3:f:166:VAL:HG23	2.20	0.41
1:g:440:MET:CE	1:g:443:MET:HE3	2.51	0.41
1:o:224:ARG:NH1	1:o:224:ARG:HB2	2.35	0.41
1:o:280:TRP:HH2	1:o:344:PHE:HE2	1.68	0.41
1:x:421:LYS:HD2	1:x:427:ILE:HG12	2.01	0.41
1:0:106:TRP:HA	1:x:482:VAL:HG12	2.02	0.41
2:1:18:LEU:HB3	2:1:82:PHE:CD2	2.56	0.41
1:3:72:ASP:OD1	1:3:77:ILE:HB	2.20	0.41
1:3:159:VAL:O	1:3:368:VAL:HG12	2.20	0.41
1:3:395:VAL:HG11	1:3:408:PHE:HE2	1.86	0.41
1:3:398:ASP:HB2	1:3:425:LYS:HB3	2.02	0.41
2:4:58:VAL:HG11	2:4:72:ARG:HD2	2.03	0.41
3:5:145:HIS:HD2	3:5:146:PRO:HD2	1.85	0.41
4:A:317:ILE:HG22	4:A:319:LEU:HD12	2.03	0.41
4:B:88:MET:HE3	4:B:231:LEU:HB2	2.01	0.41
4:B:558:SER:OG	4:B:560:ILE:O	2.37	0.41
4:C:224:PRO:HG3	4:C:258:TRP:HD1	1.84	0.41
4:D:447:LEU:HD11	4:D:453:PHE:CE2	2.55	0.41
4:E:75:ALA:HB2	4:E:87:TYR:HB3	2.03	0.41
4:E:542:ARG:HH21	3:f:17:GLN:HB3	1.85	0.41
5:G:156:SER:O	5:G:160:ILE:HG12	2.20	0.41
5:H:200:ARG:HD2	1:c:414:ARG:HH21	1.85	0.41
5:J:156:SER:O	5:J:160:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:94:ARG:CZ	5:m:70:LEU:HD21	2.51	0.41
2:P:50:ARG:HA	2:P:86:ASP:OD1	2.20	0.41
3:T:19:GLU:OE1	3:T:19:GLU:HA	2.21	0.41
1:U:125:LYS:HD3	1:U:125:LYS:O	2.20	0.41
1:U:586:ASP:OD1	1:U:593:ARG:NH1	2.54	0.41
2:Z:13:ARG:HA	2:Z:86:ASP:O	2.20	0.41
2:Z:13:ARG:HD2	2:Z:13:ARG:N	2.35	0.41
3:b:148:LEU:HD11	3:b:155:VAL:HG22	2.03	0.41
3:f:61:LYS:HA	3:f:126:TYR:CD1	2.55	0.41
3:j:50:LYS:NZ	3:j:52:THR:OG1	2.43	0.41
3:j:56:LEU:O	3:j:134:GLY:HA2	2.21	0.41
2:l:63:ARG:HB3	2:l:68:MET:HG3	2.03	0.41
1:o:382:ARG:HG2	1:o:382:ARG:HH11	1.84	0.41
1:u:410:GLU:HB3	1:u:411:GLU:OE1	2.20	0.41
3:w:28:GLU:HG2	3:w:32:TRP:NE1	2.36	0.41
3:w:106:MET:HG2	3:w:107:LYS:N	2.34	0.41
3:w:116:THR:OG1	3:w:126:TYR:HB2	2.20	0.41
1:x:278:GLU:HG2	1:x:330:ILE:HG12	2.02	0.41
1:x:450:LEU:HA	1:x:450:LEU:HD23	1.80	0.41
2:y:35:PHE:HD2	2:y:68:MET:HE1	1.86	0.41
3:z:145:HIS:HD2	3:z:146:PRO:HD2	1.85	0.41
1:0:370:ARG:O	1:0:373:ARG:HB3	2.19	0.41
1:0:595:GLU:HG3	1:0:599:ARG:NH1	2.36	0.41
1:3:395:VAL:HG11	1:3:408:PHE:CE2	2.56	0.41
1:6:117:ASP:OD2	1:6:139:LYS:NZ	2.36	0.41
4:D:22:PRO:HD2	4:D:25:ALA:HB3	2.03	0.41
4:E:319:LEU:HD21	4:E:369:TYR:HB2	2.02	0.41
4:F:546:GLY:HA3	3:z:19:GLU:HG3	2.02	0.41
5:L:34:PHE:CZ	5:L:38:THR:HG21	2.56	0.41
5:L:129:LEU:HD23	5:L:129:LEU:HA	1.87	0.41
3:T:110:GLY:O	3:T:135:VAL:HG11	2.21	0.41
3:T:148:LEU:HD11	3:T:155:VAL:HG22	2.02	0.41
1:U:167:GLU:O	1:U:181:SER:HA	2.21	0.41
1:U:398:ASP:OD1	1:U:426:GLN:HG2	2.21	0.41
2:V:36:PRO:O	2:V:63:ARG:NE	2.53	0.41
2:V:92:LEU:HD12	2:Z:8:ASN:ND2	2.35	0.41
5:W:27:ILE:HG22	5:W:138:LEU:HD11	2.03	0.41
5:W:78:MET:CE	5:W:105:VAL:HG23	2.50	0.41
1:Y:147:LEU:N	1:Y:148:PRO:HD2	2.36	0.41
1:Y:401:ALA:HA	1:Y:425:LYS:HB2	2.02	0.41
1:o:369:ILE:HG22	1:o:373:ARG:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:385:LYS:O	1:o:389:ILE:HG13	2.20	0.41
1:u:354:ILE:HG12	1:u:494:ALA:CB	2.50	0.41
1:u:401:ALA:HA	1:u:425:LYS:HB2	2.02	0.41
1:u:444:SER:O	1:u:448:GLN:HG2	2.20	0.41
1:0:357:PHE:HA	1:0:486:LYS:NZ	2.36	0.41
3:2:86:ARG:HG3	3:n:101:PRO:HB2	2.02	0.41
1:3:247:ASP:OD1	1:3:248:GLU:N	2.51	0.41
1:3:578:LEU:HA	1:3:581:LEU:HD12	2.01	0.41
1:6:449:MET:HG3	1:U:97:PHE:CE2	2.56	0.41
4:B:456:ILE:HD12	4:B:534:VAL:HG11	2.03	0.41
4:D:77:PRO:HG2	4:E:268:TYR:CE1	2.56	0.41
5:I:36:GLU:HA	5:I:66:TYR:CE2	2.55	0.41
2:N:15:VAL:HG22	2:N:26:THR:O	2.20	0.41
2:O:75:GLU:HG3	2:O:92:LEU:HD21	2.03	0.41
2:P:45:MET:HB2	2:P:96:GLU:OE2	2.20	0.41
1:Y:536:GLU:O	1:Y:541:ARG:NH1	2.53	0.41
3:b:33:LEU:HD12	3:b:165:LEU:HD12	2.02	0.41
1:c:144:VAL:HG11	1:c:177:GLU:HB3	2.03	0.41
1:c:354:ILE:HG12	1:c:494:ALA:CB	2.50	0.41
1:c:482:VAL:HA	1:c:485:ASN:OD1	2.21	0.41
5:e:3:PRO:O	5:e:6:VAL:HG22	2.20	0.41
5:e:13:ARG:HB2	3:z:99:GLU:OE2	2.21	0.41
3:f:209:ALA:HB3	3:f:212:ALA:HB2	2.02	0.41
1:g:597:VAL:O	1:g:601:ARG:HG3	2.20	0.41
2:h:57:ILE:HD12	2:h:57:ILE:HA	1.94	0.41
2:h:93:THR:HA	2:h:97:LEU:HD13	2.01	0.41
3:n:159:ALA:HB1	3:q:38:ARG:HH12	1.86	0.41
2:s:90:ALA:C	2:s:91:ARG:HD3	2.45	0.41
1:u:59:ARG:HD3	1:x:257:ARG:O	2.20	0.41
1:x:261:SER:HB3	1:x:264:ARG:HG2	2.01	0.41
1:x:377:ASP:OD1	1:x:377:ASP:C	2.63	0.41
1:0:371:TRP:CD1	1:0:372:MET:H	2.39	0.41
2:1:92:LEU:HD21	2:1:94:ALA:HB3	2.02	0.41
3:2:37:THR:O	3:2:41:VAL:HG23	2.20	0.41
1:3:129:LYS:HB2	1:3:130:PRO:HD3	2.03	0.41
1:3:139:LYS:HE2	1:3:555:ALA:O	2.21	0.41
1:3:400:GLY:HA2	5:S:184:ASP:OD1	2.20	0.41
1:3:413:ALA:HB3	5:S:204:GLN:OE1	2.21	0.41
1:3:565:LEU:O	1:3:569:ILE:HG13	2.21	0.41
1:6:332:THR:N	1:6:335:ASP:O	2.53	0.41
2:7:22:GLY:O	2:7:72:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:349:ARG:NH2	4:F:415:GLY:O	2.54	0.41
4:C:454:GLY:N	4:C:568:ALA:O	2.42	0.41
4:D:247:LEU:CB	4:D:266:MET:HE1	2.48	0.41
4:D:449:MET:HA	4:D:450:PRO:HD3	1.96	0.41
4:E:331:LEU:HB3	4:E:343:THR:HG23	2.03	0.41
4:E:568:ALA:HB1	4:E:573:GLU:HB3	2.02	0.41
4:F:304:VAL:HG22	4:F:305:GLU:H	1.85	0.41
5:G:6:VAL:O	5:G:9:PRO:HD2	2.20	0.41
5:L:78:MET:HG3	5:L:79:ARG:H	1.85	0.41
2:M:4:VAL:HG22	2:M:43:TRP:CE2	2.55	0.41
2:O:43:TRP:CE3	2:O:59:LYS:HD2	2.56	0.41
2:P:98:GLY:O	2:P:101:ARG:HG2	2.20	0.41
2:Q:63:ARG:HH11	2:Q:63:ARG:HG2	1.85	0.41
5:S:141:LEU:HD12	5:S:142:LEU:HD12	2.02	0.41
3:T:66:GLU:OE2	3:T:66:GLU:N	2.54	0.41
2:V:23:THR:C	2:V:70:ILE:HG22	2.46	0.41
2:V:68:MET:HE3	2:V:68:MET:HB3	1.98	0.41
5:W:136:ASP:OD2	5:W:136:ASP:N	2.50	0.41
1:Y:248:GLU:O	1:Y:252:TRP:CB	2.69	0.41
1:Y:354:ILE:HG12	1:Y:494:ALA:CB	2.51	0.41
1:c:154:SER:HA	1:c:183:TYR:HE1	1.86	0.41
1:c:251:ASP:OD1	1:c:275:ARG:NH2	2.27	0.41
1:c:385:LYS:O	1:c:389:ILE:HG13	2.21	0.41
2:d:113:ALA:O	2:d:117:THR:HG23	2.20	0.41
5:e:7:PHE:CZ	5:e:143:ALA:HA	2.55	0.41
3:f:48:TYR:CE1	3:f:156:GLN:HG3	2.56	0.41
1:g:124:LYS:HZ2	1:k:520:ASN:HA	1.85	0.41
5:i:18:CYS:HA	5:i:166:TRP:CZ2	2.55	0.41
5:i:37:ARG:HA	5:i:37:ARG:HD3	1.82	0.41
5:i:91:PRO:O	5:i:91:PRO:HD2	2.20	0.41
1:k:153:ARG:NH1	1:k:156:GLU:OE2	2.51	0.41
1:k:166:ILE:HG21	1:k:498:GLN:CD	2.46	0.41
1:k:170:TYR:HB3	1:k:344:PHE:CE1	2.56	0.41
1:k:170:TYR:HB3	1:k:344:PHE:HE1	1.85	0.41
1:k:247:ASP:CG	1:k:248:GLU:H	2.29	0.41
1:k:251:ASP:OD2	1:k:275:ARG:NH2	2.30	0.41
1:k:502:GLN:O	1:k:506:ILE:HG13	2.21	0.41
2:l:68:MET:SD	2:l:68:MET:N	2.94	0.41
2:l:104:ILE:O	2:l:108:GLN:HG3	2.21	0.41
5:m:105:VAL:HG22	5:m:115:PHE:CD1	2.55	0.41
1:o:361:ARG:HD3	1:r:72:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:r:430:ASN:HA	1:r:433:ARG:HH12	1.86	0.41
2:s:100:PHE:O	2:s:104:ILE:HG12	2.21	0.41
3:t:9:LEU:HD11	3:t:30:LEU:HG	2.02	0.41
3:t:24:TRP:CD1	3:t:173:ALA:HB1	2.55	0.41
3:t:39:GLU:HG2	3:t:168:TRP:CH2	2.56	0.41
1:u:103:SER:O	1:u:107:ILE:HG13	2.21	0.41
1:u:129:LYS:HA	1:u:129:LYS:HD3	1.85	0.41
1:u:183:TYR:CE2	1:u:185:SER:HA	2.56	0.41
1:u:210:LYS:HG2	1:u:276:LEU:O	2.21	0.41
1:u:248:GLU:O	1:u:252:TRP:CB	2.68	0.41
2:v:50:ARG:HG3	2:v:51:SER:O	2.21	0.41
1:x:127:ASP:C	1:x:130:PRO:HD2	2.45	0.41
1:x:348:ARG:HH21	1:x:539:ILE:HD12	1.86	0.41
1:x:385:LYS:O	1:x:389:ILE:HG13	2.20	0.41
1:x:569:ILE:HG21	1:x:581:LEU:CD2	2.51	0.41
3:z:116:THR:OG1	3:z:126:TYR:HB2	2.20	0.41
1:0:230:LYS:HG3	1:0:334:ARG:HH11	1.86	0.41
1:0:369:ILE:HG22	1:0:373:ARG:HB2	2.02	0.41
1:0:577:GLY:O	1:0:581:LEU:HB2	2.20	0.41
1:3:100:ILE:HG12	1:3:372:MET:HB3	2.03	0.41
1:3:103:SER:O	1:3:107:ILE:HG13	2.21	0.41
1:6:108:ILE:HG13	1:6:109:GLY:N	2.35	0.41
2:7:8:ASN:HA	2:7:91:ARG:HH21	1.85	0.41
2:7:82:PHE:HB3	2:7:86:ASP:OD2	2.19	0.41
4:A:26:SER:HB3	4:A:441:ARG:O	2.20	0.41
4:B:536:LYS:HD2	4:B:539:ARG:HE	1.86	0.41
4:C:10:SER:OG	4:C:24:THR:O	2.31	0.41
4:E:51:ILE:HG13	4:E:420:LEU:HD12	2.03	0.41
4:E:73:VAL:CG1	4:E:87:TYR:HB2	2.51	0.41
5:H:21:PRO:HD3	3:t:128:TYR:CZ	2.55	0.41
5:I:102:ALA:HA	5:I:117:PRO:CG	2.52	0.41
5:J:2:LYS:HB3	5:J:137:SER:OG	2.21	0.41
5:K:42:ARG:HG2	5:K:128:LEU:HD23	2.03	0.41
5:K:141:LEU:O	5:K:145:THR:OG1	2.37	0.41
5:K:183:LEU:HD23	5:K:183:LEU:HA	1.92	0.41
2:M:58:VAL:HA	2:M:74:GLN:HE22	1.86	0.41
2:M:91:ARG:NH2	2:O:93:THR:OG1	2.54	0.41
2:Q:51:SER:O	2:Q:52:ASP:HB2	2.21	0.41
1:U:371:TRP:CD1	1:U:372:MET:N	2.89	0.41
2:V:18:LEU:HB3	2:V:82:PHE:HD2	1.86	0.41
1:Y:59:ARG:NE	1:c:257:ARG:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:139:LYS:HE2	1:Y:555:ALA:O	2.21	0.41
1:Y:161:VAL:HG21	1:Y:186:TRP:CD1	2.56	0.41
1:Y:484:THR:OG1	1:Y:487:LEU:HD12	2.21	0.41
1:c:582:ASP:HB2	1:c:604:ASN:HD22	1.86	0.41
5:i:50:GLY:HA2	5:i:120:ALA:HA	2.03	0.41
3:j:148:LEU:HD11	3:j:155:VAL:HG22	2.02	0.41
1:k:280:TRP:HH2	1:k:344:PHE:HE2	1.68	0.41
1:k:407:GLU:O	1:k:411:GLU:HG2	2.21	0.41
3:n:62:GLN:HB2	3:n:125:PHE:O	2.21	0.41
3:n:159:ALA:H	3:q:144:ARG:NH2	2.19	0.41
1:o:401:ALA:HB1	1:o:427:ILE:CG1	2.51	0.41
1:u:64:ARG:HG2	1:u:247:ASP:OD2	2.21	0.41
1:u:251:ASP:OD1	1:u:275:ARG:NH2	2.54	0.41
1:u:435:LEU:HA	1:u:435:LEU:HD23	1.87	0.41
1:u:492:ARG:O	1:u:496:GLN:HG2	2.21	0.41
1:x:132:GLU:HG2	1:x:136:LYS:HE3	2.02	0.41
1:x:139:LYS:HA	1:x:139:LYS:HD2	1.77	0.41
3:z:78:LEU:HB3	3:z:136:GLN:HG2	2.03	0.41
1:0:597:VAL:O	1:0:601:ARG:HG3	2.20	0.40
1:3:99:VAL:HG22	1:3:376:GLN:NE2	2.36	0.40
1:3:122:PRO:HG2	1:3:125:LYS:HD3	2.03	0.40
4:B:251:GLU:HB2	4:B:257:ALA:HB3	2.03	0.40
4:C:272:ALA:HB3	4:C:316:VAL:HG21	2.03	0.40
4:C:346:LEU:HD23	4:C:396:PRO:HB2	2.03	0.40
4:C:542:ARG:NH1	3:T:24:TRP:HZ3	2.19	0.40
4:E:41:PRO:HA	4:E:438:LEU:HD12	2.02	0.40
4:E:87:TYR:HE1	4:E:96:ILE:HG13	1.86	0.40
5:J:103:GLN:HG3	5:J:104:TYR:CD2	2.55	0.40
2:Q:58:VAL:CG2	2:Q:70:ILE:HD11	2.51	0.40
3:T:23:ARG:HB2	3:T:24:TRP:CE3	2.56	0.40
3:T:46:SER:HB3	3:T:204:THR:H	1.86	0.40
1:U:407:GLU:O	1:U:411:GLU:HG2	2.21	0.40
1:Y:187:ARG:HD3	1:Y:249:ALA:HB1	2.03	0.40
1:Y:230:LYS:HG3	1:Y:334:ARG:HH11	1.86	0.40
1:Y:385:LYS:O	1:Y:389:ILE:HG13	2.21	0.40
1:Y:483:ALA:HA	1:c:105:ASN:HB3	2.03	0.40
1:Y:492:ARG:O	1:Y:496:GLN:HG2	2.21	0.40
1:Y:578:LEU:O	1:Y:581:LEU:HB2	2.21	0.40
1:Y:582:ASP:OD1	1:Y:583:LEU:N	2.53	0.40
3:b:159:ALA:H	3:w:144:ARG:NH2	2.19	0.40
1:c:407:GLU:O	1:c:411:GLU:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:56:GLU:OE2	2:h:72:ARG:NH1	2.54	0.40
3:j:19:GLU:OE1	3:j:19:GLU:HA	2.21	0.40
3:n:69:ILE:N	3:n:142:ALA:O	2.40	0.40
1:r:40:GLU:HG3	1:r:41:GLU:H	1.86	0.40
1:r:482:VAL:HA	1:r:485:ASN:OD1	2.20	0.40
1:u:332:THR:N	1:u:335:ASP:O	2.52	0.40
1:x:445:ARG:O	1:x:449:MET:HG2	2.20	0.40
1:0:279:CYS:HB3	1:0:329:ALA:HB3	2.02	0.40
1:0:286:ARG:NH2	1:3:218:CYS:O	2.47	0.40
1:0:489:ASP:OD2	1:3:112:LYS:HD3	2.21	0.40
1:3:598:LYS:HE3	1:3:598:LYS:HB3	1.92	0.40
3:5:155:VAL:HG12	3:5:157:MET:H	1.86	0.40
4:A:459:GLU:OE2	4:B:550:ARG:NH1	2.47	0.40
4:C:304:VAL:HG22	4:C:305:GLU:H	1.86	0.40
4:E:462:THR:HG23	4:E:537:MET:HE1	2.02	0.40
4:E:558:SER:OG	4:E:560:ILE:O	2.36	0.40
4:F:88:MET:HE1	4:F:241:ALA:HB1	2.02	0.40
5:I:102:ALA:HB2	5:I:119:GLU:OE2	2.21	0.40
5:J:43:CYS:HB2	5:J:129:LEU:HD11	2.04	0.40
2:M:65:VAL:HG12	2:M:66:ASP:N	2.37	0.40
2:N:36:PRO:O	2:N:63:ARG:HD3	2.21	0.40
5:S:32:ILE:O	5:S:36:GLU:HG3	2.22	0.40
1:U:345:ARG:NH1	1:U:508:GLN:HG3	2.36	0.40
1:Y:369:ILE:O	1:Y:372:MET:N	2.54	0.40
2:Z:83:ASN:HA	2:Z:84:PRO:HD2	1.90	0.40
5:a:18:CYS:HA	5:a:166:TRP:CZ2	2.56	0.40
1:c:324:MET:HE2	1:c:324:MET:HB2	1.98	0.40
1:c:394:LYS:O	1:c:431:VAL:HG23	2.21	0.40
5:e:20:GLU:HG3	3:f:114:HIS:CD2	2.56	0.40
1:g:489:ASP:OD2	1:k:112:LYS:HD3	2.21	0.40
3:n:19:GLU:HA	3:n:19:GLU:OE1	2.21	0.40
1:o:354:ILE:HG12	1:o:494:ALA:HB3	2.02	0.40
1:o:393:ASN:HD22	1:o:412:VAL:HG12	1.86	0.40
1:r:127:ASP:C	1:r:130:PRO:HD2	2.46	0.40
1:r:161:VAL:HG21	1:r:186:TRP:CG	2.56	0.40
3:w:32:TRP:HA	3:w:32:TRP:CE3	2.57	0.40
3:w:149:THR:HG22	3:w:150:THR:HG23	2.04	0.40
1:x:129:LYS:HB2	1:x:130:PRO:HD3	2.04	0.40
1:x:374:ASP:OD1	1:x:375:ILE:HG12	2.21	0.40
1:0:46:HIS:HB2	1:0:336:LEU:HD23	2.03	0.40
1:0:400:GLY:HA3	5:L:184:ASP:OD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:247:ASP:CG	1:3:248:GLU:H	2.29	0.40
3:5:144:ARG:NH2	3:X:159:ALA:H	2.19	0.40
1:6:327:ARG:NH1	1:6:339:GLU:OE2	2.53	0.40
4:D:412:LEU:O	4:E:309:PRO:HG3	2.22	0.40
4:E:474:ALA:O	4:E:478:ARG:HG3	2.21	0.40
4:F:391:THR:HA	4:F:396:PRO:HB3	2.03	0.40
4:F:457:LEU:HD12	4:F:457:LEU:HA	1.89	0.40
5:G:34:PHE:CZ	5:G:38:THR:HG21	2.56	0.40
5:J:29:GLU:OE2	5:e:148:LYS:HE2	2.21	0.40
5:J:39:ARG:HB2	5:J:190:THR:HG21	2.03	0.40
2:N:14:LEU:HD21	2:N:25:LEU:HD13	2.02	0.40
2:P:92:LEU:HD21	2:P:94:ALA:HB3	2.03	0.40
2:R:104:ILE:O	2:R:108:GLN:OE1	2.39	0.40
3:T:48:TYR:CE2	3:T:143:TRP:HB3	2.57	0.40
1:U:100:ILE:HA	1:U:372:MET:HE1	2.03	0.40
1:U:111:GLU:HG3	1:U:155:PHE:CD2	2.56	0.40
5:W:91:PRO:O	5:W:91:PRO:HD2	2.21	0.40
3:X:48:TYR:CE1	3:X:156:GLN:HG3	2.56	0.40
1:Y:445:ARG:O	1:Y:449:MET:HG2	2.21	0.40
5:a:116:VAL:HG12	5:a:117:PRO:HD3	2.03	0.40
5:e:116:VAL:HG12	5:e:117:PRO:HD3	2.03	0.40
1:g:247:ASP:OD1	1:g:248:GLU:HG2	2.21	0.40
2:h:50:ARG:HG2	2:h:54:ALA:O	2.21	0.40
1:k:270:LYS:HE3	1:k:270:LYS:HB3	1.93	0.40
3:n:166:VAL:O	3:n:170:LEU:HG	2.21	0.40
1:o:382:ARG:NH1	1:o:382:ARG:HG2	2.35	0.40
1:o:537:ASN:OD1	1:r:176:GLY:N	2.44	0.40
1:r:63:ASN:ND2	1:r:364:LEU:HB3	2.36	0.40
1:r:407:GLU:O	1:r:411:GLU:HG2	2.21	0.40
1:u:361:ARG:HB3	1:x:252:TRP:CZ3	2.56	0.40
1:x:139:LYS:HE3	1:x:555:ALA:O	2.21	0.40
1:0:406:GLU:OE2	1:0:409:ARG:NH2	2.50	0.40
3:2:50:LYS:HD2	3:2:143:TRP:CD2	2.57	0.40
4:B:438:LEU:O	4:B:557:ASN:HA	2.21	0.40
4:D:12:GLU:CD	4:D:28:ARG:H	2.29	0.40
4:F:417:LEU:HD23	4:F:417:LEU:HA	1.98	0.40
5:H:39:ARG:HB2	5:H:190:THR:HG21	2.03	0.40
5:I:21:PRO:HD3	3:w:128:TYR:OH	2.22	0.40
5:K:23:ALA:O	5:K:27:ILE:HG13	2.22	0.40
2:N:90:ALA:HA	2:N:91:ARG:NH1	2.37	0.40
5:S:20:GLU:HG3	3:X:114:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:261:SER:HB3	1:U:264:ARG:HG2	2.04	0.40
5:W:37:ARG:HA	5:W:37:ARG:HD3	1.82	0.40
3:X:170:LEU:HB3	3:X:189:HIS:CE1	2.56	0.40
1:Y:103:SER:O	1:Y:107:ILE:HG13	2.21	0.40
1:Y:163:LEU:HD22	1:Y:365:PRO:HG2	2.04	0.40
1:Y:361:ARG:HB3	1:c:252:TRP:CZ3	2.57	0.40
1:Y:556:THR:HG22	1:Y:559:GLN:HG3	2.02	0.40
3:f:70:GLN:NE2	3:w:202:THR:O	2.54	0.40
1:g:332:THR:N	1:g:335:ASP:O	2.51	0.40
1:k:127:ASP:C	1:k:130:PRO:HD2	2.47	0.40
1:k:401:ALA:HB1	1:k:427:ILE:HD11	2.04	0.40
5:m:205:PHE:CZ	1:x:92:GLN:HB2	2.56	0.40
3:n:171:TYR:CE1	3:n:190:TYR:HB2	2.56	0.40
1:o:556:THR:HG22	1:o:559:GLN:HG3	2.04	0.40
1:o:595:GLU:HG3	1:o:599:ARG:NH1	2.36	0.40
3:q:117:TYR:HD2	3:q:125:PHE:HB3	1.87	0.40
1:r:147:LEU:N	1:r:148:PRO:HD2	2.36	0.40
2:s:96:GLU:O	2:s:100:PHE:CD1	2.74	0.40
1:u:141:LEU:HD22	1:u:177:GLU:OE2	2.21	0.40
1:u:436:ALA:O	1:u:440:MET:HG2	2.21	0.40
3:w:145:HIS:CE1	3:w:155:VAL:HG13	2.57	0.40
1:x:407:GLU:O	1:x:411:GLU:HG2	2.20	0.40
1:0:492:ARG:HD3	1:0:492:ARG:HA	1.93	0.40
1:3:92:GLN:HE21	1:3:387:LEU:HD23	1.86	0.40
1:3:165:TRP:CE3	1:3:351:LEU:HB3	2.57	0.40
1:3:195:SER:HA	1:3:202:ASP:OD2	2.21	0.40
1:3:583:LEU:HD21	1:6:599:ARG:HH22	1.85	0.40
3:5:79:LYS:HE3	3:5:79:LYS:HB2	1.72	0.40
3:5:157:MET:HE3	3:5:157:MET:HB2	2.01	0.40
1:6:73:TYR:HD1	1:6:77:ILE:O	2.04	0.40
4:C:415:GLY:O	4:D:349:ARG:NH2	2.54	0.40
4:D:233:SER:C	4:D:234:LEU:HD22	2.46	0.40
4:D:454:GLY:O	4:D:542:ARG:HA	2.21	0.40
4:F:272:ALA:HB3	4:F:316:VAL:HG21	2.03	0.40
2:N:51:SER:O	2:N:52:ASP:HB2	2.22	0.40
2:O:48:LEU:HD22	2:O:88:ILE:HD12	2.03	0.40
5:S:34:PHE:CZ	5:S:38:THR:HG21	2.57	0.40
3:T:11:ARG:HH11	3:t:31:GLU:HG3	1.86	0.40
3:T:106:MET:HE1	3:T:128:TYR:CZ	2.57	0.40
1:U:59:ARG:HH21	1:U:364:LEU:HD21	1.86	0.40
1:U:177:GLU:HA	1:U:178:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:182:ARG:HD2	1:U:184:GLU:OE1	2.22	0.40
1:U:211:TRP:HB3	1:U:273:ARG:HH21	1.87	0.40
1:U:577:GLY:O	1:U:581:LEU:HG	2.22	0.40
1:Y:266:VAL:HG11	1:Y:270:LYS:HE2	2.03	0.40
2:Z:55:ARG:HH21	2:d:9:ASN:ND2	2.19	0.40
1:c:398:ASP:HB3	1:c:425:LYS:HE2	2.04	0.40
1:c:565:LEU:O	1:c:569:ILE:HG13	2.22	0.40
2:d:4:VAL:HG22	2:d:43:TRP:NE1	2.36	0.40
3:f:148:LEU:HD11	3:f:155:VAL:HG22	2.02	0.40
1:g:46:HIS:HB2	1:g:336:LEU:HD23	2.02	0.40
1:g:179:ILE:HG23	1:g:505:LEU:HD13	2.03	0.40
1:g:230:LYS:HG3	1:g:334:ARG:HH11	1.87	0.40
5:i:105:VAL:HG22	5:i:115:PHE:CD2	2.56	0.40
3:n:71:LEU:HG	3:n:117:TYR:CE1	2.57	0.40
2:s:48:LEU:HD12	2:s:87:ARG:O	2.21	0.40
1:u:230:LYS:HE3	1:u:334:ARG:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	535/781 (68%)	516 (96%)	17 (3%)	2 (0%)	30	62
1	3	535/781 (68%)	520 (97%)	13 (2%)	2 (0%)	30	62
1	6	535/781 (68%)	516 (96%)	17 (3%)	2 (0%)	30	62
1	U	535/781 (68%)	517 (97%)	16 (3%)	2 (0%)	30	62
1	Y	535/781 (68%)	523 (98%)	10 (2%)	2 (0%)	30	62
1	c	535/781 (68%)	519 (97%)	14 (3%)	2 (0%)	30	62
1	g	535/781 (68%)	518 (97%)	15 (3%)	2 (0%)	30	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	k	535/781 (68%)	518 (97%)	15 (3%)	2 (0%)	30	62
1	o	535/781 (68%)	519 (97%)	14 (3%)	2 (0%)	30	62
1	r	535/781 (68%)	517 (97%)	16 (3%)	2 (0%)	30	62
1	u	535/781 (68%)	520 (97%)	13 (2%)	2 (0%)	30	62
1	x	535/781 (68%)	520 (97%)	13 (2%)	2 (0%)	30	62
2	1	114/439 (26%)	106 (93%)	7 (6%)	1 (1%)	14	45
2	4	114/439 (26%)	107 (94%)	6 (5%)	1 (1%)	14	45
2	7	114/439 (26%)	106 (93%)	7 (6%)	1 (1%)	14	45
2	M	114/439 (26%)	108 (95%)	5 (4%)	1 (1%)	14	45
2	N	114/439 (26%)	105 (92%)	8 (7%)	1 (1%)	14	45
2	O	114/439 (26%)	106 (93%)	7 (6%)	1 (1%)	14	45
2	P	114/439 (26%)	107 (94%)	6 (5%)	1 (1%)	14	45
2	Q	114/439 (26%)	105 (92%)	8 (7%)	1 (1%)	14	45
2	R	114/439 (26%)	105 (92%)	8 (7%)	1 (1%)	14	45
2	V	114/439 (26%)	105 (92%)	8 (7%)	1 (1%)	14	45
2	Z	114/439 (26%)	107 (94%)	6 (5%)	1 (1%)	14	45
2	d	114/439 (26%)	105 (92%)	8 (7%)	1 (1%)	14	45
2	h	114/439 (26%)	107 (94%)	6 (5%)	1 (1%)	14	45
2	l	114/439 (26%)	106 (93%)	7 (6%)	1 (1%)	14	45
2	p	114/439 (26%)	107 (94%)	6 (5%)	1 (1%)	14	45
2	s	114/439 (26%)	108 (95%)	5 (4%)	1 (1%)	14	45
2	v	114/439 (26%)	107 (94%)	6 (5%)	1 (1%)	14	45
2	y	114/439 (26%)	106 (93%)	7 (6%)	1 (1%)	14	45
3	2	211/220 (96%)	200 (95%)	11 (5%)	0	100	100
3	5	211/220 (96%)	202 (96%)	9 (4%)	0	100	100
3	T	211/220 (96%)	196 (93%)	15 (7%)	0	100	100
3	X	211/220 (96%)	198 (94%)	13 (6%)	0	100	100
3	b	211/220 (96%)	196 (93%)	15 (7%)	0	100	100
3	f	211/220 (96%)	199 (94%)	12 (6%)	0	100	100
3	j	211/220 (96%)	197 (93%)	14 (7%)	0	100	100
3	n	211/220 (96%)	193 (92%)	18 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	q	211/220 (96%)	203 (96%)	8 (4%)	0	100	100
3	t	211/220 (96%)	199 (94%)	12 (6%)	0	100	100
3	w	211/220 (96%)	201 (95%)	10 (5%)	0	100	100
3	z	211/220 (96%)	202 (96%)	9 (4%)	0	100	100
4	A	512/577 (89%)	483 (94%)	24 (5%)	5 (1%)	12	43
4	B	512/577 (89%)	480 (94%)	27 (5%)	5 (1%)	12	43
4	C	512/577 (89%)	477 (93%)	30 (6%)	5 (1%)	12	43
4	D	512/577 (89%)	480 (94%)	27 (5%)	5 (1%)	12	43
4	E	512/577 (89%)	481 (94%)	26 (5%)	5 (1%)	12	43
4	F	512/577 (89%)	479 (94%)	28 (6%)	5 (1%)	12	43
5	G	202/206 (98%)	198 (98%)	4 (2%)	0	100	100
5	H	202/206 (98%)	199 (98%)	3 (2%)	0	100	100
5	I	202/206 (98%)	194 (96%)	8 (4%)	0	100	100
5	J	202/206 (98%)	195 (96%)	7 (4%)	0	100	100
5	K	202/206 (98%)	197 (98%)	5 (2%)	0	100	100
5	L	202/206 (98%)	194 (96%)	8 (4%)	0	100	100
5	S	202/206 (98%)	199 (98%)	3 (2%)	0	100	100
5	W	202/206 (98%)	199 (98%)	3 (2%)	0	100	100
5	a	202/206 (98%)	196 (97%)	6 (3%)	0	100	100
5	e	202/206 (98%)	198 (98%)	4 (2%)	0	100	100
5	i	202/206 (98%)	198 (98%)	4 (2%)	0	100	100
5	m	202/206 (98%)	199 (98%)	3 (2%)	0	100	100
All	All	16500/25848 (64%)	15768 (96%)	660 (4%)	72 (0%)	31	62

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	576	VAL
1	3	576	VAL
1	6	576	VAL
4	A	109	PRO
4	A	113	PRO
4	A	144	PRO
4	B	109	PRO

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Mol	Chain	Res	Type
4	B	113	PRO
4	B	144	PRO
4	C	109	PRO
4	C	113	PRO
4	C	144	PRO
4	D	109	PRO
4	D	113	PRO
4	D	144	PRO
4	E	109	PRO
4	E	113	PRO
4	E	144	PRO
4	F	109	PRO
4	F	113	PRO
4	F	144	PRO
1	U	576	VAL
1	Y	576	VAL
1	c	576	VAL
1	g	576	VAL
1	k	576	VAL
1	o	576	VAL
1	r	576	VAL
1	u	576	VAL
1	x	576	VAL
4	A	143	GLU
4	B	143	GLU
4	C	143	GLU
4	D	143	GLU
4	E	143	GLU
4	F	143	GLU
2	1	65	VAL
2	4	65	VAL
2	M	65	VAL
2	N	65	VAL
2	P	65	VAL
2	Q	65	VAL
2	V	65	VAL
2	Z	65	VAL
2	h	65	VAL
2	l	65	VAL
2	s	65	VAL
2	v	65	VAL
2	y	65	VAL

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Mol	Chain	Res	Type
1	3	260	TYR
2	7	65	VAL
4	A	125	VAL
4	B	125	VAL
4	C	125	VAL
4	D	125	VAL
4	E	125	VAL
4	F	125	VAL
2	O	65	VAL
2	R	65	VAL
1	U	260	TYR
1	c	260	TYR
2	d	65	VAL
1	k	260	TYR
2	p	65	VAL
1	x	260	TYR
1	6	260	TYR
1	o	260	TYR
1	r	260	TYR
1	0	260	TYR
1	Y	260	TYR
1	g	260	TYR
1	u	260	TYR

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	0	432/657 (66%)	432 (100%)	0	100	100
1	3	432/657 (66%)	432 (100%)	0	100	100
1	6	432/657 (66%)	431 (100%)	1 (0%)	87	87
1	U	432/657 (66%)	431 (100%)	1 (0%)	87	87
1	Y	432/657 (66%)	432 (100%)	0	100	100
1	c	432/657 (66%)	432 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	g	432/657 (66%)	431 (100%)	1 (0%)	87	87
1	k	432/657 (66%)	432 (100%)	0	100	100
1	o	432/657 (66%)	432 (100%)	0	100	100
1	r	432/657 (66%)	431 (100%)	1 (0%)	87	87
1	u	432/657 (66%)	432 (100%)	0	100	100
1	x	432/657 (66%)	432 (100%)	0	100	100
2	1	84/333 (25%)	84 (100%)	0	100	100
2	4	84/333 (25%)	83 (99%)	1 (1%)	63	72
2	7	84/333 (25%)	84 (100%)	0	100	100
2	M	84/333 (25%)	84 (100%)	0	100	100
2	N	84/333 (25%)	82 (98%)	2 (2%)	43	62
2	O	84/333 (25%)	84 (100%)	0	100	100
2	P	84/333 (25%)	84 (100%)	0	100	100
2	Q	84/333 (25%)	84 (100%)	0	100	100
2	R	84/333 (25%)	84 (100%)	0	100	100
2	V	84/333 (25%)	84 (100%)	0	100	100
2	Z	84/333 (25%)	83 (99%)	1 (1%)	63	72
2	d	84/333 (25%)	84 (100%)	0	100	100
2	h	84/333 (25%)	84 (100%)	0	100	100
2	l	84/333 (25%)	82 (98%)	2 (2%)	43	62
2	p	84/333 (25%)	84 (100%)	0	100	100
2	s	84/333 (25%)	84 (100%)	0	100	100
2	v	84/333 (25%)	84 (100%)	0	100	100
2	y	84/333 (25%)	84 (100%)	0	100	100
3	2	167/169 (99%)	167 (100%)	0	100	100
3	5	167/169 (99%)	167 (100%)	0	100	100
3	T	167/169 (99%)	167 (100%)	0	100	100
3	X	167/169 (99%)	167 (100%)	0	100	100
3	b	167/169 (99%)	167 (100%)	0	100	100
3	f	167/169 (99%)	167 (100%)	0	100	100
3	j	167/169 (99%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	n	167/169 (99%)	167 (100%)	0	100	100
3	q	167/169 (99%)	167 (100%)	0	100	100
3	t	167/169 (99%)	167 (100%)	0	100	100
3	w	167/169 (99%)	167 (100%)	0	100	100
3	z	167/169 (99%)	167 (100%)	0	100	100
4	A	366/464 (79%)	366 (100%)	0	100	100
4	B	366/464 (79%)	366 (100%)	0	100	100
4	C	366/464 (79%)	366 (100%)	0	100	100
4	D	366/464 (79%)	366 (100%)	0	100	100
4	E	366/464 (79%)	366 (100%)	0	100	100
4	F	366/464 (79%)	366 (100%)	0	100	100
5	G	170/172 (99%)	170 (100%)	0	100	100
5	H	170/172 (99%)	170 (100%)	0	100	100
5	I	170/172 (99%)	170 (100%)	0	100	100
5	J	170/172 (99%)	170 (100%)	0	100	100
5	K	170/172 (99%)	170 (100%)	0	100	100
5	L	170/172 (99%)	170 (100%)	0	100	100
5	S	170/172 (99%)	170 (100%)	0	100	100
5	W	170/172 (99%)	170 (100%)	0	100	100
5	a	170/172 (99%)	169 (99%)	1 (1%)	78	79
5	e	170/172 (99%)	170 (100%)	0	100	100
5	i	170/172 (99%)	170 (100%)	0	100	100
5	m	170/172 (99%)	170 (100%)	0	100	100
All	All	12936/20754 (62%)	12925 (100%)	11 (0%)	87	89

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	4	9	ASN
1	6	430	ASN
2	N	9	ASN
2	N	47	THR
1	U	485	ASN
2	Z	9	ASN

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Mol	Chain	Res	Type
5	a	204	GLN
1	g	430	ASN
2	l	9	ASN
2	l	47	THR
1	r	391	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	602	GLN
2	1	74	GLN
3	2	70	GLN
3	2	145	HIS
1	3	376	GLN
1	3	452	GLN
2	4	8	ASN
2	4	108	GLN
3	5	145	HIS
1	6	60	GLN
1	6	502	GLN
1	6	602	GLN
2	7	8	ASN
4	A	70	GLN
4	A	328	HIS
4	A	410	HIS
4	A	572	GLN
4	B	70	GLN
4	B	328	HIS
4	B	433	GLN
4	B	483	ASN
4	B	572	GLN
4	C	298	ASN
4	C	410	HIS
4	C	433	GLN
4	C	477	GLN
4	C	486	ASN
4	C	572	GLN
4	D	70	GLN
4	D	328	HIS
4	D	410	HIS
4	D	572	GLN
4	E	27	GLN

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Mol	Chain	Res	Type
4	E	70	GLN
4	E	328	HIS
4	E	410	HIS
4	E	433	GLN
4	E	572	GLN
4	F	298	ASN
4	F	328	HIS
4	F	410	HIS
4	F	433	GLN
4	F	477	GLN
4	F	486	ASN
4	F	572	GLN
5	H	89	GLN
5	I	12	HIS
5	I	103	GLN
5	J	195	GLN
5	K	89	GLN
5	K	107	GLN
2	M	85	ASN
2	P	74	GLN
2	P	108	GLN
5	S	12	HIS
5	S	77	ASN
3	T	111	GLN
1	U	376	GLN
1	U	502	GLN
2	V	74	GLN
5	W	12	HIS
5	W	194	GLN
3	X	182	ASN
1	Y	66	GLN
1	Y	485	ASN
2	Z	74	GLN
2	Z	108	GLN
5	a	12	HIS
5	a	48	ASN
5	a	107	GLN
5	a	194	GLN
5	a	204	GLN
1	c	46	HIS
1	c	92	GLN
1	c	426	GLN

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Mol	Chain	Res	Type
1	c	448	GLN
1	c	452	GLN
1	c	502	GLN
2	d	9	ASN
5	e	12	HIS
5	e	77	ASN
3	f	70	GLN
3	f	208	GLN
1	g	485	ASN
2	h	74	GLN
5	i	12	HIS
5	i	194	GLN
3	j	111	GLN
1	k	46	HIS
1	k	393	ASN
1	k	452	GLN
1	k	498	GLN
5	m	12	HIS
5	m	48	ASN
5	m	194	GLN
1	o	430	ASN
1	o	502	GLN
1	o	602	GLN
2	p	74	GLN
3	q	145	HIS
1	r	393	ASN
2	s	74	GLN
2	s	108	GLN
2	s	115	GLN
3	t	70	GLN
3	t	145	HIS
1	u	66	GLN
1	u	498	GLN
2	v	8	ASN
3	w	145	HIS
1	x	63	ASN
1	x	66	GLN
1	x	92	GLN
1	x	426	GLN
1	x	448	GLN
1	x	452	GLN
1	x	496	GLN

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Mol	Chain	Res	Type
1	x	498	GLN
1	x	502	GLN
2	y	9	ASN
2	y	74	GLN
2	y	108	GLN
3	z	145	HIS
3	z	200	GLN

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.

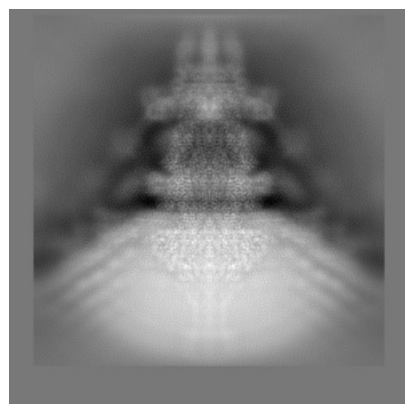
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36463. These allow visual inspection of the internal detail of the map and identification of artifacts.

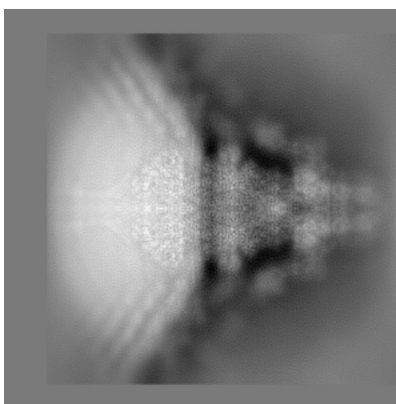
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

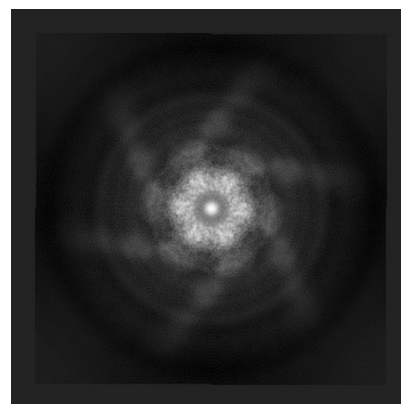
6.1.1 Primary map



X

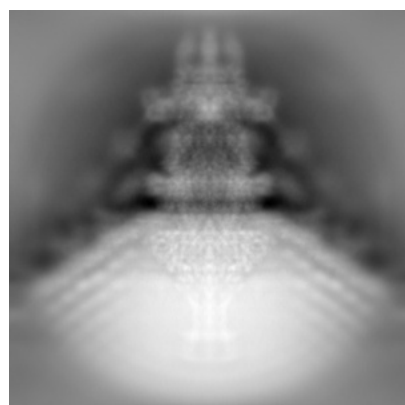


Y

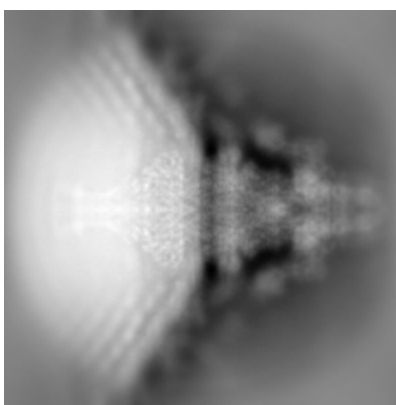


Z

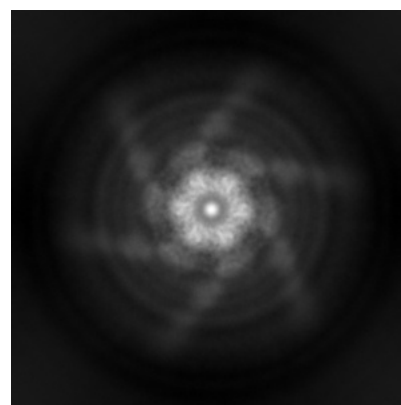
6.1.2 Raw map



X



Y

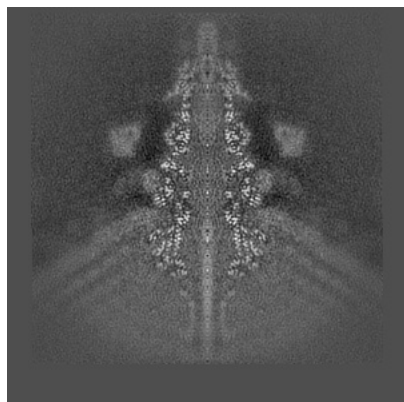


Z

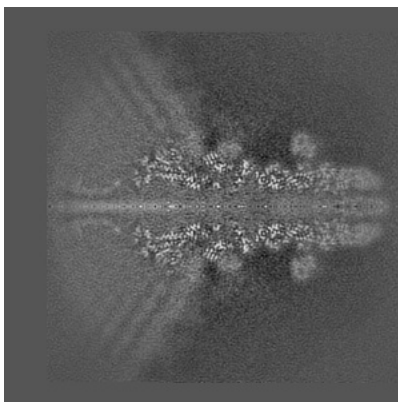
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

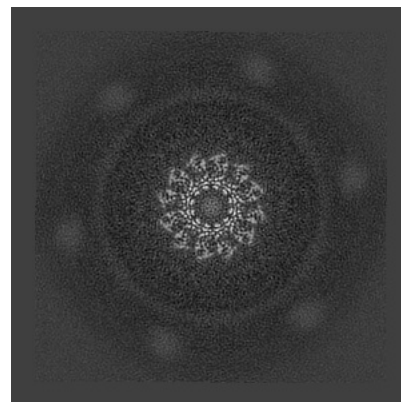
6.2.1 Primary map



X Index: 200

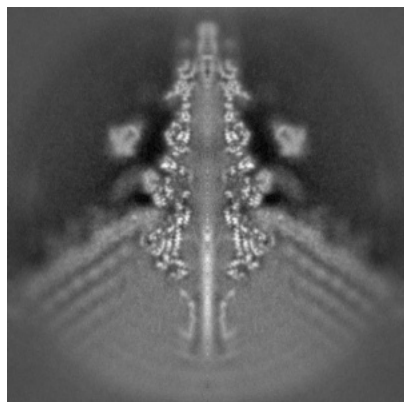


Y Index: 200

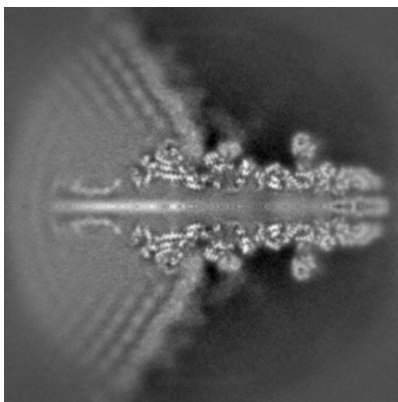


Z Index: 200

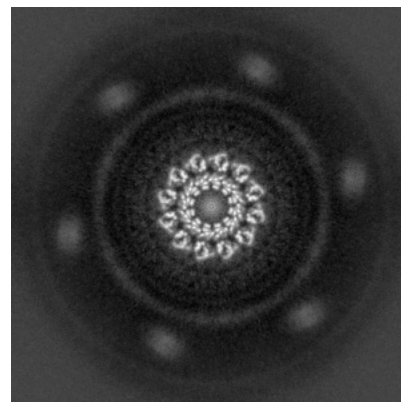
6.2.2 Raw map



X Index: 200



Y Index: 200

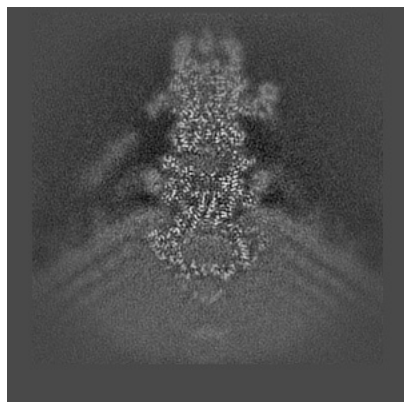


Z Index: 200

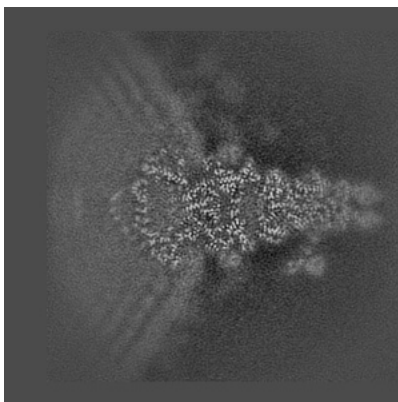
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

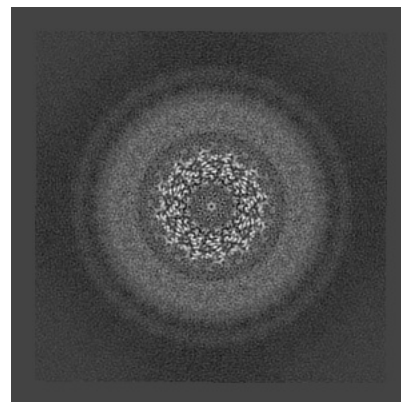
6.3.1 Primary map



X Index: 181

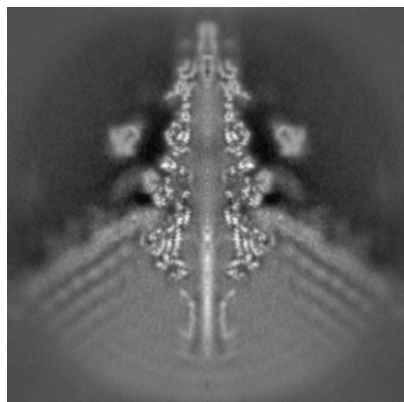


Y Index: 220

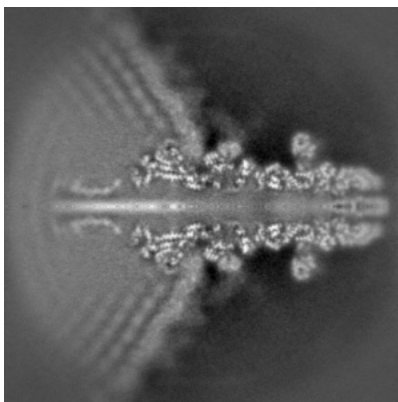


Z Index: 176

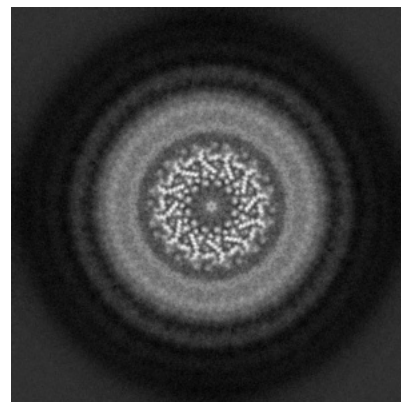
6.3.2 Raw map



X Index: 200



Y Index: 200

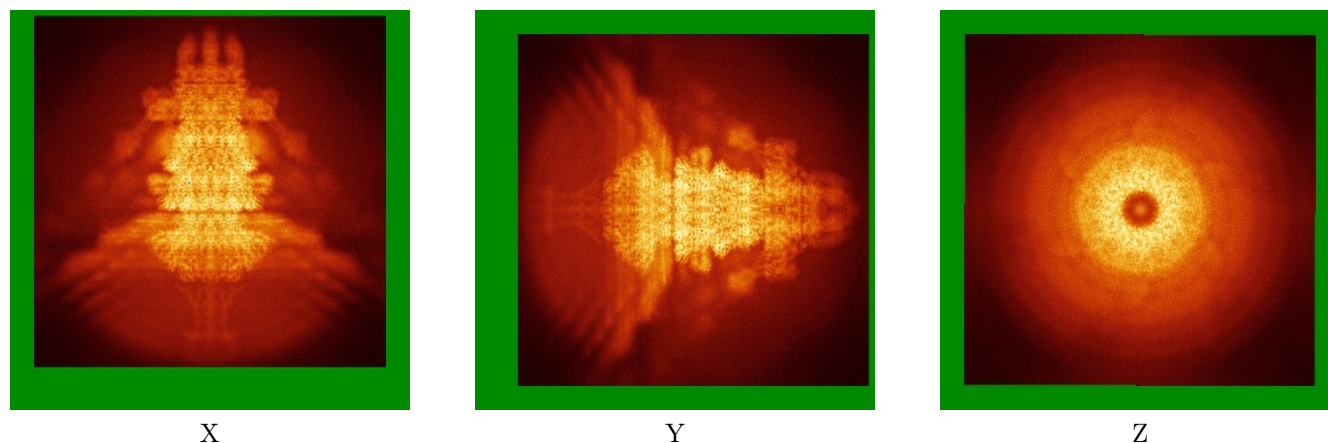


Z Index: 176

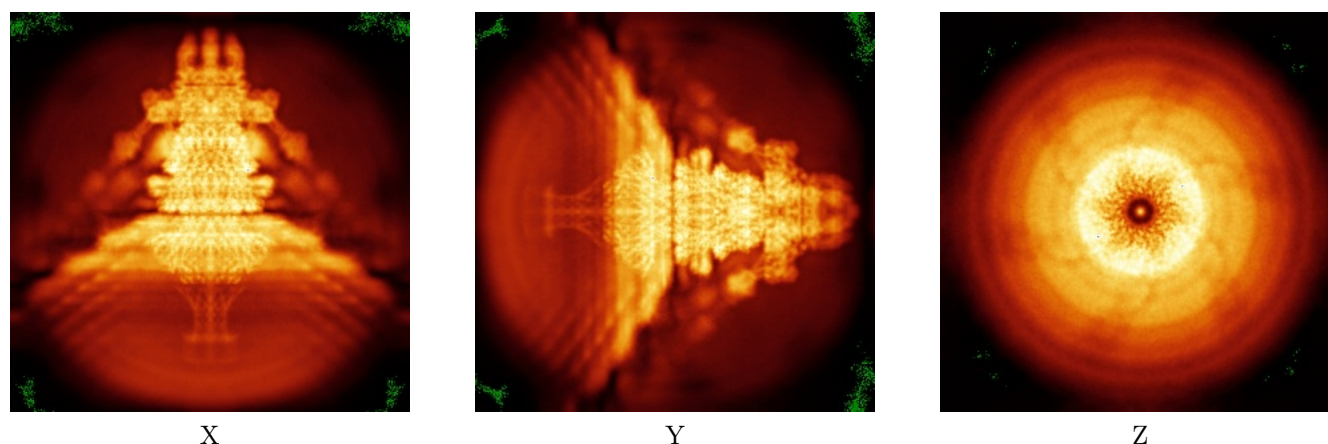
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

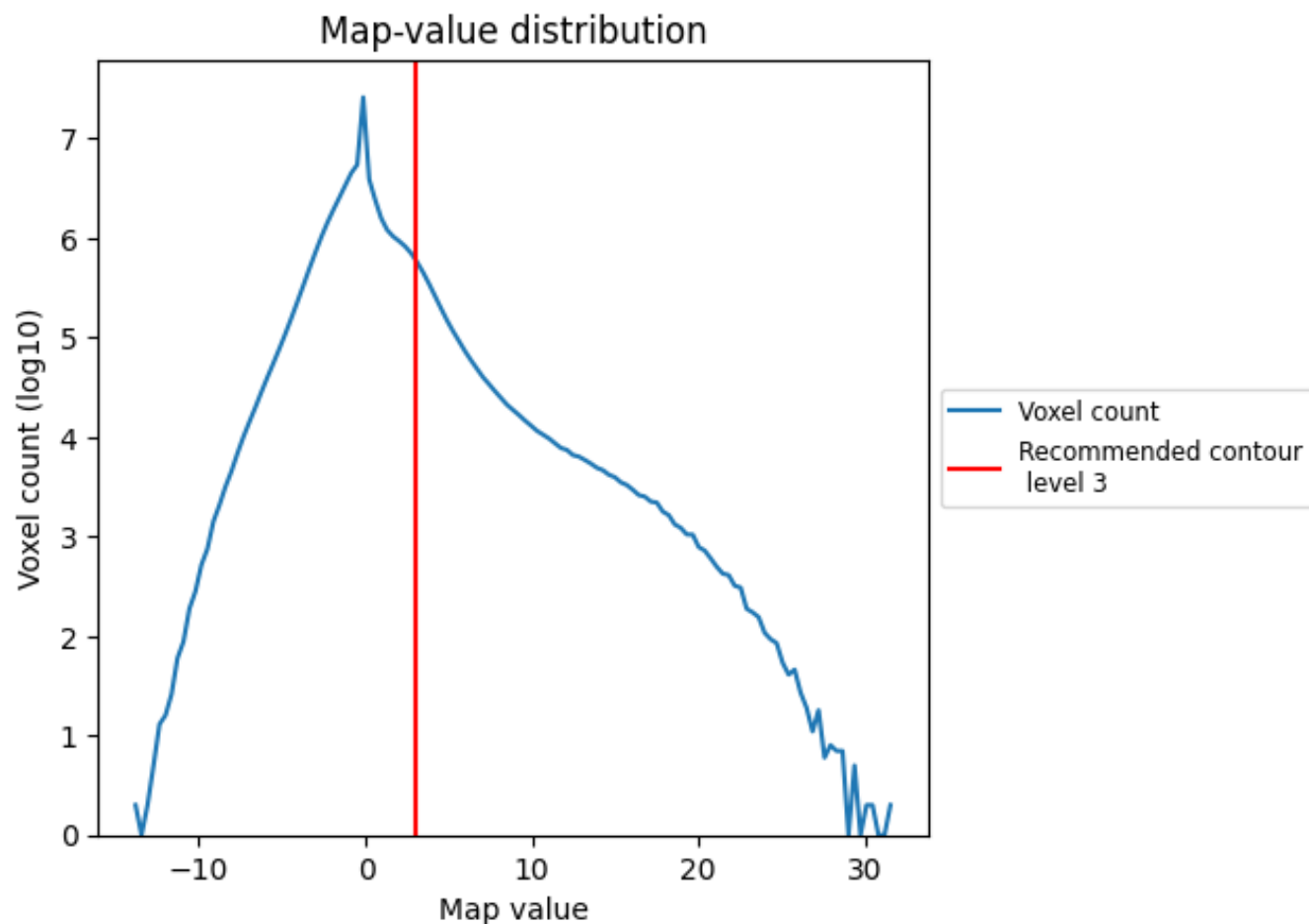
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

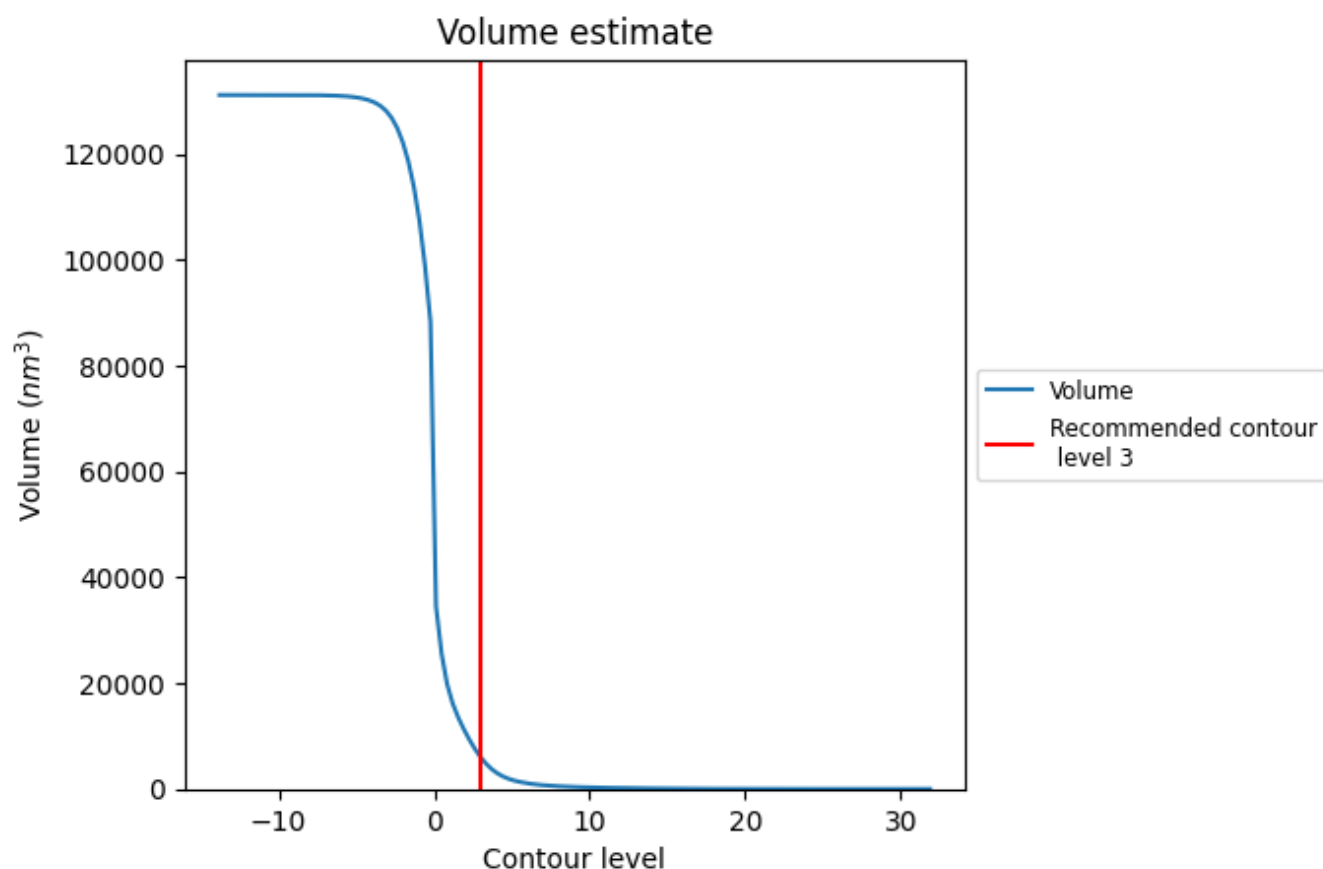
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

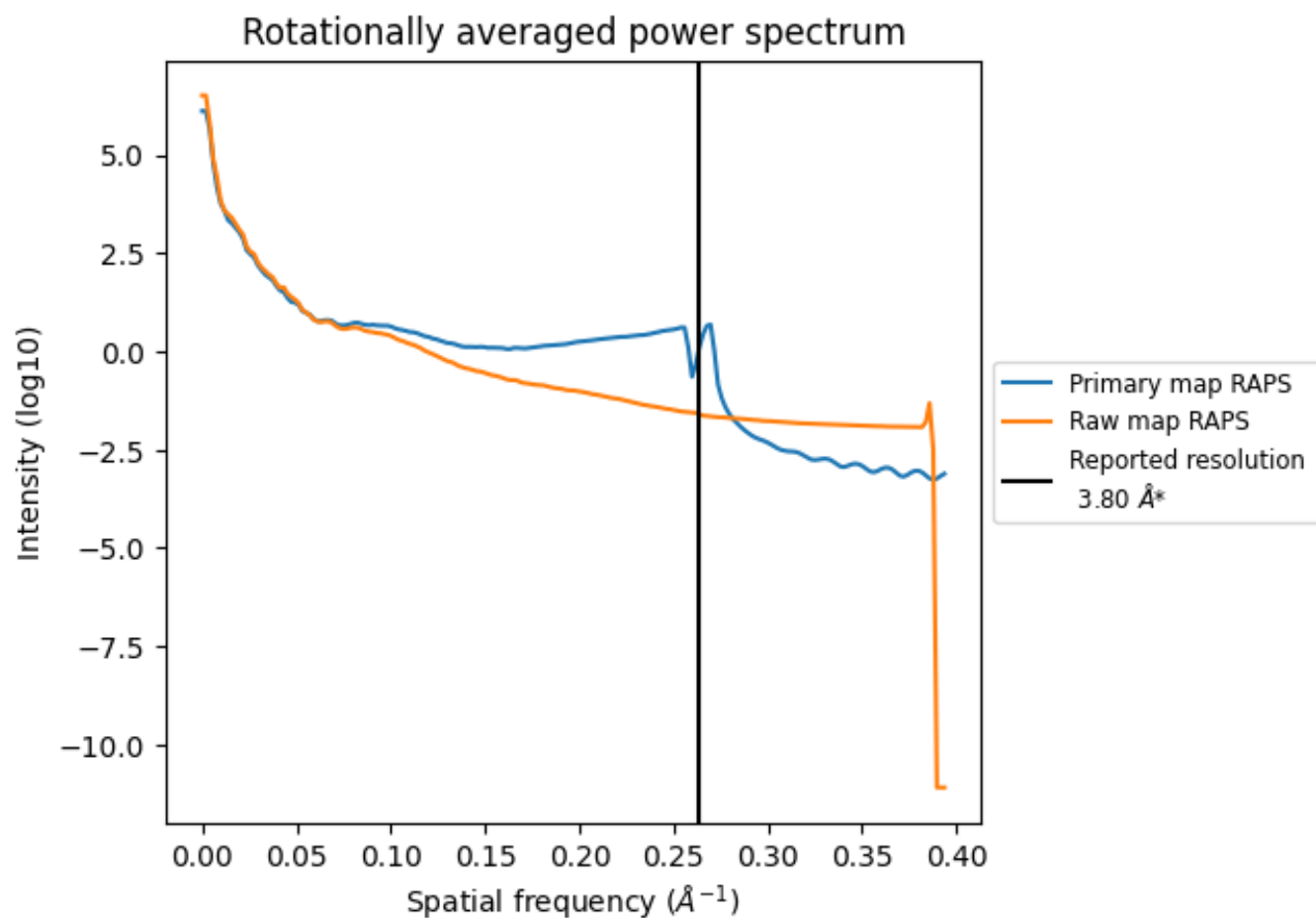
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5957 nm^3 ; this corresponds to an approximate mass of 5381 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 ⓘ

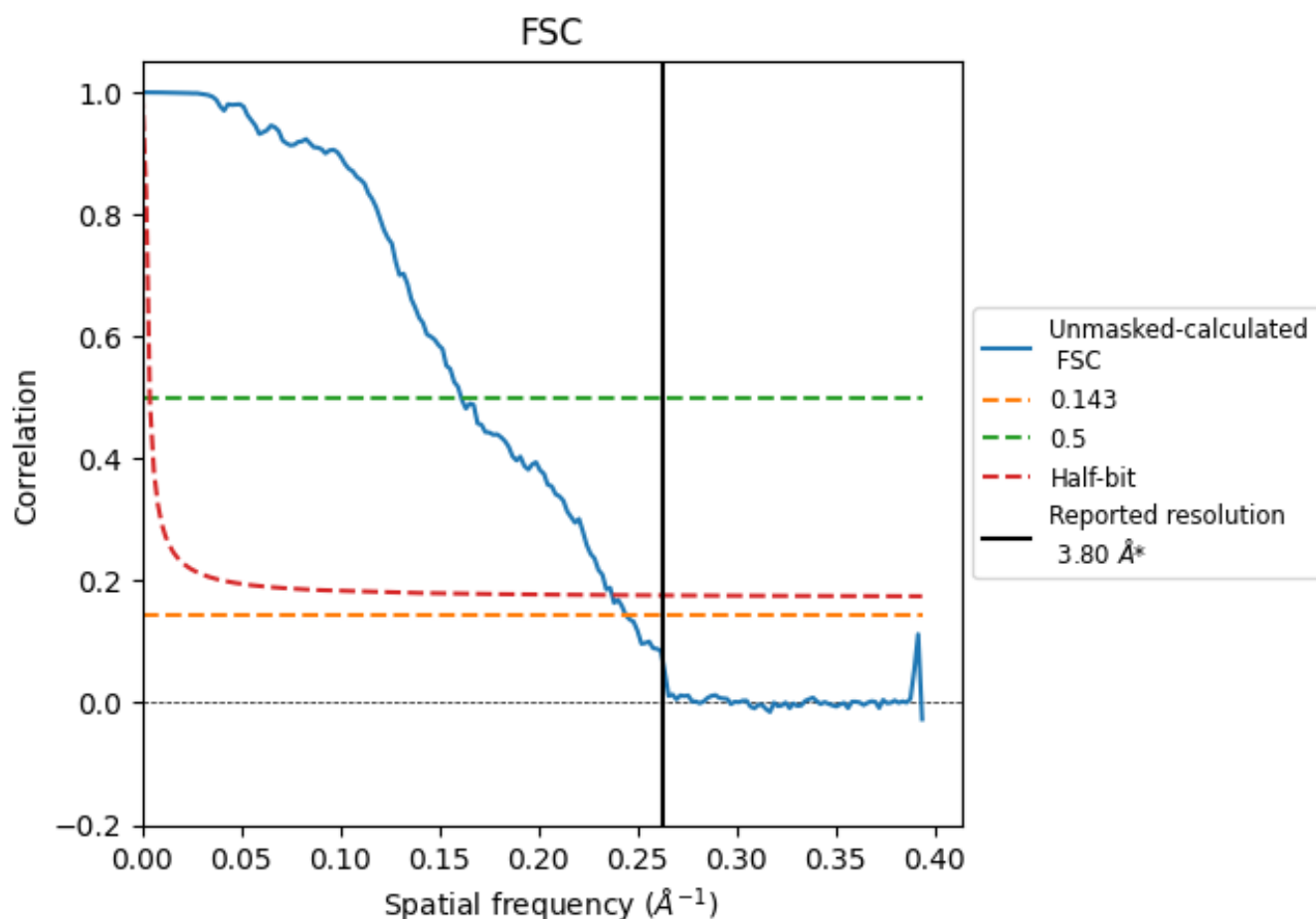


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.10	6.21	4.22

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

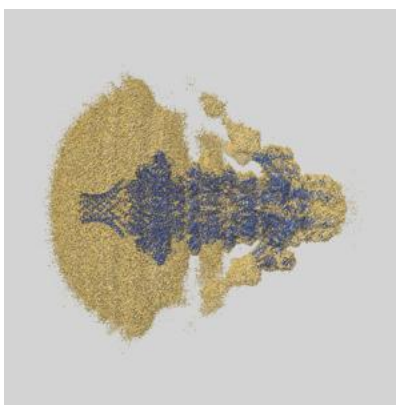
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36463 and PDB model 8JOV. Per-residue inclusion information can be found in section [3](#) on page [10](#).

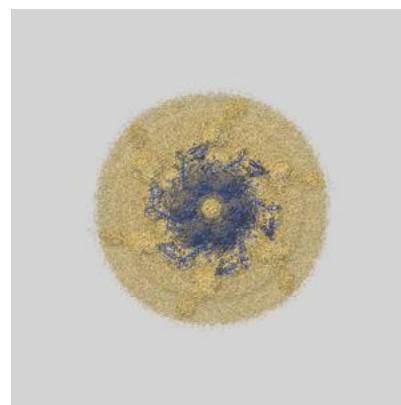
9.1 Map-model overlay [i](#)



X



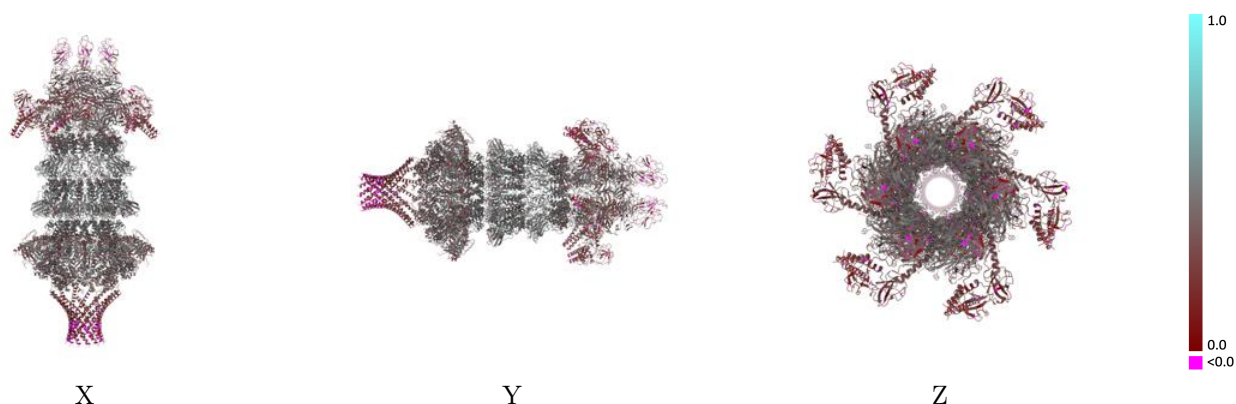
Y



Z

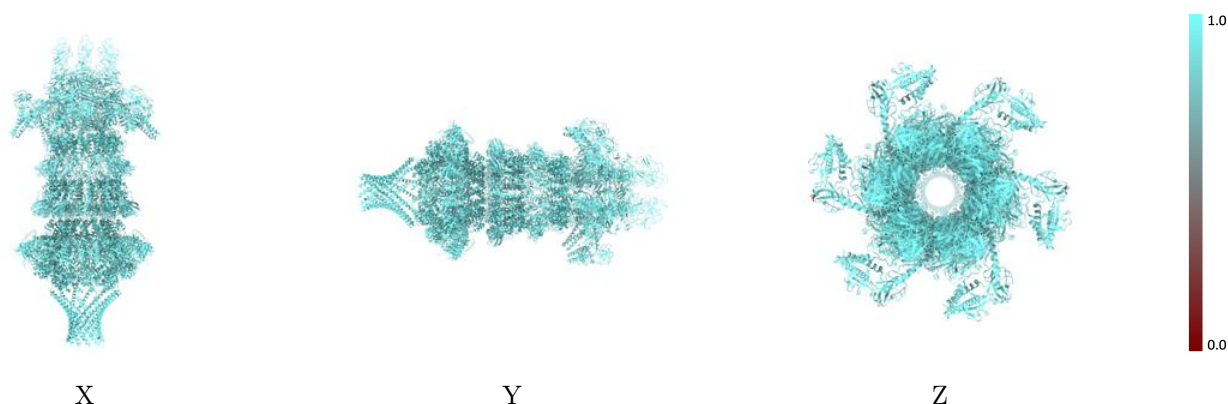
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



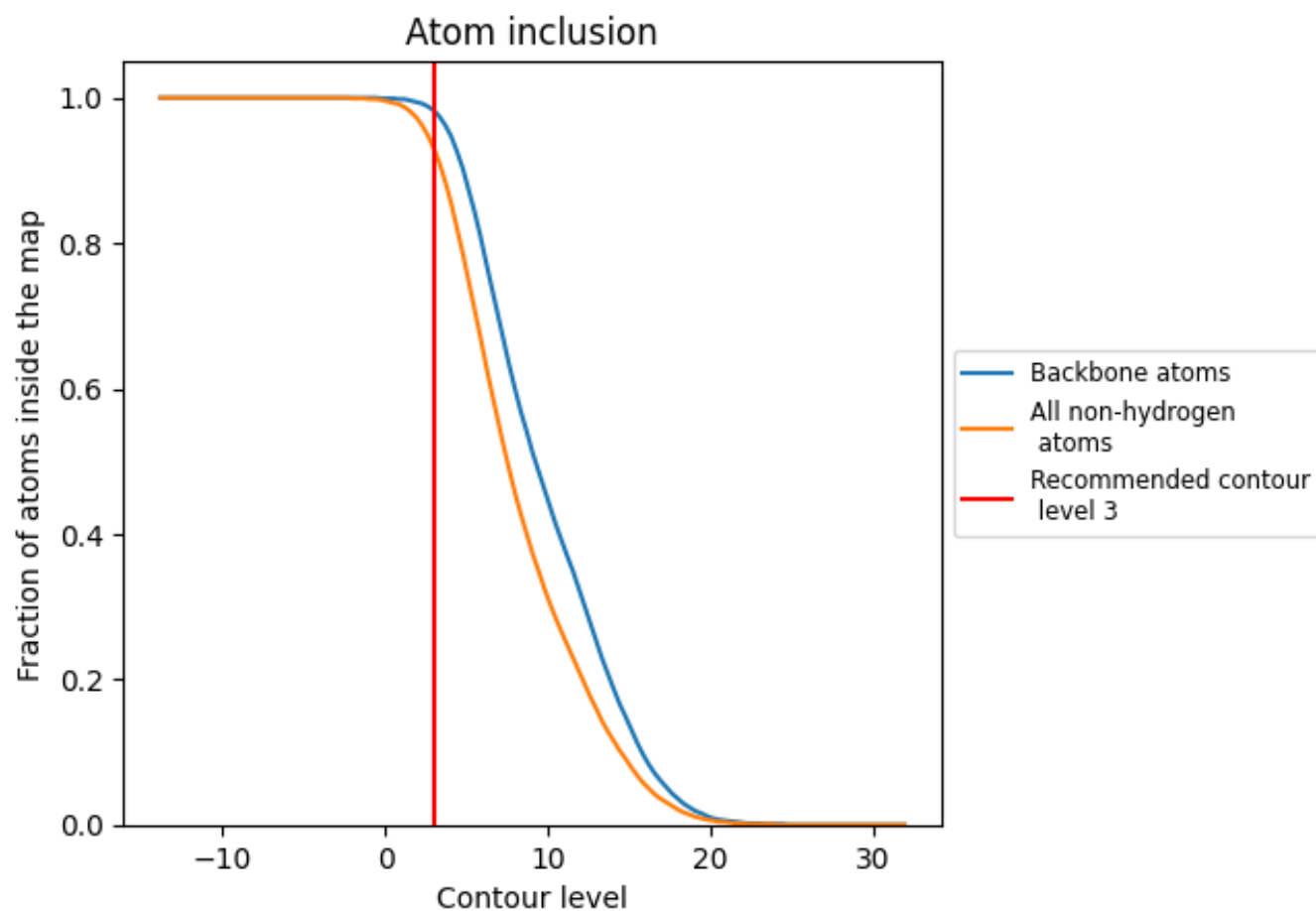
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9290	 0.4050
0	 0.9310	 0.4100
1	 0.8900	 0.2720
2	 0.9530	 0.4690
3	 0.9280	 0.4080
4	 0.9040	 0.3510
5	 0.9550	 0.4700
6	 0.9260	 0.4120
7	 0.9040	 0.2300
A	 0.9350	 0.3860
B	 0.9390	 0.3850
C	 0.9330	 0.3850
D	 0.9360	 0.3880
E	 0.9400	 0.3870
F	 0.9340	 0.3860
G	 0.9180	 0.4580
H	 0.9190	 0.4520
I	 0.9170	 0.4500
J	 0.9150	 0.4550
K	 0.9190	 0.4530
L	 0.9170	 0.4520
M	 0.9040	 0.2770
N	 0.9100	 0.3410
O	 0.9030	 0.2240
P	 0.8900	 0.2780
Q	 0.9010	 0.3440
R	 0.9040	 0.2240
S	 0.9310	 0.4620
T	 0.9560	 0.4550
U	 0.9270	 0.4060
V	 0.8850	 0.2670
W	 0.9240	 0.4530
X	 0.9580	 0.4570
Y	 0.9280	 0.4100
Z	 0.9080	 0.3480



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Chain	Atom inclusion	Q-score
a	 0.9240	 0.4570
b	 0.9530	 0.4550
c	 0.9280	 0.4070
d	 0.9040	 0.2370
e	 0.9290	 0.4610
f	 0.9570	 0.4560
g	 0.9300	 0.4110
h	 0.8970	 0.2730
i	 0.9210	 0.4530
j	 0.9530	 0.4540
k	 0.9250	 0.4060
l	 0.9050	 0.3390
m	 0.9270	 0.4590
n	 0.9510	 0.4500
o	 0.9260	 0.4110
p	 0.9060	 0.2290
q	 0.9530	 0.4670
r	 0.9310	 0.4080
s	 0.8940	 0.2790
t	 0.9550	 0.4690
u	 0.9250	 0.4090
v	 0.9050	 0.3440
w	 0.9550	 0.4700
x	 0.9260	 0.4080
y	 0.9140	 0.2330
z	 0.9560	 0.4690