



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 11:43 AM UTC

PDB ID : 8U11 / pdb_00008u11
EMDB ID : EMD-41792
Title : In situ cryo-EM structure of bacteriophage P22 gp1:gp5:gp4: gp10: gp9 N-term complex in conformation 2 at 3.1Å resolution
Authors : Iglesias, S.; Feng-Hou, C.; Cingolani, G.
Deposited on : 2023-08-30
Resolution : 3.10 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

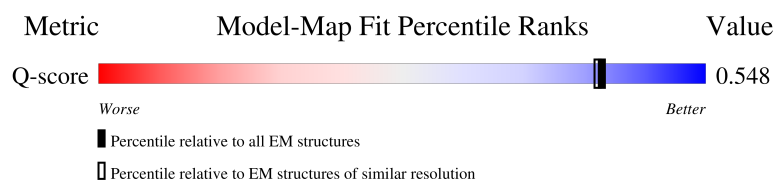
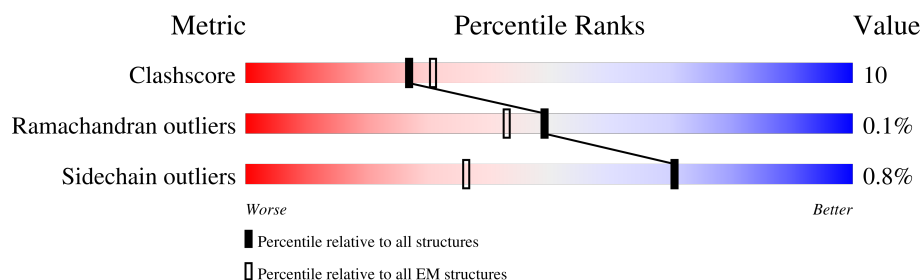
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	1	472	5% 74% 26%
1	2	472	8% 69% 31%
1	3	472	7% 76% 23%
1	4	472	5% 74% 26%

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Mol	Chain	Length	Quality of chain
1	5	472	
1	6	472	
2	10	667	
2	11	667	
2	12	667	
2	13	667	
2	14	667	
2	15	667	
2	16	667	
2	17	667	
2	18	667	
2	19	667	
2	20	667	
2	21	667	
2	22	667	
2	23	667	
2	24	667	
2	7	667	
2	8	667	
2	9	667	
3	a	725	
3	b	725	
3	c	725	
3	d	725	
3	e	725	

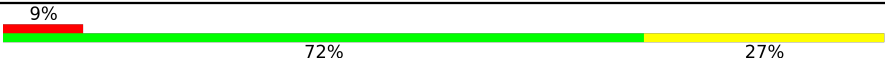
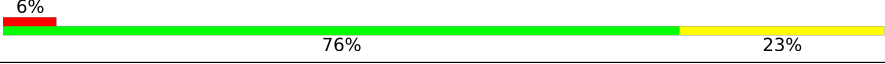
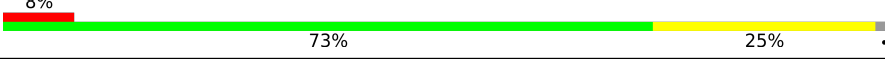
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Mol	Chain	Length	Quality of chain
3	f	725	
3	g	725	
3	h	725	
3	i	725	
3	j	725	
3	k	725	
3	l	725	
4	m	166	
4	n	166	
4	o	166	
4	p	166	
4	q	166	
4	r	166	
4	s	166	
4	t	166	
4	u	166	
4	v	166	
4	x	166	
4	y	166	
5	A	430	
5	B	430	
5	C	430	
5	D	430	
5	E	430	
5	F	430	

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Mol	Chain	Length	Quality of chain
5	G	430	
5	H	430	
5	I	430	
5	J	430	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 138386 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 Packaged DNA stabilization protein gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
1	2	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
1	3	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
1	4	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
1	5	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
1	6	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		

- Molecule 2 is a protein called Tail spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
2	8	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
2	9	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
2	10	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
2	11	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
2	12	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
2	13	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
2	14	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
2	15	120	Total	C	N	O	S	0	0
			934	595	156	182	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	16	120	Total 934	C 595	N 156	O 182	S 1	0	0
2	17	120	Total 934	C 595	N 156	O 182	S 1	0	0
2	18	120	Total 934	C 595	N 156	O 182	S 1	0	0
2	19	120	Total 934	C 595	N 156	O 182	S 1	0	0
2	20	120	Total 934	C 595	N 156	O 182	S 1	0	0
2	21	120	Total 934	C 595	N 156	O 182	S 1	0	0
2	22	120	Total 934	C 595	N 156	O 182	S 1	0	0
2	23	120	Total 934	C 595	N 156	O 182	S 1	0	0
2	24	120	Total 934	C 595	N 156	O 182	S 1	0	0

- Molecule 3 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	b	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	c	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	d	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	e	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	l	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	f	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	k	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	i	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	j	544	Total 4417	C 2791	N 756	O 850	S 20	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	h	544	Total	C	N	O	S	0	0
			4417	2791	756	850	20		
3	g	544	Total	C	N	O	S	0	0
			4417	2791	756	850	20		

- Molecule 4 is a protein called Peptidoglycan hydrolase gp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	y	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	m	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	n	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	o	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	p	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	q	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	r	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	s	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	t	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	u	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	v	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	x	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		

- Molecule 5 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	429	Total	C	N	O	S	0	0
			3277	2053	568	643	13		
5	C	429	Total	C	N	O	S	0	0
			3277	2053	568	643	13		
5	A	429	Total	C	N	O	S	0	0
			3277	2053	568	643	13		

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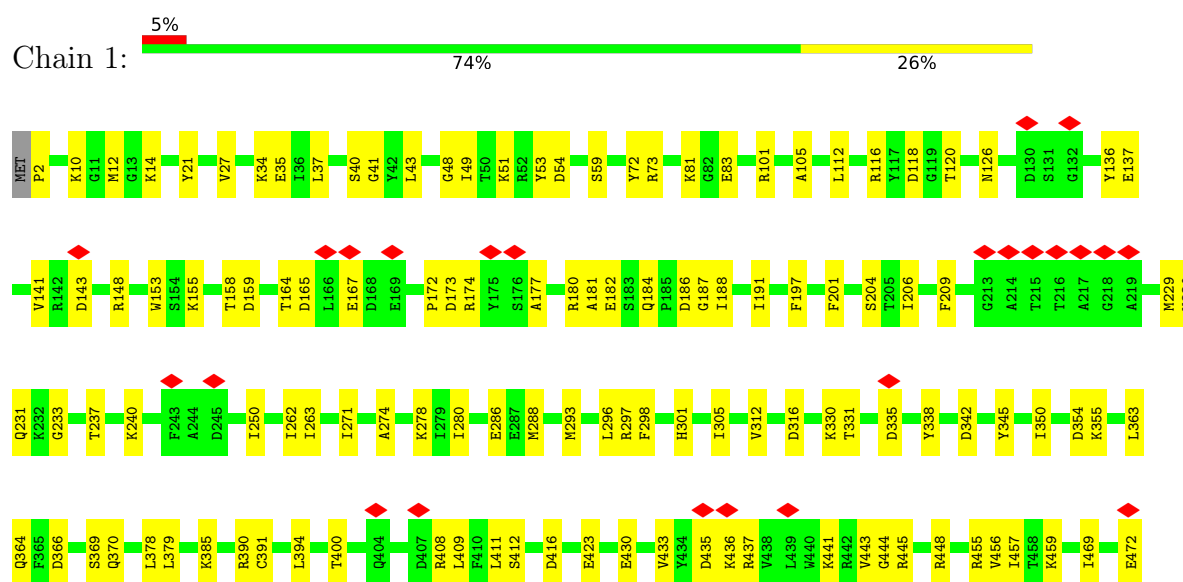
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	429	Total	C	N	O	S	0	0
			3277	2053	568	643	13		
5	I	429	Total	C	N	O	S	0	0
			3277	2053	568	643	13		
5	D	421	Total	C	N	O	S	0	0
			3219	2017	558	631	13		
5	B	421	Total	C	N	O	S	0	0
			3219	2017	558	631	13		
5	F	421	Total	C	N	O	S	0	0
			3219	2017	558	631	13		
5	H	421	Total	C	N	O	S	0	0
			3219	2017	558	631	13		
5	J	421	Total	C	N	O	S	0	0
			3219	2017	558	631	13		

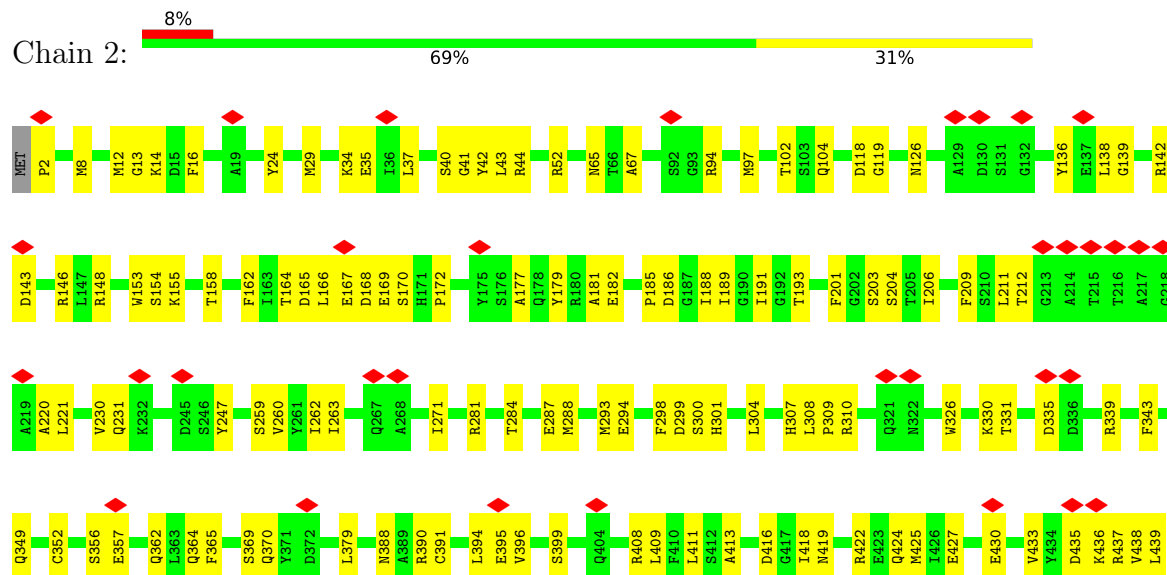
3 Residue-property plots

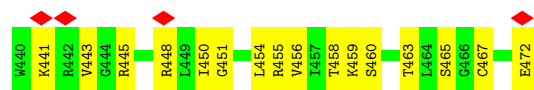
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Packaged DNA stabilization protein gp10

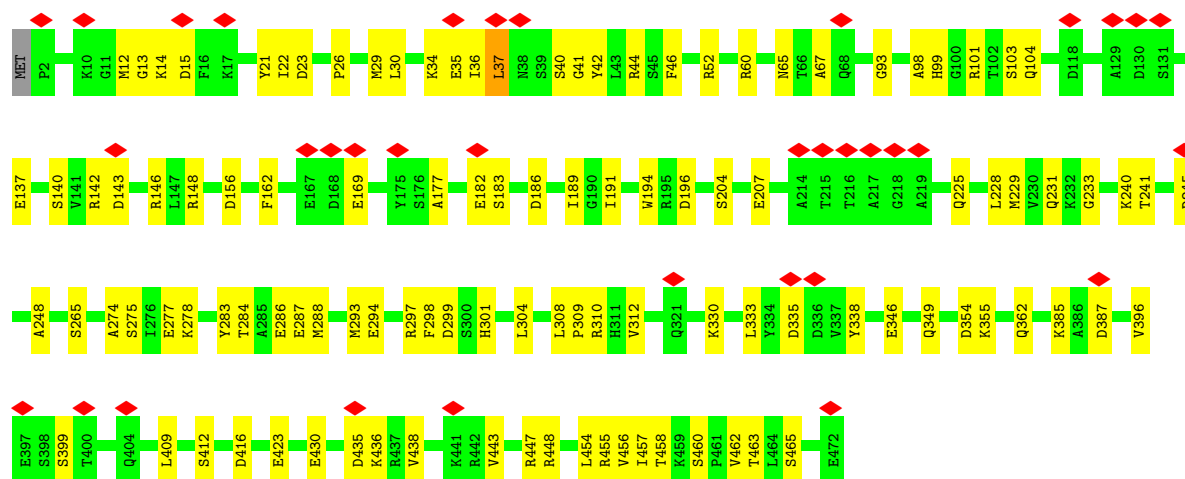
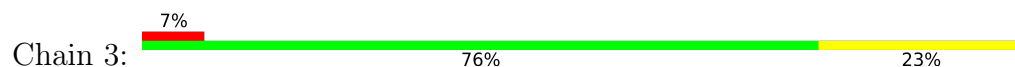


• Molecule 1: Packaged DNA stabilization protein gp10

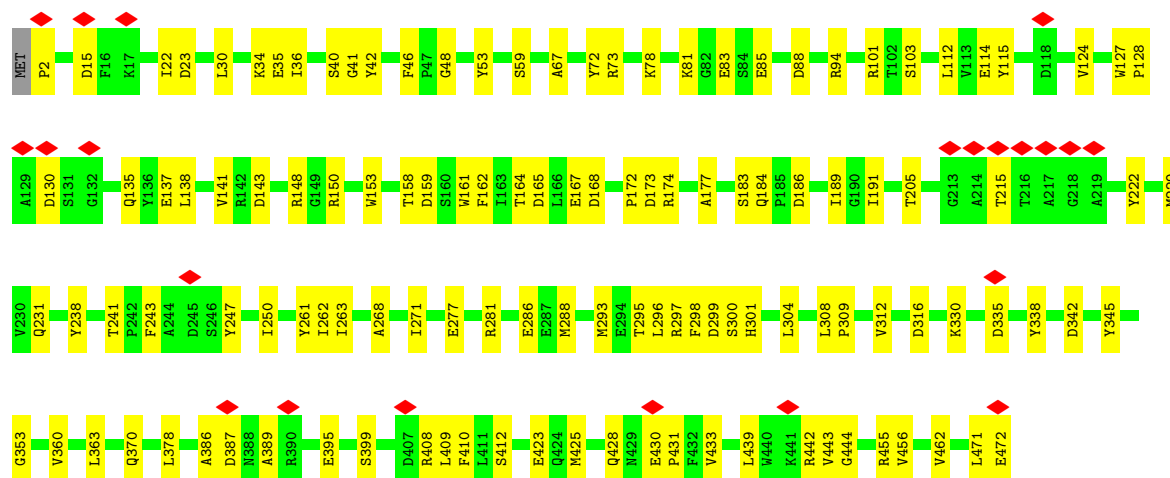
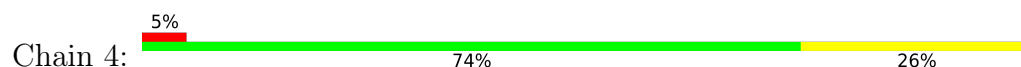




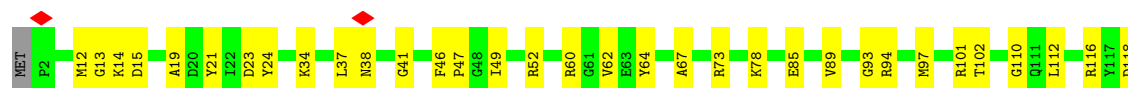
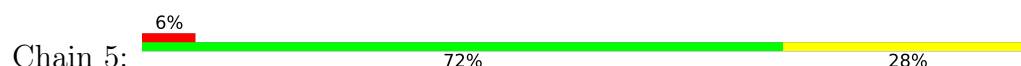
• Molecule 1: Packaged DNA stabilization protein gp10



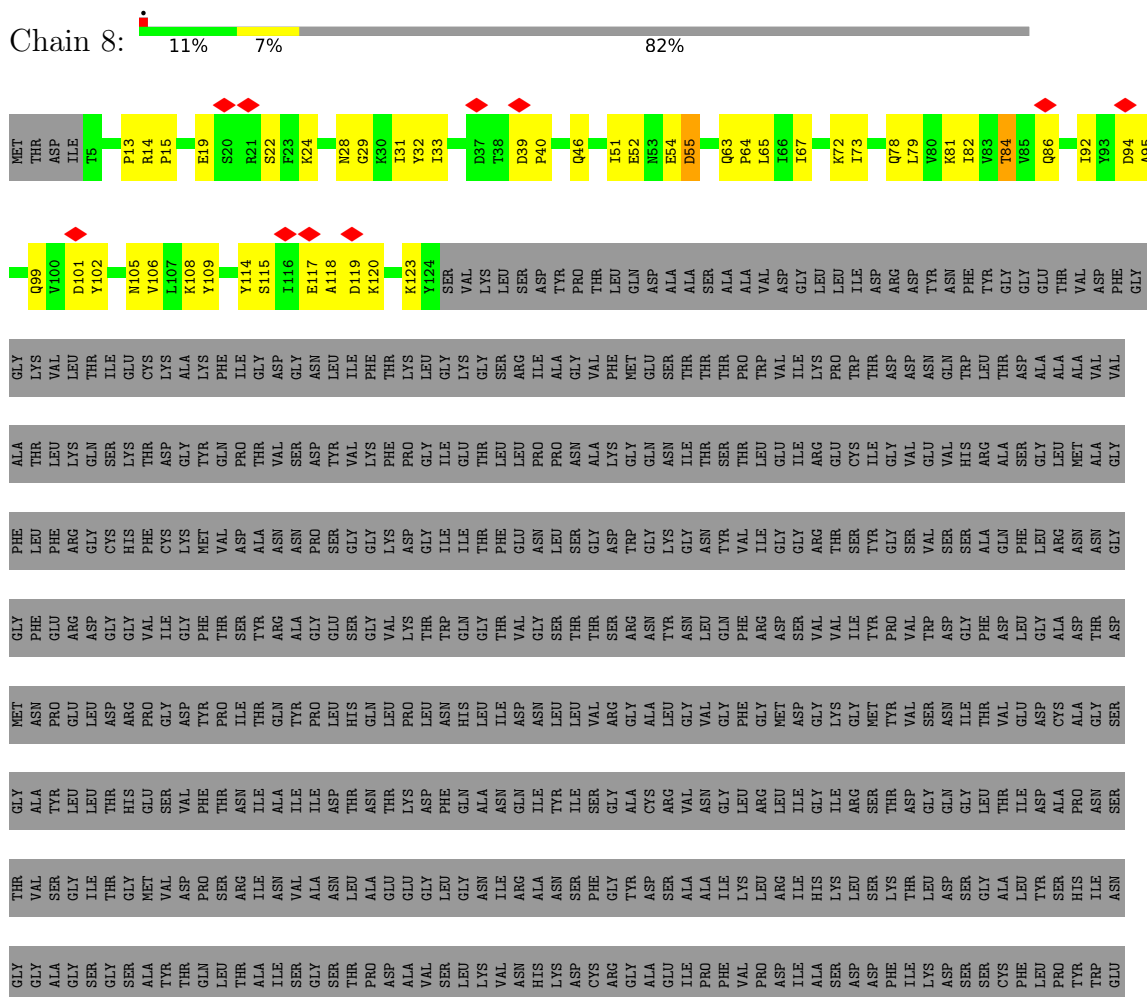
• Molecule 1: Packaged DNA stabilization protein gp10



• Molecule 1: Packaged DNA stabilization protein gp10



- Molecule 2: Tail spike protein



- Molecule 2: Tail spike protein

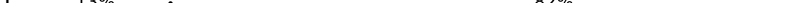
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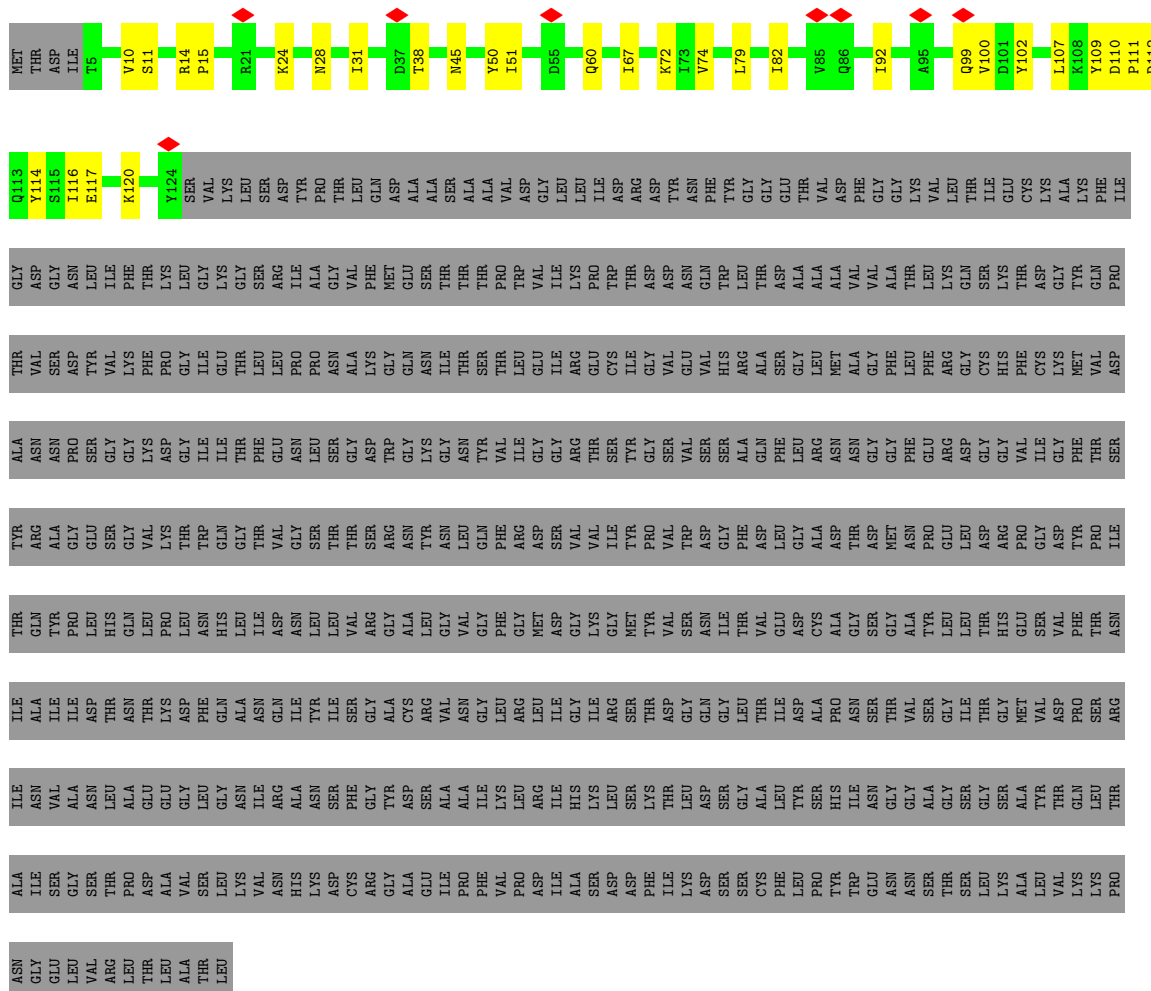
- Molecule 2: Tail spike protein

Protein	Amino Acid	Position
LEU	THR	1
ASP	ALA	2
ALA	VAL	3
ALA	ASP	4
VAL	PHE	5
VAL	GLY	6
ALA	GLY	7
THR	LYS	8
LEU	VAL	9
LYS	LEU	10
GLN	THR	11
SER	ILE	12
LYS	GLU	13
THR	CYS	14
ASP	LYS	15
GLY	ALA	16
TYR	LYS	17
GLN	PHE	18
PRO	ILE	19
THR	GLY	20
VAL	ASP	21
SER	GLY	22
ASP	ASN	23
TYR	LEU	24
VAL	ILE	25
PHE	PHE	26
PRO	LYS	27
GLY	LEU	28
ILE	GLY	29
GLU	LYS	30
THR	GLY	31
LEU	ARG	32
LEU	ILE	33
PRO	ALA	34
ASN	GLY	35
ALA	VAL	36
LYS	PHE	37
GLY	MET	38
GLN	GLU	39
ASN	SER	40
ILE	THR	41
THR	THR	42
SER	THR	43
THR	PRO	44
LEU	TRP	45
GLU	VAL	46
ILE	ILE	47
ARG	LYS	48
GLU	PRO	49
CYS	TRP	50
ILE	THR	51
GLY	ASP	52
VAL	ASN	53
GLU	VAL	54
HIS	TRP	55
MET	THR	56
ASP	ILE	57
T5	A6	58
S11	R14	59
F17	R21	60
K24	N28	61
G29	K30	62
I31	G34	63
Q35	I36	64
D37	T38	65
D39	P40	66
V41	N42	67
A44	P43	68
N45	LEU	69
Q46	SER	70
I47	ASP	71
P48	TYR	72
V49	PRO	73
Y50	THR	74
I51	THR	75
E52	GLM	76
N53	ASP	77
E54	ALA	78
D55	SER	79
G56	ALA	80
S57	ALA	81
H58	VAL	82
V59	ASP	83
Q63	GLY	84
P64	LEU	85
L65	ILE	86
I66	ASP	87
I67	ARG	88
N68	ASN	89
A69	TYR	90
V74	ASN	91
Y75	PHE	92
V76	TYR	93

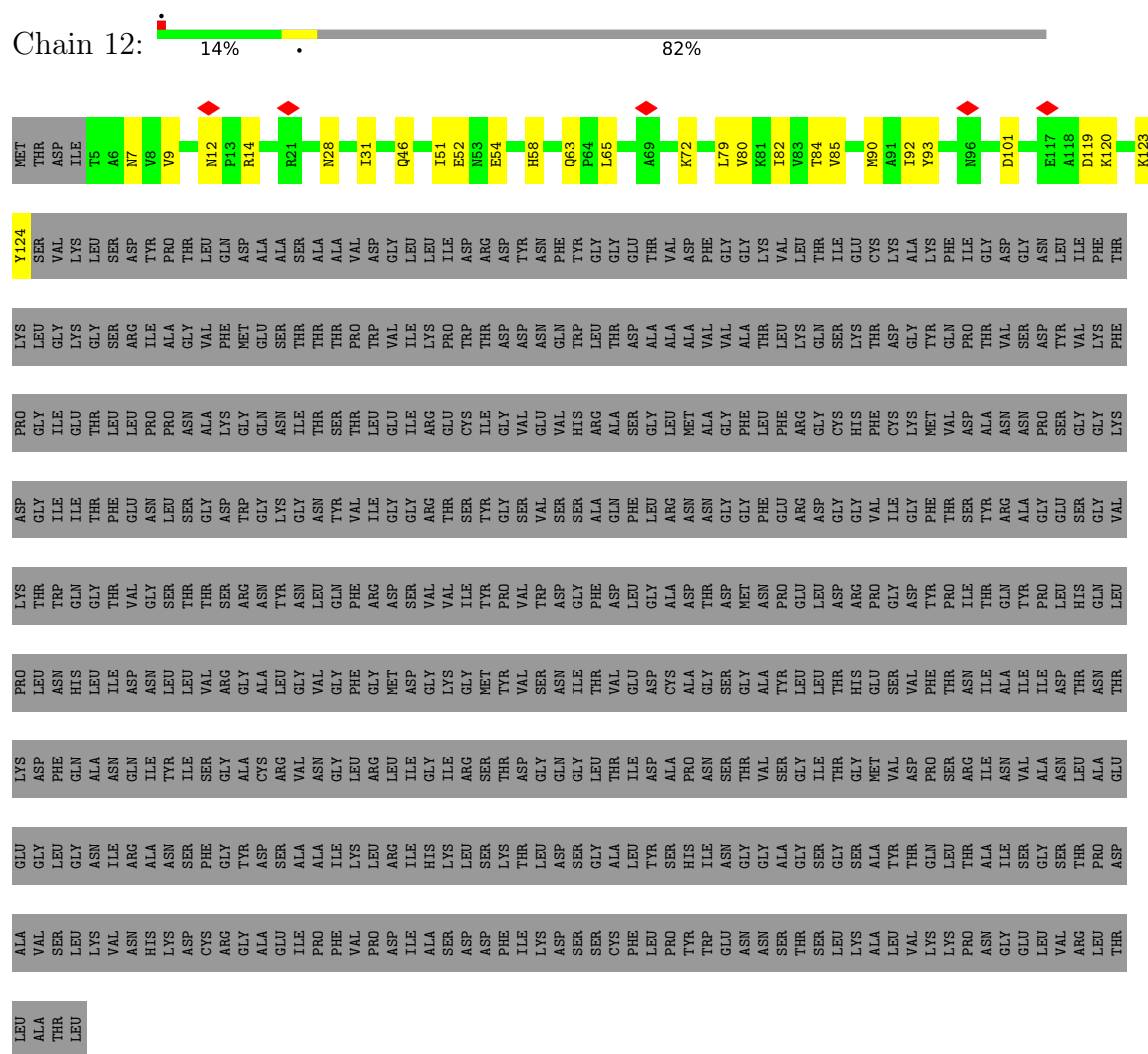
[illegible]

- Molecule 2: Tail spike protein

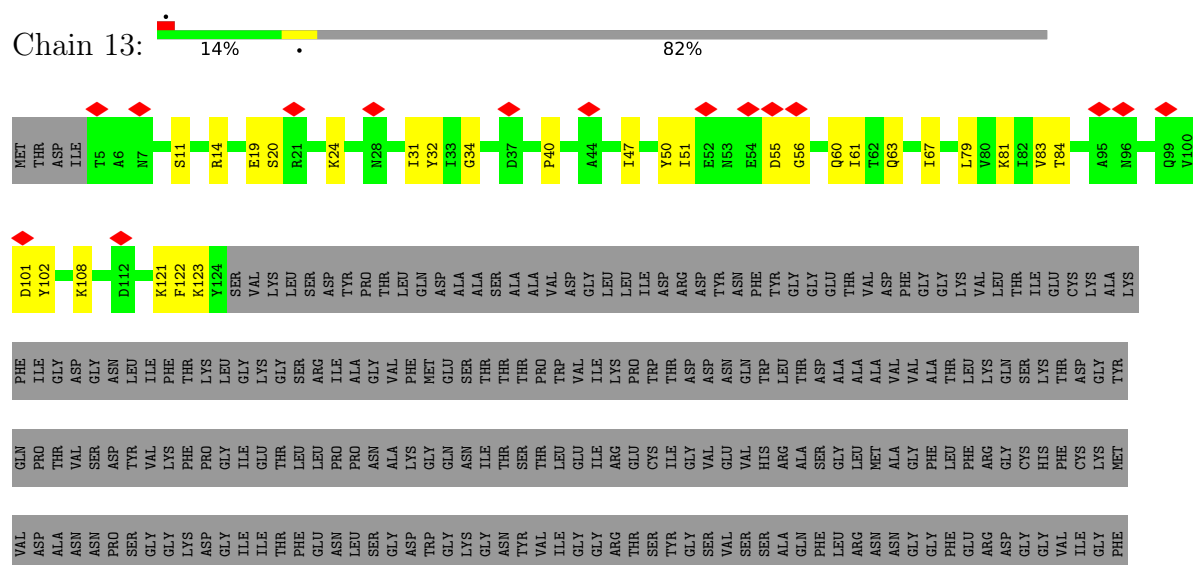
Chain 11:  13% 82%



● Molecule 2: Tail spike protein



● Molecule 2: Tail spike protein





[illegible]

- Molecule 2: Tail spike protein



- Molecule 2: Tail spike protein





[illegible]

- Molecule 2: Tail spike protein



LEU	THR	THR	LEU	LEU	ALA	PRO	ALA	ASN	GLN	GLY	GLY	LYS	PHE	THR	MET
THR	ASP	ASP	GLU	GLU	GLU	ASP	THR	THR	LEU	VAL	VAL	PHE	THR	THR	THR
LEU	ALA	ALA	GLY	GLY	GLY	VAL	LEU	LEU	LEU	THR	THR	GLY	LEU	LEU	ILE
THR	SER	SER	LEU	GLN	GLN	PHE	ASN	ASN	HIS	TRP	ILE	ILE	GLY	GLY	T5
LEU	LYS	LYS	ASN	ASN	ASN	ALA	ALA	GLN	GLN	GLY	THR	THR	LYS	LYS	A6
VAL	VAL	VAL	ARG	ARG	ARG	ASN	ASN	VAL	ILE	THR	THR	THR	LEU	LEU	N7
ASN	ASN	ASN	ALA	ALA	ILE	ILE	ASN	GLY	GLY	ASP	ASP	ARG	SER	SER	N8
HIS	HIS	HIS	ALA	ALA	ALA	ALA	ILE	ASN	ASN	ASN	PRO	ILE	TYR	TYR	Y9
LYS	LYS	LYS	ASN	ASN	THR	THR	LEU	SER	SER	SER	PRO	ALA	ALA	PRO	P15
ASP	ASP	ASP	SER	SER	ILE	ILE	LEU	THR	THR	THR	ASN	GLY	GLY	THR	P15
CYS	CYS	CYS	PHE	PHE	THR	SER	VAL	VAL	VAL	GLY	ASN	VAL	VAL	LEU	S20
ARG	ARG	GLY	THR	GLY	THR	GLY	ARG	GLY	ARG	TRP	LYS	PHE	PHE	GLN	K21
ALA	ALA	ALA	ASP	ASP	ASP	CYS	VAL	VAL	VAL	ASN	GLN	GLU	GLU	ALA	S22
SER	SER	SER	SER	SER	ARG	ARG	ARG	LEU	LEU	LYS	ASN	SER	SER	ALA	F23
ILE	ILE	ILE	ALA	ALA	VAL	VAL	VAL	GLY	GLY	GLY	ILE	THR	THR	SER	K24
PRO	PRO	PHE	ALA	ASN	ASN	GLY	GLY	VAL	PHE	ASN	THR	THR	THR	ALA	A27
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	MET	ARG	ILE	LEU	TRP	VAL	ASP	N28
ALA	ALA	HIS	HIS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ILE	VAL	VAL	GLY	Y32
SER	SER	LYS	LYS	LYS	LYS	LYS	VAL	THR	THR	THR	GLU	GLU	THR	LEU	
ASP	ASP	ASP	LEU	LEU	ARG	ARG	ASN	ASN	THR	THR	ILE	ILE	ILE	LEU	
PHE	PHE	LYS	THR	THR	THR	THR	VAL	VAL	PHE	PRO	GLY	GLY	GLY	LEU	
ILE	ILE	THR	LEU	LEU	THR	THR	ASN	ASN	ASN	THR	SER	VAL	ASN	TYR	D37
LYS	LYS	ASP	LEU	GLN	GLN	GLN	ASN	ASN	GLY	VAL	GLU	GLU	ASN	ASN	T38
SER	SER	SER	SER	ILE	ILE	ILE	ILE	ILE	SER	ILE	THR	THR	TRP	ASP	D39
ASP	ASP	ASP	SER	SER	SER	SER	SER	THR	THR	PRO	TYR	THR	THR	ARG	P40
PHE	PHE	LYS	THR	THR	THR	THR	THR	THR	TYR	ASN	GLY	GLY	ASP	ASP	V41
ILE	ILE	THR	LEU	LEU	THR	THR	VAL	VAL	VAL	VAL	SER	VAL	ASP	TYR	N42
LYS	LYS	ASP	LEU	GLN	GLN	GLN	ASN	ASN	GLY	THR	VAL	GLN	ASN	ASN	
SER	SER	SER	SER	GLY	GLY	GLY	ILE	ILE	SER	GLY	ALA	TRP	PHE	THR	Q46
CYS	CYS	GLY	ALA	THR	THR	LEU	LEU	THR	PHE	PHE	ASP	GLN	ALA	GLY	LE1
PHE	PHE	LEU	LEU	ILE	ILE	GLU	GLU	VAL	LEU	LEU	THR	ASP	ALA	THR	E52
LEU	LEU	TYR	TYR	ASP	ASP	ASP	ASP	GLY	TYR	GLY	GLY	GLY	ALA	THR	
PRO	PRO	SER	SER	ALA	ALA	CYS	CYS	ALA	ALA	ARG	LEU	LEU	ALA	VAL	
TYR	TYR	HIS	HIS	PRO	ASN	ASN	ALA	ASN	ASN	ASN	ASN	NET	ALA	ASP	
TRP	TRP	ILE	ILE	ASN	ASN	GLY	GLY	THR	THR	ASN	ASN	ALA	VAL	PHE	Q63
GLU	GLU	ASN	ASN	SER	SER	SER	SER	GLY	ASN	GLY	GLY	VAL	VAL	GLY	P64
ASN	ASN	GLY	GLY	THR	THR	GLY	GLY	THR	GLY	THR	GLY	PHE	ALA	GLY	L65
SER	SER	ALA	ALA	SER	VAL	ASN	VAL	PHE	ALA	PHE	PHE	LEU	THR	LYS	L66
THR	THR	GLY	GLY	GLY	GLY	TYR	TYR	ARG	LEU	ARG	THR	PHE	LEU	VAL	L67
SER	SER	SER	SER	ILE	ILE	LEU	LEU	ASP	GLY	ASP	GLY	GLY	LYS	LEU	
LEU	LEU	GLY	GLY	THR	THR	THR	THR	THR	THR	LEU	GLN	GLN	THR	THR	I73
ALA	ALA	ALA	ALA	ALA	ALA	GLU	GLY	PRO	HIS	ARG	GLY	CYS	SER	ILE	
LEU	LEU	TYR	TYR	VAL	VAL	SER	VAL	VAL	SER	VAL	ILE	CYS	THR	THR	K81
VAL	VAL	THR	THR	ASP	ASP	PRO	PHE	THR	PHE	THR	GLY	LYS	GLY	GLY	T82
LYS	LYS	GLN	GLN	PRO	PRO	THR	THR	THR	PHE	THR	GLY	LYS	LYS	ALA	
THR	THR	THR	THR	THR	THR	THR	THR	THR	PHE	THR	GLY	GLY	GLY	LYS	Q86
LYS	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	LYS	
PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLN	K108
ASN	ASN	ALA	ALA	ILE	ILE	ILE	ILE	THR	THR	TYR	GLY	GLY	GLY	THR	Y109
GLY	GLY	ILE	ILE	ASN	ASN	ALA	ALA	GLN	GLN	ARG	ASN	ASN	VAL	ASP	D112
GLU	GLU	SER	SER	VAL	VAL	ILE	ILE	TYR	TYR	ALA	ASN	ASN	SER	GLY	
LEU	LEU	GLY	GLY	ALA	ALA	ILE	ILE	PRO	PRO	GLY	PRO	PRO	ASP	ASN	S115
VAL	VAL	SER	SER	SER	ASN	ASN	ASN	GLU	GLY	GLY	GLY	GLY	THR	LEU	I116
ARG	ARG	THR	THR	THR	THR	THR	THR	THR	SER	SER	SER	SER	VAL	ILE	E117
															A118
															P119

- Molecule 2: Tail spike protein



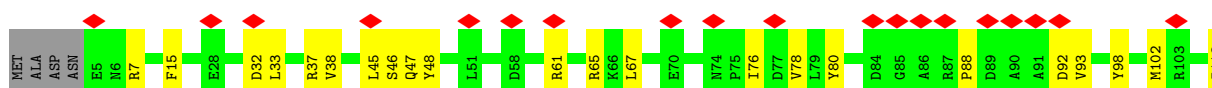
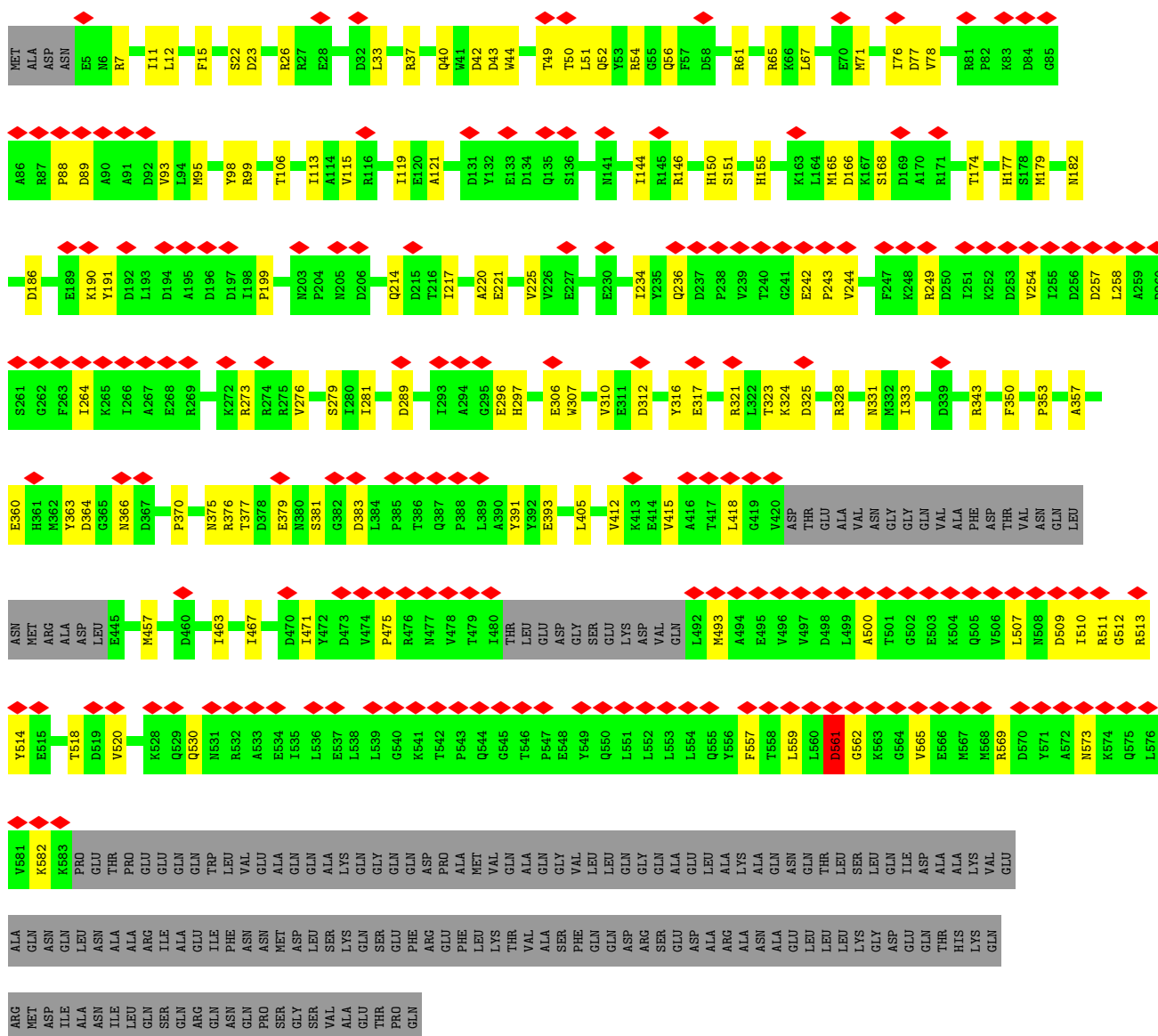
[illegible]

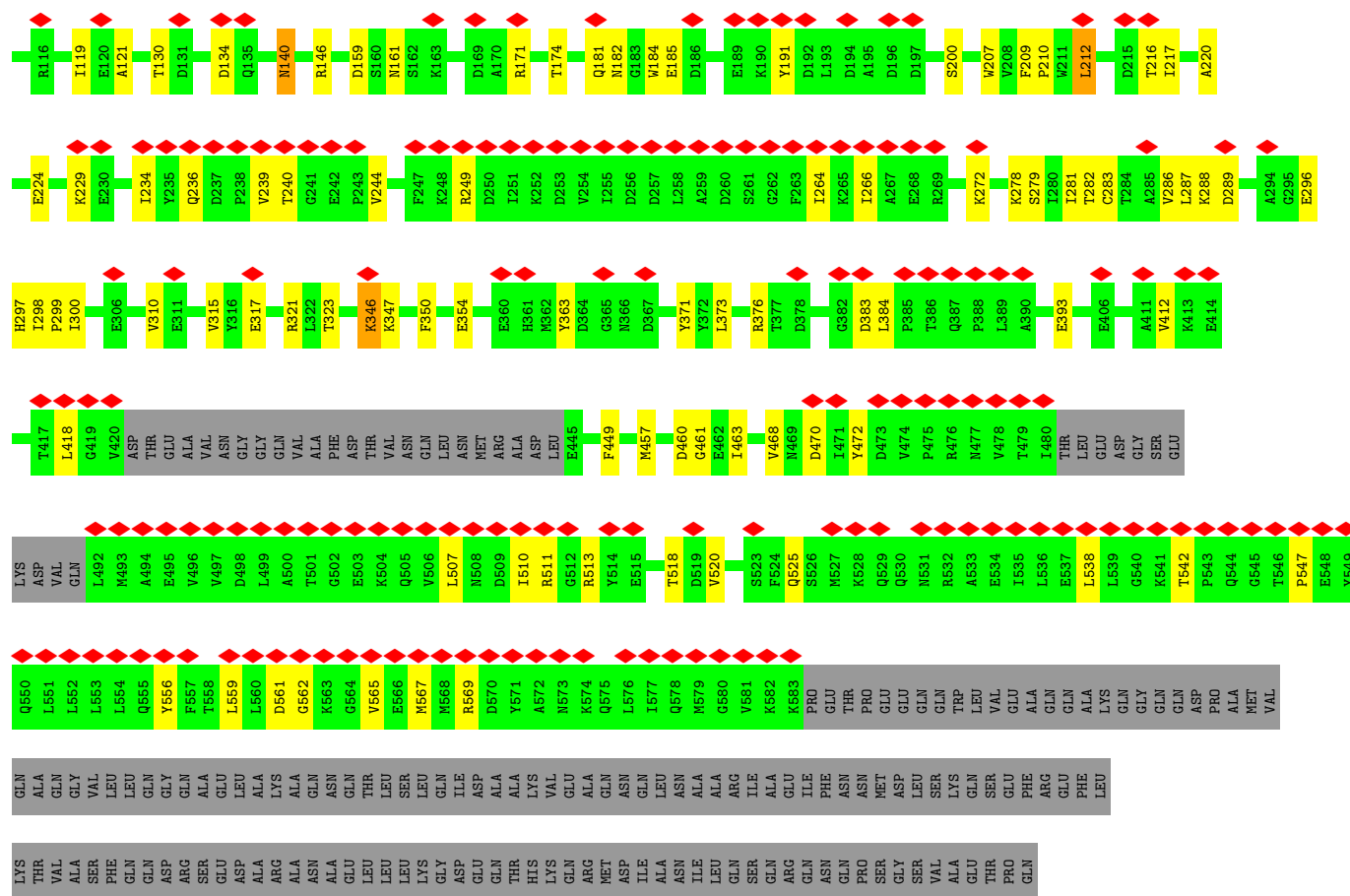
- Molecule 2: Tail spike protein



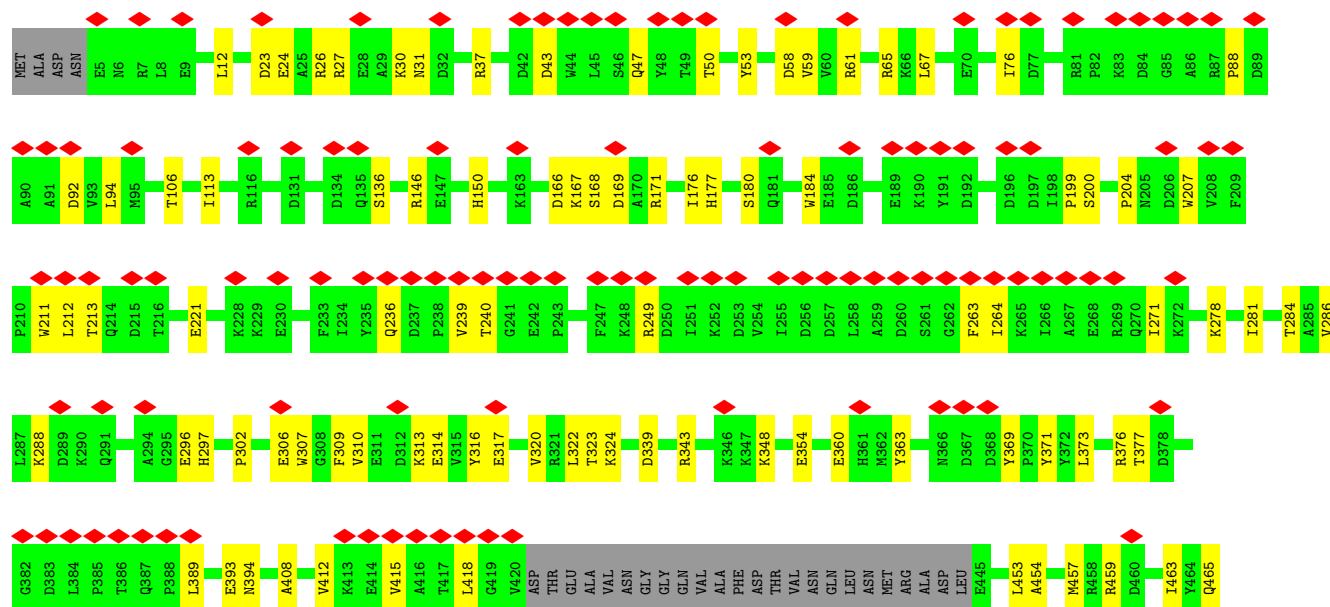
- Molecule 2: Tail spike protein

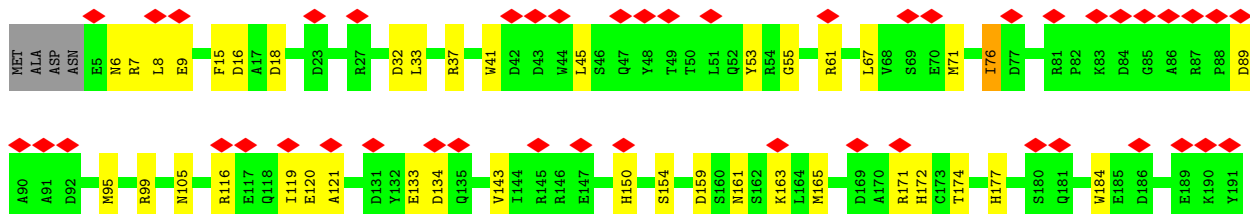


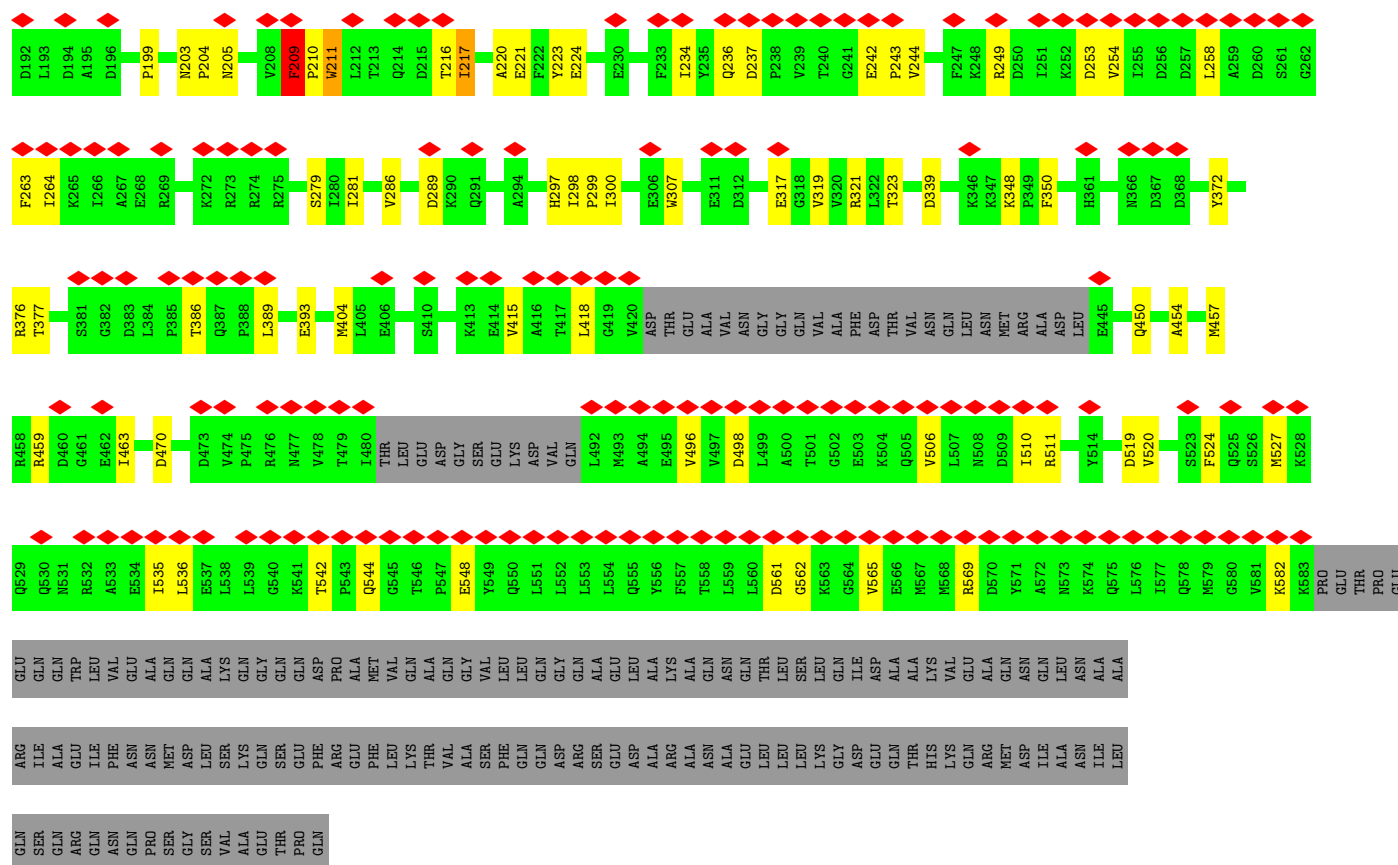




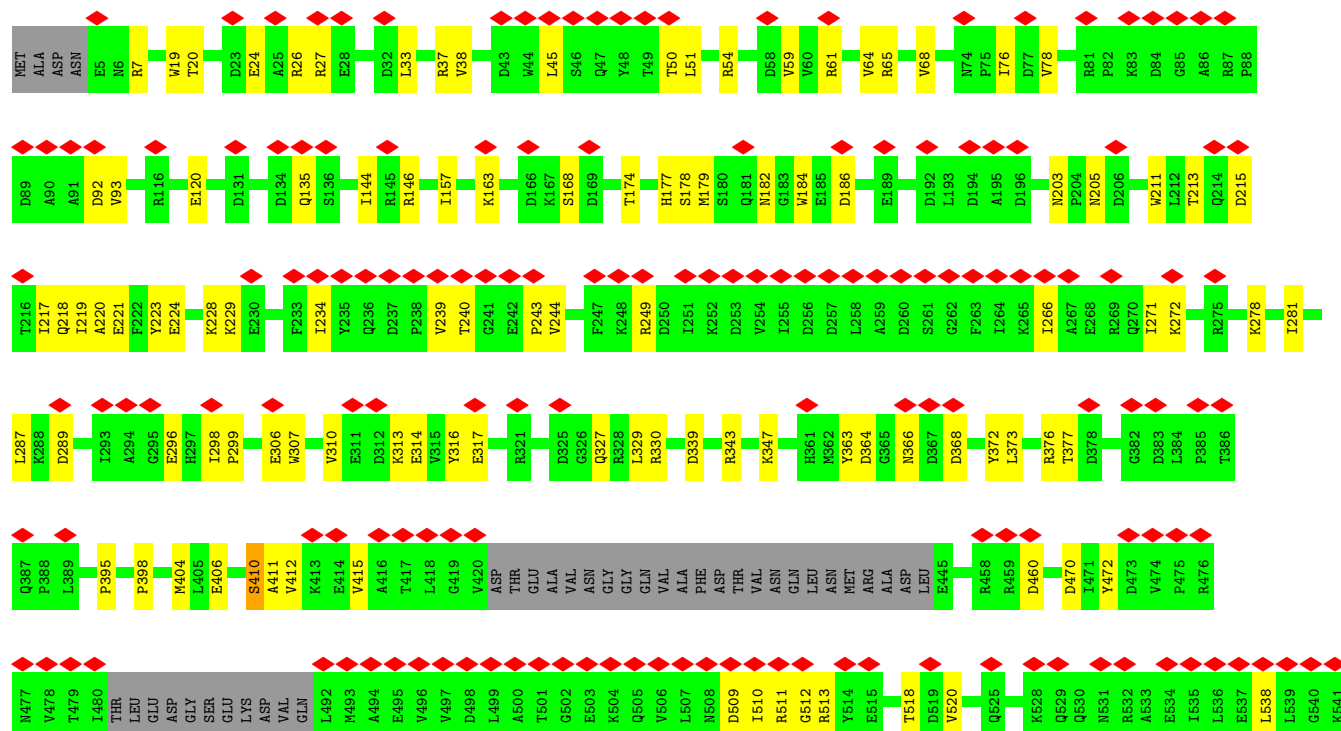
• Molecule 3: Portal protein

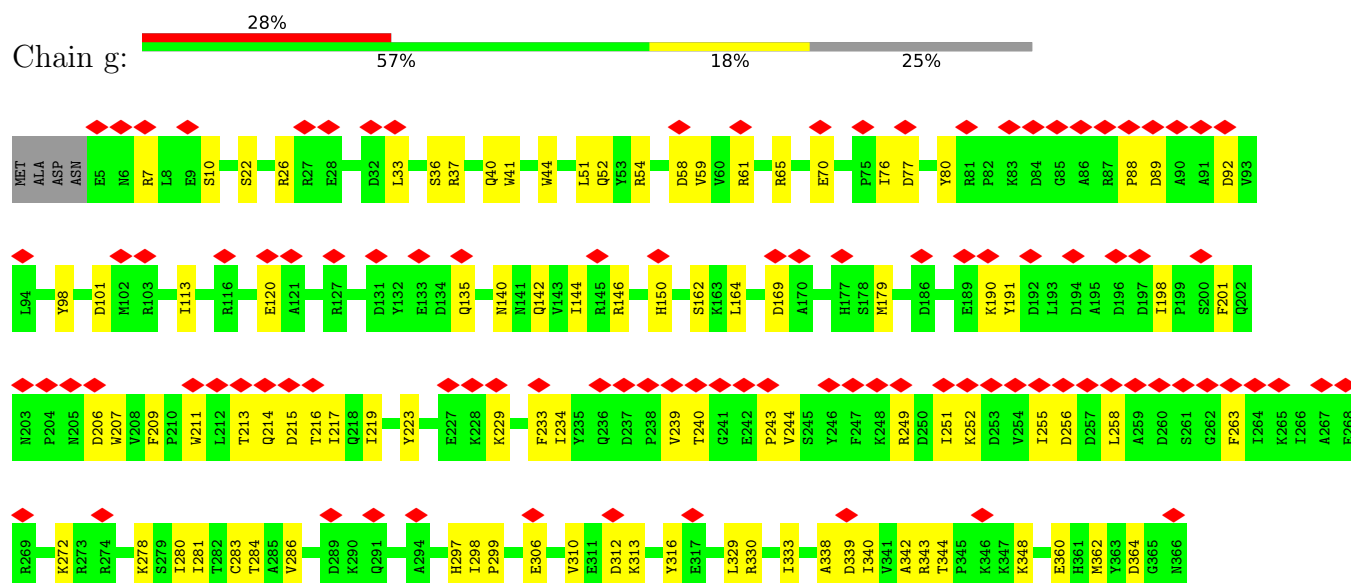
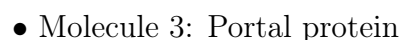


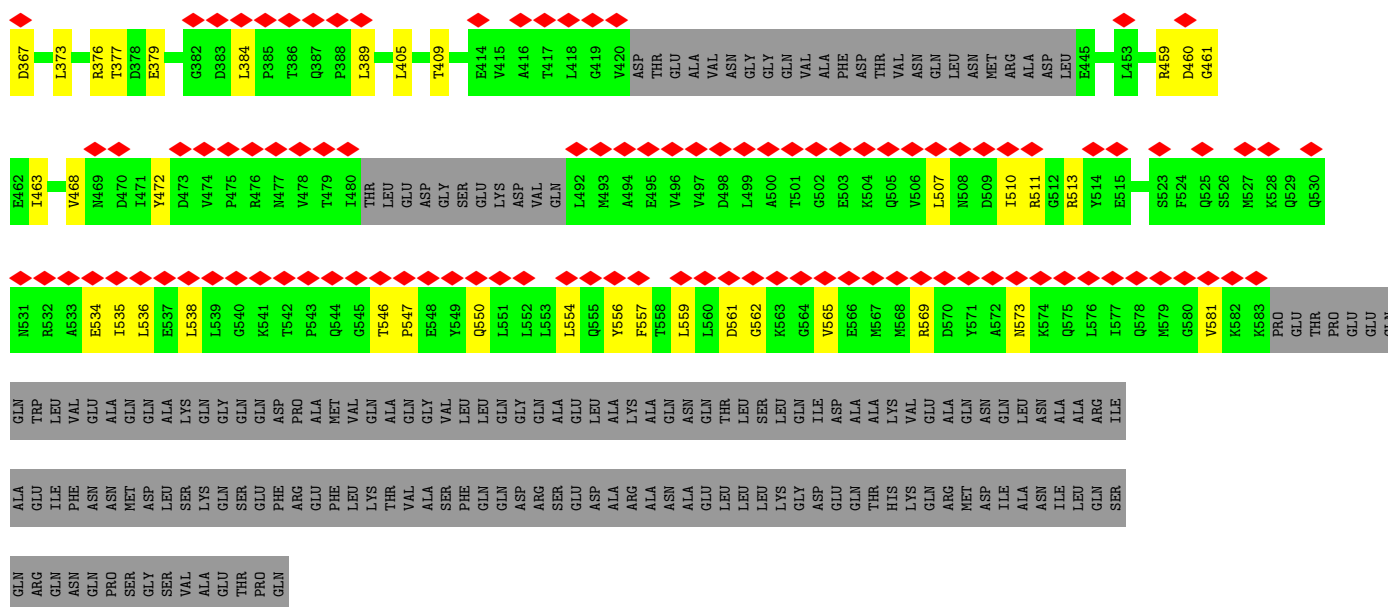




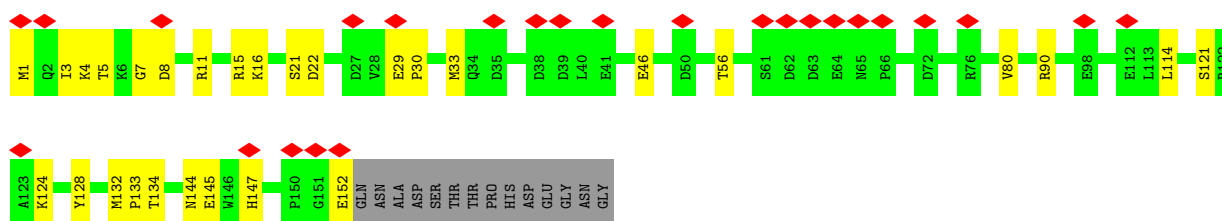
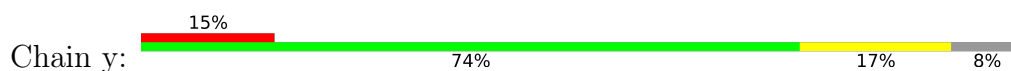
• Molecule 3: Portal protein



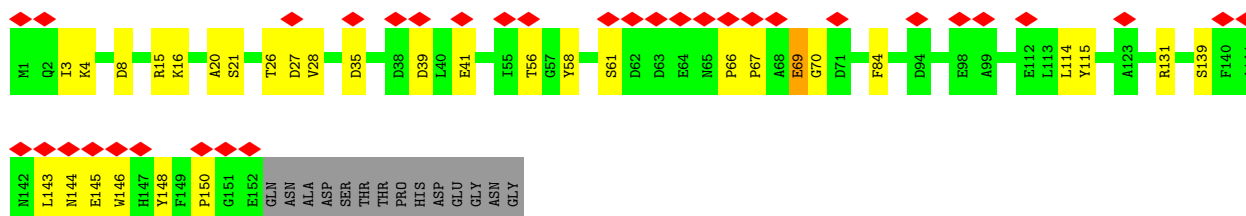
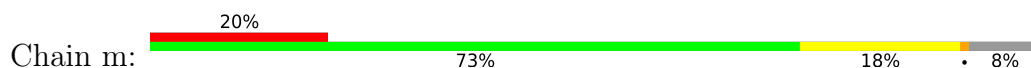




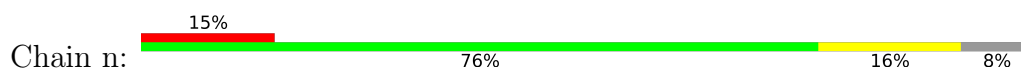
• Molecule 4: Peptidoglycan hydrolase gp4

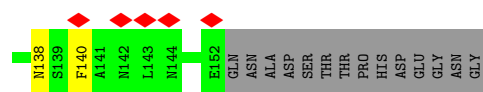


• Molecule 4: Peptidoglycan hydrolase gp4

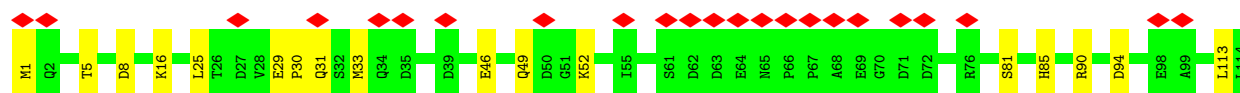
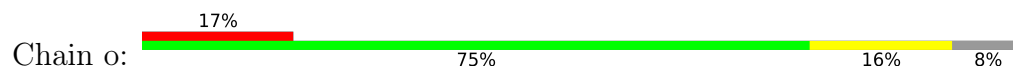


• Molecule 4: Peptidoglycan hydrolase gp4

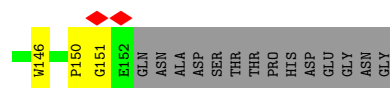
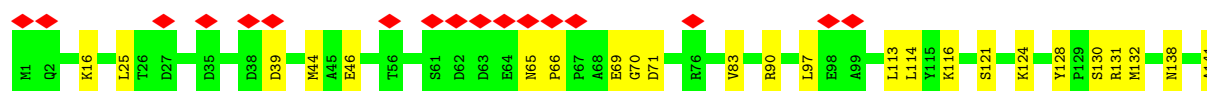
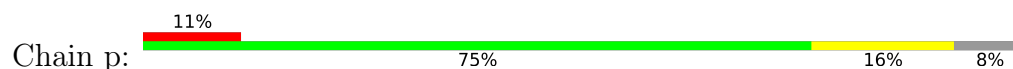




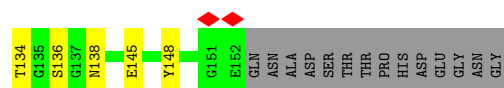
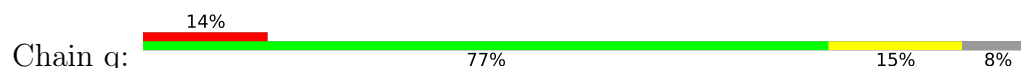
• Molecule 4: Peptidoglycan hydrolase gp4



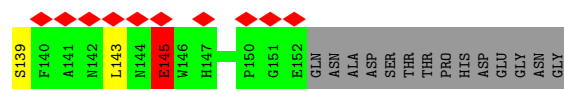
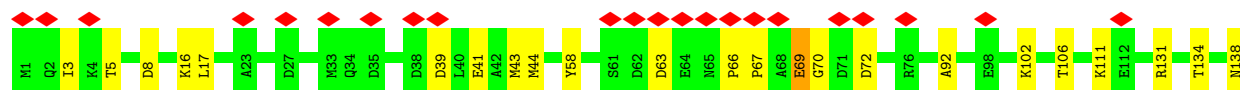
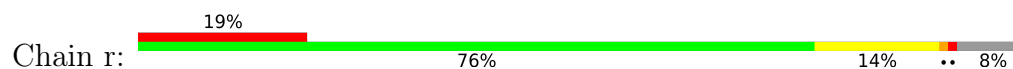
• Molecule 4: Peptidoglycan hydrolase gp4



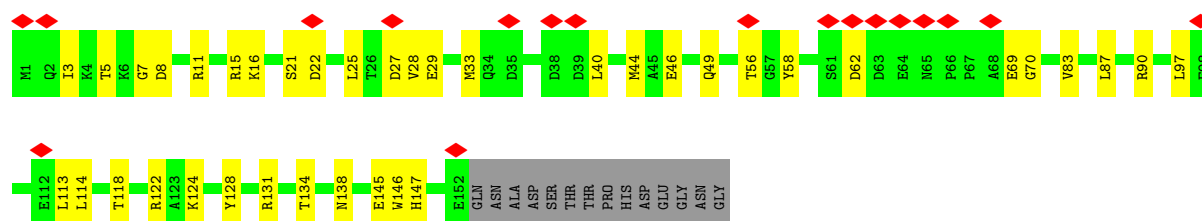
• Molecule 4: Peptidoglycan hydrolase gp4



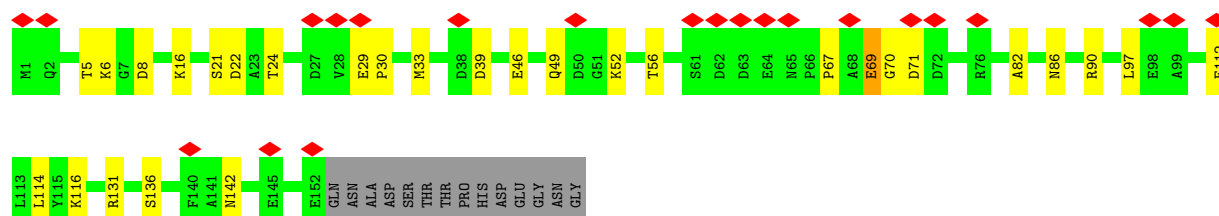
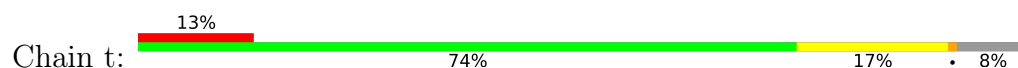
• Molecule 4: Peptidoglycan hydrolase gp4



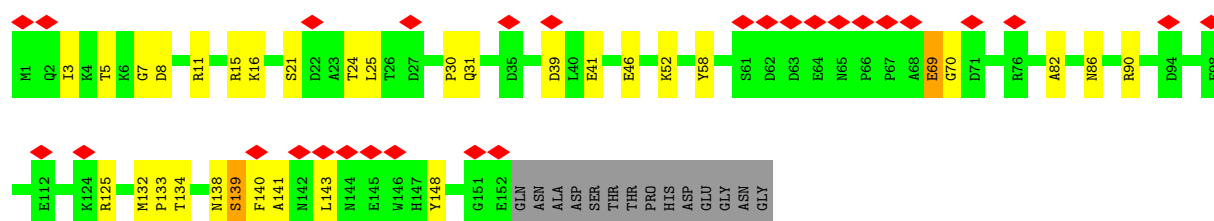
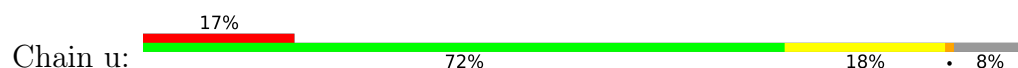
• Molecule 4: Peptidoglycan hydrolase gp4



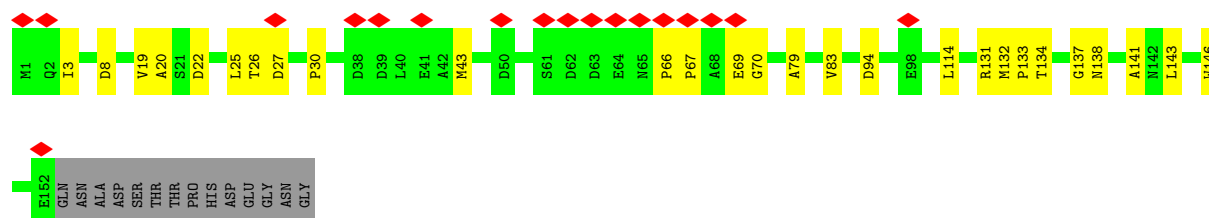
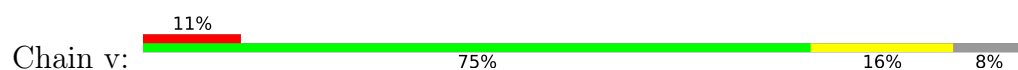
• Molecule 4: Peptidoglycan hydrolase gp4



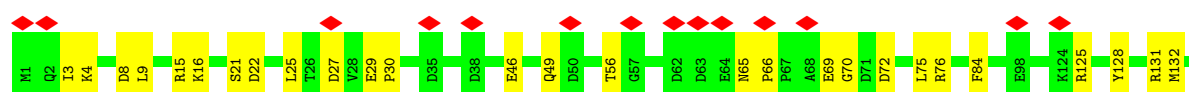
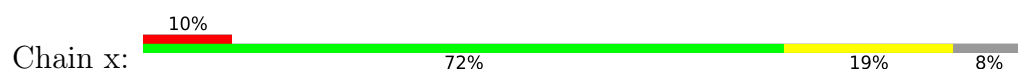
• Molecule 4: Peptidoglycan hydrolase gp4

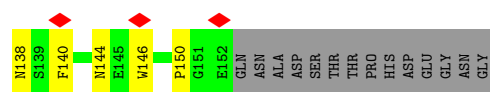


• Molecule 4: Peptidoglycan hydrolase gp4

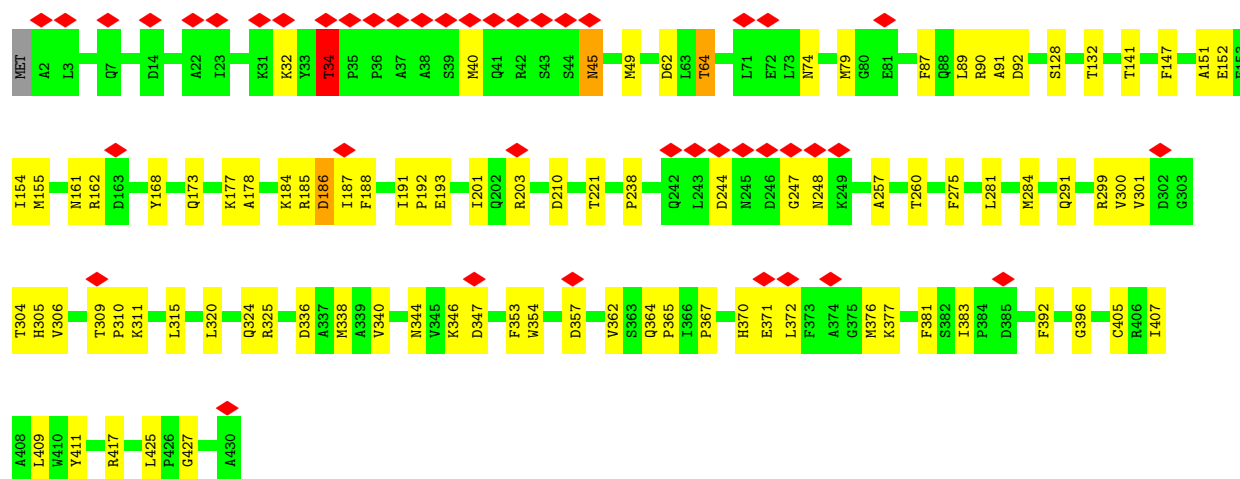
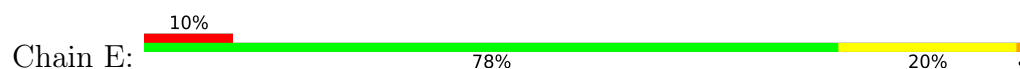


• Molecule 4: Peptidoglycan hydrolase gp4

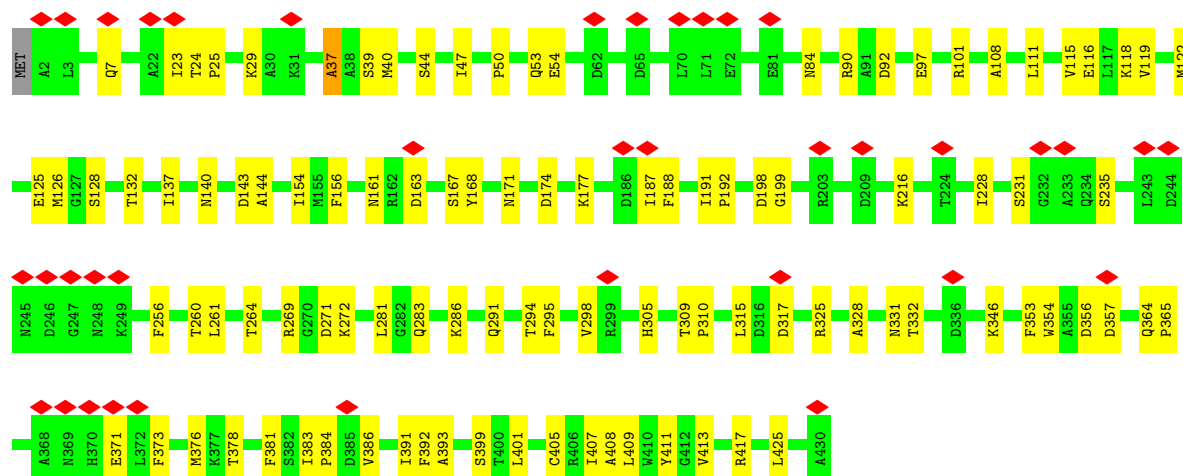
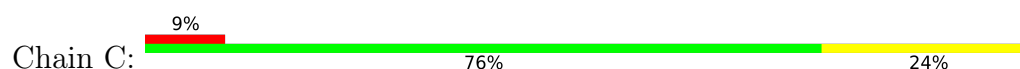




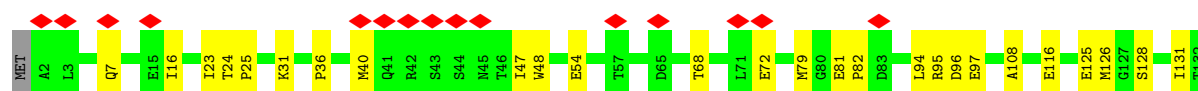
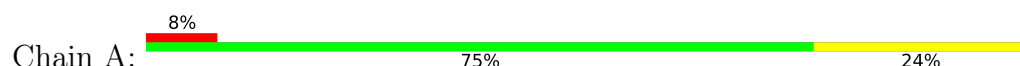
• Molecule 5: Major capsid protein

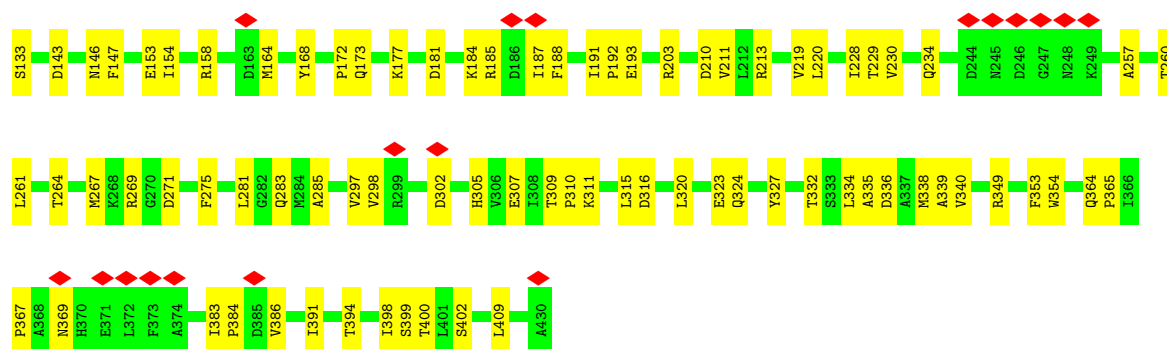


• Molecule 5: Major capsid protein

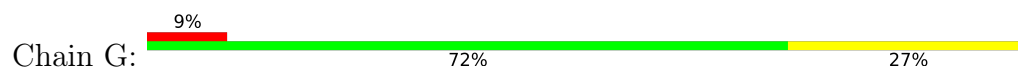


• Molecule 5: Major capsid protein

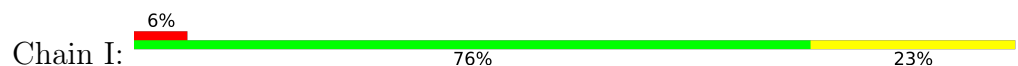




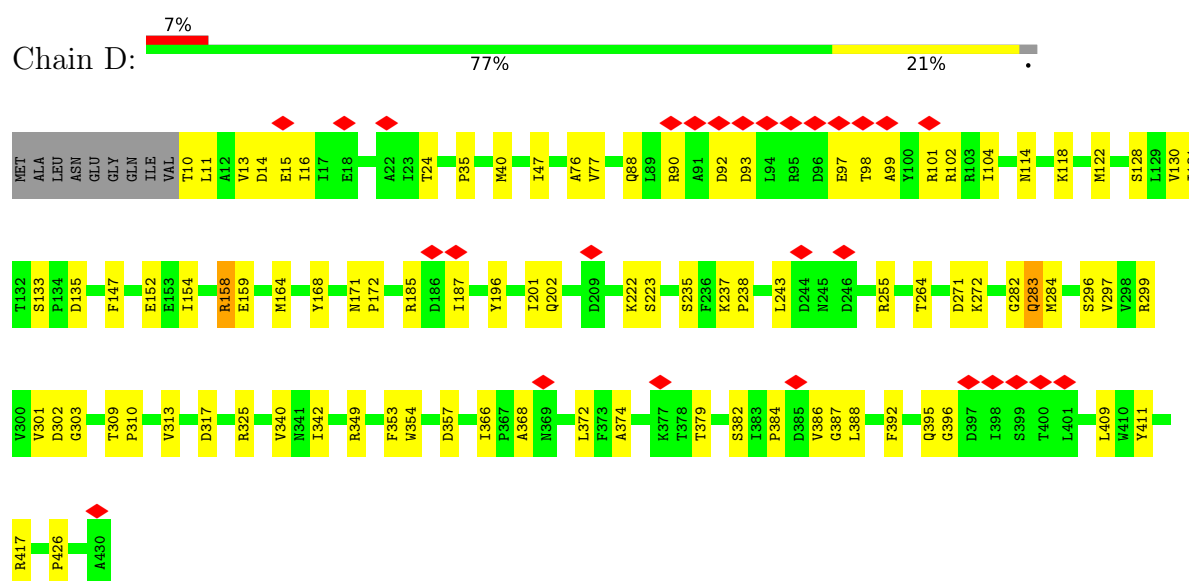
• Molecule 5: Major capsid protein



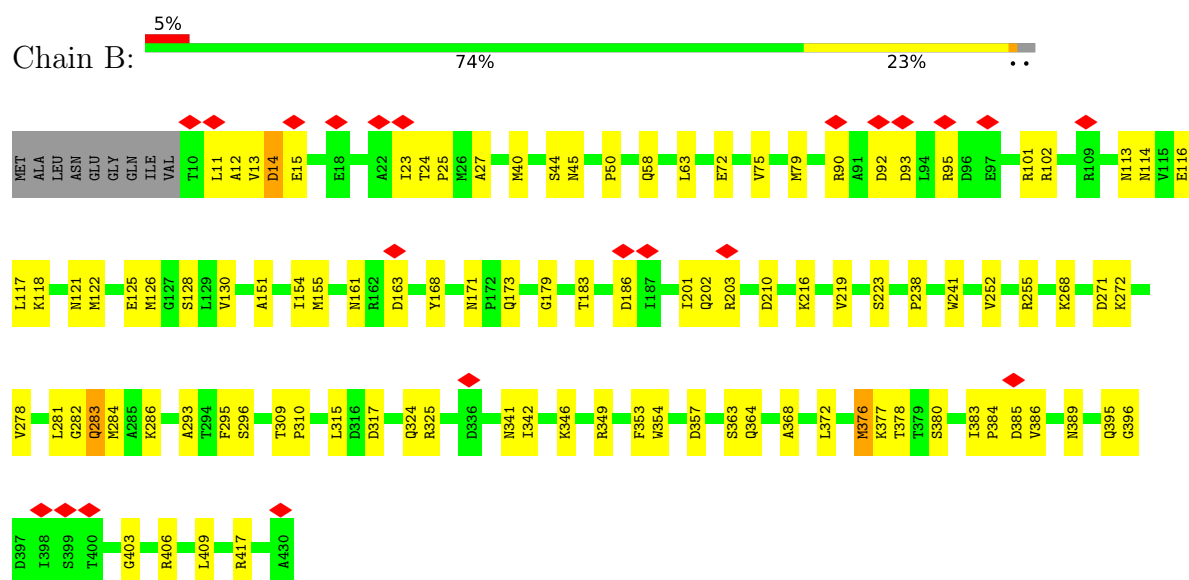
• Molecule 5: Major capsid protein



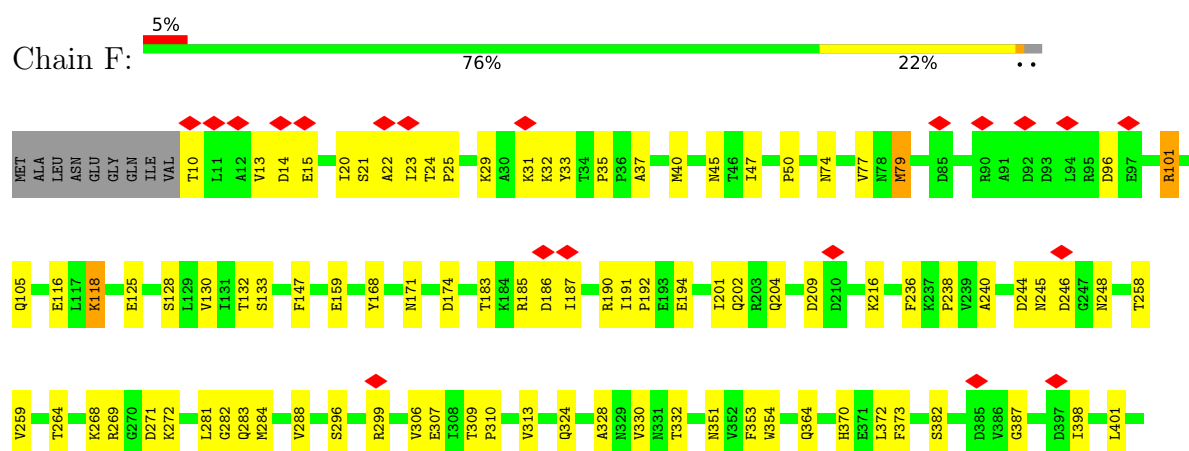
• Molecule 5: Major capsid protein



• Molecule 5: Major capsid protein

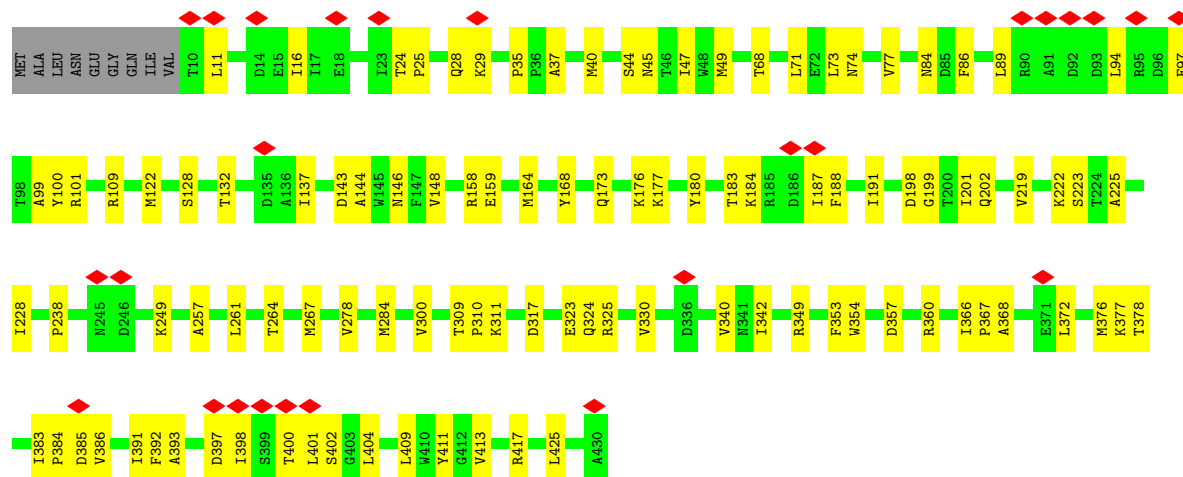
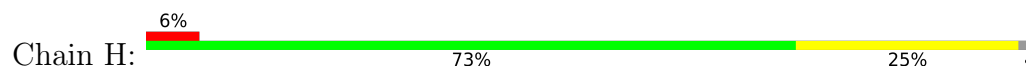


• Molecule 5: Major capsid protein

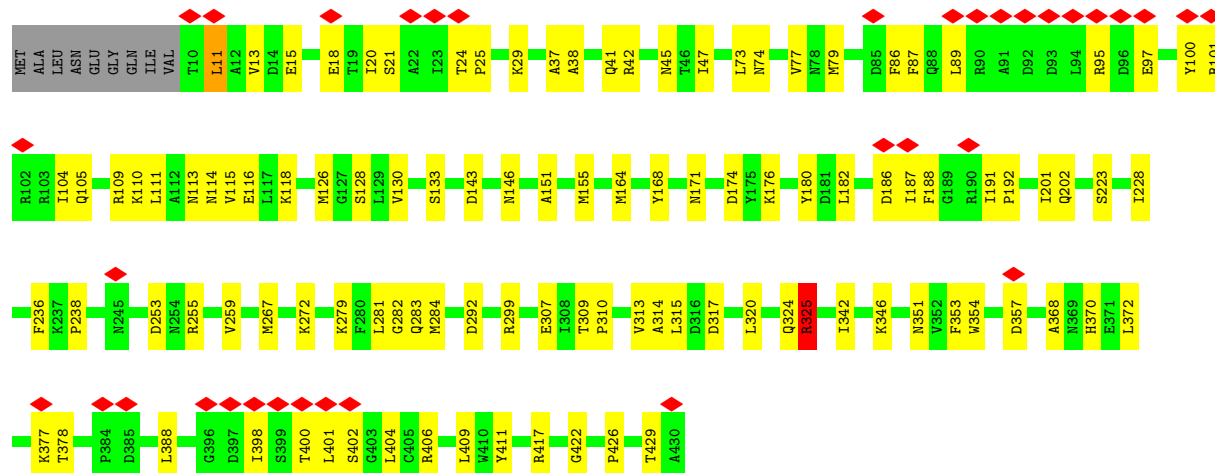




• Molecule 5: Major capsid protein



• Molecule 5: Major capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17944	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.08	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	23.428	Depositor
Minimum map value	-16.095	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	512.9599, 512.9599, 512.9599	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.165818, 1.165818, 1.165818	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	1	0.25	0/3764	0.38	0/5097
1	2	0.26	0/3764	0.41	0/5097
1	3	0.24	0/3764	0.39	0/5097
1	4	0.25	0/3764	0.41	0/5097
1	5	0.24	0/3764	0.39	0/5097
1	6	0.25	0/3764	0.39	0/5097
2	10	0.24	0/953	0.40	0/1299
2	11	0.27	0/953	0.39	0/1299
2	12	0.24	0/953	0.36	0/1299
2	13	0.21	0/953	0.37	0/1299
2	14	0.29	0/953	0.46	0/1299
2	15	0.31	0/953	0.47	0/1299
2	16	0.22	0/953	0.38	0/1299
2	17	0.27	0/953	0.40	0/1299
2	18	0.24	0/953	0.36	0/1299
2	19	0.24	0/953	0.41	0/1299
2	20	0.29	0/953	0.39	0/1299
2	21	0.29	0/953	0.41	0/1299
2	22	0.21	0/953	0.34	0/1299
2	23	0.26	0/953	0.38	0/1299
2	24	0.26	0/953	0.37	0/1299
2	7	0.22	0/953	0.41	0/1299
2	8	0.31	0/953	0.53	0/1299
2	9	0.32	0/953	0.47	0/1299
3	a	0.25	0/4512	0.38	0/6117
3	b	0.26	0/4512	0.36	0/6117
3	c	0.26	0/4512	0.44	3/6117 (0.0%)
3	d	0.26	0/4512	0.38	0/6117
3	e	0.24	0/4512	0.35	0/6117
3	f	0.24	0/4512	0.34	0/6117
3	g	0.25	0/4512	0.36	1/6117 (0.0%)
3	h	0.25	0/4512	0.36	0/6117
3	i	0.25	0/4512	0.35	0/6117
3	j	0.25	0/4512	0.37	0/6117

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	k	0.24	0/4512	0.35	0/6117
3	l	0.25	0/4512	0.36	0/6117
4	m	0.26	0/1191	0.39	0/1614
4	n	0.27	0/1191	0.35	0/1614
4	o	0.26	0/1191	0.37	0/1614
4	p	0.29	0/1191	0.39	0/1614
4	q	0.26	0/1191	0.38	0/1614
4	r	0.26	0/1191	0.39	0/1614
4	s	0.28	0/1191	0.38	0/1614
4	t	0.27	0/1191	0.38	0/1614
4	u	0.28	0/1191	0.42	0/1614
4	v	0.27	0/1191	0.37	0/1614
4	x	0.27	0/1191	0.38	0/1614
4	y	0.25	0/1191	0.36	0/1614
5	A	0.29	0/3335	0.39	0/4535
5	B	0.31	0/3277	0.43	0/4456
5	C	0.28	0/3335	0.41	0/4535
5	D	0.29	0/3277	0.41	0/4456
5	E	0.29	0/3335	0.45	2/4535 (0.0%)
5	F	0.32	0/3277	0.42	0/4456
5	G	0.31	0/3335	0.40	0/4535
5	H	0.31	0/3277	0.41	0/4456
5	I	0.29	0/3335	0.41	0/4535
5	J	0.31	0/3277	0.46	0/4456
All	All	0.27	0/141234	0.39	6/191691 (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	1	0	1
1	6	0	1
3	a	0	1
3	e	0	1
3	f	0	1
3	k	0	2
3	l	0	2
4	r	0	1
4	u	0	1
5	C	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
5	D	0	1
5	G	0	1
5	H	0	1
5	J	0	1
All	All	0	16

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	561	ASP	CB-CA-C	-16.17	89.51	111.82
3	c	561	ASP	N-CA-C	7.74	123.40	107.37
5	E	34	THR	CB-CA-C	-6.12	99.72	109.82
5	E	34	THR	N-CA-C	5.73	119.81	109.44
3	c	561	ASP	N-CA-CB	-5.36	101.03	111.11
3	g	59	VAL	N-CA-C	-5.20	108.21	113.20

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	437	ARG	Sidechain
1	6	408	ARG	Sidechain
5	C	325	ARG	Sidechain
5	D	158	ARG	Sidechain
5	G	35	PRO	Peptide
5	H	158	ARG	Sidechain
5	J	325	ARG	Sidechain
3	a	376	ARG	Sidechain
3	e	37	ARG	Sidechain
3	f	37	ARG	Sidechain
3	k	209	PHE	Peptide
3	k	211	TRP	Peptide
3	l	209	PHE	Peptide
3	l	61	ARG	Sidechain
4	r	145	GLU	Peptide
4	u	125	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	1	3683	0	3590	95	0
1	2	3683	0	3590	104	0
1	3	3683	0	3590	80	0
1	4	3683	0	3590	88	0
1	5	3683	0	3590	101	0
1	6	3683	0	3590	84	0
2	10	934	0	925	33	0
2	11	934	0	925	22	0
2	12	934	0	925	22	0
2	13	934	0	925	25	0
2	14	934	0	925	26	0
2	15	934	0	925	27	0
2	16	934	0	925	37	0
2	17	934	0	925	26	0
2	18	934	0	925	31	0
2	19	934	0	925	34	0
2	20	934	0	925	21	0
2	21	934	0	925	21	0
2	22	934	0	925	21	0
2	23	934	0	925	26	0
2	24	934	0	925	19	0
2	7	934	0	925	33	0
2	8	934	0	925	44	0
2	9	934	0	925	28	0
3	a	4417	0	4295	103	0
3	b	4417	0	4295	101	0
3	c	4417	0	4295	105	0
3	d	4417	0	4295	89	0
3	e	4417	0	4295	101	0
3	f	4417	0	4295	88	0
3	g	4417	0	4295	104	0
3	h	4417	0	4295	89	0
3	i	4417	0	4295	93	0
3	j	4417	0	4295	95	0
3	k	4417	0	4295	93	0
3	l	4417	0	4295	91	0
4	m	1166	0	1133	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	n	1166	0	1133	22	0
4	o	1166	0	1133	24	0
4	p	1166	0	1133	23	0
4	q	1166	0	1133	20	0
4	r	1166	0	1133	22	0
4	s	1166	0	1133	30	0
4	t	1166	0	1133	21	0
4	u	1166	0	1133	24	0
4	v	1166	0	1133	21	0
4	x	1166	0	1133	26	0
4	y	1166	0	1133	20	0
5	A	3277	0	3247	76	0
5	B	3219	0	3188	72	0
5	C	3277	0	3247	67	0
5	D	3219	0	3188	65	0
5	E	3277	0	3247	58	0
5	F	3219	0	3188	74	0
5	G	3277	0	3247	100	0
5	H	3219	0	3188	79	0
5	I	3277	0	3247	78	0
5	J	3219	0	3188	80	0
All	All	138386	0	135501	2716	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 10.

All (2716) 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)
5:G:367:PRO:HD2	5:G:391:ILE:HD12	1.26	1.08
5:G:366:ILE:HB	5:G:391:ILE:HD11	1.15	1.08
5:G:367:PRO:HD2	5:G:391:ILE:CD1	2.01	0.90
3:l:44:TRP:HB2	5:J:97:GLU:HG2	1.53	0.88
5:A:94:LEU:HD11	5:J:372:LEU:HD23	1.58	0.86
4:p:150:PRO:HG3	5:F:401:LEU:HD11	1.60	0.83
1:4:34:LYS:NZ	1:5:12:MET:SD	2.52	0.82
5:C:187:ILE:HG21	5:D:187:ILE:HA	1.60	0.82
5:E:34:THR:HG23	5:E:362:VAL:HG13	1.62	0.82
5:G:63:LEU:HD11	5:H:84:ASN:HD22	1.45	0.81
4:v:132:MET:HE3	4:v:133:PRO:HD2	1.62	0.80
5:I:79:MET:HE1	5:I:364:GLN:HG3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:l:342:ALA:HB2	4:u:132:MET:HE3	1.66	0.78
1:2:155:LYS:HE2	1:2:158:THR:HG21	1.66	0.77
5:D:299:ARG:HH12	5:D:301:VAL:HB	1.50	0.77
3:f:47:GLN:HE22	5:E:371:GLU:HG3	1.50	0.77
1:2:284:THR:O	1:2:288:MET:HB2	1.83	0.76
2:10:47:ILE:O	2:10:63:GLN:NE2	2.17	0.76
1:6:8:MET:HE2	1:6:467:CYS:HB2	1.68	0.76
3:c:40:GLN:HE21	3:c:331:ASN:HD21	1.33	0.76
1:4:298:PHE:O	1:4:301:HIS:HB2	1.86	0.75
3:i:376:ARG:HG3	3:i:377:THR:HG23	1.66	0.75
2:8:78:GLN:NE2	4:p:25:LEU:O	2.20	0.75
3:c:199:PRO:HD2	3:c:217:ILE:HD12	1.69	0.75
1:2:148:ARG:HH21	1:2:211:LEU:HD23	1.51	0.75
3:c:177:HIS:NE2	3:c:221:GLU:OE1	2.20	0.74
1:1:330:LYS:HD2	1:1:335:ASP:HA	1.67	0.74
5:J:228:ILE:HD13	5:J:267:MET:HE3	1.69	0.74
3:a:42:ASP:OD2	3:a:328:ARG:NH2	2.21	0.74
1:2:126:ASN:HD21	1:2:136:TYR:H	1.32	0.74
5:E:79:MET:HE1	5:E:364:GLN:HB2	1.70	0.74
3:h:209:PHE:HD2	5:G:375:GLY:H	1.36	0.74
5:C:137:ILE:HG23	5:C:177:LYS:HD2	1.69	0.74
3:k:161:ASN:HD22	3:j:183:GLY:HA3	1.52	0.74
1:3:287:GLU:HB3	1:3:309:PRO:HG3	1.70	0.73
2:19:51:ILE:HD11	2:19:61:ILE:HD12	1.69	0.73
2:22:22:SER:OG	2:22:24:LYS:NZ	2.20	0.73
2:19:33:ILE:O	2:19:63:GLN:NE2	2.22	0.73
1:2:349:GLN:NE2	1:2:362:GLN:OE1	2.21	0.73
5:E:187:ILE:HG21	5:F:187:ILE:HA	1.69	0.73
1:2:16:PHE:HB3	1:2:418:ILE:HG21	1.71	0.73
5:G:185:ARG:NH2	5:H:183:THR:O	2.22	0.73
1:2:298:PHE:O	1:2:301:HIS:HB2	1.88	0.72
2:22:14:ARG:HD3	2:22:79:LEU:HD12	1.71	0.72
1:6:159:ASP:OD1	1:6:184:GLN:NE2	2.22	0.72
5:I:302:ASP:OD1	5:I:303:GLY:N	2.22	0.72
1:5:389:ALA:HB3	1:5:446:ILE:HD12	1.70	0.72
1:6:150:ARG:NH2	1:6:173:ASP:OD1	2.22	0.72
1:6:287:GLU:HB3	1:6:309:PRO:HG3	1.71	0.72
2:10:46:GLN:HG2	2:10:63:GLN:HG2	1.72	0.72
2:24:33:ILE:HD11	2:24:49:VAL:HG11	1.71	0.72
3:f:249:ARG:HH12	3:f:513:ARG:HH12	1.37	0.72
1:5:408:ARG:NH2	2:24:93:TYR:OH	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:l:312:ASP:OD2	3:k:205:ASN:ND2	2.22	0.72
3:f:177:HIS:HB2	3:f:219:ILE:HG22	1.72	0.72
3:i:317:GLU:OE1	3:h:61:ARG:NH2	2.23	0.72
1:1:280:ILE:HG23	1:1:288:MET:HE1	1.71	0.71
3:e:177:HIS:NE2	3:e:221:GLU:OE1	2.23	0.71
3:k:216:THR:HG22	3:k:217:ILE:H	1.54	0.71
1:5:422:ARG:NH2	1:5:424:GLN:OE1	2.24	0.71
3:l:249:ARG:NH2	3:l:470:ASP:OD1	2.23	0.71
1:2:435:ASP:HB3	4:o:25:LEU:HD21	1.71	0.71
4:r:143:LEU:O	3:i:27:ARG:NH2	2.24	0.71
3:k:41:TRP:NE1	3:k:55:GLY:O	2.23	0.71
1:3:399:SER:HB3	1:3:463:THR:HB	1.73	0.71
3:d:347:LYS:NZ	3:e:393:GLU:OE1	2.23	0.71
2:11:14:ARG:HB3	2:11:72:LYS:HD3	1.72	0.70
1:3:349:GLN:NE2	1:3:362:GLN:OE1	2.24	0.70
1:2:422:ARG:NH2	1:2:424:GLN:OE1	2.25	0.70
1:4:127:TRP:O	1:4:135:GLN:NE2	2.21	0.70
3:f:40:GLN:NE2	3:f:58:ASP:OD1	2.23	0.70
5:C:118:LYS:NZ	5:C:411:TYR:OH	2.24	0.70
1:2:294:GLU:OE1	1:2:307:HIS:NE2	2.23	0.70
4:s:134:THR:O	4:s:138:ASN:ND2	2.25	0.70
5:G:367:PRO:CD	5:G:391:ILE:HD12	2.15	0.70
5:I:309:THR:HG23	5:I:310:PRO:HD3	1.74	0.70
5:I:161:ASN:HA	5:J:21:SER:HB3	1.74	0.70
2:15:33:ILE:HD11	2:15:49:VAL:HG12	1.73	0.70
3:e:23:ASP:OD1	3:e:27:ARG:NH1	2.25	0.69
3:g:37:ARG:NH1	3:g:120:GLU:OE1	2.25	0.69
1:6:98:ALA:O	1:6:104:GLN:NE2	2.25	0.69
1:6:385:LYS:NZ	1:6:387:ASP:OD2	2.25	0.69
3:b:249:ARG:HH12	3:b:513:ARG:HH12	1.40	0.69
3:a:307:TRP:NE1	3:a:314:GLU:OE2	2.21	0.69
3:e:94:LEU:HD21	3:e:465:GLN:HG3	1.75	0.69
4:v:134:THR:O	4:v:138:ASN:ND2	2.25	0.69
4:y:144:ASN:HD21	4:y:147:HIS:HB2	1.57	0.69
2:15:101:ASP:OD1	2:15:102:TYR:N	2.25	0.69
5:B:283:GLN:O	5:B:286:LYS:NZ	2.23	0.69
1:5:137:GLU:OE1	1:5:137:GLU:N	2.26	0.69
2:19:14:ARG:NH2	2:20:109:TYR:OH	2.26	0.69
3:a:249:ARG:HH12	3:a:513:ARG:HH12	1.40	0.69
3:i:45:LEU:HD11	5:G:39:SER:HB3	1.74	0.69
5:G:219:VAL:HG22	5:G:349:ARG:HG2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:22:SER:OG	3:b:26:ARG:NH2	2.25	0.69
5:I:41:GLN:O	5:I:43:SER:N	2.26	0.69
2:7:31:ILE:HD11	2:7:67:ILE:HD11	1.74	0.69
5:C:54:GLU:OE1	5:C:283:GLN:NE2	2.27	0.68
5:E:185:ARG:NH2	5:F:183:THR:O	2.25	0.68
5:D:357:ASP:OD1	5:D:417:ARG:NH1	2.26	0.68
1:2:293:MET:HE3	1:2:304:LEU:HD11	1.76	0.68
3:j:15:PHE:HE1	3:j:157:ILE:HD13	1.58	0.68
2:22:62:THR:HG22	2:22:64:PRO:HD2	1.76	0.68
3:l:47:GLN:NE2	4:u:139:SER:OG	2.27	0.68
3:h:33:LEU:O	3:h:37:ARG:HB2	1.93	0.68
2:22:47:ILE:O	2:22:63:GLN:NE2	2.26	0.68
3:a:561:ASP:OD1	3:a:569:ARG:NH1	2.27	0.68
4:o:134:THR:O	4:o:138:ASN:ND2	2.26	0.68
3:f:376:ARG:HH21	3:g:384:LEU:HD23	1.59	0.68
5:G:13:VAL:HG12	5:G:15:GLU:HG2	1.76	0.68
3:c:61:ARG:O	3:c:65:ARG:HG3	1.93	0.68
4:r:39:ASP:OD1	4:x:15:ARG:NH2	2.26	0.68
4:s:15:ARG:NH2	4:u:39:ASP:OD1	2.27	0.68
3:j:37:ARG:NH1	3:j:120:GLU:OE1	2.26	0.68
1:1:101:ARG:NH2	1:3:186:ASP:OD2	2.23	0.68
2:13:11:SER:HA	2:14:15:PRO:HG2	1.75	0.68
5:H:317:ASP:O	5:H:325:ARG:NH1	2.26	0.68
3:e:394:ASN:ND2	3:f:396:GLU:OE1	2.26	0.67
3:h:209:PHE:HB3	3:h:210:PRO:HD3	1.74	0.67
2:16:20:SER:HB3	2:18:79:LEU:HD11	1.75	0.67
2:16:51:ILE:HG22	2:16:82:ILE:HD13	1.75	0.67
2:17:31:ILE:HD12	2:17:73:ILE:HD11	1.76	0.67
1:2:37:LEU:HD13	1:6:385:LYS:HB2	1.76	0.67
3:b:220:ALA:HB3	3:b:281:ILE:HG13	1.76	0.67
3:k:177:HIS:ND1	3:k:221:GLU:OE1	2.27	0.67
2:16:20:SER:O	2:18:68:ASN:ND2	2.27	0.67
5:C:357:ASP:OD1	5:C:417:ARG:NH1	2.27	0.67
1:3:162:PHE:HA	1:3:177:ALA:O	1.94	0.67
2:11:38:THR:OG1	2:11:45:ASN:ND2	2.28	0.67
3:l:575:GLN:O	3:l:579:MET:HG3	1.94	0.67
3:j:249:ARG:NH2	3:j:470:ASP:OD1	2.27	0.67
1:6:27:VAL:HB	1:6:378:LEU:HB2	1.77	0.67
5:C:198:ASP:OD1	5:C:199:GLY:N	2.28	0.67
3:i:510:ILE:HG23	3:i:512:GLY:H	1.60	0.67
3:h:40:GLN:NE2	3:h:58:ASP:OD1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:13:14:ARG:NH1	2:14:101:ASP:OD1	2.28	0.66
3:l:249:ARG:HH12	3:l:513:ARG:HH12	1.42	0.66
1:2:142:ARG:HH21	1:2:189:ILE:HG23	1.60	0.66
3:k:376:ARG:HD3	3:k:377:THR:HG23	1.77	0.66
5:D:164:MET:HE2	5:D:357:ASP:HB3	1.76	0.66
4:y:132:MET:HE3	4:y:133:PRO:HD2	1.77	0.66
5:H:122:MET:HE2	5:H:413:VAL:HG23	1.76	0.66
3:h:6:ASN:HB3	3:h:9:GLU:HB2	1.76	0.66
4:x:29:GLU:HG2	4:x:30:PRO:HD2	1.76	0.66
1:2:14:LYS:NZ	1:3:399:SER:OG	2.20	0.66
1:6:36:ILE:HG22	1:6:37:LEU:HG	1.76	0.66
2:11:31:ILE:HG12	2:11:92:ILE:HD13	1.77	0.66
2:13:81:LYS:NZ	2:14:108:LYS:O	2.29	0.66
3:e:24:GLU:OE1	3:e:313:LYS:NZ	2.26	0.66
5:D:99:ALA:HA	5:D:102:ARG:HD2	1.77	0.66
4:u:134:THR:O	4:u:138:ASN:ND2	2.28	0.66
1:2:455:ARG:NE	2:8:54:GLU:OE2	2.28	0.66
3:a:61:ARG:NH2	3:b:317:GLU:OE1	2.28	0.66
5:G:187:ILE:HG21	5:H:187:ILE:HA	1.78	0.66
3:l:339:ASP:OD2	4:t:131:ARG:NH2	2.27	0.66
5:G:41:GLN:NE2	5:G:44:SER:OG	2.25	0.66
5:F:238:PRO:HD2	5:F:324:GLN:HB3	1.76	0.65
1:3:15:ASP:HB2	1:3:22:ILE:HD13	1.77	0.65
5:G:203:ARG:HH12	5:G:212:LEU:HD23	1.61	0.65
1:5:390:ARG:NH2	1:5:472:GLU:OE1	2.30	0.65
2:19:106:VAL:HG23	2:19:107:LEU:HD12	1.78	0.65
3:h:41:TRP:NE1	3:h:55:GLY:O	2.29	0.65
2:15:33:ILE:HG22	2:15:90:MET:HG3	1.77	0.65
3:d:61:ARG:NH2	3:e:317:GLU:OE1	2.29	0.65
3:d:146:ARG:NH2	3:d:460:ASP:OD2	2.30	0.65
5:G:366:ILE:HB	5:G:391:ILE:CD1	2.09	0.65
2:7:14:ARG:NH2	2:8:109:TYR:OH	2.30	0.65
4:x:146:TRP:HZ3	5:H:97:GLU:HA	1.62	0.65
2:20:51:ILE:HG22	2:20:82:ILE:HD13	1.77	0.65
3:i:249:ARG:NH2	3:i:470:ASP:OD1	2.30	0.65
3:i:327:GLN:HE22	3:i:330:ARG:HD3	1.61	0.65
3:h:376:ARG:HG3	3:h:377:THR:HG23	1.78	0.65
1:5:126:ASN:HD21	1:5:136:TYR:H	1.45	0.64
2:16:52:GLU:HB3	2:16:81:LYS:HE3	1.79	0.64
3:b:99:ARG:NH1	3:b:530:GLN:OE1	2.29	0.64
4:r:63:ASP:OD1	4:x:4:LYS:NZ	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:334:LEU:HA	5:G:338:MET:HE1	1.78	0.64
3:b:205:ASN:ND2	3:c:312:ASP:OD2	2.30	0.64
5:B:40:MET:HG2	5:B:45:ASN:HA	1.77	0.64
2:16:31:ILE:HB	2:16:65:LEU:HB2	1.79	0.64
5:C:132:THR:HG22	5:C:425:LEU:HB2	1.79	0.64
3:b:281:ILE:HG22	3:b:286:VAL:HG22	1.79	0.64
1:2:65:ASN:ND2	1:2:104:GLN:OE1	2.20	0.64
1:6:35:GLU:HA	1:6:40:SER:HA	1.79	0.64
2:19:117:GLU:O	2:19:121:LYS:HG2	1.97	0.64
3:e:307:TRP:NE1	3:e:314:GLU:OE2	2.27	0.64
3:k:249:ARG:NH2	3:k:470:ASP:OD1	2.31	0.64
3:i:37:ARG:NH1	3:i:120:GLU:OE1	2.31	0.64
4:p:121:SER:O	4:p:124:LYS:NZ	2.30	0.64
3:f:310:VAL:HG12	3:f:311:GLU:HG3	1.80	0.64
5:J:346:LYS:NZ	5:J:429:THR:O	2.30	0.64
2:16:52:GLU:OE2	2:16:58:HIS:NE2	2.31	0.64
2:23:38:THR:OG1	2:23:45:ASN:ND2	2.30	0.64
3:b:509:ASP:HB2	3:b:513:ARG:HH21	1.63	0.64
3:d:220:ALA:HB3	3:d:281:ILE:HG13	1.79	0.64
4:o:49:GLN:O	4:o:52:LYS:NZ	2.30	0.64
3:f:559:LEU:HD11	3:g:538:LEU:HD21	1.80	0.64
1:1:137:GLU:N	1:1:137:GLU:OE2	2.31	0.64
3:b:41:TRP:NE1	3:b:55:GLY:O	2.30	0.64
4:m:150:PRO:HB3	5:D:92:ASP:HA	1.80	0.64
3:i:33:LEU:O	3:i:37:ARG:HB2	1.97	0.64
5:D:309:THR:HG23	5:D:310:PRO:HD3	1.79	0.64
1:4:247:TYR:HB2	1:4:263:ILE:HD12	1.80	0.64
1:5:165:ASP:OD2	1:5:174:ARG:NH1	2.30	0.64
3:k:519:ASP:OD1	3:j:525:GLN:NE2	2.31	0.64
4:m:66:PRO:HB2	4:m:67:PRO:HD3	1.80	0.64
5:D:114:ASN:O	5:D:118:LYS:HG3	1.98	0.64
5:F:204:GLN:HG2	5:F:209:ASP:HA	1.79	0.64
1:3:52:ARG:NH1	1:3:346:GLU:OE2	2.28	0.63
3:a:6:ASN:HB3	3:a:9:GLU:HB2	1.79	0.63
3:d:184:TRP:HB2	3:d:217:ILE:HG21	1.78	0.63
4:v:69:GLU:OE1	4:v:70:GLY:N	2.30	0.63
3:c:177:HIS:HB3	3:c:179:MET:HE3	1.81	0.63
2:19:22:SER:OG	2:19:24:LYS:NZ	2.31	0.63
2:20:52:GLU:OE1	2:20:81:LYS:NZ	2.23	0.63
3:c:249:ARG:HH12	3:c:513:ARG:HH12	1.46	0.63
3:h:249:ARG:NH2	3:h:470:ASP:OD1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:258:LEU:HB3	3:a:263:PHE:HB2	1.80	0.63
3:d:33:LEU:HG	3:d:121:ALA:HB2	1.79	0.63
5:G:203:ARG:NH2	5:G:210:ASP:OD1	2.30	0.63
5:I:244:ASP:OD1	5:I:248:ASN:N	2.28	0.63
4:t:39:ASP:OD1	4:u:15:ARG:NH2	2.32	0.63
1:1:43:LEU:HD22	1:1:379:LEU:HD21	1.81	0.63
2:12:14:ARG:HD2	2:12:79:LEU:HD23	1.81	0.63
5:E:300:VAL:HG22	5:E:306:VAL:HG12	1.81	0.63
1:2:34:LYS:NZ	1:6:23:ASP:OD1	2.32	0.63
1:4:412:SER:HB3	1:4:423:GLU:HG2	1.80	0.63
1:5:429:ASN:OD1	1:5:430:GLU:N	2.30	0.63
2:16:14:ARG:NH1	2:17:101:ASP:OD1	2.32	0.63
4:p:39:ASP:OD2	4:r:16:LYS:NZ	2.27	0.63
1:1:165:ASP:OD2	1:1:174:ARG:NH1	2.32	0.63
3:g:44:TRP:O	5:F:96:ASP:HB2	1.99	0.63
5:C:228:ILE:HD11	5:C:261:LEU:HD13	1.81	0.63
1:2:287:GLU:HB3	1:2:309:PRO:HG3	1.81	0.63
2:10:14:ARG:NH2	2:11:109:TYR:OH	2.32	0.63
3:d:7:ARG:NH2	3:d:224:GLU:OE2	2.31	0.63
5:D:76:ALA:O	5:D:255:ARG:NH2	2.30	0.63
1:1:412:SER:HB3	1:1:423:GLU:HG2	1.80	0.62
2:18:96:ASN:ND2	4:v:30:PRO:O	2.31	0.62
1:1:286:GLU:OE2	1:1:286:GLU:N	2.28	0.62
1:4:137:GLU:OE1	1:4:137:GLU:N	2.32	0.62
2:18:94:ASP:OD1	2:18:95:ALA:N	2.29	0.62
3:a:234:ILE:HD13	3:a:244:VAL:HG13	1.81	0.62
1:3:330:LYS:HD2	1:3:335:ASP:HA	1.81	0.62
4:n:134:THR:O	4:n:138:ASN:ND2	2.32	0.62
3:e:567:MET:HE2	3:f:582:LYS:HG3	1.81	0.62
1:1:83:GLU:N	1:1:83:GLU:OE2	2.32	0.62
1:1:159:ASP:OD2	1:1:184:GLN:NE2	2.32	0.62
1:2:369:SER:HB3	1:2:459:LYS:HG2	1.80	0.62
4:n:39:ASP:OD2	4:o:16:LYS:NZ	2.25	0.62
3:g:550:GLN:HE22	3:g:581:VAL:HG21	1.63	0.62
5:H:400:THR:HG23	5:H:402:SER:HB2	1.80	0.62
1:4:35:GLU:HA	1:4:40:SER:HA	1.81	0.62
1:5:287:GLU:HB3	1:5:309:PRO:HG3	1.80	0.62
2:8:31:ILE:HG22	2:8:92:ILE:HG12	1.82	0.62
3:a:214:GLN:HA	3:b:313:LYS:HE3	1.82	0.62
3:d:561:ASP:OD2	3:d:569:ARG:NH2	2.33	0.62
3:f:146:ARG:NH2	3:f:460:ASP:OD2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:47:ILE:HD13	5:B:11:LEU:HD12	1.82	0.62
1:4:277:GLU:OE2	1:6:297:ARG:NH2	2.32	0.62
3:a:37:ARG:NH1	3:a:120:GLU:OE1	2.32	0.62
3:a:473:ASP:OD2	3:a:505:GLN:NE2	2.33	0.62
3:l:42:ASP:OD2	3:l:328:ARG:NH2	2.29	0.62
3:l:212:LEU:HD21	5:J:377:LYS:HB3	1.81	0.62
4:r:39:ASP:OD2	4:x:16:LYS:NZ	2.27	0.62
3:j:307:TRP:NE1	3:j:314:GLU:OE2	2.25	0.62
1:1:51:LYS:NZ	1:1:53:TYR:O	2.33	0.62
3:k:76:ILE:HG22	3:k:457:MET:HG3	1.80	0.62
3:i:7:ARG:NH2	3:i:224:GLU:OE2	2.33	0.62
1:1:116:ARG:NH1	1:1:118:ASP:OD2	2.32	0.62
2:22:16:ILE:HD11	2:23:23:PHE:HE1	1.64	0.62
3:a:205:ASN:ND2	3:b:312:ASP:OD2	2.32	0.62
4:x:46:GLU:O	4:x:49:GLN:NE2	2.30	0.62
2:19:11:SER:HA	2:20:15:PRO:HG2	1.82	0.62
3:g:561:ASP:OD2	3:g:569:ARG:NH2	2.33	0.62
1:3:293:MET:HE3	1:3:304:LEU:HD11	1.81	0.61
4:q:46:GLU:OE2	4:q:90:ARG:NH2	2.32	0.61
5:E:203:ARG:NH2	5:E:210:ASP:OD1	2.33	0.61
1:4:15:ASP:HB2	1:4:22:ILE:HD13	1.82	0.61
3:a:205:ASN:HB3	3:b:311:GLU:HB3	1.81	0.61
5:H:261:LEU:HD12	5:H:264:THR:HG22	1.81	0.61
1:3:44:ARG:NH1	1:3:463:THR:OG1	2.33	0.61
4:n:3:ILE:HG23	4:n:8:ASP:HB3	1.83	0.61
2:15:19:GLU:HG3	2:15:24:LYS:HG3	1.82	0.61
5:B:58:GLN:HE21	5:B:63:LEU:HD13	1.66	0.61
1:2:2:PRO:HD2	1:2:472:GLU:HA	1.82	0.61
1:3:455:ARG:NH1	2:21:37:ASP:OD1	2.33	0.61
1:6:439:LEU:HD21	4:m:26:THR:HG23	1.82	0.61
2:16:99:GLN:HE21	2:16:102:TYR:HB2	1.65	0.61
3:d:249:ARG:NH2	3:d:470:ASP:OD1	2.33	0.61
3:h:23:ASP:OD1	3:h:26:ARG:NH1	2.34	0.61
5:C:125:GLU:OE1	5:C:269:ARG:NH1	2.32	0.61
3:d:542:THR:HG21	3:d:547:PRO:HB2	1.83	0.61
4:o:131:ARG:NH2	3:g:339:ASP:OD2	2.30	0.61
4:o:145:GLU:OE1	3:g:207:TRP:NE1	2.33	0.61
4:r:69:GLU:OE1	4:r:70:GLY:N	2.34	0.61
5:D:223:SER:HB3	5:D:342:ILE:HG21	1.81	0.61
5:B:171:ASN:HD22	5:B:349:ARG:HB3	1.66	0.61
3:c:577:ILE:HD11	3:c:582:LYS:HE2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:7:ARG:NH2	3:k:224:GLU:OE2	2.33	0.61
1:1:12:MET:HE1	1:5:34:LYS:HE3	1.81	0.61
1:3:241:THR:HG21	1:3:294:GLU:HA	1.80	0.61
3:b:146:ARG:NH2	3:b:460:ASP:OD2	2.28	0.61
5:G:45:ASN:ND2	5:G:79:MET:O	2.31	0.61
5:I:47:ILE:HG12	5:J:11:LEU:HB2	1.80	0.61
1:3:146:ARG:NH1	1:3:169:GLU:OE2	2.32	0.61
3:i:38:VAL:HG23	3:j:310:VAL:HG21	1.83	0.61
4:u:69:GLU:OE1	4:u:70:GLY:N	2.34	0.61
4:o:132:MET:HE3	3:f:53:TYR:CD1	2.36	0.60
3:d:249:ARG:HH12	3:d:513:ARG:HH12	1.47	0.60
5:J:236:PHE:CZ	5:J:259:VAL:HG12	2.36	0.60
1:6:180:ARG:HD3	1:6:182:GLU:HG2	1.83	0.60
1:6:408:ARG:HG2	1:6:425:MET:HB3	1.83	0.60
4:y:5:THR:N	4:y:8:ASP:OD2	2.32	0.60
3:e:369:TYR:O	3:f:348:LYS:NZ	2.30	0.60
5:B:203:ARG:NH2	5:B:210:ASP:OD1	2.34	0.60
5:B:272:LYS:NZ	5:B:296:SER:OG	2.30	0.60
4:o:142:ASN:C	4:o:144:ASN:H	2.10	0.60
3:k:236:GLN:HB3	3:k:264:ILE:HG13	1.83	0.60
3:i:411:ALA:O	3:i:415:VAL:HG23	2.01	0.60
5:E:152:GLU:OE2	5:E:162:ARG:NH1	2.34	0.60
5:I:113:ASN:OD1	5:I:216:LYS:NZ	2.34	0.60
1:2:399:SER:HB3	1:2:463:THR:HB	1.83	0.60
1:6:442:ARG:NH2	4:m:35:ASP:OD2	2.30	0.60
2:23:36:ILE:HG21	2:23:105:ASN:HD22	1.66	0.60
3:a:186:ASP:OD2	3:b:171:ARG:NH2	2.35	0.60
3:j:210:PRO:HA	5:H:377:LYS:HD2	1.83	0.60
3:h:69:SER:O	3:h:73:GLN:HG3	2.01	0.60
3:h:249:ARG:HH12	3:h:513:ARG:HH12	1.49	0.60
5:E:187:ILE:HG12	5:F:187:ILE:HG13	1.83	0.60
1:4:161:TRP:HH2	1:4:222:TYR:HD2	1.50	0.60
3:a:554:LEU:HD22	3:l:567:MET:HE2	1.82	0.60
3:i:562:GLY:H	3:i:565:VAL:HG23	1.67	0.60
3:j:249:ARG:HH12	3:j:513:ARG:HH22	1.48	0.60
1:2:43:LEU:HD13	1:2:379:LEU:HD22	1.84	0.60
3:l:251:ILE:HG23	3:l:252:LYS:HG2	1.84	0.60
1:1:298:PHE:O	1:1:301:HIS:HB2	2.02	0.60
1:1:435:ASP:OD1	1:3:448:ARG:NH2	2.32	0.60
3:f:24:GLU:OE1	3:f:313:LYS:NZ	2.28	0.60
5:J:253:ASP:OD2	5:J:255:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:388:ASN:OD1	1:2:445:ARG:NH1	2.35	0.60
1:3:194:TRP:NE1	1:3:245:ASP:O	2.27	0.60
3:e:323:THR:HB	3:e:412:VAL:HG13	1.84	0.60
4:r:143:LEU:HD21	3:i:24:GLU:HG2	1.83	0.60
3:j:234:ILE:HD13	3:j:244:VAL:HG22	1.84	0.60
5:I:24:THR:HG23	5:I:116:GLU:HB2	1.83	0.60
1:6:298:PHE:O	1:6:301:HIS:HB2	2.01	0.59
2:21:117:GLU:O	2:21:121:LYS:HG2	2.01	0.59
3:k:159:ASP:OD2	3:k:171:ARG:NH1	2.34	0.59
4:x:144:ASN:ND2	5:H:97:GLU:O	2.35	0.59
2:19:32:TYR:HD2	2:19:41:VAL:HG22	1.67	0.59
3:g:367:ASP:OD1	4:x:125:ARG:NH1	2.33	0.59
1:4:430:GLU:HG3	1:4:431:PRO:HD2	1.84	0.59
2:8:123:LYS:O	2:9:123:LYS:NZ	2.36	0.59
3:b:33:LEU:O	3:b:37:ARG:HB2	2.02	0.59
5:A:133:SER:HB2	5:A:147:PHE:HE1	1.67	0.59
1:1:430:GLU:HB3	1:1:433:VAL:HB	1.83	0.59
1:4:164:THR:HA	1:4:172:PRO:HA	1.83	0.59
3:h:16:ASP:O	3:h:20:THR:HG23	2.02	0.59
5:A:133:SER:HB2	5:A:147:PHE:CE1	2.38	0.59
5:G:261:LEU:HD12	5:G:264:THR:HG22	1.85	0.59
5:J:111:LEU:O	5:J:115:VAL:HG23	2.01	0.59
1:1:237:THR:O	1:1:240:LYS:NZ	2.35	0.59
1:2:35:GLU:N	1:2:35:GLU:OE2	2.35	0.59
1:3:443:VAL:HG13	4:x:25:LEU:HD12	1.84	0.59
2:22:77:GLY:O	2:23:21:ARG:NH2	2.35	0.59
3:a:550:GLN:HE22	3:a:581:VAL:HG21	1.66	0.59
2:7:101:ASP:OD2	2:9:14:ARG:NH1	2.35	0.59
3:a:15:PHE:HD1	3:a:174:THR:HG21	1.68	0.59
3:k:154:SER:HB2	3:k:204:PRO:HB2	1.85	0.59
3:g:376:ARG:HD3	3:g:377:THR:HG23	1.84	0.59
5:C:90:ARG:NH2	5:C:92:ASP:OD2	2.33	0.59
1:2:67:ALA:HA	1:6:186:ASP:HB2	1.84	0.59
3:c:22:SER:OG	3:c:26:ARG:NH2	2.36	0.59
5:F:23:ILE:HG12	5:F:25:PRO:HD3	1.84	0.59
2:7:8:VAL:HG11	2:8:86:GLN:HA	1.84	0.59
3:a:281:ILE:HG22	3:a:286:VAL:HG12	1.83	0.59
3:b:61:ARG:NH2	3:c:317:GLU:OE1	2.36	0.59
3:l:15:PHE:HD1	3:l:174:THR:HG21	1.68	0.59
2:13:60:GLN:C	2:13:61:ILE:HD13	2.27	0.59
5:G:369:ASN:ND2	5:G:369:ASN:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:171:ASN:ND2	5:F:351:ASN:OD1	2.36	0.59
1:6:364:GLN:NE2	1:6:366:ASP:OD1	2.36	0.59
3:c:15:PHE:HD1	3:c:174:THR:HG21	1.68	0.59
3:d:371:TYR:HA	3:e:348:LYS:HB3	1.84	0.59
3:d:376:ARG:NH1	3:e:354:GLU:OE1	2.35	0.58
4:s:40:LEU:HD13	4:s:87:LEU:HD22	1.84	0.58
5:I:125:GLU:OE1	5:I:269:ARG:NH1	2.35	0.58
5:H:164:MET:HG3	5:H:357:ASP:HB3	1.85	0.58
1:3:229:MET:HE2	1:3:231:GLN:HG2	1.85	0.58
2:9:120:LYS:HD2	2:9:120:LYS:O	2.03	0.58
3:k:99:ARG:NH1	3:k:524:PHE:O	2.35	0.58
3:j:239:VAL:HG12	3:j:240:THR:HG22	1.85	0.58
5:D:13:VAL:HG12	5:D:14:ASP:H	1.68	0.58
2:18:52:GLU:OE1	2:18:58:HIS:NE2	2.35	0.58
3:i:157:ILE:HB	3:i:174:THR:HG23	1.84	0.58
1:1:201:PHE:CE1	1:1:240:LYS:HD2	2.38	0.58
2:9:123:LYS:HD3	2:9:123:LYS:N	2.18	0.58
2:10:11:SER:HA	2:11:15:PRO:HG2	1.84	0.58
4:u:16:LYS:HA	4:u:16:LYS:HE3	1.84	0.58
4:u:46:GLU:OE1	4:u:90:ARG:NH2	2.36	0.58
5:A:335:ALA:H	5:A:338:MET:HE2	1.67	0.58
5:H:223:SER:OG	5:H:342:ILE:HG21	2.02	0.58
1:2:12:MET:HE2	1:3:36:ILE:HG23	1.85	0.58
1:4:430:GLU:HB3	1:4:433:VAL:HB	1.86	0.58
1:5:168:ASP:OD1	1:5:170:SER:OG	2.21	0.58
4:m:69:GLU:OE1	4:m:70:GLY:N	2.37	0.58
3:e:376:ARG:NH1	3:f:378:ASP:OD2	2.36	0.58
3:e:463:ILE:O	3:e:467:ILE:HG13	2.03	0.58
3:k:53:TYR:O	4:v:131:ARG:NH1	2.32	0.58
2:13:50:TYR:HE1	2:13:60:GLN:HG2	1.69	0.58
3:c:186:ASP:OD2	3:d:171:ARG:NE	2.37	0.58
3:i:307:TRP:NE1	3:i:314:GLU:OE2	2.36	0.58
5:C:37:ALA:O	5:C:364:GLN:NE2	2.37	0.58
5:B:121:ASN:O	5:B:125:GLU:HG3	2.04	0.58
2:16:38:THR:O	2:16:102:TYR:OH	2.22	0.58
3:b:296:GLU:HG3	3:b:466:SER:HB2	1.85	0.58
5:J:309:THR:HG22	5:J:310:PRO:HD3	1.84	0.58
1:3:204:SER:H	1:3:233:GLY:HA3	1.68	0.58
2:13:108:LYS:HZ3	2:15:113:GLN:HB3	1.69	0.58
4:m:146:TRP:CD1	5:D:97:GLU:HG2	2.39	0.58
3:e:236:GLN:HB3	3:e:264:ILE:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:l:146:ARG:NH2	3:l:460:ASP:OD2	2.37	0.58
3:l:317:GLU:OE1	3:k:61:ARG:NH2	2.36	0.58
3:j:323:THR:HB	3:j:412:VAL:HG13	1.85	0.58
1:2:299:ASP:OD1	1:6:281:ARG:NH2	2.33	0.58
3:c:363:TYR:HE1	3:d:350:PHE:HE1	1.52	0.58
3:e:168:SER:OG	3:e:459:ARG:NH1	2.36	0.58
3:e:281:ILE:HG22	3:e:286:VAL:HG12	1.84	0.58
3:l:41:TRP:NE1	3:l:55:GLY:O	2.33	0.58
3:l:281:ILE:HG22	3:l:286:VAL:HG23	1.84	0.58
5:B:161:ASN:ND2	5:B:163:ASP:OD1	2.36	0.58
5:J:238:PRO:HD2	5:J:324:GLN:HB3	1.84	0.58
2:7:31:ILE:HB	2:7:65:LEU:HB2	1.84	0.58
2:22:14:ARG:NH2	2:23:109:TYR:OH	2.37	0.58
3:b:243:PRO:HA	3:b:510:ILE:HG13	1.85	0.58
3:k:561:ASP:OD1	3:k:569:ARG:NH1	2.37	0.58
3:i:538:LEU:HD21	3:h:559:LEU:HD11	1.86	0.58
1:6:312:VAL:HG21	1:6:338:TYR:HB3	1.86	0.57
2:10:42:ASN:OD1	2:10:45:ASN:N	2.37	0.57
2:13:31:ILE:HG13	2:13:67:ILE:HD11	1.86	0.57
3:a:78:VAL:HG13	3:a:518:THR:HG23	1.86	0.57
3:a:157:ILE:HB	3:a:174:THR:HG23	1.86	0.57
3:c:561:ASP:HB3	3:d:88:PRO:O	2.02	0.57
3:f:550:GLN:HE22	3:f:581:VAL:HG21	1.68	0.57
3:i:203:ASN:OD1	3:i:218:GLN:NE2	2.37	0.57
3:j:47:GLN:N	3:j:47:GLN:OE1	2.36	0.57
5:I:181:ASP:HA	5:I:184:LYS:HE3	1.87	0.57
4:y:29:GLU:HG2	4:y:30:PRO:HD2	1.85	0.57
3:j:43:ASP:OD2	3:j:46:SER:OG	2.20	0.57
3:g:249:ARG:HH12	3:g:513:ARG:HH12	1.51	0.57
5:I:185:ARG:HD2	5:J:186:ASP:HA	1.85	0.57
3:d:562:GLY:H	3:d:565:VAL:HG23	1.67	0.57
3:b:40:GLN:NE2	3:b:58:ASP:OD1	2.36	0.57
4:m:3:ILE:HG23	4:m:8:ASP:HB3	1.87	0.57
3:l:327:GLN:HE22	3:l:330:ARG:HD3	1.69	0.57
1:3:423:GLU:O	2:21:99:GLN:NE2	2.36	0.57
1:6:162:PHE:HA	1:6:177:ALA:O	2.04	0.57
2:9:74:VAL:HG12	2:9:79:LEU:HD23	1.85	0.57
3:a:33:LEU:O	3:a:37:ARG:HB2	2.05	0.57
3:a:305:GLY:O	3:a:452:ASN:ND2	2.37	0.57
3:l:458:ARG:NH1	3:k:105:ASN:OD1	2.38	0.57
3:i:51:LEU:HD13	5:H:94:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:u:3:ILE:HG23	4:u:8:ASP:HB3	1.86	0.57
5:A:285:ALA:HB2	5:B:113:ASN:HD21	1.69	0.57
5:I:217:LEU:O	5:I:349:ARG:NH2	2.38	0.57
1:4:277:GLU:OE1	1:6:300:SER:N	2.38	0.57
3:k:165:MET:HE3	3:k:307:TRP:HB3	1.87	0.57
3:j:339:ASP:OD2	4:x:131:ARG:NH2	2.35	0.57
5:A:40:MET:HB2	5:A:367:PRO:HG3	1.86	0.57
5:G:400:THR:O	5:G:402:SER:N	2.36	0.57
5:H:143:ASP:OD1	5:H:143:ASP:N	2.38	0.57
4:y:46:GLU:OE2	4:y:90:ARG:NH2	2.38	0.57
3:d:236:GLN:HB3	3:d:264:ILE:HG13	1.86	0.57
5:G:75:VAL:HB	5:G:255:ARG:HE	1.70	0.57
2:8:24:LYS:NZ	4:p:71:ASP:OD1	2.36	0.57
4:m:131:ARG:NH2	3:e:339:ASP:OD2	2.37	0.57
3:c:40:GLN:NE2	3:c:331:ASN:HD21	2.02	0.57
3:l:221:GLU:HG2	3:l:280:ILE:HD13	1.85	0.57
4:q:16:LYS:HA	4:q:16:LYS:HE3	1.87	0.57
3:k:297:HIS:HB2	3:k:463:ILE:HG12	1.87	0.57
3:e:561:ASP:OD2	3:e:569:ARG:NH2	2.38	0.57
3:k:317:GLU:OE1	3:j:61:ARG:NH2	2.37	0.57
3:i:146:ARG:NH2	3:i:460:ASP:OD2	2.37	0.57
3:i:229:LYS:HG2	3:i:272:LYS:HB2	1.86	0.57
3:h:306:GLU:OE2	3:g:65:ARG:NE	2.38	0.57
5:C:364:GLN:HG2	5:C:365:PRO:HD2	1.87	0.57
5:A:399:SER:O	5:J:406:ARG:NH1	2.34	0.57
1:6:388:ASN:OD1	1:6:445:ARG:NH2	2.38	0.57
4:y:4:LYS:NZ	4:q:63:ASP:OD1	2.37	0.57
4:s:146:TRP:HZ2	5:B:11:LEU:HD22	1.69	0.57
3:j:7:ARG:NH2	3:j:224:GLU:OE1	2.38	0.57
5:H:40:MET:HE2	5:H:45:ASN:HA	1.86	0.57
1:5:143:ASP:HB3	1:5:191:ILE:HG22	1.86	0.56
2:10:38:THR:HB	2:10:45:ASN:HD21	1.69	0.56
4:m:39:ASP:OD2	4:n:16:LYS:NZ	2.29	0.56
3:e:213:THR:HB	5:D:379:THR:OG1	2.05	0.56
3:f:306:GLU:O	3:f:316:TYR:HA	2.05	0.56
4:s:146:TRP:CZ2	5:B:11:LEU:HD22	2.39	0.56
1:1:400:THR:OG1	1:1:433:VAL:O	2.21	0.56
1:1:448:ARG:HD3	4:u:25:LEU:HD12	1.86	0.56
1:6:374:GLN:HB3	1:6:459:LYS:HG2	1.87	0.56
2:8:28:ASN:N	2:8:67:ILE:O	2.38	0.56
2:13:19:GLU:OE2	2:13:24:LYS:NZ	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:o:142:ASN:O	4:o:143:LEU:HB2	2.05	0.56
4:q:20:ALA:HA	4:q:26:THR:HB	1.87	0.56
5:H:180:TYR:HE1	5:H:184:LYS:HD3	1.69	0.56
1:1:143:ASP:HB3	1:1:191:ILE:HG22	1.86	0.56
2:11:10:VAL:HG13	2:12:90:MET:HE2	1.88	0.56
2:12:52:GLU:OE1	2:12:58:HIS:NE2	2.39	0.56
2:15:46:GLN:HE21	2:15:63:GLN:HG2	1.70	0.56
3:a:38:VAL:HG23	3:b:310:VAL:HG21	1.87	0.56
3:a:567:MET:HE2	3:b:554:LEU:HD22	1.87	0.56
4:n:131:ARG:NH2	3:f:339:ASP:OD2	2.35	0.56
4:p:46:GLU:OE2	4:p:90:ARG:NH2	2.37	0.56
3:j:44:TRP:HE1	4:x:146:TRP:CD1	2.22	0.56
3:h:234:ILE:HD13	3:h:244:VAL:HG13	1.87	0.56
4:x:138:ASN:O	4:x:140:PHE:N	2.39	0.56
4:x:146:TRP:CZ3	5:H:97:GLU:HA	2.40	0.56
5:A:31:LYS:HD2	5:A:164:MET:HE2	1.86	0.56
5:B:380:SER:OG	5:B:389:ASN:OD1	2.22	0.56
5:F:24:THR:HA	5:F:116:GLU:OE2	2.05	0.56
5:J:171:ASN:ND2	5:J:174:ASP:OD2	2.37	0.56
1:2:142:ARG:NH2	1:2:189:ILE:HG23	2.19	0.56
1:5:316:ASP:O	1:5:320:SER:OG	2.23	0.56
2:23:36:ILE:HG22	2:23:37:ASP:OD1	2.06	0.56
3:d:37:ARG:NH1	3:e:309:PHE:O	2.39	0.56
4:o:115:TYR:OH	3:e:360:GLU:OE2	2.22	0.56
3:j:561:ASP:OD2	3:j:569:ARG:NH2	2.38	0.56
5:J:357:ASP:OD1	5:J:417:ARG:NH1	2.38	0.56
2:16:111:PRO:HB2	2:18:7:ASN:ND2	2.19	0.56
2:19:108:LYS:NZ	2:21:52:GLU:OE1	2.38	0.56
2:21:46:GLN:CD	2:21:63:GLN:HG2	2.30	0.56
2:23:31:ILE:HG13	2:23:67:ILE:HD11	1.88	0.56
3:b:15:PHE:HD1	3:b:174:THR:HG21	1.71	0.56
3:c:376:ARG:NH1	3:d:354:GLU:OE2	2.39	0.56
4:q:145:GLU:OE2	5:B:377:LYS:NZ	2.38	0.56
4:s:46:GLU:O	4:s:49:GLN:NE2	2.32	0.56
5:G:7:GLN:NE2	5:F:240:ALA:O	2.39	0.56
1:2:165:ASP:OD1	1:2:166:LEU:N	2.39	0.56
1:6:237:THR:O	1:6:240:LYS:NZ	2.38	0.56
2:18:46:GLN:HG2	2:18:63:GLN:HG2	1.88	0.56
3:a:171:ARG:NH2	3:l:182:ASN:OD1	2.33	0.56
3:d:363:TYR:OH	3:d:373:LEU:O	2.23	0.56
3:f:61:ARG:NH1	3:g:306:GLU:OE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j:109:ILE:O	3:j:113:ILE:HG13	2.05	0.56
5:E:244:ASP:OD1	5:E:248:ASN:N	2.24	0.56
5:A:7:GLN:HB3	5:J:74:ASN:HD22	1.70	0.56
5:F:244:ASP:OD1	5:F:248:ASN:N	2.38	0.56
1:5:126:ASN:HD21	1:5:136:TYR:N	2.02	0.56
1:5:164:THR:HA	1:5:172:PRO:HA	1.87	0.56
2:24:84:THR:HG22	2:24:85:VAL:H	1.71	0.56
3:e:556:TYR:HH	3:f:542:THR:HG1	1.54	0.56
4:q:1:MET:O	4:q:4:LYS:NZ	2.36	0.56
5:A:398:ILE:O	5:J:406:ARG:NH1	2.38	0.56
1:1:37:LEU:HD12	1:3:385:LYS:HB2	1.88	0.56
1:5:274:ALA:O	1:5:278:LYS:HG2	2.05	0.56
1:6:164:THR:HA	1:6:172:PRO:HA	1.88	0.56
1:6:412:SER:HB3	1:6:423:GLU:HG2	1.88	0.56
2:23:78:GLN:NE2	4:s:25:LEU:O	2.38	0.56
3:e:376:ARG:HD3	3:e:377:THR:HG23	1.86	0.56
3:j:159:ASP:OD1	3:j:171:ARG:NH2	2.39	0.56
1:2:419:ASN:OD1	2:8:51:ILE:HD11	2.05	0.56
1:6:63:GLU:OE1	1:6:99:HIS:ND1	2.37	0.56
3:a:87:ARG:NH1	3:a:89:ASP:OD1	2.38	0.56
3:e:167:LYS:HG2	3:e:302:PRO:HG3	1.88	0.56
1:4:150:ARG:NH2	1:4:173:ASP:OD1	2.39	0.56
1:4:410:PHE:HE1	1:4:425:MET:HE2	1.70	0.56
2:12:65:LEU:HD13	2:12:82:ILE:HD12	1.88	0.56
3:d:209:PHE:HB3	5:D:13:VAL:HG13	1.88	0.56
4:v:27:ASP:OD1	4:v:27:ASP:N	2.39	0.56
5:D:133:SER:HB2	5:D:147:PHE:HE1	1.71	0.56
5:B:24:THR:OG1	5:B:385:ASP:OD2	2.22	0.56
1:2:164:THR:HA	1:2:172:PRO:HA	1.86	0.55
1:3:447:ARG:HD3	4:v:25:LEU:HB2	1.87	0.55
2:8:33:ILE:HD12	2:8:84:THR:HG21	1.87	0.55
2:16:114:TYR:OH	2:18:119:ASP:OD1	2.20	0.55
3:e:562:GLY:H	3:e:565:VAL:HG23	1.71	0.55
3:k:211:TRP:HZ3	5:I:35:PRO:HB3	1.70	0.55
3:h:281:ILE:HG22	3:h:286:VAL:HG22	1.87	0.55
3:a:249:ARG:NH2	3:a:470:ASP:OD1	2.39	0.55
3:i:239:VAL:HG12	3:i:240:THR:HG22	1.87	0.55
5:C:271:ASP:OD1	5:C:272:LYS:N	2.39	0.55
5:A:264:THR:O	5:A:264:THR:OG1	2.21	0.55
1:6:428:GLN:HA	1:6:438:VAL:HG21	1.89	0.55
2:14:11:SER:OG	2:14:12:ASN:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:133:SER:HB2	5:G:147:PHE:CE1	2.42	0.55
5:H:168:TYR:CD2	5:H:353:PHE:HB3	2.42	0.55
2:9:112:ASP:OD1	2:9:112:ASP:N	2.36	0.55
3:b:76:ILE:HG22	3:b:457:MET:HG3	1.88	0.55
3:d:67:LEU:HD13	3:d:418:LEU:HD22	1.87	0.55
5:C:399:SER:O	5:B:406:ARG:NH1	2.40	0.55
5:F:31:LYS:NZ	5:F:33:TYR:HB2	2.21	0.55
1:2:201:PHE:HD1	1:2:206:ILE:HG12	1.70	0.55
3:c:61:ARG:NH2	3:d:317:GLU:OE1	2.39	0.55
3:c:236:GLN:HB3	3:c:264:ILE:HG13	1.89	0.55
3:k:527:MET:HA	3:k:527:MET:HE2	1.88	0.55
5:A:228:ILE:HD13	5:A:267:MET:HE3	1.89	0.55
5:A:261:LEU:HD12	5:A:264:THR:HG22	1.89	0.55
1:2:339:ARG:NH2	1:2:357:GLU:OE1	2.39	0.55
1:4:127:TRP:HE3	1:4:128:PRO:HD2	1.72	0.55
2:12:51:ILE:HG23	2:12:80:VAL:HB	1.87	0.55
2:20:5:THR:O	2:20:5:THR:OG1	2.24	0.55
3:b:561:ASP:OD2	3:b:569:ARG:NH2	2.40	0.55
3:h:76:ILE:HG22	3:h:457:MET:HG3	1.89	0.55
5:E:260:THR:HG23	5:E:305:HIS:CE1	2.41	0.55
5:H:24:THR:O	5:H:28:GLN:HG2	2.05	0.55
5:H:368:ALA:HB3	5:H:378:THR:HG21	1.89	0.55
2:8:31:ILE:HG23	2:8:67:ILE:HD11	1.89	0.55
2:10:31:ILE:HB	2:10:65:LEU:HB2	1.89	0.55
4:s:46:GLU:OE2	4:s:90:ARG:NH2	2.39	0.55
4:u:7:GLY:O	4:u:11:ARG:HG3	2.05	0.55
3:g:206:ASP:OD1	5:F:105:GLN:NE2	2.40	0.55
3:g:214:GLN:NE2	5:F:382:SER:O	2.36	0.55
5:G:299:ARG:HD2	5:G:301:VAL:HG12	1.88	0.55
1:2:281:ARG:NH2	1:3:299:ASP:OD1	2.37	0.55
1:5:284:THR:OG1	1:5:286:GLU:O	2.20	0.55
3:a:249:ARG:HH12	3:a:513:ARG:NH1	2.04	0.55
3:j:454:ALA:O	3:j:458:ARG:HG3	2.07	0.55
1:1:12:MET:HE3	1:1:21:TYR:HB3	1.88	0.55
1:1:59:SER:OG	1:1:342:ASP:OD2	2.22	0.55
1:2:148:ARG:HA	1:6:182:GLU:O	2.06	0.55
1:3:26:PRO:HB2	1:3:29:MET:HB2	1.89	0.55
1:4:73:ARG:NH2	1:4:342:ASP:O	2.39	0.55
2:10:30:LYS:HZ1	2:10:64:PRO:HB3	1.71	0.55
3:a:136:SER:O	3:a:136:SER:OG	2.23	0.55
3:c:279:SER:OG	3:c:289:ASP:O	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:454:ALA:HB1	3:e:520:VAL:HG21	1.89	0.55
4:v:3:ILE:HG23	4:v:8:ASP:HB3	1.89	0.55
5:G:104:ILE:HD13	5:G:407:ILE:HD11	1.89	0.55
5:J:168:TYR:CD2	5:J:353:PHE:HB3	2.42	0.55
5:J:388:LEU:HD13	5:J:409:LEU:HD11	1.88	0.55
1:4:78:LYS:NZ	1:4:85:GLU:OE2	2.26	0.55
1:4:143:ASP:HB3	1:4:191:ILE:HG22	1.88	0.55
1:5:62:VAL:HG23	1:5:73:ARG:HG2	1.88	0.55
2:8:51:ILE:HG22	2:8:82:ILE:HD13	1.90	0.55
4:o:145:GLU:HB3	3:g:44:TRP:HE1	1.72	0.55
3:l:383:ASP:OD1	3:l:384:LEU:N	2.41	0.55
3:i:376:ARG:HD3	4:t:112:GLU:OE2	2.06	0.55
3:j:542:THR:HG21	3:j:547:PRO:HB2	1.89	0.55
5:B:168:TYR:CD2	5:B:353:PHE:HB3	2.42	0.55
1:5:423:GLU:OE2	1:5:455:ARG:NH2	2.37	0.54
1:6:262:ILE:HG13	1:6:271:ILE:HG13	1.88	0.54
2:22:81:LYS:NZ	2:23:108:LYS:O	2.31	0.54
3:k:16:ASP:OD2	5:I:101:ARG:NH2	2.40	0.54
5:D:384:PRO:O	5:D:386:VAL:N	2.40	0.54
5:F:128:SER:HB2	5:F:310:PRO:HG3	1.88	0.54
5:J:223:SER:OG	5:J:342:ILE:HG21	2.07	0.54
1:4:30:LEU:HD11	1:4:46:PHE:HD1	1.72	0.54
1:5:390:ARG:HD3	4:s:97:LEU:HD21	1.88	0.54
2:14:28:ASN:N	2:14:67:ILE:O	2.39	0.54
3:a:383:ASP:OD1	3:a:384:LEU:N	2.40	0.54
3:a:398:PRO:HB3	3:l:395:PRO:HD2	1.87	0.54
4:u:5:THR:OG1	4:u:8:ASP:OD2	2.24	0.54
1:2:14:LYS:HB2	1:2:418:ILE:HG12	1.89	0.54
2:14:46:GLN:CD	2:14:63:GLN:HG2	2.32	0.54
3:h:213:THR:HG22	3:h:214:GLN:H	1.72	0.54
3:g:40:GLN:NE2	3:g:58:ASP:OD1	2.40	0.54
5:E:396:GLY:O	5:D:395:GLN:NE2	2.39	0.54
5:I:7:GLN:NE2	5:H:74:ASN:HB3	2.23	0.54
1:3:29:MET:HE1	1:3:462:VAL:HB	1.90	0.54
1:4:48:GLY:O	1:4:363:LEU:HA	2.08	0.54
3:l:44:TRP:CE3	5:J:97:GLU:HB2	2.43	0.54
3:g:234:ILE:HD13	3:g:244:VAL:HG13	1.90	0.54
5:H:137:ILE:HG22	5:H:177:LYS:HB3	1.89	0.54
2:21:21:ARG:NH1	4:x:27:ASP:OD1	2.41	0.54
3:a:239:VAL:HG12	3:a:240:THR:HG22	1.90	0.54
3:h:246:TYR:CZ	3:h:273:ARG:HD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:261:LEU:HD13	5:H:267:MET:HE1	1.90	0.54
5:J:309:THR:CG2	5:J:310:PRO:HD3	2.38	0.54
1:2:396:VAL:HG23	1:2:438:VAL:HB	1.88	0.54
3:b:37:ARG:NH1	3:b:120:GLU:OE1	2.41	0.54
3:d:556:TYR:OH	3:e:542:THR:OG1	2.21	0.54
3:e:284:THR:HG21	5:D:387:GLY:HA2	1.89	0.54
3:k:542:THR:HG23	3:j:552:LEU:HD21	1.88	0.54
5:E:161:ASN:HA	5:F:21:SER:HB2	1.88	0.54
5:I:74:ASN:HD21	5:I:251:ASN:HD22	1.54	0.54
5:J:281:LEU:HD11	5:J:315:LEU:HB2	1.89	0.54
3:c:15:PHE:CD1	3:c:174:THR:HG21	2.42	0.54
3:d:281:ILE:HG22	3:d:286:VAL:HG22	1.88	0.54
3:j:146:ARG:NH2	3:j:460:ASP:OD2	2.40	0.54
3:h:215:ASP:N	3:h:215:ASP:OD1	2.41	0.54
5:C:376:MET:HB3	5:C:393:ALA:HB1	1.90	0.54
2:17:42:ASN:HB3	2:17:45:ASN:OD1	2.07	0.54
2:22:83:VAL:HG12	2:24:9:VAL:HG22	1.88	0.54
3:e:376:ARG:HH21	3:f:385:PRO:HD3	1.72	0.54
3:i:363:TYR:OH	3:i:373:LEU:O	2.23	0.54
5:E:188:PHE:HB3	5:E:193:GLU:HG2	1.90	0.54
5:I:37:ALA:O	5:I:364:GLN:NE2	2.32	0.54
1:1:435:ASP:HB3	4:v:25:LEU:HD21	1.89	0.54
1:2:331:THR:OG1	1:2:370:GLN:OE1	2.23	0.54
1:2:409:LEU:HD21	1:2:454:LEU:HD12	1.89	0.54
1:6:72:TYR:HD2	1:6:79:LEU:HD21	1.73	0.54
2:12:31:ILE:HB	2:12:65:LEU:HB2	1.89	0.54
2:19:50:TYR:HD2	2:19:58:HIS:HB3	1.73	0.54
2:19:88:HIS:CE1	2:19:106:VAL:HG21	2.42	0.54
2:22:113:GLN:O	2:22:117:GLU:HG2	2.08	0.54
3:l:69:SER:O	3:l:73:GLN:HG3	2.08	0.54
3:f:211:TRP:HB3	3:g:313:LYS:HE3	1.88	0.54
3:j:376:ARG:HG2	3:j:377:THR:HG23	1.90	0.54
5:G:146:ASN:HB2	5:H:180:TYR:CE2	2.43	0.54
5:J:47:ILE:HG23	5:J:77:VAL:HG23	1.90	0.54
2:20:46:GLN:CD	2:20:63:GLN:HG2	2.33	0.54
3:a:360:GLU:OE2	4:q:115:TYR:OH	2.25	0.54
4:r:3:ILE:HG23	4:r:8:ASP:HB3	1.90	0.54
3:k:562:GLY:H	3:k:565:VAL:HG23	1.72	0.54
3:h:93:VAL:O	3:h:97:MET:HG3	2.08	0.54
5:H:143:ASP:HA	5:H:146:ASN:HB2	1.89	0.54
1:4:167:GLU:OE2	1:4:174:ARG:NH2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:430:GLU:HG3	1:5:431:PRO:HD2	1.90	0.53
2:19:16:ILE:HD11	2:20:23:PHE:HE1	1.73	0.53
3:a:182:ASN:OD1	3:b:171:ARG:NH2	2.41	0.53
3:b:203:ASN:OD1	3:b:218:GLN:NE2	2.41	0.53
3:l:51:LEU:HD11	4:u:141:ALA:HB2	1.90	0.53
3:i:20:THR:HG21	5:G:382:SER:HB3	1.90	0.53
3:i:37:ARG:HD3	3:j:310:VAL:HG22	1.91	0.53
5:A:316:ASP:OD1	5:A:332:THR:HA	2.08	0.53
5:H:89:LEU:HD11	5:H:100:TYR:CD1	2.43	0.53
1:1:408:ARG:NH2	2:18:93:TYR:OH	2.35	0.53
1:3:283:TYR:HE2	1:3:308:LEU:HD13	1.73	0.53
1:5:49:ILE:HD12	1:5:370:GLN:HG2	1.90	0.53
1:5:442:ARG:NH2	4:s:21:SER:OG	2.41	0.53
2:7:42:ASN:HB2	2:7:45:ASN:HB2	1.90	0.53
3:a:363:TYR:OH	3:a:373:LEU:O	2.26	0.53
3:c:23:ASP:HA	3:c:26:ARG:NH1	2.23	0.53
4:o:126:ALA:O	3:f:343:ARG:NH2	2.34	0.53
3:i:234:ILE:HG22	3:i:266:ILE:HB	1.90	0.53
5:E:357:ASP:OD2	5:E:417:ARG:NH1	2.35	0.53
5:A:125:GLU:OE1	5:A:269:ARG:NE	2.42	0.53
5:G:95:ARG:HD2	5:F:37:ALA:HB1	1.90	0.53
1:1:301:HIS:ND1	1:1:316:ASP:OD2	2.41	0.53
1:1:394:LEU:HD23	1:1:411:LEU:HD21	1.89	0.53
2:10:30:LYS:NZ	2:10:64:PRO:HB3	2.22	0.53
2:13:50:TYR:HB2	2:13:83:VAL:HG23	1.90	0.53
3:a:465:GLN:O	3:a:469:ASN:ND2	2.40	0.53
1:3:354:ASP:OD1	1:3:355:LYS:N	2.40	0.53
2:17:51:ILE:HG22	2:17:82:ILE:HD13	1.89	0.53
4:n:46:GLU:OE2	4:n:90:ARG:NH2	2.28	0.53
3:e:323:THR:HG22	3:e:415:VAL:HG13	1.91	0.53
3:i:92:ASP:OD1	3:i:93:VAL:N	2.42	0.53
4:t:46:GLU:OE2	4:t:90:ARG:NH2	2.41	0.53
5:E:151:ALA:O	5:E:155:MET:HG3	2.08	0.53
5:G:146:ASN:HB2	5:H:180:TYR:HE2	1.73	0.53
1:1:126:ASN:ND2	1:1:136:TYR:O	2.42	0.53
1:2:97:MET:HE2	1:2:104:GLN:HE21	1.73	0.53
1:2:139:GLY:HA3	1:2:155:LYS:HE3	1.91	0.53
2:8:46:GLN:CD	2:8:63:GLN:HG2	2.32	0.53
3:d:65:ARG:NE	3:e:306:GLU:OE2	2.42	0.53
3:i:215:ASP:N	3:i:215:ASP:OD1	2.41	0.53
3:j:221:GLU:OE2	3:j:278:LYS:NZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:394:THR:HG21	5:J:372:LEU:HA	1.88	0.53
5:J:171:ASN:ND2	5:J:351:ASN:OD1	2.42	0.53
1:1:297:ARG:NH2	1:3:277:GLU:OE2	2.29	0.53
2:9:14:ARG:HG3	2:9:14:ARG:HH11	1.73	0.53
3:b:335:SER:OG	4:s:131:ARG:NH1	2.42	0.53
3:c:76:ILE:HG23	3:c:520:VAL:HG13	1.91	0.53
3:k:67:LEU:HD13	3:k:418:LEU:HD22	1.89	0.53
3:i:327:GLN:NE2	3:i:330:ARG:HD3	2.23	0.53
3:h:209:PHE:HZ	5:G:370:HIS:HD1	1.54	0.53
3:h:538:LEU:HD21	3:g:559:LEU:HD11	1.91	0.53
5:C:373:PHE:HA	5:C:376:MET:HG3	1.90	0.53
5:J:143:ASP:HA	5:J:146:ASN:HB2	1.90	0.53
1:1:126:ASN:HD21	1:1:136:TYR:H	1.55	0.53
1:5:34:LYS:O	1:5:41:GLY:N	2.42	0.53
1:5:139:GLY:H	1:5:155:LYS:HD2	1.73	0.53
1:5:156:ASP:OD1	1:5:156:ASP:N	2.42	0.53
1:5:262:ILE:HG13	1:5:271:ILE:HG13	1.91	0.53
1:6:261:TYR:HB3	1:6:268:ALA:HB1	1.90	0.53
3:b:364:ASP:OD1	3:b:366:ASN:ND2	2.41	0.53
3:b:510:ILE:HG23	3:b:512:GLY:H	1.72	0.53
3:l:227:GLU:OE2	3:l:272:LYS:NZ	2.42	0.53
3:l:510:ILE:HG12	3:l:511:ARG:H	1.74	0.53
5:G:133:SER:HB3	5:G:426:PRO:HA	1.90	0.53
5:I:237:LYS:HG2	5:I:320:LEU:HD23	1.91	0.53
5:D:317:ASP:O	5:D:325:ARG:NH1	2.39	0.53
1:2:143:ASP:HB3	1:2:191:ILE:HG22	1.91	0.53
1:4:297:ARG:NH2	1:5:277:GLU:OE1	2.37	0.53
1:6:141:VAL:HG22	1:6:153:TRP:CD1	2.43	0.53
2:19:43:PRO:HA	2:19:46:GLN:HG3	1.90	0.53
3:j:244:VAL:H	3:j:510:ILE:HG13	1.74	0.53
5:A:229:THR:HG22	5:A:339:ALA:HA	1.90	0.53
5:I:68:THR:H	5:J:87:PHE:HA	1.74	0.53
5:D:88:GLN:OE1	5:D:90:ARG:NH2	2.42	0.53
1:1:186:ASP:OD2	1:5:101:ARG:NH1	2.26	0.53
2:10:49:VAL:HG12	2:10:84:THR:HG22	1.89	0.53
3:a:374:LEU:HD11	3:b:350:PHE:HB3	1.90	0.53
3:c:557:PHE:HE1	3:c:573:ASN:CG	2.17	0.53
3:k:71:MET:HE3	3:k:450:GLN:HG2	1.90	0.53
3:j:27:ARG:HH22	5:H:101:ARG:NH1	2.07	0.53
5:B:223:SER:HB3	5:B:342:ILE:HG21	1.90	0.53
5:B:357:ASP:OD1	5:B:417:ARG:NH1	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:258:THR:HA	5:F:306:VAL:O	2.09	0.53
1:2:259:SER:OG	1:2:260:VAL:N	2.42	0.53
2:14:14:ARG:HG2	2:14:14:ARG:HH11	1.73	0.53
2:19:81:LYS:NZ	2:20:108:LYS:O	2.35	0.53
3:a:525:GLN:NE2	3:b:519:ASP:OD1	2.42	0.53
3:d:323:THR:HB	3:d:412:VAL:HG13	1.90	0.53
4:o:5:THR:OG1	4:o:8:ASP:OD2	2.27	0.53
3:f:81:ARG:NH2	3:f:519:ASP:OD2	2.30	0.53
3:f:376:ARG:HD3	3:f:377:THR:HG23	1.90	0.53
3:h:30:LYS:HE3	3:h:205:ASN:O	2.09	0.53
5:C:171:ASN:ND2	5:C:174:ASP:OD1	2.39	0.53
5:D:168:TYR:CD2	5:D:353:PHE:HB3	2.44	0.53
5:F:79:MET:HE1	5:F:364:GLN:HB2	1.90	0.53
1:1:186:ASP:HB2	1:5:67:ALA:HA	1.91	0.52
1:3:36:ILE:HD11	1:3:42:TYR:CD1	2.44	0.52
1:5:112:LEU:HB3	1:5:124:VAL:HB	1.92	0.52
2:9:35:GLN:O	2:9:38:THR:OG1	2.27	0.52
2:16:99:GLN:NE2	2:16:102:TYR:HB2	2.24	0.52
3:b:296:GLU:OE2	3:b:514:TYR:OH	2.26	0.52
3:c:323:THR:HG22	3:c:415:VAL:HG13	1.91	0.52
3:l:44:TRP:CZ3	3:l:45:LEU:HD23	2.43	0.52
4:s:11:ARG:HG3	4:s:33:MET:HE1	1.91	0.52
5:C:116:GLU:HG2	5:C:216:LYS:HD2	1.89	0.52
5:D:159:GLU:OE1	5:D:284:MET:HB3	2.09	0.52
5:D:302:ASP:OD1	5:D:303:GLY:N	2.33	0.52
2:7:55:ASP:OD1	2:7:56:GLY:N	2.41	0.52
2:11:99:GLN:NE2	2:11:102:TYR:HB2	2.24	0.52
2:16:51:ILE:HG12	2:16:59:VAL:HG22	1.92	0.52
3:b:7:ARG:NH2	3:b:224:GLU:OE1	2.41	0.52
3:d:76:ILE:HG22	3:d:457:MET:HG3	1.89	0.52
3:d:234:ILE:HD13	3:d:244:VAL:HG22	1.91	0.52
4:s:3:ILE:HG23	4:s:8:ASP:HB3	1.91	0.52
3:j:157:ILE:HB	3:j:174:THR:HG23	1.91	0.52
3:g:213:THR:O	3:g:214:GLN:HG3	2.09	0.52
5:F:25:PRO:O	5:F:29:LYS:HG2	2.09	0.52
1:5:47:PRO:HB3	1:5:365:PHE:HA	1.92	0.52
2:8:14:ARG:HH11	2:8:14:ARG:HG3	1.75	0.52
3:d:200:SER:H	3:d:282:THR:HG23	1.74	0.52
3:h:418:LEU:HD23	3:h:446:THR:HG22	1.91	0.52
5:C:260:THR:HA	5:C:305:HIS:HD2	1.74	0.52
5:C:405:CYS:HB2	5:B:372:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:168:TYR:CD2	5:G:353:PHE:HB3	2.43	0.52
1:1:155:LYS:HE2	1:1:158:THR:HG21	1.92	0.52
2:15:68:ASN:HB2	2:15:74:VAL:HG13	1.90	0.52
3:b:53:TYR:O	4:s:131:ARG:NH1	2.41	0.52
3:f:220:ALA:HB3	3:f:281:ILE:HG13	1.91	0.52
3:k:15:PHE:HD1	3:k:174:THR:HG21	1.75	0.52
3:h:561:ASP:OD2	3:h:569:ARG:NH2	2.42	0.52
5:I:8:ILE:HG21	5:H:249:LYS:HG3	1.90	0.52
1:1:164:THR:HA	1:1:172:PRO:HA	1.90	0.52
1:6:446:ILE:H	1:6:446:ILE:HD12	1.74	0.52
2:7:51:ILE:HG12	2:7:59:VAL:HG12	1.91	0.52
2:15:46:GLN:HE21	2:15:63:GLN:CG	2.22	0.52
3:d:525:GLN:NE2	3:e:519:ASP:OD1	2.43	0.52
4:q:46:GLU:O	4:q:49:GLN:NE2	2.39	0.52
3:j:113:ILE:HD13	3:j:150:HIS:CE1	2.45	0.52
5:C:126:MET:O	5:C:126:MET:HG3	2.10	0.52
5:G:188:PHE:HD1	5:G:192:PRO:HB2	1.75	0.52
5:I:25:PRO:HD2	5:I:116:GLU:OE2	2.09	0.52
5:H:257:ALA:HB2	5:H:311:LYS:HG3	1.91	0.52
2:8:117:GLU:H	2:8:117:GLU:CD	2.18	0.52
3:c:325:ASP:OD2	4:q:136:SER:OG	2.27	0.52
3:k:348:LYS:HB2	3:j:372:TYR:CE1	2.44	0.52
5:A:365:PRO:HB3	5:A:391:ILE:HD11	1.90	0.52
5:H:128:SER:HB2	5:H:310:PRO:HG3	1.91	0.52
1:5:60:ARG:HH22	1:5:89:VAL:HG12	1.75	0.52
2:9:33:ILE:HG22	2:9:90:MET:HG3	1.91	0.52
2:16:11:SER:HA	2:17:15:PRO:HG3	1.92	0.52
4:m:145:GLU:OE1	3:e:31:ASN:ND2	2.31	0.52
3:e:306:GLU:O	3:e:316:TYR:HA	2.09	0.52
3:i:19:TRP:O	3:i:26:ARG:NH2	2.37	0.52
3:i:364:ASP:OD1	3:i:366:ASN:ND2	2.43	0.52
5:G:40:MET:HB3	5:G:45:ASN:HA	1.91	0.52
5:F:40:MET:HG2	5:F:45:ASN:HA	1.91	0.52
1:1:229:MET:HE1	1:5:196:ASP:HB2	1.91	0.52
1:3:30:LEU:HD11	1:3:46:PHE:HD1	1.75	0.52
3:c:190:LYS:HG2	3:c:191:TYR:CD1	2.45	0.52
3:d:229:LYS:HG3	3:d:272:LYS:HG3	1.91	0.52
3:l:557:PHE:HD1	3:l:573:ASN:HD21	1.58	0.52
3:g:209:PHE:HA	5:F:101:ARG:HG2	1.91	0.52
5:A:173:GLN:HG3	5:A:177:LYS:HE3	1.92	0.52
5:G:392:PHE:HE1	5:G:405:CYS:HB2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:130:VAL:HG21	5:F:272:LYS:HB3	1.91	0.52
1:2:167:GLU:OE1	1:2:167:GLU:N	2.42	0.52
3:k:161:ASN:HB3	3:k:171:ARG:HH12	1.74	0.52
3:i:33:LEU:HD22	3:i:37:ARG:HH11	1.75	0.52
3:h:317:GLU:OE1	3:g:61:ARG:NH2	2.42	0.52
3:g:211:TRP:O	3:g:213:THR:N	2.42	0.52
1:1:297:ARG:HH22	1:3:277:GLU:CD	2.17	0.52
1:2:12:MET:SD	1:3:34:LYS:NZ	2.82	0.52
1:3:265:SER:O	1:3:265:SER:OG	2.25	0.52
3:h:323:THR:HG22	3:h:415:VAL:HG13	1.92	0.52
5:G:62:ASP:OD1	5:I:400:THR:HG22	2.10	0.52
5:B:363:SER:O	5:B:364:GLN:NE2	2.42	0.52
5:H:238:PRO:HD2	5:H:324:GLN:HB3	1.92	0.52
2:10:36:ILE:HG22	2:10:37:ASP:OD1	2.10	0.51
2:13:108:LYS:NZ	2:15:113:GLN:HB3	2.25	0.51
2:22:74:VAL:HG12	2:22:79:LEU:HD22	1.91	0.51
3:a:323:THR:HB	3:a:412:VAL:HG13	1.92	0.51
3:b:561:ASP:OD1	3:b:569:ARG:NH1	2.43	0.51
3:l:271:ILE:HG23	3:k:134:ASP:HB3	1.92	0.51
3:h:33:LEU:HD22	3:h:37:ARG:HH11	1.74	0.51
5:A:36:PRO:HG2	5:B:13:VAL:CG1	2.39	0.51
5:A:97:GLU:OE1	5:J:370:HIS:NE2	2.39	0.51
5:F:236:PHE:CZ	5:F:259:VAL:HG12	2.45	0.51
1:1:2:PRO:HD2	1:1:472:GLU:HA	1.92	0.51
1:2:206:ILE:HD13	1:2:263:ILE:HD11	1.92	0.51
2:20:52:GLU:HB3	2:20:81:LYS:HD3	1.93	0.51
3:a:18:ASP:OD2	3:a:172:HIS:HE1	1.93	0.51
3:b:274:ARG:HH11	3:b:274:ARG:HG3	1.75	0.51
3:f:45:LEU:HD12	5:E:365:PRO:HG2	1.93	0.51
3:k:121:ALA:O	3:k:321:ARG:NH2	2.43	0.51
3:k:281:ILE:HG22	3:k:286:VAL:HG22	1.92	0.51
3:h:15:PHE:HE1	3:h:157:ILE:HD13	1.75	0.51
3:h:542:THR:HG1	3:g:556:TYR:HH	1.59	0.51
3:g:33:LEU:O	3:g:37:ARG:HB2	2.10	0.51
3:g:213:THR:O	3:g:215:ASP:N	2.43	0.51
3:g:213:THR:C	3:g:215:ASP:H	2.17	0.51
4:x:9:LEU:HD22	4:x:84:PHE:HB3	1.90	0.51
5:A:320:LEU:HD22	5:A:324:GLN:HB3	1.91	0.51
5:G:39:SER:HB2	5:H:11:LEU:HD13	1.91	0.51
5:I:284:MET:CE	5:J:109:ARG:HG2	2.40	0.51
1:6:368:SER:OG	1:6:460:SER:O	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:86:GLN:HB3	2:7:112:ASP:HB2	1.92	0.51
2:10:51:ILE:HG12	2:10:59:VAL:HB	1.93	0.51
2:23:28:ASN:N	2:23:67:ILE:O	2.43	0.51
3:b:144:ILE:HD11	3:b:467:ILE:HG22	1.90	0.51
3:c:507:LEU:HD23	3:c:507:LEU:H	1.75	0.51
3:k:339:ASP:OD2	4:v:131:ARG:NH2	2.28	0.51
3:h:67:LEU:HD13	3:h:418:LEU:HD22	1.92	0.51
5:G:101:ARG:O	5:G:105:GLN:HG3	2.11	0.51
5:B:309:THR:HG22	5:B:310:PRO:HD3	1.92	0.51
1:1:231:GLN:NE2	1:5:194:TRP:O	2.42	0.51
1:2:390:ARG:HD3	4:p:97:LEU:HD21	1.92	0.51
2:17:99:GLN:NE2	2:17:102:TYR:HB2	2.24	0.51
2:21:36:ILE:HA	2:21:89:SER:HB3	1.92	0.51
5:C:50:PRO:HB2	5:D:16:ILE:HD13	1.93	0.51
5:C:168:TYR:CD2	5:C:353:PHE:HB3	2.45	0.51
5:A:7:GLN:HB3	5:J:74:ASN:ND2	2.25	0.51
2:23:119:ASP:OD1	2:24:114:TYR:OH	2.28	0.51
3:e:200:SER:HB2	5:D:382:SER:HB2	1.92	0.51
3:k:203:ASN:ND2	5:I:389:ASN:HD21	2.08	0.51
5:E:178:ALA:HB3	5:E:201:ILE:HD11	1.92	0.51
5:A:79:MET:HE1	5:A:364:GLN:HB2	1.91	0.51
5:D:271:ASP:O	5:D:297:VAL:HG12	2.10	0.51
5:D:299:ARG:HB3	5:D:299:ARG:NH1	2.25	0.51
1:2:34:LYS:H	1:2:41:GLY:HA2	1.74	0.51
2:18:73:ILE:HG21	2:18:82:ILE:HD12	1.91	0.51
4:q:7:GLY:N	4:q:69:GLU:OE1	2.44	0.51
3:i:135:GLN:NE2	3:j:296:GLU:OE2	2.39	0.51
3:i:313:LYS:HE3	3:h:211:TRP:CH2	2.46	0.51
3:g:239:VAL:HG12	3:g:240:THR:HG22	1.92	0.51
5:J:279:LYS:NZ	5:J:292:ASP:OD1	2.32	0.51
1:1:369:SER:HB3	1:1:459:LYS:HG2	1.93	0.51
1:4:330:LYS:HD2	1:4:335:ASP:HA	1.92	0.51
2:22:19:GLU:HG3	2:22:24:LYS:HG2	1.93	0.51
3:a:43:ASP:OD1	3:a:47:GLN:HG3	2.10	0.51
3:a:507:LEU:HD23	3:a:507:LEU:H	1.75	0.51
3:c:115:VAL:O	3:c:119:ILE:HD12	2.10	0.51
3:l:22:SER:OG	3:l:26:ARG:NH2	2.44	0.51
3:l:454:ALA:HB1	3:l:520:VAL:HG21	1.91	0.51
5:J:201:ILE:HG13	5:J:202:GLN:H	1.74	0.51
1:1:167:GLU:OE1	1:1:167:GLU:N	2.44	0.51
1:5:388:ASN:OD1	1:5:445:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:280:ILE:HG23	1:6:288:MET:HE1	1.91	0.51
2:13:55:ASP:OD1	2:13:56:GLY:N	2.44	0.51
2:16:26:VAL:HG13	2:16:94:ASP:HA	1.92	0.51
3:c:357:ALA:O	3:c:375:ASN:ND2	2.44	0.51
3:l:387:GLN:HG3	3:k:386:THR:HG21	1.93	0.51
3:k:171:ARG:NH2	3:j:182:ASN:OD1	2.38	0.51
3:k:234:ILE:HD13	3:k:244:VAL:HG13	1.92	0.51
3:g:297:HIS:HB3	3:g:459:ARG:NH2	2.26	0.51
5:A:153:GLU:OE1	5:B:173:GLN:NE2	2.43	0.51
5:G:377:LYS:O	5:G:393:ALA:HA	2.11	0.51
5:I:76:ALA:O	5:I:255:ARG:NH1	2.43	0.51
5:B:75:VAL:HB	5:B:255:ARG:HD3	1.93	0.51
1:1:206:ILE:HD13	1:1:263:ILE:HD11	1.92	0.51
1:1:274:ALA:O	1:1:278:LYS:HG3	2.10	0.51
1:2:448:ARG:NH1	1:3:435:ASP:OD1	2.44	0.51
2:10:107:LEU:HD21	2:11:112:ASP:HB3	1.92	0.51
4:r:134:THR:O	4:r:138:ASN:ND2	2.39	0.51
5:E:168:TYR:CD2	5:E:353:PHE:HB3	2.45	0.51
5:E:367:PRO:HG2	5:E:370:HIS:HD2	1.75	0.51
5:A:234:GLN:HE21	5:A:260:THR:H	1.58	0.51
2:18:33:ILE:HG22	2:18:90:MET:HG3	1.92	0.51
2:21:51:ILE:HG13	2:21:61:ILE:HD13	1.92	0.51
4:n:27:ASP:OD1	4:n:28:VAL:N	2.36	0.51
3:d:46:SER:O	3:d:47:GLN:HB2	2.11	0.51
3:d:310:VAL:HG23	3:d:315:VAL:HG21	1.93	0.51
3:j:33:LEU:HD22	3:j:37:ARG:HH11	1.75	0.51
3:j:49:THR:HG22	5:H:398:ILE:HD12	1.92	0.51
5:E:40:MET:HB3	5:E:45:ASN:HB3	1.93	0.51
5:G:7:GLN:NE2	5:F:74:ASN:OD1	2.44	0.51
5:G:399:SER:O	5:F:406:ARG:NH1	2.34	0.51
5:I:7:GLN:HE22	5:H:74:ASN:HB3	1.76	0.51
1:2:44:ARG:HH11	1:2:44:ARG:HG3	1.76	0.50
2:8:99:GLN:NE2	2:8:102:TYR:HB2	2.26	0.50
2:16:52:GLU:HG3	2:16:58:HIS:CD2	2.46	0.50
2:18:33:ILE:HD11	2:18:49:VAL:HG11	1.93	0.50
3:b:237:ASP:H	3:b:243:PRO:HD3	1.77	0.50
3:c:381:SER:OG	3:c:383:ASP:O	2.29	0.50
3:d:45:LEU:HG	5:C:39:SER:O	2.11	0.50
3:e:76:ILE:HG22	3:e:457:MET:HG3	1.94	0.50
4:s:16:LYS:HE2	4:s:16:LYS:HA	1.92	0.50
3:i:395:PRO:HD2	3:j:398:PRO:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j:206:ASP:HB2	5:H:377:LYS:NZ	2.26	0.50
5:G:182:LEU:O	5:G:185:ARG:HB2	2.11	0.50
1:2:330:LYS:HD2	1:2:335:ASP:HA	1.93	0.50
1:5:46:PHE:CE2	1:5:329:LEU:HD11	2.47	0.50
1:6:279:ILE:O	1:6:282:SER:OG	2.26	0.50
2:23:49:VAL:HG23	2:23:84:THR:HB	1.92	0.50
3:c:144:ILE:HD11	3:c:467:ILE:HG22	1.92	0.50
3:d:244:VAL:H	3:d:510:ILE:HG13	1.75	0.50
3:d:559:LEU:HD11	3:e:538:LEU:HD21	1.92	0.50
3:f:205:ASN:ND2	3:g:312:ASP:OD2	2.40	0.50
3:i:310:VAL:HG22	3:h:37:ARG:HD3	1.93	0.50
4:t:30:PRO:HA	4:t:33:MET:HB2	1.91	0.50
5:E:49:MET:HE3	5:F:15:GLU:HB3	1.93	0.50
5:C:235:SER:OG	5:C:317:ASP:OD2	2.27	0.50
5:G:329:ASN:N	5:G:329:ASN:OD1	2.43	0.50
5:H:201:ILE:HG13	5:H:202:GLN:H	1.76	0.50
1:4:53:TYR:CZ	1:4:83:GLU:HB3	2.45	0.50
2:17:46:GLN:CD	2:17:63:GLN:HG2	2.36	0.50
3:c:182:ASN:OD1	3:d:171:ARG:NH2	2.44	0.50
3:l:256:ASP:OD1	3:l:256:ASP:N	2.41	0.50
3:g:507:LEU:HD23	3:g:507:LEU:H	1.75	0.50
5:F:201:ILE:HG13	5:F:202:GLN:H	1.75	0.50
5:F:281:LEU:HD23	5:F:288:VAL:HA	1.93	0.50
1:3:35:GLU:HA	1:3:40:SER:HA	1.94	0.50
1:4:241:THR:HG22	1:4:293:MET:HE2	1.94	0.50
2:15:122:PHE:C	2:15:123:LYS:HD3	2.36	0.50
3:c:7:ARG:HE	3:c:11:ILE:HD11	1.76	0.50
3:c:234:ILE:HD13	3:c:244:VAL:HG22	1.93	0.50
3:e:61:ARG:NH2	3:f:317:GLU:OE1	2.45	0.50
3:e:510:ILE:HG23	3:e:512:GLY:H	1.74	0.50
3:l:76:ILE:HG23	3:l:520:VAL:HG13	1.92	0.50
3:i:211:TRP:O	3:i:213:THR:N	2.41	0.50
3:h:89:ASP:HB3	3:g:561:ASP:HB3	1.93	0.50
3:g:468:VAL:HG22	3:g:472:TYR:CD2	2.46	0.50
5:A:210:ASP:OD1	5:A:211:VAL:N	2.45	0.50
1:4:138:LEU:HD11	1:4:172:PRO:HG3	1.92	0.50
2:7:17:PHE:CE1	2:7:73:ILE:HD11	2.47	0.50
2:16:33:ILE:HG22	2:16:47:ILE:HG12	1.94	0.50
2:21:33:ILE:HG22	2:21:90:MET:HB2	1.92	0.50
3:a:562:GLY:H	3:a:565:VAL:HG23	1.76	0.50
3:c:249:ARG:HH22	3:c:273:ARG:HH12	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:119:ILE:HD13	3:d:449:PHE:HD2	1.76	0.50
3:f:15:PHE:HD1	3:f:174:THR:HG21	1.76	0.50
3:f:209:PHE:HB3	3:f:211:TRP:CD2	2.46	0.50
3:i:182:ASN:OD1	3:j:171:ARG:NH1	2.36	0.50
4:t:56:THR:HG22	4:t:114:LEU:HD22	1.92	0.50
3:h:223:TYR:CE2	3:h:278:LYS:HD3	2.46	0.50
5:E:281:LEU:HD11	5:E:315:LEU:HB2	1.94	0.50
5:F:330:VAL:HG12	5:F:332:THR:H	1.77	0.50
1:5:158:THR:O	1:5:180:ARG:NH2	2.45	0.50
2:16:42:ASN:OD1	2:16:45:ASN:N	2.44	0.50
3:b:249:ARG:HH22	3:b:273:ARG:HH12	1.60	0.50
3:c:33:LEU:HG	3:c:121:ALA:HB2	1.94	0.50
4:r:111:LYS:NZ	3:g:379:GLU:OE1	2.35	0.50
3:k:211:TRP:CZ3	5:I:35:PRO:HB3	2.46	0.50
3:j:15:PHE:HD1	3:j:174:THR:HG21	1.76	0.50
3:j:19:TRP:O	3:j:26:ARG:NH2	2.43	0.50
5:D:47:ILE:HG23	5:D:77:VAL:HG23	1.94	0.50
1:1:48:GLY:O	1:1:363:LEU:HA	2.12	0.50
1:2:162:PHE:HA	1:2:177:ALA:O	2.11	0.50
1:6:126:ASN:HD21	1:6:136:TYR:N	2.09	0.50
2:10:114:TYR:OH	2:12:119:ASP:OD1	2.29	0.50
2:23:39:ASP:O	2:23:45:ASN:ND2	2.45	0.50
3:b:507:LEU:HD23	3:b:507:LEU:H	1.77	0.50
3:f:319:VAL:HG23	3:f:418:LEU:HD13	1.94	0.50
5:C:331:ASN:OD1	5:C:332:THR:N	2.44	0.50
5:A:23:ILE:HG13	5:A:25:PRO:HD3	1.93	0.50
5:B:201:ILE:HG13	5:B:202:GLN:H	1.76	0.50
1:1:455:ARG:NH2	2:17:54:GLU:HG3	2.27	0.50
1:2:439:LEU:HD21	1:2:441:LYS:HE2	1.93	0.50
1:3:196:ASP:N	1:3:196:ASP:OD1	2.43	0.50
2:7:11:SER:HA	2:8:15:PRO:HG2	1.93	0.50
2:20:28:ASN:N	2:20:67:ILE:O	2.44	0.50
3:d:159:ASP:OD2	3:d:171:ARG:NH1	2.44	0.50
3:f:76:ILE:HG22	3:f:457:MET:HG3	1.94	0.50
3:h:239:VAL:HG12	3:h:240:THR:HG22	1.94	0.50
5:C:161:ASN:ND2	5:C:163:ASP:OD2	2.45	0.50
1:6:34:LYS:O	1:6:41:GLY:N	2.45	0.50
2:13:47:ILE:O	2:13:63:GLN:NE2	2.44	0.50
3:c:306:GLU:O	3:c:316:TYR:HA	2.11	0.50
3:c:333:ILE:HG21	3:c:405:LEU:HB2	1.94	0.50
3:d:46:SER:C	3:d:48:TYR:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:275:PHE:CD1	5:A:340:VAL:HG12	2.46	0.50
5:A:400:THR:O	5:A:402:SER:N	2.45	0.50
5:G:7:GLN:HG2	5:F:240:ALA:HB1	1.94	0.50
5:D:388:LEU:HB3	5:D:409:LEU:HD11	1.94	0.50
5:B:278:VAL:HG23	5:B:293:ALA:HB3	1.94	0.50
5:F:133:SER:HB3	5:F:426:PRO:HA	1.94	0.50
1:2:118:ASP:OD1	1:2:119:GLY:N	2.45	0.49
2:9:46:GLN:CD	2:9:63:GLN:HG2	2.37	0.49
2:22:31:ILE:HB	2:22:65:LEU:HB2	1.94	0.49
3:g:297:HIS:HB2	3:g:463:ILE:HG12	1.94	0.49
5:A:72:GLU:OE2	5:B:102:ARG:NH1	2.37	0.49
1:5:173:ASP:HB3	1:5:177:ALA:HB2	1.93	0.49
2:9:33:ILE:HD11	2:9:49:VAL:HG12	1.93	0.49
2:10:30:LYS:HE2	2:10:30:LYS:HA	1.94	0.49
2:14:16:ILE:HD11	2:14:72:LYS:NZ	2.27	0.49
2:17:24:LYS:NZ	4:t:71:ASP:OD1	2.42	0.49
2:19:32:TYR:HE1	2:19:64:PRO:HB3	1.76	0.49
2:20:124:TYR:HE1	2:21:121:LYS:HZ1	1.60	0.49
2:21:35:GLN:O	2:21:38:THR:OG1	2.26	0.49
3:f:36:SER:O	3:f:36:SER:OG	2.30	0.49
3:f:383:ASP:OD1	3:f:384:LEU:N	2.46	0.49
3:f:561:ASP:OD2	3:f:569:ARG:NH2	2.45	0.49
3:k:32:ASP:OD2	3:k:321:ARG:NE	2.44	0.49
3:h:561:ASP:OD1	3:h:569:ARG:NH1	2.44	0.49
1:2:158:THR:HA	1:3:101:ARG:HH22	1.76	0.49
1:4:231:GLN:NE2	1:6:194:TRP:O	2.45	0.49
2:17:28:ASN:N	2:17:67:ILE:O	2.45	0.49
2:18:46:GLN:CD	2:18:63:GLN:HG2	2.37	0.49
3:c:67:LEU:HD13	3:c:418:LEU:HD22	1.94	0.49
3:l:249:ARG:NH1	3:l:513:ARG:HH22	2.10	0.49
3:i:45:LEU:HD13	5:H:11:LEU:HD22	1.92	0.49
5:A:36:PRO:HG2	5:B:13:VAL:HG11	1.94	0.49
5:B:116:GLU:HG2	5:B:216:LYS:HD2	1.94	0.49
5:J:101:ARG:O	5:J:105:GLN:HG3	2.12	0.49
1:1:408:ARG:HH22	2:18:93:TYR:HH	1.57	0.49
1:2:206:ILE:HB	1:2:230:VAL:HB	1.93	0.49
1:5:331:THR:OG1	1:5:370:GLN:OE1	2.19	0.49
1:6:155:LYS:HE2	1:6:158:THR:HG21	1.94	0.49
2:8:55:ASP:OD1	2:8:55:ASP:N	2.31	0.49
3:b:254:VAL:O	3:b:258:LEU:HD23	2.12	0.49
3:f:32:ASP:OD1	3:f:324:LYS:NZ	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:242:GLU:N	3:k:242:GLU:OE1	2.46	0.49
5:B:376:MET:HB2	5:B:395:GLN:HB3	1.94	0.49
5:F:171:ASN:ND2	5:F:174:ASP:OD2	2.39	0.49
5:J:299:ARG:NH1	5:J:307:GLU:OE1	2.45	0.49
2:17:105:ASN:HB3	2:17:108:LYS:HG3	1.94	0.49
3:b:159:ASP:OD2	3:b:171:ARG:NH1	2.45	0.49
3:d:134:ASP:HB3	3:e:271:ILE:HG23	1.94	0.49
3:l:367:ASP:OD1	4:q:125:ARG:NH2	2.41	0.49
5:C:7:GLN:HE22	5:B:50:PRO:HA	1.78	0.49
5:A:302:ASP:HB2	5:A:305:HIS:HB2	1.95	0.49
1:1:105:ALA:HB1	1:1:112:LEU:HD11	1.95	0.49
1:4:312:VAL:HG21	1:4:338:TYR:HB3	1.93	0.49
1:5:46:PHE:CD2	1:5:329:LEU:HD21	2.48	0.49
2:20:32:TYR:HB3	2:20:40:PRO:HB2	1.95	0.49
3:l:209:PHE:H	5:J:101:ARG:NH2	2.10	0.49
3:h:19:TRP:O	3:h:26:ARG:NH2	2.40	0.49
4:v:20:ALA:HA	4:v:26:THR:OG1	2.11	0.49
5:G:53:GLN:HG2	5:G:72:GLU:HG3	1.94	0.49
5:F:309:THR:CG2	5:F:310:PRO:HD3	2.43	0.49
5:J:282:GLY:O	5:J:284:MET:N	2.45	0.49
1:2:395:GLU:OE2	1:2:437:ARG:HD2	2.12	0.49
1:2:430:GLU:HB3	1:2:433:VAL:HB	1.95	0.49
2:11:116:ILE:HG13	2:11:117:GLU:N	2.28	0.49
2:18:55:ASP:OD1	2:18:55:ASP:N	2.44	0.49
2:19:113:GLN:O	2:19:117:GLU:HG2	2.12	0.49
3:a:395:PRO:HD2	3:b:398:PRO:HB3	1.94	0.49
4:q:67:PRO:HB2	4:q:69:GLU:O	2.13	0.49
3:f:38:VAL:HG22	3:g:310:VAL:HG21	1.95	0.49
3:f:561:ASP:CG	3:g:88:PRO:HB2	2.37	0.49
3:i:243:PRO:HA	3:i:510:ILE:HG13	1.93	0.49
3:h:209:PHE:HB3	3:h:210:PRO:CD	2.41	0.49
5:A:384:PRO:O	5:A:386:VAL:N	2.45	0.49
5:D:201:ILE:HG13	5:D:202:GLN:H	1.77	0.49
5:B:223:SER:OG	5:B:271:ASP:OD2	2.27	0.49
5:J:101:ARG:H	5:J:101:ARG:HD2	1.78	0.49
1:2:35:GLU:HA	1:2:40:SER:HA	1.95	0.49
1:6:250:ILE:HG13	1:6:293:MET:SD	2.52	0.49
2:9:96:ASN:ND2	4:o:30:PRO:O	2.45	0.49
2:11:110:ASP:OD1	2:11:111:PRO:HD2	2.11	0.49
2:17:24:LYS:HD2	4:t:67:PRO:HG2	1.94	0.49
2:23:52:GLU:OE1	2:23:58:HIS:NE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:24:55:ASP:OD1	2:24:57:SER:OG	2.29	0.49
3:a:343:ARG:HD2	4:s:128:TYR:CZ	2.48	0.49
3:b:42:ASP:HB2	3:b:44:TRP:CZ3	2.48	0.49
3:d:181:GLN:O	3:d:185:GLU:HG2	2.13	0.49
5:H:35:PRO:HG2	5:H:40:MET:SD	2.53	0.49
5:H:383:ILE:HG13	5:H:409:LEU:HD22	1.93	0.49
1:3:409:LEU:HD12	1:3:456:VAL:HG22	1.94	0.49
2:9:98:SER:HB2	4:o:31:GLN:HG3	1.95	0.49
2:19:88:HIS:NE2	2:19:106:VAL:HG21	2.28	0.49
4:y:121:SER:O	4:y:124:LYS:NZ	2.46	0.49
4:m:144:ASN:ND2	5:D:98:THR:HG22	2.28	0.49
3:l:327:GLN:NE2	3:l:330:ARG:HD3	2.28	0.49
3:j:220:ALA:HB3	3:j:281:ILE:HG13	1.94	0.49
5:E:187:ILE:O	5:E:188:PHE:HD1	1.96	0.49
5:I:39:SER:C	5:I:41:GLN:H	2.21	0.49
5:I:284:MET:HE2	5:J:20:ILE:HG21	1.95	0.49
1:5:423:GLU:O	2:24:99:GLN:NE2	2.43	0.49
1:6:112:LEU:HB3	1:6:124:VAL:HB	1.94	0.49
2:10:101:ASP:OD1	2:10:102:TYR:N	2.42	0.49
2:24:87:GLY:HA2	2:24:107:LEU:HD13	1.95	0.49
3:e:363:TYR:OH	3:e:373:LEU:O	2.30	0.49
3:i:347:LYS:NZ	3:j:393:GLU:OE1	2.37	0.49
3:g:7:ARG:HH11	3:g:7:ARG:HG3	1.78	0.49
3:g:198:ILE:HG23	3:g:217:ILE:HG23	1.95	0.49
4:x:21:SER:OG	4:x:22:ASP:N	2.44	0.49
5:I:278:VAL:HG23	5:I:293:ALA:HB3	1.94	0.49
5:J:45:ASN:HB3	5:J:79:MET:HE2	1.94	0.49
5:J:110:LYS:HD2	5:J:113:ASN:HD22	1.78	0.49
1:1:173:ASP:HB3	1:1:177:ALA:HB2	1.94	0.48
1:1:455:ARG:HH11	1:1:457:ILE:HD11	1.78	0.48
1:2:154:SER:HB2	1:2:188:ILE:HG13	1.94	0.48
1:4:389:ALA:HB1	1:4:471:LEU:HD22	1.95	0.48
2:8:31:ILE:HD11	2:8:73:ILE:HG12	1.95	0.48
3:j:562:GLY:H	3:j:565:VAL:HG23	1.77	0.48
5:E:90:ARG:HD2	5:E:92:ASP:HB2	1.95	0.48
5:I:188:PHE:HA	5:I:192:PRO:HB2	1.94	0.48
5:B:44:SER:O	5:B:44:SER:OG	2.23	0.48
5:H:47:ILE:HG23	5:H:77:VAL:HG23	1.94	0.48
5:H:366:ILE:HB	5:H:391:ILE:HG21	1.94	0.48
1:6:443:VAL:HG12	1:6:444:GLY:H	1.78	0.48
2:9:51:ILE:HG23	2:9:80:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:12:28:ASN:OD1	4:q:66:PRO:HB3	2.13	0.48
3:c:325:ASP:CG	4:q:136:SER:HG	2.19	0.48
3:e:67:LEU:HD13	3:e:418:LEU:HD22	1.95	0.48
3:k:211:TRP:HH2	5:I:47:ILE:HD12	1.77	0.48
3:k:348:LYS:HB2	3:j:372:TYR:HE1	1.76	0.48
4:s:62:ASP:OD1	4:s:62:ASP:N	2.45	0.48
3:h:190:LYS:HG2	3:h:191:TYR:CD1	2.48	0.48
5:B:295:PHE:HD2	5:B:310:PRO:HD2	1.78	0.48
5:J:182:LEU:HD12	5:J:201:ILE:HG22	1.95	0.48
1:1:394:LEU:HD13	1:1:469:ILE:HD12	1.94	0.48
1:2:168:ASP:OD1	1:2:170:SER:OG	2.29	0.48
1:6:293:MET:HE3	1:6:304:LEU:HD11	1.95	0.48
2:14:16:ILE:HD11	2:14:72:LYS:HZ3	1.78	0.48
2:16:23:PHE:CD1	2:18:25:ALA:HB2	2.48	0.48
3:e:169:ASP:OD1	3:e:169:ASP:N	2.35	0.48
3:j:249:ARG:NH1	3:j:513:ARG:HH22	2.12	0.48
5:G:364:GLN:NE2	5:G:366:ILE:O	2.46	0.48
5:F:370:HIS:HD1	5:F:372:LEU:H	1.61	0.48
1:3:284:THR:O	1:3:288:MET:HB2	2.14	0.48
1:3:333:LEU:HD22	1:3:457:ILE:HD13	1.96	0.48
2:8:105:ASN:HB3	2:8:108:LYS:HG3	1.95	0.48
2:8:117:GLU:OE2	2:8:117:GLU:N	2.37	0.48
3:b:42:ASP:HB2	3:b:44:TRP:HZ3	1.78	0.48
4:o:29:GLU:OE1	4:o:31:GLN:NE2	2.46	0.48
3:e:371:TYR:OH	3:f:360:GLU:OE1	2.28	0.48
5:C:167:SER:OG	5:C:356:ASP:OD1	2.30	0.48
5:C:309:THR:HG22	5:C:310:PRO:HD3	1.96	0.48
5:A:230:VAL:HG13	5:A:336:ASP:O	2.14	0.48
5:H:278:VAL:HG13	5:H:330:VAL:HG13	1.94	0.48
1:4:286:GLU:C	1:4:288:MET:H	2.21	0.48
1:6:53:TYR:CZ	1:6:83:GLU:HB3	2.48	0.48
2:10:94:ASP:OD1	2:10:98:SER:N	2.46	0.48
3:a:50:THR:OG1	3:a:51:LEU:N	2.46	0.48
3:c:78:VAL:HG13	3:c:518:THR:HG23	1.95	0.48
3:d:212:LEU:HD12	5:D:14:ASP:O	2.14	0.48
3:j:44:TRP:CZ3	3:j:45:LEU:HB3	2.49	0.48
3:h:243:PRO:HB3	3:h:510:ILE:HG13	1.95	0.48
3:g:219:ILE:HD11	3:g:280:ILE:HG23	1.96	0.48
5:G:89:LEU:HD13	5:G:94:LEU:HD21	1.96	0.48
5:G:376:MET:HG2	5:G:395:GLN:HB2	1.95	0.48
5:G:391:ILE:HG22	5:G:392:PHE:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:272:LYS:NZ	5:F:296:SER:OG	2.35	0.48
1:2:52:ARG:HD2	1:2:362:GLN:HB3	1.95	0.48
1:4:94:ARG:HB2	1:4:238:TYR:CE2	2.49	0.48
2:9:120:LYS:HD2	2:9:120:LYS:C	2.38	0.48
3:a:163:LYS:HB3	3:l:150:HIS:CD2	2.48	0.48
3:a:381:SER:O	3:a:381:SER:OG	2.26	0.48
3:a:538:LEU:HD21	3:l:559:LEU:HD11	1.95	0.48
3:c:106:THR:OG1	3:c:146:ARG:O	2.28	0.48
3:d:468:VAL:HG13	3:d:472:TYR:HB2	1.96	0.48
3:k:33:LEU:HG	3:k:121:ALA:HB2	1.94	0.48
4:t:136:SER:O	4:t:142:ASN:ND2	2.46	0.48
3:j:33:LEU:HG	3:j:121:ALA:HB2	1.96	0.48
5:A:281:LEU:HD11	5:A:315:LEU:HB2	1.95	0.48
5:F:309:THR:HG23	5:F:310:PRO:HD3	1.94	0.48
5:J:25:PRO:HD2	5:J:116:GLU:OE2	2.14	0.48
1:2:231:GLN:NE2	1:3:245:ASP:OD1	2.47	0.48
1:5:46:PHE:CD1	1:5:47:PRO:HD2	2.48	0.48
2:13:20:SER:O	2:15:68:ASN:ND2	2.47	0.48
2:24:96:ASN:ND2	4:u:30:PRO:O	2.46	0.48
3:a:67:LEU:HD13	3:a:418:LEU:HD22	1.95	0.48
3:a:106:THR:OG1	3:a:146:ARG:O	2.27	0.48
3:c:99:ARG:NH2	3:c:530:GLN:OE1	2.41	0.48
1:2:271:ILE:HG22	1:2:326:TRP:HZ2	1.78	0.48
1:3:225:GLN:HG3	1:3:228:LEU:HD13	1.95	0.48
2:11:51:ILE:HG22	2:11:82:ILE:HD13	1.96	0.48
2:15:31:ILE:HD12	2:15:73:ILE:HD11	1.96	0.48
3:f:50:THR:OG1	3:f:51:LEU:N	2.47	0.48
3:k:15:PHE:CD1	3:k:174:THR:HG21	2.48	0.48
3:i:249:ARG:HH12	3:i:513:ARG:HH22	1.61	0.48
3:g:22:SER:OG	3:g:26:ARG:NH2	2.47	0.48
5:E:74:ASN:OD1	5:E:74:ASN:N	2.45	0.48
5:G:53:GLN:OE1	5:H:99:ALA:HB1	2.13	0.48
5:H:198:ASP:OD1	5:H:199:GLY:N	2.47	0.48
5:J:128:SER:HB2	5:J:310:PRO:HG3	1.96	0.48
1:1:148:ARG:HA	1:3:182:GLU:O	2.13	0.48
1:6:48:GLY:O	1:6:363:LEU:HA	2.14	0.48
2:11:92:ILE:HG22	2:11:100:VAL:HB	1.96	0.48
2:17:102:TYR:O	2:17:103:ILE:HD13	2.14	0.48
2:19:123:LYS:HA	2:19:123:LYS:HD3	1.72	0.48
2:22:14:ARG:NH1	2:23:101:ASP:OD1	2.46	0.48
3:l:78:VAL:HG13	3:l:518:THR:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:561:ASP:OD2	3:i:569:ARG:NH2	2.47	0.48
3:j:106:THR:OG1	3:j:146:ARG:O	2.28	0.48
3:j:177:HIS:NE2	3:j:221:GLU:OE1	2.47	0.48
4:u:21:SER:HG	4:u:24:THR:HG1	1.60	0.48
3:g:146:ARG:NH2	3:g:460:ASP:OD2	2.47	0.48
5:A:68:THR:OG1	5:A:323:GLU:OE1	2.31	0.48
5:F:133:SER:HB2	5:F:147:PHE:HE1	1.79	0.48
5:F:353:PHE:CZ	5:F:422:GLY:HA3	2.48	0.48
5:H:225:ALA:HB1	5:H:228:ILE:HD12	1.96	0.48
1:1:390:ARG:HA	1:1:445:ARG:HA	1.96	0.48
1:3:409:LEU:HD21	1:3:454:LEU:HD12	1.95	0.48
1:4:59:SER:OG	1:4:342:ASP:OD2	2.31	0.48
2:7:94:ASP:OD1	2:7:96:ASN:N	2.42	0.48
2:10:38:THR:HB	2:10:45:ASN:ND2	2.29	0.48
2:11:116:ILE:HG13	2:11:117:GLU:H	1.78	0.48
3:b:239:VAL:HG12	3:b:240:THR:HG22	1.96	0.48
3:c:95:MET:HE2	3:c:99:ARG:NH2	2.29	0.48
3:k:220:ALA:HB3	3:k:281:ILE:HG13	1.96	0.48
3:j:93:VAL:HG12	3:j:97:MET:HE3	1.95	0.48
3:h:15:PHE:HD1	3:h:174:THR:HG21	1.79	0.48
5:I:52:GLU:HB2	5:J:18:GLU:HA	1.96	0.48
5:B:27:ALA:HB2	5:B:116:GLU:HA	1.95	0.48
1:3:297:ARG:HA	1:3:301:HIS:O	2.13	0.47
1:5:400:THR:OG1	1:5:433:VAL:O	2.27	0.47
2:8:31:ILE:CG1	2:8:65:LEU:HB2	2.44	0.47
2:9:78:GLN:HA	2:9:78:GLN:OE1	2.14	0.47
2:9:84:THR:HG22	2:9:85:VAL:H	1.78	0.47
2:14:24:LYS:HZ2	4:n:67:PRO:HD2	1.79	0.47
2:16:107:LEU:HD21	2:17:112:ASP:HB2	1.96	0.47
2:16:124:TYR:C	2:17:123:LYS:HG2	2.39	0.47
3:e:136:SER:O	3:e:136:SER:OG	2.31	0.47
3:f:249:ARG:NH1	3:f:513:ARG:HH22	2.12	0.47
4:s:27:ASP:OD1	4:s:28:VAL:N	2.46	0.47
3:g:77:ASP:OD1	3:g:98:TYR:OH	2.27	0.47
3:g:213:THR:OG1	3:g:214:GLN:N	2.45	0.47
1:1:354:ASP:OD1	1:1:355:LYS:N	2.47	0.47
1:6:88:ASP:O	1:6:115:TYR:OH	2.27	0.47
2:8:101:ASP:C	2:8:101:ASP:OD1	2.57	0.47
2:10:55:ASP:OD1	2:10:56:GLY:N	2.48	0.47
2:15:18:THR:HA	2:15:25:ALA:HA	1.95	0.47
2:16:83:VAL:HG12	2:18:9:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:23:68:ASN:OD1	2:23:70:ALA:N	2.34	0.47
3:e:239:VAL:HG12	3:e:240:THR:HG22	1.95	0.47
3:i:559:LEU:HD11	3:j:538:LEU:HD21	1.95	0.47
4:t:69:GLU:OE1	4:t:70:GLY:N	2.47	0.47
3:h:263:PHE:HZ	3:h:496:VAL:HG11	1.79	0.47
5:A:48:TRP:O	5:B:12:ALA:HA	2.14	0.47
5:I:349:ARG:HE	5:I:349:ARG:HB3	1.53	0.47
5:B:179:GLY:O	5:B:183:THR:HG23	2.14	0.47
1:2:212:THR:N	1:2:221:LEU:O	2.30	0.47
1:3:143:ASP:HB3	1:3:191:ILE:HG22	1.96	0.47
1:4:353:GLY:HA2	1:4:360:VAL:HG22	1.96	0.47
2:19:32:TYR:CE2	2:19:41:VAL:HG13	2.49	0.47
3:b:129:VAL:HG23	3:b:145:ARG:HG3	1.96	0.47
3:b:282:THR:HG22	3:b:284:THR:H	1.79	0.47
3:d:113:ILE:HD11	3:e:307:TRP:HZ3	1.78	0.47
3:e:296:GLU:HG3	3:e:466:SER:HB3	1.96	0.47
4:q:134:THR:O	4:q:138:ASN:ND2	2.42	0.47
3:i:177:HIS:HB2	3:i:219:ILE:HG22	1.96	0.47
3:h:237:ASP:HB2	3:h:243:PRO:HD3	1.96	0.47
3:h:322:LEU:HD22	3:g:58:ASP:OD2	2.14	0.47
5:D:282:GLY:O	5:D:284:MET:N	2.46	0.47
1:1:126:ASN:HD21	1:1:136:TYR:N	2.11	0.47
1:5:60:ARG:HD2	1:5:93:GLY:O	2.14	0.47
2:16:42:ASN:HB3	2:16:45:ASN:HB2	1.95	0.47
2:17:10:VAL:HG13	2:18:90:MET:HE2	1.96	0.47
3:d:279:SER:OG	3:d:289:ASP:O	2.29	0.47
3:f:507:LEU:H	3:f:507:LEU:HD23	1.79	0.47
3:f:561:ASP:HB3	3:g:89:ASP:HB3	1.96	0.47
3:g:249:ARG:HH12	3:g:513:ARG:NH1	2.12	0.47
5:E:405:CYS:HB3	5:D:372:LEU:HD21	1.96	0.47
5:G:79:MET:HE1	5:G:364:GLN:HB3	1.96	0.47
5:D:243:LEU:H	5:D:243:LEU:HD12	1.79	0.47
5:B:128:SER:HB2	5:B:310:PRO:HG3	1.96	0.47
5:F:50:PRO:HA	5:F:74:ASN:HB3	1.96	0.47
1:3:430:GLU:HB3	1:3:436:LYS:HE2	1.96	0.47
1:5:330:LYS:HD2	1:5:335:ASP:HA	1.96	0.47
2:9:18:THR:HA	2:9:25:ALA:HA	1.94	0.47
2:14:116:ILE:HG13	2:14:117:GLU:OE1	2.14	0.47
2:15:90:MET:HE3	2:15:92:ILE:HD11	1.96	0.47
2:19:8:VAL:HG11	2:20:86:GLN:HA	1.96	0.47
3:b:297:HIS:HB2	3:b:463:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:51:LEU:HD12	3:c:51:LEU:HA	1.74	0.47
4:p:132:MET:HE1	3:g:338:ALA:HB1	1.96	0.47
3:l:67:LEU:HD13	3:l:418:LEU:HD22	1.96	0.47
3:k:199:PRO:HD2	3:k:217:ILE:HG23	1.96	0.47
3:k:253:ASP:HB3	3:k:506:VAL:HG21	1.95	0.47
4:t:82:ALA:O	4:t:86:ASN:ND2	2.33	0.47
3:h:15:PHE:CD1	3:h:174:THR:HG21	2.50	0.47
5:E:191:ILE:HB	5:E:192:PRO:HD3	1.96	0.47
1:2:185:PRO:O	1:3:101:ARG:HD3	2.15	0.47
1:2:430:GLU:OE1	1:2:436:LYS:NZ	2.30	0.47
1:3:458:THR:HB	1:3:460:SER:H	1.79	0.47
1:4:83:GLU:OE1	1:4:83:GLU:N	2.42	0.47
1:4:409:LEU:HD12	1:4:456:VAL:HG22	1.97	0.47
2:13:14:ARG:NH2	2:14:109:TYR:OH	2.47	0.47
2:19:86:GLN:OE1	2:19:86:GLN:N	2.48	0.47
3:a:310:VAL:HG21	3:l:38:VAL:HG23	1.95	0.47
3:c:510:ILE:HG23	3:c:512:GLY:H	1.80	0.47
4:u:132:MET:HG2	4:u:133:PRO:HD2	1.97	0.47
3:g:557:PHE:HE1	3:g:573:ASN:CG	2.23	0.47
5:E:346:LYS:HE2	5:E:427:GLY:O	2.14	0.47
5:G:34:THR:C	5:G:36:PRO:HD2	2.39	0.47
1:1:159:ASP:HA	1:1:188:ILE:HB	1.96	0.47
1:1:312:VAL:HG21	1:1:338:TYR:HB3	1.95	0.47
2:7:34:GLY:HA2	2:7:46:GLN:HA	1.97	0.47
2:8:19:GLU:HB2	2:8:22:SER:O	2.14	0.47
2:13:123:LYS:HA	2:13:123:LYS:HD3	1.74	0.47
2:22:22:SER:HG	2:22:24:LYS:NZ	2.10	0.47
2:23:32:TYR:HB3	2:23:40:PRO:HB2	1.97	0.47
3:a:76:ILE:HG23	3:a:520:VAL:HG13	1.97	0.47
3:a:113:ILE:HD13	3:a:150:HIS:CE1	2.49	0.47
3:e:65:ARG:NH2	3:f:306:GLU:OE2	2.43	0.47
4:p:130:SER:HB3	4:p:151:GLY:HA3	1.96	0.47
3:l:93:VAL:HG12	3:l:97:MET:HE3	1.97	0.47
3:k:37:ARG:NH1	3:k:120:GLU:OE1	2.48	0.47
3:k:393:GLU:HG3	3:j:391:TYR:CZ	2.49	0.47
5:C:128:SER:HB2	5:C:310:PRO:HG3	1.95	0.47
5:G:159:GLU:OE1	5:G:284:MET:HB3	2.15	0.47
5:I:128:SER:HB2	5:I:310:PRO:HG3	1.95	0.47
5:I:321:SER:OG	5:I:323:GLU:OE2	2.18	0.47
5:D:264:THR:O	5:D:264:THR:OG1	2.30	0.47
5:B:23:ILE:HG12	5:B:25:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:368:ALA:HB3	5:B:378:THR:HG21	1.95	0.47
5:B:383:ILE:HG13	5:B:409:LEU:HD22	1.96	0.47
5:F:282:GLY:O	5:F:284:MET:N	2.47	0.47
1:1:423:GLU:OE2	1:1:455:ARG:NH2	2.48	0.47
1:5:412:SER:HB3	1:5:423:GLU:HG2	1.97	0.47
1:6:143:ASP:OD2	1:6:191:ILE:HG22	2.15	0.47
2:8:72:LYS:HB2	2:8:79:LEU:HD22	1.97	0.47
2:16:36:ILE:HD13	2:16:105:ASN:HD21	1.79	0.47
3:c:76:ILE:HG22	3:c:457:MET:HG3	1.95	0.47
3:k:223:TYR:CE2	3:k:300:ILE:HD11	2.50	0.47
4:t:5:THR:OG1	4:t:8:ASP:OD2	2.32	0.47
3:h:546:THR:OG1	3:h:547:PRO:HD3	2.15	0.47
4:v:79:ALA:O	4:v:83:VAL:HG23	2.14	0.47
3:g:179:MET:O	3:g:216:THR:HA	2.15	0.47
5:C:7:GLN:HE21	5:B:72:GLU:HG2	1.79	0.47
1:1:53:TYR:CZ	1:1:83:GLU:HB3	2.49	0.47
1:1:181:ALA:O	1:5:148:ARG:NH1	2.47	0.47
1:4:297:ARG:HH22	1:5:277:GLU:CD	2.21	0.47
1:5:110:GLY:HA2	1:5:141:VAL:H	1.80	0.47
2:21:33:ILE:HD11	2:21:49:VAL:CG1	2.45	0.47
4:y:1:MET:HE2	4:y:80:VAL:HG11	1.96	0.47
3:c:297:HIS:HB2	3:c:463:ILE:HG12	1.97	0.47
3:c:561:ASP:OD1	3:c:561:ASP:N	2.48	0.47
3:d:191:TYR:OH	3:d:278:LYS:NZ	2.47	0.47
3:e:476:ARG:HH12	3:e:510:ILE:HG21	1.80	0.47
3:l:333:ILE:HG21	3:l:405:LEU:HB2	1.97	0.47
5:G:281:LEU:HD23	5:G:286:LYS:HD2	1.97	0.47
5:G:376:MET:HB3	5:G:393:ALA:HB1	1.95	0.47
5:D:238:PRO:HG3	5:D:313:VAL:HG21	1.96	0.47
2:17:9:VAL:HG11	2:18:108:LYS:HZ2	1.80	0.47
4:n:131:ARG:NH1	3:f:53:TYR:O	2.46	0.47
3:l:305:GLY:O	3:l:452:ASN:ND2	2.48	0.47
3:h:273:ARG:HD3	3:h:275:ARG:HE	1.80	0.47
5:C:29:LYS:NZ	5:C:356:ASP:OD2	2.37	0.47
5:C:154:ILE:HD13	5:C:291:GLN:OE1	2.15	0.47
5:B:171:ASN:ND2	5:B:349:ARG:HB3	2.29	0.47
5:H:401:LEU:O	5:H:401:LEU:HD23	2.14	0.47
1:2:138:LEU:HG	1:2:153:TRP:HZ2	1.81	0.46
1:3:34:LYS:H	1:3:41:GLY:HA2	1.80	0.46
1:6:394:LEU:HD23	1:6:411:LEU:HD21	1.96	0.46
2:10:74:VAL:HG12	2:10:79:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:13:122:PHE:HB2	2:14:122:PHE:CE2	2.50	0.46
2:15:123:LYS:HD3	2:15:123:LYS:N	2.30	0.46
3:d:78:VAL:HG13	3:d:518:THR:HG23	1.96	0.46
3:d:383:ASP:OD1	3:d:384:LEU:N	2.47	0.46
3:k:263:PHE:HZ	3:k:496:VAL:HG11	1.79	0.46
3:g:41:TRP:CE3	3:g:54:ARG:HD3	2.50	0.46
3:g:162:SER:OG	3:g:169:ASP:OD1	2.27	0.46
5:C:119:VAL:HA	5:C:413:VAL:HG11	1.97	0.46
5:A:143:ASP:HA	5:A:146:ASN:HB2	1.98	0.46
5:G:41:GLN:HE22	5:G:44:SER:HG	1.60	0.46
5:F:125:GLU:OE1	5:F:269:ARG:NH1	2.38	0.46
1:1:345:TYR:HD1	1:1:350:ILE:HG13	1.80	0.46
1:1:391:CYS:SG	1:1:469:ILE:HD11	2.54	0.46
1:1:409:LEU:HD12	1:1:456:VAL:HG22	1.97	0.46
1:2:247:TYR:HB2	1:2:263:ILE:HD12	1.97	0.46
1:2:394:LEU:HD22	1:2:411:LEU:HD21	1.98	0.46
1:4:23:ASP:OD1	1:6:34:LYS:NZ	2.47	0.46
3:a:311:GLU:HB3	3:l:205:ASN:HB2	1.96	0.46
3:a:468:VAL:HG22	3:a:472:TYR:CD2	2.51	0.46
3:b:561:ASP:HB2	3:c:88:PRO:O	2.15	0.46
3:e:58:ASP:OD1	3:e:59:VAL:N	2.48	0.46
3:e:113:ILE:HD13	3:e:150:HIS:CE1	2.50	0.46
3:e:200:SER:HB2	5:D:382:SER:CB	2.44	0.46
3:e:559:LEU:HD11	3:f:538:LEU:HD21	1.97	0.46
3:f:212:LEU:HG	3:f:213:THR:HG23	1.98	0.46
4:x:3:ILE:HG23	4:x:8:ASP:HB3	1.96	0.46
5:A:257:ALA:HB2	5:A:311:LYS:HG3	1.97	0.46
5:G:38:ALA:O	5:G:41:GLN:HG3	2.16	0.46
5:G:52:GLU:OE1	5:H:109:ARG:NH1	2.48	0.46
1:4:261:TYR:HB3	1:4:268:ALA:HB1	1.95	0.46
1:5:298:PHE:O	1:5:301:HIS:HB2	2.15	0.46
2:11:28:ASN:N	2:11:67:ILE:O	2.49	0.46
2:22:35:GLN:O	2:22:38:THR:OG1	2.33	0.46
2:23:14:ARG:HE	2:24:103:ILE:HG12	1.81	0.46
3:b:179:MET:HE3	3:b:179:MET:HB2	1.83	0.46
3:d:140:ASN:O	3:d:140:ASN:ND2	2.32	0.46
3:e:166:ASP:OD1	3:e:168:SER:HB2	2.15	0.46
3:f:323:THR:HG22	3:f:415:VAL:HG13	1.97	0.46
4:r:5:THR:OG1	4:r:8:ASP:OD2	2.33	0.46
3:k:203:ASN:HD21	5:I:389:ASN:HD21	1.63	0.46
5:A:131:ILE:HD11	5:A:154:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:34:THR:O	5:G:36:PRO:HD2	2.16	0.46
5:F:191:ILE:HB	5:F:192:PRO:HD3	1.98	0.46
1:1:204:SER:H	1:1:233:GLY:HA3	1.81	0.46
1:3:14:LYS:HE2	1:3:21:TYR:HE1	1.80	0.46
1:3:36:ILE:HG22	1:3:37:LEU:HD22	1.96	0.46
1:4:158:THR:O	1:4:159:ASP:HB2	2.15	0.46
2:9:52:GLU:HG3	2:9:58:HIS:CD2	2.50	0.46
2:14:88:HIS:CE1	2:14:106:VAL:HG21	2.51	0.46
2:16:82:ILE:HB	2:18:10:VAL:CG1	2.45	0.46
2:18:51:ILE:HB	2:18:59:VAL:HG13	1.96	0.46
3:f:246:TYR:CZ	3:f:273:ARG:HD2	2.50	0.46
4:r:131:ARG:NH2	3:i:339:ASP:OD2	2.38	0.46
5:A:7:GLN:NE2	5:J:73:LEU:O	2.47	0.46
5:G:54:GLU:HG3	5:G:327:TYR:CE1	2.51	0.46
5:I:42:ARG:NH2	5:I:371:GLU:OE2	2.49	0.46
1:4:293:MET:HE3	1:4:304:LEU:HD11	1.98	0.46
1:5:181:ALA:HB3	1:5:184:GLN:HE21	1.81	0.46
2:9:28:ASN:N	2:9:28:ASN:OD1	2.49	0.46
3:e:176:ILE:HG21	3:e:204:PRO:HG3	1.96	0.46
3:f:242:GLU:OE1	3:f:242:GLU:N	2.49	0.46
3:i:24:GLU:OE1	3:i:313:LYS:HE2	2.15	0.46
5:I:190:ARG:O	5:I:194:GLU:HG3	2.15	0.46
5:H:86:PHE:CZ	5:H:404:LEU:HD22	2.50	0.46
5:H:376:MET:HE3	5:H:393:ALA:HB1	1.97	0.46
1:4:101:ARG:HH22	1:5:182:GLU:HA	1.81	0.46
1:4:127:TRP:CE3	1:4:128:PRO:HD2	2.50	0.46
1:4:262:ILE:HG12	1:4:271:ILE:HG13	1.96	0.46
2:7:124:TYR:C	2:8:123:LYS:HG2	2.40	0.46
2:22:31:ILE:HG12	2:22:92:ILE:HG23	1.96	0.46
4:m:143:LEU:HD13	5:D:14:ASP:CG	2.41	0.46
3:d:216:THR:O	3:d:216:THR:OG1	2.33	0.46
4:s:56:THR:HG22	4:s:114:LEU:HD22	1.98	0.46
3:i:372:TYR:CE2	3:j:348:LYS:HB2	2.51	0.46
5:G:37:ALA:C	5:G:39:SER:H	2.24	0.46
5:G:43:SER:O	5:G:45:ASN:N	2.47	0.46
5:I:95:ARG:HD2	5:H:37:ALA:HB1	1.97	0.46
5:I:257:ALA:HB2	5:I:311:LYS:HG3	1.97	0.46
5:F:79:MET:HE2	5:F:364:GLN:HG3	1.98	0.46
1:1:180:ARG:HB3	1:1:182:GLU:HG2	1.98	0.46
1:3:286:GLU:C	1:3:288:MET:H	2.22	0.46
3:d:282:THR:HG22	3:d:283:CYS:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:l:212:LEU:HD23	3:l:212:LEU:HA	1.87	0.46
3:l:323:THR:HG22	3:l:415:VAL:HG13	1.98	0.46
3:j:306:GLU:O	3:j:316:TYR:HA	2.16	0.46
5:G:87:PHE:HB3	5:G:405:CYS:SG	2.56	0.46
5:B:384:PRO:O	5:B:386:VAL:N	2.47	0.46
5:J:130:VAL:HG21	5:J:272:LYS:HB3	1.96	0.46
1:1:10:LYS:HB3	1:1:10:LYS:HE2	1.66	0.46
1:2:126:ASN:HD21	1:2:136:TYR:N	2.08	0.46
1:2:300:SER:N	1:6:277:GLU:OE1	2.48	0.46
1:4:300:SER:N	1:5:277:GLU:OE1	2.47	0.46
2:16:87:GLY:H	2:16:111:PRO:HD2	1.80	0.46
3:b:93:VAL:HG12	3:b:97:MET:HE3	1.97	0.46
3:d:182:ASN:OD1	3:e:171:ARG:NH2	2.34	0.46
3:e:211:TRP:CH2	3:e:212:LEU:HG	2.50	0.46
3:e:263:PHE:HZ	3:e:496:VAL:HG11	1.80	0.46
3:l:237:ASP:HB2	3:l:243:PRO:HG3	1.98	0.46
4:q:118:THR:HG22	4:q:122:ARG:HE	1.81	0.46
3:f:15:PHE:CD1	3:f:174:THR:HG21	2.49	0.46
3:k:95:MET:O	3:k:99:ARG:HG3	2.16	0.46
3:k:119:ILE:O	3:k:319:VAL:HG12	2.16	0.46
3:i:203:ASN:ND2	3:i:205:ASN:O	2.49	0.46
3:h:88:PRO:HB2	3:g:561:ASP:OD2	2.16	0.46
5:E:383:ILE:HG13	5:E:409:LEU:HD22	1.96	0.46
5:I:171:ASN:ND2	5:I:174:ASP:OD2	2.41	0.46
5:B:93:ASP:C	5:B:95:ARG:H	2.23	0.46
1:5:64:TYR:HB2	1:5:344:MET:HE2	1.98	0.46
2:12:46:GLN:CD	2:12:63:GLN:HG2	2.41	0.46
2:15:31:ILE:HB	2:15:65:LEU:HB2	1.98	0.46
2:15:53:ASN:OD1	2:15:53:ASN:N	2.48	0.46
3:c:51:LEU:O	3:c:54:ARG:NH1	2.49	0.46
3:c:376:ARG:HG2	3:c:377:THR:HG23	1.97	0.46
3:d:38:VAL:HG23	3:e:310:VAL:HG21	1.98	0.46
3:e:184:TRP:CE2	3:e:199:PRO:HD3	2.50	0.46
3:f:297:HIS:HB3	3:f:459:ARG:NH2	2.31	0.46
3:f:418:LEU:HD21	3:f:449:PHE:CE2	2.50	0.46
3:k:211:TRP:CZ2	5:J:13:VAL:HG21	2.50	0.46
3:i:61:ARG:NH2	3:j:317:GLU:OE1	2.48	0.46
3:i:220:ALA:HB3	3:i:281:ILE:HG13	1.97	0.46
5:C:143:ASP:OD1	5:C:144:ALA:N	2.49	0.46
5:G:94:LEU:HD12	5:F:373:PHE:HE1	1.81	0.46
5:G:354:TRP:CD1	5:G:354:TRP:C	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:74:ASN:ND2	5:I:251:ASN:HD22	2.14	0.46
5:D:171:ASN:ND2	5:D:349:ARG:HB3	2.30	0.46
5:B:238:PRO:HD2	5:B:324:GLN:HB3	1.98	0.46
5:F:264:THR:HG21	5:F:306:VAL:HG13	1.98	0.46
1:4:408:ARG:NH2	1:4:425:MET:SD	2.89	0.46
1:6:203:SER:HA	1:6:233:GLY:HA3	1.97	0.46
1:6:273:THR:O	1:6:277:GLU:HG3	2.15	0.46
2:7:106:VAL:HG12	2:7:107:LEU:HD22	1.96	0.46
2:10:40:PRO:O	2:10:46:GLN:HG3	2.15	0.46
2:22:20:SER:O	2:24:68:ASN:ND2	2.49	0.46
3:a:566:GLU:HA	3:a:569:ARG:HH12	1.80	0.46
3:b:332:MET:HE2	3:b:333:ILE:HG13	1.98	0.46
3:d:61:ARG:O	3:d:65:ARG:HG3	2.16	0.46
3:l:71:MET:HE2	3:l:71:MET:HB3	1.76	0.46
4:r:43:MET:HE3	4:r:44:MET:HE2	1.98	0.46
3:k:279:SER:OG	3:k:289:ASP:O	2.22	0.46
3:i:234:ILE:HD13	3:i:244:VAL:HG22	1.98	0.46
1:4:395:GLU:HB2	1:4:439:LEU:HD12	1.98	0.45
1:4:399:SER:HB2	1:5:21:TYR:CZ	2.50	0.45
2:15:43:PRO:HA	2:15:46:GLN:OE1	2.15	0.45
2:23:36:ILE:HG21	2:23:105:ASN:ND2	2.32	0.45
3:b:305:GLY:O	3:b:452:ASN:ND2	2.49	0.45
3:c:93:VAL:HG11	3:c:475:PRO:HD2	1.98	0.45
3:c:99:ARG:HG2	3:c:99:ARG:HH11	1.80	0.45
3:c:363:TYR:HE1	3:d:350:PHE:CE1	2.34	0.45
4:p:138:ASN:ND2	3:g:52:GLN:O	2.49	0.45
3:i:144:ILE:HD12	3:i:472:TYR:CZ	2.50	0.45
5:E:221:THR:HA	5:E:347:ASP:OD1	2.16	0.45
5:G:128:SER:HG	5:G:418:PRO:C	2.24	0.45
5:I:309:THR:CG2	5:I:310:PRO:HD3	2.43	0.45
5:F:190:ARG:NH1	5:F:194:GLU:OE1	2.49	0.45
1:1:51:LYS:NZ	1:1:54:ASP:OD1	2.47	0.45
1:1:400:THR:HG21	1:1:436:LYS:HB2	1.98	0.45
1:2:179:TYR:HE1	1:2:220:ALA:HB1	1.81	0.45
1:2:409:LEU:HD12	1:2:456:VAL:HG22	1.97	0.45
1:4:101:ARG:NH2	1:5:182:GLU:HA	2.31	0.45
2:8:94:ASP:OD1	2:8:95:ALA:N	2.42	0.45
2:12:92:ILE:HD12	2:12:101:ASP:HB3	1.97	0.45
2:19:35:GLN:O	2:19:38:THR:HG22	2.16	0.45
2:20:9:VAL:HA	2:21:83:VAL:HG12	1.98	0.45
2:21:31:ILE:HB	2:21:65:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:30:LYS:HD2	3:a:154:SER:HB3	1.97	0.45
3:a:225:VAL:HG12	3:a:276:VAL:HG22	1.98	0.45
3:a:542:THR:HG1	3:l:556:TYR:HH	1.63	0.45
3:b:227:GLU:OE2	3:b:274:ARG:NH1	2.48	0.45
3:b:391:TYR:CZ	3:c:393:GLU:HG3	2.51	0.45
4:n:97:LEU:HD12	4:n:97:LEU:HA	1.86	0.45
3:d:98:TYR:O	3:d:102:MET:HB2	2.16	0.45
3:f:93:VAL:HG11	3:f:475:PRO:HD2	1.98	0.45
3:i:542:THR:OG1	3:h:556:TYR:OH	2.29	0.45
4:t:22:ASP:OD1	4:t:22:ASP:N	2.44	0.45
3:j:198:ILE:HD12	3:j:217:ILE:HD11	1.98	0.45
5:E:344:ASN:O	5:E:344:ASN:ND2	2.48	0.45
5:A:47:ILE:CD1	5:B:11:LEU:HD12	2.46	0.45
5:D:24:THR:O	5:D:24:THR:OG1	2.29	0.45
5:D:130:VAL:HG21	5:D:272:LYS:HB3	1.96	0.45
5:J:24:THR:HA	5:J:116:GLU:OE1	2.16	0.45
1:2:13:GLY:HA3	1:2:24:TYR:CZ	2.52	0.45
1:3:183:SER:HB3	1:3:207:GLU:OE2	2.16	0.45
2:8:52:GLU:OE1	2:8:81:LYS:NZ	2.41	0.45
2:8:119:ASP:HA	2:9:122:PHE:HZ	1.81	0.45
3:a:45:LEU:HG	3:a:208:VAL:HG12	1.98	0.45
3:c:510:ILE:HG12	3:c:511:ARG:H	1.81	0.45
3:d:207:TRP:NE1	5:D:15:GLU:OE1	2.49	0.45
3:d:239:VAL:HG12	3:d:240:THR:HG22	1.99	0.45
3:e:542:THR:HG21	3:e:547:PRO:HB2	1.99	0.45
3:h:383:ASP:OD1	3:h:384:LEU:N	2.49	0.45
5:G:228:ILE:HD12	5:G:267:MET:HE3	1.98	0.45
1:2:413:ALA:HB1	1:2:450:ILE:HD11	1.98	0.45
1:5:52:ARG:HH11	1:5:52:ARG:HG3	1.81	0.45
1:5:284:THR:OG1	1:5:287:GLU:OE1	2.35	0.45
2:9:122:PHE:C	2:9:123:LYS:HD3	2.41	0.45
2:16:122:PHE:CE1	2:18:122:PHE:HB2	2.51	0.45
2:17:84:THR:OG1	2:17:85:VAL:N	2.50	0.45
3:c:165:MET:HE2	3:c:307:TRP:HB3	1.98	0.45
3:c:199:PRO:HG2	3:c:217:ILE:HG23	1.97	0.45
3:c:559:LEU:HD11	3:d:538:LEU:HD21	1.97	0.45
4:p:113:LEU:HD23	4:p:113:LEU:HA	1.80	0.45
3:h:33:LEU:HG	3:h:121:ALA:HB2	1.98	0.45
5:E:62:ASP:OD1	5:E:64:THR:OG1	2.33	0.45
5:I:203:ARG:HH22	5:I:212:LEU:HG	1.81	0.45
5:I:384:PRO:O	5:I:386:VAL:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:378:LEU:HD13	1:4:455:ARG:HB2	1.98	0.45
1:6:51:LYS:HE3	1:6:359:VAL:HG12	1.98	0.45
1:6:116:ARG:NH1	1:6:118:ASP:OD2	2.50	0.45
2:14:7:ASN:OD1	2:14:7:ASN:N	2.49	0.45
3:c:220:ALA:HB3	3:c:281:ILE:HG12	1.98	0.45
3:l:559:LEU:HD23	3:l:559:LEU:HA	1.84	0.45
5:A:181:ASP:HA	5:A:184:LYS:HE2	1.99	0.45
5:G:40:MET:HE2	5:G:47:ILE:HD12	1.98	0.45
5:G:230:VAL:HB	5:G:336:ASP:O	2.17	0.45
5:D:272:LYS:NZ	5:D:296:SER:OG	2.40	0.45
5:D:309:THR:CG2	5:D:310:PRO:HD3	2.46	0.45
2:7:17:PHE:CE2	2:9:12:ASN:HB3	2.52	0.45
2:7:109:TYR:O	2:7:111:PRO:HD3	2.17	0.45
2:15:47:ILE:O	2:15:63:GLN:NE2	2.50	0.45
2:16:8:VAL:HG11	2:17:86:GLN:HA	1.98	0.45
3:c:321:ARG:HA	3:c:324:LYS:HE2	1.99	0.45
3:c:323:THR:HB	3:c:412:VAL:HG13	1.99	0.45
3:c:562:GLY:H	3:c:565:VAL:CG2	2.30	0.45
3:g:233:PHE:HE2	3:g:255:ILE:HD11	1.82	0.45
5:C:156:PHE:HE2	5:D:172:PRO:HG3	1.82	0.45
5:C:391:ILE:HG22	5:C:408:ALA:HB3	1.98	0.45
5:J:368:ALA:HB3	5:J:378:THR:HG21	1.98	0.45
1:3:60:ARG:HD2	1:3:93:GLY:O	2.16	0.45
2:10:112:ASP:OD1	2:10:112:ASP:C	2.60	0.45
2:19:111:PRO:HB2	2:21:7:ASN:ND2	2.31	0.45
3:a:561:ASP:CG	3:b:88:PRO:HB2	2.42	0.45
3:b:234:ILE:HD13	3:b:244:VAL:HG22	1.98	0.45
4:m:27:ASP:OD1	4:m:27:ASP:N	2.41	0.45
3:l:44:TRP:O	3:l:48:TYR:HB2	2.16	0.45
4:r:41:GLU:OE2	4:r:58:TYR:OH	2.23	0.45
3:k:209:PHE:HB3	3:k:210:PRO:HD3	1.99	0.45
3:i:184:TRP:HB2	3:i:217:ILE:HG21	1.98	0.45
4:t:16:LYS:HA	4:t:16:LYS:HE3	1.99	0.45
3:j:77:ASP:OD1	3:j:98:TYR:OH	2.33	0.45
3:h:128:LEU:HD11	3:h:460:ASP:OD1	2.16	0.45
5:E:184:LYS:O	5:E:184:LYS:HG2	2.16	0.45
5:A:191:ILE:HB	5:A:192:PRO:HD3	1.99	0.45
5:I:225:ALA:HB1	5:I:228:ILE:HD12	1.99	0.45
5:D:118:LYS:HD3	5:D:411:TYR:HE2	1.82	0.45
5:F:185:ARG:HA	5:F:185:ARG:HD3	1.76	0.45
1:3:23:ASP:HB2	1:3:275:SER:OG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:94:ARG:NH2	1:5:342:ASP:OD2	2.42	0.45
2:11:24:LYS:HB3	2:11:24:LYS:HE3	1.86	0.45
2:11:31:ILE:HG12	2:11:92:ILE:CD1	2.44	0.45
3:d:159:ASP:OD1	3:d:161:ASN:N	2.48	0.45
3:f:22:SER:OG	3:f:26:ARG:NH2	2.50	0.45
3:g:550:GLN:NE2	3:g:581:VAL:HG21	2.31	0.45
5:A:168:TYR:CD2	5:A:353:PHE:HB3	2.52	0.45
5:A:309:THR:CG2	5:A:310:PRO:HD3	2.46	0.45
1:2:419:ASN:CG	2:8:51:ILE:HD11	2.41	0.45
1:4:67:ALA:HA	1:5:186:ASP:HB2	1.99	0.45
2:8:92:ILE:HD12	2:8:101:ASP:OD1	2.17	0.45
2:15:33:ILE:HD11	2:15:49:VAL:CG1	2.43	0.45
3:c:242:GLU:N	3:c:242:GLU:OE1	2.50	0.45
3:c:249:ARG:NH1	3:c:513:ARG:HH22	2.14	0.45
3:d:61:ARG:HG2	3:e:322:LEU:HD11	1.99	0.45
3:e:561:ASP:OD2	3:f:88:PRO:HB2	2.17	0.45
3:k:350:PHE:HE1	3:j:363:TYR:HE2	1.64	0.45
4:s:113:LEU:HD23	4:s:113:LEU:HA	1.80	0.45
3:i:544:GLN:OE1	3:i:544:GLN:N	2.50	0.45
3:j:165:MET:HE3	3:j:165:MET:HB2	1.90	0.45
5:E:154:ILE:HD13	5:E:291:GLN:OE1	2.16	0.45
5:E:284:MET:HG2	5:F:22:ALA:HB2	1.98	0.45
5:E:309:THR:CG2	5:E:310:PRO:HD3	2.47	0.45
5:E:370:HIS:HD1	5:E:372:LEU:H	1.64	0.45
5:A:354:TRP:CD1	5:A:354:TRP:C	2.95	0.45
5:I:214:SER:HB3	5:I:217:LEU:HG	1.99	0.45
5:B:317:ASP:O	5:B:325:ARG:NH1	2.47	0.45
5:F:159:GLU:OE1	5:F:284:MET:HB3	2.17	0.45
5:F:245:ASN:OD1	5:F:246:ASP:N	2.50	0.45
5:F:268:LYS:HG2	5:F:271:ASP:OD2	2.16	0.45
5:J:114:ASN:O	5:J:118:LYS:HG3	2.16	0.45
1:4:299:ASP:OD2	1:5:278:LYS:HE2	2.17	0.45
1:4:386:ALA:O	1:4:389:ALA:HB2	2.17	0.45
2:14:90:MET:HE3	2:14:90:MET:HB2	1.84	0.45
3:a:306:GLU:O	3:a:316:TYR:HA	2.16	0.45
4:y:33:MET:HE3	4:y:33:MET:HB3	1.85	0.45
3:b:101:ASP:HB2	3:b:144:ILE:O	2.17	0.45
3:b:159:ASP:OD1	3:b:161:ASN:N	2.42	0.45
3:d:510:ILE:HG12	3:d:511:ARG:N	2.32	0.45
3:d:567:MET:HE2	3:e:554:LEU:HD22	1.98	0.45
3:e:496:VAL:O	3:e:508:ASN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:211:TRP:HE3	3:k:211:TRP:H	1.65	0.45
4:s:5:THR:H	4:s:8:ASP:HB2	1.82	0.45
3:h:97:MET:HE3	3:h:472:TYR:CD2	2.52	0.45
3:g:333:ILE:HG21	3:g:405:LEU:HB2	1.99	0.45
5:C:122:MET:HE2	5:C:122:MET:HB2	1.82	0.45
5:A:188:PHE:HB3	5:A:193:GLU:HG3	1.99	0.45
5:G:158:ARG:NH2	5:G:283:GLN:HB2	2.32	0.45
1:5:78:LYS:HD2	1:5:85:GLU:CD	2.42	0.44
1:5:345:TYR:OH	1:5:348:ASN:HA	2.17	0.44
2:12:72:LYS:HD3	2:12:79:LEU:HD21	1.99	0.44
2:13:32:TYR:HB3	2:13:40:PRO:HB2	2.00	0.44
2:21:35:GLN:HG2	2:21:45:ASN:O	2.17	0.44
4:m:139:SER:HB2	3:d:210:PRO:HB3	2.00	0.44
4:m:146:TRP:HZ2	4:m:150:PRO:HD3	1.82	0.44
3:d:32:ASP:OD2	3:d:321:ARG:NE	2.49	0.44
3:l:44:TRP:HZ3	3:l:45:LEU:HD23	1.82	0.44
3:i:398:PRO:HB3	3:h:395:PRO:HD2	1.99	0.44
4:t:29:GLU:HG2	4:t:30:PRO:HD2	1.99	0.44
3:j:383:ASP:OD1	3:j:384:LEU:N	2.49	0.44
3:j:459:ARG:HG2	3:j:459:ARG:HH11	1.82	0.44
3:h:254:VAL:O	3:h:258:LEU:HD23	2.17	0.44
3:h:353:PRO:HG3	3:g:373:LEU:HD13	1.97	0.44
5:A:95:ARG:HD2	5:J:37:ALA:HB1	1.98	0.44
5:A:298:VAL:HG22	5:A:307:GLU:HG2	1.99	0.44
5:I:231:SER:O	5:I:231:SER:OG	2.34	0.44
5:H:68:THR:HB	5:H:323:GLU:OE1	2.17	0.44
1:1:184:GLN:NE2	1:1:187:GLY:O	2.43	0.44
2:7:40:PRO:HG3	2:7:89:SER:OG	2.17	0.44
2:16:111:PRO:HB2	2:18:7:ASN:HD21	1.82	0.44
3:a:566:GLU:HA	3:a:569:ARG:NH1	2.33	0.44
3:b:159:ASP:OD1	3:b:160:SER:N	2.50	0.44
3:c:509:ASP:HB3	3:c:513:ARG:HH21	1.82	0.44
4:o:142:ASN:C	4:o:144:ASN:N	2.75	0.44
3:f:35:PHE:CZ	3:f:40:GLN:HG2	2.51	0.44
3:k:254:VAL:O	3:k:258:LEU:HD23	2.17	0.44
3:i:509:ASP:HB3	3:i:513:ARG:HH21	1.82	0.44
3:i:510:ILE:HG12	3:i:511:ARG:H	1.81	0.44
3:g:562:GLY:H	3:g:565:VAL:HG23	1.81	0.44
5:E:275:PHE:CD1	5:E:340:VAL:HG22	2.52	0.44
5:C:191:ILE:HB	5:C:192:PRO:HD3	1.99	0.44
5:H:354:TRP:C	5:H:354:TRP:CD1	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:100:TYR:O	5:J:104:ILE:HG12	2.18	0.44
1:1:416:ASP:OD1	1:1:416:ASP:N	2.49	0.44
1:3:416:ASP:OD1	1:3:416:ASP:N	2.51	0.44
2:23:68:ASN:HD22	2:23:74:VAL:CG1	2.31	0.44
3:a:209:PHE:CG	3:a:210:PRO:HD2	2.51	0.44
3:a:319:VAL:HG23	3:a:418:LEU:HD13	1.99	0.44
3:a:389:LEU:HD12	3:a:389:LEU:HA	1.78	0.44
3:a:554:LEU:HD12	3:a:557:PHE:HD2	1.82	0.44
3:l:306:GLU:O	3:l:316:TYR:HA	2.17	0.44
3:i:219:ILE:HD11	3:i:287:LEU:HD12	1.99	0.44
3:h:554:LEU:HD22	3:h:567:MET:HE2	1.98	0.44
3:g:198:ILE:HG23	3:g:217:ILE:HD12	2.00	0.44
5:C:23:ILE:HG23	5:C:25:PRO:HD3	1.99	0.44
5:C:40:MET:HE1	5:C:47:ILE:HD11	2.00	0.44
5:A:334:LEU:HA	5:A:338:MET:HE1	1.99	0.44
5:B:117:LEU:HD23	5:B:117:LEU:HA	1.84	0.44
5:J:126:MET:HE3	5:J:126:MET:HB3	1.92	0.44
1:2:165:ASP:HB3	1:2:168:ASP:O	2.17	0.44
1:2:203:SER:O	1:2:204:SER:OG	2.30	0.44
1:2:408:ARG:HG2	1:2:427:GLU:HG2	2.00	0.44
2:15:74:VAL:HG12	2:15:79:LEU:HD23	1.99	0.44
2:19:52:GLU:OE1	2:19:58:HIS:NE2	2.42	0.44
3:e:408:ALA:O	3:e:412:VAL:HG23	2.17	0.44
4:p:116:LYS:HB2	4:p:116:LYS:HE3	1.81	0.44
4:s:69:GLU:OE1	4:s:70:GLY:N	2.50	0.44
3:i:64:VAL:O	3:i:68:VAL:HG23	2.17	0.44
3:g:243:PRO:HA	3:g:510:ILE:HG13	1.99	0.44
5:C:84:ASN:HA	5:C:407:ILE:O	2.17	0.44
5:I:115:VAL:HG22	5:I:411:TYR:CZ	2.52	0.44
5:I:133:SER:O	5:I:428:GLN:N	2.34	0.44
5:B:281:LEU:HD11	5:B:315:LEU:HB2	1.99	0.44
5:F:299:ARG:NH2	5:F:307:GLU:OE1	2.49	0.44
5:J:176:LYS:HE2	5:J:176:LYS:HB3	1.71	0.44
1:1:262:ILE:HG13	1:1:271:ILE:HG13	1.98	0.44
1:4:281:ARG:NH1	1:6:298:PHE:HB2	2.33	0.44
2:14:45:ASN:OD1	2:14:45:ASN:N	2.50	0.44
2:22:36:ILE:HG22	2:22:37:ASP:OD1	2.17	0.44
3:a:174:THR:HB	3:a:222:PHE:HD1	1.83	0.44
3:a:203:ASN:OD1	3:a:218:GLN:NE2	2.51	0.44
3:a:364:ASP:OD1	3:a:366:ASN:ND2	2.51	0.44
4:y:128:TYR:CZ	3:c:343:ARG:HD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:157:ILE:HB	3:b:174:THR:HG23	1.99	0.44
3:l:418:LEU:HD21	3:l:449:PHE:CE2	2.52	0.44
3:f:367:ASP:OD1	3:g:348:LYS:NZ	2.47	0.44
3:k:18:ASP:OD2	3:k:172:HIS:HE1	2.01	0.44
4:s:145:GLU:OE1	4:s:147:HIS:NE2	2.50	0.44
3:i:249:ARG:NH1	3:i:513:ARG:HH22	2.16	0.44
3:g:258:LEU:HB3	3:g:263:PHE:HB2	1.98	0.44
5:A:81:GLU:HG3	5:A:82:PRO:HD2	1.99	0.44
5:A:185:ARG:HG3	5:B:186:ASP:HA	1.99	0.44
5:G:63:LEU:HD11	5:H:84:ASN:ND2	2.24	0.44
5:G:171:ASN:ND2	5:G:174:ASP:OD2	2.46	0.44
5:G:391:ILE:CG2	5:G:392:PHE:N	2.80	0.44
5:F:171:ASN:ND2	5:F:171:ASN:H	2.15	0.44
1:1:34:LYS:H	1:1:41:GLY:HA2	1.83	0.44
1:2:391:CYS:SG	1:2:443:VAL:HB	2.57	0.44
1:4:308:LEU:HB3	1:4:309:PRO:HD2	1.99	0.44
2:8:31:ILE:HG13	2:8:65:LEU:HB2	1.99	0.44
2:12:54:GLU:H	2:12:54:GLU:CD	2.24	0.44
2:14:31:ILE:HG23	2:14:67:ILE:HD11	1.98	0.44
2:16:43:PRO:HA	2:16:46:GLN:CD	2.43	0.44
2:16:121:LYS:HE3	2:18:124:TYR:CE1	2.52	0.44
3:a:266:ILE:HD13	3:a:266:ILE:HA	1.86	0.44
3:a:561:ASP:HB2	3:b:88:PRO:O	2.18	0.44
4:y:3:ILE:HG23	4:y:8:ASP:HB2	2.00	0.44
3:c:49:THR:HG22	3:c:50:THR:HG23	1.99	0.44
3:c:562:GLY:H	3:c:565:VAL:HG22	1.83	0.44
4:n:56:THR:HG22	4:n:114:LEU:HD22	2.00	0.44
3:d:507:LEU:HD23	3:d:507:LEU:H	1.82	0.44
4:p:128:TYR:CE1	3:g:343:ARG:HD2	2.52	0.44
3:f:573:ASN:OD1	3:f:582:LYS:NZ	2.39	0.44
4:r:17:LEU:HD21	4:r:92:ALA:HB2	1.98	0.44
3:k:45:LEU:HD13	4:v:146:TRP:CD1	2.53	0.44
3:k:184:TRP:HB2	3:k:217:ILE:HG21	2.00	0.44
3:i:271:ILE:HG23	3:h:134:ASP:HB3	2.00	0.44
3:j:54:ARG:HB3	4:v:137:GLY:HA3	1.99	0.44
4:u:143:LEU:HA	4:u:143:LEU:HD23	1.78	0.44
3:h:271:ILE:HD12	3:h:511:ARG:HH11	1.83	0.44
4:v:66:PRO:HB2	4:v:67:PRO:HD3	2.00	0.44
5:A:228:ILE:HG23	5:A:340:VAL:CG2	2.46	0.44
5:G:203:ARG:HH22	5:G:212:LEU:HD21	1.82	0.44
5:G:241:TRP:CE3	5:G:249:LYS:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:86:PHE:CZ	5:J:404:LEU:HD22	2.51	0.44
1:4:189:ILE:H	1:4:189:ILE:HG12	1.52	0.44
1:5:116:ARG:HD3	1:5:120:THR:HG23	2.00	0.44
1:5:395:GLU:HG2	1:5:439:LEU:HD12	1.99	0.44
1:6:409:LEU:HB2	1:6:428:GLN:HG2	1.99	0.44
1:6:443:VAL:HG13	4:n:25:LEU:HD12	2.00	0.44
2:10:42:ASN:OD1	2:10:45:ASN:HB2	2.17	0.44
2:11:50:TYR:HA	2:11:60:GLN:HA	1.99	0.44
2:15:94:ASP:HB2	2:15:100:VAL:HG23	2.00	0.44
3:c:391:TYR:CZ	3:d:393:GLU:HG3	2.53	0.44
4:n:140:PHE:HD2	3:e:47:GLN:HE22	1.64	0.44
3:e:546:THR:OG1	3:e:547:PRO:HD3	2.18	0.44
3:l:561:ASP:OD1	3:l:569:ARG:NH1	2.51	0.44
3:k:37:ARG:NH2	3:k:116:ARG:HD3	2.33	0.44
3:h:209:PHE:CD2	5:G:374:ALA:HA	2.53	0.44
5:F:168:TYR:CD2	5:F:353:PHE:HB3	2.53	0.44
5:H:267:MET:O	5:H:300:VAL:HG21	2.18	0.44
1:1:34:LYS:O	1:1:41:GLY:N	2.51	0.44
1:1:423:GLU:O	2:18:99:GLN:NE2	2.41	0.44
1:2:186:ASP:OD2	1:3:67:ALA:HA	2.18	0.44
1:2:413:ALA:HA	1:2:451:GLY:O	2.18	0.44
1:3:312:VAL:HG21	1:3:338:TYR:HB3	1.99	0.44
1:4:161:TRP:HH2	1:4:222:TYR:CD2	2.34	0.44
2:7:43:PRO:HA	2:7:46:GLN:NE2	2.33	0.44
2:9:47:ILE:HD11	2:9:88:HIS:HB3	1.99	0.44
2:10:34:GLY:N	2:10:40:PRO:HB3	2.32	0.44
2:11:74:VAL:HG12	2:11:79:LEU:HD23	1.99	0.44
2:13:47:ILE:HD11	2:13:84:THR:HG21	1.98	0.44
2:18:46:GLN:CG	2:18:63:GLN:HG2	2.48	0.44
3:a:531:ASN:O	3:a:535:ILE:HG12	2.18	0.44
3:k:177:HIS:CE1	3:k:221:GLU:OE1	2.70	0.44
3:g:101:ASP:HB2	3:g:144:ILE:O	2.18	0.44
3:g:223:TYR:CE2	3:g:278:LYS:HD3	2.52	0.44
5:C:354:TRP:C	5:C:354:TRP:CD1	2.96	0.44
5:I:191:ILE:HB	5:I:192:PRO:HD3	1.99	0.44
5:B:268:LYS:NZ	5:B:271:ASP:OD1	2.36	0.44
1:2:395:GLU:HG2	1:2:439:LEU:HD12	2.00	0.44
1:3:12:MET:HE2	1:3:12:MET:HB2	1.73	0.44
1:4:112:LEU:HB3	1:4:124:VAL:HB	1.99	0.44
1:6:262:ILE:HG13	1:6:271:ILE:CG1	2.48	0.44
2:12:120:LYS:HE2	2:12:120:LYS:HB3	1.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:15:68:ASN:HB2	2:15:74:VAL:CG1	2.48	0.44
3:b:116:ARG:NE	3:b:120:GLU:OE2	2.49	0.44
3:d:249:ARG:NH1	3:d:513:ARG:HH22	2.15	0.44
4:o:132:MET:SD	3:f:342:ALA:HB2	2.58	0.44
3:e:468:VAL:HG22	3:e:472:TYR:CD2	2.52	0.44
3:l:297:HIS:HB3	3:l:459:ARG:NH2	2.32	0.44
3:l:321:ARG:HA	3:l:324:LYS:HE2	2.00	0.44
3:f:45:LEU:HD23	3:f:45:LEU:HA	1.67	0.44
3:f:229:LYS:HA	3:f:272:LYS:HA	2.00	0.44
3:f:468:VAL:HG22	3:f:472:TYR:CD2	2.53	0.44
3:f:567:MET:HE2	3:g:554:LEU:HD22	1.99	0.44
3:i:296:GLU:OE2	3:h:135:GLN:NE2	2.47	0.44
5:C:384:PRO:O	5:C:386:VAL:N	2.50	0.44
5:G:342:ILE:HG13	5:G:342:ILE:O	2.17	0.44
5:I:38:ALA:O	5:I:41:GLN:HB2	2.18	0.44
5:I:91:ALA:O	5:H:367:PRO:HD2	2.18	0.44
5:D:128:SER:HB2	5:D:310:PRO:HG3	1.99	0.44
5:J:187:ILE:C	5:J:188:PHE:HD1	2.25	0.44
1:4:36:ILE:HD11	1:4:42:TYR:CD1	2.52	0.43
1:4:299:ASP:OD1	1:5:278:LYS:HD3	2.18	0.43
3:a:93:VAL:HG12	3:a:97:MET:HE3	1.99	0.43
3:a:297:HIS:HB2	3:a:463:ILE:HG12	2.00	0.43
3:c:225:VAL:HG12	3:c:276:VAL:HG22	1.99	0.43
4:p:97:LEU:HD12	4:p:97:LEU:HA	1.87	0.43
4:s:7:GLY:HA3	4:s:69:GLU:CD	2.42	0.43
4:s:44:MET:HG2	4:s:58:TYR:CG	2.53	0.43
3:g:546:THR:OG1	3:g:547:PRO:HD3	2.18	0.43
5:E:185:ARG:HG3	5:F:186:ASP:HA	1.99	0.43
5:E:354:TRP:C	5:E:354:TRP:CD1	2.96	0.43
5:G:191:ILE:HB	5:G:192:PRO:HD3	2.00	0.43
5:I:143:ASP:OD1	5:I:143:ASP:N	2.50	0.43
5:D:104:ILE:HD12	5:D:392:PHE:HE2	1.82	0.43
5:B:346:LYS:HB3	5:B:346:LYS:HE3	1.78	0.43
5:B:396:GLY:HA2	5:B:403:GLY:HA2	2.00	0.43
5:H:132:THR:HG22	5:H:425:LEU:HB2	2.00	0.43
5:J:398:ILE:C	5:J:401:LEU:H	2.26	0.43
5:J:409:LEU:HG	5:J:411:TYR:CD1	2.53	0.43
1:1:27:VAL:HB	1:1:378:LEU:HB2	2.00	0.43
1:5:127:TRP:O	1:5:135:GLN:NE2	2.39	0.43
2:10:83:VAL:HG12	2:12:9:VAL:HG22	1.99	0.43
3:b:101:ASP:OD1	3:b:101:ASP:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:m:41:GLU:OE2	4:m:58:TYR:OH	2.29	0.43
3:d:561:ASP:OD2	3:e:88:PRO:HB2	2.18	0.43
4:o:46:GLU:OE2	4:o:90:ARG:NH2	2.43	0.43
3:f:71:MET:HE3	3:f:71:MET:HB3	1.88	0.43
3:i:343:ARG:HD2	4:x:128:TYR:CZ	2.53	0.43
3:j:92:ASP:OD1	3:j:93:VAL:N	2.50	0.43
3:h:71:MET:HE2	3:h:71:MET:HB3	1.81	0.43
3:h:249:ARG:HH12	3:h:513:ARG:NH1	2.14	0.43
3:h:566:GLU:HA	3:h:569:ARG:NH1	2.33	0.43
5:E:257:ALA:HB2	5:E:311:LYS:HG3	2.00	0.43
5:E:320:LEU:HD23	5:E:325:ARG:HA	1.98	0.43
5:C:281:LEU:HD23	5:C:281:LEU:HA	1.82	0.43
5:F:132:THR:HG22	5:F:425:LEU:HB2	2.00	0.43
5:F:216:LYS:HE2	5:F:216:LYS:HB3	1.72	0.43
5:H:397:ASP:OD1	5:H:398:ILE:N	2.51	0.43
2:13:50:TYR:CE1	2:13:60:GLN:HG2	2.50	0.43
2:17:124:TYR:C	2:18:123:LYS:HG2	2.44	0.43
2:18:33:ILE:HD11	2:18:49:VAL:CG1	2.48	0.43
3:b:354:GLU:H	3:b:354:GLU:HG2	1.65	0.43
4:m:56:THR:HG22	4:m:114:LEU:HD22	2.00	0.43
4:n:16:LYS:HA	4:n:16:LYS:HD3	1.82	0.43
4:o:33:MET:HE2	4:o:33:MET:HB2	1.91	0.43
3:f:249:ARG:HH12	3:f:513:ARG:NH1	2.09	0.43
3:f:561:ASP:OD2	3:g:88:PRO:HB2	2.17	0.43
4:s:124:LYS:HE2	4:s:124:LYS:HB2	1.76	0.43
3:j:227:GLU:OE2	3:j:272:LYS:NZ	2.45	0.43
3:g:201:PHE:HA	3:g:283:CYS:SG	2.58	0.43
3:g:306:GLU:O	3:g:316:TYR:HA	2.18	0.43
3:g:329:LEU:HD23	3:g:329:LEU:HA	1.82	0.43
3:g:330:ARG:NH1	3:g:409:THR:OG1	2.48	0.43
3:g:536:LEU:HD23	3:g:536:LEU:HA	1.81	0.43
1:1:250:ILE:HG13	1:1:293:MET:SD	2.59	0.43
1:1:416:ASP:HB3	1:5:435:ASP:OD1	2.19	0.43
1:4:2:PRO:HD2	1:4:472:GLU:HA	2.01	0.43
1:5:183:SER:O	1:5:183:SER:OG	2.32	0.43
2:9:33:ILE:HD11	2:9:49:VAL:CG1	2.49	0.43
2:12:84:THR:OG1	2:12:85:VAL:N	2.41	0.43
2:23:46:GLN:HG2	2:23:63:GLN:HG2	2.01	0.43
3:a:363:TYR:HE2	3:b:350:PHE:HE1	1.67	0.43
4:y:16:LYS:NZ	4:q:94:ASP:OD1	2.48	0.43
3:b:297:HIS:HB3	3:b:459:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:556:TYR:HE1	3:e:538:LEU:HD22	1.84	0.43
3:l:8:LEU:HD23	3:l:12:LEU:HG	1.99	0.43
3:l:473:ASP:OD2	3:l:505:GLN:NE2	2.52	0.43
3:l:510:ILE:HG12	3:l:511:ARG:N	2.33	0.43
3:k:510:ILE:HG12	3:k:511:ARG:H	1.83	0.43
3:i:177:HIS:NE2	3:i:221:GLU:OE1	2.42	0.43
3:j:177:HIS:HB2	3:j:219:ILE:HG22	2.00	0.43
3:g:92:ASP:OD1	3:g:92:ASP:N	2.51	0.43
1:2:146:ARG:O	1:2:193:THR:HG21	2.18	0.43
1:4:173:ASP:HB3	1:4:177:ALA:HB2	2.00	0.43
1:4:250:ILE:HG13	1:4:293:MET:SD	2.59	0.43
1:5:310:ARG:C	1:5:311:HIS:HD2	2.26	0.43
2:10:49:VAL:HG13	2:10:63:GLN:HE22	1.84	0.43
2:10:123:LYS:HB2	2:12:123:LYS:HB2	2.00	0.43
3:b:561:ASP:CG	3:c:88:PRO:HB2	2.43	0.43
3:d:76:ILE:HG23	3:d:520:VAL:HG13	2.00	0.43
3:e:221:GLU:OE2	3:e:278:LYS:NZ	2.35	0.43
3:e:297:HIS:HB2	3:e:463:ILE:HG12	2.01	0.43
3:k:297:HIS:HB3	3:k:459:ARG:NH2	2.33	0.43
3:j:46:SER:HA	3:j:49:THR:HG23	2.01	0.43
3:h:559:LEU:HD23	3:h:559:LEU:HA	1.87	0.43
3:g:164:LEU:HD23	3:g:164:LEU:HA	1.83	0.43
3:g:233:PHE:CE2	3:g:255:ILE:HD11	2.54	0.43
5:E:377:LYS:HE2	5:D:374:ALA:HB1	2.01	0.43
5:G:309:THR:CG2	5:G:310:PRO:HD3	2.49	0.43
5:I:94:LEU:HD11	5:H:372:LEU:HD22	2.00	0.43
5:D:386:VAL:HG12	5:D:388:LEU:HD13	2.00	0.43
5:B:13:VAL:O	5:B:14:ASP:C	2.62	0.43
5:H:384:PRO:O	5:H:386:VAL:N	2.52	0.43
1:2:399:SER:HB2	1:6:21:TYR:CZ	2.53	0.43
1:3:98:ALA:O	1:3:104:GLN:NE2	2.51	0.43
1:5:330:LYS:NZ	1:5:376:GLU:OE1	2.36	0.43
1:6:103:SER:OG	1:6:104:GLN:N	2.52	0.43
1:6:308:LEU:HB3	1:6:309:PRO:HD2	2.00	0.43
2:7:13:PRO:HG2	2:8:106:VAL:HG12	2.00	0.43
2:7:120:LYS:HA	2:7:120:LYS:HD3	1.73	0.43
2:8:32:TYR:CE2	2:8:64:PRO:HB3	2.54	0.43
2:17:9:VAL:HG11	2:18:108:LYS:NZ	2.34	0.43
2:24:31:ILE:HG12	2:24:92:ILE:HG23	2.01	0.43
3:a:406:GLU:OE1	3:a:406:GLU:HA	2.18	0.43
3:b:159:ASP:OD1	3:b:159:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:373:LEU:HD13	3:c:353:PRO:HG3	2.01	0.43
3:d:287:LEU:C	3:d:288:LYS:HD2	2.44	0.43
3:e:297:HIS:HB3	3:e:459:ARG:NH2	2.34	0.43
3:j:468:VAL:HG22	3:j:472:TYR:CD2	2.53	0.43
5:C:295:PHE:HD2	5:C:310:PRO:HD2	1.83	0.43
5:A:54:GLU:HG3	5:A:327:TYR:CE2	2.54	0.43
5:A:203:ARG:HD3	5:A:203:ARG:HA	1.86	0.43
5:G:126:MET:HE2	5:G:126:MET:HB3	1.86	0.43
5:I:295:PHE:HD2	5:I:310:PRO:HD2	1.83	0.43
5:D:235:SER:HG	5:D:237:LYS:HZ1	1.64	0.43
1:6:140:SER:O	1:6:156:ASP:N	2.40	0.43
1:6:152:ALA:HA	1:6:162:PHE:O	2.19	0.43
2:7:35:GLN:O	2:7:38:THR:OG1	2.33	0.43
2:8:82:ILE:HD13	2:8:82:ILE:HA	1.82	0.43
4:m:66:PRO:CB	4:m:67:PRO:HD3	2.49	0.43
3:e:389:LEU:HD23	3:e:389:LEU:HA	1.81	0.43
3:l:94:LEU:HD21	3:l:465:GLN:HG3	2.01	0.43
3:f:118:GLN:NE2	3:f:304:PHE:O	2.49	0.43
3:f:251:ILE:HG23	3:f:252:LYS:HG2	2.01	0.43
4:r:72:ASP:N	4:r:72:ASP:OD1	2.51	0.43
3:i:186:ASP:OD2	3:j:171:ARG:NH1	2.52	0.43
3:i:543:PRO:O	3:i:548:GLU:HB2	2.19	0.43
3:h:92:ASP:OD1	3:h:93:VAL:N	2.50	0.43
5:E:381:PHE:HB2	5:E:392:PHE:HB2	2.00	0.43
5:C:256:PHE:CE1	5:C:298:VAL:HG21	2.53	0.43
5:C:378:THR:HG22	5:C:393:ALA:HB2	2.00	0.43
5:A:234:GLN:NE2	5:A:260:THR:H	2.17	0.43
5:G:24:THR:O	5:G:24:THR:OG1	2.24	0.43
5:I:72:GLU:OE2	5:J:95:ARG:NE	2.52	0.43
5:I:264:THR:O	5:I:264:THR:OG1	2.32	0.43
5:F:202:GLN:OE1	5:F:202:GLN:HA	2.19	0.43
5:H:49:MET:HE1	5:H:360:ARG:NH1	2.33	0.43
1:1:141:VAL:HG22	1:1:153:TRP:CD1	2.54	0.43
1:1:435:ASP:CG	1:3:448:ARG:HH21	2.26	0.43
1:5:427:GLU:H	1:5:427:GLU:CD	2.27	0.43
1:6:247:TYR:O	1:6:263:ILE:HG13	2.19	0.43
2:17:32:TYR:CE1	2:17:64:PRO:HB3	2.54	0.43
2:20:124:TYR:C	2:21:123:LYS:HG2	2.43	0.43
3:a:150:HIS:CD2	3:b:163:LYS:HB3	2.54	0.43
3:b:559:LEU:HD23	3:b:559:LEU:HA	1.87	0.43
3:e:249:ARG:NH2	3:e:470:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:l:342:ALA:HB2	4:u:132:MET:CE	2.44	0.43
3:l:348:LYS:HB2	3:k:372:TYR:CE2	2.54	0.43
3:k:404:MET:SD	3:j:337:ASN:HB3	2.58	0.43
3:j:546:THR:OG1	3:j:547:PRO:HD3	2.18	0.43
3:h:468:VAL:HG22	3:h:472:TYR:CD2	2.54	0.43
5:E:299:ARG:HG2	5:E:301:VAL:HG12	2.00	0.43
5:C:24:THR:HB	5:C:116:GLU:HB2	2.01	0.43
5:C:231:SER:OG	5:C:260:THR:O	2.37	0.43
5:D:135:ASP:OD1	5:D:135:ASP:N	2.50	0.43
5:H:173:GLN:O	5:H:177:LYS:HD3	2.19	0.43
1:4:301:HIS:ND1	1:4:316:ASP:OD2	2.52	0.43
1:5:312:VAL:HG21	1:5:338:TYR:HB3	2.00	0.43
1:5:398:SER:HA	1:5:463:THR:O	2.19	0.43
2:10:121:LYS:HD2	2:12:124:TYR:CE2	2.53	0.43
3:a:514:TYR:HE2	3:l:135:GLN:HB3	1.84	0.43
4:y:152:GLU:HG2	3:c:50:THR:H	1.84	0.43
3:c:71:MET:HE2	3:c:71:MET:HB3	1.82	0.43
3:l:319:VAL:HG23	3:l:418:LEU:HD13	2.01	0.43
3:i:65:ARG:HH11	3:j:418:LEU:HA	1.83	0.43
3:j:408:ALA:O	3:j:412:VAL:HG23	2.18	0.43
3:j:507:LEU:HD23	3:j:507:LEU:H	1.83	0.43
3:h:213:THR:HB	5:G:379:THR:HG22	2.01	0.43
5:C:108:ALA:HB1	5:C:384:PRO:HD3	2.00	0.43
5:A:158:ARG:NH2	5:A:283:GLN:OE1	2.48	0.43
5:G:94:LEU:HD12	5:F:373:PHE:CE1	2.54	0.43
5:I:168:TYR:CD2	5:I:353:PHE:HB3	2.53	0.43
5:B:372:LEU:HD12	5:B:372:LEU:HA	1.85	0.43
5:H:191:ILE:HG23	5:H:202:GLN:HG2	2.01	0.43
1:4:443:VAL:HG12	1:4:444:GLY:H	1.83	0.43
1:5:13:GLY:HA3	1:5:24:TYR:HE2	1.84	0.43
1:5:102:THR:O	1:5:102:THR:OG1	2.34	0.43
1:5:447:ARG:HH12	4:s:29:GLU:HG3	1.83	0.43
1:6:188:ILE:HD12	1:6:188:ILE:HA	1.87	0.43
2:10:53:ASN:ND2	2:10:57:SER:HB2	2.33	0.43
3:a:47:GLN:O	5:A:369:ASN:HB2	2.19	0.43
3:a:550:GLN:NE2	3:a:581:VAL:HG21	2.33	0.43
4:y:56:THR:HG22	4:y:114:LEU:HD22	2.01	0.43
3:e:271:ILE:HD12	3:e:511:ARG:HH11	1.84	0.43
4:p:138:ASN:HB3	4:p:141:ALA:HB3	2.01	0.43
3:k:323:THR:HG22	3:k:415:VAL:HG13	2.01	0.43
3:j:33:LEU:O	3:j:37:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:209:PHE:CE2	5:G:374:ALA:HA	2.54	0.43
3:g:113:ILE:HD13	3:g:150:HIS:CE1	2.54	0.43
3:g:298:ILE:HA	3:g:299:PRO:HD3	1.91	0.43
5:C:281:LEU:HD11	5:C:315:LEU:HB2	2.00	0.43
5:A:172:PRO:HA	5:A:213:ARG:HD2	2.00	0.43
5:F:31:LYS:HZ1	5:F:33:TYR:HB2	1.83	0.43
1:5:15:ASP:O	1:5:19:ALA:N	2.44	0.42
1:6:146:ARG:NH2	1:6:149:GLY:HA2	2.34	0.42
2:24:98:SER:HB2	4:u:31:GLN:HG3	2.00	0.42
3:a:109:ILE:HD13	3:b:165:MET:H	1.84	0.42
3:a:236:GLN:HB3	3:a:264:ILE:HG13	2.01	0.42
4:m:115:TYR:OH	3:c:360:GLU:OE2	2.34	0.42
3:e:180:SER:OG	3:f:161:ASN:HB2	2.19	0.42
3:e:249:ARG:NH1	3:e:513:ARG:HH22	2.17	0.42
4:p:132:MET:SD	3:g:342:ALA:HB2	2.59	0.42
3:f:33:LEU:HG	3:f:121:ALA:HB2	2.01	0.42
3:f:371:TYR:OH	3:g:360:GLU:OE1	2.36	0.42
3:k:237:ASP:HB2	3:k:243:PRO:HD3	2.01	0.42
3:k:510:ILE:HG12	3:k:511:ARG:N	2.34	0.42
3:i:228:LYS:HB2	3:i:228:LYS:HE2	1.76	0.42
3:j:76:ILE:O	3:j:457:MET:HE3	2.19	0.42
3:h:297:HIS:HB2	3:h:463:ILE:HG12	2.01	0.42
3:h:510:ILE:HG12	3:h:511:ARG:N	2.34	0.42
4:x:150:PRO:HB2	5:H:401:LEU:HD21	2.00	0.42
5:D:354:TRP:CD1	5:D:354:TRP:C	2.96	0.42
5:B:241:TRP:HA	5:B:252:VAL:HG23	2.01	0.42
1:1:379:LEU:HD23	1:1:379:LEU:HA	1.63	0.42
1:2:29:MET:HE3	1:2:379:LEU:HD11	2.01	0.42
1:2:155:LYS:HB3	1:2:158:THR:OG1	2.19	0.42
1:5:60:ARG:NH2	1:5:89:VAL:HG12	2.34	0.42
1:5:126:ASN:ND2	1:5:136:TYR:O	2.52	0.42
2:14:13:PRO:HG2	2:15:103:ILE:CD1	2.49	0.42
2:19:39:ASP:OD1	2:19:41:VAL:HG23	2.19	0.42
2:24:117:GLU:O	2:24:121:LYS:HB2	2.19	0.42
3:a:101:ASP:OD1	3:a:101:ASP:N	2.52	0.42
3:a:554:LEU:HD21	3:l:564:GLY:C	2.44	0.42
4:y:134:THR:HG22	4:y:145:GLU:C	2.43	0.42
3:b:76:ILE:HG23	3:b:520:VAL:HG13	2.00	0.42
3:c:257:ASP:OD1	3:c:257:ASP:N	2.50	0.42
3:d:310:VAL:HG23	3:d:315:VAL:CG2	2.49	0.42
3:d:346:LYS:H	3:d:346:LYS:HG2	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:o:1:MET:HE2	4:o:1:MET:HB2	1.92	0.42
3:l:239:VAL:HG12	3:l:240:THR:HG22	2.01	0.42
4:q:69:GLU:CD	4:q:70:GLY:N	2.76	0.42
3:f:24:GLU:O	3:f:28:GLU:HG3	2.19	0.42
3:k:6:ASN:HD22	3:k:9:GLU:HG2	1.84	0.42
5:C:383:ILE:HD13	5:C:383:ILE:HA	1.90	0.42
5:B:151:ALA:O	5:B:154:ILE:HG22	2.20	0.42
5:H:144:ALA:O	5:H:148:VAL:HG23	2.19	0.42
1:l:14:LYS:HE3	1:l:416:ASP:O	2.18	0.42
1:l:364:GLN:NE2	1:l:366:ASP:OD2	2.52	0.42
1:4:345:TYR:CE2	1:5:258:PRO:HD3	2.54	0.42
2:11:11:SER:O	2:12:90:MET:HE1	2.19	0.42
2:16:121:LYS:HE3	2:18:124:TYR:HE1	1.85	0.42
2:24:46:GLN:CD	2:24:63:GLN:HG2	2.44	0.42
3:b:199:PRO:HD2	3:b:217:ILE:HG23	2.00	0.42
4:m:4:LYS:HE3	4:m:4:LYS:HB2	1.90	0.42
3:c:40:GLN:HG3	3:c:56:GLN:NE2	2.34	0.42
3:c:165:MET:HE3	3:c:165:MET:HB2	1.88	0.42
3:l:310:VAL:HG12	3:l:311:GLU:HG3	2.00	0.42
3:l:363:TYR:OH	3:l:373:LEU:O	2.33	0.42
3:f:546:THR:OG1	3:f:547:PRO:HD3	2.19	0.42
4:r:66:PRO:HB2	4:r:67:PRO:HD3	2.00	0.42
3:h:242:GLU:O	3:h:242:GLU:HG2	2.19	0.42
3:g:219:ILE:HD11	3:g:280:ILE:CG2	2.48	0.42
5:C:111:LEU:O	5:C:115:VAL:HG23	2.19	0.42
5:A:24:THR:HB	5:A:116:GLU:HG3	2.00	0.42
5:I:296:SER:O	5:I:309:THR:HG22	2.19	0.42
1:3:12:MET:HG3	1:3:13:GLY:N	2.35	0.42
1:4:165:ASP:OD1	1:4:174:ARG:NH1	2.52	0.42
1:6:338:TYR:HE2	1:6:343:PHE:HZ	1.66	0.42
2:8:31:ILE:CG2	2:8:67:ILE:HD11	2.49	0.42
2:14:114:TYR:O	2:14:114:TYR:HD1	2.03	0.42
2:15:50:TYR:HE1	2:15:60:GLN:HE21	1.67	0.42
2:16:107:LEU:HD23	2:16:109:TYR:CE1	2.54	0.42
3:b:207:TRP:CE2	5:B:101:ARG:HD3	2.53	0.42
3:e:30:LYS:HB3	3:e:30:LYS:HE3	1.81	0.42
3:e:92:ASP:OD1	3:e:92:ASP:N	2.53	0.42
3:l:76:ILE:HG22	3:l:457:MET:HG3	2.00	0.42
3:l:178:SER:HA	3:l:217:ILE:O	2.19	0.42
3:l:561:ASP:OD2	3:l:569:ARG:NH2	2.53	0.42
3:f:297:HIS:HB2	3:f:463:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:78:VAL:HG13	3:i:518:THR:HG23	2.00	0.42
3:i:306:GLU:O	3:i:316:TYR:HA	2.20	0.42
3:g:559:LEU:HD23	3:g:559:LEU:HA	1.81	0.42
4:x:128:TYR:CD1	4:x:132:MET:HG2	2.54	0.42
5:E:32:LYS:HA	5:E:32:LYS:HD3	1.91	0.42
5:C:97:GLU:OE2	5:C:101:ARG:NH2	2.52	0.42
5:C:346:LYS:HE3	5:C:346:LYS:HB2	1.81	0.42
5:A:271:ASP:O	5:A:297:VAL:HG12	2.20	0.42
5:G:273:ILE:HD11	5:G:308:ILE:HG21	2.01	0.42
5:D:395:GLN:HG2	5:D:396:GLY:H	1.84	0.42
5:F:118:LYS:HB2	5:F:118:LYS:HE3	1.79	0.42
1:2:441:LYS:HA	1:2:441:LYS:HD3	1.83	0.42
1:3:298:PHE:O	1:3:301:HIS:HB2	2.19	0.42
1:4:103:SER:OG	1:4:114:GLU:HB3	2.19	0.42
1:4:148:ARG:HA	1:5:182:GLU:O	2.20	0.42
1:5:389:ALA:HB1	1:5:471:LEU:HD22	2.00	0.42
1:6:354:ASP:OD1	1:6:355:LYS:N	2.52	0.42
2:8:114:TYR:HA	2:8:117:GLU:OE1	2.19	0.42
2:10:123:LYS:HA	2:10:123:LYS:HD3	1.73	0.42
2:17:14:ARG:HG2	2:17:14:ARG:HH11	1.85	0.42
2:24:36:ILE:HA	2:24:89:SER:HB3	2.02	0.42
4:y:21:SER:OG	4:y:22:ASP:N	2.52	0.42
3:c:243:PRO:HA	3:c:510:ILE:HG13	2.01	0.42
3:c:257:ASP:OD2	3:c:500:ALA:HA	2.19	0.42
3:c:379:GLU:HB3	4:n:109:TYR:CD2	2.54	0.42
3:l:98:TYR:CE1	3:l:102:MET:HG3	2.54	0.42
3:f:329:LEU:HD23	3:f:329:LEU:HA	1.84	0.42
3:k:389:LEU:HD12	3:k:389:LEU:HA	1.81	0.42
4:s:118:THR:O	4:s:122:ARG:HG3	2.19	0.42
3:i:298:ILE:HA	3:i:299:PRO:HD3	1.87	0.42
5:I:201:ILE:O	5:I:202:GLN:HG2	2.19	0.42
5:D:133:SER:HB3	5:D:426:PRO:HA	2.01	0.42
5:F:32:LYS:HE2	5:F:387:GLY:H	1.84	0.42
5:F:236:PHE:HZ	5:F:259:VAL:HG12	1.84	0.42
1:1:72:TYR:CE2	1:1:81:LYS:HB2	2.55	0.42
1:6:297:ARG:HA	1:6:301:HIS:O	2.18	0.42
2:7:28:ASN:ND2	2:7:28:ASN:O	2.53	0.42
2:7:87:GLY:N	2:7:111:PRO:HD2	2.34	0.42
3:a:89:ASP:HB3	3:l:561:ASP:HB3	2.01	0.42
3:b:26:ARG:O	3:b:30:LYS:HG3	2.19	0.42
3:b:468:VAL:HG22	3:b:472:TYR:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:296:GLU:OE2	3:c:514:TYR:OH	2.36	0.42
3:c:364:ASP:OD1	3:c:366:ASN:ND2	2.52	0.42
3:e:271:ILE:HD12	3:e:511:ARG:NH1	2.34	0.42
4:p:69:GLU:OE2	4:p:70:GLY:N	2.52	0.42
3:k:71:MET:HE2	3:k:71:MET:HB3	1.92	0.42
3:i:223:TYR:CD2	3:i:278:LYS:HG3	2.54	0.42
3:j:536:LEU:HD23	3:j:536:LEU:HA	1.88	0.42
3:g:244:VAL:HB	3:g:511:ARG:HB2	2.02	0.42
3:g:389:LEU:HA	3:g:389:LEU:HD23	1.76	0.42
5:I:185:ARG:CD	5:J:186:ASP:HA	2.49	0.42
5:I:256:PHE:CE1	5:I:298:VAL:HG21	2.54	0.42
5:D:366:ILE:O	5:D:368:ALA:N	2.50	0.42
5:B:122:MET:HE3	5:B:126:MET:SD	2.60	0.42
5:B:219:VAL:HA	5:B:349:ARG:HA	2.01	0.42
5:H:398:ILE:HA	5:H:401:LEU:H	1.84	0.42
1:1:443:VAL:HG12	1:1:444:GLY:H	1.84	0.42
1:2:42:TYR:CB	1:2:465:SER:HB3	2.49	0.42
1:3:103:SER:OG	1:3:104:GLN:N	2.52	0.42
1:4:183:SER:HB2	1:6:148:ARG:HH21	1.84	0.42
1:4:296:LEU:HD23	1:4:296:LEU:HA	1.81	0.42
2:13:83:VAL:HG12	2:15:9:VAL:HG22	2.01	0.42
2:14:24:LYS:NZ	4:n:67:PRO:HD2	2.34	0.42
2:20:117:GLU:OE2	2:20:117:GLU:N	2.44	0.42
3:b:223:TYR:CE2	3:b:278:LYS:HD3	2.54	0.42
3:b:249:ARG:NH2	3:b:273:ARG:HH12	2.18	0.42
4:r:131:ARG:HG2	3:i:54:ARG:NH1	2.34	0.42
3:k:163:LYS:HB3	3:j:150:HIS:CD2	2.54	0.42
4:t:97:LEU:HD23	4:t:97:LEU:HA	1.86	0.42
3:j:329:LEU:HD23	3:j:329:LEU:HA	1.92	0.42
3:j:418:LEU:HD21	3:j:449:PHE:CE2	2.55	0.42
4:u:41:GLU:OE2	4:u:58:TYR:OH	2.31	0.42
3:h:59:VAL:HG13	3:h:412:VAL:HG11	2.00	0.42
4:x:72:ASP:OD1	4:x:72:ASP:N	2.52	0.42
5:E:132:THR:HG22	5:E:425:LEU:HB2	2.02	0.42
5:A:228:ILE:HG23	5:A:340:VAL:HG22	2.01	0.42
5:A:383:ILE:HG13	5:A:409:LEU:HD22	2.02	0.42
5:G:153:GLU:OE1	5:H:176:LYS:HD3	2.20	0.42
5:G:373:PHE:HE2	5:G:391:ILE:CG2	2.32	0.42
5:I:168:TYR:HB3	5:I:211:VAL:HG22	2.02	0.42
1:1:73:ARG:NH2	1:1:342:ASP:O	2.50	0.42
1:3:447:ARG:NH1	4:v:22:ASP:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:121:LYS:HE3	2:7:122:PHE:CZ	2.55	0.42
3:a:510:ILE:HG12	3:a:511:ARG:N	2.34	0.42
4:y:7:GLY:O	4:y:11:ARG:HG3	2.19	0.42
4:m:15:ARG:HB2	4:m:21:SER:HB3	2.00	0.42
3:c:42:ASP:CG	3:c:328:ARG:HH21	2.26	0.42
3:e:26:ARG:O	3:e:30:LYS:HG3	2.20	0.42
3:e:510:ILE:HG23	3:e:512:GLY:N	2.34	0.42
4:t:49:GLN:O	4:t:52:LYS:HG2	2.20	0.42
5:E:128:SER:HB2	5:E:310:PRO:HG3	2.01	0.42
5:A:128:SER:HB2	5:A:310:PRO:HG3	2.02	0.42
5:I:47:ILE:O	5:I:76:ALA:HA	2.20	0.42
5:I:48:TRP:HA	5:I:75:VAL:O	2.19	0.42
5:D:185:ARG:HA	5:D:185:ARG:HD3	1.83	0.42
1:4:34:LYS:O	1:4:41:GLY:N	2.53	0.42
1:5:204:SER:H	1:5:233:GLY:HA3	1.85	0.42
2:8:114:TYR:CE1	2:8:118:ALA:HB2	2.55	0.42
2:10:36:ILE:CG2	2:10:105:ASN:HD22	2.33	0.42
2:14:40:PRO:O	2:14:46:GLN:NE2	2.50	0.42
2:19:79:LEU:HD11	2:20:20:SER:HB2	2.01	0.42
2:20:108:LYS:HE3	2:20:108:LYS:HB3	1.92	0.42
3:a:561:ASP:OD2	3:a:569:ARG:NH2	2.53	0.42
4:n:128:TYR:CE1	3:e:343:ARG:HD2	2.55	0.42
3:f:478:VAL:HG22	3:f:492:LEU:O	2.20	0.42
3:i:563:LYS:HA	3:i:563:LYS:HD2	1.91	0.42
4:v:114:LEU:HD23	4:v:114:LEU:HA	1.78	0.42
3:g:190:LYS:HD2	3:g:191:TYR:CE1	2.54	0.42
5:E:336:ASP:O	5:E:338:MET:N	2.51	0.42
5:C:40:MET:HE2	5:C:40:MET:HB3	1.80	0.42
5:C:401:LEU:HD23	5:C:401:LEU:HA	1.91	0.42
5:A:108:ALA:HB1	5:A:384:PRO:HD3	2.02	0.42
5:G:40:MET:SD	5:G:79:MET:HG3	2.60	0.42
5:G:365:PRO:O	5:G:366:ILE:HG12	2.19	0.42
5:I:295:PHE:CE2	5:I:312:PRO:HG3	2.54	0.42
5:I:378:THR:HB	5:I:391:ILE:HG23	2.02	0.42
5:D:131:ILE:HD11	5:D:154:ILE:HG21	2.02	0.42
5:B:130:VAL:HG21	5:B:272:LYS:HB3	2.00	0.42
5:J:29:LYS:HE2	5:J:29:LYS:HB2	1.84	0.42
5:J:353:PHE:CZ	5:J:422:GLY:HA3	2.54	0.42
5:J:354:TRP:CD1	5:J:354:TRP:C	2.97	0.42
1:6:284:THR:O	1:6:288:MET:CB	2.68	0.42
2:13:34:GLY:HA3	2:13:40:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:19:94:ASP:OD1	2:19:98:SER:N	2.52	0.42
2:20:65:LEU:HD22	2:20:73:ILE:HD13	2.01	0.42
2:20:112:ASP:OD1	2:20:115:SER:HB3	2.19	0.42
3:a:249:ARG:NH1	3:a:513:ARG:HH22	2.17	0.42
3:a:251:ILE:HG23	3:a:252:LYS:HG2	2.02	0.42
4:m:148:TYR:CD1	3:e:43:ASP:HB2	2.55	0.42
3:c:467:ILE:O	3:c:471:ILE:HG12	2.20	0.42
3:k:133:GLU:HB3	3:k:143:VAL:HG13	2.01	0.42
3:k:184:TRP:CZ2	3:k:199:PRO:HD3	2.54	0.42
3:k:321:ARG:HE	3:k:321:ARG:HB2	1.64	0.42
3:g:33:LEU:HD22	3:g:37:ARG:NH1	2.35	0.42
3:g:256:ASP:OD1	3:g:256:ASP:N	2.47	0.42
5:G:279:LYS:NZ	5:G:292:ASP:OD1	2.50	0.42
5:B:90:ARG:NH2	5:B:92:ASP:HB3	2.35	0.42
5:J:133:SER:HB3	5:J:426:PRO:HA	2.01	0.42
1:1:385:LYS:HG3	1:5:37:LEU:HD12	2.02	0.41
1:2:390:ARG:NH2	1:2:472:GLU:OE1	2.53	0.41
1:2:408:ARG:HA	1:2:427:GLU:HA	2.02	0.41
1:3:140:SER:HB2	1:3:156:ASP:HB2	2.02	0.41
1:3:240:LYS:HA	1:3:248:ALA:O	2.20	0.41
2:7:115:SER:HA	2:8:114:TYR:OH	2.19	0.41
2:10:31:ILE:HG13	2:10:67:ILE:HD11	2.01	0.41
2:13:79:LEU:HD11	2:14:20:SER:HB2	2.02	0.41
4:y:144:ASN:ND2	4:y:147:HIS:HB2	2.28	0.41
4:m:41:GLU:OE1	4:m:61:SER:OG	2.37	0.41
3:c:166:ASP:OD1	3:c:168:SER:OG	2.35	0.41
3:d:229:LYS:HA	3:d:272:LYS:HA	2.02	0.41
3:d:559:LEU:HD23	3:d:559:LEU:HA	1.82	0.41
3:e:320:VAL:O	3:e:324:LYS:HG3	2.19	0.41
4:r:102:LYS:HA	4:r:102:LYS:HD2	1.92	0.41
3:k:298:ILE:HA	3:k:299:PRO:HD3	1.86	0.41
3:i:343:ARG:HD2	4:x:128:TYR:CE1	2.55	0.41
5:E:173:GLN:HG3	5:E:177:LYS:HE3	2.01	0.41
5:E:392:PHE:HD1	5:E:407:ILE:HG12	1.84	0.41
5:C:381:PHE:HB2	5:C:392:PHE:HB2	2.01	0.41
5:B:171:ASN:OD1	5:B:171:ASN:N	2.42	0.41
1:2:458:THR:HB	1:2:460:SER:H	1.85	0.41
2:8:39:ASP:HA	2:8:40:PRO:HD3	1.88	0.41
2:11:99:GLN:HE21	2:11:102:TYR:HB2	1.85	0.41
2:13:121:LYS:HE3	2:13:122:PHE:CZ	2.55	0.41
2:16:94:ASP:N	2:16:94:ASP:OD1	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:21:86:GLN:HG2	2:21:87:GLY:O	2.20	0.41
2:23:112:ASP:OD1	2:23:115:SER:HB3	2.19	0.41
4:n:29:GLU:HG2	4:n:30:PRO:HD2	2.01	0.41
3:d:298:ILE:HG22	3:d:300:ILE:HG12	2.02	0.41
3:e:207:TRP:HB2	5:D:101:ARG:HG2	2.01	0.41
3:k:8:LEU:HG	3:k:286:VAL:HG23	2.01	0.41
3:k:544:GLN:HG3	3:k:548:GLU:OE1	2.19	0.41
3:j:254:VAL:O	3:j:258:LEU:HD23	2.20	0.41
3:g:7:ARG:HG3	3:g:7:ARG:NH1	2.35	0.41
3:g:51:LEU:HD23	3:g:51:LEU:HA	1.84	0.41
5:C:44:SER:O	5:C:44:SER:OG	2.36	0.41
5:C:53:GLN:OE1	5:D:99:ALA:HB1	2.20	0.41
5:C:383:ILE:HG13	5:C:409:LEU:HD13	2.02	0.41
5:G:173:GLN:HE21	5:G:177:LYS:HE2	1.84	0.41
5:F:313:VAL:HB	5:F:328:ALA:HA	2.01	0.41
5:H:357:ASP:OD1	5:H:417:ARG:NH1	2.44	0.41
1:1:116:ARG:HD3	1:1:120:THR:HB	2.03	0.41
1:1:297:ARG:HA	1:1:301:HIS:O	2.21	0.41
1:3:14:LYS:HD2	1:3:416:ASP:O	2.20	0.41
1:3:274:ALA:O	1:3:278:LYS:HG3	2.20	0.41
1:5:436:LYS:HA	1:5:436:LYS:HD2	1.89	0.41
1:6:391:CYS:SG	1:6:446:ILE:HD11	2.60	0.41
2:7:46:GLN:CD	2:7:63:GLN:HG2	2.45	0.41
2:13:51:ILE:HG23	2:13:61:ILE:CG1	2.50	0.41
2:18:117:GLU:O	2:18:121:LYS:HB2	2.20	0.41
2:23:34:GLY:N	2:23:40:PRO:HB3	2.35	0.41
3:a:22:SER:OG	3:a:26:ARG:NH2	2.49	0.41
3:a:92:ASP:OD1	3:a:93:VAL:N	2.54	0.41
3:c:166:ASP:OD1	3:c:166:ASP:C	2.63	0.41
3:c:249:ARG:NH2	3:c:273:ARG:HH12	2.17	0.41
3:d:15:PHE:CD1	3:d:174:THR:HG21	2.55	0.41
3:l:107:ALA:O	3:l:111:VAL:HG23	2.20	0.41
3:f:445:GLU:HG3	3:f:446:THR:N	2.35	0.41
3:k:33:LEU:HD22	3:k:37:ARG:HH11	1.85	0.41
3:g:535:ILE:HD13	3:g:535:ILE:HA	1.89	0.41
5:G:39:SER:OG	5:G:47:ILE:HD11	2.20	0.41
5:G:66:LYS:HZ3	5:G:66:LYS:HG3	1.79	0.41
5:D:35:PRO:HG2	5:D:40:MET:HE2	2.02	0.41
5:H:71:LEU:HD21	5:H:73:LEU:HD21	2.01	0.41
1:2:409:LEU:O	1:2:425:MET:HA	2.20	0.41
1:5:14:LYS:HE3	1:5:416:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:49:ILE:HD11	1:6:338:TYR:OH	2.20	0.41
2:19:120:LYS:HD3	2:19:120:LYS:HA	1.86	0.41
2:21:39:ASP:OD1	2:21:39:ASP:C	2.62	0.41
2:22:42:ASN:OD1	2:22:45:ASN:N	2.53	0.41
3:b:15:PHE:CD1	3:b:174:THR:HG21	2.53	0.41
4:m:20:ALA:HB1	4:m:28:VAL:HG22	2.02	0.41
3:c:12:LEU:HD23	3:c:12:LEU:HA	1.85	0.41
3:c:43:ASP:OD1	3:c:43:ASP:C	2.64	0.41
3:d:510:ILE:HG12	3:d:511:ARG:H	1.83	0.41
3:e:453:LEU:O	3:e:457:MET:HG2	2.20	0.41
3:l:163:LYS:HB3	3:k:150:HIS:CD2	2.55	0.41
3:k:76:ILE:HG23	3:k:520:VAL:HG13	2.02	0.41
3:k:209:PHE:CD2	5:l:36:PRO:HB3	2.56	0.41
3:k:536:LEU:HD23	3:k:536:LEU:HA	1.90	0.41
3:i:76:ILE:HG23	3:i:520:VAL:HG13	2.02	0.41
3:i:178:SER:C	3:i:179:MET:HG3	2.45	0.41
3:h:220:ALA:HB3	3:h:281:ILE:HG13	2.02	0.41
5:E:409:LEU:HG	5:E:411:TYR:HD2	1.85	0.41
5:C:188:PHE:HA	5:C:192:PRO:HB2	2.02	0.41
5:A:96:ASP:N	5:J:41:GLN:OE1	2.54	0.41
5:G:275:PHE:CD1	5:G:340:VAL:HG22	2.54	0.41
5:F:40:MET:HE2	5:F:45:ASN:HA	2.02	0.41
5:H:222:LYS:HB3	5:H:222:LYS:HE2	1.78	0.41
1:1:197:PHE:HA	1:1:209:PHE:O	2.19	0.41
1:2:182:GLU:O	1:3:148:ARG:HA	2.20	0.41
2:7:23:PHE:CD1	2:9:25:ALA:HB2	2.55	0.41
2:23:68:ASN:OD1	2:23:68:ASN:C	2.63	0.41
2:23:115:SER:HB2	2:24:114:TYR:CE1	2.55	0.41
3:b:30:LYS:HB3	3:b:30:LYS:HE2	1.83	0.41
4:m:39:ASP:OD1	4:n:15:ARG:NH2	2.54	0.41
3:e:493:MET:HE2	3:e:493:MET:HB2	1.84	0.41
4:p:131:ARG:NH2	3:h:339:ASP:OD2	2.37	0.41
4:p:146:TRP:CE2	5:F:398:ILE:HD12	2.56	0.41
4:r:102:LYS:HE3	4:r:106:THR:OG1	2.21	0.41
4:u:52:LYS:HZ3	4:u:52:LYS:HB2	1.85	0.41
3:h:30:LYS:HD2	3:h:207:TRP:HE1	1.85	0.41
3:h:319:VAL:HG23	3:h:418:LEU:HD13	2.03	0.41
4:v:141:ALA:HB1	4:v:146:TRP:HB3	2.02	0.41
5:G:130:VAL:HA	5:G:423:VAL:O	2.21	0.41
5:F:47:ILE:HG23	5:F:77:VAL:HG22	2.03	0.41
5:J:38:ALA:O	5:J:42:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:400:THR:HG23	5:J:402:SER:HB2	2.03	0.41
1:4:34:LYS:HG2	1:4:36:ILE:HD13	2.02	0.41
1:4:141:VAL:HG22	1:4:153:TRP:CD1	2.55	0.41
1:5:23:ASP:OD1	1:5:23:ASP:N	2.52	0.41
1:5:47:PRO:HG3	1:5:365:PHE:CE1	2.55	0.41
1:6:408:ARG:HH21	1:6:425:MET:HB2	1.85	0.41
2:7:116:ILE:H	2:7:116:ILE:HG13	1.70	0.41
2:8:29:GLY:HA3	2:8:67:ILE:HD12	2.02	0.41
2:12:31:ILE:HD13	2:12:31:ILE:HA	1.83	0.41
2:14:14:ARG:HG2	2:14:14:ARG:NH1	2.36	0.41
2:16:36:ILE:HD12	2:16:110:ASP:HB2	2.02	0.41
2:21:85:VAL:HG23	2:21:86:GLN:OE1	2.21	0.41
2:22:114:TYR:OH	2:24:119:ASP:OD1	2.33	0.41
3:b:78:VAL:HG13	3:b:518:THR:HG23	2.03	0.41
3:b:342:ALA:HB2	4:q:132:MET:SD	2.61	0.41
3:b:557:PHE:HA	3:b:569:ARG:HG3	2.02	0.41
3:c:151:SER:O	3:c:155:HIS:HB2	2.21	0.41
3:d:80:TYR:OH	3:d:461:GLY:O	2.37	0.41
3:e:288:LYS:HB3	3:e:288:LYS:HE2	1.77	0.41
3:i:406:GLU:O	3:i:410:SER:OG	2.34	0.41
3:j:243:PRO:HA	3:j:510:ILE:HG13	2.03	0.41
5:E:238:PRO:HD2	5:E:324:GLN:HG2	2.03	0.41
5:A:219:VAL:HG22	5:A:349:ARG:HG2	2.03	0.41
5:B:354:TRP:CD1	5:B:354:TRP:C	2.98	0.41
1:2:181:ALA:HA	1:2:209:PHE:HZ	1.85	0.41
1:4:442:ARG:NH2	4:y:21:SER:OG	2.54	0.41
2:11:107:LEU:HD23	2:11:107:LEU:HA	1.83	0.41
2:15:52:GLU:HG3	2:15:58:HIS:CD2	2.56	0.41
2:19:23:PHE:CD1	2:21:25:ALA:HB2	2.56	0.41
2:20:123:LYS:HA	2:20:123:LYS:HD3	1.88	0.41
3:a:391:TYR:CZ	3:b:393:GLU:HG3	2.55	0.41
3:b:263:PHE:HZ	3:b:496:VAL:HG11	1.85	0.41
3:b:333:ILE:HG21	3:b:405:LEU:HB2	2.03	0.41
4:m:84:PHE:CD1	4:m:84:PHE:C	2.99	0.41
3:c:33:LEU:O	3:c:37:ARG:HB2	2.21	0.41
3:c:43:ASP:HB3	4:q:148:TYR:CD1	2.54	0.41
3:e:167:LYS:N	3:e:167:LYS:HD2	2.35	0.41
3:l:329:LEU:HD23	3:l:329:LEU:HA	1.81	0.41
3:l:352:TRP:CD1	3:k:376:ARG:HB2	2.56	0.41
3:f:271:ILE:HD12	3:f:511:ARG:NH1	2.35	0.41
4:t:116:LYS:HB2	4:t:116:LYS:HE3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:80:TYR:OH	3:h:461:GLY:O	2.37	0.41
5:A:298:VAL:CG1	5:A:309:THR:HB	2.51	0.41
5:G:125:GLU:OE1	5:G:269:ARG:NH1	2.51	0.41
5:I:354:TRP:CD1	5:I:354:TRP:C	2.99	0.41
5:F:35:PRO:HG2	5:F:40:MET:SD	2.61	0.41
5:F:268:LYS:NZ	5:F:271:ASP:OD1	2.45	0.41
5:J:79:MET:HE3	5:J:79:MET:HB2	1.69	0.41
5:J:238:PRO:HG3	5:J:313:VAL:HG21	2.02	0.41
1:4:243:PHE:HA	1:4:295:THR:HG21	2.03	0.41
1:5:167:GLU:OE2	1:5:174:ARG:NH2	2.54	0.41
2:10:17:PHE:HD2	2:12:12:ASN:HD22	1.67	0.41
3:a:12:LEU:HD23	3:a:12:LEU:HA	1.89	0.41
3:a:373:LEU:HA	3:b:351:PHE:O	2.21	0.41
3:a:542:THR:HG23	3:l:552:LEU:HD21	2.01	0.41
3:d:266:ILE:HD13	3:d:266:ILE:HA	1.84	0.41
4:o:94:ASP:OD1	4:p:16:LYS:HD2	2.20	0.41
3:e:249:ARG:HH12	3:e:513:ARG:HH22	1.68	0.41
3:k:89:ASP:HB3	3:j:561:ASP:HB3	2.03	0.41
3:i:7:ARG:HD3	3:i:289:ASP:OD1	2.20	0.41
3:i:45:LEU:HD23	3:i:45:LEU:HA	1.92	0.41
4:u:133:PRO:HA	4:u:148:TYR:HA	2.01	0.41
5:E:184:LYS:O	5:E:186:ASP:N	2.54	0.41
5:B:154:ILE:HD12	5:B:154:ILE:HA	1.87	0.41
5:F:191:ILE:HG12	5:F:202:GLN:NE2	2.35	0.41
5:H:159:GLU:OE1	5:H:284:MET:HB3	2.21	0.41
1:1:35:GLU:HA	1:1:40:SER:HA	2.03	0.41
1:1:49:ILE:HG12	1:1:363:LEU:HD12	2.02	0.41
1:1:206:ILE:HB	1:1:230:VAL:HB	2.01	0.41
1:1:331:THR:OG1	1:1:370:GLN:OE1	2.35	0.41
1:2:294:GLU:O	1:2:304:LEU:HD12	2.21	0.41
1:3:42:TYR:CB	1:3:465:SER:HB3	2.50	0.41
1:3:283:TYR:OH	1:3:310:ARG:HB2	2.21	0.41
1:3:308:LEU:HB3	1:3:309:PRO:HD2	2.02	0.41
1:4:88:ASP:O	1:4:115:TYR:OH	2.24	0.41
1:4:277:GLU:O	1:4:281:ARG:HG3	2.21	0.41
1:5:166:LEU:HA	1:5:166:LEU:HD23	1.84	0.41
1:5:416:ASP:N	1:5:416:ASP:OD1	2.51	0.41
1:6:34:LYS:H	1:6:41:GLY:HA2	1.85	0.41
2:14:78:GLN:HE21	4:n:26:THR:HA	1.86	0.41
2:17:36:ILE:HD13	2:17:105:ASN:ND2	2.35	0.41
2:19:46:GLN:CD	2:19:63:GLN:HG2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:32:ASP:OD1	3:b:324:LYS:NZ	2.49	0.41
3:b:329:LEU:HD23	3:b:329:LEU:HA	1.83	0.41
3:c:77:ASP:OD1	3:c:98:TYR:OH	2.35	0.41
3:c:89:ASP:OD1	3:c:89:ASP:C	2.64	0.41
3:c:254:VAL:O	3:c:258:LEU:HD23	2.20	0.41
3:c:370:PRO:HG3	4:n:124:LYS:O	2.20	0.41
3:d:92:ASP:OD1	3:d:93:VAL:N	2.52	0.41
3:d:346:LYS:HB3	3:d:346:LYS:HE3	1.85	0.41
4:o:113:LEU:HD23	4:o:113:LEU:HA	1.85	0.41
3:e:106:THR:OG1	3:e:146:ARG:O	2.34	0.41
3:e:560:LEU:HD11	3:f:534:GLU:OE2	2.21	0.41
3:l:164:LEU:HD23	3:l:164:LEU:HA	1.81	0.41
3:f:77:ASP:HA	3:f:457:MET:HE2	2.02	0.41
3:f:158:TRP:CD2	3:f:167:LYS:HG2	2.56	0.41
3:f:174:THR:HB	3:f:222:PHE:HD1	1.86	0.41
3:f:510:ILE:HG23	3:f:512:GLY:H	1.86	0.41
3:f:560:LEU:HD11	3:g:534:GLU:OE2	2.21	0.41
3:f:562:GLY:H	3:f:565:VAL:HG23	1.85	0.41
3:k:535:ILE:HD13	3:k:535:ILE:HA	1.88	0.41
4:s:21:SER:OG	4:s:22:ASP:N	2.54	0.41
4:s:44:MET:HE1	4:s:83:VAL:HG13	2.02	0.41
3:i:163:LYS:HB3	3:h:150:HIS:CD2	2.55	0.41
3:j:184:TRP:CZ3	3:j:199:PRO:HG3	2.56	0.41
4:u:82:ALA:O	4:u:86:ASN:ND2	2.44	0.41
3:h:208:VAL:HG12	3:h:209:PHE:HB2	2.03	0.41
3:g:61:ARG:O	3:g:65:ARG:HG3	2.21	0.41
3:g:80:TYR:OH	3:g:461:GLY:O	2.35	0.41
3:g:281:ILE:HG13	3:g:286:VAL:HG22	2.03	0.41
3:g:362:MET:HE2	3:g:362:MET:HB3	1.82	0.41
4:x:69:GLU:OE1	4:x:70:GLY:N	2.53	0.41
4:x:76:ARG:H	4:x:76:ARG:HG2	1.57	0.41
5:E:87:PHE:CZ	5:E:89:LEU:HG	2.56	0.41
5:A:126:MET:HE2	5:A:126:MET:HB3	1.88	0.41
5:A:309:THR:HG23	5:A:310:PRO:HD3	2.02	0.41
5:G:185:ARG:HG2	5:H:188:PHE:HE1	1.86	0.41
5:I:142:ALA:HB3	5:J:180:TYR:HE1	1.86	0.41
5:B:282:GLY:O	5:B:284:MET:N	2.53	0.41
5:J:143:ASP:N	5:J:143:ASP:OD1	2.54	0.41
1:2:308:LEU:O	1:2:310:ARG:N	2.55	0.41
1:4:72:TYR:OH	1:4:81:LYS:HD2	2.21	0.41
1:5:118:ASP:OD1	1:5:120:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:258:PRO:HB2	1:5:280:ILE:HG21	2.01	0.41
1:6:208:TYR:O	1:6:225:GLN:N	2.52	0.41
2:8:115:SER:HA	2:9:114:TYR:CE2	2.56	0.41
2:13:101:ASP:OD1	2:13:102:TYR:N	2.53	0.41
2:16:79:LEU:HD11	2:17:20:SER:HB2	2.03	0.41
2:19:14:ARG:NH1	2:19:80:VAL:O	2.53	0.41
2:24:51:ILE:HG23	2:24:80:VAL:HB	2.02	0.41
3:b:37:ARG:HD3	3:c:310:VAL:HG22	2.03	0.41
3:b:77:ASP:HA	3:b:457:MET:HE2	2.03	0.41
4:m:131:ARG:NH1	3:e:53:TYR:O	2.54	0.41
3:c:113:ILE:HD13	3:c:150:HIS:NE2	2.36	0.41
3:k:454:ALA:HB1	3:k:520:VAL:HG21	2.03	0.41
3:j:53:TYR:O	4:x:131:ARG:NH1	2.51	0.41
4:v:94:ASP:OD1	4:v:94:ASP:N	2.54	0.41
3:g:364:ASP:OD1	3:g:364:ASP:N	2.53	0.41
5:I:162:ARG:HE	5:I:162:ARG:HB2	1.68	0.41
5:H:25:PRO:O	5:H:29:LYS:HG3	2.21	0.41
5:J:182:LEU:HD23	5:J:182:LEU:HA	1.88	0.41
5:J:320:LEU:HB2	5:J:325:ARG:HD3	2.02	0.41
1:2:8:MET:SD	1:2:467:CYS:HB2	2.61	0.40
1:2:94:ARG:HE	1:2:94:ARG:HB3	1.72	0.40
1:3:137:GLU:HA	1:3:137:GLU:OE2	2.22	0.40
1:4:408:ARG:NH2	2:12:93:TYR:OH	2.44	0.40
1:5:288:MET:HE3	1:5:288:MET:HB3	1.98	0.40
2:7:34:GLY:N	2:7:40:PRO:HB3	2.36	0.40
2:11:114:TYR:HB2	2:12:7:ASN:OD1	2.21	0.40
2:19:106:VAL:HG23	2:19:107:LEU:CD1	2.49	0.40
3:c:363:TYR:CE1	3:d:350:PHE:HE1	2.34	0.40
4:p:65:ASN:HA	4:p:66:PRO:HD3	1.92	0.40
3:i:59:VAL:HG13	3:i:412:VAL:HG11	2.02	0.40
4:t:6:LYS:HE2	4:t:71:ASP:HB2	2.03	0.40
4:t:21:SER:O	4:t:24:THR:HG22	2.21	0.40
3:j:115:VAL:O	3:j:119:ILE:HG13	2.20	0.40
3:h:205:ASN:C	3:h:207:TRP:HD1	2.29	0.40
4:v:143:LEU:HD23	4:v:143:LEU:HA	1.80	0.40
3:g:36:SER:O	3:g:36:SER:OG	2.38	0.40
5:A:210:ASP:OD1	5:A:210:ASP:C	2.64	0.40
5:B:79:MET:HE1	5:B:364:GLN:HB2	2.03	0.40
5:B:151:ALA:O	5:B:155:MET:HG3	2.21	0.40
5:F:354:TRP:CD1	5:F:354:TRP:C	2.99	0.40
5:H:44:SER:O	5:H:44:SER:OG	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:164:MET:SD	5:J:357:ASP:HB3	2.62	0.40
5:J:191:ILE:HB	5:J:192:PRO:HD3	2.02	0.40
1:1:296:LEU:HD12	1:1:305:ILE:HD11	2.03	0.40
1:1:390:ARG:HD3	4:t:97:LEU:HD11	2.03	0.40
1:1:441:LYS:HE3	4:v:19:VAL:HG13	2.03	0.40
1:3:412:SER:HB3	1:3:423:GLU:HG3	2.02	0.40
1:4:428:GLN:NE2	1:4:462:VAL:HG13	2.36	0.40
1:5:188:ILE:HD12	1:5:188:ILE:HA	1.82	0.40
1:5:308:LEU:HB3	1:5:309:PRO:HD2	2.02	0.40
1:5:343:PHE:CD1	1:5:352:CYS:HB3	2.57	0.40
1:5:402:VAL:O	1:5:402:VAL:HG23	2.22	0.40
2:7:17:PHE:HE1	2:7:73:ILE:HD11	1.86	0.40
2:14:51:ILE:HG22	2:14:82:ILE:HD13	2.04	0.40
2:16:117:GLU:O	2:16:121:LYS:HB3	2.21	0.40
2:17:112:ASP:OD1	2:17:112:ASP:C	2.64	0.40
2:19:34:GLY:HA3	2:19:40:PRO:HB3	2.02	0.40
2:19:117:GLU:HB3	2:19:121:LYS:NZ	2.35	0.40
3:a:88:PRO:HB2	3:l:561:ASP:CG	2.46	0.40
3:a:237:ASP:HB3	3:a:240:THR:O	2.22	0.40
3:b:177:HIS:HB2	3:b:219:ILE:HG22	2.02	0.40
3:b:198:ILE:HA	3:b:199:PRO:HD3	1.96	0.40
3:b:374:LEU:HD11	3:c:350:PHE:CD1	2.56	0.40
3:d:298:ILE:HA	3:d:299:PRO:HD3	1.94	0.40
3:e:12:LEU:HD23	3:e:12:LEU:HA	1.89	0.40
3:f:113:ILE:HD13	3:f:150:HIS:CE1	2.56	0.40
3:i:561:ASP:OD2	3:j:88:PRO:HB2	2.22	0.40
3:i:561:ASP:OD1	3:i:569:ARG:NH1	2.55	0.40
4:u:140:PHE:O	4:u:141:ALA:C	2.65	0.40
3:h:229:LYS:HA	3:h:272:LYS:HA	2.04	0.40
5:C:286:LYS:HE3	5:C:328:ALA:O	2.22	0.40
5:A:220:LEU:HD12	5:A:220:LEU:HA	1.91	0.40
5:G:236:PHE:HZ	5:G:259:VAL:HG22	1.86	0.40
5:I:24:THR:O	5:I:28:GLN:HG3	2.21	0.40
5:D:122:MET:HE2	5:D:122:MET:HB2	1.81	0.40
5:D:196:TYR:CD1	5:D:196:TYR:C	2.98	0.40
5:H:409:LEU:HG	5:H:411:TYR:HD1	1.86	0.40
1:2:262:ILE:HG13	1:2:271:ILE:HG13	2.04	0.40
1:3:65:ASN:HA	1:3:99:HIS:CD2	2.56	0.40
1:3:396:VAL:HG23	1:3:438:VAL:HB	2.02	0.40
1:4:229:MET:HE3	1:4:231:GLN:HG2	2.04	0.40
4:y:15:ARG:HH11	4:y:15:ARG:HG2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:44:TRP:CD1	3:c:44:TRP:H	2.38	0.40
4:n:33:MET:HE2	4:n:33:MET:HB2	1.88	0.40
3:d:297:HIS:HB2	3:d:463:ILE:HG12	2.03	0.40
3:l:265:LYS:HB2	3:l:265:LYS:HE3	1.86	0.40
3:l:389:LEU:HD23	3:l:389:LEU:HA	1.86	0.40
4:r:16:LYS:HD3	4:r:16:LYS:HA	1.79	0.40
4:r:139:SER:HB2	4:r:145:GLU:CD	2.46	0.40
3:i:415:VAL:HG22	3:h:58:ASP:O	2.22	0.40
3:i:559:LEU:HD23	3:i:559:LEU:HA	1.75	0.40
3:j:12:LEU:HD23	3:j:12:LEU:HA	1.92	0.40
3:j:181:GLN:HE22	3:j:198:ILE:HD11	1.86	0.40
3:j:205:ASN:HB3	5:H:392:PHE:CD1	2.56	0.40
3:j:257:ASP:OD1	3:j:257:ASP:N	2.52	0.40
3:j:559:LEU:HD23	3:j:559:LEU:HA	1.82	0.40
3:g:251:ILE:HG23	3:g:252:LYS:HG2	2.03	0.40
3:g:340:ILE:O	3:g:344:THR:OG1	2.36	0.40
4:x:56:THR:HB	4:x:75:LEU:HD23	2.03	0.40
5:E:244:ASP:OD1	5:E:247:GLY:N	2.54	0.40
5:C:128:SER:O	5:C:294:THR:OG1	2.31	0.40
5:I:403:GLY:HA3	5:H:372:LEU:HD23	2.04	0.40
5:H:219:VAL:HA	5:H:349:ARG:HA	2.03	0.40
5:J:314:ALA:HB3	5:J:317:ASP:HB2	2.02	0.40
1:2:343:PHE:CD1	1:2:352:CYS:HB3	2.57	0.40
1:2:364:GLN:HG2	1:2:365:PHE:N	2.37	0.40
1:2:416:ASP:OD1	1:2:416:ASP:N	2.54	0.40
1:3:142:ARG:NH1	1:3:189:ILE:O	2.54	0.40
1:4:186:ASP:HB2	1:6:67:ALA:HA	2.03	0.40
1:4:338:TYR:HE1	1:4:370:GLN:OE1	2.05	0.40
1:6:2:PRO:HD2	1:6:472:GLU:HA	2.04	0.40
1:6:416:ASP:OD1	1:6:416:ASP:N	2.49	0.40
2:7:20:SER:HB3	2:9:79:LEU:HD11	2.02	0.40
2:7:51:ILE:O	2:7:51:ILE:HG13	2.20	0.40
2:8:14:ARG:HG3	2:8:14:ARG:NH1	2.36	0.40
2:23:105:ASN:OD1	2:23:107:LEU:N	2.54	0.40
3:a:33:LEU:HD22	3:a:37:ARG:NH1	2.36	0.40
3:a:44:TRP:HH2	3:a:207:TRP:CZ3	2.40	0.40
3:a:209:PHE:O	3:a:211:TRP:N	2.48	0.40
3:b:113:ILE:HD13	3:b:150:HIS:CE1	2.56	0.40
3:e:550:GLN:OE1	3:e:581:VAL:HG21	2.21	0.40
4:p:114:LEU:HD23	4:p:114:LEU:HA	1.81	0.40
3:l:288:LYS:HD2	3:l:288:LYS:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:l:298:ILE:HA	3:l:299:PRO:HD3	1.90	0.40
3:f:249:ARG:NH2	3:f:470:ASP:OD1	2.53	0.40
3:i:223:TYR:CE2	3:i:278:LYS:HG3	2.57	0.40
3:i:404:MET:HG3	3:h:341:VAL:HG21	2.01	0.40
3:j:493:MET:HE2	3:j:493:MET:HB2	1.90	0.40
3:j:510:ILE:HG12	3:j:511:ARG:N	2.37	0.40
3:h:162:SER:OG	3:h:169:ASP:OD1	2.30	0.40
3:g:140:ASN:O	3:g:142:GLN:HG3	2.21	0.40
3:g:229:LYS:HA	3:g:272:LYS:HA	2.03	0.40
5:C:264:THR:O	5:C:264:THR:OG1	2.35	0.40
5:A:187:ILE:HD12	5:A:187:ILE:HA	1.90	0.40
5:G:40:MET:HB2	5:G:79:MET:HE3	2.04	0.40
5:I:182:LEU:HD23	5:I:182:LEU:HA	1.88	0.40
5:D:222:LYS:HE2	5:D:222:LYS:HB2	1.79	0.40
5:B:126:MET:HE2	5:B:126:MET:HB3	1.79	0.40
5:H:309:THR:CG2	5:H:310:PRO:HD3	2.52	0.40
5:J:89:LEU:HD23	5:J:89:LEU:HA	1.88	0.40
5:J:151:ALA:O	5:J:155:MET:HG3	2.21	0.40
1:4:143:ASP:O	1:4:153:TRP:HA	2.22	0.40
1:4:162:PHE:HA	1:4:177:ALA:O	2.21	0.40
1:4:165:ASP:OD2	1:4:168:ASP:N	2.29	0.40
1:6:204:SER:H	1:6:233:GLY:HA3	1.86	0.40
2:8:13:PRO:O	2:8:14:ARG:HB2	2.22	0.40
3:a:557:PHE:HA	3:a:569:ARG:HG3	2.03	0.40
3:b:165:MET:HE2	3:b:165:MET:HB2	1.99	0.40
3:b:237:ASP:HB2	3:b:243:PRO:HG3	2.02	0.40
4:m:16:LYS:HD3	4:m:16:LYS:HA	1.79	0.40
3:c:510:ILE:HG12	3:c:511:ARG:N	2.37	0.40
4:o:81:SER:O	4:o:85:HIS:ND1	2.48	0.40
4:p:44:MET:HE3	4:p:83:VAL:HG13	2.02	0.40
3:l:47:GLN:H	3:l:47:GLN:HG2	1.68	0.40
3:i:329:LEU:HD23	3:i:329:LEU:HA	1.86	0.40
3:h:306:GLU:O	3:h:316:TYR:HA	2.21	0.40
3:g:213:THR:C	3:g:215:ASP:N	2.80	0.40
5:E:90:ARG:HG2	5:E:91:ALA:N	2.37	0.40
5:G:236:PHE:CZ	5:G:259:VAL:HG22	2.57	0.40
5:I:77:VAL:HB	5:I:414:ASN:OD1	2.21	0.40
5:B:114:ASN:O	5:B:118:LYS:HG2	2.21	0.40
5:F:116:GLU:CD	5:F:216:LYS:HD2	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	469/472 (99%)	427 (91%)	42 (9%)	0	100	100
1	2	469/472 (99%)	435 (93%)	34 (7%)	0	100	100
1	3	469/472 (99%)	428 (91%)	41 (9%)	0	100	100
1	4	469/472 (99%)	425 (91%)	44 (9%)	0	100	100
1	5	469/472 (99%)	425 (91%)	44 (9%)	0	100	100
1	6	469/472 (99%)	437 (93%)	32 (7%)	0	100	100
2	10	118/667 (18%)	108 (92%)	10 (8%)	0	100	100
2	11	118/667 (18%)	112 (95%)	6 (5%)	0	100	100
2	12	118/667 (18%)	114 (97%)	4 (3%)	0	100	100
2	13	118/667 (18%)	113 (96%)	5 (4%)	0	100	100
2	14	118/667 (18%)	112 (95%)	6 (5%)	0	100	100
2	15	118/667 (18%)	111 (94%)	7 (6%)	0	100	100
2	16	118/667 (18%)	111 (94%)	7 (6%)	0	100	100
2	17	118/667 (18%)	110 (93%)	8 (7%)	0	100	100
2	18	118/667 (18%)	108 (92%)	10 (8%)	0	100	100
2	19	118/667 (18%)	112 (95%)	6 (5%)	0	100	100
2	20	118/667 (18%)	111 (94%)	7 (6%)	0	100	100
2	21	118/667 (18%)	111 (94%)	7 (6%)	0	100	100
2	22	118/667 (18%)	110 (93%)	8 (7%)	0	100	100
2	23	118/667 (18%)	110 (93%)	8 (7%)	0	100	100
2	24	118/667 (18%)	114 (97%)	4 (3%)	0	100	100
2	7	118/667 (18%)	111 (94%)	7 (6%)	0	100	100
2	8	118/667 (18%)	110 (93%)	8 (7%)	0	100	100
2	9	118/667 (18%)	113 (96%)	5 (4%)	0	100	100
3	a	538/725 (74%)	511 (95%)	27 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	b	538/725 (74%)	512 (95%)	26 (5%)	0	100	100
3	c	538/725 (74%)	508 (94%)	28 (5%)	2 (0%)	30	61
3	d	538/725 (74%)	508 (94%)	30 (6%)	0	100	100
3	e	538/725 (74%)	511 (95%)	26 (5%)	1 (0%)	43	73
3	f	538/725 (74%)	507 (94%)	31 (6%)	0	100	100
3	g	538/725 (74%)	505 (94%)	33 (6%)	0	100	100
3	h	538/725 (74%)	510 (95%)	27 (5%)	1 (0%)	43	73
3	i	538/725 (74%)	513 (95%)	25 (5%)	0	100	100
3	j	538/725 (74%)	513 (95%)	25 (5%)	0	100	100
3	k	538/725 (74%)	507 (94%)	29 (5%)	2 (0%)	30	61
3	l	538/725 (74%)	508 (94%)	30 (6%)	0	100	100
4	m	150/166 (90%)	143 (95%)	7 (5%)	0	100	100
4	n	150/166 (90%)	147 (98%)	3 (2%)	0	100	100
4	o	150/166 (90%)	141 (94%)	9 (6%)	0	100	100
4	p	150/166 (90%)	147 (98%)	3 (2%)	0	100	100
4	q	150/166 (90%)	142 (95%)	8 (5%)	0	100	100
4	r	150/166 (90%)	142 (95%)	7 (5%)	1 (1%)	18	49
4	s	150/166 (90%)	147 (98%)	3 (2%)	0	100	100
4	t	150/166 (90%)	149 (99%)	1 (1%)	0	100	100
4	u	150/166 (90%)	141 (94%)	8 (5%)	1 (1%)	18	49
4	v	150/166 (90%)	145 (97%)	5 (3%)	0	100	100
4	x	150/166 (90%)	144 (96%)	5 (3%)	1 (1%)	18	49
4	y	150/166 (90%)	143 (95%)	7 (5%)	0	100	100
5	A	427/430 (99%)	392 (92%)	35 (8%)	0	100	100
5	B	419/430 (97%)	396 (94%)	22 (5%)	1 (0%)	43	73
5	C	427/430 (99%)	400 (94%)	25 (6%)	2 (0%)	24	57
5	D	419/430 (97%)	405 (97%)	13 (3%)	1 (0%)	43	73
5	E	427/430 (99%)	396 (93%)	31 (7%)	0	100	100
5	F	419/430 (97%)	397 (95%)	21 (5%)	1 (0%)	43	73
5	G	427/430 (99%)	387 (91%)	39 (9%)	1 (0%)	43	73
5	H	419/430 (97%)	398 (95%)	20 (5%)	1 (0%)	43	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I	427/430 (99%)	396 (93%)	31 (7%)	0	100	100
5	J	419/430 (97%)	397 (95%)	21 (5%)	1 (0%)	43	73
All	All	17424/29830 (58%)	16386 (94%)	1021 (6%)	17 (0%)	49	78

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	r	145	GLU
3	k	209	PHE
3	h	209	PHE
5	C	37	ALA
5	F	283	GLN
5	J	283	GLN
3	e	50	THR
5	D	283	GLN
5	B	283	GLN
5	H	385	ASP
3	c	214	GLN
3	c	52	GLN
4	u	139	SER
5	C	140	ASN
3	k	217	ILE
4	x	66	PRO
5	G	366	ILE

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	1	394/395 (100%)	394 (100%)	0	100	100
1	2	394/395 (100%)	391 (99%)	3 (1%)	73	81
1	3	394/395 (100%)	392 (100%)	2 (0%)	81	85
1	4	394/395 (100%)	389 (99%)	5 (1%)	61	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5	394/395 (100%)	391 (99%)	3 (1%)	73	81
1	6	394/395 (100%)	389 (99%)	5 (1%)	61	77
2	10	103/548 (19%)	102 (99%)	1 (1%)	68	79
2	11	103/548 (19%)	102 (99%)	1 (1%)	68	79
2	12	103/548 (19%)	103 (100%)	0	100	100
2	13	103/548 (19%)	103 (100%)	0	100	100
2	14	103/548 (19%)	101 (98%)	2 (2%)	50	73
2	15	103/548 (19%)	102 (99%)	1 (1%)	68	79
2	16	103/548 (19%)	103 (100%)	0	100	100
2	17	103/548 (19%)	102 (99%)	1 (1%)	68	79
2	18	103/548 (19%)	102 (99%)	1 (1%)	68	79
2	19	103/548 (19%)	103 (100%)	0	100	100
2	20	103/548 (19%)	102 (99%)	1 (1%)	68	79
2	21	103/548 (19%)	101 (98%)	2 (2%)	50	73
2	22	103/548 (19%)	103 (100%)	0	100	100
2	23	103/548 (19%)	103 (100%)	0	100	100
2	24	103/548 (19%)	103 (100%)	0	100	100
2	7	103/548 (19%)	103 (100%)	0	100	100
2	8	103/548 (19%)	100 (97%)	3 (3%)	37	66
2	9	103/548 (19%)	102 (99%)	1 (1%)	68	79
3	a	480/630 (76%)	477 (99%)	3 (1%)	78	83
3	b	480/630 (76%)	475 (99%)	5 (1%)	68	79
3	c	480/630 (76%)	477 (99%)	3 (1%)	78	83
3	d	480/630 (76%)	475 (99%)	5 (1%)	68	79
3	e	480/630 (76%)	479 (100%)	1 (0%)	87	89
3	f	480/630 (76%)	478 (100%)	2 (0%)	84	86
3	g	480/630 (76%)	475 (99%)	5 (1%)	68	79
3	h	480/630 (76%)	478 (100%)	2 (0%)	84	86
3	i	480/630 (76%)	475 (99%)	5 (1%)	68	79
3	j	480/630 (76%)	476 (99%)	4 (1%)	73	81
3	k	480/630 (76%)	477 (99%)	3 (1%)	78	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	l	480/630 (76%)	478 (100%)	2 (0%)	84	86
4	m	120/131 (92%)	119 (99%)	1 (1%)	73	81
4	n	120/131 (92%)	119 (99%)	1 (1%)	73	81
4	o	120/131 (92%)	120 (100%)	0	100	100
4	p	120/131 (92%)	120 (100%)	0	100	100
4	q	120/131 (92%)	120 (100%)	0	100	100
4	r	120/131 (92%)	119 (99%)	1 (1%)	73	81
4	s	120/131 (92%)	120 (100%)	0	100	100
4	t	120/131 (92%)	119 (99%)	1 (1%)	73	81
4	u	120/131 (92%)	119 (99%)	1 (1%)	73	81
4	v	120/131 (92%)	119 (99%)	1 (1%)	73	81
4	x	120/131 (92%)	119 (99%)	1 (1%)	73	81
4	y	120/131 (92%)	120 (100%)	0	100	100
5	A	351/352 (100%)	350 (100%)	1 (0%)	86	87
5	B	345/352 (98%)	341 (99%)	4 (1%)	63	78
5	C	351/352 (100%)	350 (100%)	1 (0%)	86	87
5	D	345/352 (98%)	338 (98%)	7 (2%)	48	72
5	E	351/352 (100%)	343 (98%)	8 (2%)	44	70
5	F	345/352 (98%)	338 (98%)	7 (2%)	48	72
5	G	351/352 (100%)	348 (99%)	3 (1%)	70	80
5	H	345/352 (98%)	343 (99%)	2 (1%)	78	83
5	I	351/352 (100%)	349 (99%)	2 (1%)	78	83
5	J	345/352 (98%)	342 (99%)	3 (1%)	70	80
All	All	14898/24886 (60%)	14781 (99%)	117 (1%)	70	81

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	102	THR
1	2	169	GLU
1	2	356	SER
1	3	37	LEU
1	3	387	ASP
1	4	130	ASP

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Mol	Chain	Res	Type
1	4	184	GLN
1	4	205	THR
1	4	215	THR
1	4	387	ASP
1	5	38	ASN
1	5	97	MET
1	5	439	LEU
1	6	101	ARG
1	6	275	SER
1	6	294	GLU
1	6	372	ASP
1	6	408	ARG
2	8	55	ASP
2	8	84	THR
2	8	120	LYS
2	9	57	SER
2	10	24	LYS
2	11	120	LYS
2	14	92	ILE
2	14	116	ILE
2	15	36	ILE
2	17	78	GLN
2	18	61	ILE
2	20	24	LYS
2	21	49	VAL
2	21	57	SER
3	a	230	GLU
3	a	271	ILE
3	a	374	LEU
3	b	189	GLU
3	b	208	VAL
3	b	279	SER
3	b	354	GLU
3	b	413	LYS
4	m	69	GLU
3	c	493	MET
3	c	561	ASP
3	c	569	ARG
4	n	69	GLU
3	d	130	THR
3	d	140	ASN
3	d	212	LEU

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Mol	Chain	Res	Type
3	d	296	GLU
3	d	346	LYS
3	e	470	ASP
3	l	58	ASP
3	l	264	ILE
3	f	368	ASP
3	f	520	VAL
4	r	69	GLU
3	k	76	ILE
3	k	498	ASP
3	k	582	LYS
3	i	50	THR
3	i	168	SER
3	i	368	ASP
3	i	410	SER
3	i	565	VAL
4	t	69	GLU
3	j	56	GLN
3	j	134	ASP
3	j	347	LYS
3	j	396	GLU
4	u	69	GLU
3	h	270	GLN
3	h	550	GLN
4	v	43	MET
3	g	10	SER
3	g	70	GLU
3	g	76	ILE
3	g	135	GLN
3	g	284	THR
4	x	65	ASN
5	E	34	THR
5	E	45	ASN
5	E	64	THR
5	E	141	THR
5	E	147	PHE
5	E	186	ASP
5	E	304	THR
5	E	376	MET
5	C	371	GLU
5	A	16	ILE
5	G	86	PHE

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Mol	Chain	Res	Type
5	G	135	ASP
5	G	405	CYS
5	I	106	SER
5	I	130	VAL
5	D	10	THR
5	D	11	LEU
5	D	93	ASP
5	D	152	GLU
5	D	158	ARG
5	D	283	GLN
5	D	340	VAL
5	B	14	ASP
5	B	15	GLU
5	B	341	ASN
5	B	376	MET
5	F	10	THR
5	F	13	VAL
5	F	14	ASP
5	F	20	ILE
5	F	79	MET
5	F	101	ARG
5	F	118	LYS
5	H	16	ILE
5	H	340	VAL
5	J	11	LEU
5	J	15	GLU
5	J	325	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (178) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	5	GLN
1	1	126	ASN
1	2	126	ASN
1	2	364	GLN
1	4	171	HIS
1	4	184	GLN
1	4	321	GLN
1	4	322	ASN
1	5	126	ASN
1	5	225	GLN
1	5	377	HIS

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Mol	Chain	Res	Type
1	6	69	ASN
1	6	377	HIS
1	6	468	GLN
2	7	46	GLN
2	7	53	ASN
2	8	46	GLN
2	8	99	GLN
2	9	58	HIS
2	10	53	ASN
2	10	63	GLN
2	11	7	ASN
2	11	45	ASN
2	11	113	GLN
2	12	88	HIS
2	13	63	GLN
2	13	99	GLN
2	15	46	GLN
2	15	60	GLN
2	16	46	GLN
2	16	60	GLN
2	18	86	GLN
2	18	113	GLN
2	19	46	GLN
2	19	99	GLN
2	20	42	ASN
2	21	53	ASN
2	22	86	GLN
2	22	88	HIS
2	23	12	ASN
2	23	45	ASN
2	23	60	GLN
3	a	56	GLN
3	a	172	HIS
3	a	218	GLN
3	a	355	GLN
3	a	361	HIS
3	a	575	GLN
4	y	86	ASN
4	y	147	HIS
3	b	31	ASN
3	b	47	GLN
3	b	56	GLN

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Mol	Chain	Res	Type
3	b	177	HIS
3	b	380	ASN
3	b	450	GLN
3	b	477	ASN
4	m	65	ASN
3	c	31	ASN
3	c	40	GLN
3	c	56	GLN
3	c	135	GLN
3	c	270	GLN
3	c	366	ASN
3	c	394	ASN
3	c	469	ASN
4	n	86	ASN
4	n	142	ASN
3	d	74	ASN
3	d	142	GLN
3	d	181	GLN
3	d	214	GLN
3	d	380	ASN
3	d	450	GLN
4	o	31	GLN
4	o	65	ASN
4	o	144	ASN
3	e	181	GLN
3	e	361	HIS
4	p	34	GLN
3	l	52	GLN
3	l	135	GLN
3	l	141	ASN
3	l	181	GLN
3	l	205	ASN
3	l	361	HIS
3	l	477	ASN
3	l	573	ASN
3	f	47	GLN
3	f	74	ASN
3	f	182	ASN
3	f	477	ASN
3	f	575	GLN
4	r	65	ASN
4	r	147	HIS

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Mol	Chain	Res	Type
3	k	355	GLN
4	s	31	GLN
3	i	74	ASN
3	i	203	ASN
3	i	218	GLN
3	i	361	HIS
3	j	74	ASN
3	j	181	GLN
3	j	205	ASN
4	u	117	GLN
3	h	6	ASN
3	h	141	ASN
3	h	142	GLN
3	h	361	HIS
3	h	450	GLN
3	h	465	GLN
3	h	573	ASN
3	h	575	GLN
3	g	47	GLN
3	g	73	GLN
3	g	74	ASN
3	g	141	ASN
3	g	150	HIS
3	g	327	GLN
3	g	575	GLN
4	x	65	ASN
5	E	4	ASN
5	E	53	GLN
5	E	105	GLN
5	E	121	ASN
5	E	305	HIS
5	E	344	ASN
5	E	389	ASN
5	C	4	ASN
5	C	7	GLN
5	C	41	GLN
5	C	74	ASN
5	C	88	GLN
5	C	251	ASN
5	C	305	HIS
5	A	4	ASN
5	A	7	GLN

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Mol	Chain	Res	Type
5	A	58	GLN
5	A	248	ASN
5	G	4	ASN
5	G	88	GLN
5	G	121	ASN
5	G	146	ASN
5	G	248	ASN
5	I	4	ASN
5	I	45	ASN
5	I	74	ASN
5	I	161	ASN
5	I	171	ASN
5	I	248	ASN
5	I	389	ASN
5	I	395	GLN
5	D	58	GLN
5	D	84	ASN
5	D	146	ASN
5	B	41	GLN
5	B	74	ASN
5	B	113	ASN
5	B	161	ASN
5	B	287	ASN
5	B	305	HIS
5	B	324	GLN
5	F	28	GLN
5	F	41	GLN
5	F	146	ASN
5	F	171	ASN
5	F	341	ASN
5	H	45	ASN
5	H	84	ASN
5	H	105	GLN
5	H	114	ASN
5	H	121	ASN
5	H	291	GLN
5	J	58	GLN
5	J	171	ASN
5	J	251	ASN
5	J	395	GLN
5	J	414	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

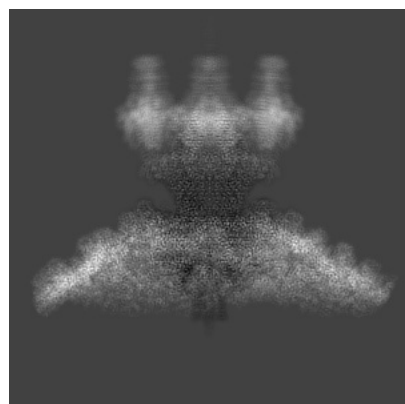
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41792. These allow visual inspection of the internal detail of the map and identification of artifacts.

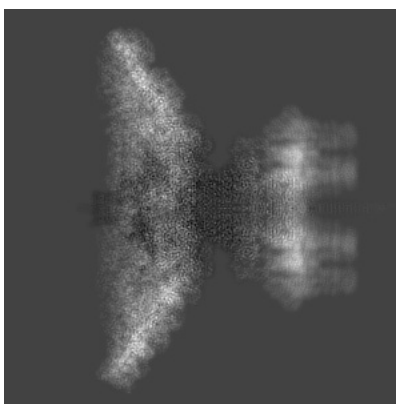
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

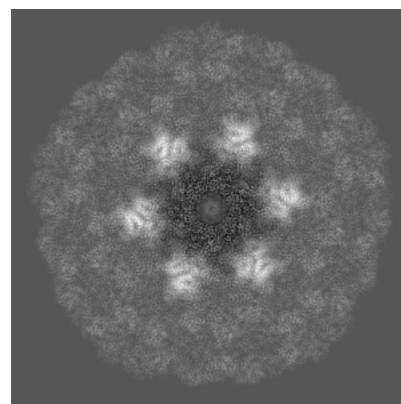
6.1.1 Primary map



X

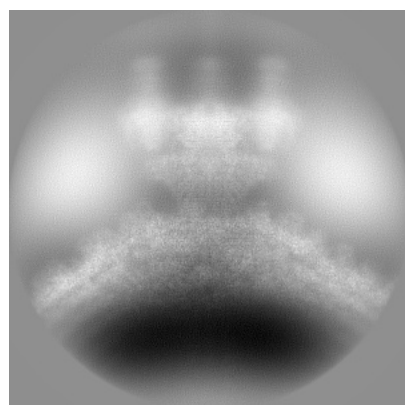


Y

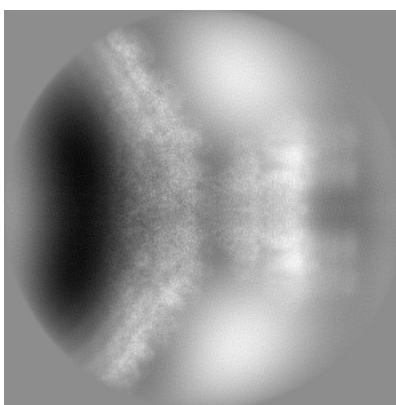


Z

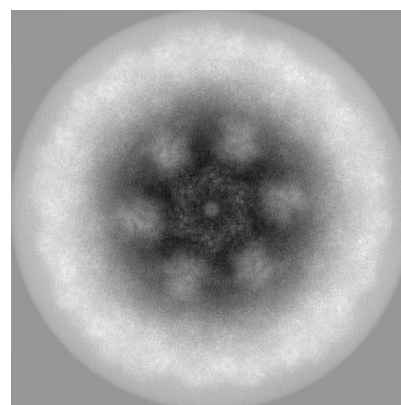
6.1.2 Raw map



X



Y

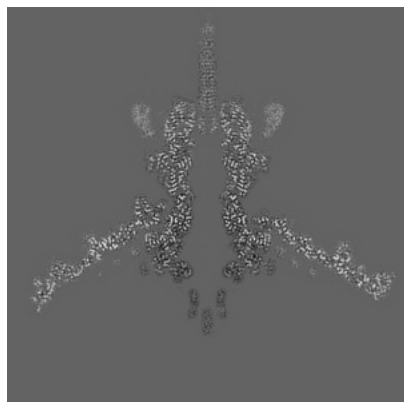


Z

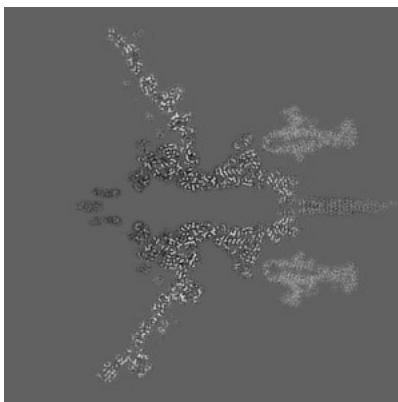
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

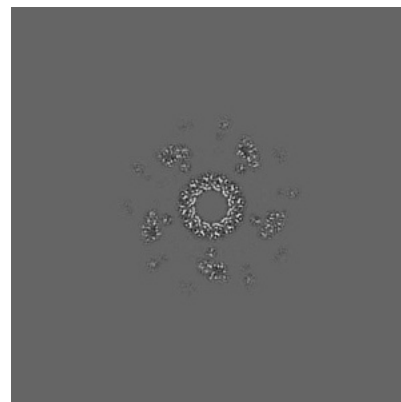
6.2.1 Primary map



X Index: 220

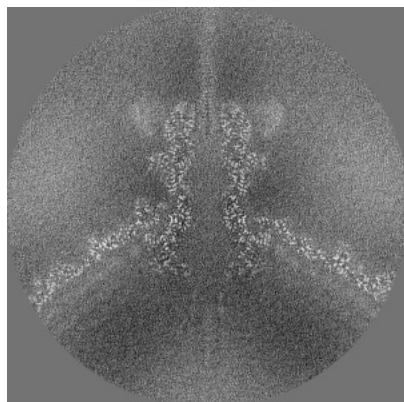


Y Index: 220

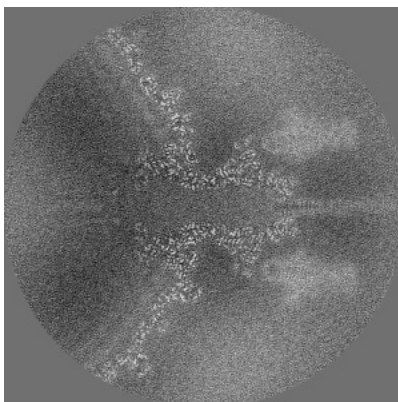


Z Index: 220

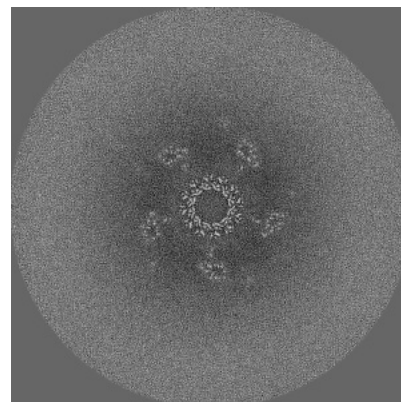
6.2.2 Raw map



X Index: 220



Y Index: 220

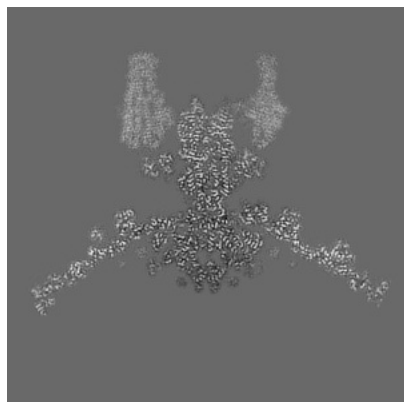


Z Index: 220

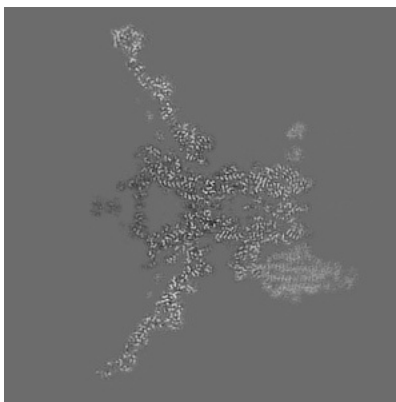
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

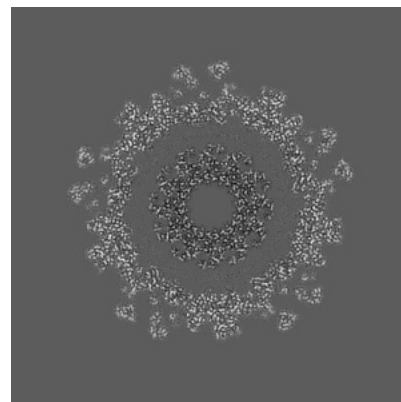
6.3.1 Primary map



X Index: 188

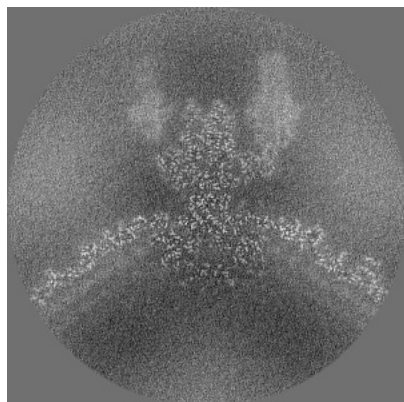


Y Index: 202

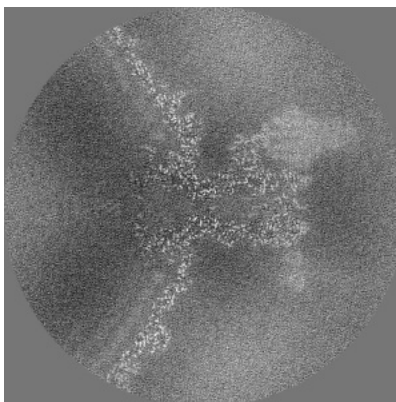


Z Index: 177

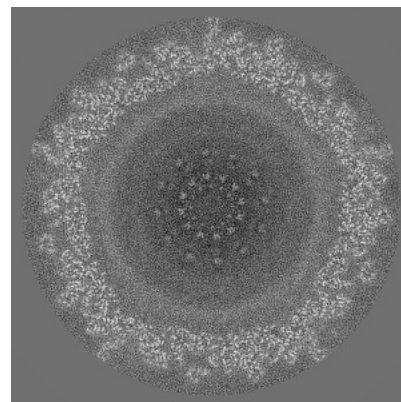
6.3.2 Raw map



X Index: 247



Y Index: 236

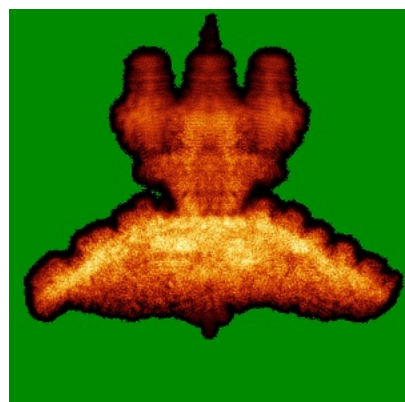


Z Index: 144

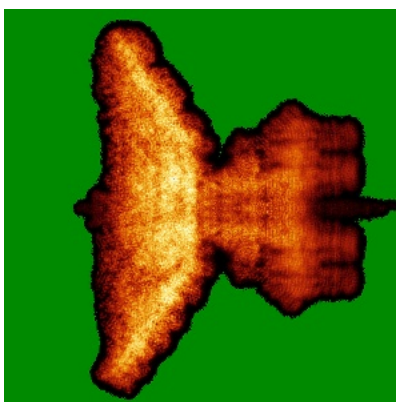
The images above show the largest variance slices of the map in three orthogonal directions.

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

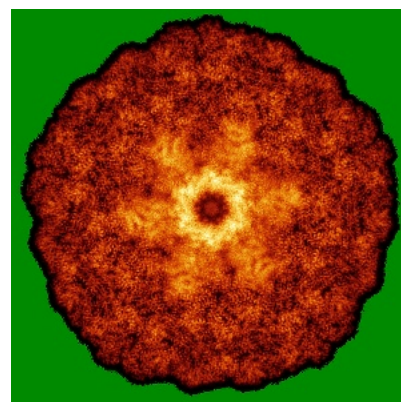
6.4.1 Primary map



X

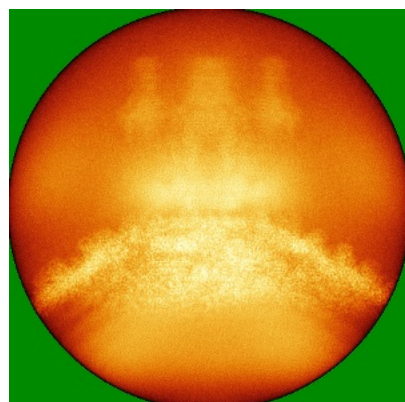


Y

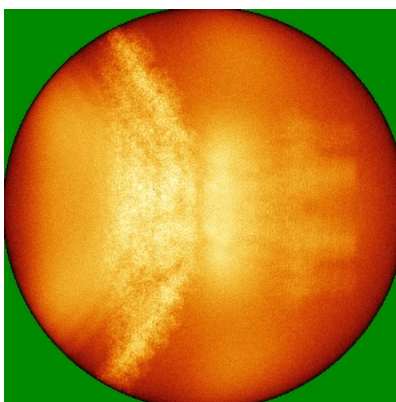


Z

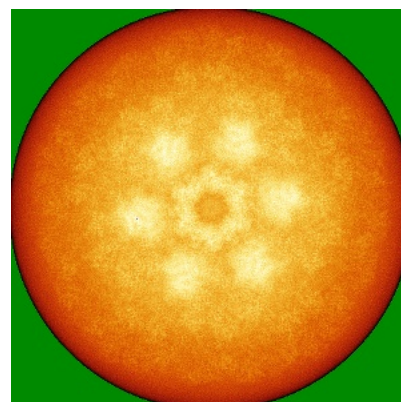
6.4.2 Raw map



X



Y

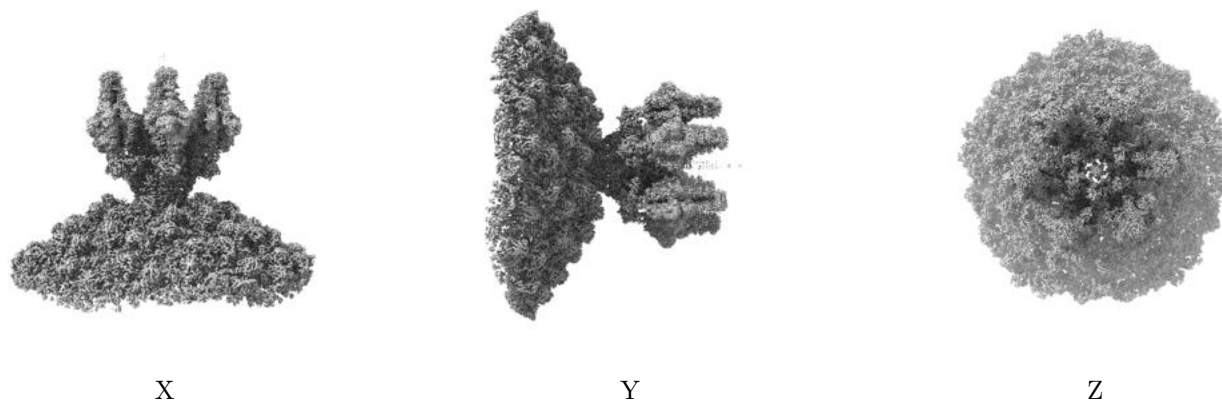


Z

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

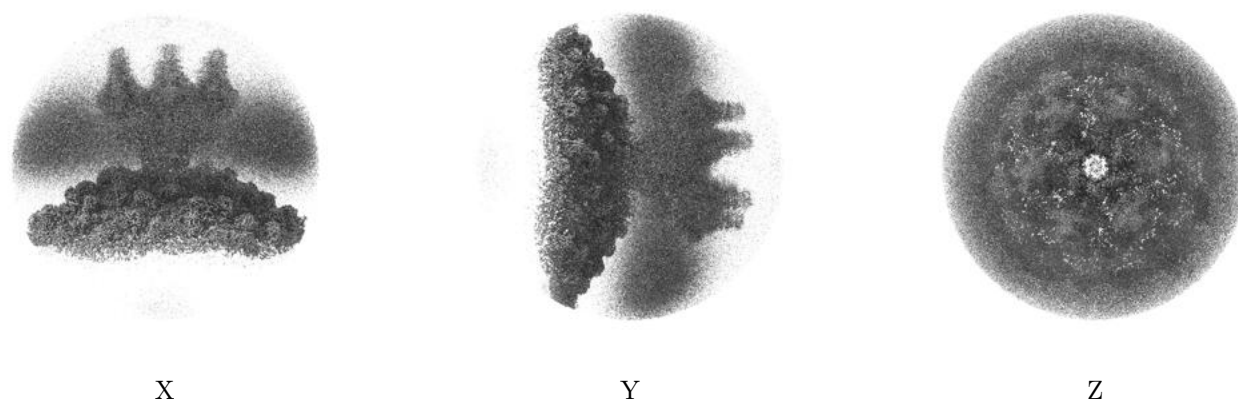
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

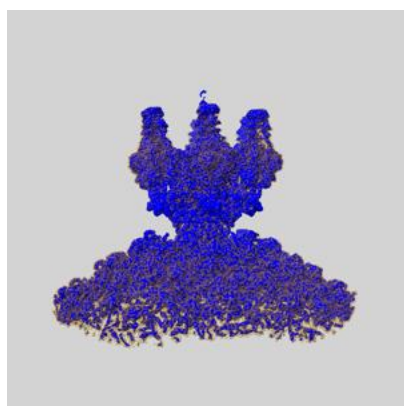
6.6 Mask visualisation [i](#)

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

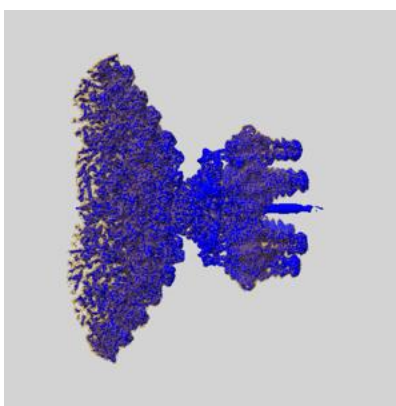
A mask typically either:

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

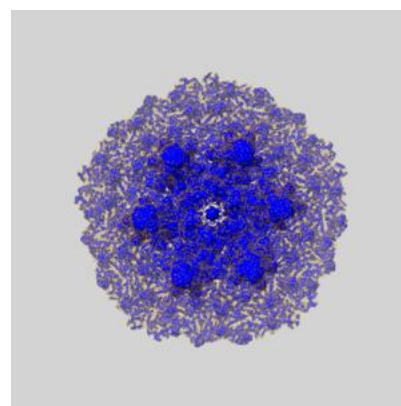
6.6.1 emd_41792_msk_1.map [i](#)



X



Y

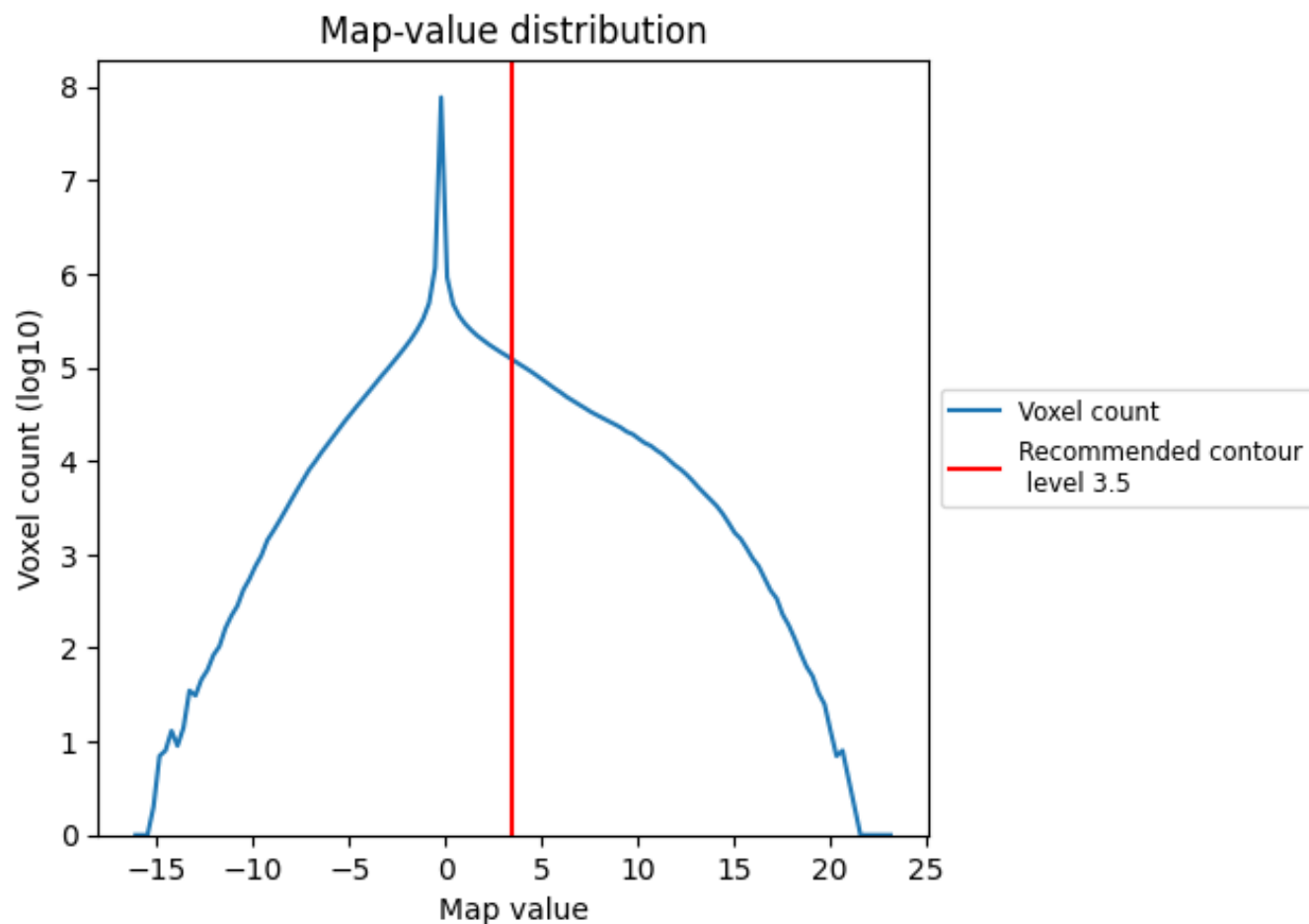


Z

7 Map analysis [i](#)

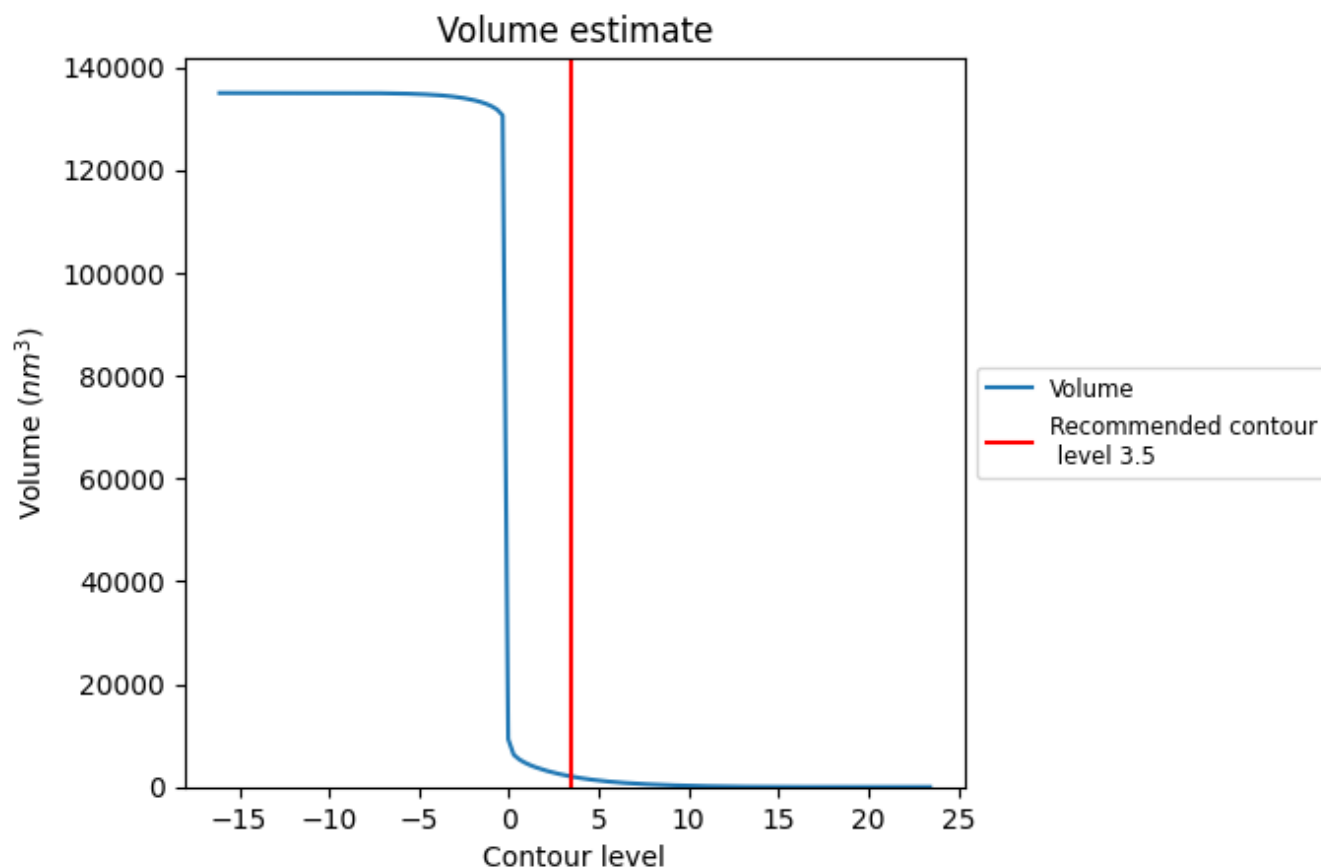
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

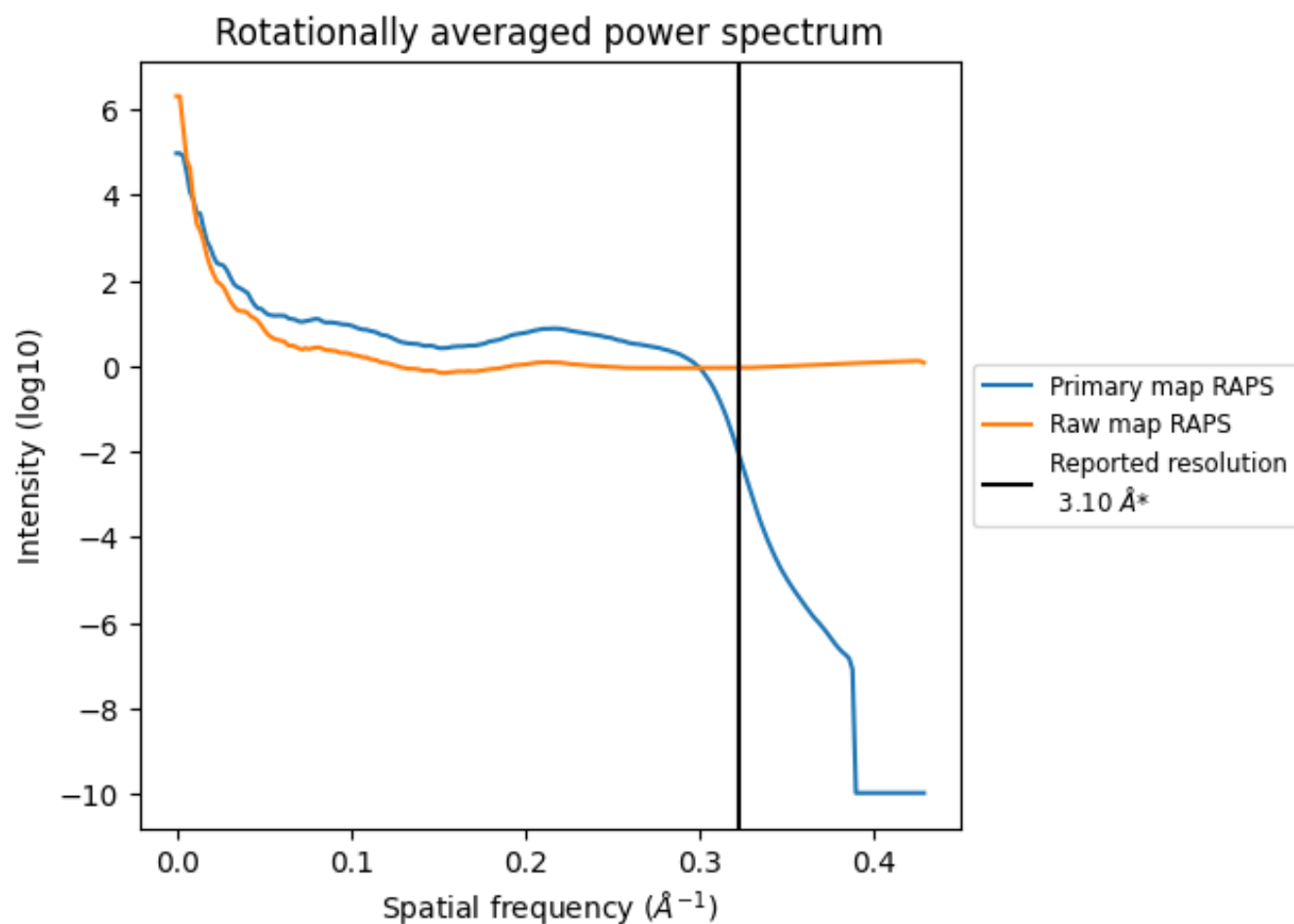
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2023 nm^3 ; this corresponds to an approximate mass of 1827 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 ⓘ

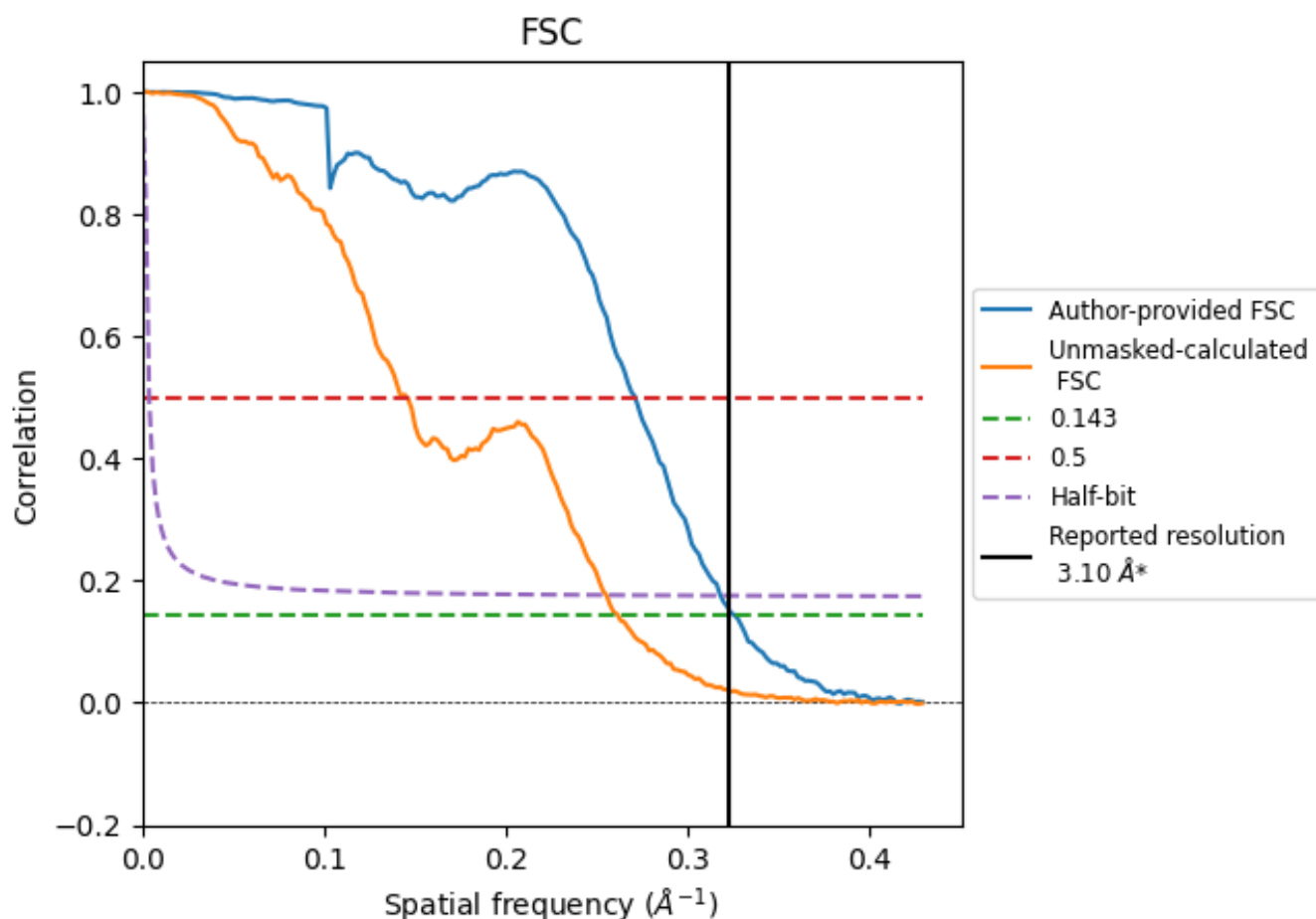


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

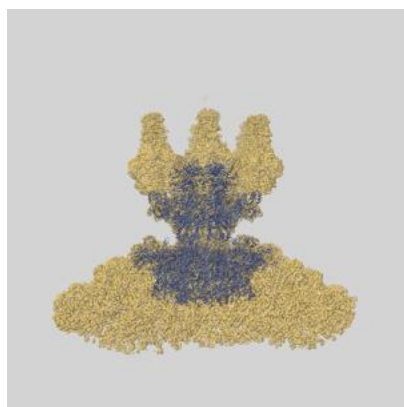
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.69	3.14
Unmasked-calculated*	3.82	7.03	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 3.1 by more than 10 %

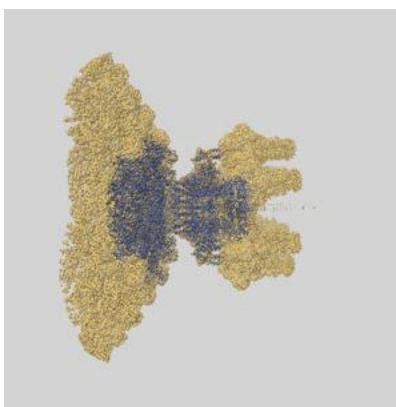
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41792 and PDB model 8U11. Per-residue inclusion information can be found in section [3](#) on page [10](#).

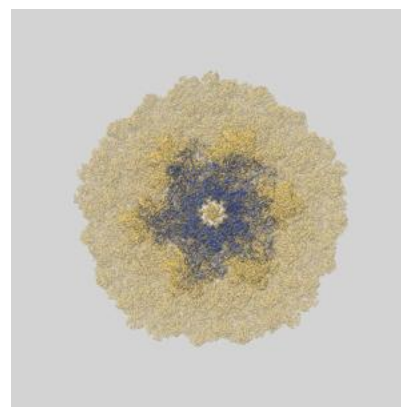
9.1 Map-model overlay [i](#)



X



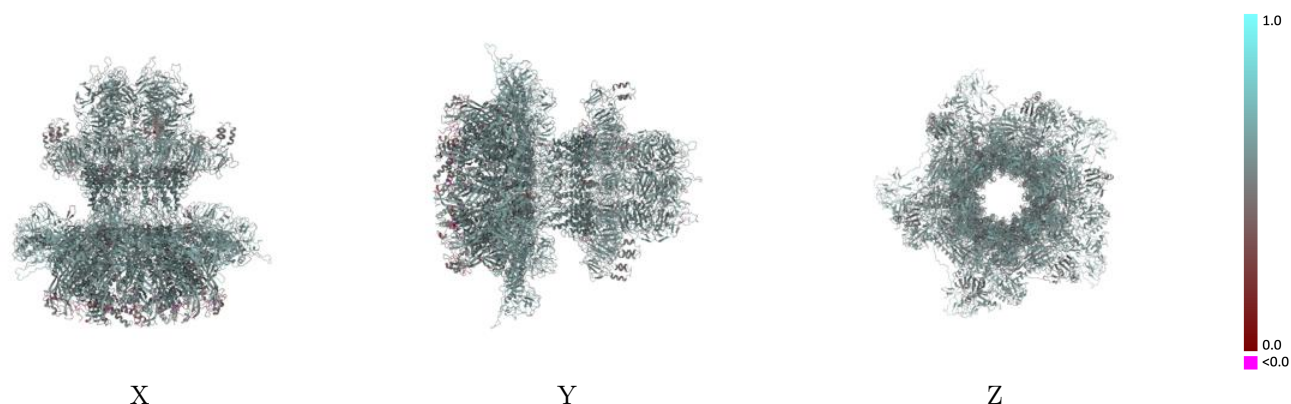
Y



Z

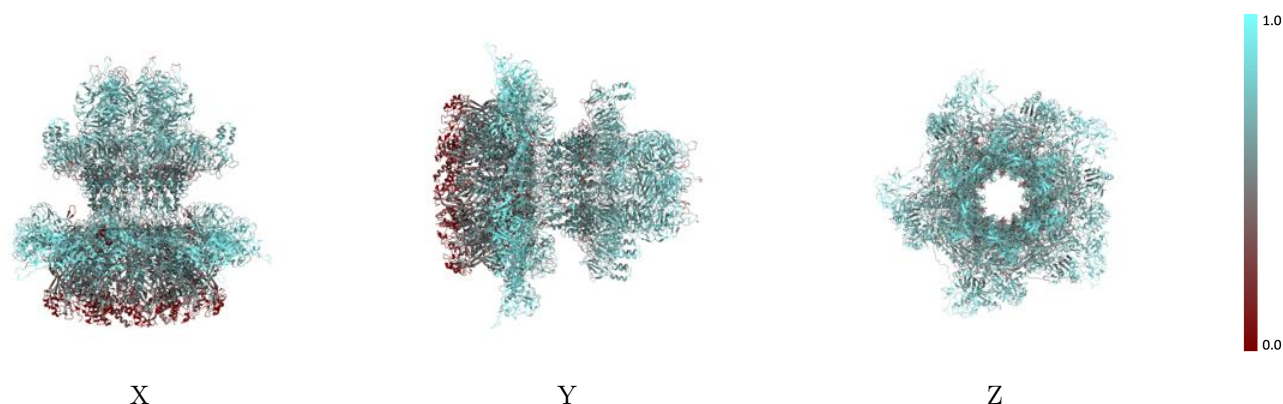
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



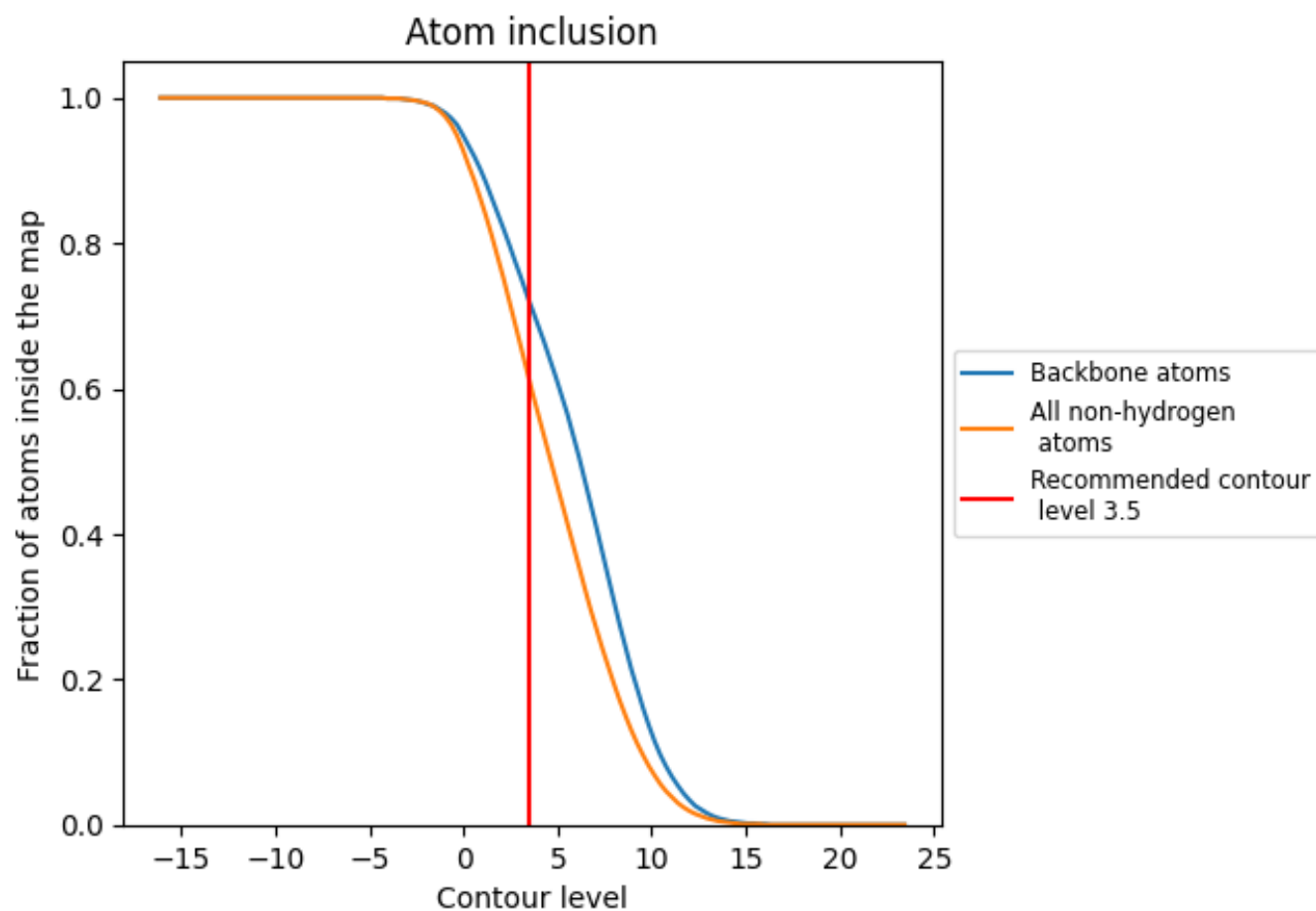
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 61% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6110	 0.5480
1	 0.7130	 0.5540
10	 0.6170	 0.5120
11	 0.6600	 0.5390
12	 0.6840	 0.5530
13	 0.6150	 0.5050
14	 0.6530	 0.5390
15	 0.6830	 0.5480
16	 0.6110	 0.5040
17	 0.6710	 0.5410
18	 0.6670	 0.5480
19	 0.6320	 0.5150
2	 0.6970	 0.5500
20	 0.6600	 0.5440
21	 0.7070	 0.5460
22	 0.6040	 0.5120
23	 0.6540	 0.5450
24	 0.6910	 0.5450
3	 0.7000	 0.5540
4	 0.7100	 0.5550
5	 0.7080	 0.5540
6	 0.7110	 0.5540
7	 0.6230	 0.5120
8	 0.6570	 0.5440
9	 0.6820	 0.5420
A	 0.7100	 0.5650
B	 0.7790	 0.5690
C	 0.7020	 0.5700
D	 0.7470	 0.5630
E	 0.6770	 0.5630
F	 0.7730	 0.5680
G	 0.6870	 0.5570
H	 0.7680	 0.5690
I	 0.7040	 0.5670
J	 0.7510	 0.5580



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Chain	Atom inclusion	Q-score
a	 0.4830	 0.5380
b	 0.4930	 0.5390
c	 0.5000	 0.5390
d	 0.4880	 0.5410
e	 0.4710	 0.5410
f	 0.4900	 0.5370
g	 0.4780	 0.5390
h	 0.4800	 0.5330
i	 0.4930	 0.5430
j	 0.4770	 0.5360
k	 0.4750	 0.5320
l	 0.4620	 0.5270
m	 0.5620	 0.5350
n	 0.6170	 0.5610
o	 0.6010	 0.5520
p	 0.6320	 0.5650
q	 0.6240	 0.5550
r	 0.5800	 0.5380
s	 0.6340	 0.5740
t	 0.6250	 0.5650
u	 0.6030	 0.5490
v	 0.6120	 0.5550
x	 0.6450	 0.5650
y	 0.6320	 0.5640