



Full wwPDB EM Validation Report ⓘ

Jul 7, 2026 – 10:55 am BST

PDB ID : 9SYS / pdb_00009sys
EMDB ID : EMD-55352
Title : Special vertex of bacteriophage LUZ19 computed in C1 symmetry
Authors : Stefanik Sobotkova, A.; Cienikova, Z.; Mironova, Y.; Fuzik, T.; Plevka, P.;
Novacek, J.; Hlavenkova, Z.
Deposited on : 2025-10-14
Resolution : 4.01 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.dev133
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) : 2.50

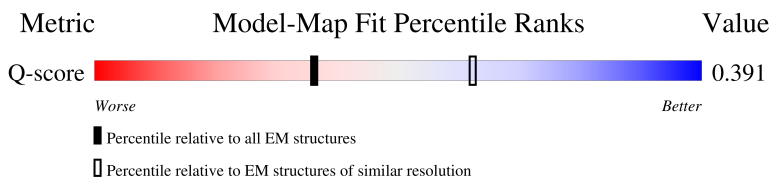
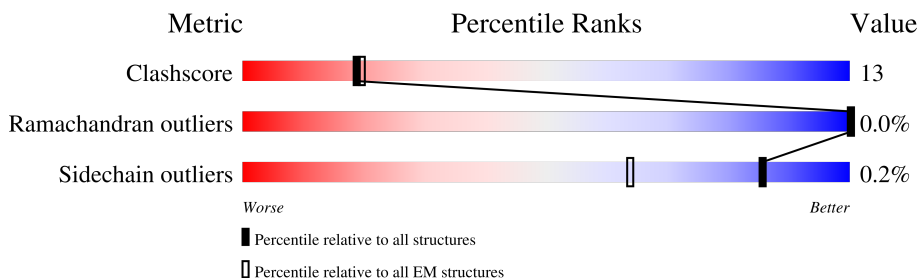
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.01 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.



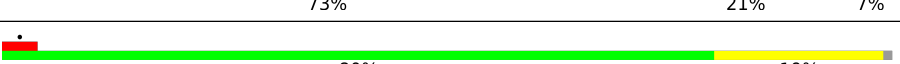
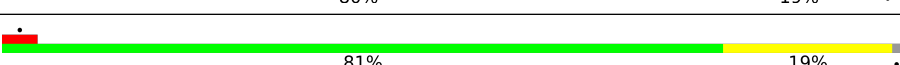
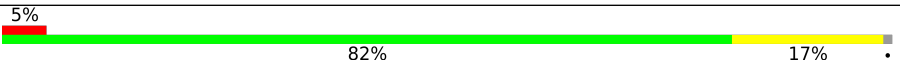
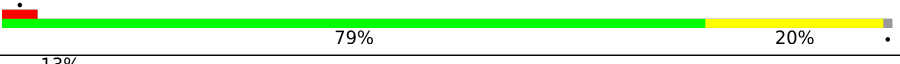
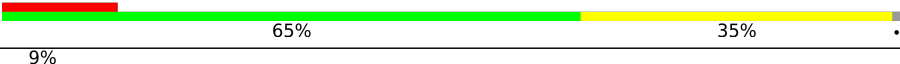
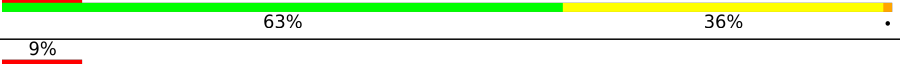
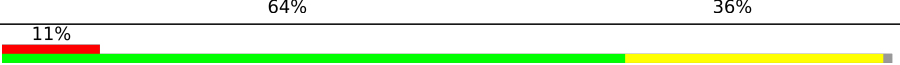
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6765 (3.51 - 4.51)

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

Mol	Chain	Length	Quality of chain
1	A	335	5% 82% 17% .
1	B	335	6% 74% 26% .
1	C	335	. 72% 28% .
1	D	335	. 73% 26% .

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Mol	Chain	Length	Quality of chain
1	E	335	
1	F	335	
1	G	335	
1	H	335	
1	I	335	
1	J	335	
1	K	335	
1	L	335	
1	M	335	
1	N	335	
1	O	335	
2	P	184	
2	Q	184	
2	R	184	
2	S	184	
2	T	184	
2	U	184	
2	V	184	
2	W	184	
2	X	184	
2	k	184	
2	l	184	
2	m	184	
3	Y	510	
3	Z	510	

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Mol	Chain	Length	Quality of chain
3	a	510	
3	b	510	
3	c	510	
3	d	510	
3	e	510	
3	f	510	
3	g	510	
3	h	510	
3	i	510	
3	j	510	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 98061 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	333	Total	C	N	O	S	0	0
			2643	1668	469	498	8		
1	B	333	Total	C	N	O	S	0	0
			2643	1668	469	498	8		
1	C	333	Total	C	N	O	S	0	0
			2643	1668	469	498	8		
1	D	333	Total	C	N	O	S	0	0
			2643	1668	469	498	8		
1	E	333	Total	C	N	O	S	0	0
			2643	1668	469	498	8		
1	F	313	Total	C	N	O	S	0	0
			2487	1571	442	466	8		
1	G	313	Total	C	N	O	S	0	0
			2487	1571	442	466	8		
1	H	313	Total	C	N	O	S	0	0
			2487	1571	442	466	8		
1	I	313	Total	C	N	O	S	0	0
			2487	1571	442	466	8		
1	J	313	Total	C	N	O	S	0	0
			2487	1571	442	466	8		
1	K	333	Total	C	N	O	S	0	0
			2643	1668	469	498	8		
1	L	333	Total	C	N	O	S	0	0
			2643	1668	469	498	8		
1	M	333	Total	C	N	O	S	0	0
			2643	1668	469	498	8		
1	N	333	Total	C	N	O	S	0	0
			2643	1668	469	498	8		
1	O	333	Total	C	N	O	S	0	0
			2643	1668	469	498	8		

- Molecule 2 is a protein called Tail tubular protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	183	Total	C	N	O	S	0	0
			1488	941	273	270	4		
2	Q	184	Total	C	N	O	S	0	0
			1496	945	274	273	4		
2	R	184	Total	C	N	O	S	0	0
			1496	945	274	273	4		
2	S	184	Total	C	N	O	S	0	0
			1496	945	274	273	4		
2	T	182	Total	C	N	O	S	0	0
			1477	935	269	269	4		
2	U	182	Total	C	N	O	S	0	0
			1477	935	269	269	4		
2	V	183	Total	C	N	O	S	0	0
			1488	941	273	270	4		
2	W	183	Total	C	N	O	S	0	0
			1488	941	273	270	4		
2	X	184	Total	C	N	O	S	0	0
			1496	945	274	273	4		
2	k	184	Total	C	N	O	S	0	0
			1496	945	274	273	4		
2	l	184	Total	C	N	O	S	0	0
			1496	945	274	273	4		
2	m	183	Total	C	N	O	S	0	0
			1488	941	273	270	4		

- Molecule 3 is a protein called Head-tail connector protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Y	444	Total	C	N	O	S	0	0
			3443	2172	597	660	14		
3	Z	444	Total	C	N	O	S	0	0
			3443	2172	597	660	14		
3	a	444	Total	C	N	O	S	0	0
			3443	2172	597	660	14		
3	b	444	Total	C	N	O	S	0	0
			3443	2172	597	660	14		
3	c	444	Total	C	N	O	S	0	0
			3443	2172	597	660	14		
3	d	445	Total	C	N	O	S	0	0
			3447	2174	598	661	14		
3	e	444	Total	C	N	O	S	0	0
			3443	2172	597	660	14		
3	f	444	Total	C	N	O	S	0	0
			3443	2172	597	660	14		

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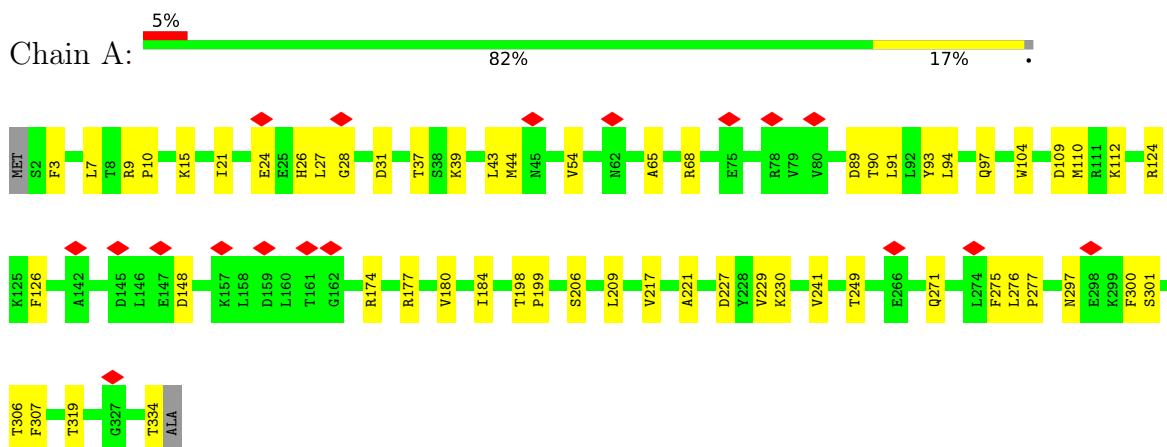
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	g	443	Total	C	N	O	S	0	0
			3436	2168	596	658	14		
3	h	444	Total	C	N	O	S	0	0
			3443	2172	597	660	14		
3	i	444	Total	C	N	O	S	0	0
			3440	2170	597	659	14		
3	j	445	Total	C	N	O	S	0	0
			3447	2174	598	661	14		

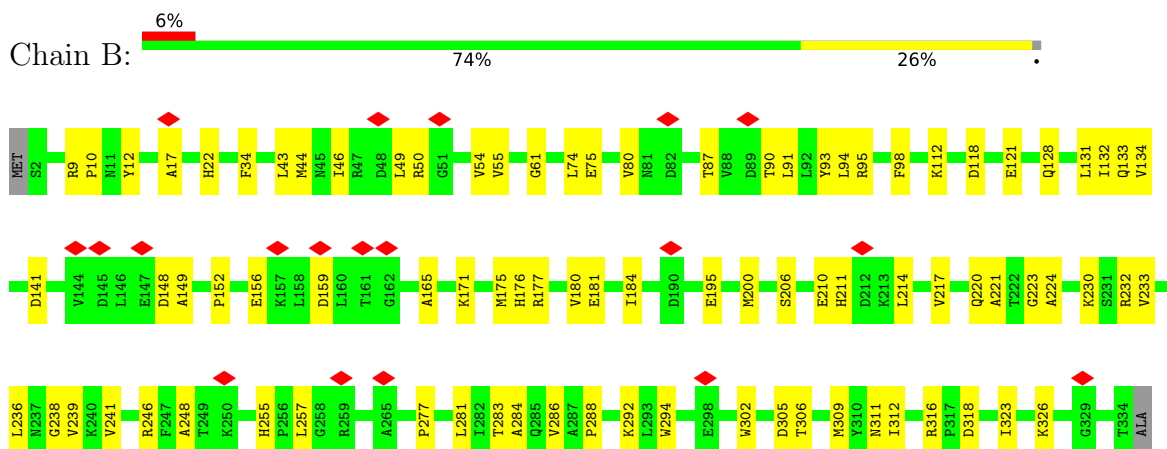
3 Residue-property plots

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

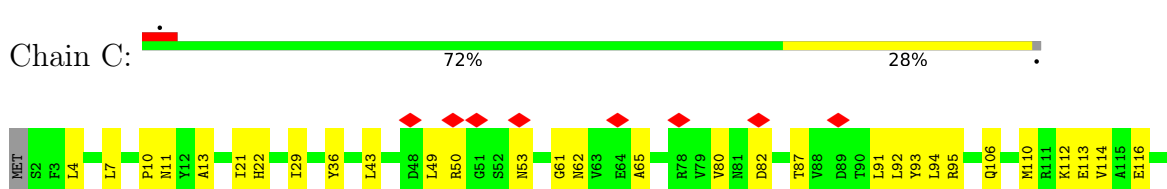
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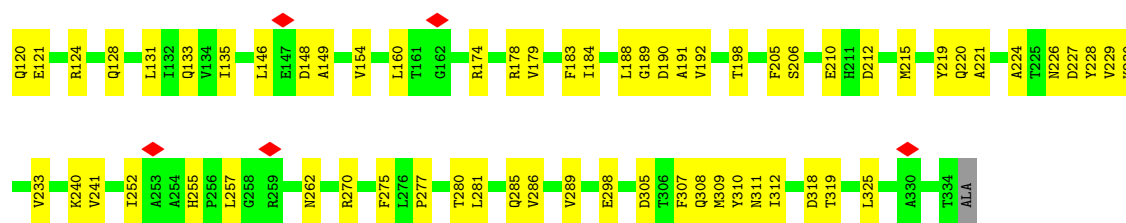


- Molecule 1: Major capsid protein

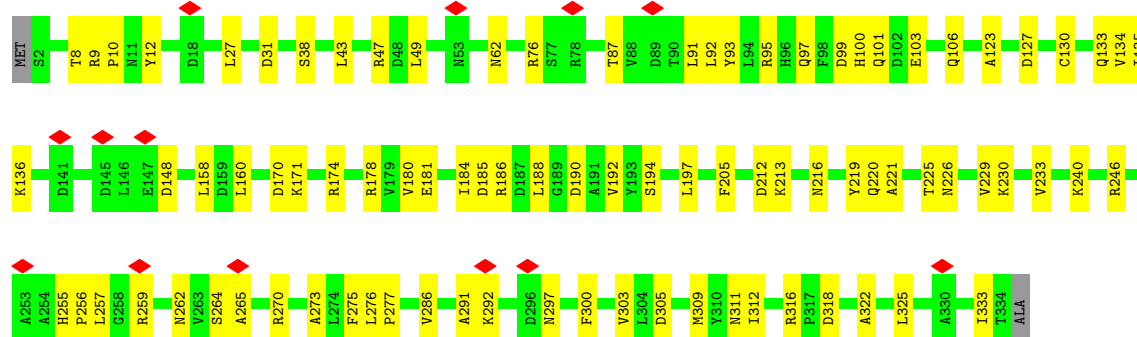


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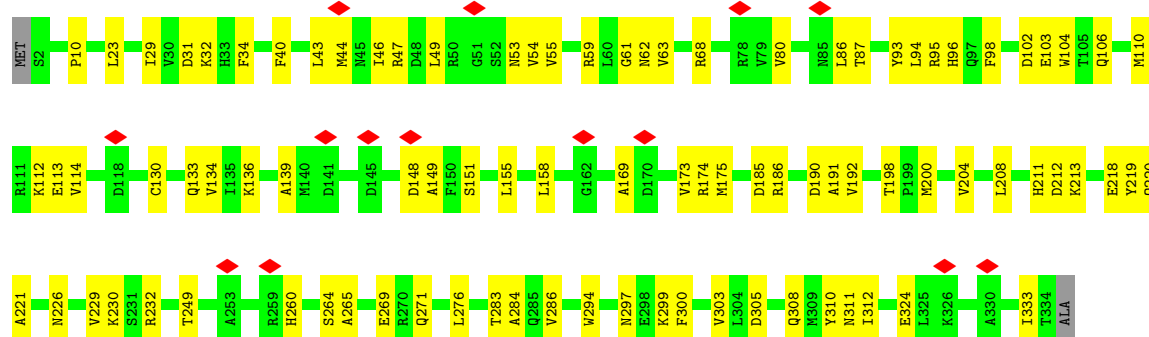




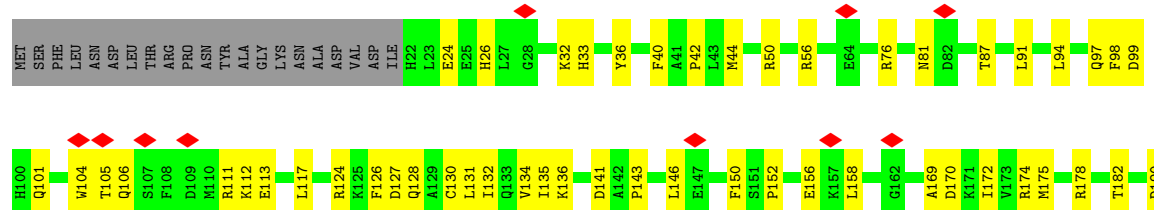
• Molecule 1: Major capsid protein

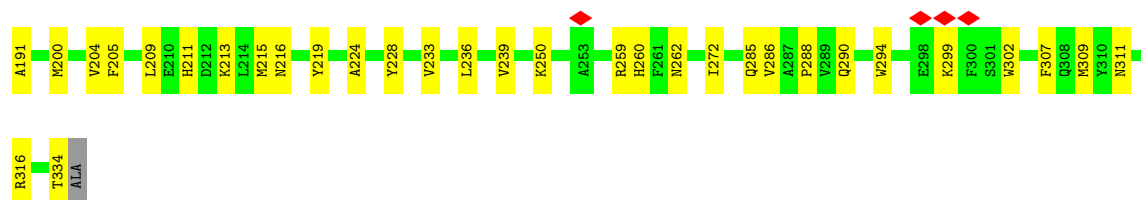


• Molecule 1: Major capsid protein



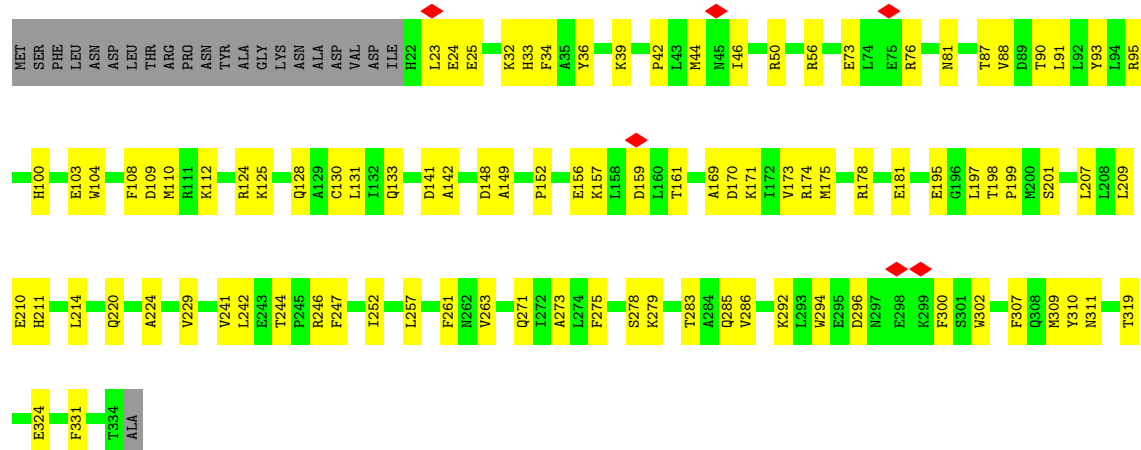
• Molecule 1: Major capsid protein





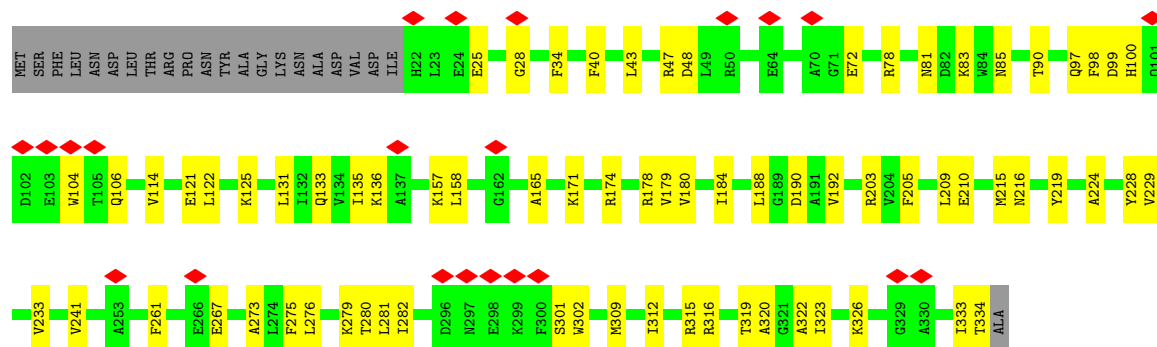
• Molecule 1: Major capsid protein

Chain G: 65% 28% 7%



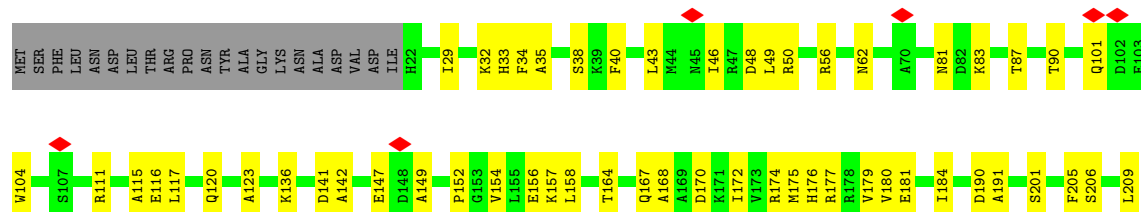
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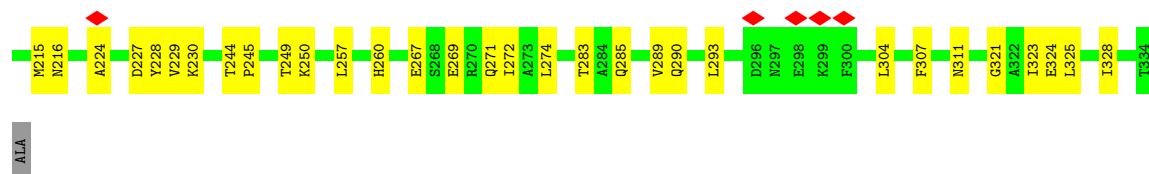
Chain H: 7% 72% 22% 7%



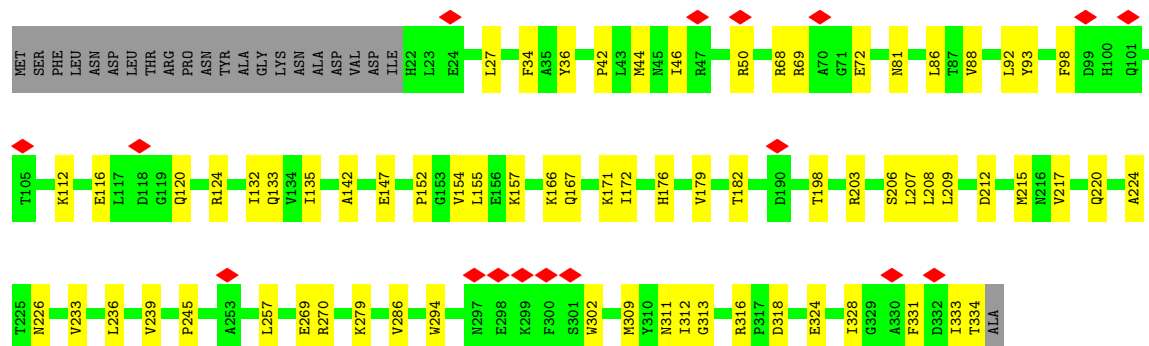
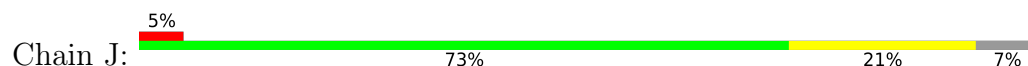
• Molecule 1: Major capsid protein

Chain I: 68% 26% 7%

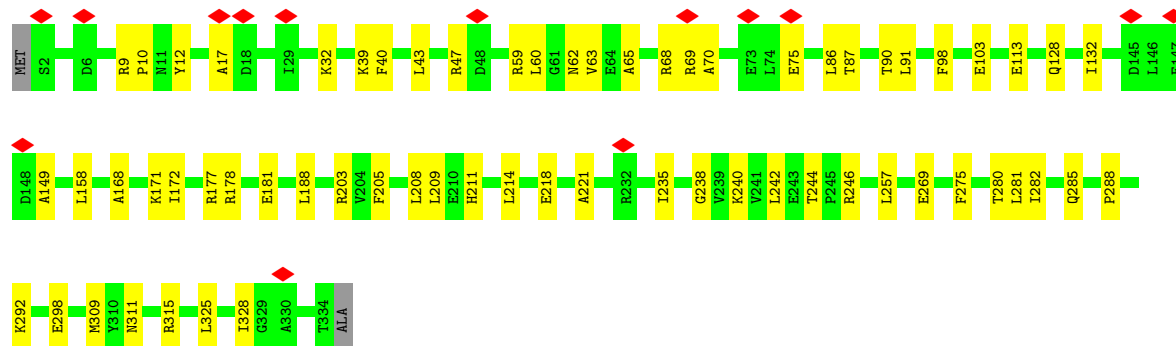
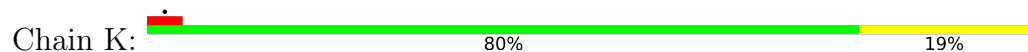




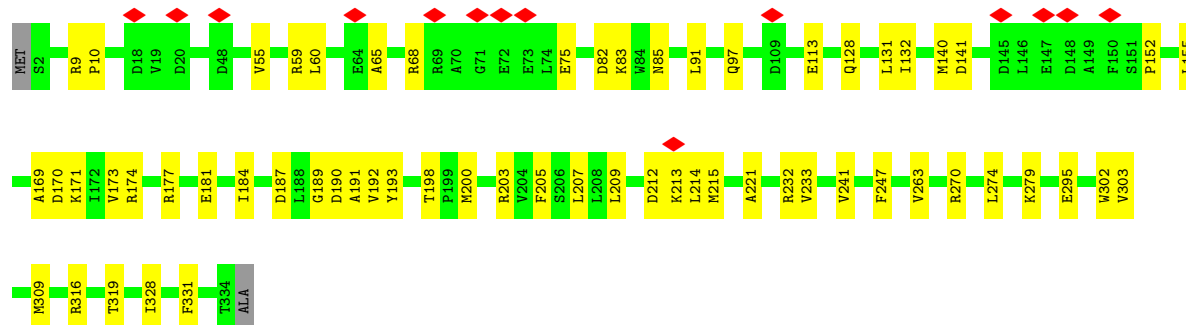
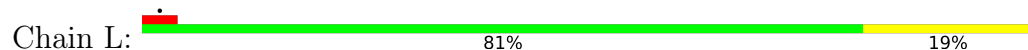
- Molecule 1: Major capsid protein



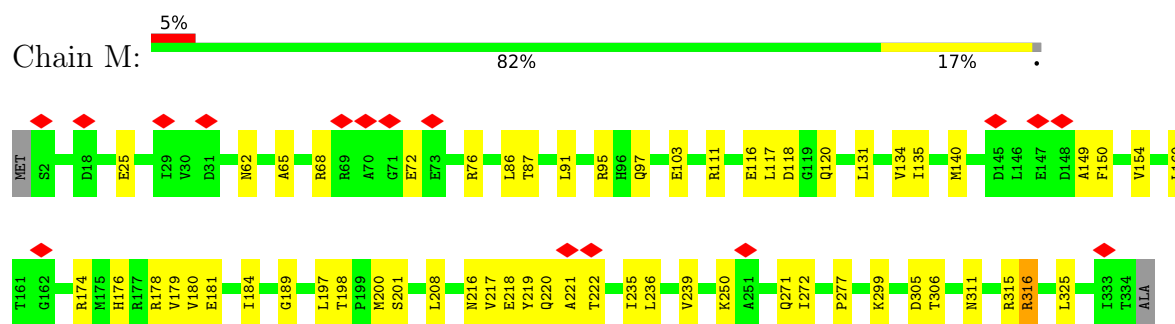
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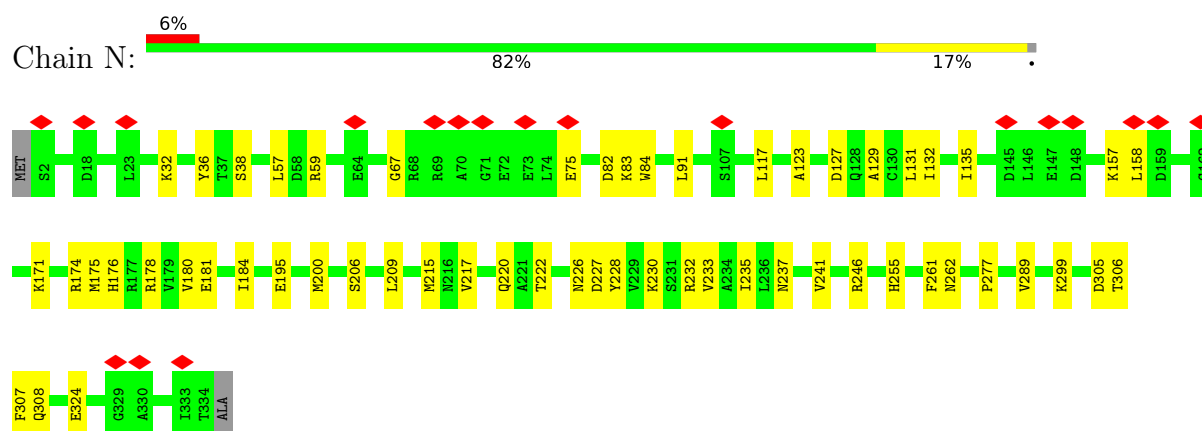
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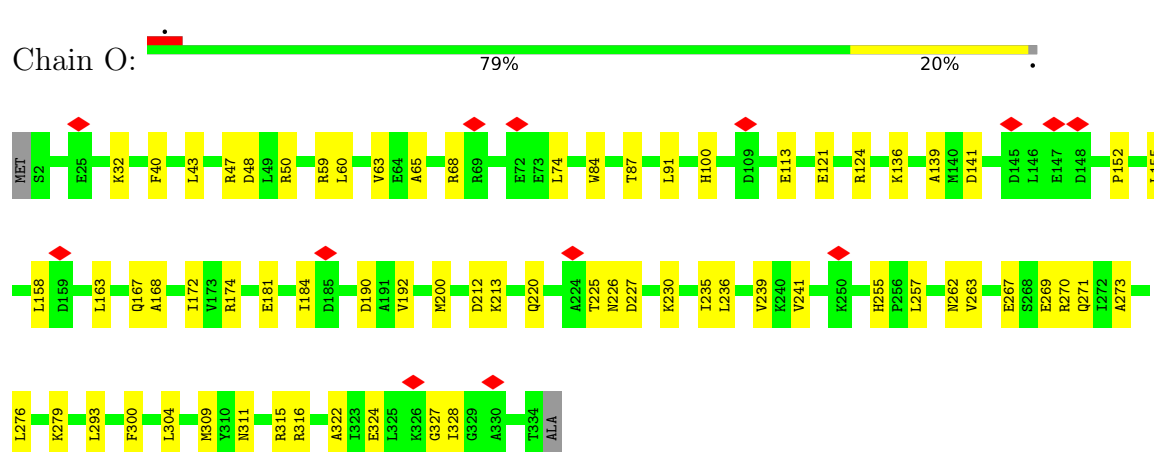
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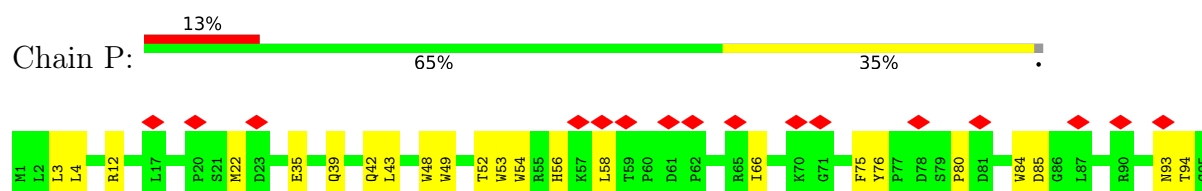
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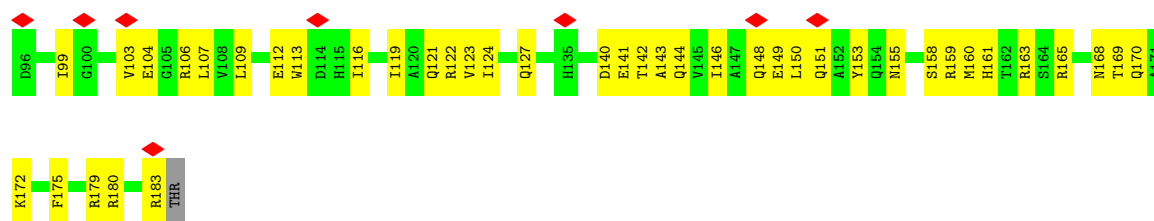


- Molecule 1: Major capsid protein

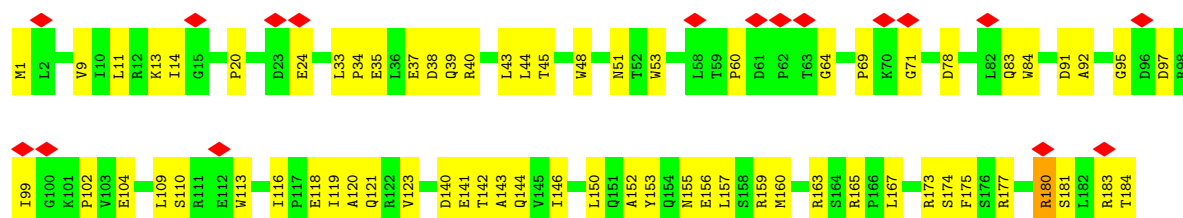


- Molecule 2: Tail tubular protein A

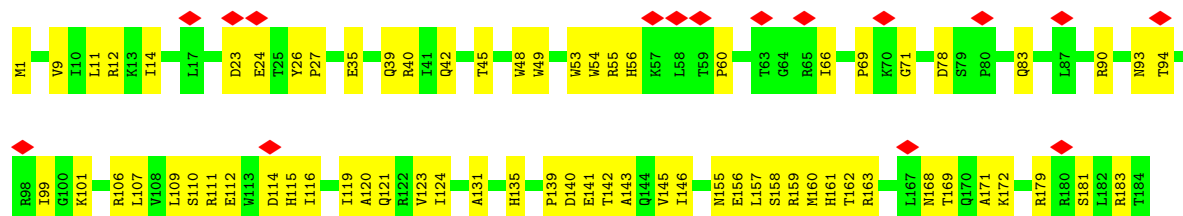




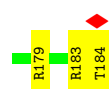
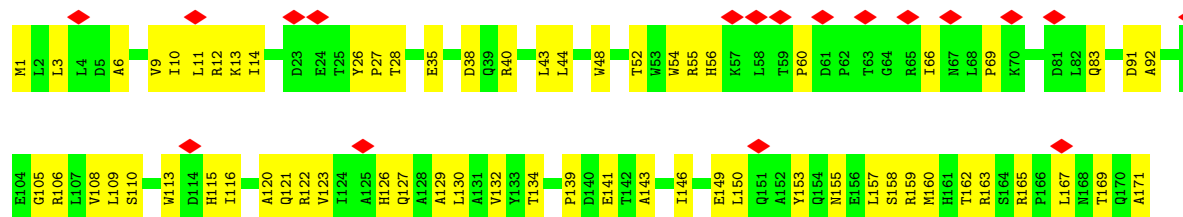
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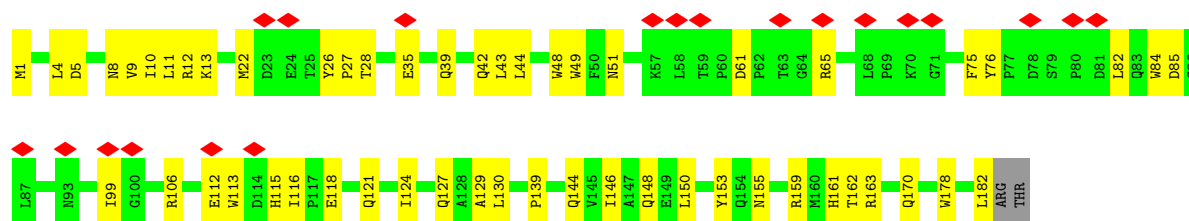


• Molecule 2: Tail tubular protein A

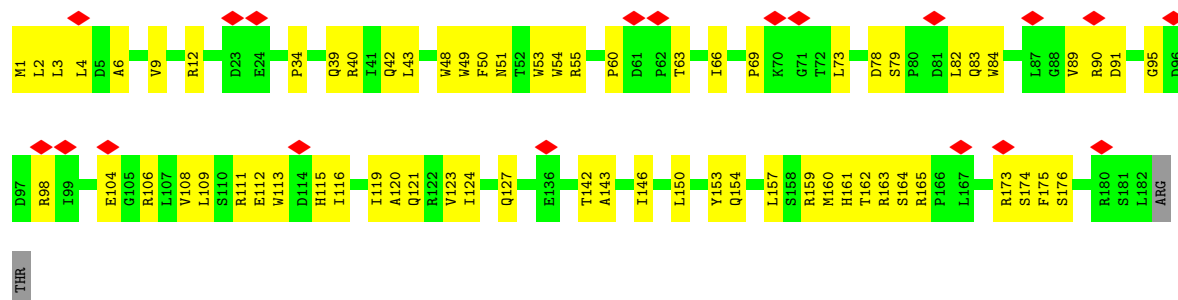


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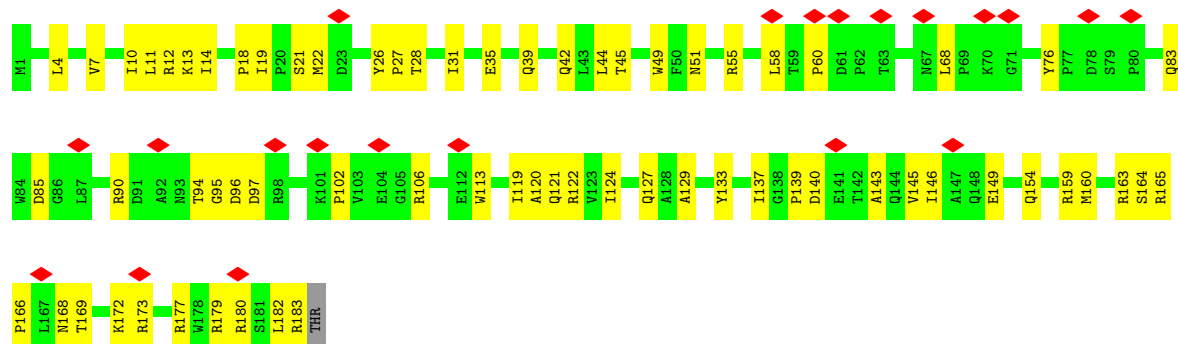




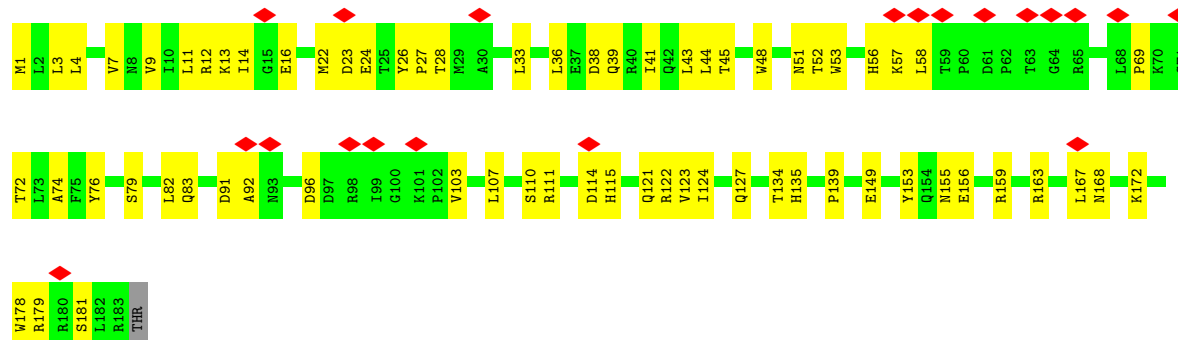
• Molecule 2: Tail tubular protein A



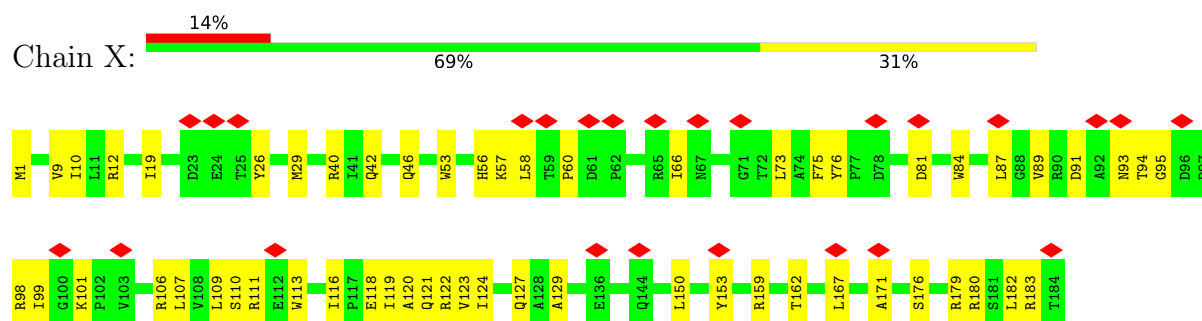
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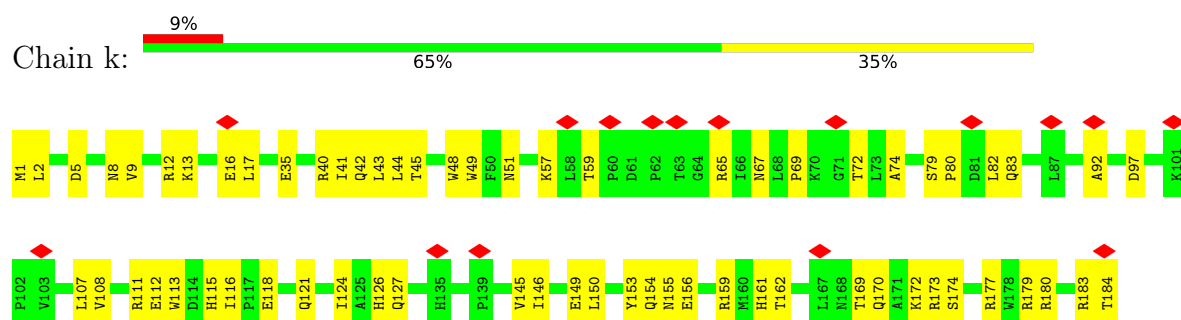
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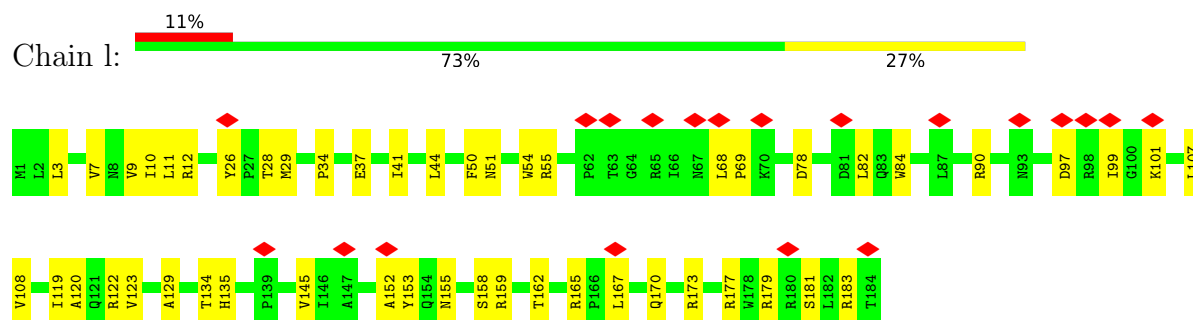
- Molecule 2: Tail tubular protein A



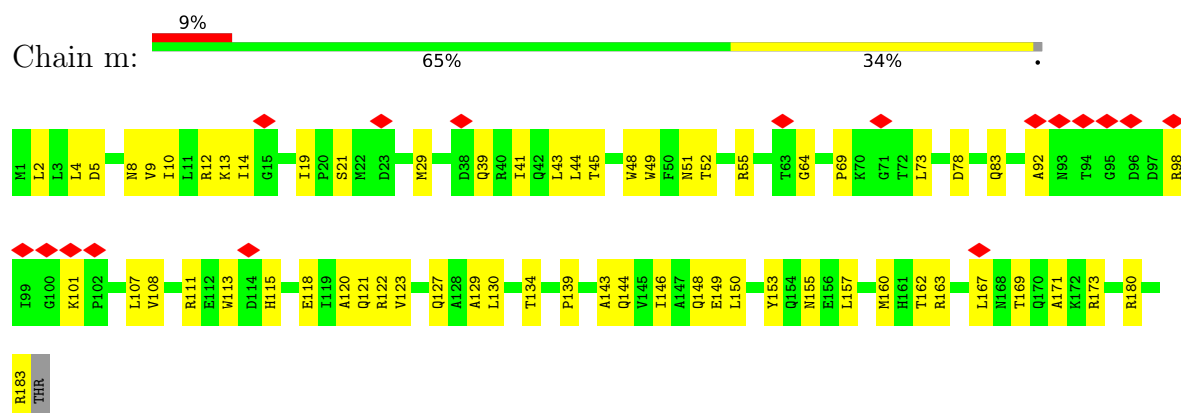
- Molecule 2: Tail tubular protein A



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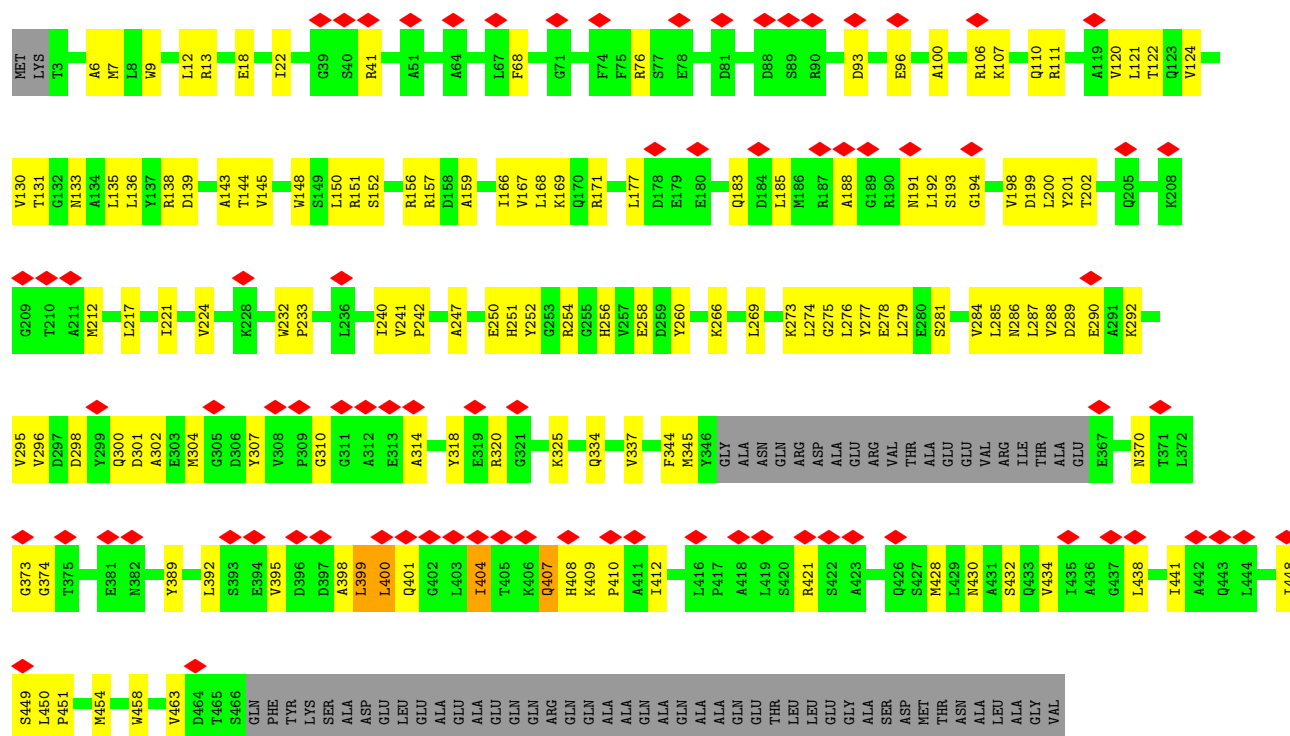


- Molecule 2: Tail tubular protein A

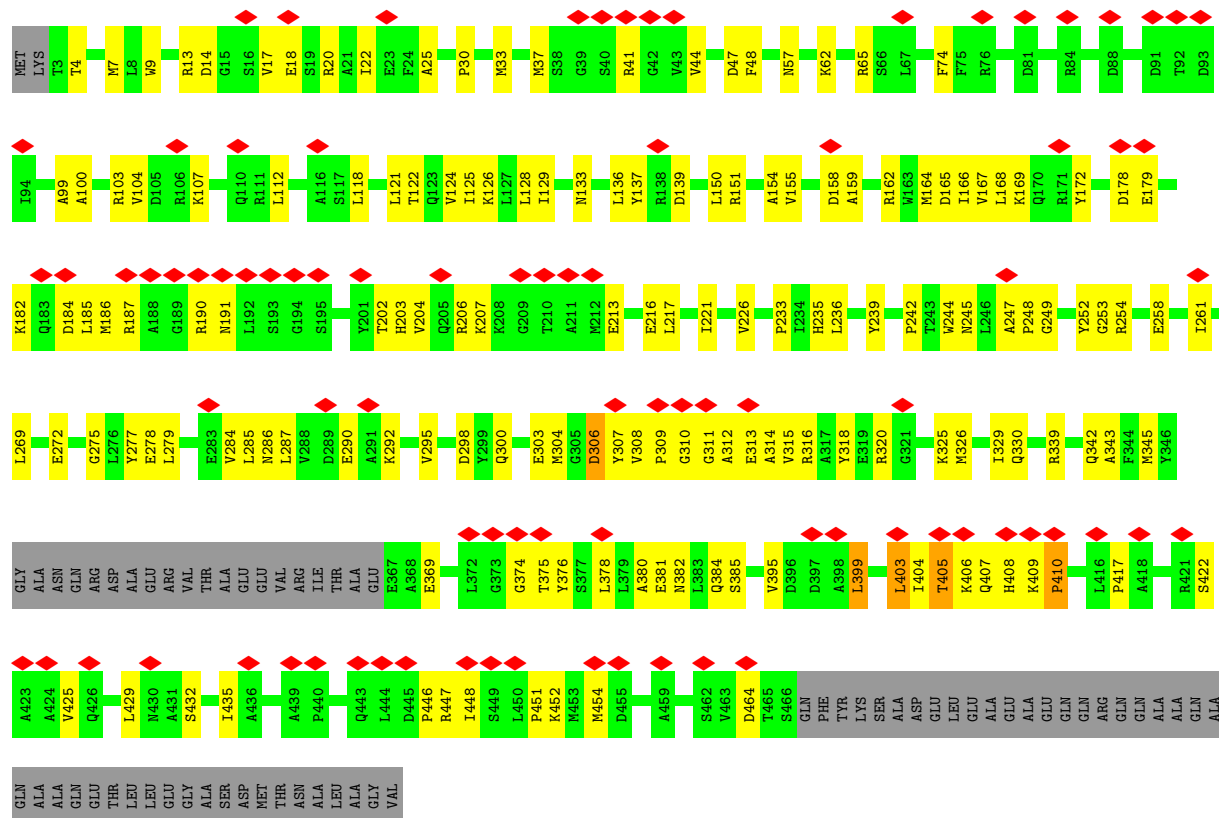


- Molecule 3: Head-tail connector protein

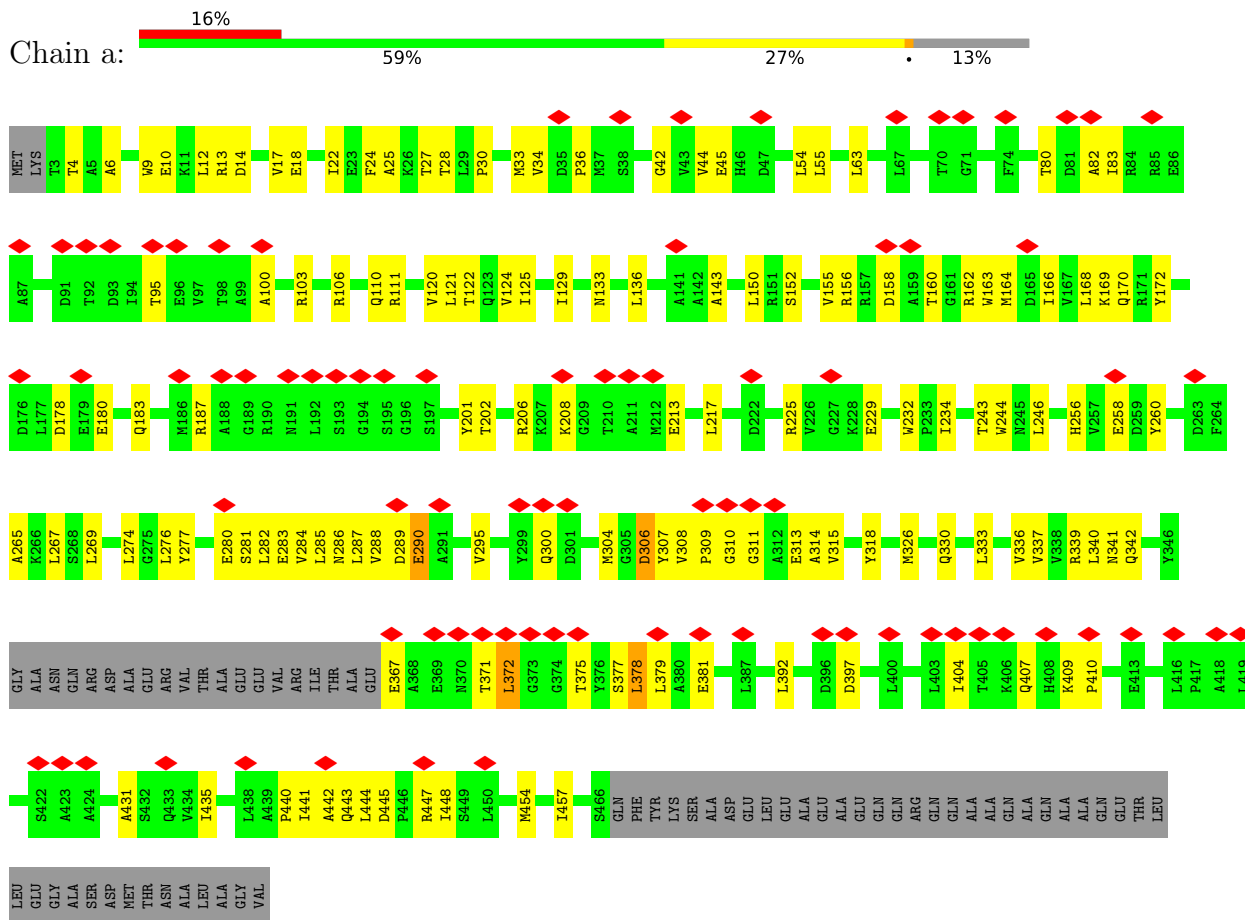




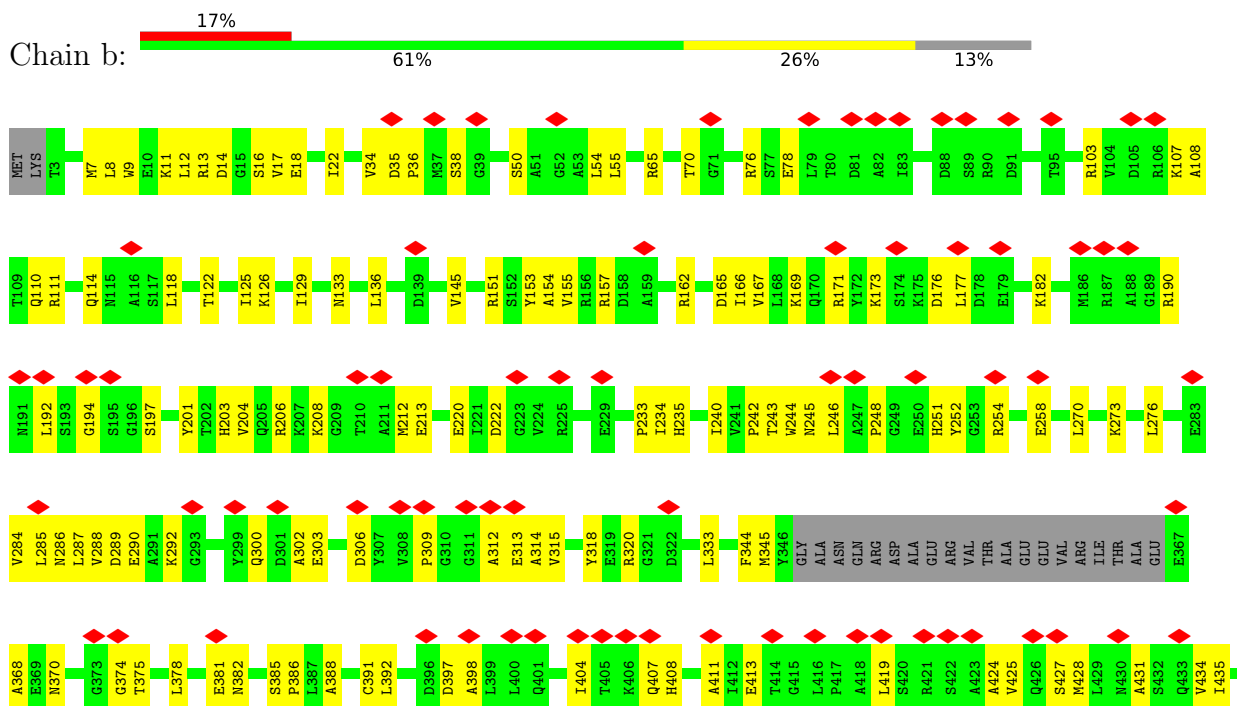
• Molecule 3: Head-tail connector protein

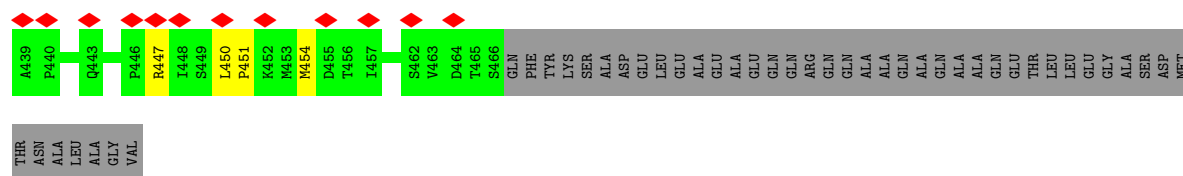


Chain a:

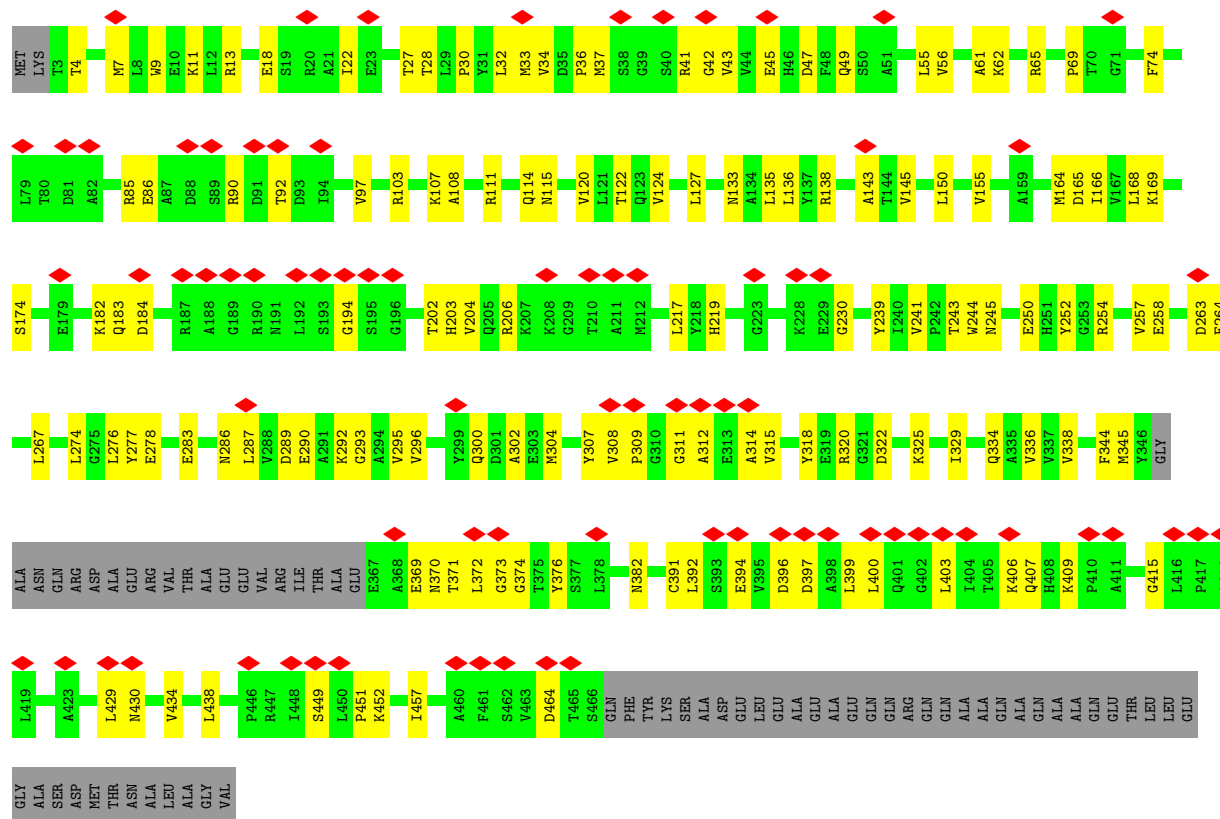


Chain b:

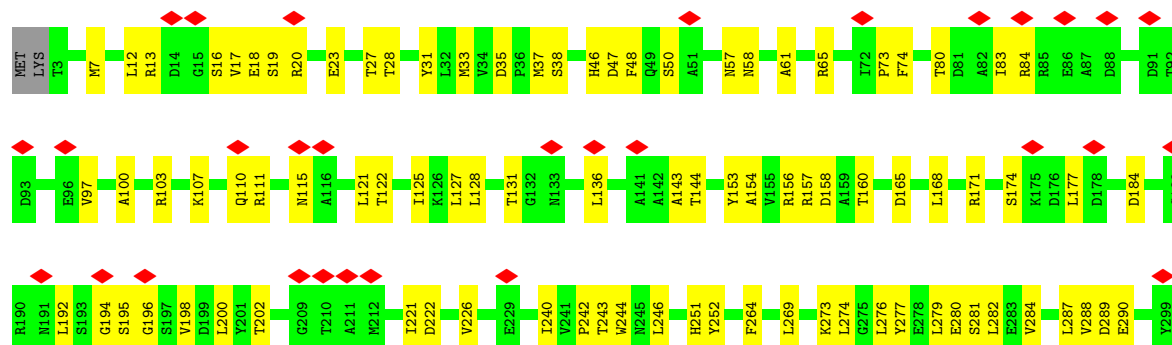


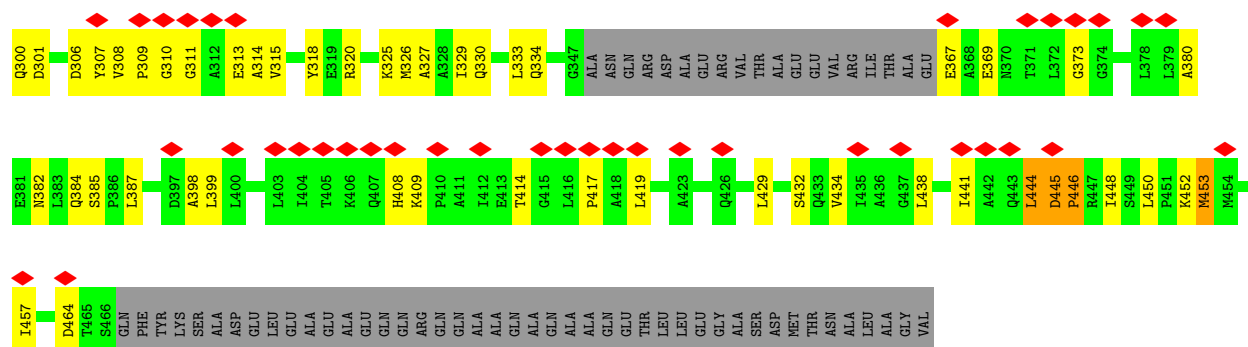


• Molecule 3: Head-tail connector protein

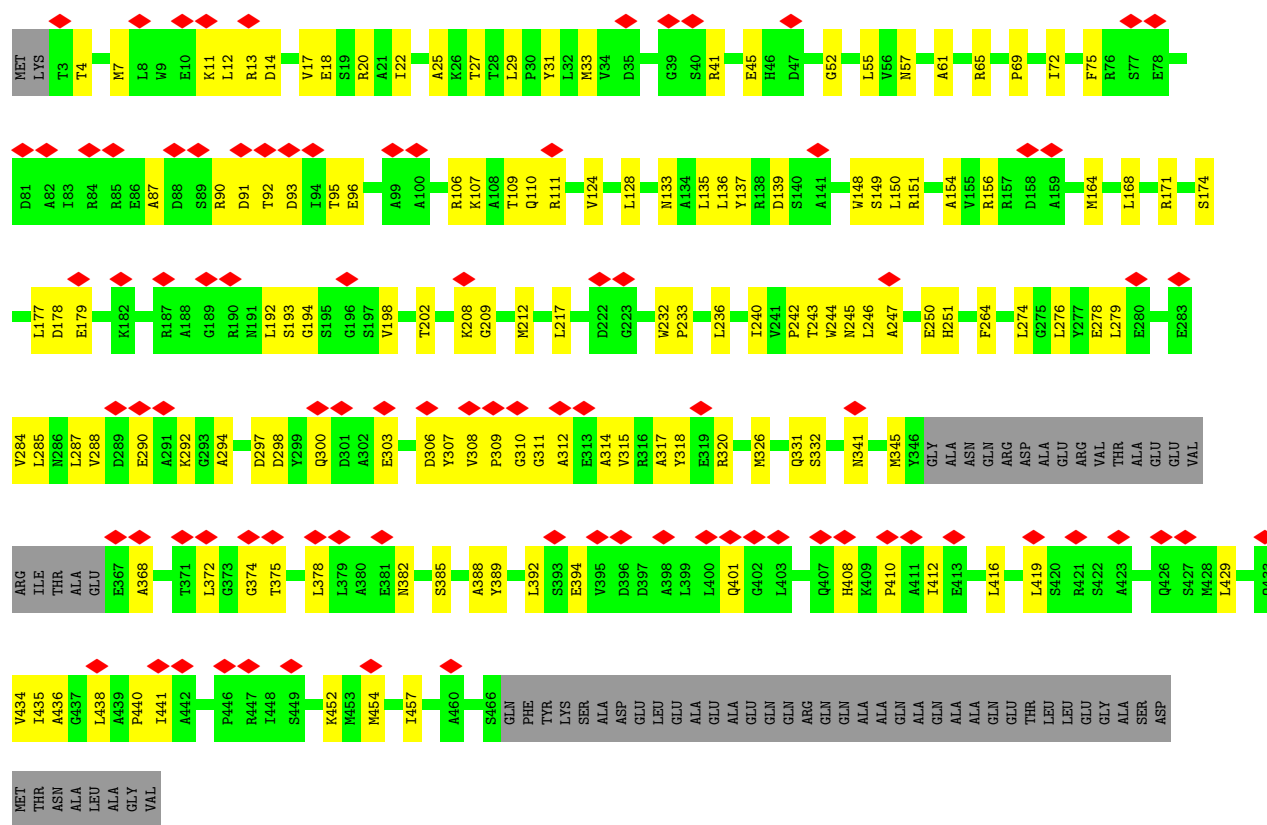


• Molecule 3: Head-tail connector protein

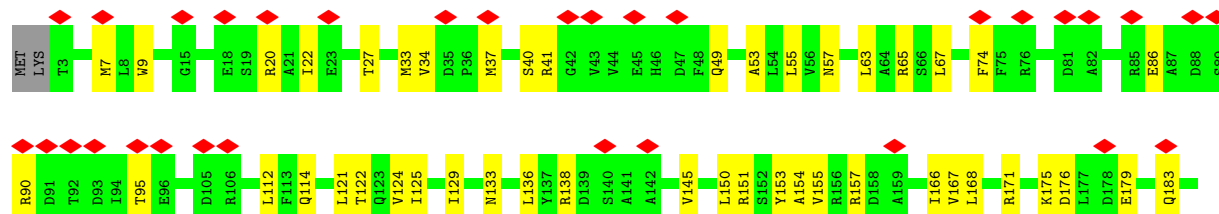




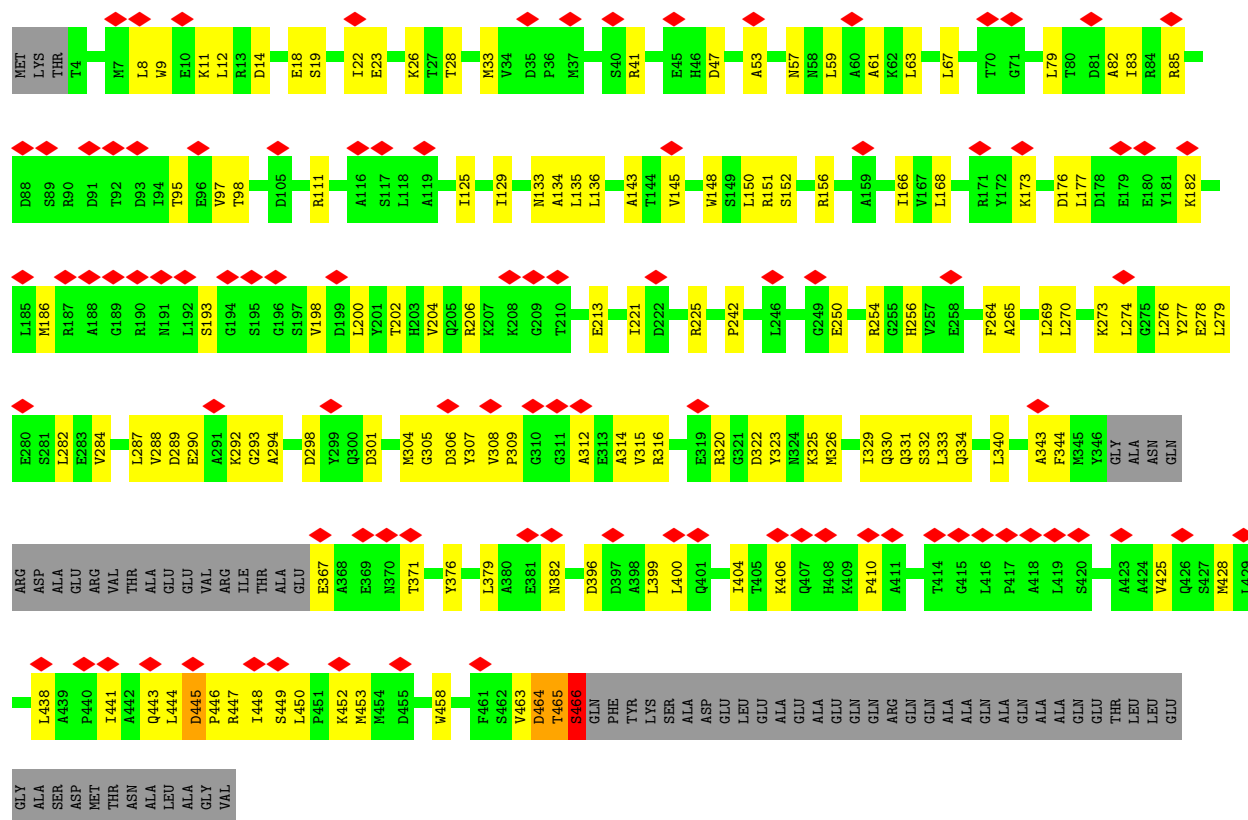
• Molecule 3: Head-tail connector protein



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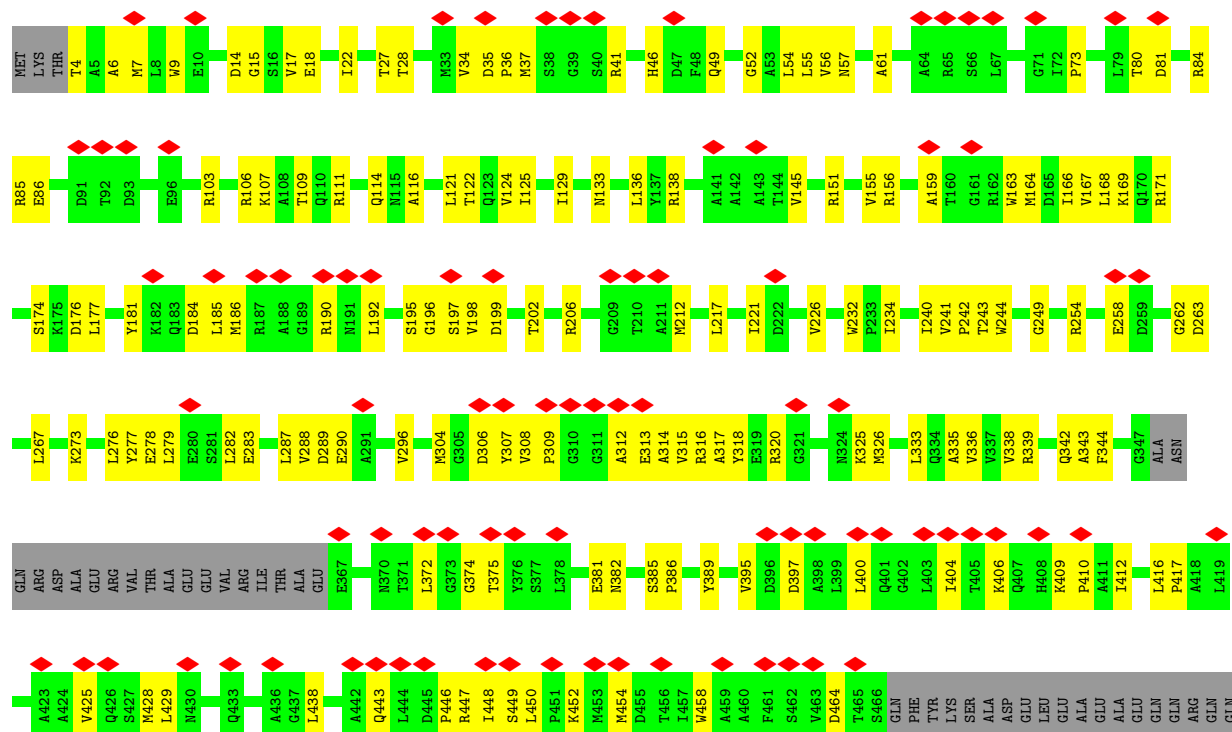


- Molecule 3: Head-tail connector protein



- Molecule 3: Head-tail connector protein

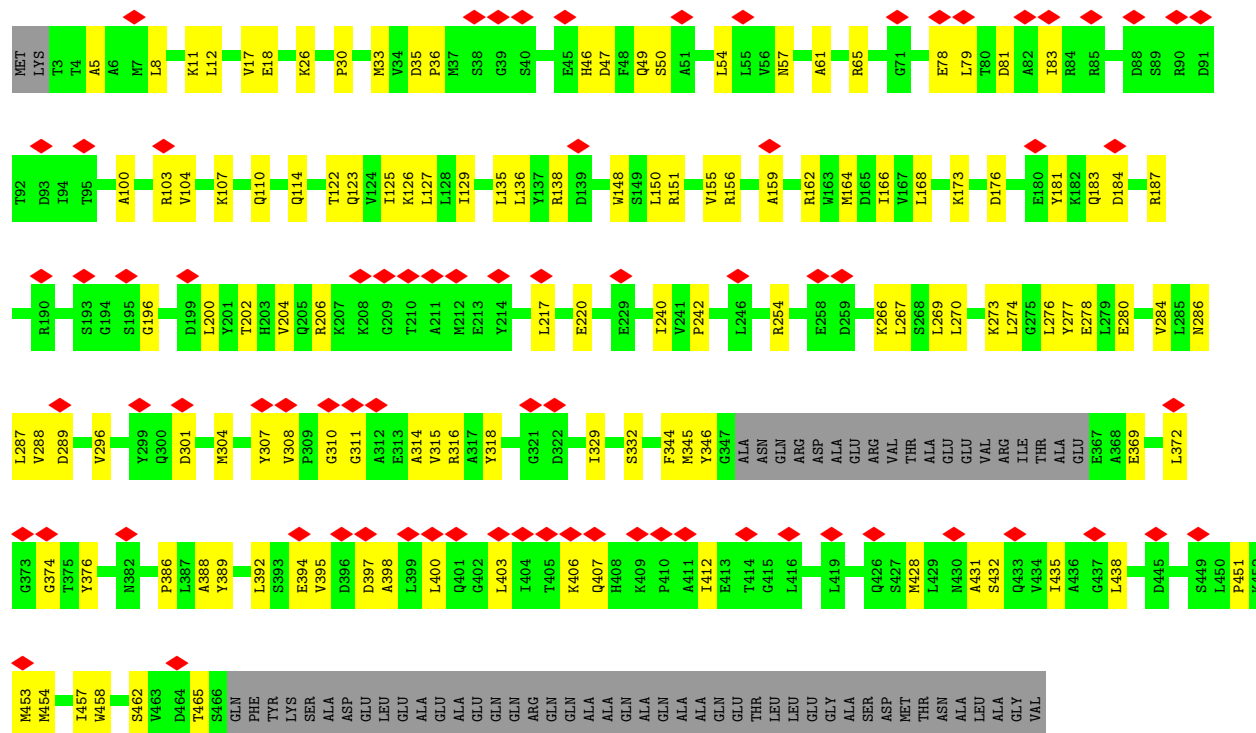




ALA
ALA
GLN
ALA
GLN
ALA
ALA
GLN
GLU
THR
LEU
LEU
GLY
ALA
SER
ASP
MET
THR
ASN
ALA
LEU
ALA
GLY
VAL

• Molecule 3: Head-tail connector protein

Chain j:  15% 63% 24% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21683	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 ($e^-/\text{\AA}^2$)	94	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.124	Depositor
Minimum map value	-0.088	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0195	Depositor
Map size ($\text{\AA}$)	445.12003, 445.12003, 445.12003	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.16	0/2692	0.31	0/3643
1	B	0.12	0/2692	0.29	0/3643
1	C	0.12	0/2692	0.29	0/3643
1	D	0.12	0/2692	0.30	0/3643
1	E	0.12	0/2692	0.32	0/3643
1	F	0.17	0/2533	0.33	0/3426
1	G	0.13	0/2533	0.33	0/3426
1	H	0.11	0/2533	0.28	0/3426
1	I	0.12	0/2533	0.31	0/3426
1	J	0.12	0/2533	0.30	0/3426
1	K	0.11	0/2692	0.29	0/3643
1	L	0.11	0/2692	0.27	0/3643
1	M	0.12	0/2692	0.31	1/3643 (0.0%)
1	N	0.12	0/2692	0.30	0/3643
1	O	0.16	0/2692	0.34	0/3643
2	P	0.20	0/1526	0.38	0/2079
2	Q	0.18	0/1534	0.43	2/2089 (0.1%)
2	R	0.14	0/1534	0.35	0/2089
2	S	0.16	0/1534	0.37	0/2089
2	T	0.19	0/1515	0.38	1/2065 (0.0%)
2	U	0.11	0/1515	0.30	0/2065
2	V	0.12	0/1526	0.33	0/2079
2	W	0.14	0/1526	0.33	0/2079
2	X	0.13	0/1534	0.33	0/2089
2	k	0.13	0/1534	0.34	0/2089
2	l	0.12	0/1534	0.32	0/2089
2	m	0.14	0/1526	0.40	0/2079
3	Y	0.33	2/3503 (0.1%)	0.51	9/4750 (0.2%)
3	Z	0.34	1/3503 (0.0%)	0.50	3/4750 (0.1%)
3	a	0.25	0/3503	0.46	1/4750 (0.0%)
3	b	0.13	0/3503	0.35	0/4750
3	c	0.16	0/3503	0.33	0/4750
3	d	0.36	1/3507 (0.0%)	0.50	6/4755 (0.1%)
3	e	0.13	0/3503	0.32	0/4750

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	f	0.15	0/3503	0.38	0/4750
3	g	0.36	1/3496 (0.0%)	0.59	5/4740 (0.1%)
3	h	0.13	0/3503	0.33	0/4750
3	i	0.14	0/3500	0.37	0/4745
3	j	0.12	0/3507	0.34	0/4755
All	All	0.19	5/99957 (0.0%)	0.37	28/135535 (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
3	a	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	d	446	PRO	N-CD	15.49	1.69	1.47
3	Z	410	PRO	N-CD	-12.38	1.30	1.47
3	g	446	PRO	N-CD	11.62	1.64	1.47
3	Y	410	PRO	N-CD	-9.29	1.34	1.47
3	Y	399	LEU	CA-C	9.13	1.64	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	g	464	ASP	N-CA-C	12.92	126.21	110.19
3	g	445	ASP	N-CA-C	10.68	122.71	109.57
3	d	446	PRO	CA-N-CD	-9.91	98.12	112.00
3	Y	407	GLN	N-CA-CB	9.48	123.82	110.17
3	d	446	PRO	N-CA-CB	8.34	112.01	103.25
2	Q	181	SER	N-CA-C	-7.95	102.61	113.18
3	d	445	ASP	N-CA-C	7.82	127.09	109.81
3	a	372	LEU	N-CA-CB	-7.79	98.40	111.17
3	d	453	MET	N-CA-C	-7.42	102.35	111.40
3	d	444	LEU	N-CA-C	7.03	119.60	111.02
3	g	466	SER	N-CA-CB	-7.01	98.58	110.50
3	Y	407	GLN	N-CA-C	-6.77	100.95	110.50
3	g	446	PRO	CA-N-CD	-6.74	102.56	112.00
3	Y	400	LEU	N-CA-C	-6.46	104.32	111.36
1	M	316	ARG	N-CA-CB	-5.80	100.83	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	448	ILE	N-CA-C	-5.78	108.22	113.71
3	Z	410	PRO	CA-N-CD	5.62	119.87	112.00
3	Y	399	LEU	CA-C-O	5.41	127.87	121.17
3	Y	398	ALA	N-CA-C	5.36	119.80	113.16
3	d	398	ALA	N-CA-C	-5.27	106.71	112.72
2	T	178	TRP	N-CA-C	-5.27	105.62	111.36
3	Y	399	LEU	CB-CA-C	-5.25	102.30	111.23
2	Q	180	ARG	CB-CA-C	5.16	120.70	110.65
3	Y	404	ILE	N-CA-C	5.11	116.64	108.87
3	Z	405	THR	N-CA-C	-5.11	105.79	111.36
3	g	446	PRO	N-CA-CB	5.04	110.08	103.42
3	Z	306	ASP	CA-CB-CG	5.03	117.63	112.60
3	Y	410	PRO	CA-N-CD	5.02	119.03	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	a	306	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2643	0	2632	50	0
1	B	2643	0	2632	71	0
1	C	2643	0	2632	77	0
1	D	2643	0	2632	72	0
1	E	2643	0	2632	77	0
1	F	2487	0	2484	66	0
1	G	2487	0	2484	82	0
1	H	2487	0	2484	61	0
1	I	2487	0	2484	68	0
1	J	2487	0	2484	52	0
1	K	2643	0	2632	47	0
1	L	2643	0	2632	45	0
1	M	2643	0	2632	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	2643	0	2632	39	0
1	O	2643	0	2632	50	0
2	P	1488	0	1480	49	0
2	Q	1496	0	1487	60	0
2	R	1496	0	1487	61	0
2	S	1496	0	1487	65	0
2	T	1477	0	1467	45	0
2	U	1477	0	1467	57	0
2	V	1488	0	1480	70	0
2	W	1488	0	1480	58	0
2	X	1496	0	1487	58	0
2	k	1496	0	1487	64	0
2	l	1496	0	1487	42	0
2	m	1488	0	1480	50	0
3	Y	3443	0	3443	141	0
3	Z	3443	0	3443	152	0
3	a	3443	0	3443	126	0
3	b	3443	0	3443	107	0
3	c	3443	0	3443	119	0
3	d	3447	0	3446	126	0
3	e	3443	0	3443	126	0
3	f	3443	0	3443	115	0
3	g	3436	0	3436	119	0
3	h	3443	0	3443	113	0
3	i	3440	0	3439	134	0
3	j	3447	0	3446	107	0
All	All	98061	0	97827	2525	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 13.

All (2525) 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)
3:g:444:LEU:CD2	3:g:445:ASP:OD1	1.75	1.33
3:d:446:PRO:CD	3:d:446:PRO:N	1.69	1.31
3:Y:399:LEU:O	3:Y:399:LEU:HD12	1.42	1.18
3:g:444:LEU:HD23	3:g:445:ASP:OD1	1.41	1.15
3:g:464:ASP:OD1	3:g:465:THR:N	1.81	1.12
3:g:444:LEU:HD21	3:g:445:ASP:OD1	1.50	1.11
3:d:448:ILE:HG21	3:d:452:LYS:HE3	1.37	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:400:LEU:HD11	3:Y:401:GLN:NE2	1.73	1.04
3:Y:400:LEU:CD1	3:Y:401:GLN:CD	2.43	0.92
3:a:308:VAL:HG12	3:a:310:GLY:H	1.36	0.90
3:Y:100:ALA:CB	3:Y:399:LEU:HD23	2.01	0.90
3:Y:392:LEU:HD22	3:Y:409:LYS:HE2	1.51	0.90
3:Z:307:TYR:HB3	3:Z:312:ALA:HB2	1.50	0.90
3:Y:399:LEU:O	3:Y:399:LEU:CD1	2.20	0.90
3:g:444:LEU:HD23	3:g:445:ASP:N	1.87	0.89
3:Y:400:LEU:HD11	3:Y:401:GLN:CD	1.96	0.89
3:f:311:GLY:HA2	3:f:315:VAL:H	1.40	0.85
3:i:37:MET:HE1	3:i:169:LYS:HG3	1.60	0.84
1:B:49:LEU:HD11	1:B:286:VAL:HG22	1.60	0.83
3:f:53:ALA:O	3:f:57:ASN:ND2	2.10	0.83
3:f:286:ASN:HD21	3:g:304:MET:HA	1.43	0.83
3:Y:100:ALA:HB1	3:Y:399:LEU:HD23	1.58	0.83
3:Y:399:LEU:HD12	3:Y:399:LEU:C	2.03	0.83
3:Z:447:ARG:HG3	3:Z:448:ILE:N	1.93	0.83
2:k:43:LEU:HG	2:k:48:TRP:HE1	1.44	0.82
3:d:307:TYR:HD2	2:l:159:ARG:HE	1.25	0.81
2:Q:173:ARG:HH22	2:Q:177:ARG:HH22	1.28	0.81
3:h:318:TYR:HE1	3:h:320:ARG:HB2	1.46	0.80
2:U:123:VAL:HG12	2:U:153:TYR:HB3	1.63	0.80
1:E:158:LEU:HB2	1:E:175:MET:HE1	1.63	0.80
3:e:288:VAL:HG12	3:e:315:VAL:HG22	1.62	0.80
3:d:300:GLN:NE2	3:d:306:ASP:OD1	2.14	0.80
1:J:220:GLN:HE22	1:J:226:ASN:HB2	1.48	0.79
3:Z:447:ARG:HG3	3:Z:448:ILE:H	1.43	0.79
1:K:47:ARG:HE	1:K:282:ILE:HD11	1.46	0.79
3:h:183:GLN:HA	3:h:186:MET:HE1	1.62	0.79
3:e:33:MET:HB3	3:e:151:ARG:HD2	1.64	0.78
3:a:289:ASP:H	3:a:314:ALA:HB1	1.47	0.78
3:g:458:TRP:HE3	3:g:463:VAL:HG13	1.48	0.78
3:Y:400:LEU:HD12	3:Y:401:GLN:N	1.97	0.78
3:Y:290:GLU:HG3	3:Z:308:VAL:HG11	1.66	0.77
3:b:171:ARG:HD2	3:b:197:SER:HB3	1.65	0.77
3:b:254:ARG:HH12	3:c:41:ARG:HH12	1.32	0.77
3:Y:266:LYS:NZ	3:Z:278:GLU:OE1	2.17	0.77
3:f:287:LEU:HB2	3:f:316:ARG:H	1.51	0.76
2:X:19:ILE:HD13	2:X:29:MET:HE3	1.66	0.76
1:O:163:LEU:HA	1:O:167:GLN:HE21	1.50	0.76
3:j:403:LEU:HD11	3:j:407:GLN:HE21	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:451:PRO:HA	3:f:454:MET:HG2	1.68	0.75
1:M:116:GLU:HG3	1:M:120:GLN:HE22	1.52	0.75
2:Q:123:VAL:HG11	2:Q:157:LEU:HD22	1.69	0.75
2:X:56:HIS:HB3	2:X:107:LEU:HD13	1.66	0.75
3:Y:400:LEU:HD12	3:Y:401:GLN:CD	2.10	0.75
3:a:283:GLU:HG2	3:a:285:LEU:HD13	1.69	0.75
1:E:32:LYS:HD3	1:E:113:GLU:HB3	1.68	0.74
1:A:297:ASN:O	1:G:95:ARG:NH2	2.21	0.74
1:F:112:LYS:NZ	3:i:15:GLY:O	2.19	0.74
1:G:50:ARG:HH12	1:G:286:VAL:HG13	1.52	0.74
3:f:308:VAL:HA	3:f:312:ALA:HB3	1.69	0.74
2:R:163:ARG:HH21	2:S:106:ARG:HH22	1.34	0.74
2:V:180:ARG:HA	2:V:183:ARG:HG2	1.69	0.74
3:d:445:ASP:OD1	3:d:445:ASP:O	2.06	0.74
1:F:136:LYS:NZ	1:F:260:HIS:O	2.21	0.74
3:d:37:MET:HG2	3:d:171:ARG:HB2	1.69	0.74
3:h:76:ARG:HB3	3:h:421:ARG:HH21	1.52	0.74
1:L:113:GLU:OE2	1:L:113:GLU:N	2.21	0.74
2:W:163:ARG:HG3	3:a:307:TYR:HE2	1.52	0.74
3:Y:325:LYS:NZ	3:Z:318:TYR:O	2.19	0.73
3:i:449:SER:OG	3:i:452:LYS:NZ	2.20	0.73
2:S:69:PRO:HG2	2:S:109:LEU:HD21	1.70	0.73
1:B:112:LYS:NZ	3:a:201:TYR:OH	2.22	0.73
2:S:11:LEU:HD21	2:S:28:THR:HG21	1.68	0.73
3:c:111:ARG:HH11	3:c:394:GLU:HB3	1.54	0.73
1:B:224:ALA:HB1	1:K:221:ALA:HB1	1.71	0.73
2:S:122:ARG:HH12	2:T:42:GLN:HG2	1.54	0.73
3:Z:403:LEU:HD21	3:Z:409:LYS:HE2	1.70	0.73
2:P:175:PHE:HA	3:d:279:LEU:HD23	1.70	0.72
1:C:36:TYR:O	1:C:120:GLN:NE2	2.21	0.72
1:B:50:ARG:HB3	2:k:183:ARG:HB2	1.70	0.72
3:g:79:LEU:HA	3:g:83:ILE:HD11	1.72	0.72
2:T:127:GLN:HG2	2:T:150:LEU:HD11	1.71	0.72
2:m:123:VAL:HG21	2:m:157:LEU:HD22	1.72	0.71
3:Z:184:ASP:HA	3:Z:187:ARG:HD2	1.72	0.71
1:C:174:ARG:HE	1:H:334:THR:HA	1.53	0.71
1:M:116:GLU:O	1:M:120:GLN:NE2	2.24	0.71
3:d:310:GLY:HA2	3:d:313:GLU:HB3	1.71	0.71
1:B:49:LEU:HD23	1:B:284:ALA:HB1	1.73	0.71
2:U:40:ARG:HA	2:U:124:ILE:HD13	1.72	0.71
3:i:156:ARG:HH12	3:j:173:LYS:HG3	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:173:ARG:HG3	3:f:301:ASP:HB3	1.72	0.70
1:H:209:LEU:HD13	1:H:215:MET:HE3	1.73	0.70
3:a:156:ARG:NH2	3:b:176:ASP:OD1	2.24	0.70
2:k:113:TRP:O	2:k:121:GLN:NE2	2.24	0.70
1:E:110:MET:HE3	1:O:60:LEU:HD21	1.74	0.70
3:Z:4:THR:H	3:Z:7:MET:HE3	1.56	0.70
3:Y:110:GLN:NE2	3:j:78:GLU:OE2	2.23	0.70
2:R:1:MET:N	2:R:121:GLN:OE1	2.24	0.70
1:D:316:ARG:NH2	1:I:32:LYS:O	2.25	0.70
2:T:144:GLN:O	2:T:148:GLN:NE2	2.23	0.70
3:f:74:PHE:O	3:f:384:GLN:NE2	2.25	0.70
3:d:74:PHE:O	3:d:384:GLN:NE2	2.24	0.70
2:Q:113:TRP:O	2:Q:121:GLN:NE2	2.25	0.70
2:U:113:TRP:O	2:U:121:GLN:NE2	2.22	0.70
3:Z:404:ILE:HG13	3:Z:407:GLN:H	1.56	0.70
3:h:79:LEU:HA	3:h:83:ILE:HD11	1.74	0.69
3:Y:284:VAL:HG21	3:j:276:LEU:HD23	1.73	0.69
1:E:230:LYS:HD3	1:E:232:ARG:HH21	1.56	0.69
3:Y:247:ALA:HB3	3:Y:250:GLU:HG3	1.75	0.69
3:Z:325:LYS:NZ	3:a:318:TYR:O	2.23	0.69
3:e:308:VAL:HA	3:e:312:ALA:HB3	1.74	0.69
1:C:221:ALA:HB1	1:H:224:ALA:HB1	1.74	0.69
1:C:224:ALA:HB1	1:M:221:ALA:HB1	1.73	0.69
1:K:32:LYS:HZ2	1:K:113:GLU:HG3	1.56	0.69
3:b:370:ASN:HD21	3:c:62:LYS:HE3	1.57	0.69
2:l:10:ILE:HG22	2:l:129:ALA:HB2	1.73	0.69
1:O:190:ASP:OD2	3:h:190:ARG:NH2	2.26	0.69
3:d:277:TYR:O	3:d:281:SER:HB2	1.92	0.69
3:e:4:THR:HG22	3:e:7:MET:HE1	1.75	0.69
1:C:36:TYR:H	1:C:120:GLN:HE21	1.41	0.69
1:I:50:ARG:HE	3:d:192:LEU:HA	1.57	0.69
2:W:134:THR:HG23	2:W:139:PRO:HG3	1.74	0.69
3:Y:100:ALA:HB3	3:Y:399:LEU:HD23	1.73	0.69
2:k:172:LYS:HG3	2:k:173:ARG:H	1.58	0.69
3:a:162:ARG:HB2	3:a:206:ARG:HH22	1.56	0.69
3:b:288:VAL:HG22	3:b:315:VAL:HG22	1.72	0.69
3:g:274:LEU:HB2	3:g:329:ILE:HG21	1.74	0.69
3:g:316:ARG:HH12	3:h:308:VAL:HG22	1.58	0.69
3:i:374:GLY:HA3	3:j:122:THR:HG21	1.72	0.69
3:Z:290:GLU:OE2	3:a:308:VAL:HG13	1.92	0.69
3:b:258:GLU:OE2	2:m:183:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:289:ASP:HB2	3:c:314:ALA:HA	1.75	0.69
1:G:207:LEU:HD21	1:G:331:PHE:HE2	1.58	0.69
1:B:17:ALA:H	1:H:78:ARG:HH12	1.41	0.68
1:B:43:LEU:HB2	1:B:277:PRO:HB3	1.73	0.68
1:I:136:LYS:NZ	1:I:260:HIS:O	2.25	0.68
2:U:55:ARG:HH12	2:U:78:ASP:HB2	1.57	0.68
1:B:316:ARG:NH2	1:G:32:LYS:O	2.26	0.68
2:P:119:ILE:HD13	2:Q:45:THR:HG21	1.76	0.68
2:X:167:LEU:HB2	2:k:80:PRO:HD3	1.75	0.68
3:Z:318:TYR:HE1	3:Z:320:ARG:HG2	1.57	0.68
3:c:276:LEU:HD22	3:d:284:VAL:HG21	1.74	0.68
2:k:49:TRP:HE3	2:k:161:HIS:HA	1.58	0.68
3:e:192:LEU:HD12	3:e:194:GLY:H	1.57	0.68
3:h:373:GLY:HA2	3:i:61:ALA:HB2	1.76	0.68
2:V:160:MET:SD	2:W:76:TYR:OH	2.45	0.68
3:i:163:TRP:O	3:i:206:ARG:NH1	2.26	0.68
3:Y:240:ILE:HG22	3:Y:242:PRO:HD3	1.75	0.68
2:T:163:ARG:HH12	2:U:106:ARG:HH12	1.41	0.68
2:k:127:GLN:HG2	2:k:150:LEU:HD21	1.76	0.68
1:L:82:ASP:OD1	1:L:83:LYS:N	2.27	0.68
3:Z:155:VAL:HG23	3:Z:166:ILE:HG22	1.76	0.68
3:d:184:ASP:HB2	3:d:226:VAL:HG23	1.76	0.68
2:S:159:ARG:HB3	2:S:163:ARG:HH21	1.59	0.68
3:Y:254:ARG:HB3	3:Y:258:GLU:HG3	1.76	0.68
3:d:438:LEU:HD22	3:d:453:MET:HE2	1.77	0.67
1:B:133:GLN:HG3	1:B:312:ILE:HG23	1.75	0.67
1:F:91:LEU:HD12	1:F:309:MET:HB2	1.74	0.67
2:S:143:ALA:HA	2:S:146:ILE:HG22	1.76	0.67
1:C:91:LEU:HD11	1:C:307:PHE:HB2	1.77	0.67
1:C:174:ARG:HD2	1:H:333:ILE:HG12	1.76	0.67
2:S:52:THR:HG22	2:S:108:VAL:HG22	1.76	0.67
1:K:62:ASN:OD1	1:K:63:VAL:N	2.27	0.67
3:b:374:GLY:HA3	3:c:122:THR:HG21	1.75	0.67
3:c:217:LEU:HB3	3:c:230:GLY:HA3	1.77	0.67
3:e:133:ASN:HB3	3:e:150:LEU:HD21	1.76	0.67
1:D:219:TYR:HE1	1:I:216:ASN:HD22	1.41	0.67
1:H:106:GLN:O	2:m:180:ARG:NH1	2.27	0.67
2:U:163:ARG:NE	2:U:163:ARG:O	2.27	0.67
2:X:91:ASP:HB2	2:X:95:GLY:H	1.58	0.67
1:C:87:THR:O	1:C:311:ASN:ND2	2.28	0.67
1:J:147:GLU:N	1:J:147:GLU:OE2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:103:GLU:OE1	1:M:111:ARG:NH1	2.28	0.67
3:b:12:LEU:HB2	3:b:154:ALA:HB1	1.77	0.67
2:R:169:THR:HG23	2:R:171:ALA:H	1.60	0.67
2:U:162:THR:HG21	3:j:288:VAL:HG21	1.77	0.67
3:d:240:ILE:HG22	3:d:242:PRO:HD3	1.77	0.67
1:B:90:THR:HG21	1:B:257:LEU:HA	1.77	0.66
1:M:200:MET:HE1	1:M:208:LEU:HD12	1.77	0.66
3:g:447:ARG:HH21	3:h:465:THR:HB	1.59	0.66
3:Z:285:LEU:HD11	3:a:300:GLN:HB3	1.77	0.66
3:e:274:LEU:O	3:e:278:GLU:HG2	1.94	0.66
1:L:205:PHE:HE1	1:L:233:VAL:HG22	1.59	0.66
2:W:16:GLU:OE2	2:W:26:TYR:OH	2.12	0.66
2:X:118:GLU:OE2	2:X:118:GLU:N	2.24	0.66
3:h:290:GLU:HG3	3:i:309:PRO:HG3	1.78	0.66
3:c:41:ARG:NH1	3:c:42:GLY:O	2.29	0.66
3:h:258:GLU:OE2	3:i:46:HIS:NE2	2.16	0.66
1:E:49:LEU:HD11	1:E:286:VAL:HG22	1.78	0.66
2:U:91:ASP:HB3	2:U:95:GLY:H	1.61	0.66
3:h:62:LYS:NZ	3:h:345:MET:O	2.25	0.66
1:L:203:ARG:NH1	1:L:328:ILE:O	2.28	0.66
1:H:47:ARG:HE	3:b:192:LEU:HD13	1.61	0.66
1:K:128:GLN:O	1:K:132:ILE:HG12	1.96	0.66
3:e:111:ARG:NH2	3:e:394:GLU:OE2	2.29	0.66
3:j:47:ASP:OD2	3:j:49:GLN:NE2	2.29	0.66
2:m:43:LEU:HG	2:m:48:TRP:HE1	1.60	0.66
3:Z:292:LYS:HD2	3:Z:314:ALA:HB2	1.77	0.66
2:R:183:ARG:O	3:e:20:ARG:NH2	2.29	0.65
3:Z:22:ILE:HD11	3:Z:151:ARG:HH21	1.60	0.65
3:c:286:ASN:ND2	2:l:170:GLN:OE1	2.29	0.65
2:m:9:VAL:O	2:m:13:LYS:HG2	1.96	0.65
1:J:209:LEU:HA	1:J:215:MET:HE3	1.77	0.65
1:D:31:ASP:HB2	1:N:59:ARG:HG2	1.77	0.65
2:Q:35:GLU:OE2	2:Q:39:GLN:NE2	2.21	0.65
3:d:20:ARG:NH1	3:d:23:GLU:OE2	2.29	0.65
1:A:276:LEU:HD13	1:A:319:THR:HB	1.78	0.65
1:G:36:TYR:HD2	1:G:124:ARG:HG2	1.60	0.65
2:S:122:ARG:NH1	2:T:42:GLN:HG2	2.10	0.65
3:Y:404:ILE:HB	3:Y:407:GLN:CG	2.26	0.65
3:d:33:MET:HE3	3:d:131:THR:HG21	1.78	0.65
3:f:250:GLU:OE2	3:g:41:ARG:NH1	2.29	0.65
3:Y:318:TYR:OH	3:Z:315:VAL:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:169:THR:HA	3:Z:304:MET:H	1.61	0.65
3:g:404:ILE:HG22	3:g:406:LYS:H	1.60	0.65
1:I:177:ARG:NE	1:I:181:GLU:OE2	2.28	0.65
2:P:127:GLN:HG3	2:P:150:LEU:HD11	1.79	0.65
2:R:159:ARG:HD3	3:g:290:GLU:HG2	1.79	0.65
2:X:162:THR:HG21	3:a:288:VAL:HG11	1.78	0.65
3:e:294:ALA:HB3	3:e:309:PRO:HB2	1.79	0.65
2:m:55:ARG:NH2	2:m:78:ASP:OD1	2.30	0.65
1:E:136:LYS:NZ	1:E:260:HIS:O	2.30	0.65
3:Y:76:ARG:HH22	3:j:462:SER:HB3	1.59	0.65
2:Q:165:ARG:NH2	3:f:299:TYR:OH	2.29	0.65
2:U:153:TYR:HE1	2:V:42:GLN:HG3	1.62	0.65
2:X:159:ARG:NH1	3:a:290:GLU:HG2	2.12	0.65
3:g:343:ALA:HA	3:h:54:LEU:HD13	1.78	0.65
2:l:11:LEU:HD21	2:l:28:THR:HG21	1.79	0.65
2:m:9:VAL:HG23	2:m:12:ARG:HH21	1.62	0.65
1:I:90:THR:HG21	1:I:257:LEU:HA	1.79	0.64
2:P:158:SER:OG	3:e:290:GLU:O	2.13	0.64
3:Y:392:LEU:HD22	3:Y:409:LYS:CE	2.26	0.64
3:c:370:ASN:O	3:d:58:ASN:ND2	2.26	0.64
3:f:27:THR:OG1	3:f:49:GLN:NE2	2.29	0.64
3:f:276:LEU:HD22	3:g:284:VAL:HG21	1.79	0.64
1:C:135:ILE:O	1:C:270:ARG:NH1	2.29	0.64
3:Y:139:ASP:OD2	3:Y:144:THR:OG1	2.14	0.64
3:g:325:LYS:NZ	3:h:281:SER:O	2.30	0.64
2:V:49:TRP:CD1	2:V:164:SER:HB3	2.32	0.64
3:Z:307:TYR:HE2	3:Z:311:GLY:HA3	1.62	0.64
2:S:165:ARG:HE	2:S:167:LEU:HD12	1.62	0.64
3:f:37:MET:HB3	3:f:171:ARG:HH11	1.61	0.64
2:S:9:VAL:HG23	2:S:12:ARG:HH22	1.61	0.64
2:X:58:LEU:HD11	2:X:107:LEU:HD21	1.80	0.64
1:B:46:ILE:HA	1:B:283:THR:HB	1.79	0.64
3:Y:177:LEU:HD11	3:Y:198:VAL:HG21	1.80	0.64
3:b:212:MET:HE1	3:b:233:PRO:HB3	1.79	0.64
3:d:13:ARG:NH2	3:d:18:GLU:OE1	2.30	0.64
1:D:185:ASP:HA	1:I:245:PRO:HB3	1.78	0.64
3:e:212:MET:HE1	3:e:233:PRO:HB3	1.79	0.64
3:e:374:GLY:HA3	3:f:122:THR:HG21	1.80	0.64
1:D:316:ARG:NH1	1:D:318:ASP:OD2	2.31	0.64
1:E:212:ASP:OD1	1:O:213:LYS:NZ	2.30	0.64
1:G:279:LYS:HG2	1:G:319:THR:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:179:ARG:O	2:P:183:ARG:N	2.28	0.64
1:I:156:GLU:HB3	1:I:175:MET:HE3	1.78	0.64
2:Q:177:ARG:HD2	3:d:269:LEU:HD21	1.80	0.64
2:W:156:GLU:OE1	2:X:46:GLN:NE2	2.31	0.64
3:Z:254:ARG:NH1	3:Z:258:GLU:OE2	2.31	0.64
3:i:343:ALA:HA	3:j:54:LEU:HD21	1.80	0.64
2:Q:53:TRP:HE1	2:Q:109:LEU:HD12	1.63	0.63
3:j:57:ASN:OD1	3:j:126:LYS:NZ	2.29	0.63
1:J:42:PRO:HD3	3:g:193:SER:HA	1.80	0.63
2:Q:1:MET:N	2:Q:121:GLN:OE1	2.30	0.63
2:Q:91:ASP:HB3	2:Q:95:GLY:H	1.62	0.63
2:S:141:GLU:HG3	2:T:139:PRO:HG2	1.80	0.63
3:j:156:ARG:HH21	3:j:164:MET:HB3	1.63	0.63
3:i:168:LEU:HB3	3:i:202:THR:HB	1.80	0.63
2:k:145:VAL:HG11	2:l:134:THR:HG21	1.80	0.63
1:C:112:LYS:HE2	3:c:11:LYS:HE2	1.81	0.63
1:K:298:GLU:OE1	1:K:298:GLU:N	2.29	0.63
3:d:136:LEU:HB3	3:d:240:ILE:HB	1.81	0.63
3:e:45:GLU:N	3:e:45:GLU:OE1	2.32	0.63
3:h:30:PRO:HB2	3:h:44:VAL:HG13	1.81	0.63
2:R:114:ASP:OD1	2:R:115:HIS:ND1	2.32	0.63
3:b:65:ARG:HH22	3:b:70:THR:HG23	1.64	0.63
3:e:307:TYR:HE2	2:m:163:ARG:HB2	1.62	0.63
1:G:44:MET:HE2	1:G:130:CYS:HB2	1.79	0.63
2:T:153:TYR:HE2	2:U:42:GLN:HG3	1.64	0.63
3:a:307:TYR:HD1	3:a:308:VAL:HG23	1.63	0.63
2:P:35:GLU:N	2:m:12:ARG:HH12	1.97	0.63
3:b:125:ILE:O	3:b:129:ILE:HG12	1.98	0.63
3:g:410:PRO:O	3:h:114:GLN:NE2	2.32	0.63
3:h:447:ARG:NH2	3:i:464:ASP:O	2.32	0.63
3:Y:320:ARG:NH2	3:Z:286:ASN:OD1	2.31	0.63
3:a:13:ARG:NH2	3:a:18:GLU:OE1	2.32	0.63
1:F:36:TYR:OH	1:F:127:ASP:OD2	2.17	0.62
2:S:115:HIS:NE2	2:T:85:ASP:OD2	2.32	0.62
3:g:316:ARG:HH22	3:h:308:VAL:HG13	1.64	0.62
1:F:113:GLU:N	1:F:113:GLU:OE1	2.31	0.62
1:M:250:LYS:HA	1:M:250:LYS:HE3	1.79	0.62
2:X:120:ALA:O	2:X:124:ILE:HG12	1.99	0.62
3:Y:22:ILE:HD11	3:Y:151:ARG:NH1	2.13	0.62
3:b:246:LEU:HD13	3:b:378:LEU:HD11	1.80	0.62
3:i:277:TYR:CE1	3:j:284:VAL:HG22	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:1:MET:HB3	2:W:121:GLN:HE21	1.64	0.62
3:Y:374:GLY:HA3	3:Z:122:THR:HG21	1.81	0.62
3:h:273:LYS:HD3	3:i:283:GLU:HA	1.79	0.62
1:A:24:GLU:OE2	1:L:85:ASN:ND2	2.31	0.62
3:i:107:LYS:HB3	3:i:395:VAL:HG21	1.82	0.62
3:j:184:ASP:HA	3:j:187:ARG:HH11	1.64	0.62
3:b:318:TYR:HE2	3:b:320:ARG:HD3	1.64	0.62
1:E:49:LEU:HD23	1:E:284:ALA:HB1	1.81	0.62
2:W:155:ASN:HA	3:Z:290:GLU:HB3	1.81	0.62
3:Y:76:ARG:HE	3:Y:421:ARG:HH12	1.48	0.62
3:i:450:LEU:HB3	3:i:454:MET:HE2	1.82	0.62
2:W:91:ASP:HB3	2:W:96:ASP:H	1.65	0.62
3:Z:309:PRO:O	3:Z:313:GLU:HG2	1.99	0.62
1:H:188:LEU:HD11	1:H:319:THR:HG22	1.82	0.62
2:S:12:ARG:NH1	2:T:35:GLU:OE1	2.33	0.62
3:Y:287:LEU:HB3	3:Z:309:PRO:HG3	1.81	0.62
3:j:123:GLN:O	3:j:127:LEU:HD12	2.00	0.62
1:G:170:ASP:OD1	1:G:171:LYS:N	2.33	0.61
1:I:249:THR:HG23	1:I:250:LYS:HD2	1.81	0.61
1:A:221:ALA:HB1	1:F:224:ALA:HB1	1.81	0.61
2:P:151:GLN:O	2:P:155:ASN:ND2	2.27	0.61
3:b:177:LEU:O	3:b:182:LYS:NZ	2.33	0.61
3:c:311:GLY:H	3:c:314:ALA:HB3	1.63	0.61
1:L:141:ASP:HA	1:L:152:PRO:HB3	1.81	0.61
2:R:131:ALA:O	2:R:135:HIS:ND1	2.32	0.61
2:S:1:MET:SD	2:S:121:GLN:NE2	2.74	0.61
2:V:4:LEU:HD13	2:V:22:MET:HG2	1.83	0.61
3:b:7:MET:O	3:b:11:LYS:HG3	2.00	0.61
1:O:136:LYS:NZ	1:O:267:GLU:OE1	2.28	0.61
2:Q:183:ARG:HB2	3:e:45:GLU:HG3	1.82	0.61
2:W:123:VAL:HG22	2:W:153:TYR:HB3	1.83	0.61
2:X:40:ARG:HA	2:X:124:ILE:HD12	1.83	0.61
3:a:342:GLN:HG2	3:b:54:LEU:HD21	1.81	0.61
3:h:250:GLU:OE1	3:h:254:ARG:NH2	2.34	0.61
1:H:215:MET:HE1	1:H:233:VAL:HG22	1.81	0.61
3:Y:404:ILE:HB	3:Y:407:GLN:HG3	1.82	0.61
3:Z:207:LYS:HE3	3:Z:216:GLU:HB2	1.82	0.61
3:h:431:ALA:O	3:h:435:ILE:HG12	2.00	0.61
2:U:119:ILE:HD13	2:V:45:THR:HG21	1.81	0.61
2:W:159:ARG:HH21	3:a:307:TYR:HE1	1.48	0.61
3:Y:408:HIS:O	3:Y:409:LYS:HG2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:90:ARG:HH11	2:l:97:ASP:HB3	1.65	0.61
1:B:281:LEU:HB3	1:B:312:ILE:HD11	1.83	0.61
2:R:23:ASP:OD1	2:R:24:GLU:N	2.33	0.61
3:i:410:PRO:O	3:j:114:GLN:NE2	2.32	0.61
1:C:43:LEU:HB2	1:C:277:PRO:HB3	1.82	0.61
2:V:127:GLN:OE1	2:V:154:GLN:NE2	2.34	0.61
3:Z:124:VAL:HG21	3:Z:136:LEU:HD12	1.83	0.61
1:A:21:ILE:O	1:G:56:ARG:NH1	2.27	0.61
1:C:178:ARG:NH2	1:H:334:THR:OG1	2.34	0.60
1:D:226:ASN:HD22	1:D:233:VAL:HA	1.66	0.60
2:X:119:ILE:HD11	2:k:45:THR:HG21	1.84	0.60
3:Y:400:LEU:HD11	3:Y:401:GLN:HE22	1.65	0.60
3:Y:9:TRP:HD1	3:Y:167:VAL:HG13	1.66	0.60
3:a:244:TRP:CE3	3:a:379:LEU:HD21	2.36	0.60
1:C:10:PRO:O	1:I:81:ASN:ND2	2.33	0.60
1:O:212:ASP:OD1	1:O:213:LYS:N	2.33	0.60
1:G:211:HIS:HB3	1:G:214:LEU:HB2	1.83	0.60
1:H:302:TRP:HE1	2:l:183:ARG:HH12	1.49	0.60
2:Q:153:TYR:HE1	2:R:42:GLN:HG3	1.67	0.60
2:R:54:TRP:HE1	2:R:106:ARG:HH21	1.49	0.60
1:D:136:LYS:NZ	1:D:262:ASN:O	2.27	0.60
1:F:158:LEU:HD11	1:F:175:MET:HG2	1.82	0.60
1:G:100:HIS:CD2	2:X:180:ARG:HE	2.20	0.60
2:P:104:GLU:OE1	2:P:104:GLU:N	2.34	0.60
2:m:41:ILE:HD11	2:m:73:LEU:HD21	1.83	0.60
2:m:118:GLU:OE2	2:m:118:GLU:N	2.25	0.60
1:D:27:LEU:HD12	1:N:57:LEU:HB3	1.82	0.60
3:Y:130:VAL:HG12	3:Y:131:THR:HG23	1.83	0.60
3:Z:57:ASN:HA	3:Z:126:LYS:HE3	1.84	0.60
3:c:133:ASN:HD22	3:c:150:LEU:HD21	1.66	0.60
3:c:374:GLY:HA3	3:d:122:THR:HG21	1.84	0.60
3:d:121:LEU:O	3:d:125:ILE:HG12	2.01	0.60
3:f:373:GLY:HA2	3:g:61:ALA:HB2	1.84	0.60
3:g:273:LYS:NZ	3:h:283:GLU:HA	2.16	0.60
2:U:69:PRO:HB2	2:U:109:LEU:HD11	1.82	0.60
3:Z:158:ASP:OD1	3:Z:159:ALA:N	2.32	0.60
3:a:244:TRP:CZ3	3:a:379:LEU:HD11	2.36	0.60
3:i:282:LEU:HD11	3:i:326:MET:HE1	1.83	0.60
3:j:345:MET:HE1	3:j:372:LEU:HG	1.83	0.60
1:A:10:PRO:O	1:G:81:ASN:ND2	2.35	0.60
1:C:280:THR:HG22	1:C:281:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:179:VAL:HG21	1:H:323:ILE:HD11	1.83	0.60
2:V:119:ILE:HD13	2:W:45:THR:HG21	1.84	0.60
2:W:167:LEU:HD21	2:X:81:ASP:H	1.67	0.60
3:a:445:ASP:HB3	3:a:448:ILE:HG12	1.83	0.60
3:b:287:LEU:HD13	3:c:312:ALA:HB2	1.82	0.60
3:c:183:GLN:HG3	3:c:184:ASP:H	1.67	0.60
3:e:434:VAL:HG22	3:f:429:LEU:HD11	1.84	0.60
3:Y:285:LEU:HD22	3:Z:306:ASP:HB2	1.84	0.60
3:Y:310:GLY:HA2	3:Y:314:ALA:HB3	1.83	0.60
3:g:464:ASP:CG	3:g:465:THR:N	2.56	0.60
3:e:307:TYR:O	3:e:311:GLY:N	2.33	0.60
3:f:9:TRP:HD1	3:f:167:VAL:HB	1.67	0.60
3:f:313:GLU:O	3:f:316:ARG:NH2	2.34	0.60
3:d:80:THR:H	3:d:83:ILE:HD12	1.67	0.59
3:f:322:ASP:HB2	3:f:325:LYS:HD2	1.83	0.59
2:k:127:GLN:NE2	2:k:154:GLN:OE1	2.35	0.59
1:E:190:ASP:OD1	1:E:191:ALA:N	2.35	0.59
1:L:198:THR:HB	1:L:274:LEU:HD12	1.84	0.59
3:d:373:GLY:HA2	3:e:61:ALA:HB2	1.83	0.59
1:E:34:PHE:HE1	1:O:316:ARG:HH12	1.49	0.59
1:L:9:ARG:HH11	1:L:10:PRO:HD2	1.66	0.59
3:Y:373:GLY:O	3:Z:126:LYS:NZ	2.35	0.59
3:b:289:ASP:HB3	3:b:314:ALA:HB1	1.83	0.59
3:d:277:TYR:HB3	3:d:326:MET:HG2	1.83	0.59
3:e:14:ASP:OD2	3:f:41:ARG:NH1	2.35	0.59
3:g:332:SER:OG	3:h:278:GLU:OE2	2.15	0.59
3:i:124:VAL:HG11	3:i:136:LEU:HD21	1.85	0.59
3:i:438:LEU:HD23	3:j:432:SER:HB3	1.83	0.59
2:k:49:TRP:CE3	2:k:161:HIS:HA	2.37	0.59
1:H:180:VAL:O	1:H:184:ILE:HG12	2.02	0.59
3:d:177:LEU:HD11	3:d:198:VAL:HG11	1.83	0.59
3:e:29:LEU:HD12	3:e:31:TYR:HE2	1.67	0.59
3:i:254:ARG:HB3	3:i:258:GLU:HG3	1.84	0.59
1:B:93:TYR:OH	1:K:75:GLU:OE1	2.21	0.59
1:F:178:ARG:O	1:F:182:THR:HG23	2.02	0.59
3:b:290:GLU:HG3	2:k:155:ASN:HB3	1.85	0.59
3:b:425:VAL:HA	3:b:428:MET:HE3	1.84	0.59
3:g:458:TRP:HE3	3:g:463:VAL:CG1	2.13	0.59
3:h:13:ARG:NH2	3:h:18:GLU:OE2	2.35	0.59
3:h:35:ASP:HB3	3:h:151:ARG:HH21	1.68	0.59
1:B:75:GLU:OE1	1:G:93:TYR:OH	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:157:LYS:HA	1:I:324:GLU:HB2	1.85	0.59
3:b:434:VAL:HG12	3:c:429:LEU:HD11	1.84	0.59
3:i:171:ARG:HD2	3:i:197:SER:HB3	1.83	0.59
1:E:10:PRO:O	1:F:81:ASN:ND2	2.36	0.59
1:E:62:ASN:HB2	1:E:149:ALA:HB2	1.85	0.59
1:G:100:HIS:HD2	2:X:180:ARG:HE	1.48	0.59
3:f:329:ILE:HG13	3:g:282:LEU:HD23	1.85	0.59
1:M:160:LEU:HD11	1:M:325:LEU:HD23	1.85	0.59
2:R:172:LYS:HE3	3:g:298:ASP:HA	1.84	0.59
3:e:243:THR:O	3:e:382:ASN:ND2	2.36	0.59
2:m:19:ILE:HD13	2:m:29:MET:HE1	1.84	0.59
1:G:23:LEU:HD11	2:k:180:ARG:HH22	1.68	0.59
1:O:48:ASP:OD1	1:O:50:ARG:NH1	2.34	0.59
2:V:76:TYR:HD2	2:V:106:ARG:HH11	1.49	0.59
3:Y:400:LEU:CD1	3:Y:401:GLN:OE1	2.51	0.59
3:e:307:TYR:CZ	2:m:162:THR:HG23	2.37	0.59
3:h:247:ALA:HB1	3:i:34:VAL:HG21	1.85	0.59
2:m:123:VAL:HG12	2:m:153:TYR:HB3	1.84	0.59
2:U:150:LEU:O	2:U:154:GLN:HG3	2.03	0.59
3:a:307:TYR:CD1	3:a:308:VAL:HG23	2.38	0.59
1:N:200:MET:HE3	1:N:241:VAL:HG13	1.84	0.58
2:Q:118:GLU:OE1	2:Q:118:GLU:N	2.35	0.58
2:R:163:ARG:HH21	2:S:106:ARG:NH2	2.00	0.58
3:Z:62:LYS:NZ	3:Z:345:MET:O	2.36	0.58
3:h:155:VAL:HG21	3:h:241:VAL:HG21	1.85	0.58
3:i:169:LYS:HE2	3:i:199:ASP:HB2	1.84	0.58
1:D:291:ALA:H	3:f:40:SER:HB3	1.68	0.58
1:I:180:VAL:O	1:I:184:ILE:HG13	2.03	0.58
2:S:1:MET:HE1	2:S:122:ARG:HB2	1.84	0.58
3:g:134:ALA:HB3	3:g:242:PRO:HG2	1.83	0.58
1:E:219:TYR:OH	1:J:212:ASP:OD1	2.19	0.58
1:M:68:ARG:NH1	1:M:72:GLU:O	2.36	0.58
3:Y:18:GLU:OE2	3:Y:151:ARG:NH1	2.35	0.58
3:i:4:THR:HG23	3:i:6:ALA:H	1.67	0.58
1:E:32:LYS:HG2	1:O:60:LEU:HB2	1.85	0.58
1:J:50:ARG:NH1	3:f:7:MET:SD	2.77	0.58
2:R:12:ARG:NE	2:S:35:GLU:OE2	2.36	0.58
3:Z:133:ASN:HB2	3:Z:150:LEU:HD21	1.84	0.58
3:e:87:ALA:HB1	3:e:92:THR:HB	1.86	0.58
2:T:49:TRP:HD1	2:U:83:GLN:HE21	1.52	0.58
3:a:162:ARG:HB2	3:a:206:ARG:NH2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:375:THR:HA	3:e:378:LEU:HB3	1.84	0.58
1:G:131:LEU:HD22	1:G:247:PHE:HE1	1.68	0.58
1:I:289:VAL:H	3:d:7:MET:HE1	1.68	0.58
1:O:141:ASP:HA	1:O:152:PRO:HB3	1.85	0.58
2:V:119:ILE:HD12	2:V:122:ARG:HD3	1.86	0.58
3:Z:446:PRO:O	3:Z:447:ARG:HG2	2.03	0.58
3:a:12:LEU:HD11	3:a:156:ARG:HG3	1.85	0.58
2:m:64:GLY:HA2	2:m:98:ARG:HH11	1.69	0.58
1:G:90:THR:HG21	1:G:257:LEU:HA	1.86	0.58
3:Y:288:VAL:HG11	3:Y:295:VAL:HG12	1.85	0.58
3:g:67:LEU:HD11	3:g:379:LEU:HD22	1.85	0.58
3:g:168:LEU:HB3	3:g:202:THR:HB	1.86	0.58
1:D:91:LEU:HD12	1:D:309:MET:HB2	1.86	0.58
1:M:95:ARG:NE	1:M:305:ASP:OD1	2.34	0.58
2:V:113:TRP:O	2:V:121:GLN:NE2	2.37	0.58
3:h:318:TYR:HD2	3:i:306:ASP:OD2	1.87	0.58
1:D:10:PRO:O	1:J:81:ASN:ND2	2.37	0.58
1:I:205:PHE:O	1:I:209:LEU:HG	2.04	0.58
1:J:92:LEU:HD11	1:J:257:LEU:HD21	1.86	0.58
2:P:113:TRP:O	2:P:121:GLN:NE2	2.35	0.58
3:b:103:ARG:NH1	3:b:397:ASP:OD2	2.37	0.58
3:f:124:VAL:HG21	3:f:136:LEU:HD13	1.86	0.58
3:g:396:ASP:HA	3:g:400:LEU:HD13	1.84	0.58
3:i:206:ARG:HE	3:i:234:ILE:HG12	1.67	0.58
2:l:37:GLU:O	2:l:41:ILE:HG12	2.04	0.58
1:E:23:LEU:HG	1:F:56:ARG:HH21	1.68	0.57
2:P:123:VAL:HG22	2:P:153:TYR:HB3	1.86	0.57
2:W:44:LEU:HG	2:W:51:ASN:HD22	1.69	0.57
3:c:289:ASP:HA	3:d:309:PRO:HD3	1.85	0.57
3:d:128:LEU:HG	3:d:244:TRP:HB2	1.86	0.57
3:h:108:ALA:HB1	3:h:391:CYS:HB3	1.85	0.57
3:i:103:ARG:HA	3:i:106:ARG:HH12	1.69	0.57
3:j:288:VAL:HG12	3:j:315:VAL:HG12	1.85	0.57
1:A:68:ARG:HH12	1:E:300:PHE:HD1	1.52	0.57
1:D:186:ARG:HG3	1:D:188:LEU:HD13	1.85	0.57
1:D:229:VAL:HG11	1:N:220:GLN:HE22	1.69	0.57
1:C:95:ARG:NH2	1:C:305:ASP:OD2	2.32	0.57
2:Q:165:ARG:NH1	2:Q:167:LEU:HD13	2.19	0.57
2:R:120:ALA:HA	2:R:123:VAL:HG12	1.87	0.57
2:T:39:GLN:HG2	2:T:127:GLN:HB2	1.86	0.57
2:V:13:LYS:HG2	2:V:129:ALA:HB1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:53:TRP:HB2	2:W:107:LEU:HB3	1.85	0.57
3:Y:212:MET:HE1	3:Y:233:PRO:HB3	1.86	0.57
3:g:177:LEU:HD11	3:g:198:VAL:HG21	1.87	0.57
1:B:10:PRO:O	1:H:81:ASN:ND2	2.38	0.57
1:J:112:LYS:O	1:J:116:GLU:HG3	2.04	0.57
1:N:206:SER:HA	1:N:209:LEU:HD12	1.86	0.57
3:i:276:LEU:HD23	3:j:284:VAL:HG21	1.86	0.57
3:i:397:ASP:HB3	3:i:400:LEU:HB2	1.85	0.57
3:i:404:ILE:HG22	3:i:406:LYS:H	1.69	0.57
2:R:9:VAL:HG12	2:R:12:ARG:NH1	2.20	0.57
3:b:450:LEU:O	3:b:454:MET:HG3	2.05	0.57
3:e:124:VAL:HG21	3:e:136:LEU:HD12	1.86	0.57
1:C:255:HIS:HE1	1:C:257:LEU:HD13	1.70	0.57
1:I:116:GLU:O	1:I:120:GLN:HG3	2.05	0.57
2:T:113:TRP:CZ2	2:T:121:GLN:HB2	2.40	0.57
3:c:277:TYR:OH	3:d:282:LEU:O	2.21	0.57
3:e:244:TRP:HD1	3:e:245:ASN:HB2	1.68	0.57
3:f:369:GLU:HG2	3:f:376:TYR:HD1	1.70	0.57
3:h:244:TRP:CD1	3:h:245:ASN:HD22	2.22	0.57
1:D:255:HIS:HD2	1:D:257:LEU:H	1.53	0.57
1:E:230:LYS:HG3	1:O:235:ILE:HG12	1.86	0.57
1:H:43:LEU:HD23	1:H:275:PHE:HZ	1.69	0.57
2:P:122:ARG:NH2	2:Q:38:ASP:OD1	2.37	0.57
2:U:2:LEU:HD12	2:U:3:LEU:H	1.69	0.57
3:c:155:VAL:HG21	3:c:241:VAL:HG11	1.87	0.57
1:C:255:HIS:H	1:C:262:ASN:HD22	1.53	0.57
1:J:36:TYR:H	1:J:120:GLN:HG2	1.70	0.57
2:U:49:TRP:O	2:V:83:GLN:NE2	2.37	0.57
2:W:149:GLU:HG2	2:W:153:TYR:HE2	1.70	0.57
3:a:163:TRP:O	3:a:206:ARG:NH2	2.36	0.57
3:c:133:ASN:HD21	3:c:252:TYR:HB3	1.68	0.57
3:c:276:LEU:HD13	3:d:284:VAL:HG11	1.87	0.57
2:l:155:ASN:O	2:l:159:ARG:HG2	2.05	0.57
2:m:113:TRP:O	2:m:121:GLN:NE2	2.36	0.57
1:A:94:LEU:HD21	1:L:65:ALA:HA	1.87	0.57
1:A:104:TRP:HH2	1:G:307:PHE:HE2	1.51	0.57
1:I:50:ARG:NH2	3:d:195:SER:O	2.36	0.57
1:L:212:ASP:OD1	1:L:213:LYS:N	2.38	0.57
1:O:40:PHE:HB2	1:O:43:LEU:HD13	1.85	0.57
2:U:159:ARG:HG2	3:Y:307:TYR:CD2	2.39	0.57
3:Y:441:ILE:HD12	3:Z:432:SER:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:409:LYS:HG3	3:Z:409:LYS:O	2.04	0.57
3:c:27:THR:HG21	3:c:264:PHE:HB3	1.86	0.57
2:k:13:LYS:HD2	2:l:135:HIS:CE1	2.40	0.57
1:A:297:ASN:HD22	1:G:294:TRP:CD1	2.23	0.57
1:E:148:ASP:OD1	1:E:149:ALA:N	2.37	0.57
1:I:170:ASP:HB3	1:I:174:ARG:NH1	2.20	0.57
3:a:287:LEU:HD23	3:b:306:ASP:HB3	1.87	0.57
1:G:285:GLN:HB2	1:G:310:TYR:HA	1.87	0.56
1:I:32:LYS:HD2	1:I:117:LEU:HG	1.87	0.56
3:f:217:LEU:HD22	3:f:232:TRP:HH2	1.70	0.56
2:R:71:GLY:O	2:R:110:SER:OG	2.21	0.56
2:U:173:ARG:NH2	3:j:301:ASP:OD1	2.38	0.56
2:V:76:TYR:HD2	2:V:106:ARG:HD2	1.70	0.56
3:Y:122:THR:HG21	3:j:374:GLY:HA3	1.87	0.56
3:h:318:TYR:CE1	3:h:320:ARG:HB2	2.35	0.56
2:m:44:LEU:HD13	2:m:111:ARG:H	1.69	0.56
1:C:65:ALA:HB3	1:H:125:LYS:HE3	1.86	0.56
1:D:130:CYS:O	1:D:134:VAL:HG23	2.05	0.56
1:F:33:HIS:CD2	1:F:124:ARG:HH12	2.22	0.56
1:L:128:GLN:O	1:L:132:ILE:HG12	2.06	0.56
1:M:216:ASN:O	1:M:220:GLN:NE2	2.38	0.56
3:a:435:ILE:HG21	3:a:454:MET:HE1	1.87	0.56
3:c:289:ASP:OD1	3:c:290:GLU:N	2.37	0.56
3:d:453:MET:HE3	3:d:457:ILE:HG12	1.86	0.56
3:g:425:VAL:HA	3:g:428:MET:HE3	1.87	0.56
2:m:130:LEU:HD13	2:m:146:ILE:HG23	1.88	0.56
1:A:28:GLY:HA3	3:Y:193:SER:HB2	1.87	0.56
1:K:91:LEU:HD12	1:K:309:MET:HE2	1.87	0.56
2:P:180:ARG:HB3	2:P:180:ARG:NH1	2.21	0.56
3:c:168:LEU:HB3	3:c:202:THR:HB	1.87	0.56
3:e:93:ASP:HB3	3:e:96:GLU:HG2	1.87	0.56
1:E:133:GLN:HG3	1:E:312:ILE:HB	1.86	0.56
1:F:87:THR:O	1:F:311:ASN:ND2	2.37	0.56
1:J:167:GLN:O	1:J:171:LYS:HG2	2.06	0.56
1:K:87:THR:O	1:K:311:ASN:ND2	2.28	0.56
2:V:49:TRP:HD1	2:V:164:SER:HB3	1.70	0.56
2:V:163:ARG:HE	3:Z:307:TYR:HE1	1.52	0.56
3:i:443:GLN:HE22	3:j:435:ILE:HD12	1.71	0.56
1:B:87:THR:O	1:B:311:ASN:ND2	2.39	0.56
1:E:192:VAL:HG22	1:E:276:LEU:HD11	1.87	0.56
1:F:204:VAL:HG11	1:F:272:ILE:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:MET:HG2	1:F:228:TYR:HB2	1.87	0.56
1:J:98:PHE:O	1:J:302:TRP:N	2.38	0.56
1:L:181:GLU:HA	1:L:184:ILE:HG22	1.87	0.56
2:Q:174:SER:OG	3:d:273:LYS:NZ	2.39	0.56
2:S:120:ALA:HA	2:S:157:LEU:HD21	1.87	0.56
3:Z:47:ASP:OD1	3:Z:48:PHE:N	2.38	0.56
3:a:133:ASN:HB2	3:a:150:LEU:HD21	1.88	0.56
3:e:13:ARG:HG2	3:e:154:ALA:HB2	1.88	0.56
3:h:18:GLU:O	3:h:22:ILE:HG12	2.06	0.56
2:l:158:SER:O	2:l:162:THR:HG22	2.06	0.56
1:A:27:LEU:HD21	1:L:55:VAL:HB	1.87	0.56
1:K:240:LYS:HD3	1:K:240:LYS:N	2.21	0.56
2:P:80:PRO:HB2	2:m:167:LEU:HD12	1.86	0.56
3:Z:133:ASN:HD21	3:Z:253:GLY:H	1.52	0.56
3:Z:286:ASN:O	3:a:306:ASP:HB3	2.04	0.56
3:c:345:MET:HE2	3:c:371:THR:HB	1.88	0.56
3:e:11:LYS:HG3	3:e:12:LEU:HD12	1.88	0.56
1:B:50:ARG:HD2	2:k:183:ARG:O	2.06	0.56
1:G:285:GLN:HB2	1:G:309:MET:O	2.06	0.56
3:Z:254:ARG:HB3	3:Z:258:GLU:HG2	1.88	0.56
3:a:129:ILE:HG23	3:a:256:HIS:HB3	1.87	0.56
3:b:122:THR:O	3:b:126:LYS:HG3	2.06	0.56
3:b:312:ALA:C	3:b:314:ALA:H	2.14	0.56
3:c:322:ASP:HB2	3:c:325:LYS:HD2	1.86	0.56
3:d:318:TYR:HE2	3:e:311:GLY:HA3	1.71	0.56
3:e:278:GLU:OE2	3:e:326:MET:HE2	2.05	0.56
3:f:372:LEU:HG	3:f:375:THR:HB	1.87	0.56
3:i:18:GLU:O	3:i:22:ILE:HG12	2.06	0.56
3:i:164:MET:HE1	3:j:176:ASP:HB3	1.88	0.56
1:D:230:LYS:HB3	1:N:235:ILE:HG21	1.88	0.56
2:V:44:LEU:HD22	2:V:51:ASN:HD22	1.71	0.56
2:X:12:ARG:NE	2:k:35:GLU:OE2	2.33	0.56
3:Y:6:ALA:HA	3:Y:201:TYR:HE2	1.71	0.56
3:f:273:LYS:NZ	3:g:279:LEU:HA	2.21	0.56
3:f:292:LYS:HB3	3:f:309:PRO:HB3	1.88	0.56
3:j:296:VAL:HB	3:j:311:GLY:HA3	1.86	0.56
3:j:386:PRO:HA	3:j:389:TYR:HD1	1.71	0.56
1:B:220:GLN:HE21	1:G:229:VAL:HG21	1.71	0.56
1:C:92:LEU:HD22	1:C:257:LEU:HD11	1.88	0.56
3:a:121:LEU:O	3:a:125:ILE:HG12	2.06	0.56
3:j:369:GLU:HB2	3:j:376:TYR:HD2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:ARG:HG3	3:i:195:SER:HB3	1.87	0.55
1:L:190:ASP:OD1	1:L:191:ALA:N	2.38	0.55
3:Y:277:TYR:CE1	3:Z:284:VAL:HG12	2.40	0.55
3:d:318:TYR:HE1	3:d:320:ARG:HB2	1.70	0.55
3:e:452:LYS:HZ3	3:f:95:THR:HA	1.71	0.55
3:g:177:LEU:O	3:g:182:LYS:NZ	2.39	0.55
3:h:332:SER:OG	3:i:278:GLU:OE2	2.24	0.55
1:B:94:LEU:HD21	1:K:65:ALA:HA	1.88	0.55
1:D:221:ALA:HB1	1:I:224:ALA:HB1	1.89	0.55
1:I:170:ASP:HB3	1:I:174:ARG:HH12	1.71	0.55
2:Q:142:THR:HG22	2:R:139:PRO:HD3	1.88	0.55
3:j:79:LEU:HA	3:j:83:ILE:HD11	1.88	0.55
1:C:116:GLU:O	1:C:120:GLN:HG2	2.07	0.55
1:I:101:GLN:HA	1:I:104:TRP:CD1	2.41	0.55
1:I:154:VAL:HG21	1:I:179:VAL:HG13	1.88	0.55
2:T:118:GLU:HA	2:T:121:GLN:NE2	2.22	0.55
2:U:115:HIS:NE2	2:V:85:ASP:OD2	2.38	0.55
2:W:14:ILE:HG23	2:W:16:GLU:HG3	1.87	0.55
3:Z:20:ARG:HG2	3:Z:254:ARG:HH12	1.70	0.55
3:f:397:ASP:H	3:f:400:LEU:HD13	1.71	0.55
3:h:9:TRP:HD1	3:h:167:VAL:HG13	1.71	0.55
3:j:12:LEU:HD22	3:j:156:ARG:HB2	1.88	0.55
1:J:135:ILE:HD11	1:J:270:ARG:HB3	1.88	0.55
1:O:139:ALA:HB2	1:O:155:LEU:HD13	1.89	0.55
3:e:392:LEU:HD11	3:e:412:ILE:HD11	1.89	0.55
1:C:93:TYR:CE1	1:M:68:ARG:HB3	2.41	0.55
1:G:197:LEU:HD11	1:G:242:LEU:HB2	1.89	0.55
3:i:155:VAL:HG21	3:i:241:VAL:HG21	1.88	0.55
1:D:180:VAL:O	1:D:184:ILE:HG12	2.07	0.55
1:D:192:VAL:HG22	1:D:276:LEU:HD11	1.87	0.55
3:a:9:TRP:CZ3	3:a:169:LYS:HD3	2.42	0.55
3:g:135:LEU:HD23	3:g:168:LEU:HD13	1.89	0.55
3:j:240:ILE:HG22	3:j:242:PRO:HD3	1.89	0.55
1:J:206:SER:HA	1:J:209:LEU:HD12	1.89	0.55
3:Z:374:GLY:HA3	3:a:122:THR:HG21	1.88	0.55
3:a:283:GLU:N	3:a:283:GLU:OE2	2.40	0.55
1:D:170:ASP:O	1:D:174:ARG:HG3	2.07	0.55
1:F:190:ASP:OD1	1:F:191:ALA:N	2.40	0.55
1:M:131:LEU:HA	1:M:134:VAL:HG12	1.89	0.55
2:W:69:PRO:HG3	2:W:107:LEU:HD21	1.88	0.55
3:b:397:ASP:OD1	3:b:398:ALA:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:87:ALA:O	3:e:91:ASP:N	2.39	0.55
3:h:34:VAL:O	3:h:36:PRO:HD3	2.07	0.55
2:k:41:ILE:O	2:k:45:THR:HG23	2.07	0.55
1:C:106:GLN:NE2	3:d:194:GLY:O	2.29	0.55
1:G:207:LEU:HD21	1:G:331:PHE:CE2	2.40	0.55
1:K:168:ALA:O	1:K:172:ILE:HG12	2.07	0.55
1:M:118:ASP:HB3	1:M:306:THR:HG21	1.89	0.55
2:S:43:LEU:O	2:S:48:TRP:NE1	2.40	0.55
3:g:148:TRP:HB3	3:g:152:SER:HB2	1.89	0.55
1:D:9:ARG:HB2	1:D:12:TYR:HB2	1.87	0.54
3:Z:244:TRP:CE2	3:Z:375:THR:HG21	2.42	0.54
3:b:424:ALA:O	3:b:427:SER:OG	2.21	0.54
1:D:87:THR:O	1:D:311:ASN:ND2	2.36	0.54
1:E:174:ARG:HB3	1:J:334:THR:HG22	1.88	0.54
1:K:158:LEU:HD11	1:K:171:LYS:HG2	1.89	0.54
2:P:52:THR:HG21	2:P:54:TRP:CZ2	2.42	0.54
2:V:13:LYS:HD3	2:W:135:HIS:NE2	2.23	0.54
3:Y:107:LYS:NZ	3:j:81:ASP:OD1	2.40	0.54
3:Y:400:LEU:CD1	3:Y:401:GLN:NE2	2.55	0.54
3:a:435:ILE:HG12	3:a:457:ILE:HG21	1.88	0.54
3:c:90:ARG:NH2	3:c:92:THR:OG1	2.40	0.54
3:g:97:VAL:HG12	3:g:399:LEU:HD11	1.88	0.54
3:i:221:ILE:HG22	3:i:226:VAL:HB	1.87	0.54
3:i:313:GLU:HA	3:i:316:ARG:HH21	1.72	0.54
1:C:36:TYR:H	1:C:120:GLN:NE2	2.05	0.54
1:F:32:LYS:HD2	1:F:117:LEU:HD21	1.89	0.54
2:S:155:ASN:HD22	3:h:290:GLU:HB2	1.72	0.54
2:T:170:GLN:OE1	3:j:304:MET:N	2.35	0.54
2:U:173:ARG:HH22	3:j:301:ASP:CG	2.14	0.54
3:a:282:LEU:HD11	3:a:326:MET:HE1	1.89	0.54
3:c:290:GLU:OE2	2:l:155:ASN:HB3	2.06	0.54
3:c:308:VAL:HA	3:c:312:ALA:HB3	1.88	0.54
3:d:452:LYS:HB2	3:e:95:THR:HG21	1.90	0.54
3:e:33:MET:HG3	3:e:149:SER:HB3	1.90	0.54
3:j:431:ALA:O	3:j:435:ILE:HG12	2.07	0.54
2:X:76:TYR:HD2	2:X:106:ARG:HB3	1.73	0.54
3:Z:448:ILE:HB	3:Z:452:LYS:HD3	1.88	0.54
3:a:14:ASP:HB3	3:a:17:VAL:HG22	1.88	0.54
3:e:434:VAL:HG13	3:f:429:LEU:HD21	1.89	0.54
1:E:213:LYS:HG2	1:E:219:TYR:HE1	1.72	0.54
1:F:105:THR:OG1	1:F:106:GLN:OE1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:157:ARG:HG3	3:Y:251:HIS:HA	1.90	0.54
3:Z:178:ASP:OD1	3:Z:179:GLU:N	2.40	0.54
3:a:308:VAL:HG12	3:a:310:GLY:N	2.16	0.54
3:b:169:LYS:HG3	3:b:201:TYR:CE2	2.43	0.54
3:i:155:VAL:HG22	3:i:166:ILE:HG22	1.89	0.54
3:i:184:ASP:HB2	3:i:226:VAL:HG13	1.90	0.54
1:O:100:HIS:HB2	1:O:300:PHE:CE1	2.43	0.54
3:a:258:GLU:N	3:a:258:GLU:OE1	2.39	0.54
3:a:265:ALA:O	3:a:269:LEU:HG	2.08	0.54
3:a:277:TYR:O	3:a:281:SER:HB2	2.06	0.54
3:g:18:GLU:O	3:g:22:ILE:HG12	2.08	0.54
3:g:200:LEU:HA	3:g:221:ILE:HG13	1.90	0.54
3:h:318:TYR:CE2	3:i:312:ALA:HB2	2.43	0.54
2:k:8:ASN:O	2:k:12:ARG:HG3	2.08	0.54
1:C:148:ASP:OD1	1:C:149:ALA:N	2.40	0.54
2:P:144:GLN:O	2:P:148:GLN:HG2	2.07	0.54
2:R:49:TRP:O	2:S:83:GLN:NE2	2.41	0.54
3:Z:286:ASN:HD22	3:a:304:MET:HA	1.72	0.54
3:e:435:ILE:HA	3:e:438:LEU:HB2	1.90	0.54
3:g:298:ASP:HB2	3:h:304:MET:HE1	1.90	0.54
3:h:339:ARG:HH22	3:i:54:LEU:HD23	1.73	0.54
1:G:199:PRO:HG2	1:G:273:ALA:HB3	1.90	0.54
1:K:9:ARG:HE	1:K:10:PRO:HD2	1.73	0.54
2:P:58:LEU:HD13	2:P:103:VAL:HG23	1.88	0.54
2:S:155:ASN:O	2:S:159:ARG:HG3	2.07	0.54
2:W:163:ARG:HG3	3:a:307:TYR:CE2	2.38	0.54
3:a:80:THR:H	3:a:83:ILE:HD12	1.73	0.54
3:g:294:ALA:HB3	3:g:308:VAL:HG21	1.90	0.54
1:B:230:LYS:HG2	1:K:235:ILE:HG21	1.89	0.54
1:C:50:ARG:NH2	1:H:25:GLU:OE1	2.40	0.54
1:C:289:VAL:O	3:c:13:ARG:NH2	2.36	0.54
1:D:255:HIS:NE2	1:D:257:LEU:HD13	2.23	0.54
2:P:54:TRP:HZ3	2:P:106:ARG:HH21	1.55	0.54
2:Q:120:ALA:HA	2:Q:123:VAL:HG12	1.90	0.54
2:R:158:SER:OG	3:g:290:GLU:O	2.24	0.54
2:R:168:ASN:ND2	3:g:298:ASP:OD2	2.29	0.54
3:a:152:SER:OG	3:a:169:LYS:O	2.25	0.54
3:f:274:LEU:O	3:f:278:GLU:HG3	2.08	0.54
3:h:444:LEU:HA	3:i:454:MET:HE1	1.90	0.54
3:i:217:LEU:HD22	3:i:232:TRP:HH2	1.73	0.54
3:j:269:LEU:O	3:j:273:LYS:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:50:PHE:HA	2:m:83:GLN:HE21	1.73	0.54
1:H:48:ASP:HB2	3:b:194:GLY:HA3	1.90	0.54
1:L:177:ARG:O	1:L:181:GLU:HG2	2.08	0.54
1:N:32:LYS:HG2	1:N:117:LEU:HD21	1.89	0.54
2:S:9:VAL:O	2:S:13:LYS:HG3	2.08	0.54
2:V:76:TYR:CD2	2:V:106:ARG:HD2	2.43	0.54
3:Y:408:HIS:O	3:Y:409:LYS:CG	2.55	0.54
3:b:208:LYS:HD3	3:b:213:GLU:HG2	1.90	0.54
3:b:318:TYR:OH	3:c:315:VAL:O	2.21	0.54
3:c:287:LEU:HG	3:d:309:PRO:HA	1.89	0.54
3:c:311:GLY:N	3:c:314:ALA:HB3	2.23	0.54
3:h:103:ARG:NH2	3:h:397:ASP:OD2	2.41	0.54
1:C:62:ASN:ND2	1:H:121:GLU:OE2	2.40	0.53
1:E:151:SER:HB2	1:E:186:ARG:HH11	1.74	0.53
2:V:173:ARG:HB3	3:Y:301:ASP:OD2	2.08	0.53
2:V:165:ARG:NH2	2:V:168:ASN:OD1	2.41	0.53
2:W:26:TYR:HD1	2:W:27:PRO:HD2	1.73	0.53
3:h:133:ASN:HD21	3:h:252:TYR:HB3	1.73	0.53
3:i:138:ARG:HA	3:i:145:VAL:HG12	1.89	0.53
1:E:112:LYS:HZ1	3:h:6:ALA:C	2.15	0.53
1:H:233:VAL:HG12	1:H:241:VAL:HG21	1.91	0.53
1:I:48:ASP:OD1	1:I:49:LEU:N	2.41	0.53
1:K:275:PHE:HD2	1:K:280:THR:HG21	1.74	0.53
3:d:243:THR:HG21	3:d:246:LEU:HD12	1.89	0.53
3:d:282:LEU:HD11	3:d:326:MET:HE1	1.91	0.53
1:F:143:PRO:HB2	1:F:146:LEU:HB2	1.89	0.53
1:F:170:ASP:HB3	1:F:174:ARG:HH12	1.73	0.53
1:H:40:PHE:HA	1:H:43:LEU:HD13	1.91	0.53
1:K:68:ARG:NH1	1:K:69:ARG:O	2.41	0.53
1:L:132:ILE:HD12	1:L:263:VAL:HG21	1.91	0.53
2:Q:152:ALA:HA	2:Q:155:ASN:HD22	1.74	0.53
3:Y:441:ILE:HD11	3:Z:435:ILE:HD12	1.89	0.53
3:c:277:TYR:HE2	3:c:329:ILE:HG13	1.74	0.53
3:h:374:GLY:O	3:h:378:LEU:N	2.39	0.53
3:i:80:THR:O	3:i:84:ARG:HG3	2.07	0.53
3:i:381:GLU:O	3:i:385:SER:OG	2.26	0.53
3:j:138:ARG:NH2	3:j:394:GLU:OE2	2.40	0.53
1:G:131:LEU:HD13	1:G:247:PHE:CD1	2.44	0.53
2:Q:153:TYR:CE1	2:R:42:GLN:HG3	2.43	0.53
2:U:51:ASN:HA	2:U:111:ARG:HH11	1.72	0.53
3:b:107:LYS:O	3:b:110:GLN:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:443:GLN:NE2	3:j:435:ILE:HD12	2.22	0.53
1:D:49:LEU:HD22	1:D:286:VAL:HG12	1.90	0.53
2:T:11:LEU:HD21	2:T:28:THR:HG21	1.90	0.53
2:V:90:ARG:NE	2:V:97:ASP:OD1	2.41	0.53
2:W:23:ASP:OD1	2:W:24:GLU:N	2.41	0.53
3:f:33:MET:HE1	3:f:150:LEU:HD21	1.91	0.53
1:F:170:ASP:HB3	1:F:174:ARG:NH1	2.23	0.53
1:L:155:LEU:HD11	1:L:270:ARG:HD3	1.91	0.53
1:O:269:GLU:OE1	1:O:327:GLY:N	2.42	0.53
3:d:385:SER:HB3	3:d:414:THR:HG21	1.91	0.53
3:e:452:LYS:NZ	3:f:95:THR:HA	2.23	0.53
3:g:287:LEU:HD13	3:h:308:VAL:HA	1.90	0.53
3:h:125:ILE:O	3:h:129:ILE:HG12	2.08	0.53
3:i:111:ARG:HA	3:i:114:GLN:HG2	1.91	0.53
2:W:163:ARG:CG	3:a:307:TYR:HE2	2.22	0.53
3:Y:171:ARG:O	3:j:159:ALA:HB2	2.08	0.53
3:d:16:SER:O	3:d:20:ARG:HG2	2.09	0.53
3:d:115:ASN:HD22	3:d:144:THR:HG22	1.74	0.53
3:e:178:ASP:OD1	3:e:179:GLU:N	2.42	0.53
3:h:288:VAL:HG12	3:h:315:VAL:HG22	1.91	0.53
2:W:39:GLN:NE2	2:W:127:GLN:HG2	2.24	0.53
3:a:22:ILE:HD13	3:a:33:MET:HG3	1.90	0.53
3:e:290:GLU:HB2	3:f:308:VAL:HG21	1.91	0.53
3:h:51:ALA:O	3:h:55:LEU:HD12	2.08	0.53
2:l:82:LEU:HD21	2:l:99:ILE:HG21	1.91	0.53
1:E:230:LYS:HD3	1:E:232:ARG:NH2	2.22	0.53
1:I:190:ASP:OD1	1:I:191:ALA:N	2.42	0.53
2:T:159:ARG:HE	3:j:308:VAL:HG13	1.74	0.53
2:V:182:LEU:HD13	3:i:262:GLY:HA3	1.91	0.53
2:X:53:TRP:CZ3	2:X:109:LEU:HD22	2.44	0.53
3:b:9:TRP:HD1	3:b:167:VAL:HG13	1.74	0.53
3:j:61:ALA:O	3:j:65:ARG:HG3	2.09	0.53
3:j:308:VAL:HG12	3:j:310:GLY:N	2.24	0.53
3:j:403:LEU:HD11	3:j:407:GLN:NE2	2.24	0.53
2:m:169:THR:HG23	2:m:171:ALA:H	1.74	0.53
1:H:98:PHE:O	1:H:302:TRP:N	2.38	0.52
3:Y:76:ARG:HH21	3:Y:421:ARG:CZ	2.22	0.52
3:Y:296:VAL:HG11	3:Y:307:TYR:CE1	2.45	0.52
3:c:138:ARG:HH12	3:c:143:ALA:HA	1.73	0.52
3:f:157:ARG:NH1	3:f:251:HIS:O	2.38	0.52
3:f:286:ASN:ND2	3:g:304:MET:HE3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j:458:TRP:HE3	3:j:465:THR:HG22	1.73	0.52
1:G:246:ARG:NH1	1:G:246:ARG:HA	2.24	0.52
1:G:302:TRP:CE3	2:X:180:ARG:HD3	2.44	0.52
1:H:302:TRP:NE1	2:l:183:ARG:HH12	2.07	0.52
2:P:140:ASP:OD1	2:P:142:THR:OG1	2.27	0.52
2:Q:64:GLY:HA3	2:Q:99:ILE:HG23	1.90	0.52
2:T:61:ASP:N	2:T:65:ARG:O	2.41	0.52
3:c:369:GLU:OE1	3:d:65:ARG:NH2	2.42	0.52
3:g:225:ARG:NH1	3:g:225:ARG:HB2	2.23	0.52
3:i:52:GLY:O	3:i:56:VAL:HG23	2.09	0.52
1:K:211:HIS:HB3	1:K:214:LEU:HB3	1.91	0.52
2:U:142:THR:HG22	2:V:139:PRO:HD3	1.92	0.52
2:V:7:VAL:HA	2:V:10:ILE:HG22	1.92	0.52
2:V:172:LYS:HD3	3:j:280:GLU:OE1	2.09	0.52
2:W:9:VAL:HG12	2:W:12:ARG:HH12	1.73	0.52
3:Y:76:ARG:HE	3:Y:421:ARG:NH1	2.06	0.52
3:a:103:ARG:HA	3:a:106:ARG:NH1	2.24	0.52
3:a:160:THR:OG1	3:a:162:ARG:NH1	2.41	0.52
3:f:217:LEU:N	3:f:230:GLY:O	2.41	0.52
3:i:73:PRO:HA	3:i:109:THR:HG21	1.90	0.52
2:m:127:GLN:HG3	2:m:150:LEU:HD11	1.90	0.52
1:D:92:LEU:HD11	1:D:257:LEU:HG	1.91	0.52
2:T:9:VAL:HA	2:T:12:ARG:NE	2.25	0.52
3:Y:139:ASP:HB2	3:Y:144:THR:H	1.75	0.52
3:Z:343:ALA:HB2	3:a:54:LEU:HD11	1.92	0.52
3:d:289:ASP:HB2	3:d:314:ALA:HB1	1.91	0.52
3:g:125:ILE:O	3:g:129:ILE:HD12	2.08	0.52
3:h:339:ARG:NH1	3:h:342:GLN:OE1	2.43	0.52
3:j:125:ILE:O	3:j:129:ILE:HG12	2.09	0.52
2:m:120:ALA:HA	2:m:123:VAL:HG22	1.91	0.52
2:U:90:ARG:HB3	2:U:95:GLY:HA2	1.90	0.52
2:W:4:LEU:HD11	2:W:22:MET:HB2	1.91	0.52
3:Z:381:GLU:O	3:Z:385:SER:OG	2.26	0.52
3:b:36:PRO:HD2	3:b:151:ARG:HD2	1.92	0.52
3:b:155:VAL:HG13	3:b:166:ILE:HG22	1.91	0.52
3:f:235:HIS:CD2	3:f:408:HIS:HA	2.45	0.52
3:h:169:LYS:HD3	3:h:201:TYR:CZ	2.45	0.52
2:k:118:GLU:OE1	2:k:118:GLU:N	2.42	0.52
2:m:10:ILE:O	2:m:14:ILE:HD12	2.10	0.52
1:B:255:HIS:CE1	1:B:257:LEU:HD23	2.45	0.52
3:c:376:TYR:OH	3:c:415:GLY:O	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:288:VAL:HA	3:d:315:VAL:HA	1.91	0.52
3:e:247:ALA:HB1	3:f:34:VAL:HG21	1.92	0.52
1:J:69:ARG:N	1:J:72:GLU:OE2	2.29	0.52
2:P:75:PHE:HB3	2:P:84:TRP:CD1	2.45	0.52
2:Q:156:GLU:OE1	2:Q:159:ARG:NH2	2.42	0.52
3:f:318:TYR:OH	3:g:315:VAL:O	2.27	0.52
3:i:312:ALA:C	3:i:314:ALA:H	2.16	0.52
1:B:214:LEU:HD11	1:B:236:LEU:HD13	1.92	0.52
2:R:143:ALA:HA	2:R:146:ILE:HG22	1.92	0.52
3:Z:206:ARG:NE	3:Z:213:GLU:OE2	2.42	0.52
3:b:254:ARG:HH12	3:c:41:ARG:NH1	2.04	0.52
3:d:276:LEU:O	3:d:280:GLU:HG3	2.09	0.52
3:f:454:MET:HA	3:f:457:ILE:HG22	1.92	0.52
3:g:292:LYS:HZ1	3:g:312:ALA:HB3	1.75	0.52
2:m:144:GLN:NE2	2:m:148:GLN:OE1	2.43	0.52
1:B:292:LYS:HG2	1:B:294:TRP:HD1	1.75	0.52
2:P:12:ARG:NH1	2:Q:35:GLU:OE1	2.43	0.52
2:W:53:TRP:N	2:W:107:LEU:O	2.42	0.52
3:Y:6:ALA:HA	3:Y:201:TYR:CE2	2.45	0.52
3:Z:451:PRO:HA	3:Z:454:MET:HE2	1.91	0.52
3:c:392:LEU:HD12	3:c:409:LYS:HZ3	1.75	0.52
3:d:221:ILE:HG13	3:d:226:VAL:HG11	1.92	0.52
3:i:263:ASP:OD2	3:j:50:SER:OG	2.25	0.52
3:i:342:GLN:NE2	3:j:346:TYR:OH	2.41	0.52
3:j:5:ALA:HA	3:j:8:LEU:HD13	1.91	0.52
2:l:120:ALA:HA	2:l:123:VAL:HG22	1.92	0.52
2:R:155:ASN:O	2:R:159:ARG:HG2	2.10	0.52
2:U:50:PHE:O	2:U:111:ARG:NH1	2.43	0.52
2:V:4:LEU:HD21	2:V:21:SER:HA	1.92	0.52
2:X:127:GLN:HG3	2:X:150:LEU:HD11	1.92	0.52
3:Y:304:MET:HG2	3:j:286:ASN:HD21	1.75	0.52
3:e:7:MET:SD	3:e:7:MET:N	2.83	0.52
3:g:444:LEU:CD2	3:g:445:ASP:N	2.67	0.52
3:h:28:THR:HG21	3:h:56:VAL:HG21	1.92	0.52
1:A:91:LEU:HD11	1:A:307:PHE:HB2	1.92	0.51
1:N:132:ILE:HD11	1:N:261:PHE:HD2	1.75	0.51
1:N:157:LYS:HA	1:N:324:GLU:HB3	1.91	0.51
2:S:149:GLU:HB3	2:S:153:TYR:CZ	2.44	0.51
2:W:69:PRO:O	2:W:72:THR:OG1	2.23	0.51
3:f:179:GLU:O	3:f:183:GLN:N	2.36	0.51
1:A:334:THR:HG22	1:L:171:LYS:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:GLU:OE2	1:M:174:ARG:NE	2.39	0.51
1:J:172:ILE:HG21	1:J:208:LEU:HD11	1.93	0.51
3:Y:310:GLY:H	3:j:287:LEU:HD22	1.75	0.51
3:Y:404:ILE:HB	3:Y:407:GLN:HG2	1.91	0.51
3:a:168:LEU:HB3	3:a:202:THR:HB	1.93	0.51
3:e:410:PRO:HB2	3:f:114:GLN:HE21	1.75	0.51
1:A:31:ASP:HB2	1:L:59:ARG:HG3	1.92	0.51
1:D:158:LEU:HD11	1:D:171:LYS:HE3	1.92	0.51
1:E:62:ASN:OD1	1:E:63:VAL:N	2.43	0.51
2:S:10:ILE:O	2:S:14:ILE:HG12	2.11	0.51
2:T:106:ARG:NH2	3:i:296:VAL:HG21	2.25	0.51
2:T:130:LEU:HD12	2:T:146:ILE:HG22	1.91	0.51
2:V:120:ALA:O	2:V:124:ILE:HG12	2.10	0.51
3:Y:106:ARG:HH22	3:j:79:LEU:HD21	1.76	0.51
3:b:244:TRP:HD1	3:b:245:ASN:HB2	1.74	0.51
3:c:449:SER:HB2	3:c:451:PRO:HD2	1.92	0.51
3:d:17:VAL:HG11	3:d:252:TYR:HD2	1.76	0.51
3:e:276:LEU:HD23	3:f:284:VAL:HG11	1.91	0.51
3:i:416:LEU:HD12	3:i:417:PRO:HD2	1.93	0.51
1:B:171:LYS:O	1:B:175:MET:HG2	2.10	0.51
1:O:87:THR:O	1:O:311:ASN:ND2	2.41	0.51
2:W:111:ARG:HD3	2:W:115:HIS:HD1	1.76	0.51
3:Y:76:ARG:NH2	3:j:462:SER:HB3	2.24	0.51
3:Y:168:LEU:HB3	3:Y:202:THR:HB	1.93	0.51
3:Z:378:LEU:O	3:Z:382:ASN:ND2	2.43	0.51
3:d:35:ASP:HB3	3:d:38:SER:HB2	1.92	0.51
1:F:200:MET:HB2	1:F:272:ILE:HG22	1.93	0.51
1:M:86:LEU:HD21	1:M:311:ASN:HB3	1.92	0.51
3:Y:276:LEU:HD23	3:Z:284:VAL:HG21	1.93	0.51
3:e:14:ASP:HB3	3:e:17:VAL:HG12	1.91	0.51
3:e:307:TYR:H	3:e:310:GLY:HA3	1.76	0.51
3:h:13:ARG:NH2	3:h:150:LEU:O	2.43	0.51
2:l:68:LEU:HD21	2:l:84:TRP:HE1	1.76	0.51
1:I:56:ARG:HH12	1:I:83:LYS:HD2	1.76	0.51
1:I:111:ARG:NH2	3:d:19:SER:OG	2.43	0.51
1:L:209:LEU:HA	1:L:215:MET:HE3	1.92	0.51
2:P:4:LEU:HD21	2:P:22:MET:HB2	1.93	0.51
3:a:404:ILE:HB	3:a:407:GLN:HG2	1.90	0.51
3:d:156:ARG:HG2	3:d:165:ASP:HB3	1.92	0.51
3:e:18:GLU:O	3:e:22:ILE:HG12	2.10	0.51
3:i:35:ASP:OD1	3:i:151:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:PHE:HB2	1:B:74:LEU:HD11	1.93	0.51
1:B:141:ASP:HA	1:B:152:PRO:HB3	1.93	0.51
1:G:244:THR:HG22	1:G:246:ARG:H	1.76	0.51
3:a:120:VAL:O	3:a:124:VAL:HG23	2.11	0.51
3:g:458:TRP:CE3	3:g:463:VAL:CG1	2.93	0.51
3:i:85:ARG:NH1	3:i:86:GLU:OE2	2.44	0.51
3:j:453:MET:O	3:j:457:ILE:HG12	2.10	0.51
1:C:205:PHE:HE2	1:C:233:VAL:HB	1.75	0.51
1:G:100:HIS:HB3	2:X:176:SER:HB3	1.93	0.51
1:K:203:ARG:HD2	1:K:328:ILE:HG13	1.92	0.51
2:P:39:GLN:OE1	2:P:127:GLN:HB3	2.10	0.51
2:Q:69:PRO:HG2	2:Q:109:LEU:HD21	1.91	0.51
2:R:12:ARG:NH1	2:S:38:ASP:OD2	2.24	0.51
2:S:184:THR:OXT	3:f:20:ARG:NE	2.41	0.51
3:Z:13:ARG:NH2	3:Z:18:GLU:OE2	2.44	0.51
3:a:125:ILE:O	3:a:129:ILE:HD12	2.10	0.51
3:j:266:LYS:HE2	3:j:270:LEU:HD11	1.91	0.51
2:m:134:THR:HG23	2:m:139:PRO:HG3	1.92	0.51
1:A:31:ASP:HB3	1:L:316:ARG:HH21	1.74	0.51
1:B:17:ALA:H	1:H:78:ARG:NH1	2.07	0.51
2:Q:9:VAL:O	2:Q:13:LYS:HG2	2.10	0.51
2:S:169:THR:HG23	2:S:171:ALA:H	1.76	0.51
2:X:10:ILE:HG22	2:X:129:ALA:HB2	1.93	0.51
3:Z:277:TYR:CE1	3:a:284:VAL:HG22	2.46	0.51
3:Z:287:LEU:HB2	3:Z:316:ARG:HG2	1.92	0.51
3:Z:409:LYS:N	3:Z:410:PRO:HD3	2.24	0.51
3:e:243:THR:HG21	3:e:246:LEU:HB2	1.93	0.51
3:f:133:ASN:HD21	3:f:252:TYR:HB3	1.76	0.51
3:Y:409:LYS:HG3	3:Y:409:LYS:O	2.11	0.51
3:Y:434:VAL:HG13	3:Z:429:LEU:HD21	1.92	0.51
3:d:444:LEU:CB	3:e:454:MET:HE1	2.41	0.51
3:f:125:ILE:O	3:f:129:ILE:HD12	2.11	0.51
3:i:103:ARG:HA	3:i:106:ARG:NH1	2.24	0.51
2:k:170:GLN:H	2:k:170:GLN:CD	2.19	0.51
2:k:179:ARG:HG2	2:k:179:ARG:HH11	1.75	0.51
2:m:127:GLN:HG2	2:m:150:LEU:HD21	1.93	0.51
1:J:157:LYS:HA	1:J:324:GLU:HB2	1.93	0.50
2:Q:184:THR:OG1	3:d:20:ARG:NH2	2.38	0.50
3:Y:191:ASN:C	3:Y:192:LEU:HD23	2.35	0.50
3:j:329:ILE:O	3:j:332:SER:OG	2.22	0.50
2:m:4:LEU:HD11	2:m:21:SER:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:SER:OG	1:D:265:ALA:N	2.44	0.50
1:M:25:GLU:OE2	1:M:25:GLU:N	2.34	0.50
2:R:171:ALA:HB1	2:R:179:ARG:HH12	1.75	0.50
2:S:127:GLN:HG3	2:S:150:LEU:HD21	1.93	0.50
2:S:134:THR:OG1	2:S:139:PRO:HG3	2.11	0.50
3:d:301:ASP:OD1	3:d:301:ASP:N	2.44	0.50
3:e:174:SER:HB2	3:e:192:LEU:HD13	1.92	0.50
3:f:155:VAL:HG21	3:f:241:VAL:HG21	1.92	0.50
3:g:67:LEU:HD23	3:g:376:TYR:CE1	2.46	0.50
3:h:250:GLU:OE2	3:i:41:ARG:NH1	2.44	0.50
3:i:55:LEU:HD12	3:i:344:PHE:HB2	1.92	0.50
1:A:54:VAL:HG13	1:F:24:GLU:HA	1.94	0.50
1:B:131:LEU:HA	1:B:134:VAL:HG12	1.93	0.50
1:B:206:SER:OG	1:K:177:ARG:NE	2.43	0.50
1:C:82:ASP:HB3	1:C:146:LEU:HD11	1.92	0.50
1:E:174:ARG:HH21	1:J:334:THR:HA	1.76	0.50
1:E:297:ASN:HB3	1:F:294:TRP:CE2	2.46	0.50
1:G:108:PHE:HE2	1:G:110:MET:HE2	1.76	0.50
2:U:123:VAL:HG21	2:U:157:LEU:HD22	1.93	0.50
2:V:163:ARG:NE	3:Z:307:TYR:HE1	2.09	0.50
2:V:172:LYS:HG2	3:Y:298:ASP:OD1	2.11	0.50
3:c:18:GLU:O	3:c:22:ILE:HG12	2.11	0.50
3:c:403:LEU:HB3	3:c:406:LYS:HG3	1.93	0.50
3:e:208:LYS:NZ	3:e:209:GLY:O	2.44	0.50
3:e:318:TYR:CE1	3:f:311:GLY:HA3	2.47	0.50
3:j:162:ARG:NH1	3:j:206:ARG:HH11	2.08	0.50
2:l:122:ARG:NH2	2:l:153:TYR:HB3	2.26	0.50
2:l:173:ARG:HG2	2:l:177:ARG:HH21	1.76	0.50
1:B:54:VAL:HG13	1:G:24:GLU:HG2	1.93	0.50
1:D:43:LEU:HB2	1:D:277:PRO:HB3	1.92	0.50
1:E:93:TYR:HE1	1:O:68:ARG:HB3	1.75	0.50
1:I:170:ASP:HB3	1:I:174:ARG:NH2	2.26	0.50
2:P:180:ARG:HB3	2:P:180:ARG:HH11	1.77	0.50
2:V:143:ALA:HA	2:V:146:ILE:HG22	1.93	0.50
2:X:153:TYR:HE1	2:k:42:GLN:HG3	1.77	0.50
3:Y:430:ASN:O	3:Y:434:VAL:HG23	2.10	0.50
3:e:297:ASP:OD1	3:e:315:VAL:HG21	2.11	0.50
1:A:177:ARG:O	1:A:177:ARG:HD2	2.11	0.50
1:J:68:ARG:NH2	1:J:69:ARG:O	2.45	0.50
1:J:279:LYS:HE2	1:J:316:ARG:HG3	1.92	0.50
3:e:416:LEU:HD22	3:e:419:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:LYS:HG2	1:M:235:ILE:HG21	1.92	0.50
1:H:279:LYS:O	1:H:315:ARG:NE	2.37	0.50
1:I:62:ASN:HB2	1:I:149:ALA:HB2	1.93	0.50
1:O:192:VAL:HG22	1:O:276:LEU:HD21	1.93	0.50
2:V:160:MET:HE1	2:W:74:ALA:HB2	1.93	0.50
3:b:65:ARG:NE	3:b:65:ARG:HA	2.26	0.50
3:h:37:MET:O	3:h:171:ARG:NH1	2.45	0.50
1:B:177:ARG:HD3	1:G:209:LEU:HD12	1.94	0.50
1:B:181:GLU:HA	1:B:184:ILE:HD12	1.93	0.50
1:D:43:LEU:HD13	1:D:275:PHE:HZ	1.76	0.50
1:K:113:GLU:OE1	1:K:113:GLU:N	2.45	0.50
2:T:121:GLN:HA	2:T:124:ILE:HD12	1.94	0.50
2:U:43:LEU:HD22	2:U:124:ILE:HD11	1.92	0.50
3:Y:22:ILE:HD11	3:Y:151:ARG:HH12	1.75	0.50
3:Z:165:ASP:OD1	3:Z:203:HIS:NE2	2.45	0.50
3:Z:261:ILE:HG21	2:k:184:THR:HG21	1.94	0.50
3:Z:404:ILE:HD11	3:Z:407:GLN:HB2	1.94	0.50
3:f:373:GLY:HA3	3:g:57:ASN:OD1	2.12	0.50
3:g:292:LYS:NZ	3:g:312:ALA:HB3	2.27	0.50
3:h:374:GLY:HA3	3:i:122:THR:HG21	1.94	0.50
3:i:243:THR:O	3:i:382:ASN:ND2	2.44	0.50
3:j:274:LEU:O	3:j:278:GLU:HG3	2.10	0.50
2:l:55:ARG:NH2	2:l:78:ASP:OD2	2.45	0.50
1:C:21:ILE:HD12	1:I:56:ARG:HH22	1.76	0.50
1:N:91:LEU:HD21	1:N:307:PHE:HB2	1.93	0.50
2:Q:71:GLY:O	2:Q:110:SER:N	2.45	0.50
2:R:112:GLU:O	2:R:116:ILE:HG12	2.12	0.50
2:R:119:ILE:HD11	2:R:156:GLU:HG2	1.93	0.50
2:S:3:LEU:HG	2:S:113:TRP:CD1	2.47	0.50
2:T:115:HIS:ND1	2:T:115:HIS:O	2.42	0.50
3:Y:217:LEU:HB2	3:Y:232:TRP:HH2	1.76	0.50
3:c:136:LEU:HD11	3:c:145:VAL:HB	1.94	0.50
3:d:464:ASP:N	3:d:464:ASP:OD1	2.45	0.50
3:f:208:LYS:HA	3:f:213:GLU:HG3	1.94	0.50
3:f:333:LEU:O	3:f:337:VAL:HG22	2.11	0.50
3:h:273:LYS:NZ	3:i:279:LEU:HA	2.27	0.50
2:m:64:GLY:HA3	2:m:98:ARG:HD3	1.94	0.50
1:C:61:GLY:N	1:C:80:VAL:O	2.44	0.50
1:E:130:CYS:O	1:E:134:VAL:HG23	2.12	0.50
1:E:218:GLU:HB3	1:J:217:VAL:HG12	1.94	0.50
2:Q:11:LEU:HA	2:Q:14:ILE:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:68:PHE:CD2	3:Y:121:LEU:HD13	2.46	0.50
3:Z:233:PRO:HG2	3:Z:236:LEU:HD12	1.94	0.50
3:b:206:ARG:HE	3:b:234:ILE:HD11	1.77	0.50
3:d:320:ARG:HD2	3:e:317:ALA:HB2	1.92	0.50
3:f:167:VAL:HG22	3:f:203:HIS:CE1	2.47	0.50
3:i:4:THR:HG22	3:i:7:MET:HE1	1.94	0.50
3:i:28:THR:HG21	3:i:56:VAL:HG21	1.94	0.50
2:l:9:VAL:HA	2:l:12:ARG:HG2	1.94	0.50
1:A:37:THR:O	1:A:39:LYS:HE2	2.12	0.49
1:E:175:MET:HG2	1:J:334:THR:HG21	1.93	0.49
2:P:49:TRP:H	2:P:161:HIS:HD2	1.60	0.49
2:T:4:LEU:HB2	2:T:22:MET:HE2	1.94	0.49
3:a:274:LEU:HD21	3:a:330:GLN:HG3	1.94	0.49
3:b:240:ILE:HG22	3:b:242:PRO:HD3	1.94	0.49
3:c:307:TYR:HE1	2:k:162:THR:HG23	1.76	0.49
3:d:445:ASP:OD1	3:d:445:ASP:C	2.55	0.49
3:i:192:LEU:HD11	3:i:198:VAL:HB	1.94	0.49
2:k:156:GLU:HA	2:k:159:ARG:HH11	1.77	0.49
2:S:44:LEU:HD11	2:S:116:ILE:HD11	1.94	0.49
3:Y:12:LEU:HD11	3:Y:156:ARG:HB2	1.93	0.49
3:Z:74:PHE:CZ	3:Z:112:LEU:HD13	2.47	0.49
3:Z:408:HIS:O	3:Z:409:LYS:HG2	2.12	0.49
3:d:307:TYR:HA	2:l:162:THR:HG21	1.94	0.49
3:g:206:ARG:NE	3:g:213:GLU:OE2	2.44	0.49
3:h:244:TRP:CE2	3:h:375:THR:HG21	2.47	0.49
2:k:111:ARG:HD2	2:k:115:HIS:CE1	2.47	0.49
1:D:133:GLN:NE2	1:D:312:ILE:O	2.44	0.49
3:Z:300:GLN:HB2	3:Z:303:GLU:HB3	1.94	0.49
3:Z:446:PRO:O	3:Z:447:ARG:CG	2.60	0.49
3:a:18:GLU:O	3:a:22:ILE:HG12	2.12	0.49
3:d:330:GLN:O	3:d:334:GLN:HG2	2.12	0.49
3:f:285:LEU:HD21	3:g:301:ASP:HA	1.94	0.49
3:h:336:VAL:O	3:h:340:LEU:HG	2.11	0.49
3:h:380:ALA:HB1	3:h:414:THR:HG22	1.95	0.49
1:D:100:HIS:HB2	1:D:300:PHE:CE1	2.47	0.49
1:F:128:GLN:O	1:F:132:ILE:HG12	2.12	0.49
1:N:299:LYS:HG3	1:N:299:LYS:O	2.12	0.49
2:P:53:TRP:CH2	2:Q:95:GLY:HA3	2.47	0.49
2:S:1:MET:O	2:S:121:GLN:NE2	2.33	0.49
3:f:318:TYR:OH	3:g:315:VAL:HG23	2.12	0.49
3:g:277:TYR:CD2	3:g:326:MET:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j:173:LYS:NZ	3:j:196:GLY:O	2.34	0.49
1:A:26:HIS:HE1	3:Y:194:GLY:HA2	1.76	0.49
1:C:184:ILE:HG22	1:C:189:GLY:HA2	1.93	0.49
1:G:46:ILE:HD12	1:G:46:ILE:H	1.76	0.49
1:G:104:TRP:CH2	2:X:171:ALA:HA	2.48	0.49
3:Y:458:TRP:HE3	3:Y:463:VAL:HG21	1.77	0.49
3:Z:278:GLU:HG2	3:Z:326:MET:HE3	1.94	0.49
3:e:168:LEU:HB3	3:e:202:THR:HB	1.94	0.49
3:e:434:VAL:HG12	3:e:457:ILE:HD11	1.93	0.49
3:g:323:TYR:HA	3:g:326:MET:HE3	1.94	0.49
3:h:249:GLY:HA3	3:i:36:PRO:HB3	1.95	0.49
3:j:103:ARG:O	3:j:107:LYS:HG2	2.13	0.49
1:C:4:LEU:HA	1:C:7:LEU:HD13	1.93	0.49
1:D:95:ARG:NE	1:D:305:ASP:OD1	2.46	0.49
1:E:29:ILE:HD11	1:O:47:ARG:HH22	1.78	0.49
1:E:87:THR:O	1:E:311:ASN:ND2	2.45	0.49
1:E:204:VAL:O	1:E:208:LEU:HG	2.13	0.49
1:F:44:MET:HE1	1:F:126:PHE:HE1	1.77	0.49
1:G:220:GLN:HG3	1:G:224:ALA:HA	1.94	0.49
1:I:115:ALA:HB2	1:I:304:LEU:HD21	1.95	0.49
1:N:82:ASP:OD1	1:N:83:LYS:N	2.45	0.49
2:W:178:TRP:CZ3	3:Y:275:GLY:HA3	2.47	0.49
3:g:82:ALA:O	3:g:85:ARG:N	2.45	0.49
3:h:292:LYS:NZ	3:h:309:PRO:HB2	2.27	0.49
2:l:173:ARG:HG3	2:l:177:ARG:HE	1.77	0.49
1:E:221:ALA:HB1	1:J:224:ALA:HB1	1.93	0.49
1:I:168:ALA:O	1:I:172:ILE:HG12	2.13	0.49
2:R:35:GLU:O	2:R:39:GLN:HG2	2.12	0.49
2:V:179:ARG:HH12	2:V:182:LEU:HD23	1.78	0.49
2:V:179:ARG:NE	2:V:179:ARG:HA	2.26	0.49
2:X:93:ASN:OD1	2:X:94:THR:N	2.44	0.49
3:Z:300:GLN:OE1	3:Z:300:GLN:N	2.45	0.49
3:b:14:ASP:OD2	3:b:16:SER:OG	2.27	0.49
3:c:32:LEU:HD22	3:c:127:LEU:HD13	1.94	0.49
3:c:296:VAL:HG21	3:c:307:TYR:HE2	1.76	0.49
3:e:135:LEU:HD22	3:e:148:TRP:HE3	1.76	0.49
3:j:5:ALA:HB3	3:j:220:GLU:OE2	2.12	0.49
1:C:133:GLN:HG3	1:C:312:ILE:HB	1.95	0.49
1:E:139:ALA:HB2	1:E:155:LEU:HD22	1.95	0.49
1:F:209:LEU:HA	1:F:215:MET:HE3	1.94	0.49
1:G:87:THR:O	1:G:311:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:49:TRP:CD1	2:R:161:HIS:HA	2.48	0.49
2:R:60:PRO:HB3	2:R:66:ILE:HG13	1.94	0.49
2:U:83:GLN:NE2	2:U:84:TRP:O	2.46	0.49
2:W:44:LEU:HD23	2:W:110:SER:HA	1.95	0.49
3:Z:451:PRO:HA	3:Z:454:MET:HG2	1.94	0.49
3:a:225:ARG:HH21	3:a:229:GLU:HB2	1.77	0.49
3:e:276:LEU:CD2	3:f:284:VAL:HG11	2.43	0.49
3:e:438:LEU:HD11	3:f:428:MET:HE2	1.94	0.49
3:f:454:MET:O	3:f:458:TRP:HD1	1.94	0.49
3:h:13:ARG:NH1	3:h:153:TYR:O	2.46	0.49
3:h:339:ARG:NH2	3:i:54:LEU:HD23	2.28	0.49
2:k:2:LEU:HD23	2:k:2:LEU:H	1.77	0.49
1:C:275:PHE:HB2	1:C:280:THR:HG21	1.94	0.49
1:E:46:ILE:O	3:h:41:ARG:NH2	2.46	0.49
1:G:88:VAL:HG23	1:G:311:ASN:HB2	1.95	0.49
1:O:91:LEU:HB2	1:O:309:MET:HE3	1.95	0.49
2:R:26:TYR:HD1	2:R:27:PRO:HD2	1.77	0.49
2:S:13:LYS:HE2	2:S:126:HIS:HD2	1.78	0.49
3:Z:285:LEU:HD12	3:a:306:ASP:HB2	1.94	0.49
3:c:308:VAL:HB	3:c:309:PRO:HD3	1.95	0.49
3:d:168:LEU:HB3	3:d:202:THR:HB	1.94	0.49
1:C:198:THR:HB	1:C:241:VAL:HG12	1.94	0.49
1:C:220:GLN:HE22	1:C:226:ASN:HB2	1.78	0.49
1:E:294:TRP:NE1	1:E:305:ASP:OD2	2.43	0.49
1:K:90:THR:HG21	1:K:257:LEU:HA	1.94	0.49
2:U:39:GLN:OE1	2:U:127:GLN:NE2	2.36	0.49
3:b:270:LEU:HB3	3:b:333:LEU:HD21	1.95	0.49
3:c:290:GLU:HG2	3:d:309:PRO:HD2	1.94	0.49
3:d:444:LEU:HD22	3:e:454:MET:HE1	1.95	0.49
1:B:128:GLN:HE22	1:B:132:ILE:HD11	1.77	0.48
1:B:311:ASN:OD1	1:B:312:ILE:N	2.44	0.48
2:Q:173:ARG:HH22	2:Q:177:ARG:NH2	2.06	0.48
2:W:168:ASN:HD22	3:Z:298:ASP:HB3	1.77	0.48
2:X:159:ARG:HH11	3:a:290:GLU:HG2	1.78	0.48
3:Z:249:GLY:HA3	3:a:36:PRO:HA	1.94	0.48
3:Z:287:LEU:HD11	3:Z:318:TYR:HA	1.95	0.48
3:a:306:ASP:OD1	3:a:307:TYR:N	2.31	0.48
3:a:339:ARG:HH11	3:a:339:ARG:HG3	1.78	0.48
3:c:373:GLY:HA3	3:d:57:ASN:HB3	1.95	0.48
3:d:97:VAL:HG12	3:d:399:LEU:HD11	1.95	0.48
3:d:307:TYR:O	2:l:159:ARG:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:177:ARG:HG3	2:k:180:ARG:HH21	1.78	0.48
1:A:93:TYR:OH	1:L:75:GLU:N	2.46	0.48
1:C:93:TYR:HA	1:C:307:PHE:HB3	1.95	0.48
1:M:87:THR:O	1:M:311:ASN:ND2	2.37	0.48
1:N:158:LEU:HD11	1:N:171:LYS:HE3	1.94	0.48
2:R:162:THR:HG21	3:g:288:VAL:HG11	1.95	0.48
3:Y:232:TRP:HD1	3:Y:233:PRO:O	1.96	0.48
3:Z:277:TYR:HE2	3:Z:329:ILE:HG13	1.78	0.48
3:b:18:GLU:O	3:b:22:ILE:HG12	2.12	0.48
3:g:273:LYS:HZ1	3:h:283:GLU:HA	1.78	0.48
2:k:9:VAL:O	2:k:13:LYS:HG2	2.13	0.48
1:D:38:SER:O	3:e:7:MET:HG2	2.14	0.48
1:F:97:GLN:HE22	1:F:299:LYS:HD3	1.77	0.48
1:G:76:ARG:NE	1:G:76:ARG:HA	2.28	0.48
1:G:285:GLN:OE1	1:G:285:GLN:N	2.42	0.48
1:G:292:LYS:HG3	1:G:307:PHE:HE1	1.77	0.48
1:I:49:LEU:N	1:I:285:GLN:O	2.46	0.48
1:I:158:LEU:HB2	1:I:175:MET:HE1	1.94	0.48
1:I:269:GLU:O	1:I:325:LEU:HB2	2.13	0.48
1:L:169:ALA:O	1:L:173:VAL:HG23	2.14	0.48
1:N:255:HIS:N	1:N:262:ASN:OD1	2.40	0.48
2:Q:183:ARG:HA	3:e:45:GLU:HA	1.96	0.48
3:Y:166:ILE:HD12	3:Y:241:VAL:HG11	1.95	0.48
3:Z:184:ASP:H	3:Z:187:ARG:NH1	2.11	0.48
3:a:124:VAL:HG21	3:a:136:LEU:HD21	1.94	0.48
3:a:277:TYR:CE2	3:b:284:VAL:HG22	2.48	0.48
3:d:13:ARG:HG2	3:d:154:ALA:HB2	1.95	0.48
3:d:287:LEU:HD21	3:e:312:ALA:HA	1.95	0.48
3:e:25:ALA:HB2	3:e:33:MET:HE1	1.95	0.48
3:e:164:MET:N	3:e:164:MET:SD	2.85	0.48
3:g:111:ARG:HH21	3:g:143:ALA:HB2	1.78	0.48
3:j:8:LEU:HA	3:j:11:LYS:HG2	1.96	0.48
3:j:388:ALA:O	3:j:392:LEU:HB2	2.14	0.48
3:j:397:ASP:OD1	3:j:398:ALA:N	2.37	0.48
1:H:165:ALA:HB1	1:H:210:GLU:HG3	1.94	0.48
1:M:201:SER:HB2	1:M:271:GLN:HB3	1.95	0.48
1:N:59:ARG:HH12	1:N:84:TRP:HD1	1.61	0.48
1:O:263:VAL:HG13	1:O:267:GLU:HB2	1.95	0.48
2:T:12:ARG:NH1	2:U:34:PRO:HB2	2.29	0.48
3:Y:133:ASN:HD21	3:Y:252:TYR:HB3	1.78	0.48
3:Y:277:TYR:CZ	3:Z:284:VAL:HG12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:375:THR:HG23	3:b:378:LEU:HD23	1.96	0.48
3:b:381:GLU:O	3:b:385:SER:OG	2.30	0.48
3:e:308:VAL:O	3:e:314:ALA:HB2	2.14	0.48
3:a:206:ARG:HH11	3:a:234:ILE:HG12	1.79	0.48
3:c:4:THR:HG22	3:c:7:MET:HE1	1.95	0.48
3:e:156:ARG:HG3	3:e:251:HIS:CE1	2.49	0.48
3:f:447:ARG:HH11	3:f:447:ARG:HG3	1.79	0.48
2:m:143:ALA:HA	2:m:146:ILE:HG22	1.94	0.48
1:C:228:TYR:HB3	1:M:219:TYR:HB3	1.94	0.48
1:D:97:GLN:HG3	1:D:303:VAL:HG22	1.94	0.48
1:O:271:GLN:HG3	1:O:328:ILE:HG21	1.95	0.48
2:P:149:GLU:HG2	2:P:153:TYR:CE2	2.49	0.48
2:W:172:LYS:HE3	3:Z:298:ASP:HA	1.96	0.48
3:a:80:THR:HG22	3:a:82:ALA:H	1.78	0.48
3:a:285:LEU:HD12	3:b:302:ALA:HA	1.95	0.48
3:d:325:LYS:O	3:d:329:ILE:HG12	2.13	0.48
3:h:133:ASN:ND2	3:h:252:TYR:HB3	2.28	0.48
3:j:451:PRO:HA	3:j:454:MET:HG2	1.95	0.48
1:D:190:ASP:HB3	3:e:193:SER:HB3	1.95	0.48
1:E:211:HIS:CE1	1:E:213:LYS:HB2	2.49	0.48
1:I:50:ARG:HD3	3:d:222:ASP:OD2	2.14	0.48
1:I:274:LEU:O	1:I:321:GLY:N	2.46	0.48
2:P:56:HIS:HD2	2:P:58:LEU:HG	1.78	0.48
2:T:26:TYR:HD1	2:T:27:PRO:HD2	1.79	0.48
2:X:40:ARG:HD3	2:X:116:ILE:HD11	1.96	0.48
3:Y:124:VAL:HG21	3:Y:136:LEU:HD13	1.95	0.48
3:Z:168:LEU:HB3	3:Z:202:THR:HB	1.95	0.48
3:a:27:THR:HG22	3:a:28:THR:HG23	1.96	0.48
3:c:108:ALA:HB1	3:c:391:CYS:HB3	1.95	0.48
3:c:263:ASP:OD2	3:d:50:SER:OG	2.21	0.48
3:e:27:THR:HG21	3:e:264:PHE:HB3	1.96	0.48
3:f:274:LEU:HB2	3:f:329:ILE:HG21	1.96	0.48
1:B:232:ARG:HG2	1:B:232:ARG:HH11	1.78	0.48
1:F:76:ARG:HA	1:F:76:ARG:NE	2.29	0.48
1:H:131:LEU:O	1:H:135:ILE:HG12	2.13	0.48
2:U:73:LEU:HD13	2:U:108:VAL:HG12	1.95	0.48
2:U:143:ALA:HA	2:U:146:ILE:HG12	1.95	0.48
2:V:26:TYR:HD2	2:V:28:THR:HG22	1.79	0.48
3:Z:128:LEU:HD21	3:Z:242:PRO:HB2	1.95	0.48
3:a:225:ARG:HG2	3:a:225:ARG:HH11	1.78	0.48
3:d:84:ARG:HE	3:e:107:LYS:HZ1	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:301:ASP:OD2	2:m:173:ARG:NE	2.24	0.48
3:e:29:LEU:HD12	3:e:31:TYR:CE2	2.48	0.48
3:e:454:MET:HA	3:e:457:ILE:HG22	1.96	0.48
3:g:458:TRP:CE3	3:g:463:VAL:HG13	2.36	0.48
2:k:12:ARG:HH11	2:l:34:PRO:HB2	1.79	0.48
1:G:296:ASP:O	1:G:300:PHE:N	2.47	0.48
2:S:60:PRO:HB3	2:S:66:ILE:HG12	1.96	0.48
2:S:91:ASP:OD1	2:S:92:ALA:N	2.47	0.48
2:W:111:ARG:HD3	2:W:115:HIS:ND1	2.29	0.48
3:c:47:ASP:OD2	3:c:49:GLN:NE2	2.47	0.48
3:c:97:VAL:HA	3:c:400:LEU:HD11	1.95	0.48
3:e:247:ALA:HB3	3:e:250:GLU:HB2	1.95	0.48
3:g:289:ASP:H	3:g:314:ALA:HB1	1.78	0.48
3:h:320:ARG:HD2	3:i:317:ALA:H	1.79	0.48
1:B:217:VAL:HG22	1:K:221:ALA:HB2	1.96	0.48
1:C:94:LEU:HD13	1:M:65:ALA:HA	1.95	0.48
1:E:264:SER:OG	1:E:265:ALA:N	2.47	0.48
3:Y:13:ARG:NH1	3:Y:150:LEU:O	2.41	0.48
3:Z:9:TRP:HD1	3:Z:167:VAL:HG13	1.79	0.48
3:Z:318:TYR:CE1	3:Z:320:ARG:HG2	2.45	0.48
3:f:307:TYR:H	3:f:310:GLY:HA3	1.79	0.48
3:i:448:ILE:HD12	3:i:448:ILE:H	1.79	0.48
3:j:8:LEU:O	3:j:12:LEU:HG	2.14	0.48
1:B:236:LEU:O	1:B:239:VAL:HG22	2.14	0.47
1:C:160:LEU:HD21	1:C:325:LEU:HD12	1.96	0.47
1:D:93:TYR:OH	1:N:75:GLU:OE1	2.30	0.47
1:F:285:GLN:HE21	1:F:288:PRO:HA	1.78	0.47
1:H:281:LEU:HD12	1:H:282:ILE:N	2.29	0.47
2:P:141:GLU:HA	2:P:144:GLN:HG2	1.96	0.47
3:Z:248:PRO:HB2	3:a:36:PRO:HG3	1.96	0.47
3:e:233:PRO:HD2	3:e:236:LEU:HB2	1.96	0.47
3:e:318:TYR:HE2	3:e:320:ARG:HD3	1.78	0.47
3:f:233:PRO:HD2	3:f:236:LEU:HD22	1.96	0.47
3:g:288:VAL:H	3:h:307:TYR:HA	1.79	0.47
3:j:287:LEU:HD21	3:j:318:TYR:CD1	2.49	0.47
1:B:217:VAL:HG23	1:K:218:GLU:O	2.14	0.47
1:H:281:LEU:HD12	1:H:282:ILE:H	1.79	0.47
2:W:179:ARG:C	2:W:181:SER:H	2.21	0.47
3:g:186:MET:HE3	3:g:186:MET:HA	1.94	0.47
3:h:320:ARG:HD2	3:i:317:ALA:N	2.29	0.47
3:j:49:GLN:HG2	3:j:267:LEU:HG	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:ASN:HD21	1:D:148:ASP:HB3	1.79	0.47
1:D:205:PHE:CE1	1:D:233:VAL:HB	2.49	0.47
1:E:102:ASP:O	1:E:106:GLN:HG2	2.15	0.47
1:I:290:GLN:HE21	1:I:307:PHE:HE1	1.62	0.47
2:P:66:ILE:HD11	2:P:99:ILE:HB	1.97	0.47
2:R:141:GLU:OE2	2:S:139:PRO:HD2	2.14	0.47
2:R:159:ARG:O	2:R:163:ARG:HB2	2.14	0.47
2:S:6:ALA:O	2:S:9:VAL:HG12	2.14	0.47
2:U:119:ILE:O	2:U:123:VAL:HG13	2.14	0.47
2:X:98:ARG:O	2:X:99:ILE:HD13	2.14	0.47
3:Y:284:VAL:HG12	3:j:277:TYR:CE1	2.49	0.47
3:Y:389:TYR:HA	3:Y:409:LYS:HZ3	1.79	0.47
3:f:374:GLY:O	3:f:378:LEU:N	2.47	0.47
3:i:288:VAL:HG13	3:i:288:VAL:O	2.14	0.47
1:E:249:THR:HA	1:E:271:GLN:HE22	1.78	0.47
1:G:33:HIS:HD2	1:G:34:PHE:H	1.63	0.47
1:O:255:HIS:CE1	1:O:257:LEU:HD23	2.49	0.47
2:T:10:ILE:HG12	2:T:129:ALA:HB2	1.96	0.47
2:U:175:PHE:HA	3:i:279:LEU:HD12	1.95	0.47
2:W:3:LEU:O	2:W:7:VAL:HG23	2.15	0.47
3:c:438:LEU:HD23	3:d:432:SER:HB2	1.95	0.47
3:e:65:ARG:HG3	3:e:65:ARG:HH11	1.80	0.47
1:A:91:LEU:HD23	1:L:68:ARG:HE	1.79	0.47
1:B:61:GLY:N	1:B:80:VAL:O	2.47	0.47
1:B:118:ASP:HB3	1:B:306:THR:HG21	1.97	0.47
1:B:148:ASP:OD1	1:B:149:ALA:N	2.47	0.47
1:D:220:GLN:OE1	1:D:226:ASN:HB2	2.15	0.47
1:I:170:ASP:HB3	1:I:174:ARG:HH22	1.79	0.47
1:N:176:HIS:O	1:N:180:VAL:HG23	2.14	0.47
2:S:158:SER:O	2:S:162:THR:HG22	2.14	0.47
2:T:163:ARG:HA	3:j:307:TYR:HB3	1.96	0.47
2:V:26:TYR:CD1	2:V:27:PRO:HD2	2.48	0.47
3:Y:370:ASN:CG	3:Z:65:ARG:HH21	2.22	0.47
3:Y:389:TYR:HA	3:Y:409:LYS:NZ	2.29	0.47
3:e:55:LEU:HD21	3:e:341:ASN:OD1	2.14	0.47
3:h:170:GLN:HG3	3:h:172:TYR:CZ	2.49	0.47
3:h:434:VAL:HA	3:i:429:LEU:HD21	1.97	0.47
1:D:230:LYS:NZ	1:N:222:THR:OG1	2.35	0.47
1:E:31:ASP:HB3	1:O:316:ARG:HD3	1.96	0.47
1:F:170:ASP:OD1	1:F:211:HIS:NE2	2.47	0.47
1:I:50:ARG:NE	3:d:192:LEU:HA	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:70:ALA:O	2:l:101:LYS:NZ	2.47	0.47
2:Q:20:PRO:HG2	2:Q:24:GLU:OE2	2.13	0.47
2:Q:140:ASP:OD1	2:Q:142:THR:OG1	2.31	0.47
2:V:11:LEU:HD11	2:V:28:THR:HG21	1.96	0.47
2:W:79:SER:HB2	2:W:82:LEU:HD13	1.97	0.47
3:Z:247:ALA:HB1	3:a:34:VAL:HG11	1.96	0.47
3:e:372:LEU:HB3	3:e:375:THR:HB	1.97	0.47
3:f:154:ALA:O	3:f:166:ILE:HA	2.15	0.47
3:f:242:PRO:HA	3:f:382:ASN:HB2	1.96	0.47
3:i:273:LYS:O	3:i:277:TYR:HD1	1.97	0.47
3:j:392:LEU:HD22	3:j:412:ILE:HD11	1.96	0.47
1:E:308:GLN:HG2	1:E:310:TYR:HD2	1.79	0.47
1:G:91:LEU:HB2	1:G:309:MET:HE3	1.96	0.47
1:G:141:ASP:OD1	1:G:141:ASP:N	2.46	0.47
1:H:158:LEU:HD11	1:H:171:LYS:HB3	1.96	0.47
1:H:192:VAL:HG12	1:H:276:LEU:HD21	1.96	0.47
2:U:165:ARG:HA	2:U:165:ARG:HH11	1.80	0.47
2:V:182:LEU:HD21	3:j:47:ASP:O	2.15	0.47
2:X:9:VAL:HG12	2:X:12:ARG:HH22	1.79	0.47
2:X:179:ARG:O	2:X:183:ARG:N	2.48	0.47
3:Z:155:VAL:HG12	3:Z:252:TYR:CE1	2.50	0.47
3:Z:235:HIS:CE1	3:Z:408:HIS:HA	2.50	0.47
3:Z:244:TRP:CD2	3:Z:375:THR:HG21	2.50	0.47
3:a:155:VAL:HA	3:a:166:ILE:HG22	1.97	0.47
3:d:153:TYR:HB3	3:d:168:LEU:HD13	1.97	0.47
3:e:217:LEU:HD13	3:e:232:TRP:HZ3	1.79	0.47
3:e:408:HIS:CE1	3:e:410:PRO:HB3	2.49	0.47
3:f:345:MET:SD	3:f:371:THR:OG1	2.65	0.47
3:g:305:GLY:HA2	3:g:307:TYR:CE1	2.50	0.47
3:h:58:ASN:OD1	3:h:62:LYS:HE2	2.15	0.47
3:i:249:GLY:HA3	3:j:36:PRO:HA	1.96	0.47
3:i:447:ARG:HD2	3:i:452:LYS:HE3	1.97	0.47
3:j:183:GLN:HG3	3:j:184:ASP:N	2.29	0.47
2:k:69:PRO:O	2:k:72:THR:OG1	2.32	0.47
2:l:26:TYR:HB2	2:l:29:MET:HE1	1.97	0.47
2:m:10:ILE:HG13	2:m:129:ALA:HA	1.97	0.47
1:A:89:ASP:OD1	1:A:90:THR:N	2.48	0.47
1:G:148:ASP:OD1	1:G:149:ALA:N	2.47	0.47
2:P:49:TRP:H	2:P:49:TRP:CD1	2.32	0.47
2:Q:97:ASP:OD1	2:Q:97:ASP:N	2.47	0.47
2:R:40:ARG:HA	2:R:124:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:53:TRP:CZ3	2:V:95:GLY:HA2	2.50	0.47
2:V:145:VAL:HG11	2:W:134:THR:HG21	1.95	0.47
3:Y:188:ALA:HB2	3:Y:224:VAL:HG21	1.97	0.47
3:Y:254:ARG:HH12	3:Z:44:VAL:HG11	1.80	0.47
3:c:55:LEU:HD12	3:c:344:PHE:HB2	1.96	0.47
3:j:78:GLU:OE1	3:j:78:GLU:N	2.41	0.47
1:B:156:GLU:HB2	1:B:323:ILE:HG23	1.96	0.47
1:C:93:TYR:HE1	1:M:68:ARG:HB3	1.78	0.47
1:D:133:GLN:OE1	1:D:133:GLN:HA	2.15	0.47
1:E:59:ARG:HH11	1:E:59:ARG:HG3	1.79	0.47
1:J:44:MET:HG3	1:J:46:ILE:HG13	1.96	0.47
2:X:119:ILE:O	2:X:123:VAL:HG23	2.15	0.47
2:X:167:LEU:HB2	2:k:80:PRO:CD	2.45	0.47
3:b:13:ARG:HH11	3:b:13:ARG:HG3	1.79	0.47
3:c:36:PRO:HG2	3:c:37:MET:HE3	1.97	0.47
3:g:8:LEU:O	3:g:12:LEU:HG	2.15	0.47
3:g:438:LEU:HD22	3:g:453:MET:HE2	1.97	0.47
1:F:50:ARG:HH12	1:F:286:VAL:HG13	1.80	0.47
1:H:190:ASP:N	1:H:190:ASP:OD1	2.45	0.47
2:T:118:GLU:HA	2:T:121:GLN:CD	2.40	0.47
2:U:60:PRO:HB3	2:U:66:ILE:HG13	1.97	0.47
2:U:120:ALA:O	2:U:124:ILE:HG13	2.14	0.47
2:V:94:THR:HG23	2:V:96:ASP:H	1.80	0.47
3:c:267:LEU:HB2	3:c:336:VAL:HG11	1.97	0.47
3:f:416:LEU:HD12	3:f:417:PRO:HD2	1.97	0.47
3:i:287:LEU:HD21	3:i:318:TYR:HD1	1.80	0.47
2:k:40:ARG:O	2:k:44:LEU:HD23	2.15	0.47
2:k:126:HIS:CD2	2:k:150:LEU:HB2	2.50	0.47
2:l:119:ILE:HD13	2:m:45:THR:HG21	1.96	0.47
2:R:55:ARG:NE	2:R:78:ASP:OD2	2.42	0.46
2:S:13:LYS:HE2	2:S:126:HIS:CD2	2.50	0.46
2:V:58:LEU:HD21	2:V:68:LEU:HA	1.96	0.46
2:W:111:ARG:HG2	2:W:111:ARG:HH11	1.79	0.46
3:Y:400:LEU:HD12	3:Y:401:GLN:H	1.78	0.46
3:Z:137:TYR:HE2	3:Z:139:ASP:HB2	1.80	0.46
3:a:183:GLN:O	3:a:187:ARG:HG3	2.15	0.46
3:b:419:LEU:HD13	3:c:65:ARG:HH22	1.80	0.46
3:h:287:LEU:O	3:h:315:VAL:HA	2.14	0.46
3:i:409:LYS:HG3	3:i:409:LYS:O	2.15	0.46
1:D:197:LEU:HD12	1:D:240:LYS:HG3	1.96	0.46
2:Q:155:ASN:HA	3:f:290:GLU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:73:LEU:HD21	2:X:110:SER:HB2	1.97	0.46
3:b:292:LYS:HD3	3:b:292:LYS:HA	1.70	0.46
3:g:331:GLN:O	3:g:334:GLN:HG2	2.16	0.46
3:i:7:MET:N	3:i:7:MET:SD	2.88	0.46
1:B:95:ARG:NH2	1:B:305:ASP:OD2	2.34	0.46
1:H:72:GLU:OE1	1:H:72:GLU:N	2.48	0.46
1:I:38:SER:HB2	1:I:123:ALA:HB1	1.97	0.46
1:J:98:PHE:HB2	1:J:302:TRP:HB2	1.96	0.46
2:U:66:ILE:HD13	2:U:89:VAL:HG21	1.97	0.46
2:X:75:PHE:HD2	2:X:84:TRP:HB2	1.80	0.46
3:a:318:TYR:CD1	3:b:312:ALA:HB1	2.51	0.46
3:b:244:TRP:CE2	3:b:375:THR:HG21	2.50	0.46
3:f:206:ARG:HG3	3:f:234:ILE:HD13	1.96	0.46
3:f:286:ASN:O	3:g:306:ASP:HB3	2.14	0.46
3:g:316:ARG:HH11	3:g:316:ARG:HG3	1.81	0.46
3:i:125:ILE:O	3:i:129:ILE:HG12	2.15	0.46
2:k:44:LEU:O	2:k:51:ASN:ND2	2.48	0.46
1:J:142:ALA:HB2	1:J:152:PRO:HG3	1.96	0.46
1:O:168:ALA:O	1:O:172:ILE:HD12	2.14	0.46
2:Q:119:ILE:HG21	2:Q:160:MET:SD	2.56	0.46
2:R:54:TRP:HE1	2:R:106:ARG:NH2	2.13	0.46
2:T:75:PHE:HB3	2:T:84:TRP:CE3	2.51	0.46
3:Y:169:LYS:HD2	3:Y:201:TYR:CE1	2.50	0.46
3:Y:199:ASP:HB3	3:Y:201:TYR:HE1	1.80	0.46
3:Y:290:GLU:HG3	3:Z:308:VAL:CG1	2.43	0.46
3:Z:37:MET:HE1	3:Z:169:LYS:NZ	2.31	0.46
3:b:14:ASP:O	3:b:18:GLU:HG2	2.16	0.46
3:d:200:LEU:HD12	3:d:221:ILE:HD11	1.97	0.46
3:h:14:ASP:HB3	3:h:17:VAL:HG12	1.96	0.46
3:h:164:MET:HE3	3:i:176:ASP:OD1	2.15	0.46
2:k:9:VAL:HG23	2:k:12:ARG:NH2	2.31	0.46
2:k:59:THR:OG1	2:k:67:ASN:O	2.29	0.46
2:k:79:SER:HB2	2:k:82:LEU:HD23	1.97	0.46
1:D:135:ILE:O	1:D:270:ARG:NH1	2.46	0.46
1:D:292:LYS:N	1:D:305:ASP:O	2.49	0.46
1:H:157:LYS:HB3	1:H:326:LYS:NZ	2.31	0.46
1:H:203:ARG:HH11	1:H:203:ARG:HG3	1.80	0.46
1:N:230:LYS:HB3	1:N:232:ARG:NH2	2.31	0.46
2:S:122:ARG:HH22	2:T:42:GLN:HA	1.81	0.46
2:T:43:LEU:O	2:T:48:TRP:NE1	2.49	0.46
3:a:295:VAL:O	3:a:295:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:399:LEU:HD23	3:c:399:LEU:H	1.81	0.46
3:d:287:LEU:HD12	3:e:306:ASP:O	2.15	0.46
2:k:16:GLU:HG2	2:k:17:LEU:HD23	1.98	0.46
1:A:198:THR:HB	1:A:241:VAL:HG12	1.98	0.46
1:A:249:THR:HG22	1:A:271:GLN:HE22	1.81	0.46
1:C:95:ARG:HD3	1:M:76:ARG:NH1	2.31	0.46
1:D:229:VAL:O	1:N:237:ASN:N	2.49	0.46
1:D:292:LYS:HB3	1:D:305:ASP:HB2	1.98	0.46
1:E:95:ARG:HH21	1:E:303:VAL:HG11	1.80	0.46
1:F:156:GLU:HG3	1:F:175:MET:SD	2.55	0.46
1:H:178:ARG:HH11	1:H:178:ARG:HG3	1.80	0.46
1:J:133:GLN:HG3	1:J:312:ILE:HB	1.96	0.46
1:L:91:LEU:HD23	1:L:309:MET:HE3	1.97	0.46
3:d:12:LEU:HD22	3:d:156:ARG:HB3	1.96	0.46
3:f:449:SER:OG	3:f:451:PRO:HD2	2.15	0.46
3:j:181:TYR:CE1	3:j:200:LEU:HD11	2.51	0.46
3:j:240:ILE:HD12	3:j:386:PRO:HB2	1.96	0.46
1:C:255:HIS:H	1:C:262:ASN:ND2	2.14	0.46
1:D:225:THR:OG1	1:I:229:VAL:HG21	2.16	0.46
1:E:96:HIS:NE2	1:O:63:VAL:HG11	2.31	0.46
1:E:103:GLU:HA	1:E:106:GLN:HG3	1.98	0.46
1:F:216:ASN:HB3	1:F:219:TYR:HD1	1.80	0.46
1:L:295:GLU:HG2	1:L:302:TRP:CH2	2.51	0.46
1:N:178:ARG:HA	1:N:181:GLU:HG2	1.98	0.46
1:O:59:ARG:HH21	1:O:84:TRP:CD1	2.34	0.46
2:P:165:ARG:HE	2:P:168:ASN:HD21	1.64	0.46
2:Q:91:ASP:HB3	2:Q:95:GLY:N	2.29	0.46
3:Y:274:LEU:O	3:Y:278:GLU:HG3	2.16	0.46
3:d:47:ASP:OD1	3:d:48:PHE:N	2.44	0.46
3:e:385:SER:O	3:e:389:TYR:HD1	1.98	0.46
3:f:168:LEU:HB3	3:f:202:THR:OG1	2.16	0.46
3:h:124:VAL:HG21	3:h:136:LEU:HD21	1.98	0.46
3:h:318:TYR:OH	3:i:315:VAL:O	2.30	0.46
3:j:289:ASP:OD2	3:j:316:ARG:NH2	2.49	0.46
1:E:98:PHE:HZ	1:E:114:VAL:HG21	1.81	0.46
1:K:205:PHE:O	1:K:209:LEU:HG	2.16	0.46
1:K:242:LEU:HG	1:K:244:THR:HG23	1.96	0.46
1:L:97:GLN:HG3	1:L:303:VAL:HG22	1.98	0.46
1:N:217:VAL:HA	1:N:220:GLN:HG2	1.98	0.46
1:O:293:LEU:HD21	1:O:304:LEU:HD12	1.98	0.46
3:Y:281:SER:OG	3:Y:320:ARG:NH1	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:25:ALA:HB1	3:a:30:PRO:HA	1.98	0.46
3:b:300:GLN:NE2	3:b:303:GLU:O	2.49	0.46
3:c:345:MET:HB3	3:c:371:THR:HG21	1.98	0.46
1:A:68:ARG:HB3	1:F:91:LEU:HB3	1.97	0.46
1:F:98:PHE:CE2	1:F:111:ARG:HG3	2.51	0.46
1:G:44:MET:HB2	1:G:46:ILE:HD11	1.97	0.46
1:H:104:TRP:O	2:m:180:ARG:NH2	2.49	0.46
2:U:112:GLU:O	2:U:116:ILE:HG12	2.16	0.46
2:W:13:LYS:HE2	2:W:13:LYS:HB2	1.83	0.46
3:a:4:THR:HG23	3:a:6:ALA:H	1.81	0.46
3:c:114:GLN:OE1	3:c:115:ASN:N	2.47	0.46
3:d:318:TYR:CE1	3:d:320:ARG:HB2	2.50	0.46
3:g:59:LEU:HD12	3:g:344:PHE:O	2.14	0.46
3:h:285:LEU:HB3	3:i:306:ASP:HB2	1.97	0.46
1:A:3:PHE:CD2	1:A:7:LEU:HD21	2.52	0.46
1:O:181:GLU:HA	1:O:184:ILE:HD12	1.97	0.46
1:O:236:LEU:O	1:O:239:VAL:HG22	2.15	0.46
2:P:123:VAL:HG12	2:P:127:GLN:OE1	2.16	0.46
2:R:9:VAL:HA	2:R:12:ARG:HG2	1.98	0.46
2:W:56:HIS:HE1	2:W:58:LEU:HD23	1.81	0.46
2:W:114:ASP:OD2	2:W:115:HIS:N	2.49	0.46
3:Y:450:LEU:N	3:Y:451:PRO:HD2	2.30	0.46
3:b:17:VAL:HG11	3:b:252:TYR:HD2	1.81	0.46
3:c:292:LYS:HZ3	3:c:295:VAL:HG22	1.82	0.46
3:d:121:LEU:HD11	3:d:387:LEU:HD11	1.96	0.46
3:d:157:ARG:HG3	3:d:251:HIS:HA	1.98	0.46
3:d:276:LEU:HD23	3:e:284:VAL:HG21	1.97	0.46
3:d:444:LEU:CD2	3:e:454:MET:HE1	2.46	0.46
3:e:128:LEU:HD11	3:e:242:PRO:HB2	1.98	0.46
3:e:240:ILE:HG22	3:e:242:PRO:HD3	1.96	0.46
2:l:165:ARG:NH2	2:l:167:LEU:HD12	2.30	0.46
1:B:94:LEU:HD11	1:B:121:GLU:OE2	2.16	0.45
1:F:42:PRO:HA	3:i:190:ARG:NH1	2.32	0.45
1:F:215:MET:HE2	1:F:215:MET:HB2	1.84	0.45
2:S:11:LEU:HD23	2:S:14:ILE:HD11	1.98	0.45
2:V:39:GLN:HB2	2:V:124:ILE:HG23	1.98	0.45
2:W:57:LYS:HA	2:W:103:VAL:O	2.16	0.45
2:W:122:ARG:HH22	2:X:42:GLN:HA	1.79	0.45
3:a:286:ASN:O	3:b:306:ASP:HB2	2.15	0.45
3:c:9:TRP:CH2	3:c:169:LYS:HD3	2.51	0.45
3:d:327:ALA:HA	3:d:330:GLN:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:55:LEU:HD23	3:f:344:PHE:HB2	1.98	0.45
3:f:383:LEU:O	3:f:387:LEU:HG	2.16	0.45
2:l:3:LEU:O	2:l:7:VAL:HG23	2.16	0.45
1:C:220:GLN:HE21	1:H:229:VAL:HG21	1.81	0.45
1:G:210:GLU:OE1	1:G:210:GLU:N	2.42	0.45
1:H:136:LYS:HE2	1:H:267:GLU:OE1	2.16	0.45
2:Q:141:GLU:O	2:Q:144:GLN:HG3	2.17	0.45
2:V:31:ILE:O	2:V:35:GLU:HG3	2.16	0.45
3:Y:13:ARG:HH22	3:Y:151:ARG:HA	1.81	0.45
3:Y:392:LEU:HD13	3:Y:409:LYS:HD2	1.98	0.45
3:Z:13:ARG:HD2	3:Z:154:ALA:HB2	1.99	0.45
3:b:289:ASP:N	3:b:314:ALA:O	2.46	0.45
3:c:165:ASP:OD2	3:c:203:HIS:NE2	2.48	0.45
3:d:308:VAL:HG13	3:d:311:GLY:N	2.31	0.45
3:e:90:ARG:HD2	3:e:90:ARG:O	2.16	0.45
3:g:63:LEU:HD12	3:g:129:ILE:HD11	1.98	0.45
3:j:168:LEU:HB3	3:j:202:THR:OG1	2.16	0.45
2:k:126:HIS:CE1	2:k:146:ILE:HG23	2.52	0.45
1:A:97:GLN:OE1	1:A:301:SER:OG	2.31	0.45
1:M:150:PHE:HE2	1:M:316:ARG:HH12	1.64	0.45
1:N:131:LEU:O	1:N:135:ILE:HG12	2.17	0.45
2:P:76:TYR:CE1	2:m:160:MET:HE1	2.52	0.45
2:Q:37:GLU:OE2	2:Q:40:ARG:HD3	2.17	0.45
3:b:55:LEU:HB3	3:b:344:PHE:CD2	2.52	0.45
3:c:397:ASP:OD1	3:c:397:ASP:N	2.49	0.45
3:d:103:ARG:HG2	3:d:107:LYS:NZ	2.30	0.45
3:d:277:TYR:CE1	3:e:284:VAL:HG12	2.51	0.45
3:e:69:PRO:HB2	3:e:72:ILE:HB	1.98	0.45
3:f:270:LEU:HD21	3:g:278:GLU:HB3	1.99	0.45
3:i:372:LEU:HG	3:i:375:THR:HB	1.97	0.45
3:j:107:LYS:HA	3:j:110:GLN:HG2	1.98	0.45
3:j:155:VAL:HG22	3:j:166:ILE:HG22	1.98	0.45
1:A:217:VAL:HG12	1:L:221:ALA:HB2	1.98	0.45
1:D:297:ASN:HB3	1:J:294:TRP:CE2	2.52	0.45
1:E:104:TRP:O	1:F:50:ARG:NH2	2.49	0.45
1:K:292:LYS:HB3	1:K:292:LYS:HE2	1.69	0.45
2:R:69:PRO:HG2	2:R:107:LEU:HD21	1.98	0.45
2:V:60:PRO:HD3	2:V:102:PRO:HG3	1.99	0.45
3:Y:451:PRO:HA	3:Y:454:MET:HG2	1.97	0.45
3:b:385:SER:OG	3:b:386:PRO:HD3	2.16	0.45
3:g:26:LYS:O	3:g:47:ASP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:33:MET:O	3:g:151:ARG:NH2	2.43	0.45
2:k:112:GLU:O	2:k:116:ILE:HG12	2.16	0.45
1:C:50:ARG:NH1	3:c:43:VAL:HG13	2.32	0.45
1:I:293:LEU:HD13	1:I:304:LEU:HB2	1.99	0.45
1:N:246:ARG:NE	1:N:246:ARG:HA	2.32	0.45
2:P:85:ASP:OD2	2:m:115:HIS:NE2	2.32	0.45
2:P:107:LEU:HD21	2:P:109:LEU:HD21	1.97	0.45
2:R:42:GLN:O	2:R:45:THR:HG22	2.17	0.45
2:S:26:TYR:CD1	2:S:27:PRO:HD2	2.52	0.45
2:U:79:SER:HB2	2:U:82:LEU:HD13	1.98	0.45
3:a:111:ARG:HH21	3:a:143:ALA:HB2	1.82	0.45
3:b:447:ARG:NH2	3:c:464:ASP:OD2	2.50	0.45
3:d:287:LEU:HD11	3:e:312:ALA:N	2.31	0.45
3:d:434:VAL:HG22	3:e:429:LEU:HD11	1.97	0.45
3:h:28:THR:HG22	3:h:29:LEU:HG	1.99	0.45
3:h:168:LEU:HB3	3:h:202:THR:HB	1.98	0.45
3:h:286:ASN:HB2	3:i:304:MET:HA	1.98	0.45
3:i:186:MET:N	3:i:186:MET:SD	2.90	0.45
3:i:425:VAL:HA	3:i:428:MET:HE2	1.98	0.45
3:j:26:LYS:HA	3:j:30:PRO:HB3	1.98	0.45
2:l:145:VAL:HG21	2:m:134:THR:HG21	1.99	0.45
1:B:180:VAL:O	1:B:184:ILE:HG13	2.17	0.45
1:B:230:LYS:HA	1:K:238:GLY:HA2	1.99	0.45
1:C:298:GLU:OE1	1:D:76:ARG:NH2	2.49	0.45
1:E:40:PHE:O	1:E:44:MET:HG2	2.17	0.45
1:E:68:ARG:HB2	1:J:93:TYR:CD1	2.52	0.45
1:F:99:ASP:HB3	1:F:101:GLN:HG2	1.97	0.45
1:I:87:THR:O	1:I:311:ASN:ND2	2.44	0.45
1:K:98:PHE:HB3	1:K:103:GLU:OE2	2.17	0.45
1:L:316:ARG:HG2	1:L:319:THR:HG23	1.98	0.45
1:N:226:ASN:ND2	1:N:233:VAL:HG13	2.32	0.45
1:N:230:LYS:HB3	1:N:232:ARG:HH21	1.82	0.45
2:T:162:THR:OG1	3:i:288:VAL:HG11	2.16	0.45
2:V:12:ARG:HH11	2:V:18:PRO:HB3	1.81	0.45
3:Z:185:LEU:HD22	3:Z:190:ARG:HB2	1.98	0.45
3:Z:339:ARG:O	3:Z:342:GLN:HG3	2.16	0.45
3:e:177:LEU:HD11	3:e:198:VAL:HG11	1.98	0.45
3:f:284:VAL:O	3:f:284:VAL:HG13	2.16	0.45
3:i:156:ARG:NH1	3:j:173:LYS:HG3	2.29	0.45
2:l:54:TRP:HD1	2:m:92:ALA:HB1	1.82	0.45
2:m:8:ASN:O	2:m:12:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:ALA:O	1:G:173:VAL:HG23	2.17	0.45
1:J:34:PHE:O	1:J:124:ARG:NH2	2.50	0.45
2:P:49:TRP:N	2:P:161:HIS:HD2	2.15	0.45
2:R:111:ARG:HA	2:R:111:ARG:HD3	1.77	0.45
2:W:91:ASP:OD1	2:W:92:ALA:N	2.50	0.45
3:Y:135:LEU:HD12	3:Y:166:ILE:HD11	1.98	0.45
3:Y:217:LEU:HB2	3:Y:232:TRP:CH2	2.51	0.45
3:Y:438:LEU:O	3:Y:441:ILE:HG22	2.17	0.45
3:Z:100:ALA:HB1	3:Z:399:LEU:HD22	1.98	0.45
3:a:435:ILE:HD13	3:a:454:MET:HE1	1.99	0.45
3:b:431:ALA:O	3:b:435:ILE:HG22	2.17	0.45
3:c:103:ARG:O	3:c:107:LYS:HG3	2.17	0.45
3:c:373:GLY:HA2	3:d:61:ALA:HB2	1.99	0.45
3:g:129:ILE:HG23	3:g:256:HIS:HB3	1.98	0.45
3:g:133:ASN:HD22	3:g:150:LEU:HD21	1.82	0.45
3:h:424:ALA:O	3:h:428:MET:HE2	2.17	0.45
1:A:110:MET:HE3	1:L:60:LEU:HD21	1.98	0.45
1:A:227:ASP:OD2	1:A:230:LYS:NZ	2.47	0.45
1:C:285:GLN:HB2	1:C:309:MET:O	2.17	0.45
1:D:62:ASN:ND2	1:D:148:ASP:HB3	2.32	0.45
1:G:201:SER:HB2	1:G:247:PHE:HD2	1.81	0.45
1:I:136:LYS:HE3	1:I:267:GLU:OE2	2.16	0.45
1:I:170:ASP:HB3	1:I:174:ARG:CZ	2.47	0.45
1:N:38:SER:HB2	1:N:123:ALA:HB1	1.99	0.45
1:O:32:LYS:HD3	1:O:113:GLU:HB3	1.99	0.45
3:Y:334:GLN:HA	3:Y:337:VAL:HG22	1.99	0.45
3:Z:408:HIS:O	3:Z:409:LYS:CG	2.63	0.45
3:a:103:ARG:NH2	3:a:397:ASP:HB3	2.32	0.45
3:a:367:GLU:O	3:a:371:THR:N	2.50	0.45
3:c:166:ILE:HB	3:c:204:VAL:HB	1.98	0.45
3:c:274:LEU:O	3:c:278:GLU:HG2	2.16	0.45
3:e:440:PRO:HG2	3:e:441:ILE:HD12	1.98	0.45
3:f:447:ARG:HH12	3:g:466:SER:HB2	1.82	0.45
3:h:288:VAL:HG22	3:i:307:TYR:HD2	1.82	0.45
1:D:160:LEU:HD11	1:D:325:LEU:HB3	1.99	0.45
1:G:199:PRO:HG3	1:G:275:PHE:HE1	1.82	0.45
1:H:273:ALA:HA	1:H:322:ALA:HA	1.99	0.45
1:H:315:ARG:HD2	1:H:316:ARG:HG2	1.99	0.45
2:Q:78:ASP:HB2	2:Q:104:GLU:HG3	1.98	0.45
3:Z:325:LYS:O	3:Z:329:ILE:HG12	2.16	0.45
3:a:276:LEU:HD23	3:b:284:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:287:LEU:O	3:a:315:VAL:HA	2.16	0.45
3:c:318:TYR:CE2	3:c:320:ARG:HG2	2.51	0.45
3:h:159:ALA:HA	3:h:249:GLY:HA2	1.99	0.45
3:h:443:GLN:HG3	3:i:450:LEU:HG	1.98	0.45
2:k:149:GLU:HG2	2:k:153:TYR:CE2	2.52	0.45
2:m:69:PRO:HG3	2:m:107:LEU:HD21	1.98	0.45
1:A:3:PHE:HD2	1:A:7:LEU:HD21	1.82	0.45
1:A:43:LEU:HB2	1:A:277:PRO:HB2	1.99	0.45
1:B:94:LEU:HD13	1:B:118:ASP:OD1	2.17	0.45
1:C:121:GLU:OE2	1:C:124:ARG:NH2	2.49	0.45
1:J:88:VAL:HG12	1:J:309:MET:HE3	1.98	0.45
1:L:200:MET:HE3	1:L:241:VAL:HG13	1.99	0.45
2:P:143:ALA:HA	2:P:146:ILE:HG22	1.98	0.45
2:W:43:LEU:HD13	2:W:124:ILE:HG13	1.97	0.45
2:X:182:LEU:HD21	3:Z:48:PHE:HA	1.97	0.45
3:Y:399:LEU:CD1	3:Y:399:LEU:C	2.75	0.45
3:Z:304:MET:C	3:Z:306:ASP:H	2.25	0.45
3:c:135:LEU:HD11	3:c:239:TYR:HB3	1.98	0.45
3:d:380:ALA:HB1	3:d:414:THR:HB	1.99	0.45
3:g:270:LEU:HD21	3:h:278:GLU:HG2	1.99	0.45
2:k:74:ALA:HB3	2:k:108:VAL:HB	1.98	0.45
2:k:172:LYS:HG3	2:k:173:ARG:N	2.28	0.45
1:A:94:LEU:N	1:A:306:THR:O	2.49	0.44
1:B:91:LEU:HA	1:B:309:MET:HG2	1.98	0.44
1:B:112:LYS:NZ	3:a:6:ALA:HB1	2.32	0.44
1:B:221:ALA:HB1	1:G:224:ALA:HB1	1.99	0.44
1:B:238:GLY:N	1:G:229:VAL:O	2.50	0.44
1:C:131:LEU:O	1:C:135:ILE:HG12	2.17	0.44
1:C:289:VAL:HG22	1:C:308:GLN:OE1	2.17	0.44
1:E:169:ALA:O	1:E:173:VAL:HG22	2.17	0.44
1:H:83:LYS:HE3	1:H:85:ASN:HD21	1.83	0.44
1:J:155:LEU:HD11	1:J:270:ARG:HD3	1.99	0.44
1:M:216:ASN:OD1	1:M:217:VAL:N	2.50	0.44
2:X:66:ILE:HD12	2:X:89:VAL:HG21	1.98	0.44
3:Z:99:ALA:O	3:Z:103:ARG:HG3	2.17	0.44
3:b:78:GLU:H	3:b:411:ALA:HB1	1.82	0.44
3:c:307:TYR:CE1	2:k:162:THR:HG23	2.52	0.44
3:d:373:GLY:HA3	3:e:57:ASN:OD1	2.16	0.44
3:d:444:LEU:HB2	3:e:454:MET:HE1	1.99	0.44
3:e:401:GLN:OE1	3:e:401:GLN:N	2.39	0.44
3:f:369:GLU:HG2	3:f:376:TYR:CD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j:372:LEU:HD12	3:j:376:TYR:HB2	1.97	0.44
2:l:107:LEU:HD12	2:l:108:VAL:N	2.32	0.44
1:F:132:ILE:HA	1:F:135:ILE:HG12	1.98	0.44
1:G:209:LEU:HD23	1:G:209:LEU:HA	1.78	0.44
1:K:62:ASN:HB3	1:K:149:ALA:HB1	1.98	0.44
1:M:62:ASN:H	1:M:149:ALA:HB1	1.81	0.44
1:N:129:ALA:HA	1:N:132:ILE:HG12	1.98	0.44
2:T:1:MET:HG2	2:T:5:ASP:HB2	1.99	0.44
3:Y:68:PHE:HD2	3:Y:121:LEU:HD13	1.82	0.44
3:a:169:LYS:HD2	3:a:201:TYR:CE1	2.52	0.44
3:b:8:LEU:O	3:b:12:LEU:HG	2.17	0.44
3:e:156:ARG:NH1	3:f:176:ASP:OD1	2.50	0.44
3:g:322:ASP:HA	3:g:325:LYS:HB3	1.98	0.44
1:C:110:MET:O	1:C:114:VAL:HG23	2.17	0.44
1:C:113:GLU:HA	1:C:116:GLU:OE1	2.17	0.44
1:G:159:ASP:OD1	1:G:161:THR:OG1	2.29	0.44
1:G:285:GLN:CD	3:Y:7:MET:HE1	2.43	0.44
1:H:174:ARG:NH2	1:H:178:ARG:HH22	2.16	0.44
2:P:3:LEU:HD12	2:P:4:LEU:HD23	1.99	0.44
2:R:120:ALA:O	2:R:124:ILE:HG12	2.17	0.44
2:X:19:ILE:HG12	2:X:26:TYR:CD2	2.53	0.44
2:X:159:ARG:HH21	3:b:292:LYS:HG3	1.83	0.44
3:Z:284:VAL:O	3:Z:285:LEU:HD22	2.17	0.44
3:a:440:PRO:O	3:a:443:GLN:HG2	2.17	0.44
3:c:245:ASN:O	3:c:254:ARG:N	2.50	0.44
3:c:334:GLN:O	3:c:338:VAL:HG12	2.18	0.44
3:d:107:LYS:O	3:d:110:GLN:HG2	2.18	0.44
3:f:217:LEU:HD22	3:f:232:TRP:CH2	2.51	0.44
3:h:287:LEU:HA	3:i:306:ASP:O	2.17	0.44
3:i:27:THR:O	3:i:49:GLN:NE2	2.45	0.44
3:i:277:TYR:OH	3:i:325:LYS:HD3	2.17	0.44
3:i:333:LEU:HA	3:i:336:VAL:HG12	1.99	0.44
1:B:200:MET:HE2	1:B:200:MET:HB3	1.77	0.44
1:C:206:SER:OG	1:M:181:GLU:OE1	2.29	0.44
1:C:219:TYR:HB3	1:H:228:TYR:HB3	1.99	0.44
1:E:46:ILE:HD13	1:E:283:THR:HB	1.98	0.44
1:G:108:PHE:CE2	1:G:110:MET:HE2	2.53	0.44
1:I:46:ILE:HG12	1:I:283:THR:HB	1.99	0.44
1:L:205:PHE:CE1	1:L:233:VAL:HG22	2.47	0.44
1:O:273:ALA:HA	1:O:322:ALA:HA	1.99	0.44
2:V:49:TRP:NE1	2:W:83:GLN:HG3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:158:ASP:OD2	3:a:164:MET:HE2	2.17	0.44
3:a:318:TYR:HE1	3:b:313:GLU:H	1.65	0.44
3:b:65:ARG:HH12	3:b:118:LEU:HD21	1.82	0.44
3:c:289:ASP:N	3:c:314:ALA:O	2.50	0.44
3:e:288:VAL:HG22	3:f:307:TYR:CD1	2.52	0.44
3:g:447:ARG:HG3	3:h:466:SER:HA	2.00	0.44
2:m:49:TRP:CH2	2:m:160:MET:HG3	2.53	0.44
1:A:148:ASP:OD1	1:A:148:ASP:N	2.51	0.44
1:B:55:VAL:HG12	1:G:25:GLU:HG2	1.99	0.44
1:D:256:PRO:HB3	1:N:67:GLY:H	1.82	0.44
1:I:141:ASP:HA	1:I:152:PRO:HB3	1.98	0.44
2:W:11:LEU:HD21	2:W:28:THR:HG21	2.00	0.44
3:Y:286:ASN:O	3:Z:306:ASP:HB3	2.17	0.44
3:Z:221:ILE:HG22	3:Z:226:VAL:HB	1.99	0.44
3:b:190:ARG:NH1	3:b:222:ASP:OD2	2.50	0.44
3:c:164:MET:HG2	3:c:206:ARG:HD3	1.99	0.44
3:f:133:ASN:HB3	3:f:153:TYR:OH	2.18	0.44
3:g:14:ASP:CG	3:h:41:ARG:HH11	2.26	0.44
3:j:104:VAL:HG13	3:j:395:VAL:HG11	1.98	0.44
1:C:190:ASP:OD1	1:C:191:ALA:N	2.51	0.44
1:H:215:MET:HE1	1:H:233:VAL:CG2	2.48	0.44
1:H:261:PHE:HZ	1:H:312:ILE:HB	1.82	0.44
1:M:184:ILE:HG12	1:M:189:GLY:HA2	1.99	0.44
1:N:180:VAL:O	1:N:184:ILE:HG13	2.18	0.44
1:O:121:GLU:HA	1:O:124:ARG:HE	1.82	0.44
2:S:9:VAL:HG23	2:S:12:ARG:NH2	2.32	0.44
2:S:179:ARG:HG2	2:S:183:ARG:HH12	1.83	0.44
2:T:155:ASN:HA	3:i:290:GLU:HB2	1.99	0.44
3:Y:159:ALA:HB3	3:Z:172:TYR:HE1	1.83	0.44
3:Z:422:SER:HA	3:Z:425:VAL:HG22	1.99	0.44
3:a:260:TYR:HD1	3:b:50:SER:HB3	1.83	0.44
3:b:388:ALA:O	3:b:392:LEU:HG	2.18	0.44
3:f:22:ILE:HD11	3:f:151:ARG:HH21	1.83	0.44
3:g:448:ILE:HG23	3:g:449:SER:N	2.31	0.44
1:B:50:ARG:NH1	2:k:180:ARG:O	2.51	0.44
1:C:154:VAL:HG21	1:C:179:VAL:HG13	2.00	0.44
1:J:176:HIS:HA	1:J:179:VAL:HG12	1.99	0.44
1:M:216:ASN:ND2	1:M:218:GLU:HG3	2.32	0.44
2:R:119:ILE:HG21	2:R:160:MET:SD	2.58	0.44
2:T:163:ARG:NH1	2:U:106:ARG:HH12	2.12	0.44
2:U:43:LEU:HG	2:U:48:TRP:HE1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:153:TYR:CE1	2:V:42:GLN:HG3	2.47	0.44
2:V:145:VAL:O	2:V:149:GLU:HG2	2.18	0.44
2:X:1:MET:HE2	2:X:121:GLN:HG3	2.00	0.44
3:Y:120:VAL:HB	3:Y:145:VAL:HG23	1.99	0.44
3:Z:295:VAL:O	3:Z:295:VAL:HG12	2.17	0.44
3:a:431:ALA:O	3:a:435:ILE:HG13	2.18	0.44
3:d:307:TYR:HA	2:l:162:THR:CG2	2.48	0.44
1:B:98:PHE:O	1:B:302:TRP:N	2.48	0.44
1:C:49:LEU:HD21	1:C:53:ASN:HA	2.00	0.44
1:E:68:ARG:HB2	1:J:93:TYR:CE1	2.52	0.44
1:E:229:VAL:HG21	1:O:220:GLN:HG3	2.00	0.44
1:H:97:GLN:NE2	1:H:301:SER:OG	2.36	0.44
1:I:142:ALA:HB2	1:I:152:PRO:HD3	2.00	0.44
2:S:56:HIS:N	2:S:105:GLY:O	2.50	0.44
2:U:2:LEU:HG	2:U:4:LEU:H	1.83	0.44
3:Y:344:PHE:C	3:Y:345:MET:HG2	2.43	0.44
3:c:9:TRP:O	3:c:13:ARG:HG3	2.17	0.44
3:c:69:PRO:HD2	3:c:74:PHE:HB3	2.00	0.44
3:c:243:THR:H	3:c:382:ASN:HD22	1.66	0.44
3:h:6:ALA:HA	3:h:201:TYR:CE2	2.52	0.44
3:i:14:ASP:HB3	3:i:17:VAL:HG12	2.00	0.44
3:i:185:LEU:HD11	3:i:192:LEU:HD23	2.00	0.44
3:j:35:ASP:OD1	3:j:151:ARG:NH1	2.50	0.44
1:C:188:LEU:HD21	1:H:34:PHE:CE2	2.53	0.44
1:D:226:ASN:ND2	1:D:233:VAL:HA	2.33	0.44
1:E:94:LEU:HD21	1:O:65:ALA:HA	1.99	0.44
1:F:50:ARG:NE	1:F:50:ARG:HA	2.33	0.44
1:F:104:TRP:NE1	2:V:177:ARG:HG2	2.32	0.44
1:J:286:VAL:HB	1:J:309:MET:HE2	1.98	0.44
1:J:318:ASP:OD1	1:J:318:ASP:N	2.51	0.44
2:Q:60:PRO:HD3	2:Q:102:PRO:HG3	1.99	0.44
2:Q:83:GLN:NE2	2:Q:92:ALA:HB2	2.33	0.44
2:R:83:GLN:HE21	2:R:90:ARG:HG2	1.83	0.44
2:V:14:ILE:HG23	2:V:137:ILE:HD11	2.00	0.44
2:V:159:ARG:HD2	3:Z:307:TYR:CZ	2.53	0.44
3:Z:186:MET:HG3	3:Z:191:ASN:HB3	2.00	0.44
3:a:309:PRO:O	3:a:313:GLU:HB2	2.17	0.44
3:b:375:THR:HA	3:b:378:LEU:HB3	2.00	0.44
3:g:95:THR:HA	3:g:98:THR:HG22	1.98	0.44
3:g:367:GLU:O	3:g:371:THR:N	2.50	0.44
3:h:421:ARG:HD3	3:h:421:ARG:HA	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:81:ASP:O	3:i:85:ARG:HG2	2.17	0.44
3:i:267:LEU:HD12	3:i:336:VAL:HG13	2.00	0.44
3:i:389:TYR:CE1	3:i:412:ILE:HD12	2.53	0.44
3:j:397:ASP:H	3:j:400:LEU:HD13	1.82	0.44
1:D:194:SER:HB2	3:e:193:SER:OG	2.17	0.43
1:G:46:ILE:HA	1:G:283:THR:O	2.18	0.43
1:H:98:PHE:HZ	1:H:114:VAL:HG11	1.83	0.43
2:V:159:ARG:O	2:V:163:ARG:HD3	2.17	0.43
2:V:165:ARG:N	2:V:166:PRO:HD3	2.33	0.43
3:Z:74:PHE:HA	3:Z:417:PRO:HB3	1.99	0.43
3:a:44:VAL:N	2:k:184:THR:O	2.36	0.43
3:b:450:LEU:HB3	3:b:451:PRO:HD3	2.00	0.43
3:e:345:MET:SD	3:e:345:MET:N	2.91	0.43
3:f:138:ARG:HA	3:f:145:VAL:HG12	2.00	0.43
3:f:325:LYS:O	3:f:329:ILE:HD12	2.16	0.43
1:D:8:THR:HG23	1:D:8:THR:O	2.18	0.43
1:G:257:LEU:HA	1:G:257:LEU:HD23	1.79	0.43
1:O:270:ARG:HG2	1:O:324:GLU:HB2	1.99	0.43
2:P:42:GLN:OE1	2:m:122:ARG:NH1	2.52	0.43
2:R:69:PRO:HG2	2:R:109:LEU:HD21	1.99	0.43
2:S:163:ARG:HD2	2:T:76:TYR:OH	2.18	0.43
2:U:2:LEU:HD12	2:U:3:LEU:N	2.32	0.43
2:U:164:SER:O	2:U:164:SER:OG	2.34	0.43
3:Y:18:GLU:O	3:Y:22:ILE:HG12	2.18	0.43
3:Z:17:VAL:HG21	3:Z:252:TYR:CD2	2.54	0.43
3:Z:292:LYS:HD3	3:Z:310:GLY:HA2	1.99	0.43
3:b:35:ASP:OD2	3:b:38:SER:N	2.52	0.43
3:b:133:ASN:HB3	3:b:153:TYR:OH	2.18	0.43
3:d:19:SER:O	3:d:23:GLU:HG3	2.17	0.43
3:f:155:VAL:HG13	3:f:166:ILE:HG22	1.99	0.43
3:g:287:LEU:O	3:g:315:VAL:HG12	2.18	0.43
3:g:330:GLN:HA	3:g:333:LEU:HB2	2.00	0.43
3:h:135:LEU:HD23	3:h:168:LEU:HD13	2.00	0.43
3:i:289:ASP:HB2	3:i:313:GLU:O	2.17	0.43
2:k:12:ARG:HE	2:k:12:ARG:HB2	1.60	0.43
1:B:195:GLU:HG2	1:B:277:PRO:HD2	1.99	0.43
1:B:220:GLN:HB3	1:B:223:GLY:O	2.17	0.43
1:B:233:VAL:HG12	1:B:241:VAL:HG11	2.00	0.43
1:C:49:LEU:HD23	1:C:286:VAL:HG23	2.01	0.43
1:G:109:ASP:HB2	2:X:183:ARG:HD3	2.01	0.43
1:H:28:GLY:O	3:b:16:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:40:PHE:CZ	1:I:244:THR:HG21	2.54	0.43
1:K:43:LEU:HD21	1:K:275:PHE:CE2	2.54	0.43
3:Z:244:TRP:HB3	3:Z:254:ARG:O	2.18	0.43
3:a:170:GLN:HG3	3:a:172:TYR:HE1	1.83	0.43
3:a:441:ILE:HA	3:a:444:LEU:HD12	2.00	0.43
3:c:430:ASN:O	3:c:434:VAL:HG23	2.18	0.43
3:d:27:THR:HG21	3:d:264:PHE:HB3	2.00	0.43
3:e:287:LEU:HD13	3:f:312:ALA:HB2	2.01	0.43
3:f:167:VAL:HG22	3:f:203:HIS:ND1	2.33	0.43
1:A:199:PRO:HG3	1:A:275:PHE:HE2	1.83	0.43
1:B:9:ARG:HD3	1:B:12:TYR:CD1	2.52	0.43
1:C:227:ASP:OD1	1:C:229:VAL:HG22	2.19	0.43
1:E:269:GLU:HB2	1:E:324:GLU:OE2	2.19	0.43
1:J:50:ARG:HA	1:J:50:ARG:HD2	1.72	0.43
1:J:132:ILE:O	1:J:135:ILE:HG22	2.19	0.43
1:N:195:GLU:HG3	1:N:277:PRO:HD2	2.00	0.43
2:Q:44:LEU:HG	2:Q:51:ASN:HD22	1.82	0.43
2:Q:116:ILE:O	2:Q:121:GLN:NE2	2.52	0.43
2:Q:159:ARG:HB3	2:Q:163:ARG:HH22	1.83	0.43
2:W:153:TYR:CE1	2:X:42:GLN:HG3	2.53	0.43
3:Z:9:TRP:CD1	3:Z:167:VAL:HG13	2.53	0.43
3:Z:137:TYR:HD1	3:Z:239:TYR:CZ	2.37	0.43
3:Z:307:TYR:CE2	3:Z:311:GLY:HA3	2.46	0.43
3:c:85:ARG:HH21	3:c:86:GLU:CD	2.26	0.43
3:c:120:VAL:HB	3:c:145:VAL:HG23	1.99	0.43
3:c:302:ALA:O	2:k:169:THR:OG1	2.33	0.43
3:e:171:ARG:HE	3:e:171:ARG:HB2	1.61	0.43
2:k:1:MET:HE3	2:k:5:ASP:HB3	2.00	0.43
2:l:50:PHE:HA	2:m:83:GLN:NE2	2.33	0.43
1:H:133:GLN:HG2	1:H:261:PHE:CE1	2.53	0.43
1:I:147:GLU:H	1:I:147:GLU:CD	2.26	0.43
2:Q:177:ARG:CD	3:d:269:LEU:HD21	2.47	0.43
2:R:99:ILE:HG23	2:R:101:LYS:HZ3	1.82	0.43
2:S:160:MET:HA	2:S:163:ARG:HG2	2.00	0.43
2:U:12:ARG:CZ	2:V:35:GLU:HG2	2.49	0.43
2:V:11:LEU:HD12	2:V:19:ILE:HG13	2.01	0.43
3:a:243:THR:HG21	3:a:246:LEU:HB2	2.01	0.43
3:a:280:GLU:OE2	2:k:174:SER:HB3	2.18	0.43
3:c:28:THR:HG21	3:c:56:VAL:HG21	1.99	0.43
3:d:441:ILE:HD11	3:e:436:ALA:HB2	2.00	0.43
3:e:244:TRP:NE1	3:e:375:THR:HG21	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:203:HIS:CE1	3:h:205:GLN:HG2	2.54	0.43
3:i:240:ILE:HG22	3:i:242:PRO:HD3	2.00	0.43
3:i:335:ALA:O	3:i:338:VAL:HG12	2.18	0.43
1:A:124:ARG:NH1	1:L:187:ASP:OD2	2.52	0.43
1:C:128:GLN:HE21	1:C:252:ILE:HD11	1.83	0.43
1:D:273:ALA:HA	1:D:322:ALA:HA	2.00	0.43
1:E:299:LYS:O	1:E:299:LYS:HG3	2.17	0.43
1:H:209:LEU:HA	1:H:215:MET:HE3	2.01	0.43
1:O:158:LEU:HD13	1:O:172:ILE:HG13	2.01	0.43
2:R:181:SER:HA	3:e:20:ARG:HH12	1.84	0.43
2:U:54:TRP:CD1	2:U:54:TRP:H	2.35	0.43
2:U:63:THR:O	2:U:98:ARG:NH1	2.51	0.43
2:U:174:SER:C	2:U:176:SER:H	2.27	0.43
3:Z:326:MET:O	3:Z:330:GLN:HG3	2.18	0.43
3:a:267:LEU:HB2	3:a:336:VAL:HG11	2.00	0.43
3:a:308:VAL:HB	3:a:311:GLY:N	2.34	0.43
3:a:392:LEU:HD23	3:a:409:LYS:HD3	2.00	0.43
3:b:76:ARG:H	3:b:413:GLU:HB3	1.84	0.43
3:b:273:LYS:HE3	3:c:283:GLU:HA	2.00	0.43
3:e:285:LEU:HD13	3:f:306:ASP:HB2	2.01	0.43
3:f:296:VAL:O	3:f:300:GLN:NE2	2.40	0.43
3:i:241:VAL:O	3:i:241:VAL:HG13	2.18	0.43
3:j:150:LEU:HD23	3:j:150:LEU:HA	1.88	0.43
1:K:172:ILE:HG21	1:K:208:LEU:HD11	1.99	0.43
1:K:178:ARG:O	1:K:181:GLU:HB2	2.19	0.43
2:Q:159:ARG:HB3	2:Q:163:ARG:NH2	2.34	0.43
2:R:123:VAL:HG11	2:R:157:LEU:HD22	2.00	0.43
2:X:113:TRP:HA	2:X:116:ILE:HD12	2.01	0.43
3:Y:111:ARG:O	3:Y:138:ARG:NH2	2.44	0.43
3:Y:289:ASP:OD2	3:Y:292:LYS:N	2.37	0.43
3:Y:392:LEU:HD22	3:Y:409:LYS:CD	2.48	0.43
3:Z:164:MET:HG2	3:Z:206:ARG:HD3	2.00	0.43
3:b:289:ASP:HA	3:c:308:VAL:HG23	2.01	0.43
3:c:37:MET:HE2	3:c:37:MET:N	2.33	0.43
3:c:449:SER:O	3:c:452:LYS:HB3	2.19	0.43
3:d:27:THR:HG22	3:d:28:THR:HG23	2.00	0.43
3:j:369:GLU:HB2	3:j:376:TYR:CD2	2.52	0.43
2:k:65:ARG:NH1	2:k:97:ASP:OD2	2.51	0.43
2:l:152:ALA:O	2:l:155:ASN:HB2	2.18	0.43
1:A:334:THR:C	1:L:171:LYS:HD2	2.44	0.43
1:G:73:GLU:OE1	1:G:73:GLU:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:147:GLU:OE1	1:I:147:GLU:N	2.49	0.43
1:L:232:ARG:NE	1:L:232:ARG:HA	2.33	0.43
1:M:178:ARG:HA	1:M:181:GLU:HG2	2.01	0.43
1:M:236:LEU:O	1:M:239:VAL:HG12	2.18	0.43
2:T:182:LEU:HB3	3:h:46:HIS:HB2	2.00	0.43
2:V:55:ARG:HG2	2:V:55:ARG:O	2.18	0.43
2:W:33:LEU:HA	2:W:36:LEU:HD12	2.01	0.43
3:Z:17:VAL:HG21	3:Z:252:TYR:CE2	2.53	0.43
3:b:235:HIS:NE2	3:b:408:HIS:HA	2.33	0.43
3:g:320:ARG:NE	3:h:317:ALA:HB2	2.34	0.43
3:h:296:VAL:HG22	3:h:300:GLN:HG2	2.00	0.43
3:h:310:GLY:HA2	3:h:314:ALA:HB2	1.99	0.43
3:j:33:MET:HE3	3:j:33:MET:HB3	1.93	0.43
1:B:50:ARG:HD3	3:Z:20:ARG:NH2	2.34	0.43
1:C:308:GLN:HG2	1:C:310:TYR:CD1	2.54	0.43
1:D:47:ARG:NH1	1:I:29:ILE:HD11	2.34	0.43
1:G:142:ALA:HB2	1:G:152:PRO:HG3	2.01	0.43
3:Y:318:TYR:HE1	3:Z:313:GLU:HA	1.84	0.43
3:Z:33:MET:HG3	3:Z:33:MET:O	2.17	0.43
3:Z:408:HIS:C	3:Z:409:LYS:HG2	2.44	0.43
3:g:406:LYS:HD2	3:g:406:LYS:HA	1.80	0.43
1:B:34:PHE:CD1	1:K:188:LEU:HD21	2.53	0.43
1:B:165:ALA:HB1	1:B:210:GLU:OE1	2.18	0.43
1:D:93:TYR:HH	1:N:75:GLU:H	1.67	0.43
1:E:93:TYR:CE1	1:O:68:ARG:HB3	2.53	0.43
1:E:185:ASP:HA	1:J:245:PRO:HB3	2.01	0.43
1:F:98:PHE:O	1:F:302:TRP:N	2.36	0.43
1:F:104:TRP:HB2	2:V:173:ARG:NH1	2.34	0.43
1:F:205:PHE:CZ	1:F:233:VAL:HB	2.54	0.43
1:F:236:LEU:O	1:F:239:VAL:HG12	2.18	0.43
1:G:198:THR:HB	1:G:241:VAL:HA	2.00	0.43
1:I:40:PHE:HZ	1:I:244:THR:HG21	1.84	0.43
2:U:55:ARG:NH2	2:U:104:GLU:HB3	2.33	0.43
3:Y:400:LEU:HD12	3:Y:401:GLN:OE1	2.17	0.43
3:a:63:LEU:HD12	3:a:129:ILE:HD11	2.01	0.43
3:d:408:HIS:O	3:d:409:LYS:HG2	2.19	0.43
3:g:308:VAL:HG13	3:g:309:PRO:HD3	2.00	0.43
3:h:158:ASP:OD2	3:h:162:ARG:NH2	2.51	0.43
3:i:385:SER:OG	3:i:386:PRO:HD3	2.19	0.43
1:F:259:ARG:O	1:F:262:ASN:ND2	2.52	0.42
1:G:39:LYS:O	1:G:42:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:40:PHE:HA	1:I:43:LEU:HD12	2.01	0.42
1:I:209:LEU:HA	1:I:215:MET:SD	2.59	0.42
1:K:59:ARG:O	1:K:60:LEU:HD23	2.19	0.42
1:M:197:LEU:HD23	1:M:277:PRO:HG2	2.01	0.42
1:O:50:ARG:HG2	1:O:50:ARG:HH11	1.84	0.42
1:O:279:LYS:HA	1:O:315:ARG:HH21	1.83	0.42
2:R:141:GLU:OE1	2:S:139:PRO:HB2	2.19	0.42
2:T:49:TRP:CE3	2:T:161:HIS:HA	2.54	0.42
2:U:160:MET:HG3	2:V:76:TYR:OH	2.19	0.42
3:Y:169:LYS:HD2	3:Y:201:TYR:CZ	2.53	0.42
3:Y:200:LEU:HD12	3:Y:221:ILE:HD11	2.01	0.42
3:Z:245:ASN:O	3:Z:254:ARG:N	2.50	0.42
3:Z:292:LYS:HD3	3:Z:311:GLY:N	2.33	0.42
3:b:285:LEU:HD21	3:c:300:GLN:CD	2.44	0.42
3:f:276:LEU:HG	3:f:280:GLU:OE2	2.19	0.42
3:f:461:PHE:HB3	3:f:463:VAL:HG13	2.01	0.42
3:i:124:VAL:HG21	3:i:136:LEU:HD11	2.01	0.42
3:j:17:VAL:HG23	3:j:254:ARG:HH12	1.83	0.42
1:C:212:ASP:OD1	1:C:212:ASP:N	2.52	0.42
1:C:318:ASP:OD1	1:C:319:THR:HG23	2.19	0.42
1:E:95:ARG:HG2	1:E:305:ASP:OD1	2.19	0.42
1:F:130:CYS:O	1:F:134:VAL:HG23	2.19	0.42
1:F:216:ASN:HB3	1:F:219:TYR:CD1	2.53	0.42
1:H:281:LEU:HD11	1:H:312:ILE:CG2	2.48	0.42
1:I:325:LEU:HB3	1:I:328:ILE:HB	2.01	0.42
2:S:26:TYR:HD1	2:S:27:PRO:HD2	1.82	0.42
2:S:54:TRP:O	2:S:55:ARG:HG2	2.18	0.42
2:S:130:LEU:HD13	2:S:146:ILE:HG23	2.01	0.42
2:X:1:MET:HE1	2:X:122:ARG:HA	2.01	0.42
2:X:113:TRP:CZ2	2:X:121:GLN:HB2	2.55	0.42
3:Y:191:ASN:O	3:Y:192:LEU:HD23	2.19	0.42
3:Y:250:GLU:OE1	3:Z:41:ARG:HG3	2.20	0.42
3:Z:104:VAL:HA	3:Z:107:LYS:HZ3	1.85	0.42
3:a:156:ARG:HH22	3:b:176:ASP:CG	2.24	0.42
3:b:108:ALA:HB1	3:b:391:CYS:HB3	2.00	0.42
3:f:401:GLN:OE1	3:f:401:GLN:N	2.42	0.42
3:h:33:MET:HE3	3:h:151:ARG:HD3	2.01	0.42
3:i:244:TRP:CE2	3:i:375:THR:HG21	2.55	0.42
3:j:406:LYS:HE2	3:j:406:LYS:HB3	1.92	0.42
2:k:57:LYS:HB2	2:k:57:LYS:HE3	1.81	0.42
2:m:39:GLN:OE1	2:m:127:GLN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:52:THR:HG22	2:m:108:VAL:HG22	2.01	0.42
1:A:180:VAL:O	1:A:184:ILE:HG12	2.19	0.42
1:E:95:ARG:HH11	1:O:74:LEU:HB3	1.83	0.42
1:E:95:ARG:HD2	1:O:74:LEU:HD13	2.00	0.42
1:G:44:MET:HB2	1:G:46:ILE:CD1	2.49	0.42
1:G:133:GLN:HG2	1:G:261:PHE:CE1	2.54	0.42
1:I:272:ILE:CG2	1:I:323:ILE:HB	2.49	0.42
1:M:131:LEU:O	1:M:135:ILE:HG12	2.19	0.42
2:W:11:LEU:HA	2:W:14:ILE:HG22	2.00	0.42
3:Z:4:THR:N	3:Z:7:MET:HE3	2.29	0.42
3:Z:118:LEU:HA	3:Z:121:LEU:HD12	2.01	0.42
3:Z:287:LEU:HD21	3:Z:318:TYR:HD2	1.83	0.42
3:b:111:ARG:HA	3:b:111:ARG:HD2	1.80	0.42
3:b:166:ILE:HG13	3:b:204:VAL:HB	2.02	0.42
3:c:258:GLU:OE2	3:d:46:HIS:NE2	2.48	0.42
3:d:243:THR:H	3:d:382:ASN:ND2	2.18	0.42
3:g:19:SER:O	3:g:23:GLU:HG3	2.19	0.42
3:g:173:LYS:HB2	3:g:176:ASP:OD1	2.19	0.42
3:i:307:TYR:HD2	3:i:307:TYR:HA	1.67	0.42
2:k:156:GLU:HA	2:k:159:ARG:NH1	2.34	0.42
1:E:211:HIS:HE1	1:E:213:LYS:HE2	1.84	0.42
1:F:112:LYS:NZ	3:i:18:GLU:HG3	2.34	0.42
1:I:56:ARG:NH1	1:I:83:LYS:HD2	2.35	0.42
2:P:160:MET:HE3	2:P:160:MET:HB2	1.88	0.42
2:Q:150:LEU:HA	2:Q:153:TYR:HD2	1.83	0.42
2:W:41:ILE:O	2:W:45:THR:OG1	2.30	0.42
3:Y:269:LEU:O	3:Y:273:LYS:HG2	2.19	0.42
3:d:111:ARG:HH21	3:d:143:ALA:HB2	1.84	0.42
2:k:65:ARG:HH12	2:k:97:ASP:CG	2.28	0.42
1:B:318:ASP:OD1	1:B:318:ASP:N	2.47	0.42
1:C:50:ARG:HD2	3:c:45:GLU:HG3	2.01	0.42
1:D:333:ILE:HG22	1:N:174:ARG:HD3	2.01	0.42
1:G:156:GLU:HB3	1:G:175:MET:HE2	2.02	0.42
1:H:47:ARG:NE	3:b:192:LEU:HD13	2.32	0.42
1:K:9:ARG:HH21	1:K:10:PRO:HD2	1.84	0.42
1:L:184:ILE:HG13	1:L:189:GLY:HA3	2.02	0.42
1:N:305:ASP:OD1	1:N:306:THR:N	2.52	0.42
2:X:60:PRO:HG3	2:X:66:ILE:HG12	2.01	0.42
3:a:217:LEU:HD13	3:a:232:TRP:HH2	1.83	0.42
3:c:28:THR:HG21	3:c:257:VAL:HG11	2.00	0.42
3:d:73:PRO:O	3:d:417:PRO:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:127:LEU:O	3:d:131:THR:OG1	2.33	0.42
3:d:380:ALA:HA	3:d:384:GLN:HB3	2.01	0.42
3:f:86:GLU:O	3:f:90:ARG:HG2	2.19	0.42
3:i:121:LEU:O	3:i:125:ILE:HG12	2.19	0.42
3:j:344:PHE:C	3:j:345:MET:HG2	2.44	0.42
1:D:181:GLU:OE1	1:I:206:SER:OG	2.32	0.42
1:D:259:ARG:HA	1:D:262:ASN:ND2	2.34	0.42
1:F:141:ASP:HA	1:F:152:PRO:HB3	2.02	0.42
1:J:86:LEU:HD13	1:J:313:GLY:HA3	2.02	0.42
1:K:246:ARG:HA	1:K:246:ARG:NE	2.34	0.42
1:M:91:LEU:HD23	1:M:91:LEU:H	1.84	0.42
2:P:119:ILE:O	2:P:123:VAL:HG23	2.19	0.42
2:V:35:GLU:O	2:V:39:GLN:HG2	2.20	0.42
2:W:11:LEU:HD22	2:W:16:GLU:HB2	2.02	0.42
3:Y:148:TRP:HB3	3:Y:152:SER:HB2	2.02	0.42
3:b:162:ARG:HD2	3:b:206:ARG:NH1	2.35	0.42
3:g:22:ILE:CD1	3:g:151:ARG:HH22	2.33	0.42
3:g:59:LEU:HD22	3:g:129:ILE:HG12	2.01	0.42
3:g:445:ASP:OD1	3:g:445:ASP:O	2.38	0.42
3:h:244:TRP:CE2	3:h:256:HIS:HB2	2.55	0.42
3:i:37:MET:HB3	3:i:171:ARG:NH2	2.34	0.42
3:j:100:ALA:O	3:j:104:VAL:HG23	2.19	0.42
1:D:318:ASP:OD1	1:D:318:ASP:N	2.51	0.42
1:K:40:PHE:HZ	1:K:244:THR:HG21	1.85	0.42
1:M:97:GLN:NE2	1:M:299:LYS:HG2	2.35	0.42
2:S:123:VAL:HG11	2:S:157:LEU:CD2	2.50	0.42
2:T:82:LEU:HD21	2:T:99:ILE:HG12	2.01	0.42
3:Y:111:ARG:HH21	3:Y:143:ALA:HB2	1.85	0.42
3:Y:200:LEU:HA	3:Y:221:ILE:HG12	2.01	0.42
3:a:45:GLU:OE2	2:k:183:ARG:NH1	2.53	0.42
3:a:280:GLU:HG3	2:k:170:GLN:O	2.20	0.42
3:c:244:TRP:CZ2	3:c:372:LEU:HD11	2.55	0.42
3:d:367:GLU:N	3:d:369:GLU:OE2	2.53	0.42
3:d:448:ILE:CG2	3:d:452:LYS:HE3	2.28	0.42
3:g:166:ILE:HB	3:g:204:VAL:HB	2.02	0.42
3:g:265:ALA:O	3:g:269:LEU:HG	2.19	0.42
3:h:414:THR:HG21	3:i:116:ALA:HB2	2.00	0.42
3:i:174:SER:N	3:i:196:GLY:O	2.48	0.42
3:j:308:VAL:HG12	3:j:310:GLY:H	1.84	0.42
2:m:101:LYS:HD3	2:m:101:LYS:HA	1.86	0.42
1:A:44:MET:HE3	1:A:126:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:SER:HA	1:A:209:LEU:HD12	2.02	0.42
1:C:183:PHE:HB3	1:C:192:VAL:HG21	2.01	0.42
1:C:240:LYS:HE2	3:c:194:GLY:H	1.84	0.42
1:J:166:LYS:HA	1:J:166:LYS:HD2	1.81	0.42
1:M:117:LEU:HD23	1:M:117:LEU:HA	1.92	0.42
2:Q:83:GLN:OE1	2:Q:83:GLN:N	2.53	0.42
2:R:155:ASN:HA	3:g:290:GLU:O	2.20	0.42
2:S:10:ILE:HD11	2:S:132:VAL:HG21	2.01	0.42
2:W:163:ARG:NH1	2:X:76:TYR:OH	2.52	0.42
2:X:109:LEU:HD11	2:X:111:ARG:NH1	2.34	0.42
3:c:244:TRP:HZ2	3:c:372:LEU:HD11	1.85	0.42
3:d:369:GLU:H	3:d:369:GLU:CD	2.28	0.42
3:f:121:LEU:O	3:f:125:ILE:HG12	2.20	0.42
3:g:12:LEU:HD22	3:g:156:ARG:HB2	2.01	0.42
2:l:44:LEU:HD22	2:l:51:ASN:HD22	1.85	0.42
1:E:49:LEU:HD13	1:E:53:ASN:HA	2.00	0.42
1:E:220:GLN:OE1	1:E:226:ASN:HB2	2.20	0.42
1:J:154:VAL:HG21	1:J:182:THR:HG21	2.01	0.42
1:M:140:MET:HE2	1:M:140:MET:HB2	1.84	0.42
1:N:227:ASP:OD1	1:N:228:TYR:N	2.53	0.42
1:O:300:PHE:O	1:O:300:PHE:CD1	2.73	0.42
2:P:159:ARG:NH2	2:P:163:ARG:HH22	2.17	0.42
2:Q:143:ALA:HA	2:Q:146:ILE:HG12	2.02	0.42
2:Q:167:LEU:H	2:Q:167:LEU:HD12	1.85	0.42
2:R:145:VAL:HG11	2:S:134:THR:OG1	2.19	0.42
2:V:182:LEU:HG	3:j:46:HIS:HB2	2.02	0.42
2:W:48:TRP:O	2:W:52:THR:OG1	2.19	0.42
3:Z:380:ALA:HA	3:Z:384:GLN:HB2	2.01	0.42
3:b:136:LEU:HD11	3:b:145:VAL:HB	2.02	0.42
3:b:244:TRP:CD1	3:b:245:ASN:HB2	2.52	0.42
3:c:434:VAL:HG12	3:c:457:ILE:HD11	2.02	0.42
3:e:300:GLN:NE2	3:e:303:GLU:OE1	2.52	0.42
3:f:255:GLY:O	3:f:258:GLU:HG2	2.20	0.42
3:g:305:GLY:HA2	3:g:307:TYR:CZ	2.54	0.42
3:i:443:GLN:HB2	3:i:446:PRO:HG3	2.02	0.42
2:k:126:HIS:HD2	2:k:150:LEU:HD13	1.85	0.42
1:A:174:ARG:HD3	1:F:334:THR:HA	2.01	0.42
1:E:200:MET:HE3	1:E:200:MET:HB2	1.80	0.42
1:G:39:LYS:O	1:G:39:LYS:HD3	2.19	0.42
2:Q:43:LEU:O	2:Q:48:TRP:NE1	2.49	0.42
2:S:163:ARG:HA	3:i:307:TYR:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:127:GLN:CD	2:T:150:LEU:HD21	2.44	0.42
2:X:167:LEU:HA	3:b:303:GLU:OE2	2.19	0.42
3:Z:286:ASN:ND2	3:a:304:MET:HA	2.35	0.42
3:a:447:ARG:HD2	3:a:447:ARG:O	2.19	0.42
3:b:243:THR:O	3:b:382:ASN:ND2	2.49	0.42
3:c:111:ARG:NH1	3:c:394:GLU:HB3	2.27	0.42
3:c:292:LYS:HG3	3:c:293:GLY:H	1.84	0.42
3:d:419:LEU:HD11	3:e:65:ARG:NH2	2.35	0.42
3:f:175:LYS:HB3	3:f:175:LYS:HE2	1.75	0.42
3:f:212:MET:HE3	3:f:213:GLU:O	2.20	0.42
3:f:221:ILE:HG13	3:f:226:VAL:HG21	2.00	0.42
3:g:9:TRP:CD1	3:g:9:TRP:C	2.98	0.42
2:k:172:LYS:CG	2:k:173:ARG:H	2.30	0.42
2:m:51:ASN:OD1	2:m:52:THR:HG23	2.20	0.42
1:C:135:ILE:HB	1:C:270:ARG:HD2	2.02	0.41
1:D:220:GLN:HA	1:I:227:ASP:OD1	2.20	0.41
1:E:47:ARG:HG3	1:J:27:LEU:HD21	2.01	0.41
1:F:146:LEU:HD13	1:F:150:PHE:HE2	1.85	0.41
1:F:250:LYS:N	1:F:250:LYS:HD3	2.34	0.41
1:F:285:GLN:NE2	1:F:288:PRO:HA	2.35	0.41
1:I:35:ALA:HA	1:I:120:GLN:HE22	1.85	0.41
1:N:36:TYR:OH	1:N:127:ASP:OD1	2.31	0.41
1:N:158:LEU:HD13	1:N:175:MET:HG3	2.01	0.41
2:Q:13:LYS:HD2	2:R:135:HIS:NE2	2.35	0.41
2:Q:159:ARG:HH11	3:g:308:VAL:HB	1.85	0.41
2:S:159:ARG:HE	2:S:163:ARG:NH2	2.17	0.41
2:W:115:HIS:HA	2:X:87:LEU:HD11	2.01	0.41
2:X:56:HIS:ND1	2:X:57:LYS:N	2.68	0.41
3:Y:302:ALA:HA	3:j:284:VAL:O	2.20	0.41
3:b:201:TYR:HB2	3:b:220:GLU:O	2.20	0.41
3:e:52:GLY:HA3	3:e:264:PHE:HE2	1.85	0.41
3:e:106:ARG:HA	3:e:109:THR:HG22	2.01	0.41
3:e:345:MET:HE3	3:e:368:ALA:HA	2.02	0.41
3:f:319:GLU:OE2	3:f:323:TYR:OH	2.22	0.41
3:h:240:ILE:HD12	3:h:386:PRO:HB2	2.01	0.41
3:i:199:ASP:O	3:i:221:ILE:HG13	2.20	0.41
3:j:289:ASP:HB2	3:j:314:ALA:HB1	2.02	0.41
2:k:115:HIS:ND1	2:k:115:HIS:O	2.53	0.41
1:A:104:TRP:HB3	1:G:286:VAL:HG11	2.02	0.41
1:D:188:LEU:HD23	1:D:276:LEU:HD22	2.02	0.41
1:F:26:HIS:HE1	2:V:180:ARG:NH1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:LEU:HD23	1:F:131:LEU:HA	1.94	0.41
1:F:290:GLN:HE21	1:F:307:PHE:HE1	1.68	0.41
1:I:164:THR:OG1	1:I:167:GLN:HG3	2.20	0.41
1:I:201:SER:OG	1:I:271:GLN:HB3	2.20	0.41
1:M:272:ILE:HG22	1:M:325:LEU:HD11	2.02	0.41
2:U:6:ALA:HA	2:U:9:VAL:HG12	2.02	0.41
3:Y:428:MET:O	3:Y:432:SER:OG	2.32	0.41
3:Z:269:LEU:HA	3:Z:272:GLU:HG2	2.01	0.41
3:a:100:ALA:HA	3:a:103:ARG:HH12	1.85	0.41
3:a:333:LEU:O	3:a:337:VAL:HG23	2.20	0.41
3:e:306:ASP:C	3:e:307:TYR:CD1	2.98	0.41
3:e:454:MET:O	3:e:457:ILE:HG22	2.20	0.41
3:g:250:GLU:HG2	3:g:254:ARG:NH1	2.35	0.41
2:k:83:GLN:NE2	2:k:92:ALA:HA	2.35	0.41
1:A:109:ASP:OD2	1:A:112:LYS:HG3	2.20	0.41
1:C:11:ASN:ND2	1:C:22:HIS:HA	2.36	0.41
1:C:13:ALA:HB2	1:C:21:ILE:HD13	2.02	0.41
1:C:227:ASP:HB2	1:M:222:THR:HG23	2.02	0.41
1:D:178:ARG:HA	1:D:181:GLU:HG2	2.01	0.41
1:E:61:GLY:N	1:E:80:VAL:O	2.53	0.41
2:P:43:LEU:HD23	2:P:124:ILE:HG13	2.03	0.41
2:P:49:TRP:HH2	2:Q:84:TRP:CE3	2.38	0.41
2:R:11:LEU:HA	2:R:14:ILE:HG12	2.02	0.41
2:T:44:LEU:HD22	2:T:51:ASN:HD22	1.85	0.41
2:V:133:TYR:HH	2:V:140:ASP:CG	2.28	0.41
3:Y:107:LYS:HB3	3:Y:395:VAL:HG11	2.01	0.41
3:Z:125:ILE:O	3:Z:129:ILE:HG12	2.20	0.41
3:Z:275:GLY:O	3:Z:279:LEU:HG	2.21	0.41
3:b:34:VAL:O	3:b:36:PRO:HD3	2.20	0.41
3:c:250:GLU:OE2	3:c:254:ARG:NH2	2.45	0.41
3:e:137:TYR:HE1	3:e:139:ASP:HB2	1.85	0.41
3:f:241:VAL:HG13	3:f:241:VAL:O	2.20	0.41
3:g:136:LEU:HD11	3:g:145:VAL:HB	2.01	0.41
3:g:316:ARG:HH12	3:h:308:VAL:CG2	2.31	0.41
3:i:312:ALA:C	3:i:314:ALA:N	2.78	0.41
3:i:454:MET:O	3:i:458:TRP:CD1	2.73	0.41
1:G:157:LYS:HG3	1:G:324:GLU:HB3	2.01	0.41
1:G:252:ILE:HG12	1:G:263:VAL:HB	2.02	0.41
1:I:176:HIS:O	1:I:180:VAL:HG23	2.19	0.41
1:K:285:GLN:NE2	1:K:288:PRO:HA	2.36	0.41
1:M:198:THR:HG23	1:M:198:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:33:LEU:HB3	2:Q:34:PRO:HD3	2.03	0.41
2:R:39:GLN:HB2	2:R:124:ILE:HG23	2.01	0.41
2:X:75:PHE:HB3	2:X:84:TRP:CG	2.55	0.41
3:Z:464:ASP:OD1	3:Z:464:ASP:N	2.50	0.41
3:a:308:VAL:HB	3:a:311:GLY:H	1.85	0.41
3:c:30:PRO:O	3:c:33:MET:HG2	2.19	0.41
3:c:290:GLU:HB3	2:l:155:ASN:CG	2.45	0.41
3:i:177:LEU:HD23	3:i:181:TYR:HB3	2.02	0.41
3:i:308:VAL:HG21	3:i:312:ALA:O	2.21	0.41
1:B:246:ARG:NE	1:B:246:ARG:HA	2.36	0.41
1:C:29:ILE:HG23	1:M:315:ARG:HH21	1.86	0.41
1:E:198:THR:HG23	1:E:198:THR:O	2.20	0.41
1:F:169:ALA:HA	1:F:172:ILE:HG12	2.01	0.41
1:K:86:LEU:HD21	1:K:311:ASN:HB3	2.03	0.41
1:M:176:HIS:O	1:M:180:VAL:HG23	2.21	0.41
2:R:93:ASN:OD1	2:R:94:THR:N	2.53	0.41
2:S:113:TRP:CH2	2:S:121:GLN:HG3	2.55	0.41
2:X:60:PRO:HA	2:X:66:ILE:HA	2.03	0.41
3:Y:41:ARG:HH21	3:j:254:ARG:NH1	2.18	0.41
3:Z:133:ASN:ND2	3:Z:253:GLY:H	2.18	0.41
3:Z:137:TYR:HD1	3:Z:239:TYR:CE1	2.39	0.41
3:a:6:ALA:O	3:a:10:GLU:HG2	2.19	0.41
3:g:14:ASP:O	3:g:18:GLU:HG2	2.19	0.41
3:g:276:LEU:HD22	3:h:284:VAL:HG21	2.02	0.41
3:h:301:ASP:OD1	3:h:301:ASP:N	2.53	0.41
2:l:69:PRO:HG3	2:l:107:LEU:HD21	2.02	0.41
2:m:2:LEU:HD23	2:m:5:ASP:OD2	2.20	0.41
1:D:213:LYS:HE2	1:D:219:TYR:HE2	1.86	0.41
1:G:125:LYS:HD2	1:G:125:LYS:HA	1.84	0.41
1:J:207:LEU:HD23	1:J:207:LEU:HA	1.87	0.41
1:L:140:MET:HE3	1:L:141:ASP:H	1.85	0.41
2:P:93:ASN:OD1	2:P:94:THR:N	2.54	0.41
2:V:165:ARG:HD2	2:V:165:ARG:HA	1.91	0.41
2:X:99:ILE:HG22	2:X:101:LYS:H	1.85	0.41
2:X:159:ARG:NH2	3:b:309:PRO:O	2.53	0.41
3:Y:408:HIS:C	3:Y:409:LYS:HG2	2.45	0.41
3:Z:14:ASP:HB3	3:Z:17:VAL:HG22	2.01	0.41
3:Z:162:ARG:NE	3:Z:206:ARG:HH22	2.19	0.41
3:d:307:TYR:CD2	3:d:308:VAL:HG12	2.56	0.41
3:f:190:ARG:HB3	3:f:191:ASN:H	1.58	0.41
3:g:309:PRO:HB2	3:g:315:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:373:GLY:HA3	3:i:57:ASN:OD1	2.21	0.41
3:i:159:ALA:HA	3:i:249:GLY:HA2	2.02	0.41
3:j:204:VAL:HG12	3:j:217:LEU:HA	2.02	0.41
3:j:428:MET:HE3	3:j:431:ALA:HB3	2.02	0.41
1:A:15:LYS:HB3	1:A:15:LYS:HE2	1.80	0.41
1:B:159:ASP:HA	1:B:326:LYS:HB3	2.03	0.41
1:B:211:HIS:HB3	1:B:214:LEU:HB3	2.02	0.41
1:D:99:ASP:OD2	1:D:101:GLN:HB2	2.21	0.41
1:G:112:LYS:O	1:G:112:LYS:HD3	2.21	0.41
1:H:90:THR:O	1:H:309:MET:HG3	2.21	0.41
1:H:205:PHE:O	1:H:209:LEU:HD23	2.21	0.41
1:L:170:ASP:O	1:L:174:ARG:HG3	2.21	0.41
2:S:13:LYS:HE3	2:S:146:ILE:CD1	2.50	0.41
2:W:38:ASP:O	2:W:41:ILE:HG22	2.20	0.41
2:W:58:LEU:HD22	2:W:69:PRO:HD3	2.02	0.41
3:Y:12:LEU:HD23	3:Y:12:LEU:HA	1.92	0.41
3:Y:93:ASP:HB3	3:Y:96:GLU:OE1	2.20	0.41
3:Y:279:LEU:HD21	3:j:269:LEU:HD13	2.03	0.41
3:Z:284:VAL:C	3:Z:285:LEU:HD22	2.46	0.41
3:Z:404:ILE:HD12	3:Z:406:LYS:HB2	2.03	0.41
3:a:100:ALA:HA	3:a:103:ARG:NH1	2.36	0.41
3:a:300:GLN:HG2	3:a:306:ASP:HA	2.02	0.41
3:b:345:MET:HE1	3:b:368:ALA:HA	2.03	0.41
3:h:404:ILE:HD12	3:h:406:LYS:HB2	2.03	0.41
3:i:335:ALA:O	3:i:339:ARG:HG2	2.20	0.41
1:D:103:GLU:O	1:D:106:GLN:HG2	2.21	0.41
1:F:40:PHE:O	1:F:44:MET:HE2	2.21	0.41
1:F:213:LYS:HE2	1:F:219:TYR:CE2	2.56	0.41
1:J:333:ILE:H	1:J:333:ILE:HD12	1.86	0.41
1:M:154:VAL:HG11	1:M:179:VAL:HG13	2.02	0.41
1:O:121:GLU:HA	1:O:121:GLU:OE2	2.21	0.41
2:R:163:ARG:NH2	2:S:106:ARG:HH12	2.19	0.41
2:U:120:ALA:HA	2:U:123:VAL:HG22	2.03	0.41
2:V:26:TYR:CG	2:V:27:PRO:HD2	2.56	0.41
3:Y:183:GLN:C	3:Y:185:LEU:H	2.28	0.41
3:Y:185:LEU:HD23	3:Y:185:LEU:HA	1.81	0.41
3:Y:304:MET:CG	3:j:286:ASN:HD21	2.33	0.41
3:a:156:ARG:HH12	3:b:173:LYS:HD3	1.85	0.41
3:c:61:ALA:O	3:c:65:ARG:HG2	2.21	0.41
3:c:120:VAL:O	3:c:124:VAL:HG23	2.20	0.41
3:f:301:ASP:N	3:f:301:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ARG:NH2	1:F:205:PHE:HD2	2.19	0.41
1:B:12:TYR:CE1	1:B:22:HIS:HE1	2.39	0.41
1:B:44:MET:HE2	1:B:312:ILE:HD12	2.01	0.41
1:B:288:PRO:HG3	3:a:42:GLY:HA2	2.01	0.41
1:C:308:GLN:HG2	1:C:310:TYR:HD1	1.86	0.41
1:D:219:TYR:HB3	1:I:228:TYR:HB3	2.03	0.41
1:E:173:VAL:HG21	1:E:211:HIS:NE2	2.36	0.41
1:G:103:GLU:OE2	1:G:104:TRP:NE1	2.54	0.41
1:G:195:GLU:OE1	1:G:278:SER:OG	2.33	0.41
1:G:201:SER:HB3	1:G:271:GLN:HB3	2.02	0.41
1:H:99:ASP:OD1	1:H:100:HIS:N	2.54	0.41
1:J:88:VAL:HG13	1:J:311:ASN:OD1	2.21	0.41
1:J:226:ASN:OD1	1:J:233:VAL:HA	2.20	0.41
1:J:269:GLU:HB2	1:J:328:ILE:HG22	2.03	0.41
1:L:198:THR:HG23	1:L:198:THR:O	2.21	0.41
2:P:172:LYS:HD3	3:e:298:ASP:HA	2.02	0.41
2:S:40:ARG:NH2	2:S:110:SER:HB3	2.34	0.41
2:S:60:PRO:HA	2:S:66:ILE:HA	2.03	0.41
2:T:8:ASN:HB3	2:T:12:ARG:HH21	1.86	0.41
2:T:159:ARG:HH21	3:j:308:VAL:HG11	1.85	0.41
2:X:75:PHE:HD1	2:X:107:LEU:HG	1.86	0.41
2:X:179:ARG:HD2	2:X:179:ARG:HA	1.73	0.41
3:Z:25:ALA:HB1	3:Z:30:PRO:HA	2.02	0.41
3:Z:179:GLU:HA	3:Z:182:LYS:HE3	2.02	0.41
3:a:178:ASP:OD2	3:a:180:GLU:HG2	2.20	0.41
3:a:318:TYR:HD1	3:b:312:ALA:HB1	1.85	0.41
3:a:410:PRO:O	3:b:114:GLN:NE2	2.31	0.41
3:b:248:PRO:HG2	3:c:34:VAL:HB	2.03	0.41
3:b:345:MET:CE	3:b:368:ALA:HA	2.51	0.41
3:c:174:SER:O	3:c:182:LYS:NZ	2.54	0.41
3:c:217:LEU:HD21	3:c:219:HIS:NE2	2.36	0.41
3:c:396:ASP:OD1	3:c:396:ASP:N	2.49	0.41
3:d:274:LEU:HD13	3:d:329:ILE:HB	2.02	0.41
3:e:388:ALA:O	3:e:392:LEU:HG	2.20	0.41
3:f:136:LEU:HD23	3:f:387:LEU:HD21	2.03	0.41
3:f:153:TYR:HA	3:f:167:VAL:O	2.20	0.41
3:f:447:ARG:HG3	3:f:447:ARG:NH1	2.35	0.41
3:h:93:ASP:HB3	3:h:96:GLU:OE1	2.21	0.41
2:k:69:PRO:HG3	2:k:107:LEU:HD21	2.03	0.41
2:k:173:ARG:O	2:k:177:ARG:HB2	2.21	0.41
1:D:127:ASP:HB2	1:D:246:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:ILE:HG22	1:O:174:ARG:HD3	2.01	0.41
1:G:178:ARG:HA	1:G:181:GLU:HG3	2.03	0.41
1:H:122:LEU:HD23	1:H:122:LEU:HA	1.90	0.41
1:H:280:THR:HG21	1:H:320:ALA:HB2	2.02	0.41
1:I:325:LEU:HD23	1:I:325:LEU:HA	1.93	0.41
1:J:198:THR:HG23	1:J:198:THR:O	2.21	0.41
1:K:269:GLU:HB3	1:K:325:LEU:O	2.20	0.41
1:L:131:LEU:HD13	1:L:247:PHE:CD1	2.56	0.41
1:L:207:LEU:HD21	1:L:331:PHE:CE2	2.56	0.41
2:Q:39:GLN:OE1	2:Q:39:GLN:N	2.54	0.41
2:S:10:ILE:HG13	2:S:129:ALA:HA	2.03	0.41
2:S:163:ARG:HA	3:i:307:TYR:CE1	2.56	0.41
2:U:49:TRP:HB3	2:U:161:HIS:HD1	1.86	0.41
2:V:179:ARG:HH22	2:V:182:LEU:HB3	1.85	0.41
3:a:55:LEU:HD21	3:a:341:ASN:OD1	2.21	0.41
3:d:174:SER:N	3:d:196:GLY:O	2.54	0.41
3:d:290:GLU:HG3	2:m:155:ASN:HB3	2.02	0.41
3:e:75:PHE:CZ	3:e:392:LEU:HD21	2.56	0.41
3:f:63:LEU:O	3:f:67:LEU:HD23	2.21	0.41
3:f:155:VAL:HG22	3:f:166:ILE:HG22	2.02	0.41
3:f:428:MET:HE3	3:f:428:MET:HB2	1.83	0.41
3:i:446:PRO:HD2	3:i:448:ILE:HG13	2.02	0.41
3:j:136:LEU:HB3	3:j:240:ILE:HB	2.03	0.41
1:B:176:HIS:HD1	1:B:236:LEU:HG	1.85	0.40
1:D:38:SER:HB2	1:D:123:ALA:HB1	2.03	0.40
1:E:53:ASN:OD1	1:E:54:VAL:HG13	2.21	0.40
1:E:55:VAL:HB	1:E:86:LEU:HB3	2.03	0.40
1:H:174:ARG:CZ	1:H:178:ARG:HH22	2.34	0.40
1:I:227:ASP:OD2	1:I:230:LYS:HG3	2.20	0.40
1:J:203:ARG:NH1	1:J:331:PHE:O	2.55	0.40
1:J:236:LEU:O	1:J:239:VAL:HG12	2.21	0.40
1:K:9:ARG:HG2	1:K:12:TYR:CE1	2.56	0.40
1:K:12:TYR:HD1	1:K:17:ALA:HB1	1.86	0.40
1:K:59:ARG:NH2	1:K:315:ARG:O	2.47	0.40
1:N:209:LEU:HA	1:N:215:MET:HE2	2.03	0.40
1:O:200:MET:HE3	1:O:241:VAL:HG13	2.04	0.40
1:O:227:ASP:OD2	1:O:230:LYS:HG3	2.21	0.40
2:R:48:TRP:CZ3	3:g:293:GLY:HA3	2.56	0.40
2:R:140:ASP:OD2	2:R:142:THR:HB	2.21	0.40
2:R:179:ARG:C	2:R:181:SER:H	2.29	0.40
3:Y:296:VAL:HG22	3:Y:300:GLN:HE22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:55:LEU:HD13	3:a:340:LEU:HB3	2.03	0.40
3:f:307:TYR:HB2	3:f:309:PRO:HD2	2.03	0.40
3:g:264:PHE:CE1	3:g:340:LEU:HD21	2.56	0.40
3:h:9:TRP:CD1	3:h:167:VAL:HG13	2.54	0.40
3:h:25:ALA:HB1	3:h:30:PRO:HA	2.03	0.40
3:h:61:ALA:O	3:h:65:ARG:HG2	2.21	0.40
3:h:203:HIS:HE1	3:h:205:GLN:HE21	1.69	0.40
2:k:40:ARG:HA	2:k:124:ILE:HD13	2.03	0.40
1:F:50:ARG:NH1	1:F:286:VAL:O	2.53	0.40
1:K:280:THR:HG23	1:K:281:LEU:HG	2.03	0.40
1:L:9:ARG:HD2	1:L:9:ARG:HA	1.88	0.40
1:L:279:LYS:HE2	1:L:316:ARG:HD2	2.03	0.40
1:N:289:VAL:HA	1:N:308:GLN:HB3	2.03	0.40
1:O:225:THR:HG23	1:O:226:ASN:OD1	2.20	0.40
1:O:255:HIS:N	1:O:262:ASN:OD1	2.46	0.40
2:P:112:GLU:O	2:P:116:ILE:HG12	2.21	0.40
2:R:53:TRP:HE3	2:R:56:HIS:NE2	2.19	0.40
2:V:113:TRP:CZ2	2:V:121:GLN:HB3	2.56	0.40
2:V:179:ARG:NH2	2:V:182:LEU:HB3	2.37	0.40
3:a:442:ALA:HA	3:a:448:ILE:HD11	2.03	0.40
3:c:287:LEU:O	3:c:315:VAL:HA	2.21	0.40
3:c:399:LEU:HG	3:c:400:LEU:HG	2.02	0.40
3:c:434:VAL:CG1	3:c:457:ILE:HD11	2.51	0.40
3:d:158:ASP:OD1	3:d:160:THR:N	2.54	0.40
3:d:408:HIS:C	3:d:409:LYS:HG2	2.46	0.40
3:e:107:LYS:HD2	3:e:110:GLN:NE2	2.36	0.40
3:e:287:LEU:O	3:e:315:VAL:HA	2.22	0.40
3:g:242:PRO:HA	3:g:382:ASN:HB3	2.04	0.40
3:h:263:ASP:HB3	3:h:340:LEU:HD21	2.03	0.40
3:i:212:MET:HE2	3:i:212:MET:HB3	1.99	0.40
3:j:18:GLU:OE2	3:j:151:ARG:HG2	2.22	0.40
1:D:212:ASP:O	1:D:216:ASN:HB2	2.21	0.40
1:E:43:LEU:HB3	3:g:11:LYS:HE2	2.03	0.40
1:G:128:GLN:HB2	1:G:246:ARG:NH2	2.37	0.40
1:K:39:LYS:HE2	1:K:39:LYS:HB2	1.79	0.40
2:P:54:TRP:HZ3	2:P:106:ARG:NH2	2.18	0.40
2:Q:163:ARG:HG3	3:g:307:TYR:HD2	1.86	0.40
2:S:139:PRO:HA	2:S:143:ALA:CB	2.51	0.40
2:T:112:GLU:O	2:T:116:ILE:HG13	2.21	0.40
2:U:1:MET:N	2:U:121:GLN:OE1	2.34	0.40
2:U:174:SER:O	2:U:175:PHE:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:107:LYS:HE2	3:Z:395:VAL:HG13	2.03	0.40
3:Z:204:VAL:HA	3:Z:217:LEU:HA	2.02	0.40
3:Z:452:LYS:HE2	3:a:95:THR:OG1	2.21	0.40
3:a:281:SER:C	3:a:282:LEU:HD12	2.46	0.40
3:a:378:LEU:O	3:a:381:GLU:HG3	2.21	0.40
3:b:404:ILE:HD11	3:b:407:GLN:HE22	1.87	0.40
3:c:434:VAL:HG13	3:d:429:LEU:CD2	2.51	0.40
3:d:100:ALA:HA	3:d:103:ARG:HH12	1.86	0.40
3:e:292:LYS:HD2	3:e:292:LYS:HA	1.83	0.40
3:e:331:GLN:HG3	3:e:332:SER:N	2.37	0.40
3:f:65:ARG:HA	3:f:65:ARG:NE	2.35	0.40
3:f:444:LEU:HD13	3:g:466:SER:HB3	2.03	0.40
3:h:340:LEU:O	3:h:344:PHE:N	2.54	0.40
2:l:179:ARG:C	2:l:181:SER:H	2.30	0.40
2:m:149:GLU:OE2	2:m:153:TYR:CZ	2.74	0.40
1:A:9:ARG:H	1:A:9:ARG:HG2	1.74	0.40
1:G:302:TRP:CZ3	2:X:180:ARG:HD3	2.57	0.40
1:I:33:HIS:ND1	1:I:34:PHE:N	2.68	0.40
2:P:43:LEU:HD12	2:P:48:TRP:HE1	1.86	0.40
2:Q:175:PHE:HA	3:e:279:LEU:HD13	2.04	0.40
2:R:1:MET:HE2	2:R:1:MET:HB3	1.91	0.40
3:a:24:PHE:HE2	3:a:258:GLU:HG3	1.87	0.40
3:a:106:ARG:O	3:a:110:GLN:HG2	2.21	0.40
3:b:7:MET:HA	3:b:7:MET:HE2	2.04	0.40
3:b:165:ASP:OD1	3:b:203:HIS:NE2	2.54	0.40
3:b:276:LEU:HD11	2:l:170:GLN:HB3	2.03	0.40
3:c:434:VAL:HG13	3:d:429:LEU:HD21	2.02	0.40
3:d:329:ILE:O	3:d:333:LEU:HD13	2.20	0.40
3:e:41:ARG:HH11	3:e:41:ARG:HB3	1.86	0.40
3:f:74:PHE:CZ	3:f:112:LEU:HD13	2.56	0.40
3:g:28:THR:OG1	3:g:53:ALA:HA	2.21	0.40
3:i:9:TRP:HB2	3:i:167:VAL:HG11	2.04	0.40
3:j:451:PRO:HA	3:j:454:MET:HE2	2.04	0.40
2:l:7:VAL:HA	2:l:10:ILE:HG12	2.02	0.40
1:A:65:ALA:HA	1:F:94:LEU:HD21	2.04	0.40
1:A:229:VAL:HG12	1:L:214:LEU:HD12	2.03	0.40
1:B:128:GLN:HE21	1:B:248:ALA:HB2	1.86	0.40
1:C:215:MET:HE1	1:C:233:VAL:HG22	2.04	0.40
1:F:150:PHE:HD1	1:F:316:ARG:HH22	1.69	0.40
1:G:170:ASP:HB2	1:G:174:ARG:NH1	2.36	0.40
1:G:257:LEU:HD11	1:G:310:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:216:ASN:HB3	1:H:219:TYR:HD1	1.86	0.40
1:L:192:VAL:HG13	1:L:193:TYR:HD1	1.86	0.40
1:O:269:GLU:OE1	1:O:328:ILE:HG22	2.21	0.40
2:T:9:VAL:O	2:T:13:LYS:HG2	2.22	0.40
3:Y:256:HIS:CE1	3:Y:260:TYR:HE2	2.40	0.40
3:Y:449:SER:OG	3:Y:451:PRO:HD2	2.21	0.40
3:Z:155:VAL:HG12	3:Z:252:TYR:HE1	1.87	0.40
3:Z:369:GLU:OE1	3:Z:376:TYR:HB3	2.21	0.40
3:a:208:LYS:HA	3:a:213:GLU:HG3	2.04	0.40
3:b:157:ARG:NE	3:b:251:HIS:O	2.38	0.40
3:b:286:ASN:HD21	3:c:304:MET:HG2	1.86	0.40
3:c:9:TRP:CZ2	3:c:13:ARG:HD3	2.56	0.40
3:c:403:LEU:HB2	3:c:407:GLN:HB3	2.03	0.40
3:d:31:TYR:CD1	3:d:31:TYR:C	3.00	0.40
3:i:318:TYR:CE2	3:i:320:ARG:HB2	2.56	0.40
3:j:135:LEU:HD22	3:j:148:TRP:CE3	2.56	0.40
3:j:438:LEU:HD12	3:j:453:MET:CE	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/335 (99%)	324 (98%)	7 (2%)	0	100	100
1	B	331/335 (99%)	323 (98%)	8 (2%)	0	100	100
1	C	331/335 (99%)	321 (97%)	10 (3%)	0	100	100
1	D	331/335 (99%)	325 (98%)	6 (2%)	0	100	100
1	E	331/335 (99%)	322 (97%)	9 (3%)	0	100	100
1	F	311/335 (93%)	306 (98%)	5 (2%)	0	100	100
1	G	311/335 (93%)	298 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	311/335 (93%)	305 (98%)	6 (2%)	0	100	100
1	I	311/335 (93%)	307 (99%)	4 (1%)	0	100	100
1	J	311/335 (93%)	304 (98%)	7 (2%)	0	100	100
1	K	331/335 (99%)	323 (98%)	8 (2%)	0	100	100
1	L	331/335 (99%)	322 (97%)	9 (3%)	0	100	100
1	M	331/335 (99%)	324 (98%)	7 (2%)	0	100	100
1	N	331/335 (99%)	320 (97%)	11 (3%)	0	100	100
1	O	331/335 (99%)	318 (96%)	13 (4%)	0	100	100
2	P	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
2	Q	182/184 (99%)	176 (97%)	6 (3%)	0	100	100
2	R	182/184 (99%)	175 (96%)	7 (4%)	0	100	100
2	S	182/184 (99%)	177 (97%)	5 (3%)	0	100	100
2	T	180/184 (98%)	170 (94%)	10 (6%)	0	100	100
2	U	180/184 (98%)	173 (96%)	7 (4%)	0	100	100
2	V	181/184 (98%)	174 (96%)	7 (4%)	0	100	100
2	W	181/184 (98%)	178 (98%)	3 (2%)	0	100	100
2	X	182/184 (99%)	174 (96%)	8 (4%)	0	100	100
2	k	182/184 (99%)	170 (93%)	12 (7%)	0	100	100
2	l	182/184 (99%)	178 (98%)	4 (2%)	0	100	100
2	m	181/184 (98%)	173 (96%)	8 (4%)	0	100	100
3	Y	440/510 (86%)	424 (96%)	16 (4%)	0	100	100
3	Z	440/510 (86%)	422 (96%)	18 (4%)	0	100	100
3	a	440/510 (86%)	426 (97%)	14 (3%)	0	100	100
3	b	440/510 (86%)	419 (95%)	21 (5%)	0	100	100
3	c	440/510 (86%)	423 (96%)	17 (4%)	0	100	100
3	d	441/510 (86%)	419 (95%)	22 (5%)	0	100	100
3	e	440/510 (86%)	421 (96%)	19 (4%)	0	100	100
3	f	440/510 (86%)	424 (96%)	16 (4%)	0	100	100
3	g	439/510 (86%)	415 (94%)	23 (5%)	1 (0%)	43	75
3	h	440/510 (86%)	420 (96%)	20 (4%)	0	100	100
3	i	440/510 (86%)	420 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	j	441/510 (86%)	420 (95%)	21 (5%)	0	100	100
All	All	12322/13353 (92%)	11890 (96%)	431 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	g	465	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/282 (100%)	281 (100%)	0	100	100
1	B	281/282 (100%)	281 (100%)	0	100	100
1	C	281/282 (100%)	281 (100%)	0	100	100
1	D	281/282 (100%)	281 (100%)	0	100	100
1	E	281/282 (100%)	281 (100%)	0	100	100
1	F	264/282 (94%)	264 (100%)	0	100	100
1	G	264/282 (94%)	264 (100%)	0	100	100
1	H	264/282 (94%)	264 (100%)	0	100	100
1	I	264/282 (94%)	264 (100%)	0	100	100
1	J	264/282 (94%)	264 (100%)	0	100	100
1	K	281/282 (100%)	281 (100%)	0	100	100
1	L	281/282 (100%)	281 (100%)	0	100	100
1	M	281/282 (100%)	281 (100%)	0	100	100
1	N	281/282 (100%)	281 (100%)	0	100	100
1	O	281/282 (100%)	281 (100%)	0	100	100
2	P	159/160 (99%)	157 (99%)	2 (1%)	61	72
2	Q	160/160 (100%)	159 (99%)	1 (1%)	78	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	160/160 (100%)	160 (100%)	0	100	100
2	S	160/160 (100%)	160 (100%)	0	100	100
2	T	158/160 (99%)	158 (100%)	0	100	100
2	U	158/160 (99%)	158 (100%)	0	100	100
2	V	159/160 (99%)	159 (100%)	0	100	100
2	W	159/160 (99%)	159 (100%)	0	100	100
2	X	160/160 (100%)	160 (100%)	0	100	100
2	k	160/160 (100%)	160 (100%)	0	100	100
2	l	160/160 (100%)	160 (100%)	0	100	100
2	m	159/160 (99%)	159 (100%)	0	100	100
3	Y	362/410 (88%)	361 (100%)	1 (0%)	86	85
3	Z	362/410 (88%)	359 (99%)	3 (1%)	73	78
3	a	362/410 (88%)	357 (99%)	5 (1%)	59	71
3	b	362/410 (88%)	362 (100%)	0	100	100
3	c	362/410 (88%)	362 (100%)	0	100	100
3	d	362/410 (88%)	361 (100%)	1 (0%)	86	85
3	e	362/410 (88%)	362 (100%)	0	100	100
3	f	362/410 (88%)	361 (100%)	1 (0%)	86	85
3	g	361/410 (88%)	356 (99%)	5 (1%)	59	71
3	h	362/410 (88%)	362 (100%)	0	100	100
3	i	361/410 (88%)	360 (100%)	1 (0%)	86	85
3	j	362/410 (88%)	362 (100%)	0	100	100
All	All	10384/11070 (94%)	10364 (100%)	20 (0%)	85	87

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

Mol	Chain	Res	Type
2	P	169	THR
2	P	170	GLN
2	Q	180	ARG
3	Y	412	ILE
3	Z	399	LEU
3	Z	403	LEU
3	Z	405	THR

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Mol	Chain	Res	Type
3	a	290	GLU
3	a	372	LEU
3	a	375	THR
3	a	377	SER
3	a	378	LEU
3	d	450	LEU
3	f	191	ASN
3	g	441	ILE
3	g	443	GLN
3	g	450	LEU
3	g	452	LYS
3	g	466	SER
3	i	133	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	128	GLN
1	B	101	GLN
1	B	128	GLN
1	B	220	GLN
1	B	237	ASN
1	C	22	HIS
1	C	101	GLN
1	C	120	GLN
1	C	220	GLN
1	D	5	ASN
1	D	226	ASN
1	D	297	ASN
1	E	33	HIS
1	F	22	HIS
1	F	97	GLN
1	F	271	GLN
1	F	308	GLN
1	G	33	HIS
1	H	97	GLN
1	H	271	GLN
1	I	285	GLN
1	J	22	HIS
1	J	53	ASN
1	J	220	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	285	GLN
1	K	22	HIS
1	K	85	ASN
1	K	271	GLN
1	L	45	ASN
1	M	120	GLN
1	M	167	GLN
1	M	290	GLN
1	N	11	ASN
1	N	22	HIS
1	N	285	GLN
1	O	97	GLN
1	O	167	GLN
2	P	154	GLN
2	P	161	HIS
2	P	168	ASN
2	Q	151	GLN
2	R	83	GLN
2	S	170	GLN
2	T	126	HIS
2	T	148	GLN
2	T	154	GLN
2	U	83	GLN
2	V	51	ASN
2	W	121	GLN
2	W	168	ASN
2	X	39	GLN
2	X	127	GLN
2	X	154	GLN
2	X	161	HIS
2	X	168	ASN
3	Y	114	GLN
3	Z	114	GLN
3	Z	133	ASN
3	Z	219	HIS
3	Z	330	GLN
3	Z	370	ASN
3	Z	382	ASN
3	Z	430	ASN
3	a	49	GLN
3	a	123	GLN
3	a	382	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	a	407	GLN
3	b	430	ASN
3	c	205	GLN
3	c	330	GLN
3	c	430	ASN
3	d	58	ASN
3	d	245	ASN
3	d	251	HIS
3	d	384	GLN
3	e	407	GLN
3	e	408	HIS
3	f	286	ASN
3	f	384	GLN
3	g	115	ASN
3	g	235	HIS
3	g	256	HIS
3	h	205	GLN
3	h	330	GLN
3	i	183	GLN
3	i	443	GLN
3	j	110	GLN
3	j	123	GLN
3	j	170	GLN
2	k	8	ASN
2	k	126	HIS
2	k	127	GLN
2	k	154	GLN
2	l	127	GLN
2	l	135	HIS
2	l	155	ASN
2	m	83	GLN
2	m	93	ASN
2	m	121	GLN
2	m	126	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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.

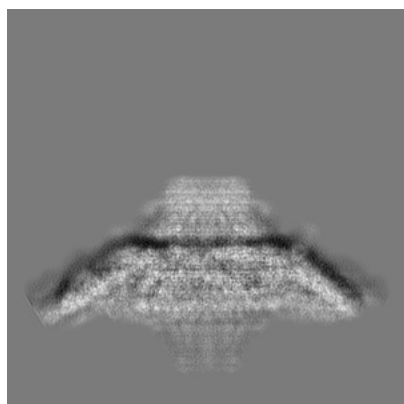
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55352. These allow visual inspection of the internal detail of the map and identification of artifacts.

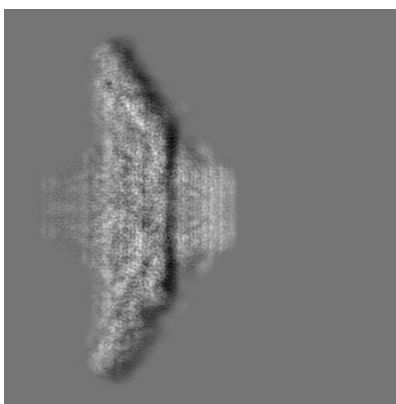
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

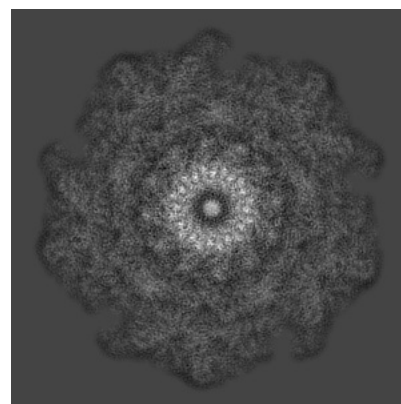
6.1.1 Primary map



X

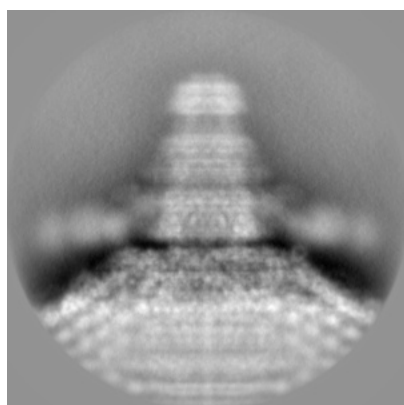


Y

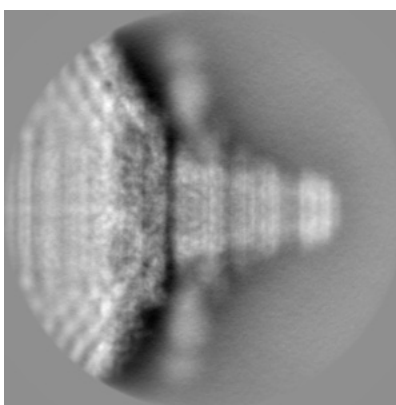


Z

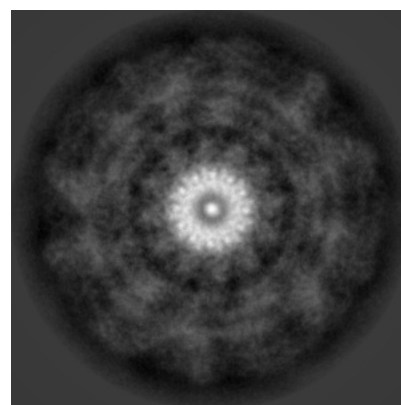
6.1.2 Raw map



X



Y

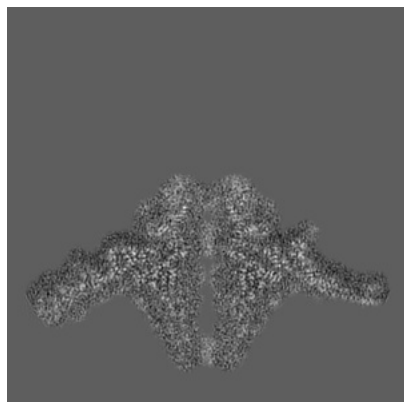


Z

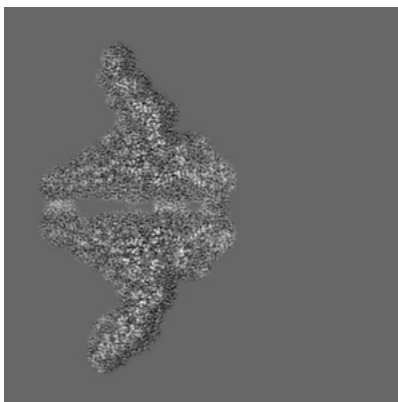
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

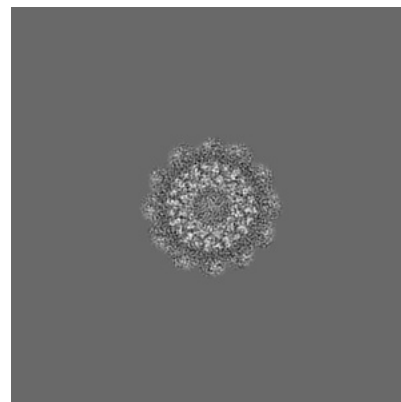
6.2.1 Primary map



X Index: 208

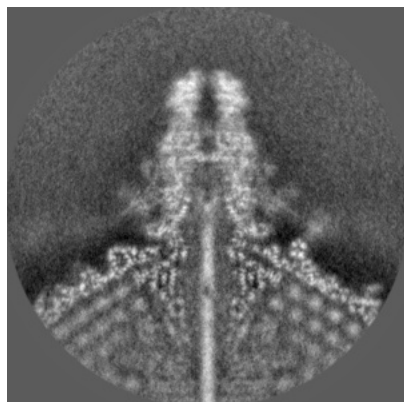


Y Index: 208

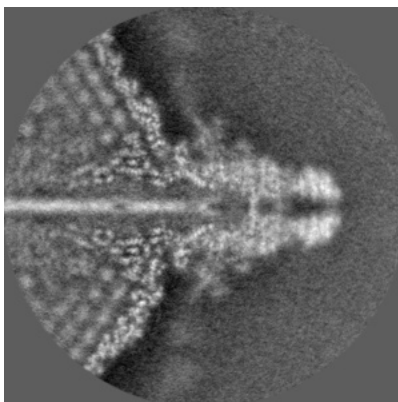


Z Index: 208

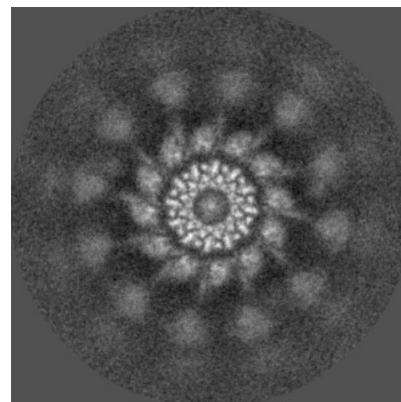
6.2.2 Raw map



X Index: 208



Y Index: 208

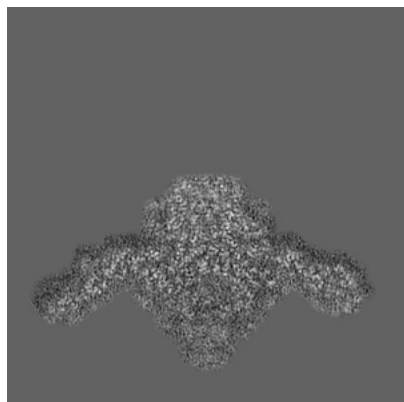


Z Index: 208

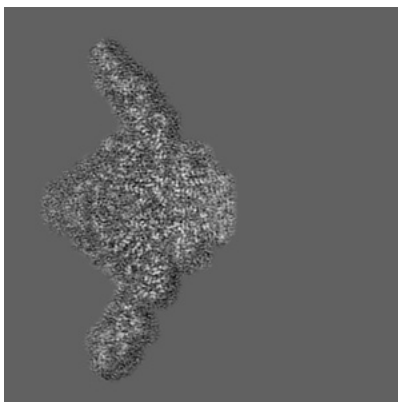
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

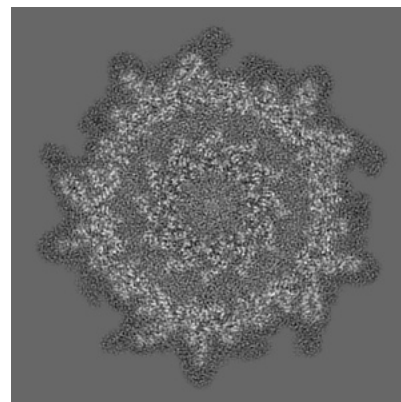
6.3.1 Primary map



X Index: 179

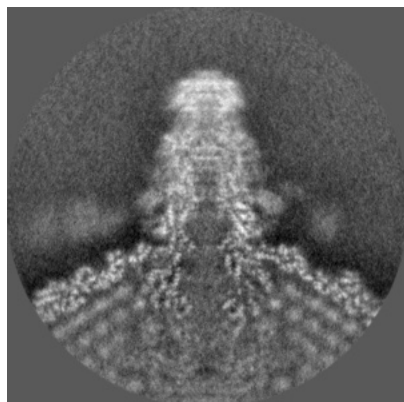


Y Index: 178

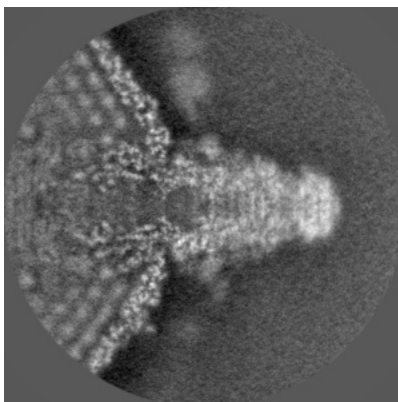


Z Index: 130

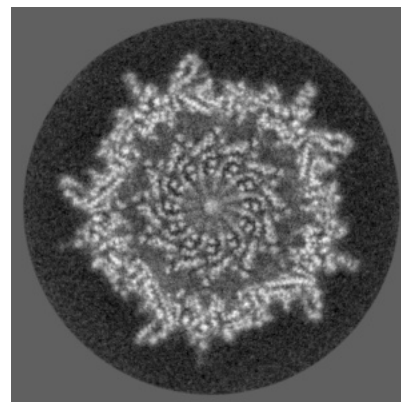
6.3.2 Raw map



X Index: 192



Y Index: 191

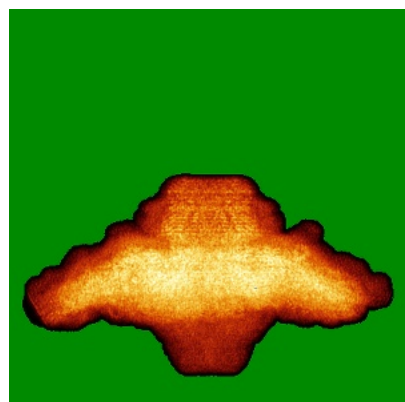


Z Index: 133

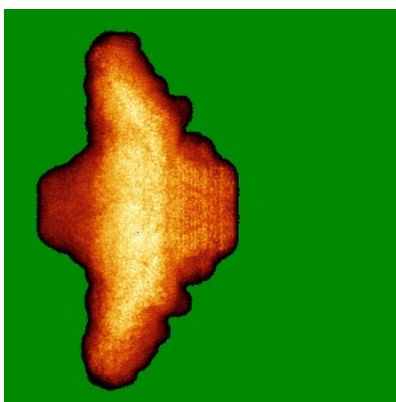
The images above show the largest variance slices of the map in three orthogonal directions.

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

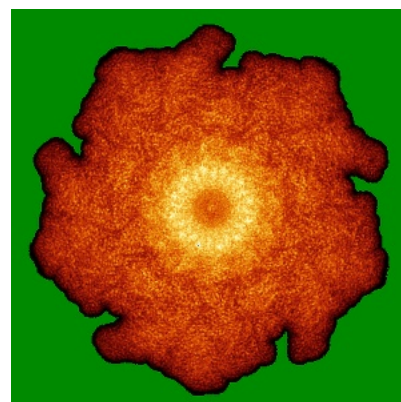
6.4.1 Primary map



X

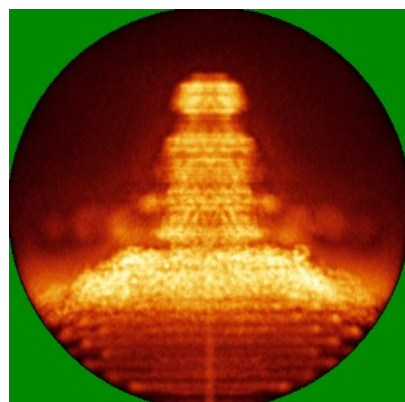


Y

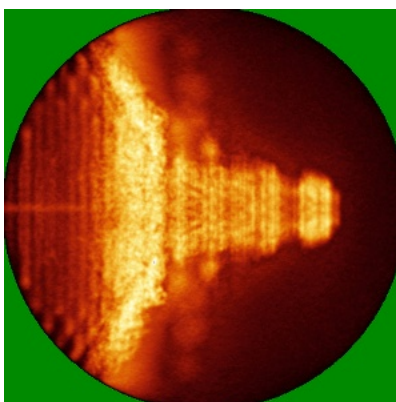


Z

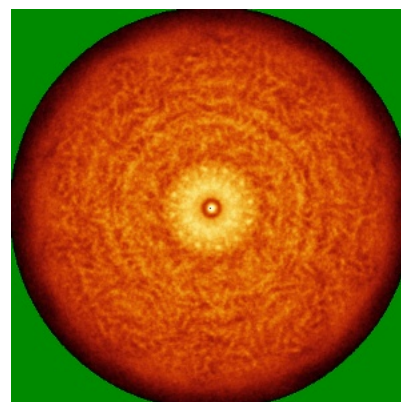
6.4.2 Raw map



X



Y

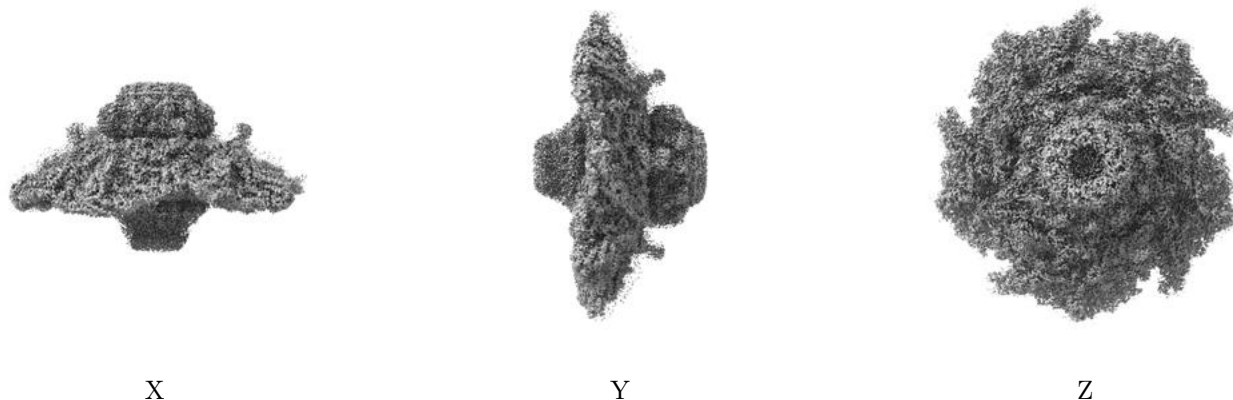


Z

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

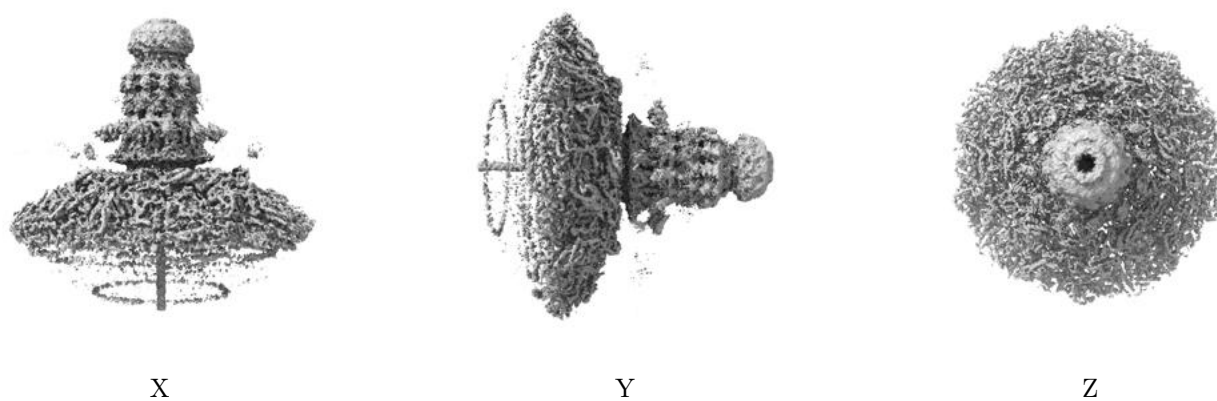
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0195. 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.

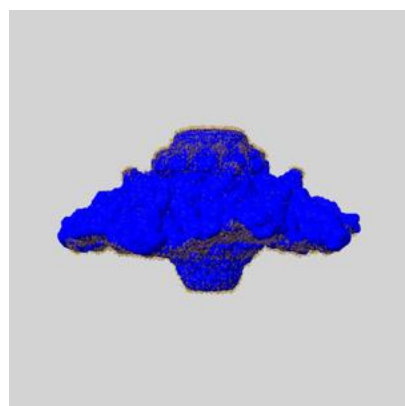
6.6 Mask visualisation [i](#)

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

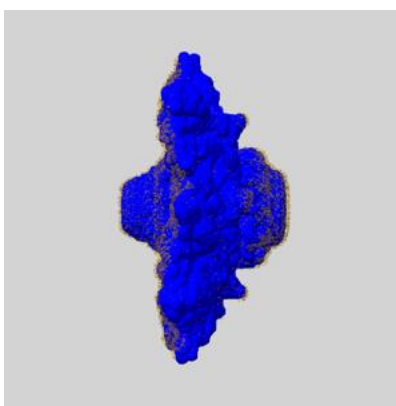
A mask typically either:

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

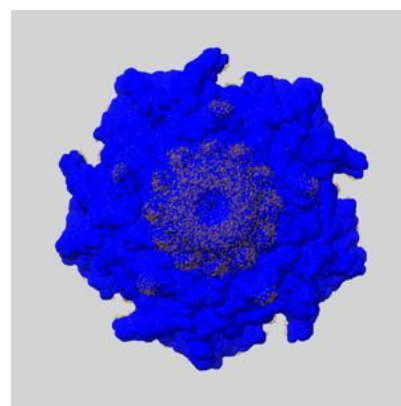
6.6.1 emd_55352_msk_1.map [i](#)



X



Y

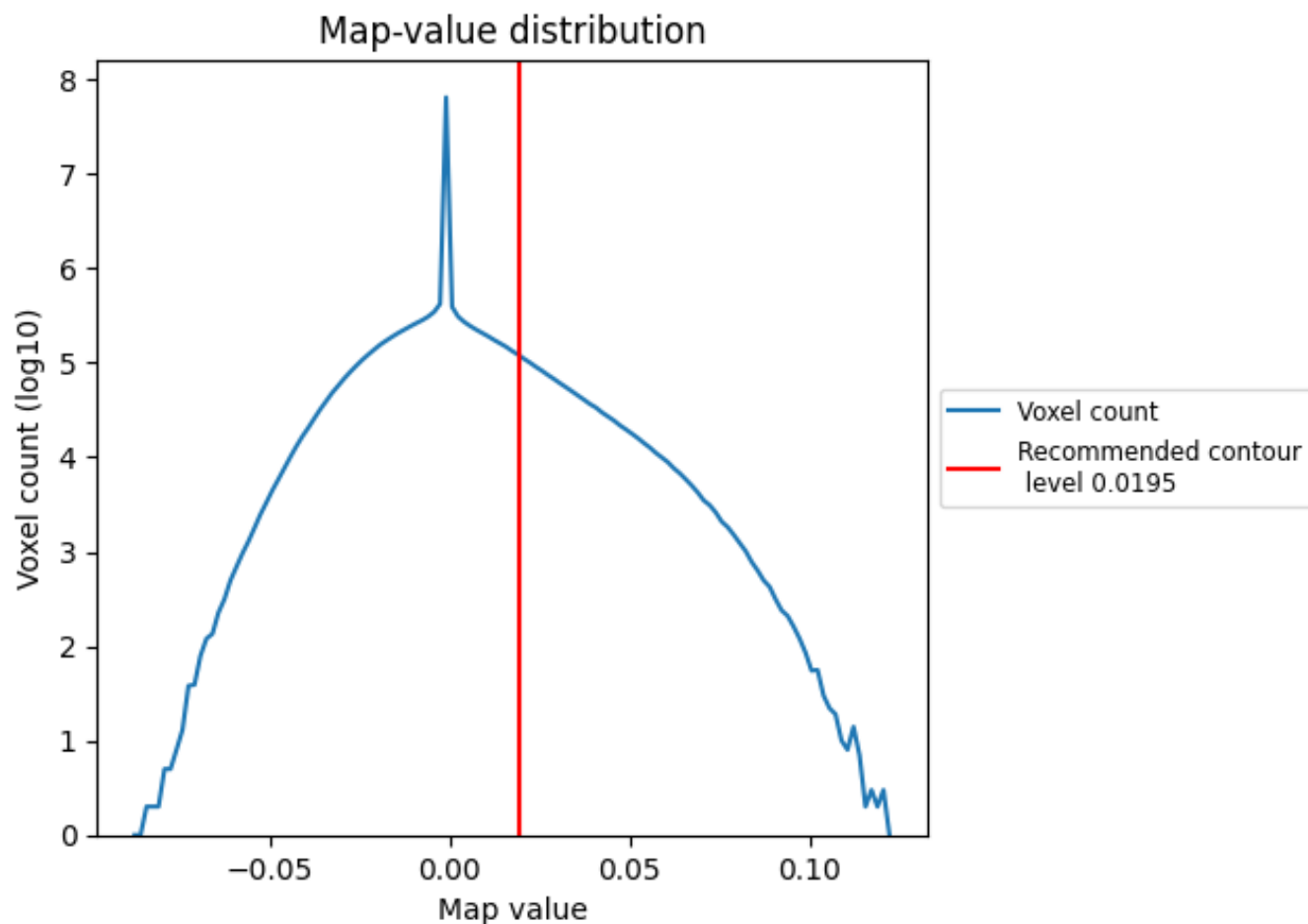


Z

7 Map analysis [i](#)

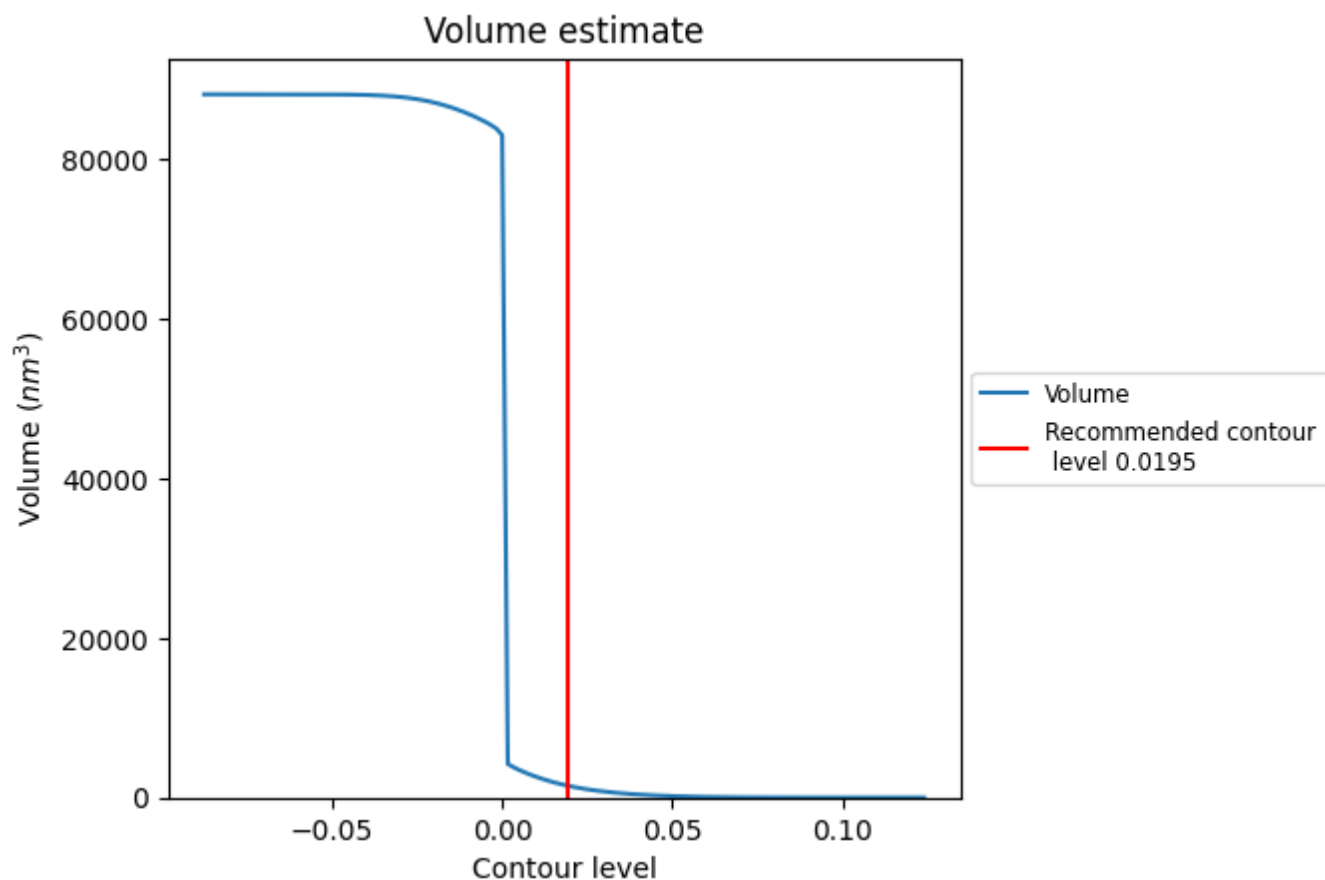
This section contains the results of statistical analysis of the map.

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.

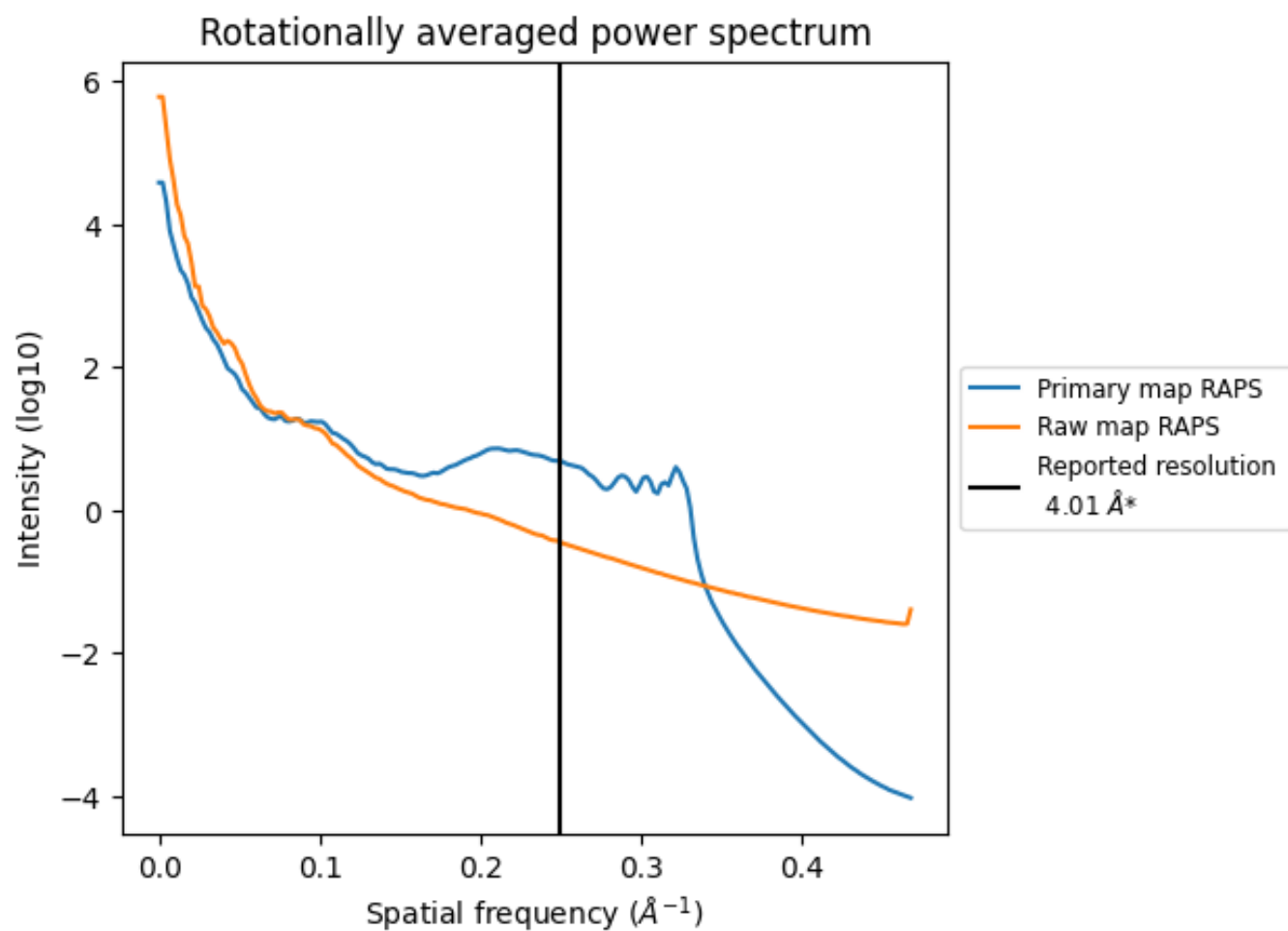
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1464 nm³; this corresponds to an approximate mass of 1323 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 ⓘ

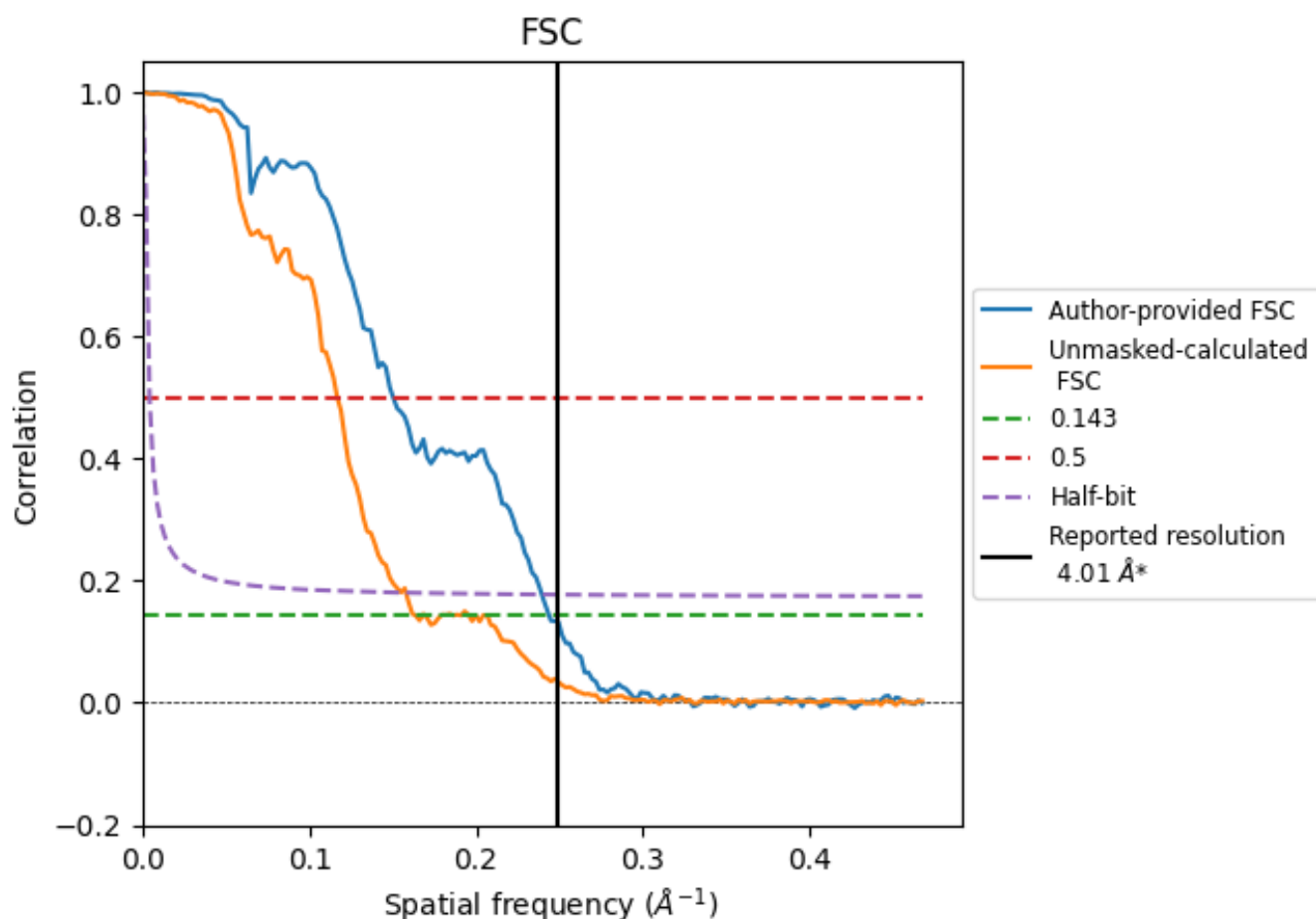


*Reported resolution corresponds to spatial frequency of 0.249 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.249 Å⁻¹

8.2 Resolution estimates [i](#)

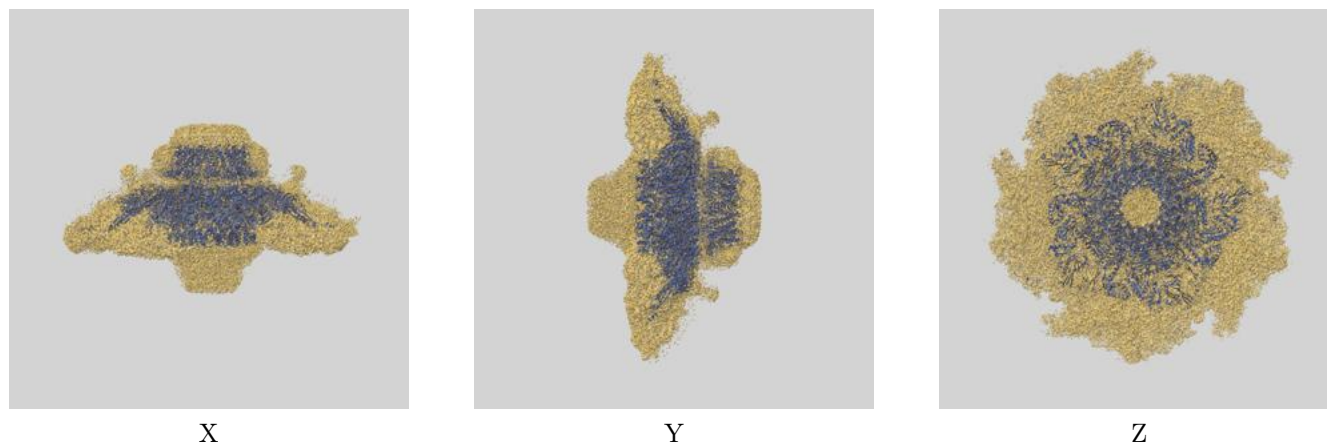
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.01	-	-
Author-provided FSC curve	4.10	6.65	4.18
Unmasked-calculated*	6.12	8.56	6.33

*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 6.12 differs from the reported value 4.01 by more than 10 %

9 Map-model fit [i](#)

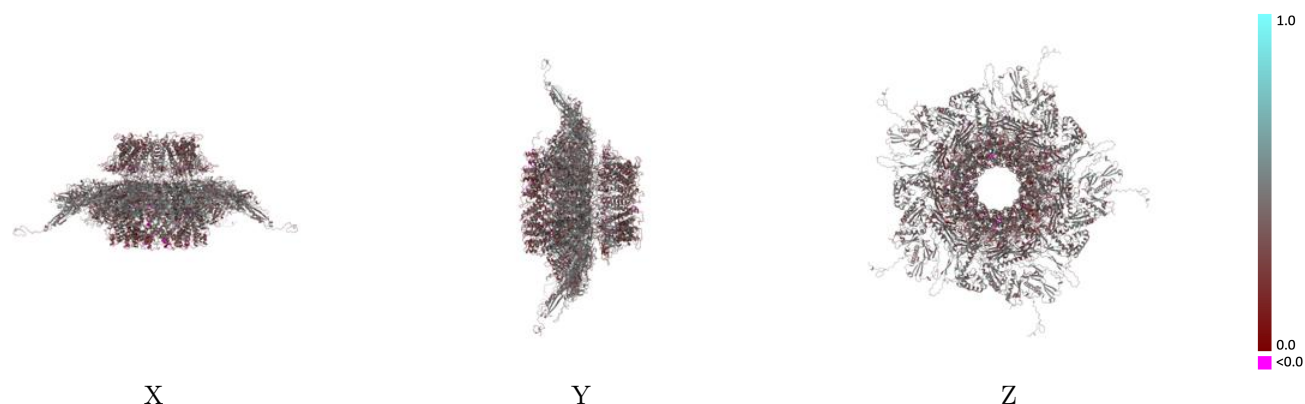
This section contains information regarding the fit between EMDB map EMD-55352 and PDB model 9SYS. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



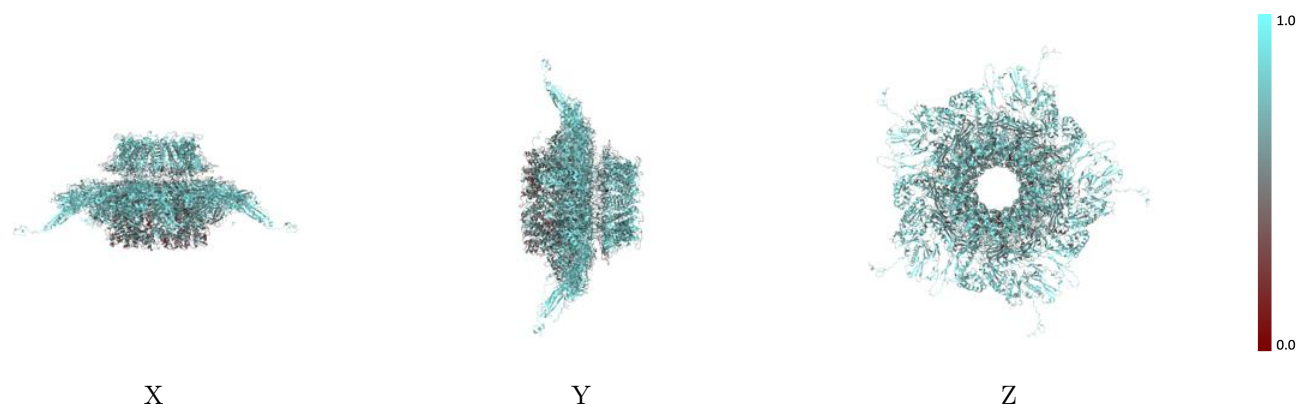
The images above show the 3D surface view of the map at the recommended contour level 0.0195 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



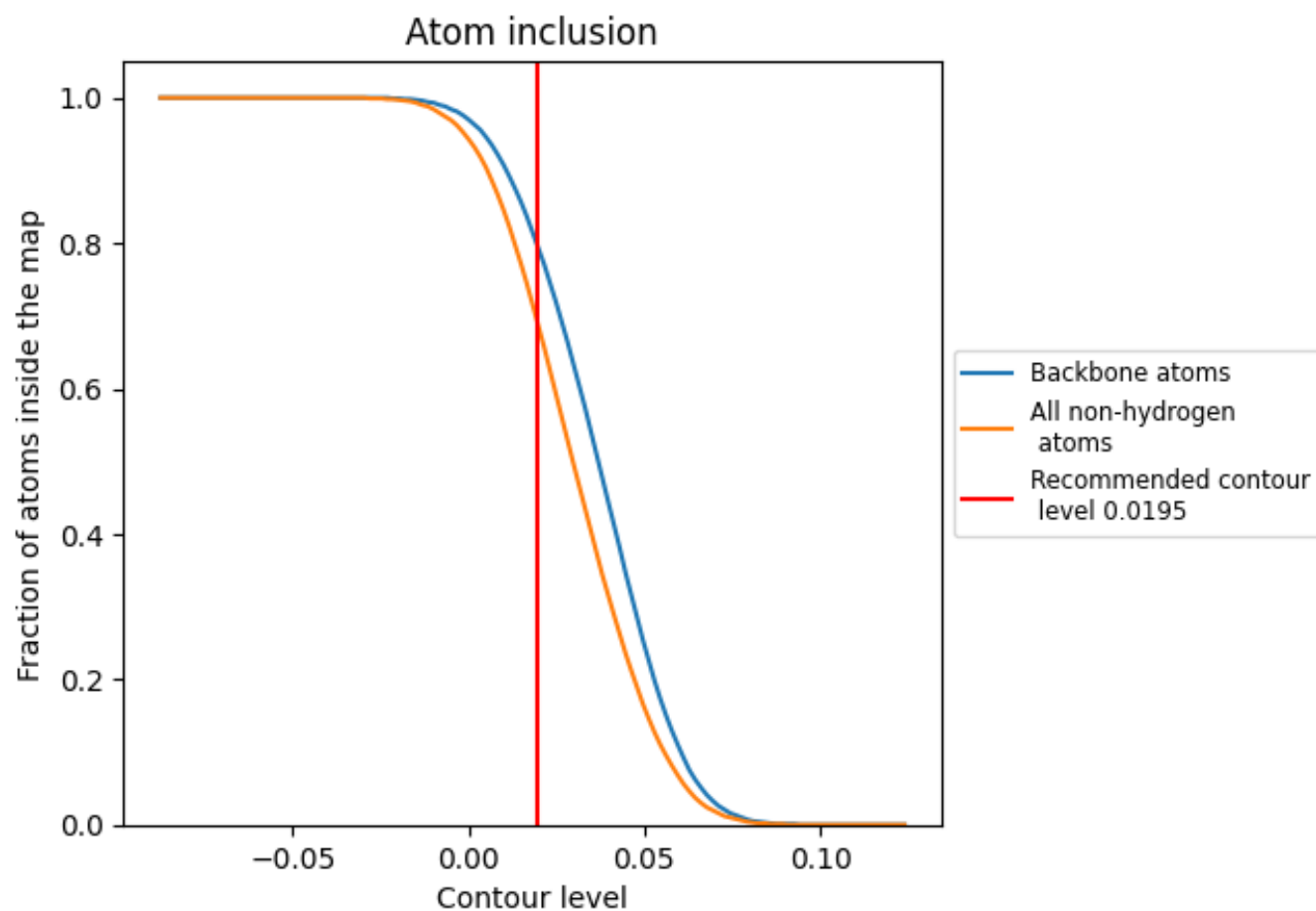
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0195).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0195) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6920	 0.3910
A	 0.7470	 0.4310
B	 0.7690	 0.4480
C	 0.7650	 0.4420
D	 0.7600	 0.4370
E	 0.7660	 0.4420
F	 0.7470	 0.4320
G	 0.7710	 0.4330
H	 0.7490	 0.4230
I	 0.7690	 0.4350
J	 0.7550	 0.4280
K	 0.7650	 0.4210
L	 0.7690	 0.4250
M	 0.7530	 0.4230
N	 0.7660	 0.4250
O	 0.7690	 0.4310
P	 0.7420	 0.3640
Q	 0.7400	 0.3520
R	 0.7300	 0.3470
S	 0.7290	 0.3460
T	 0.7290	 0.3470
U	 0.7280	 0.3560
V	 0.7150	 0.3370
W	 0.7310	 0.3560
X	 0.7240	 0.3490
Y	 0.6190	 0.3780
Z	 0.6020	 0.3670
a	 0.6180	 0.3790
b	 0.6200	 0.3740
c	 0.6280	 0.3800
d	 0.6420	 0.3860
e	 0.5960	 0.3580
f	 0.5940	 0.3590
g	 0.6050	 0.3520
h	 0.6030	 0.3650



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Chain	Atom inclusion	Q-score
i	 0.6050	 0.3700
j	 0.5990	 0.3720
k	 0.7240	 0.3640
l	 0.7360	 0.3550
m	 0.7330	 0.3580