



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:29 PM UTC

PDB ID : 7SPU / pdb_00007spu
EMDB ID : EMD-25372
Title : In situ cryo-EM structure of bacteriophage Sf6 gp3:gp7:gp5 complex in con-
formation 1 at 3.73Å resolution
Authors : Li, F.; Cingolani, G.; Hou, C.; Yang, R.
Deposited on : 2021-11-03
Resolution : 3.73 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

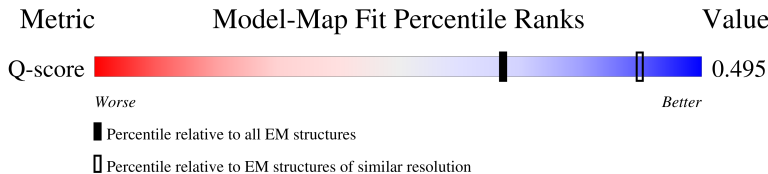
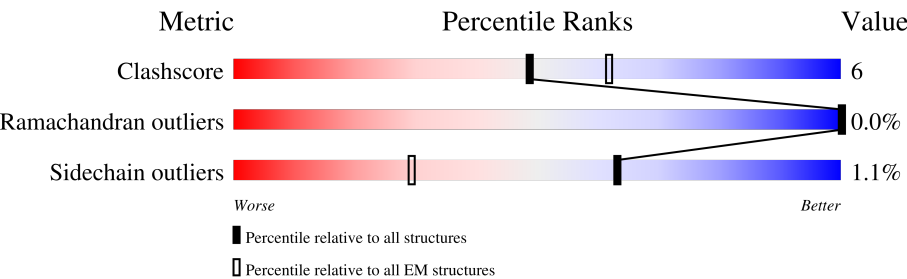
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.73 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	10415 (3.23 - 4.23)

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

Mol	Chain	Length	Quality of chain
1	0	160	30% 76% 17% 8%
1	1	160	42% 74% 24% .
1	Y	160	28% 68% 22% . 8%
1	f	160	34% 82% 16% .

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Mol	Chain	Length	Quality of chain
1	h	160	
1	n	160	
1	p	160	
1	r	160	
1	v	160	
1	w	160	
1	x	160	
1	z	160	
2	A	708	
2	B	708	
2	C	708	
2	D	708	
2	E	708	
2	F	708	
2	G	708	
2	H	708	
2	I	708	
2	J	708	
2	K	708	
2	L	708	
3	M	423	
3	N	423	
3	O	423	
3	P	423	
3	Q	423	

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Mol	Chain	Length	Quality of chain
3	R	423	20% 86% 13%
3	S	423	22% 87% 12%
3	T	423	23% 88% 11%
3	U	423	19% 88% 11%
3	V	423	21% 90% 10%
3	W	423	21% 89% 11%
3	X	423	20% 91% 8%
3	Z	423	20% 87% 12%
3	a	423	23% 83% 17%
3	b	423	18% 86% 13%
3	c	423	19% 88% 11%
3	d	423	18% 85% 14%
3	e	423	22% 86% 12%
3	g	423	23% 86% 12%
3	i	423	21% 83% 15%
3	j	423	21% 86% 13%
3	k	423	22% 85% 13%
3	l	423	20% 82% 16%
3	m	423	22% 87% 13%
3	o	423	20% 88% 12%
3	q	423	24% 84% 15%
3	s	423	19% 88% 12%
3	t	423	21% 90% 9%
3	u	423	23% 87% 13%
3	y	423	23% 88% 12%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 169896 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 Gene 7 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		
1	1	158	Total	C	N	O	S	0	0
			1232	777	202	247	6		
1	Y	148	Total	C	N	O	S	0	0
			1162	734	191	231	6		
1	f	158	Total	C	N	O	S	0	0
			1232	777	202	247	6		
1	h	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		
1	n	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		
1	p	158	Total	C	N	O	S	0	0
			1232	777	202	247	6		
1	r	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		
1	v	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		
1	w	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		
1	x	158	Total	C	N	O	S	0	0
			1232	777	202	247	6		
1	z	158	Total	C	N	O	S	0	0
			1229	774	202	247	6		

- Molecule 2 is a protein called Gene 3 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	B	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	C	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	E	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	F	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	G	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	H	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	I	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	J	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	K	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	L	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		

- Molecule 3 is a protein called Gene 5 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	N	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	O	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	P	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	Q	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	R	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	S	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	T	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	U	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	V	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		

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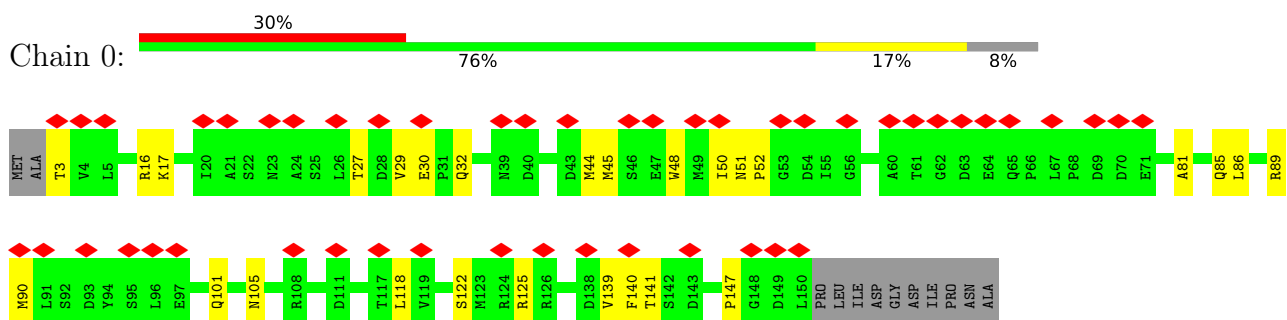
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	X	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	Z	421	Total	C	N	O	S	0	0
			3202	2013	549	630	10		
3	a	421	Total	C	N	O	S	0	0
			3202	2013	549	630	10		
3	b	421	Total	C	N	O	S	0	0
			3202	2013	549	630	10		
3	c	421	Total	C	N	O	S	0	0
			3202	2013	549	630	10		
3	d	421	Total	C	N	O	S	0	0
			3202	2013	549	630	10		
3	e	414	Total	C	N	O	S	0	0
			3149	1983	539	617	10		
3	g	414	Total	C	N	O	S	0	0
			3149	1983	539	617	10		
3	i	414	Total	C	N	O	S	0	0
			3149	1983	539	617	10		
3	j	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	k	414	Total	C	N	O	S	0	0
			3149	1983	539	617	10		
3	l	414	Total	C	N	O	S	0	0
			3149	1983	539	617	10		
3	m	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	o	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	q	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	s	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	t	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	u	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	y	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		

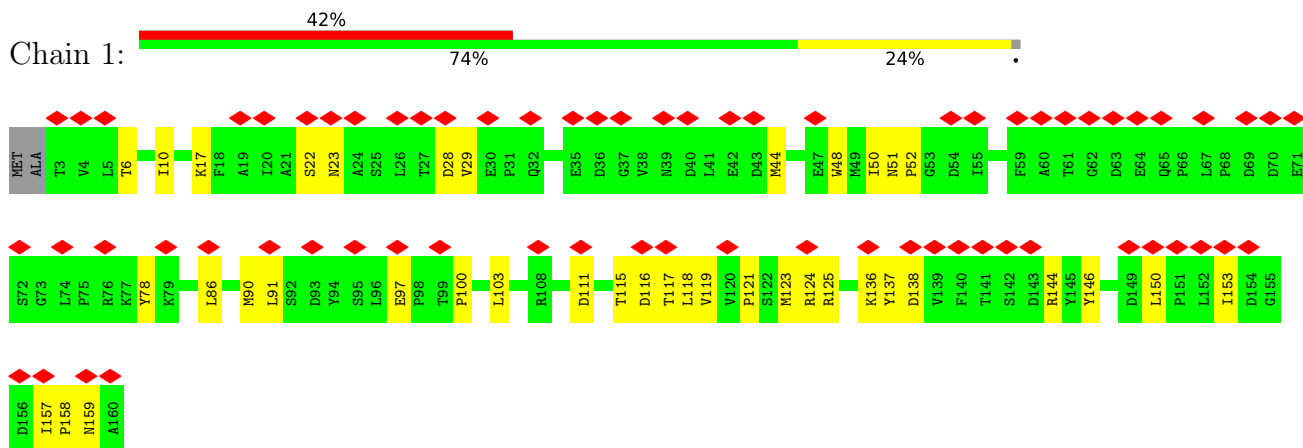
3 Residue-property plots [i](#)

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.

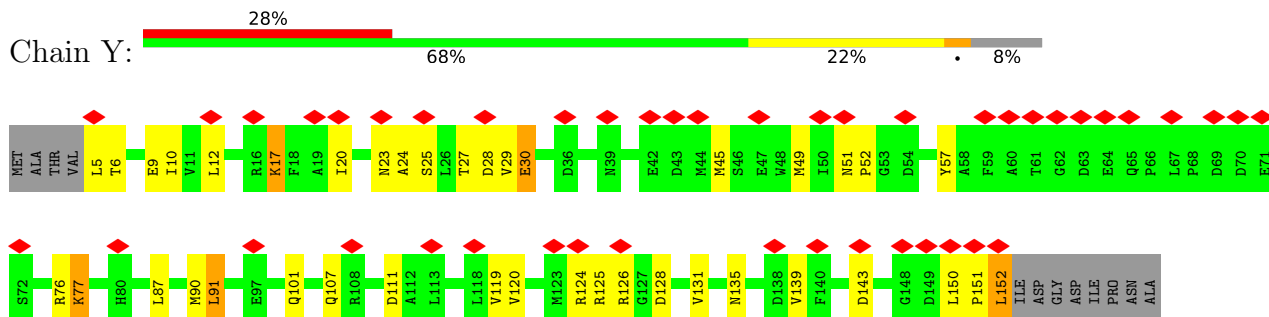
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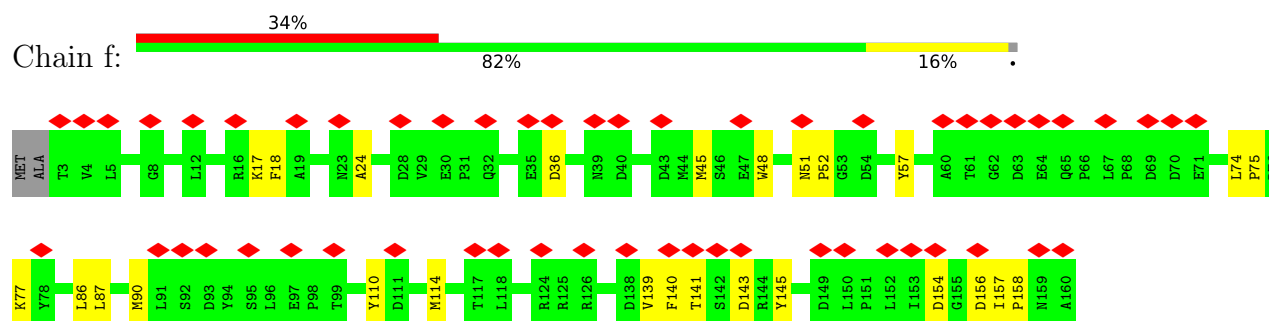
- Molecule 1: Gene 7 protein



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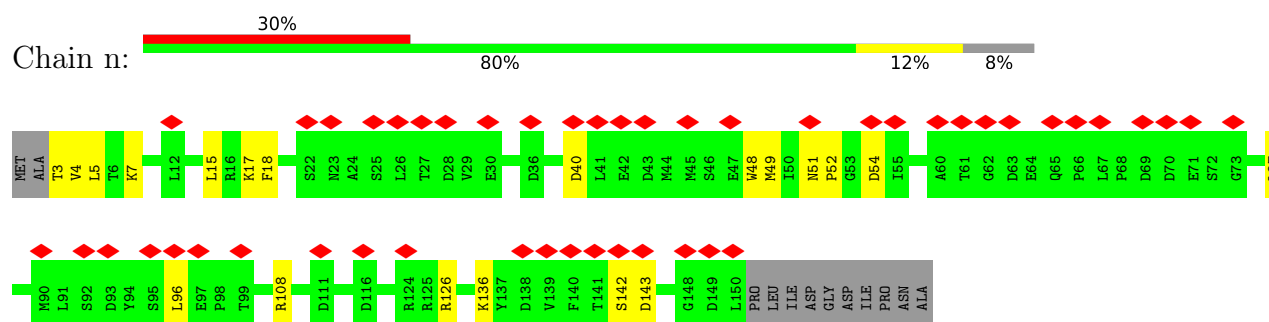
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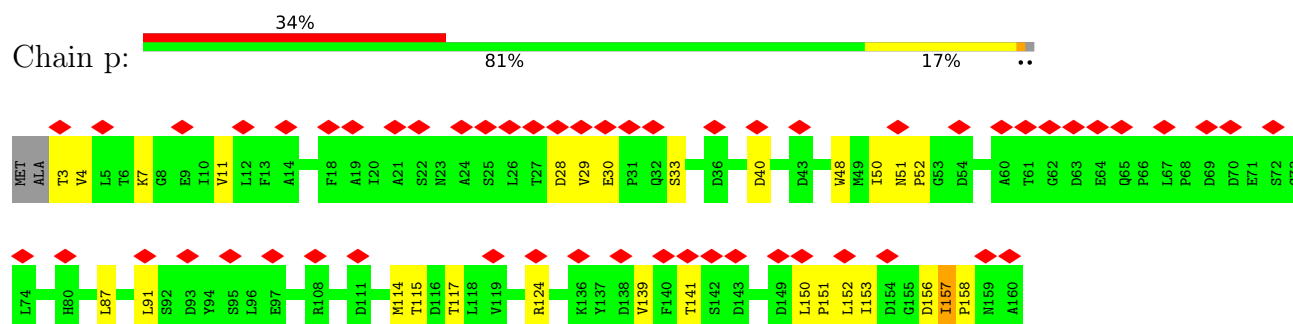
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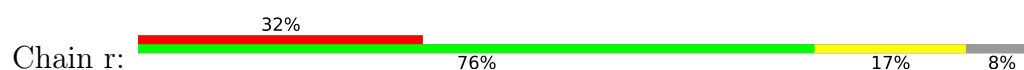
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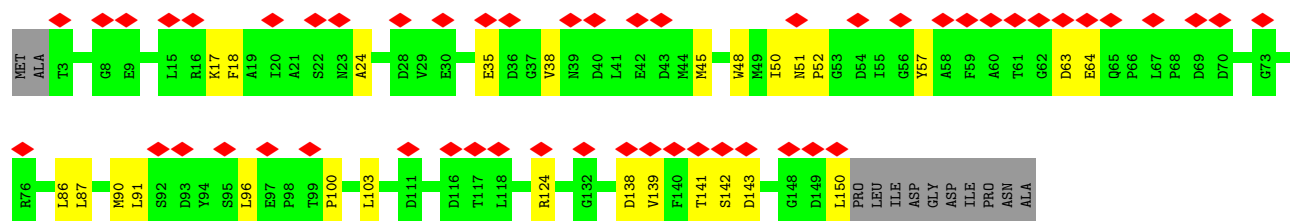


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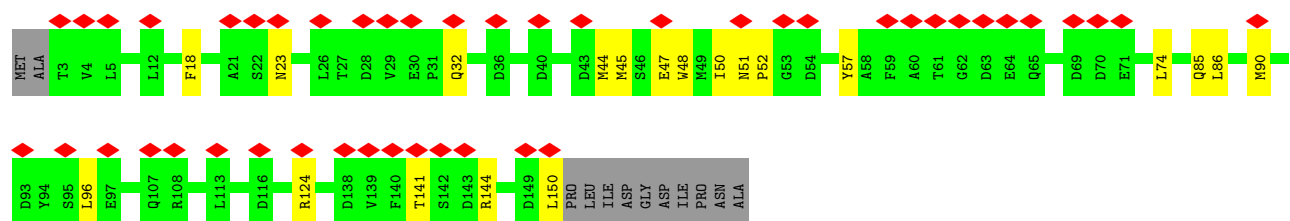
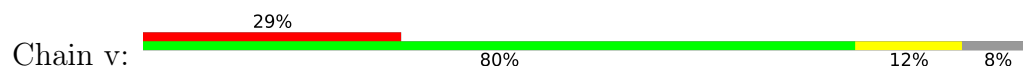


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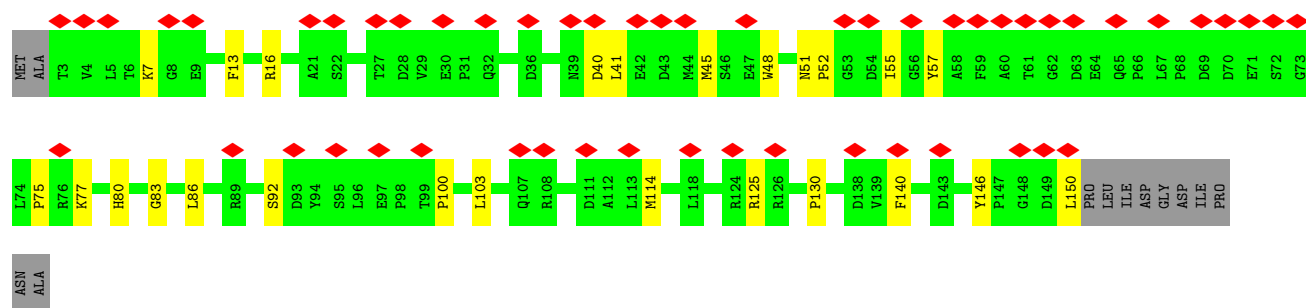
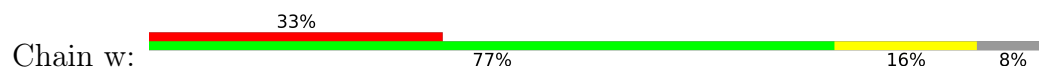




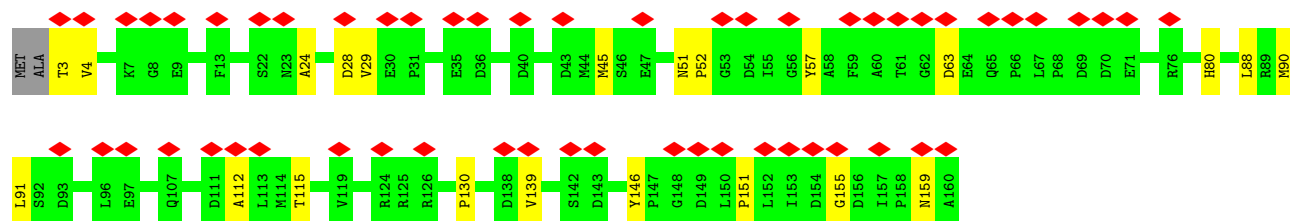
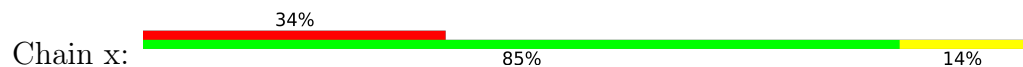
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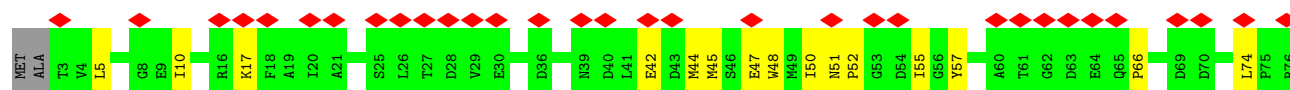
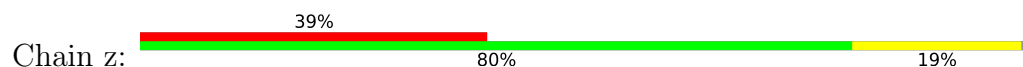
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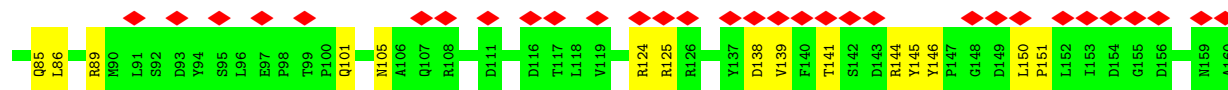


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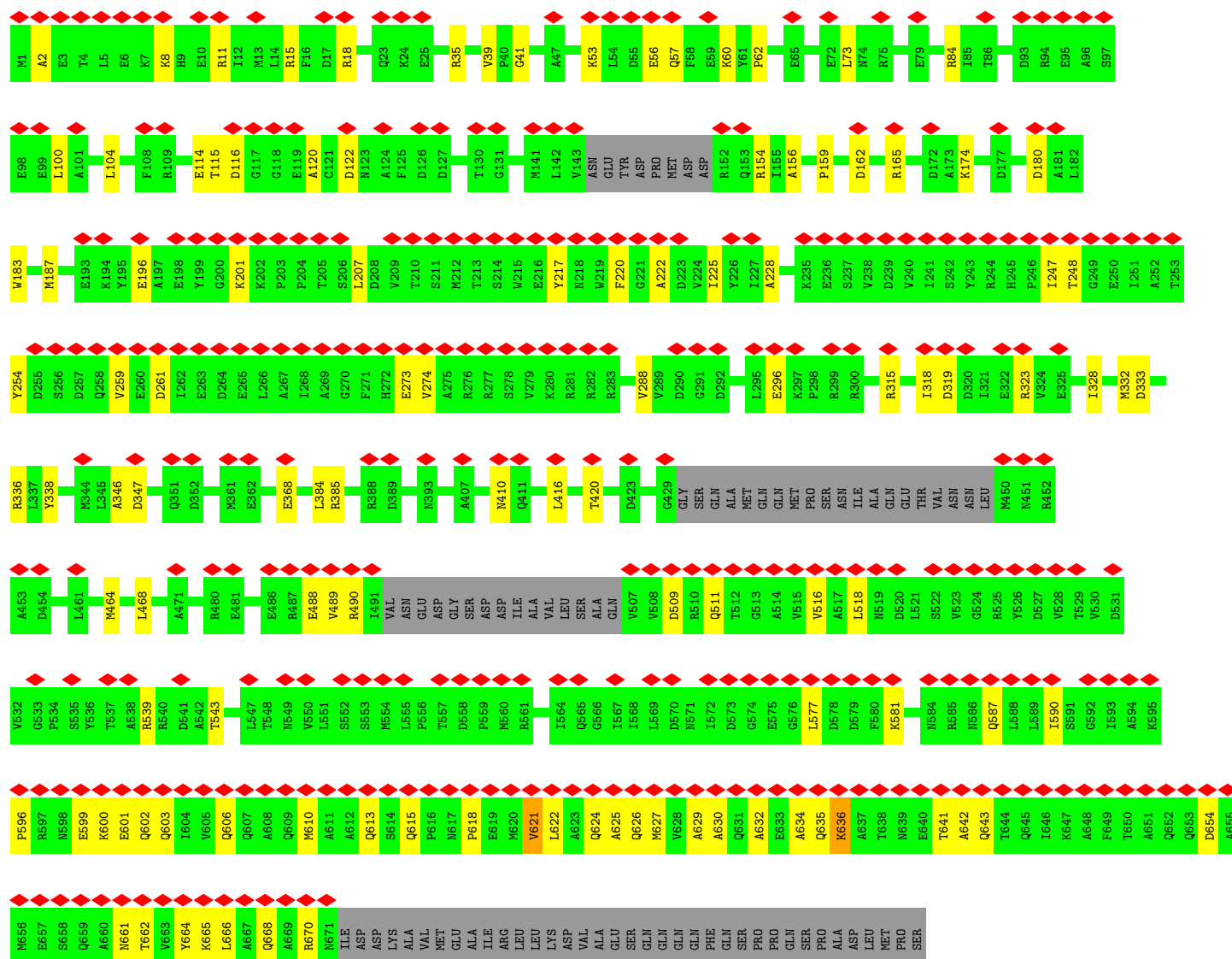
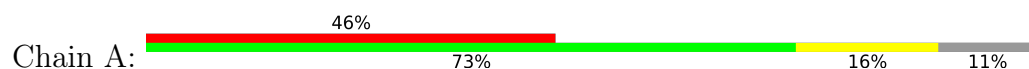


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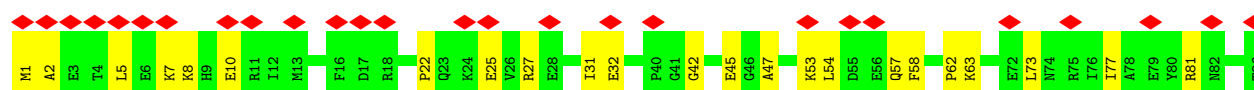
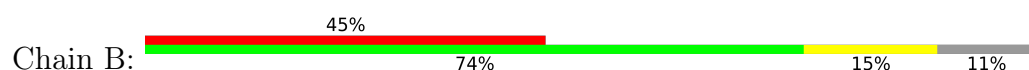


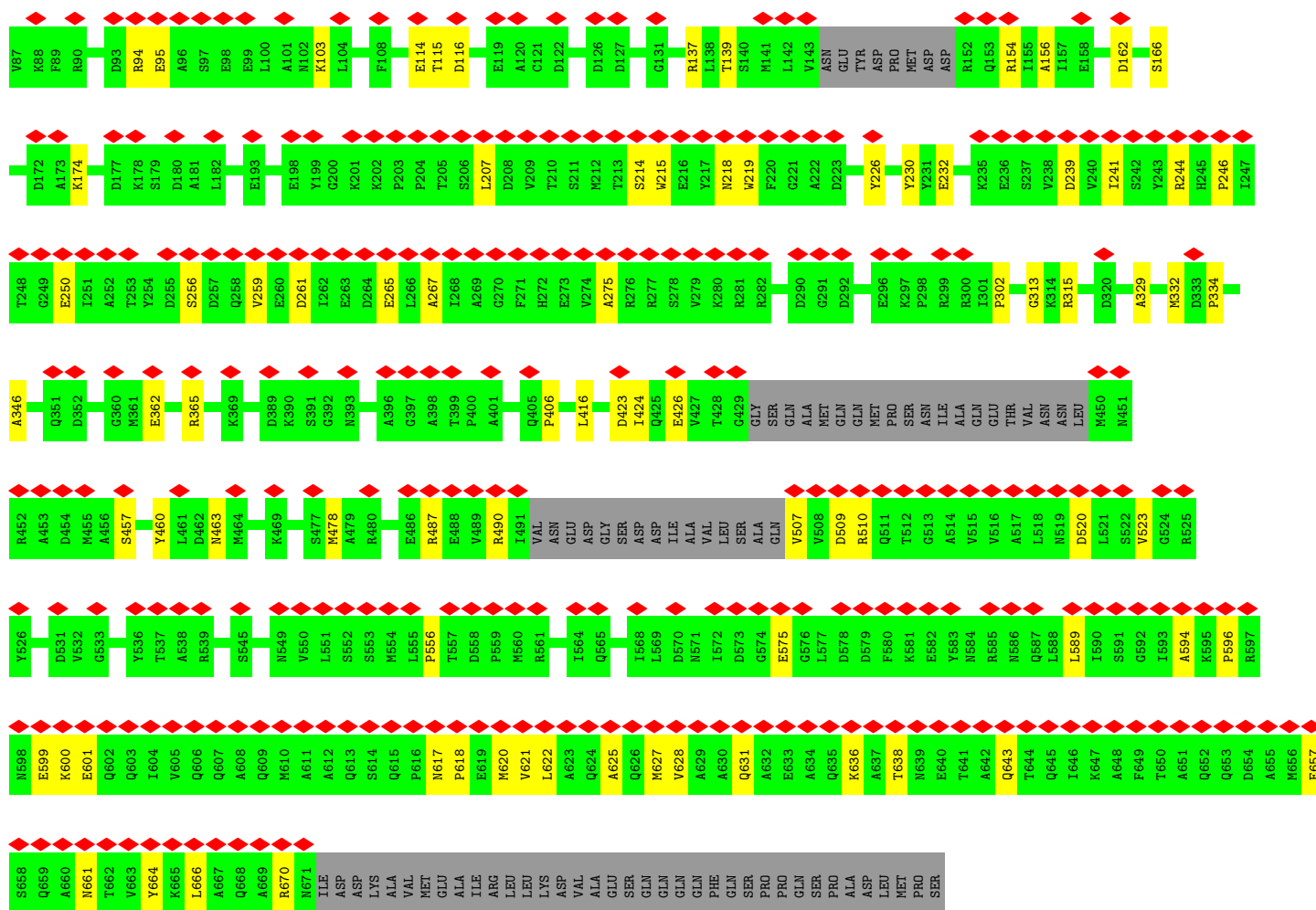


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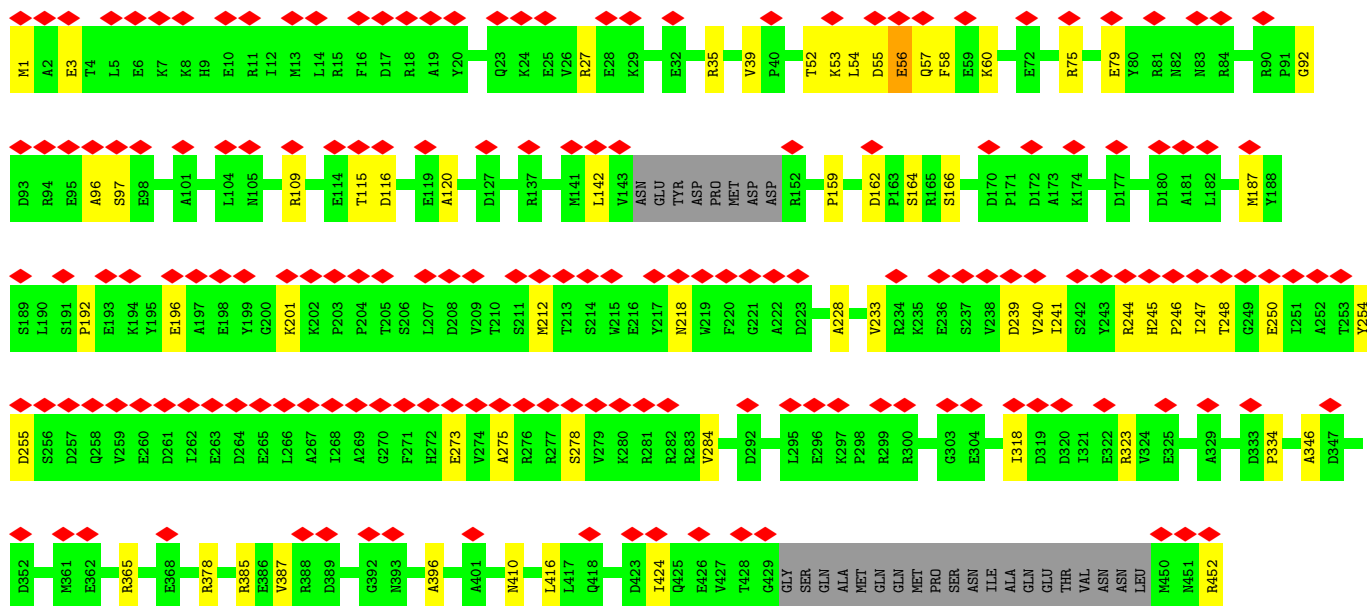
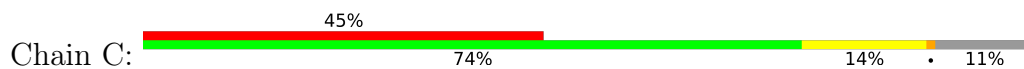


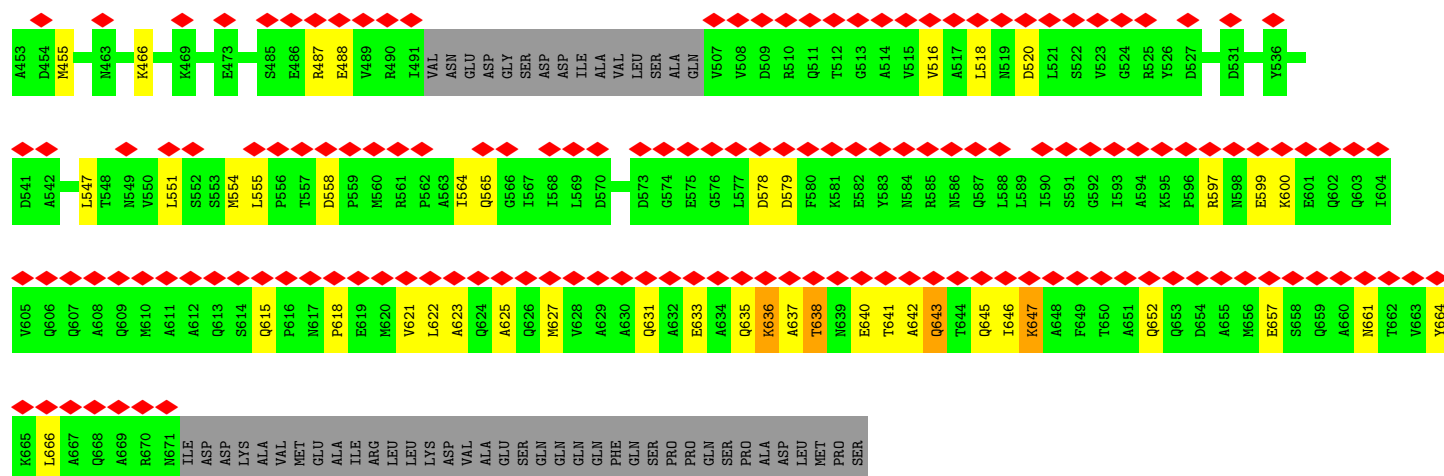
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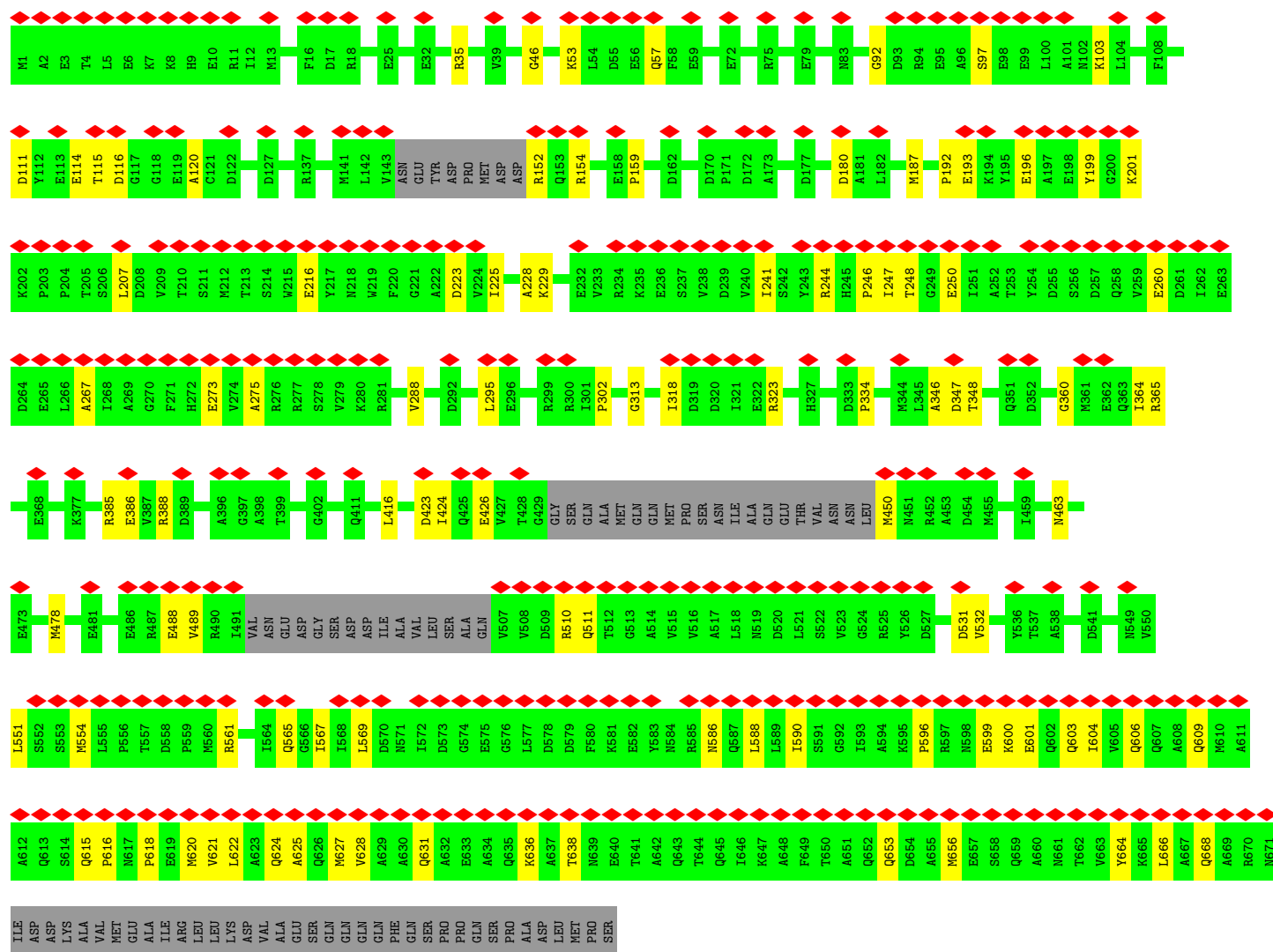
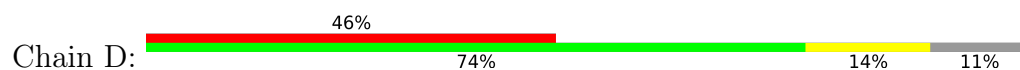


• Molecule 2: Gene 3 protein



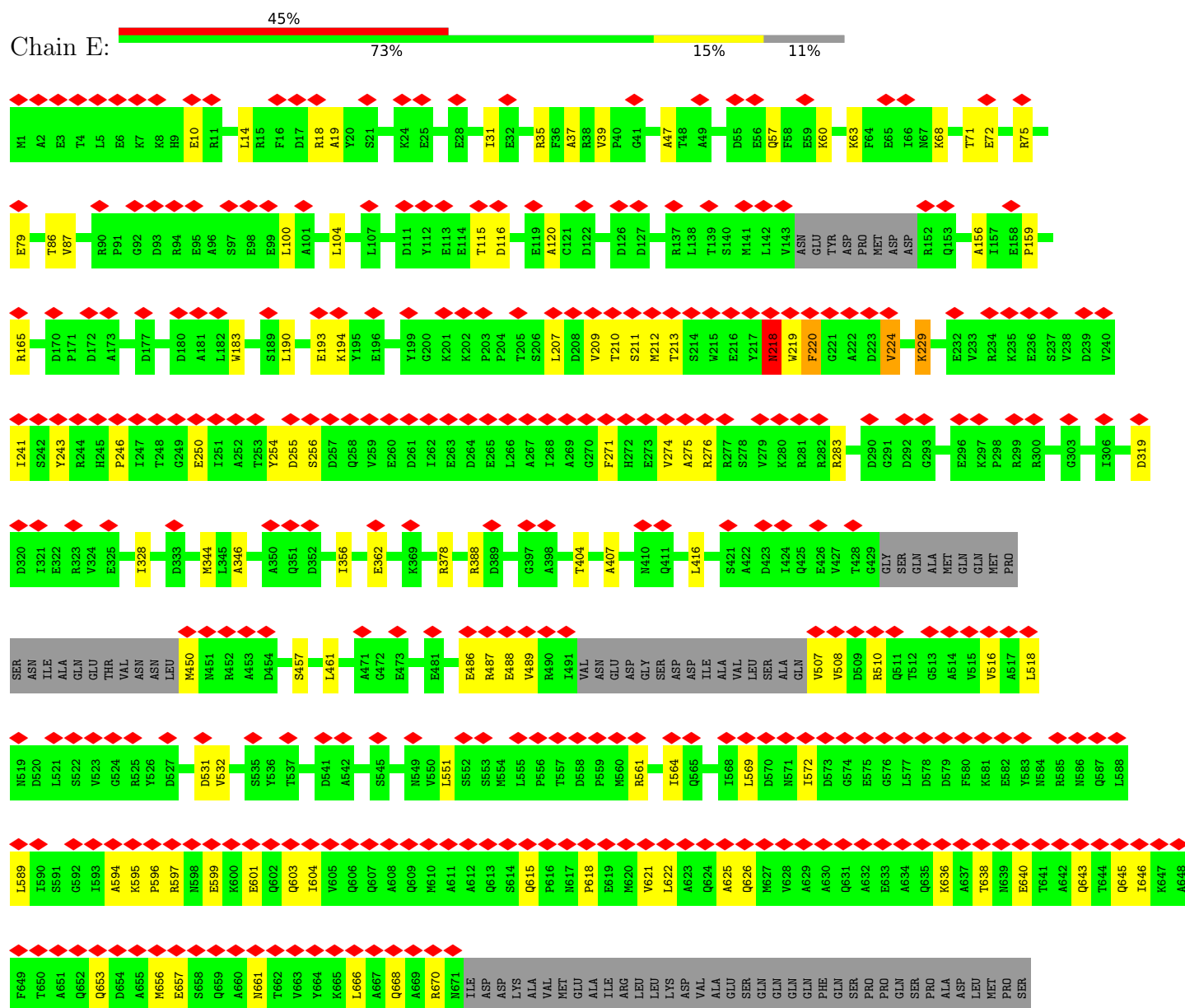


• Molecule 2: Gene 3 protein



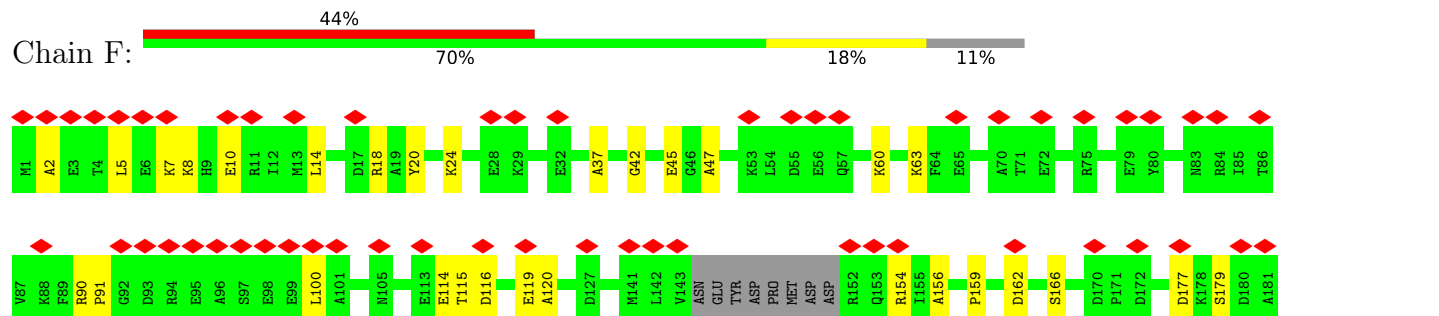
- Molecule 2: Gene 3 protein

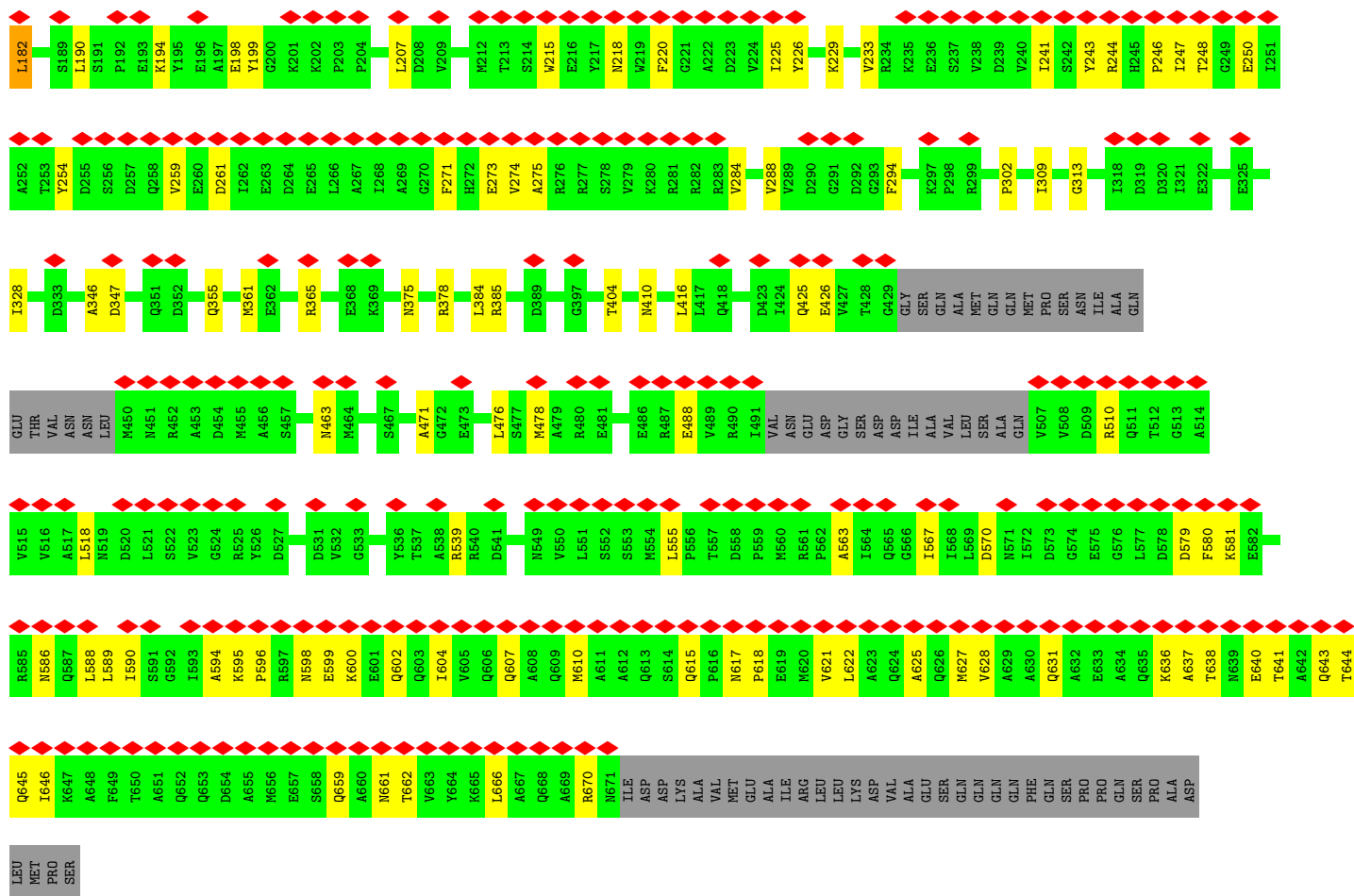
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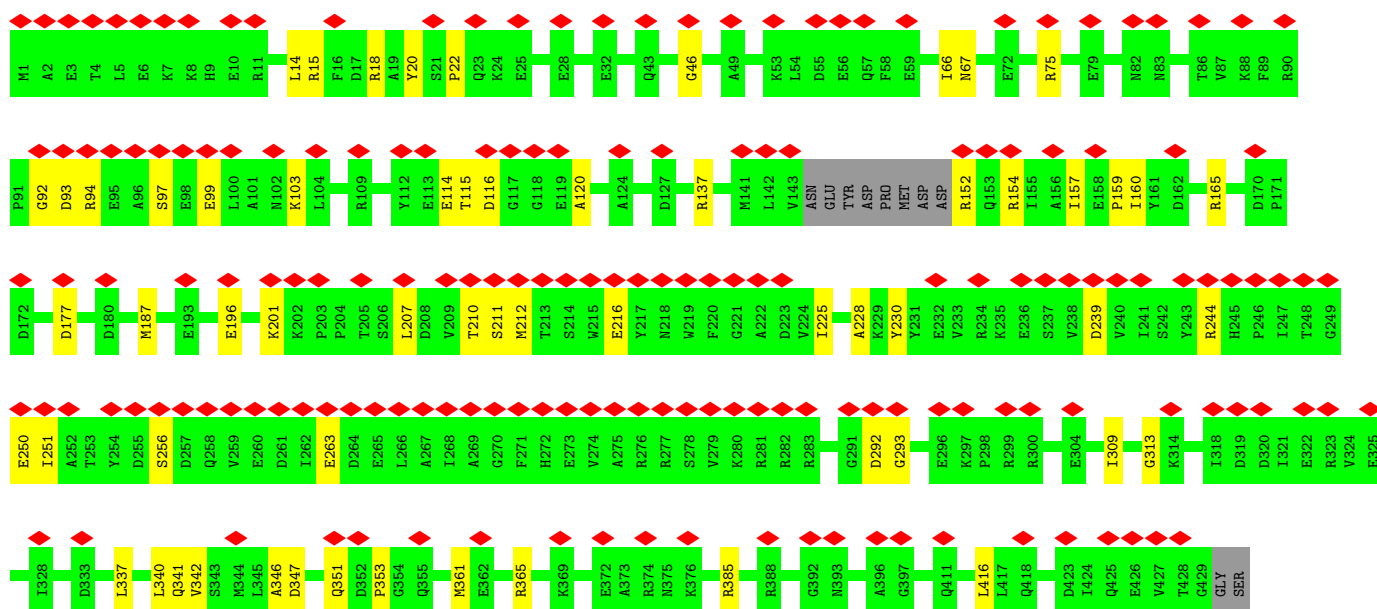
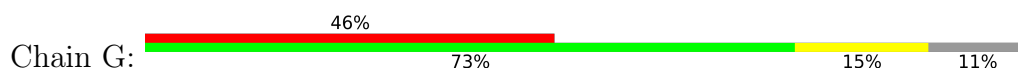
- Molecule 2: Gene 3 protein

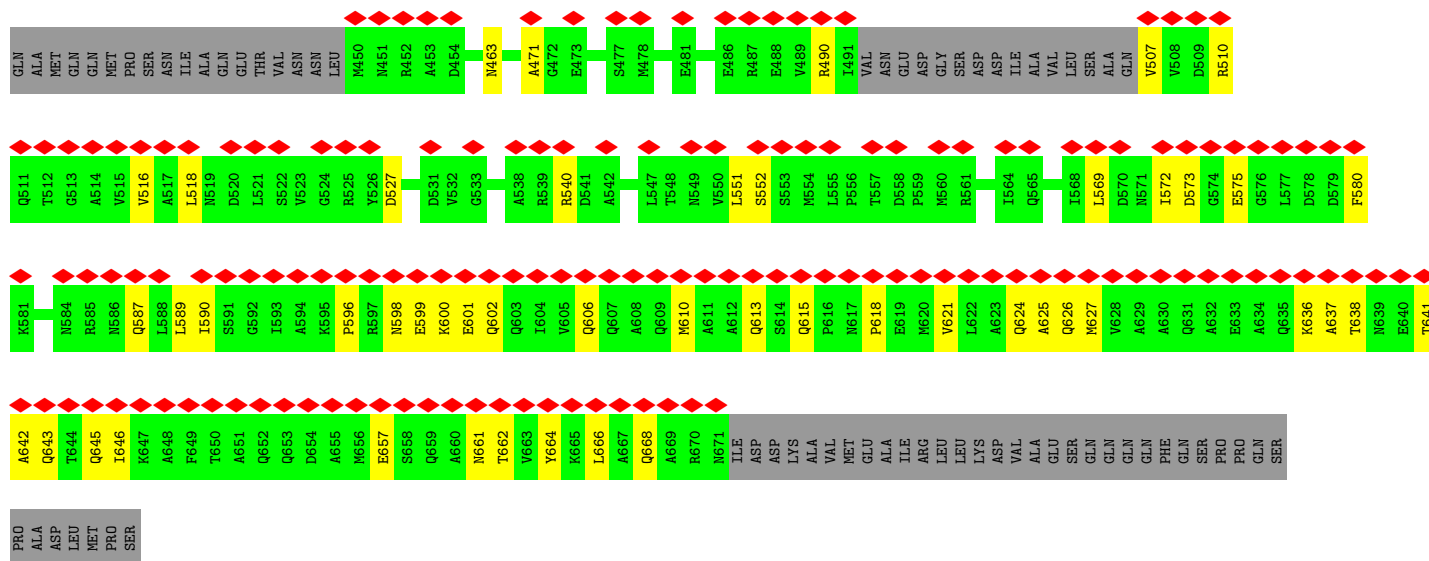
Chain F:



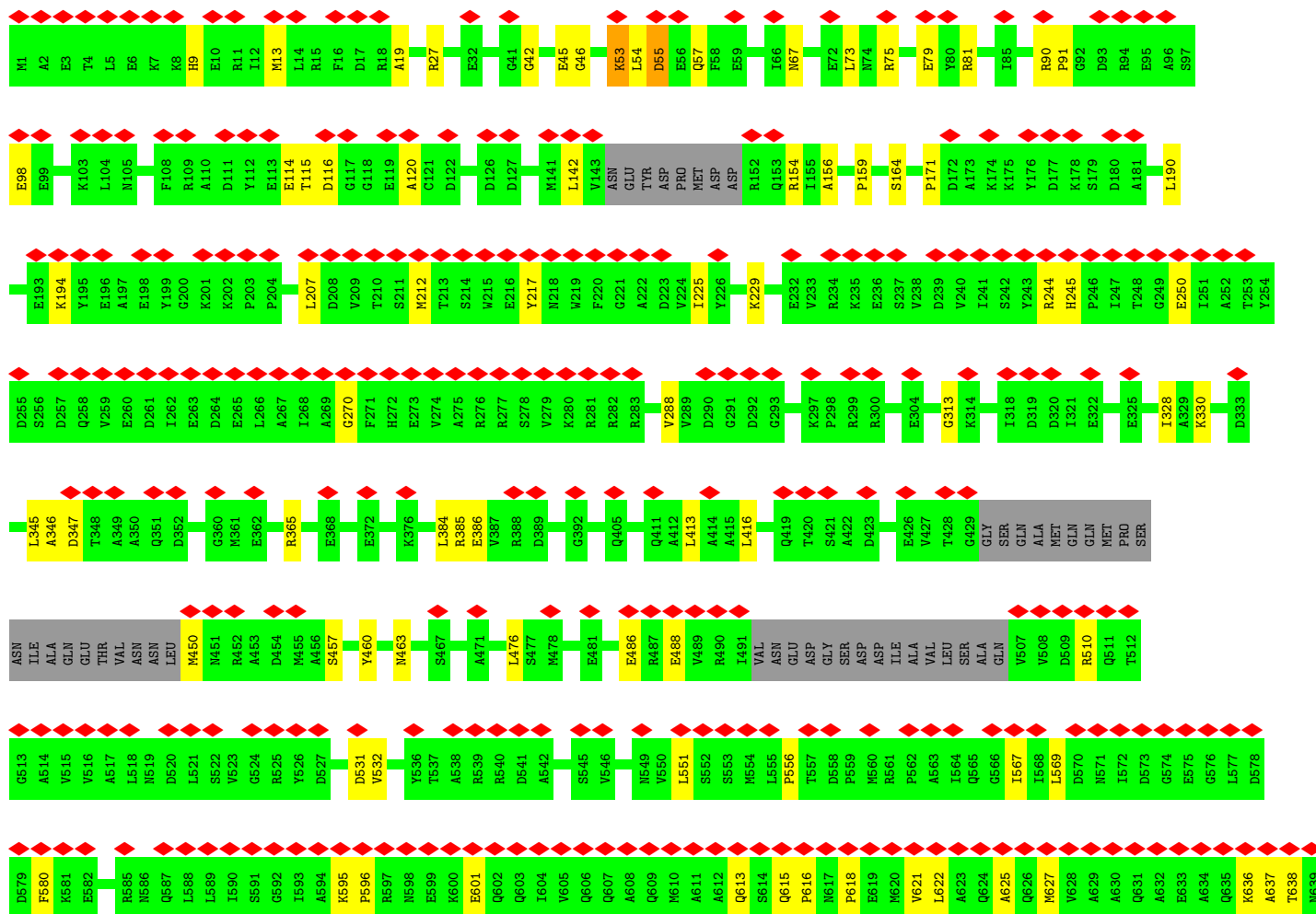


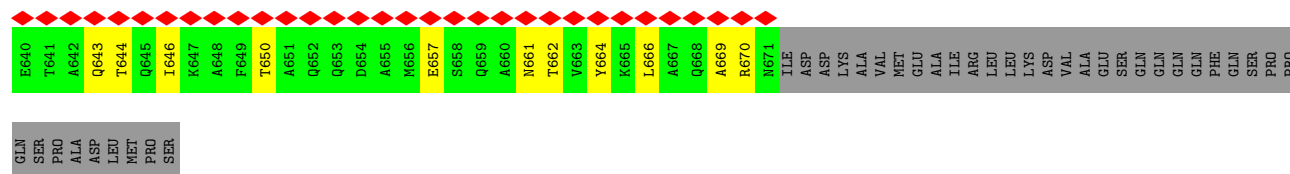
• Molecule 2: Gene 3 protein



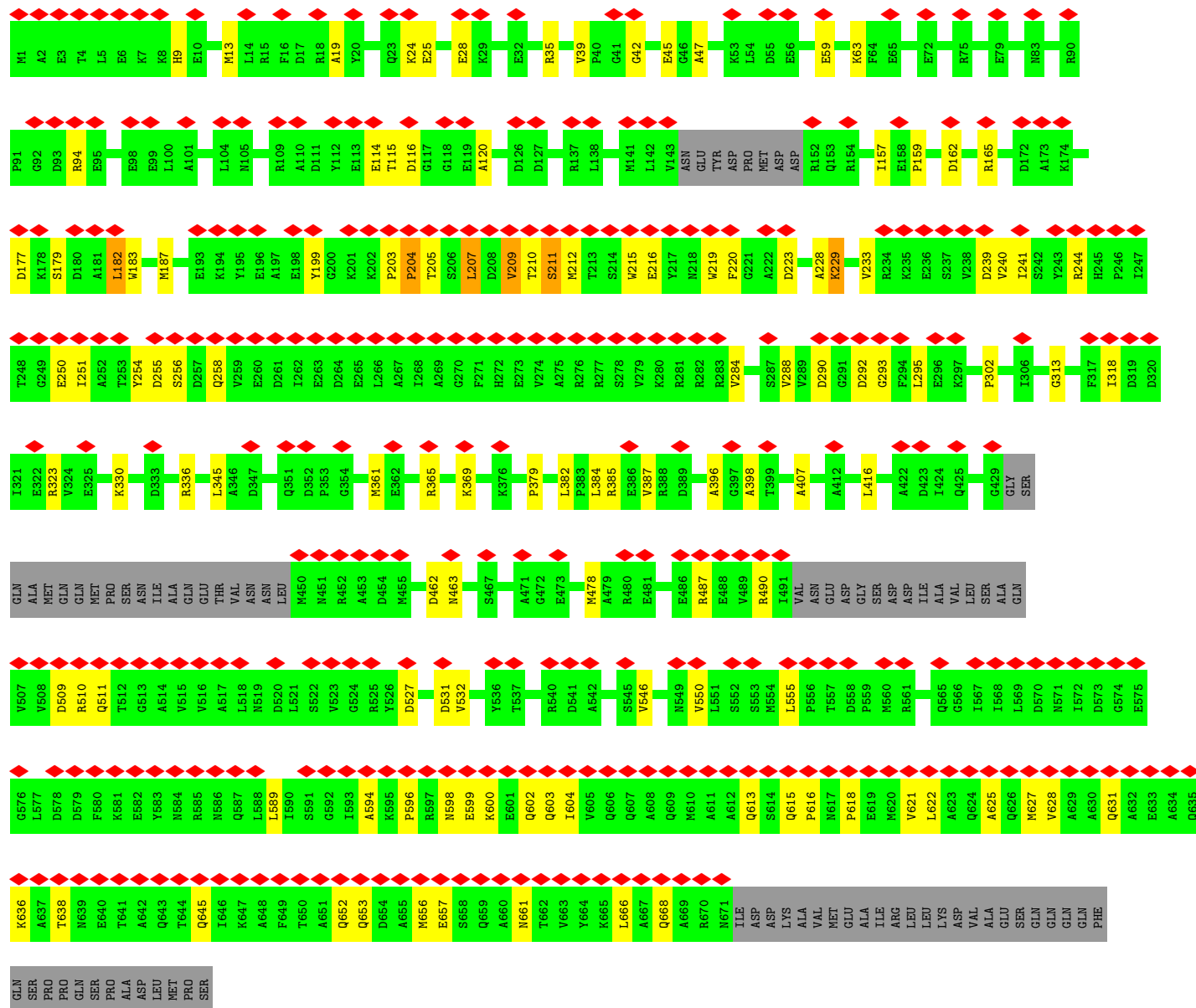


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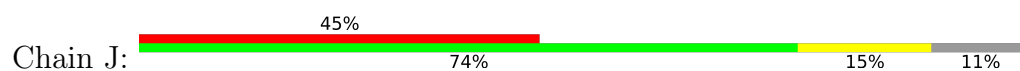


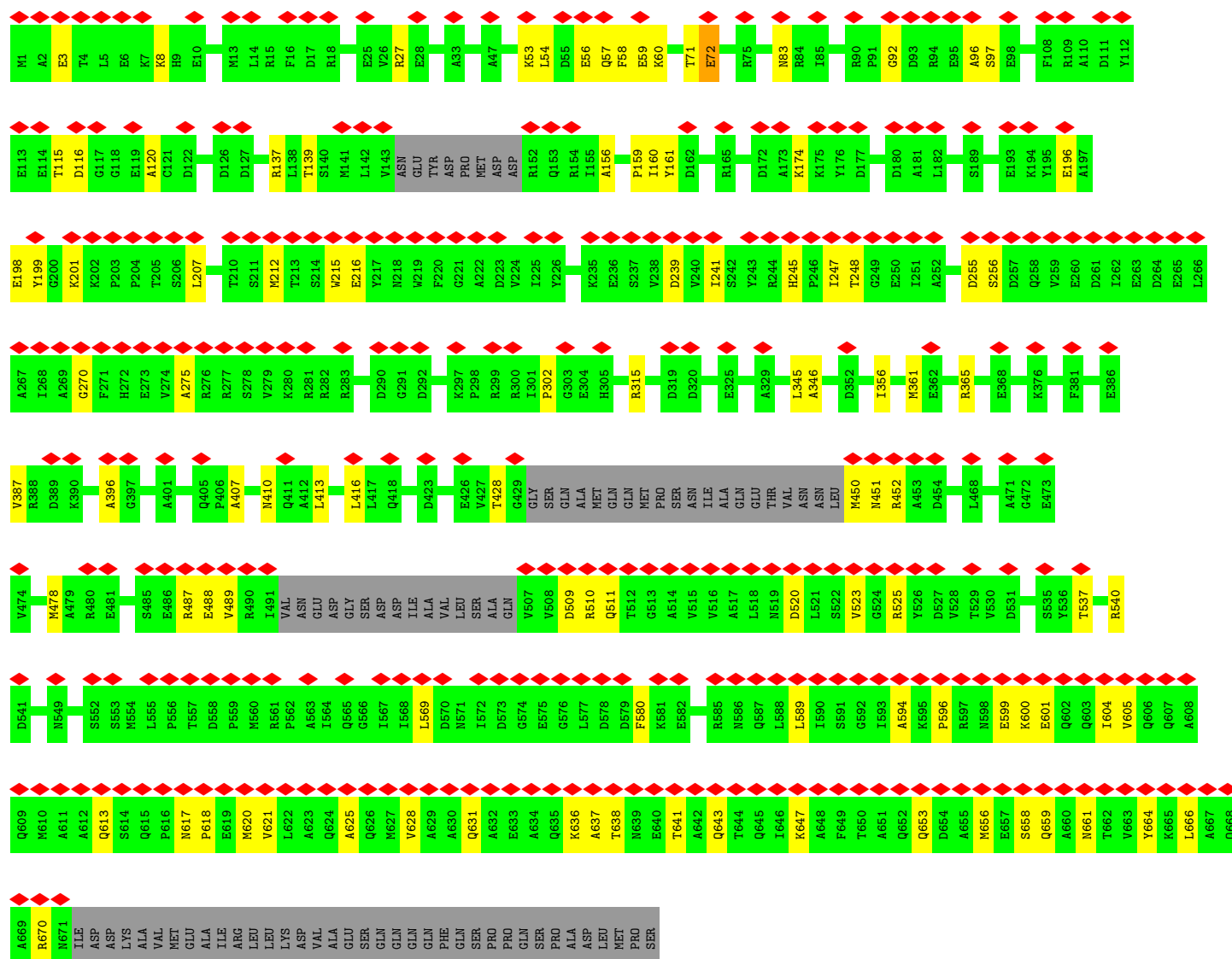


• Molecule 2: Gene 3 protein

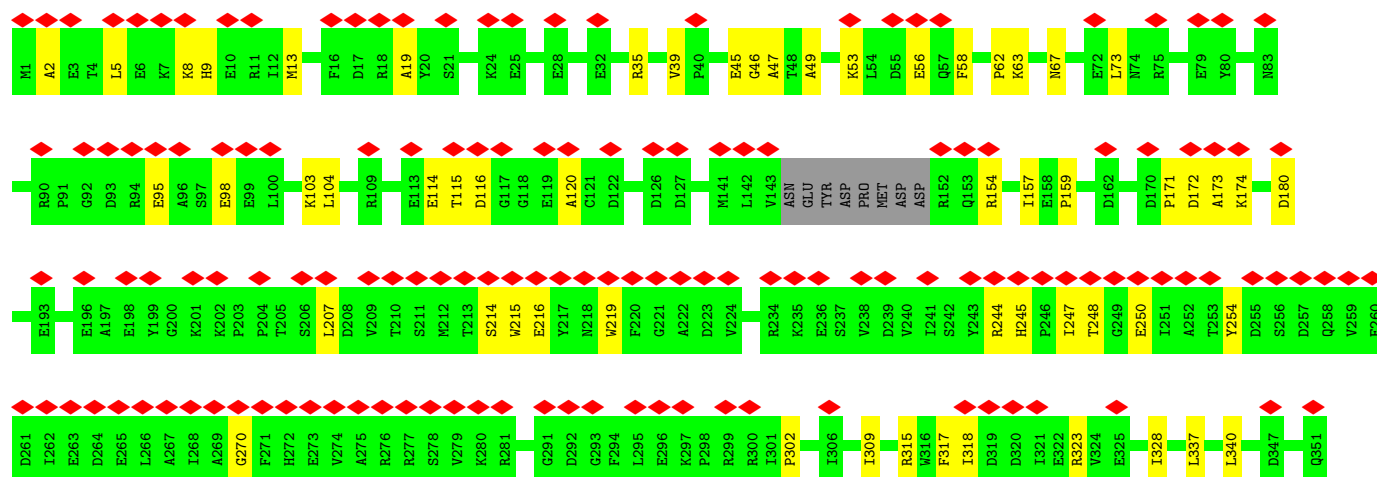
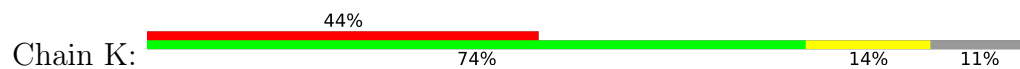


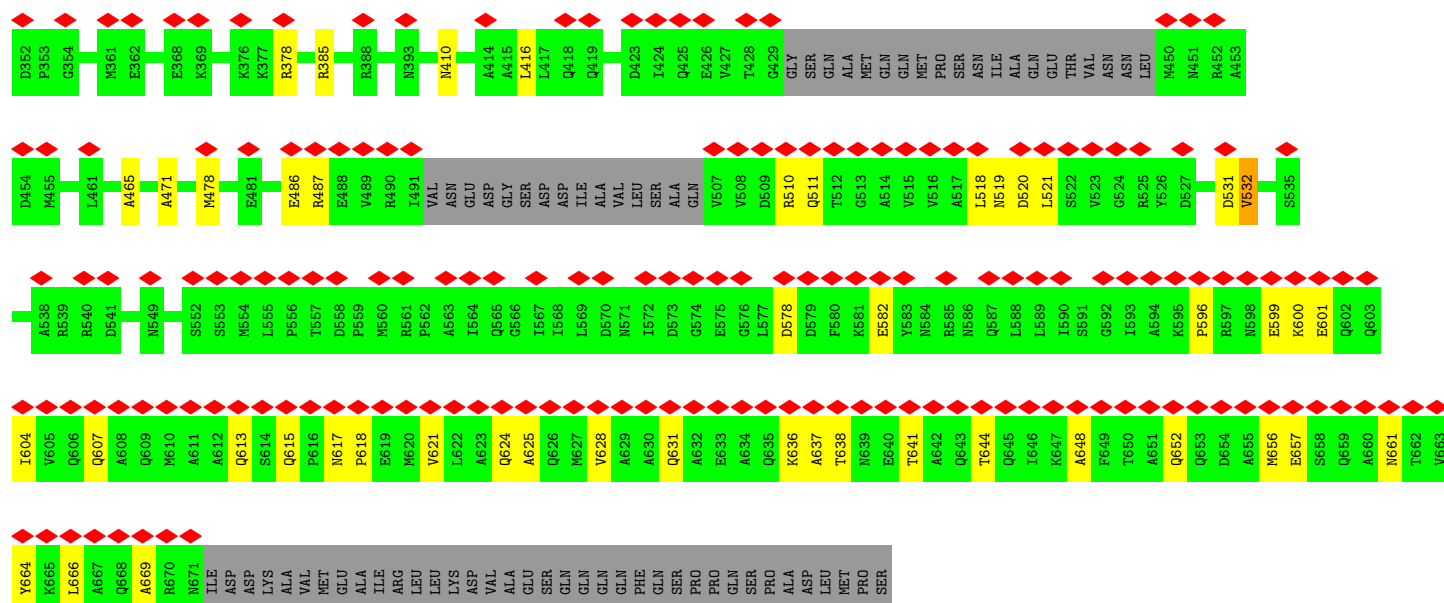
• Molecule 2: Gene 3 protein



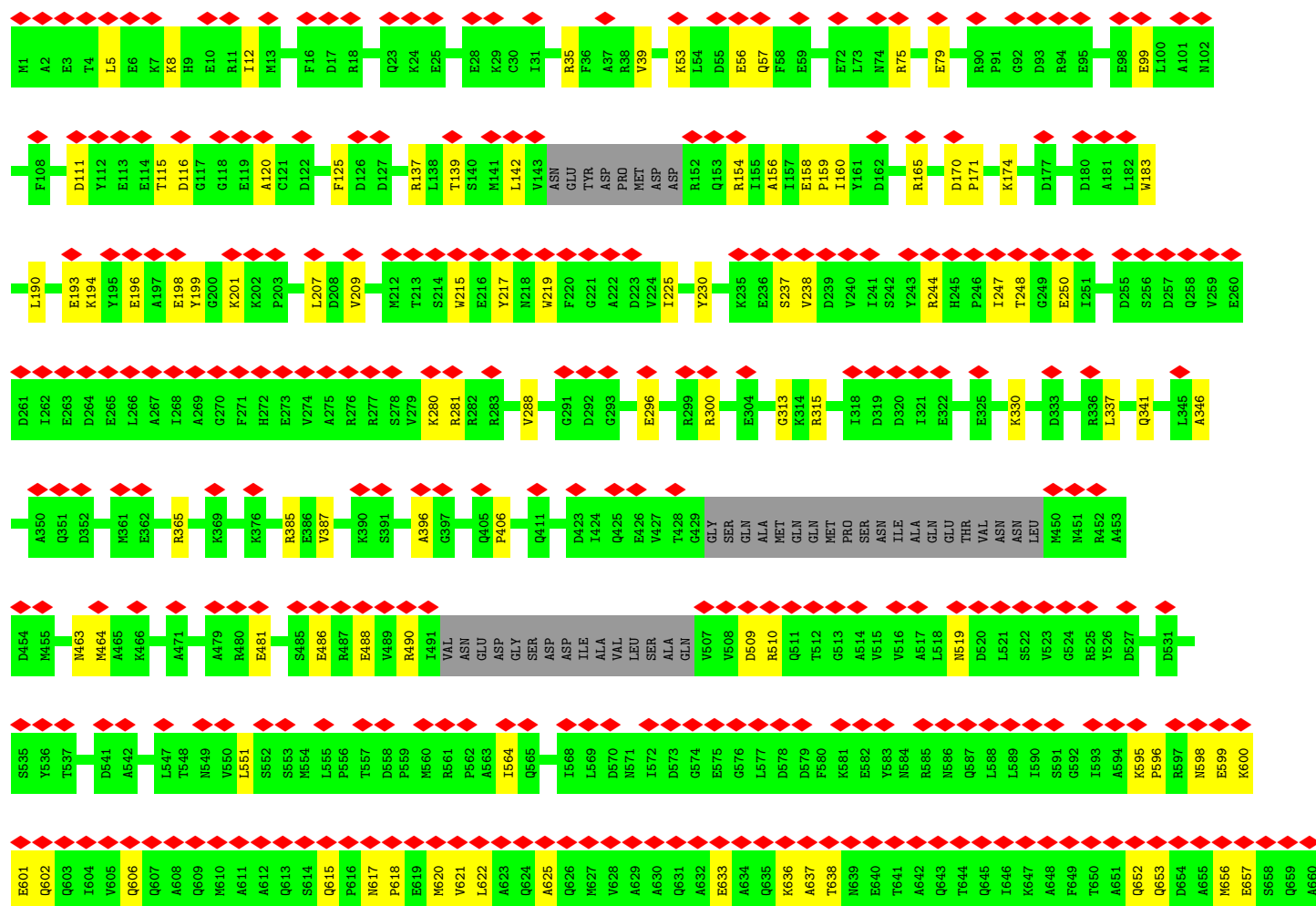
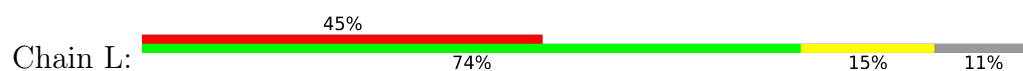


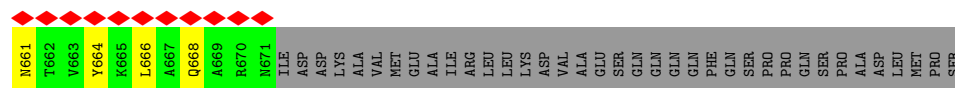
• Molecule 2: Gene 3 protein



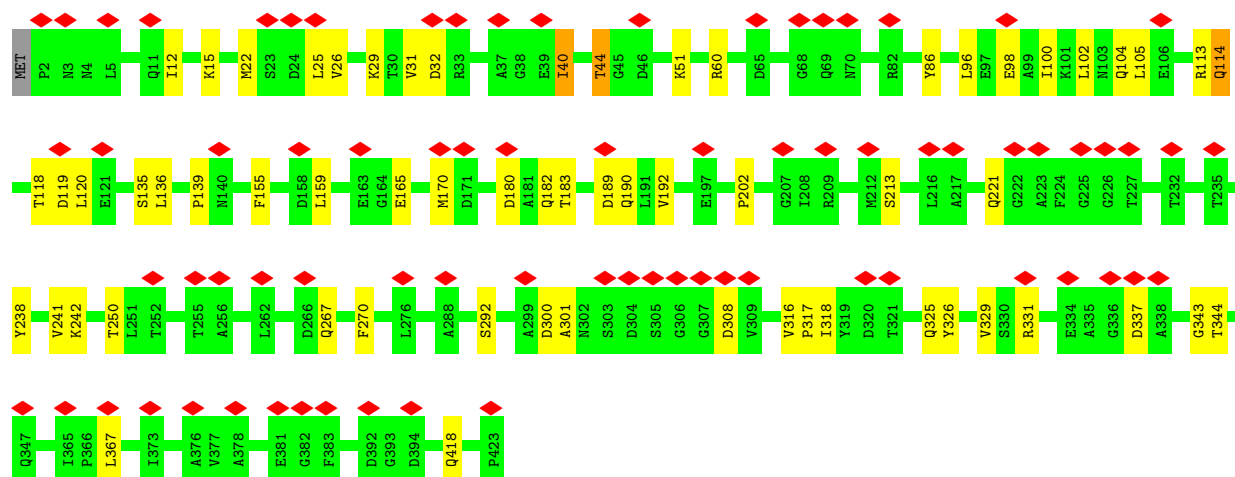
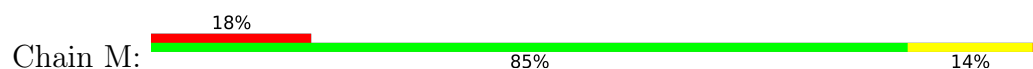


• Molecule 2: Gene 3 protein

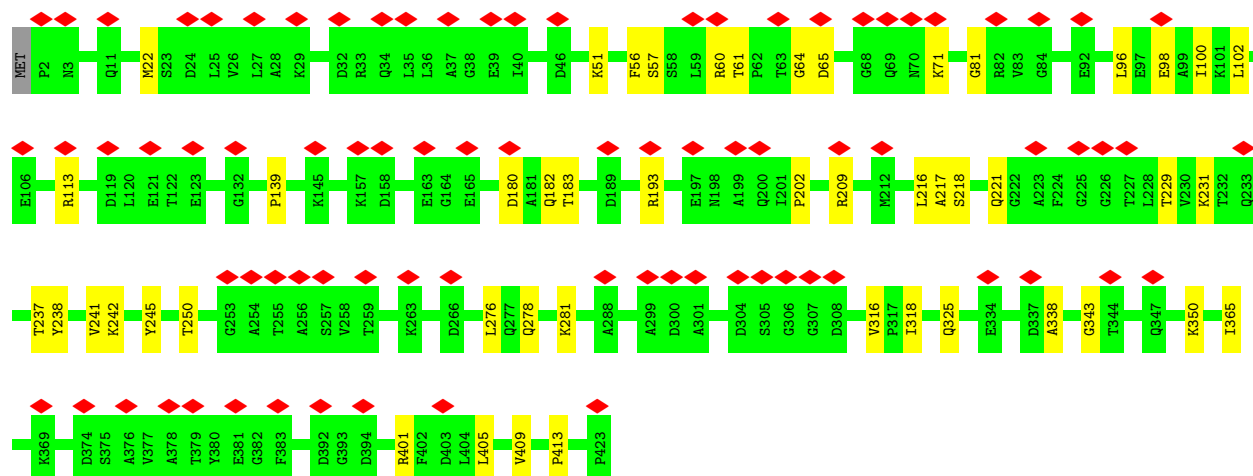
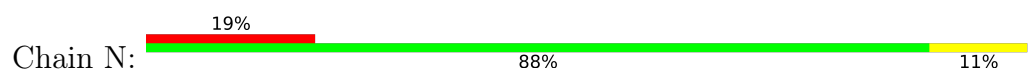




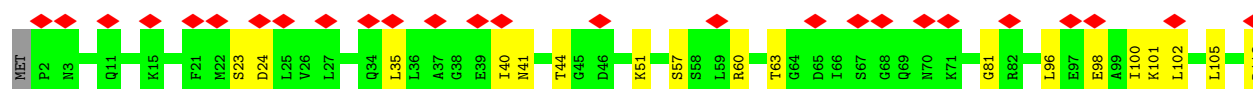
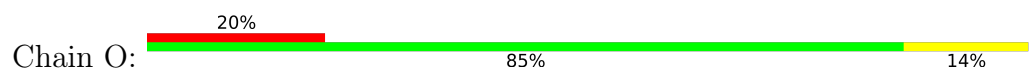
• Molecule 3: Gene 5 protein

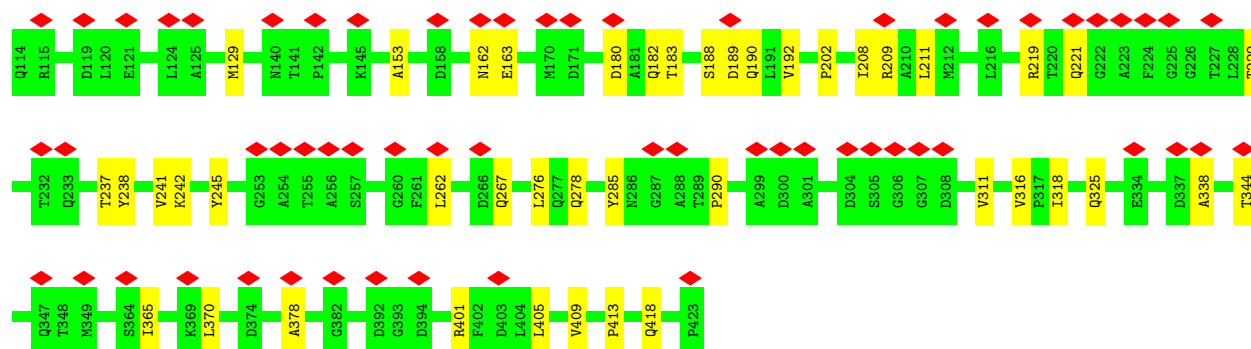


• Molecule 3: Gene 5 protein

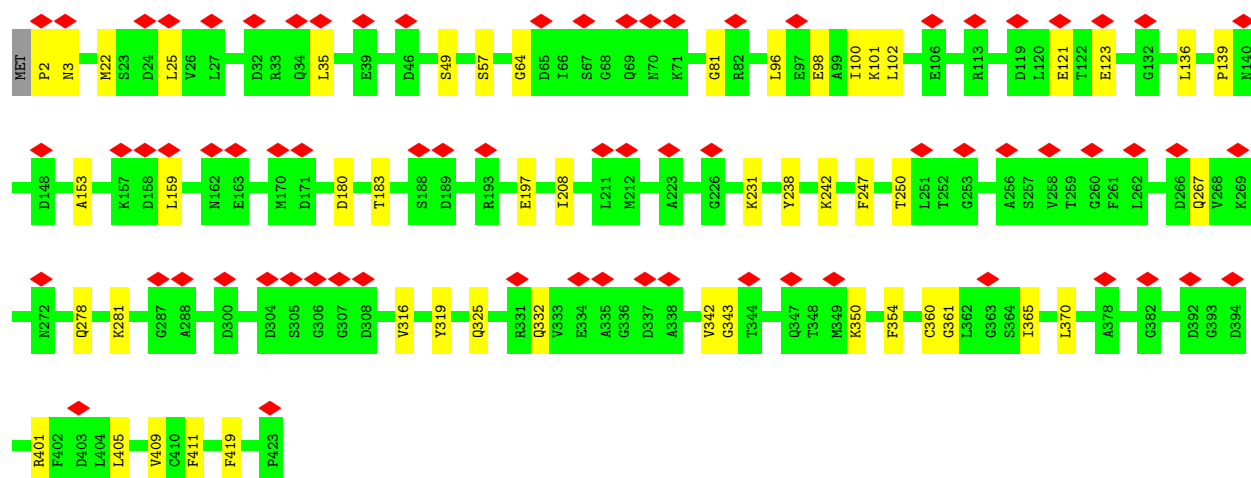
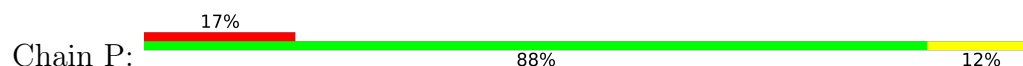


• Molecule 3: Gene 5 protein

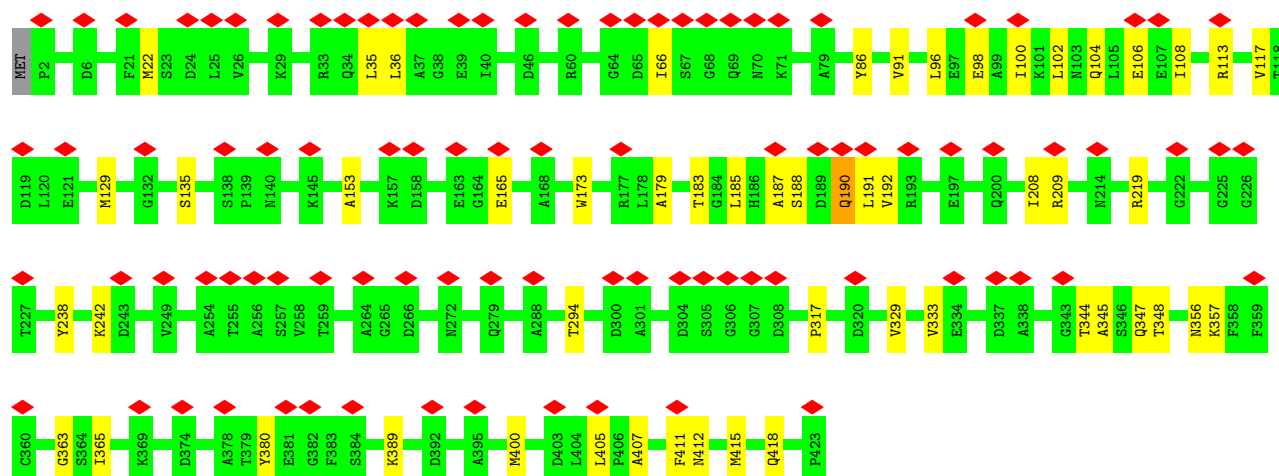
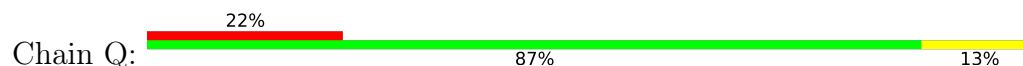




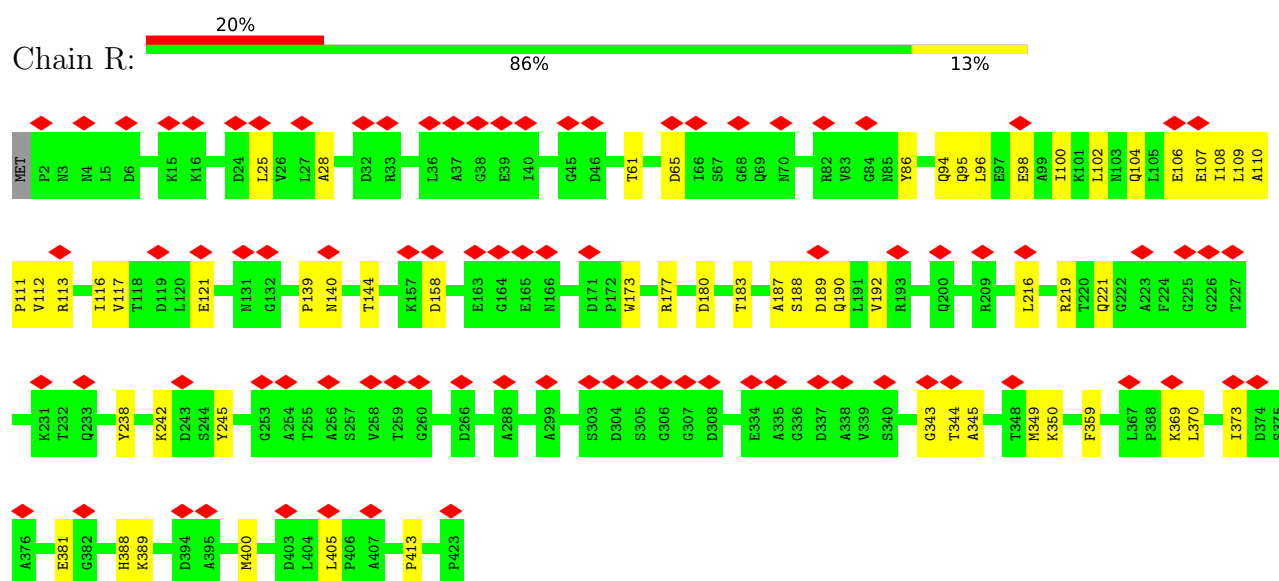
• Molecule 3: Gene 5 protein



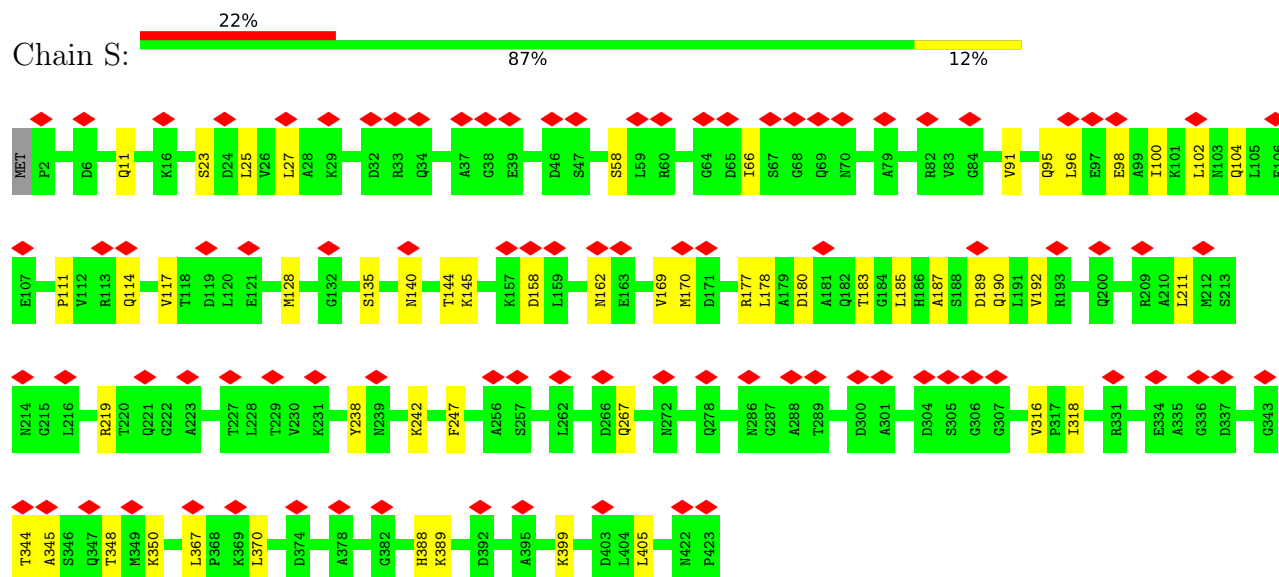
• Molecule 3: Gene 5 protein



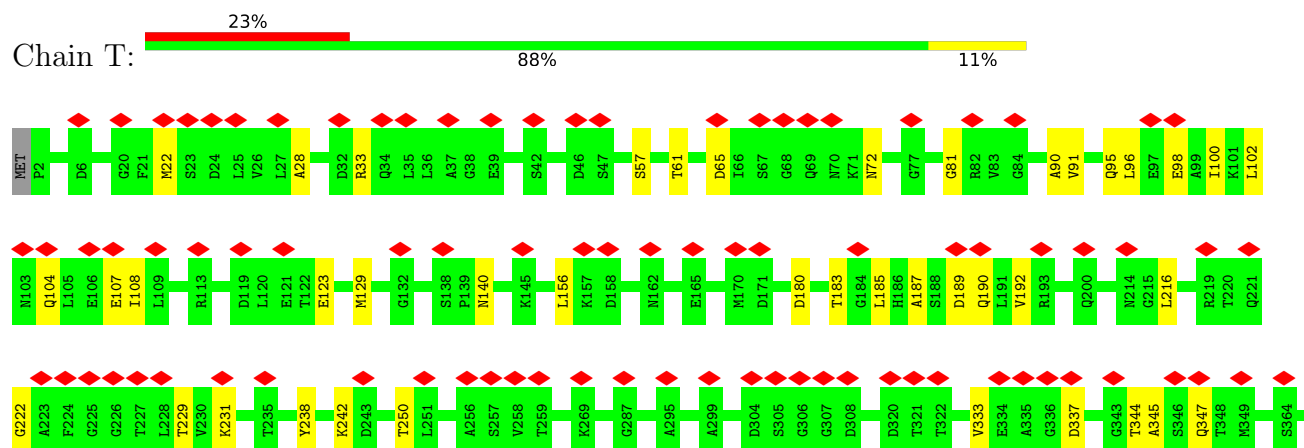
• Molecule 3: Gene 5 protein

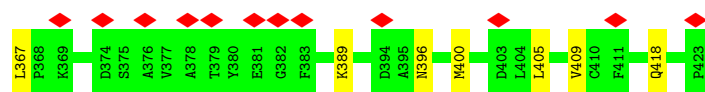


• Molecule 3: Gene 5 protein

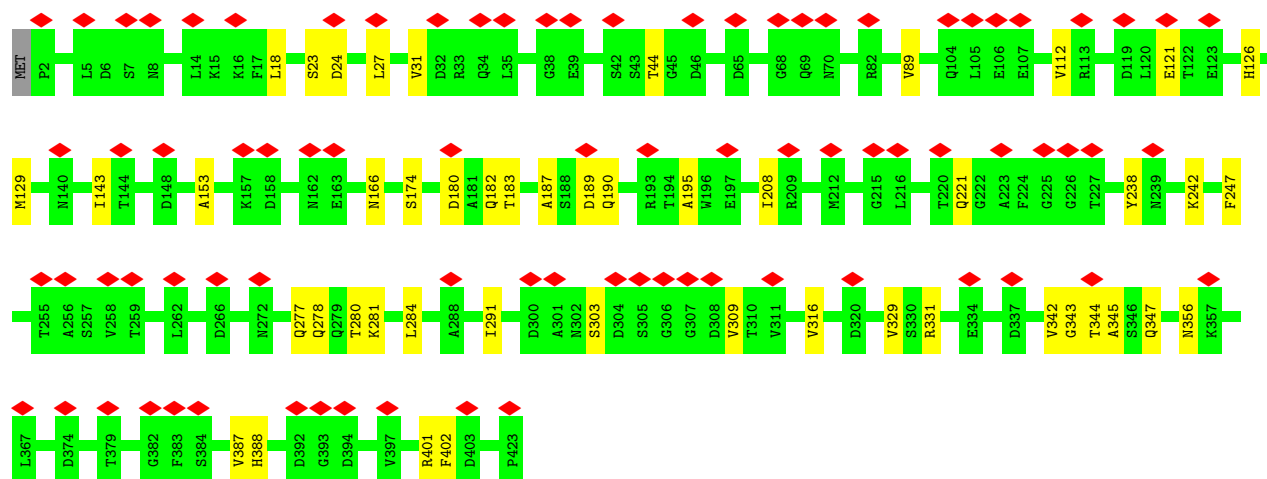
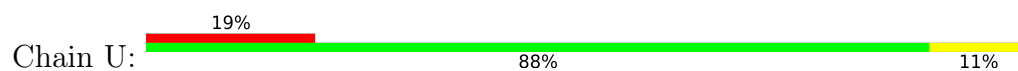


• Molecule 3: Gene 5 protein

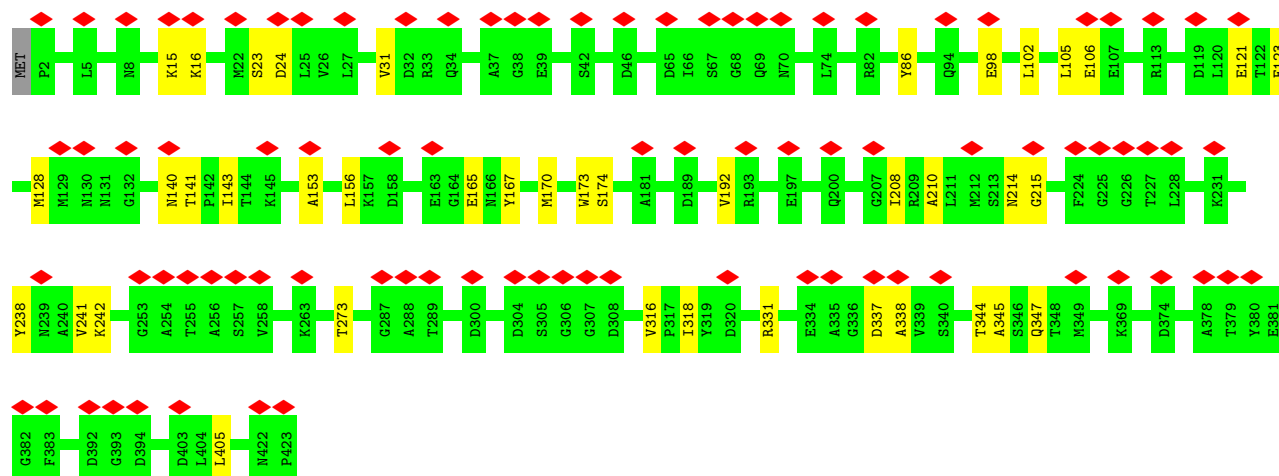
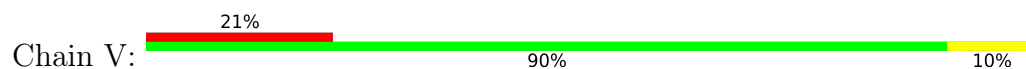




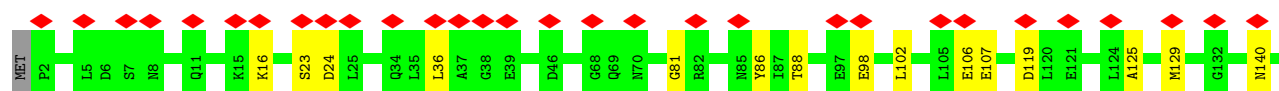
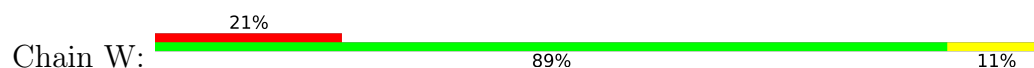
• Molecule 3: Gene 5 protein

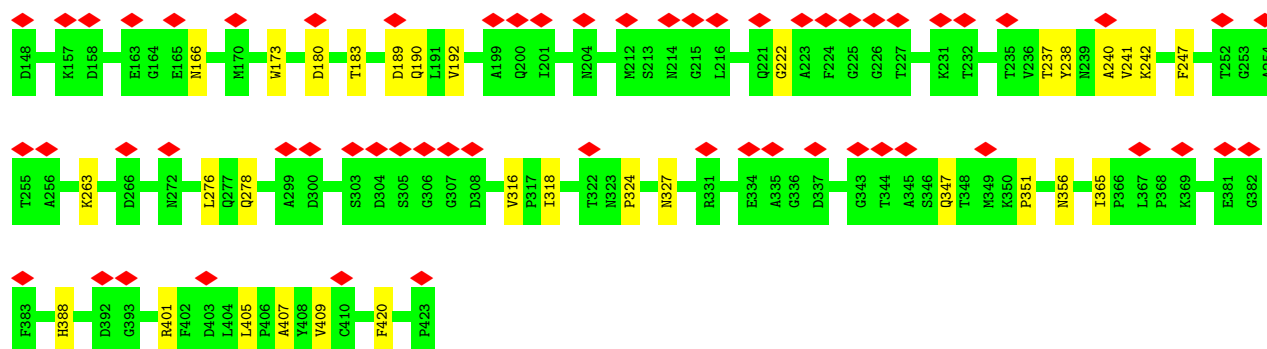


• Molecule 3: Gene 5 protein

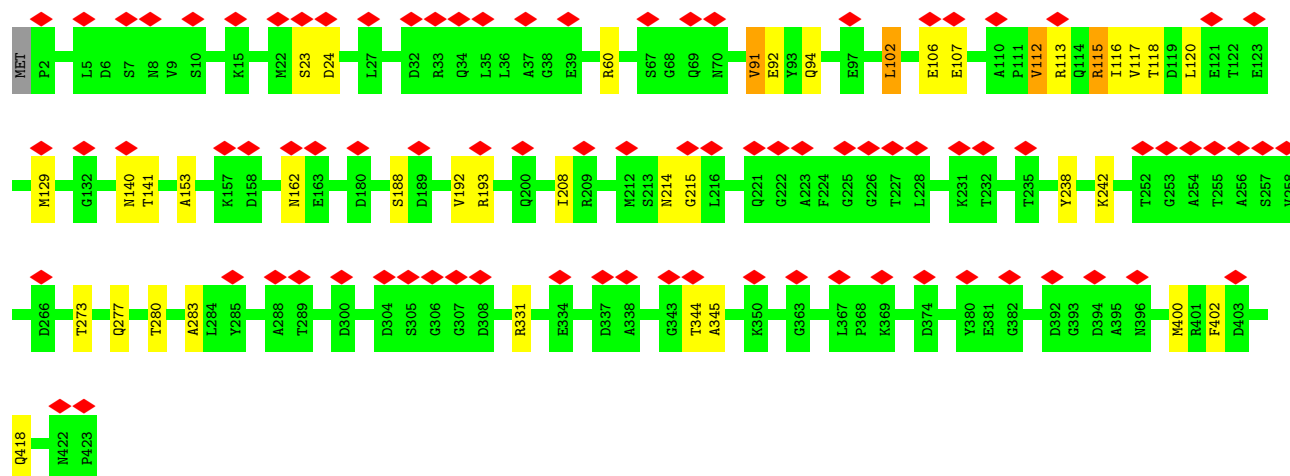


• Molecule 3: Gene 5 protein

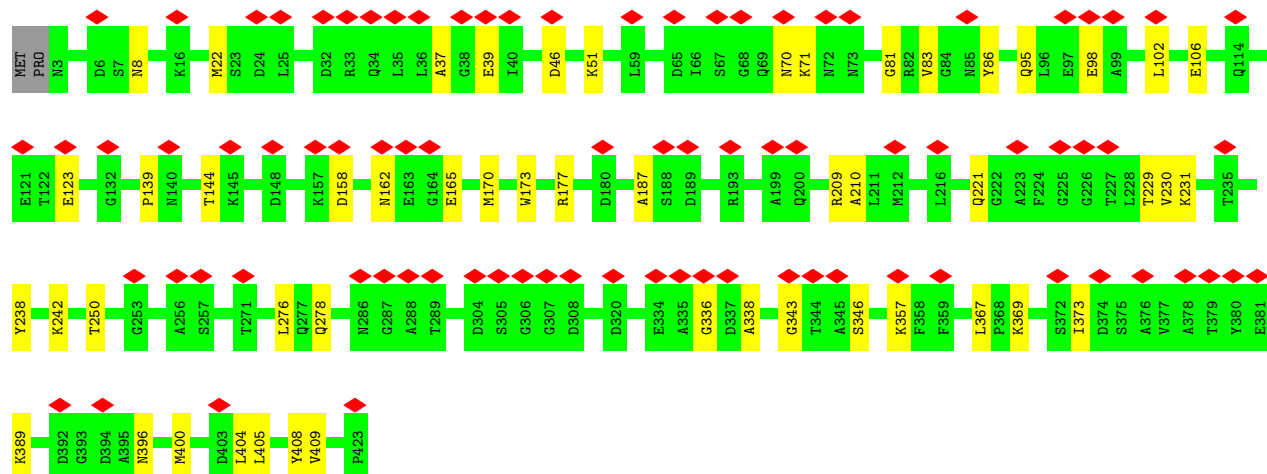
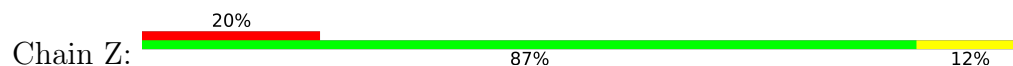




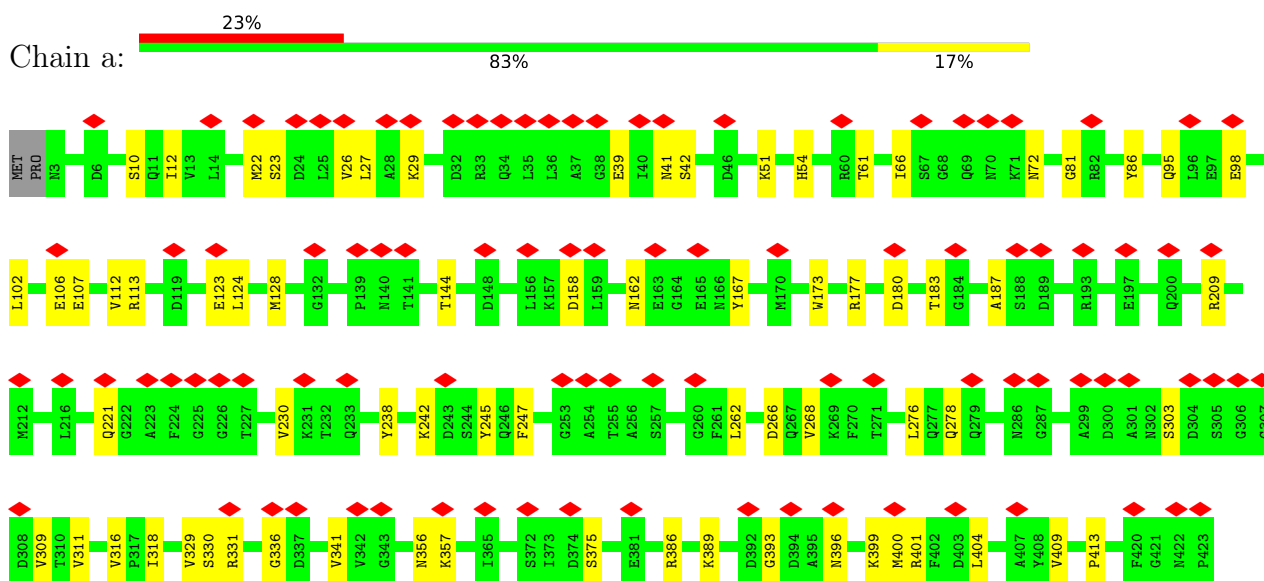
• Molecule 3: Gene 5 protein



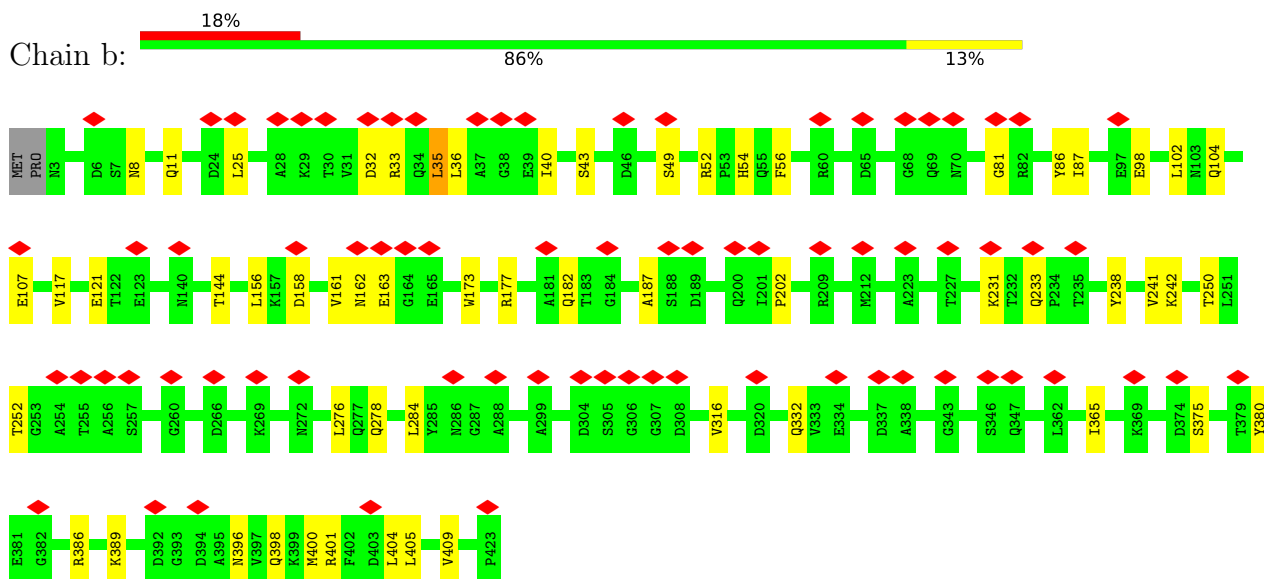
• Molecule 3: Gene 5 protein



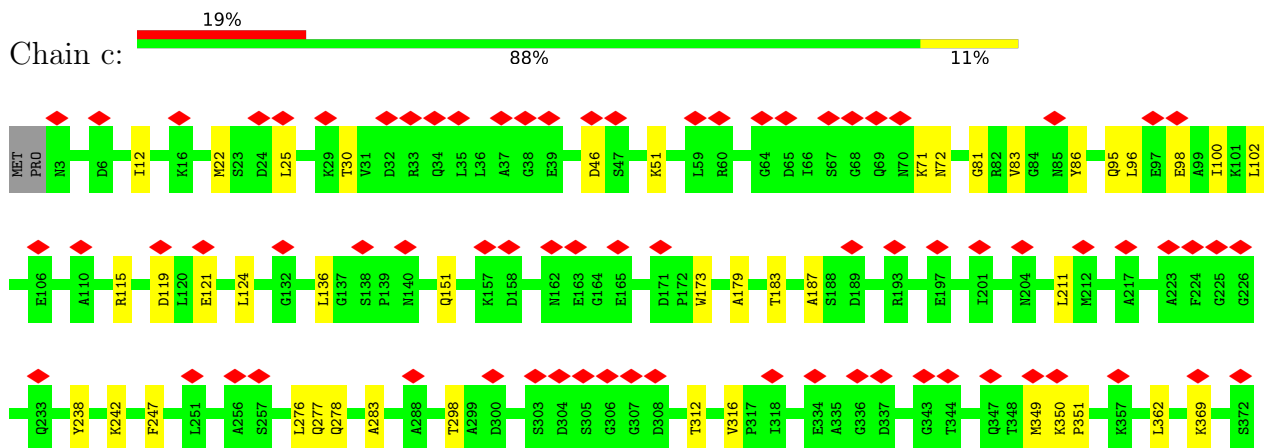
• Molecule 3: Gene 5 protein

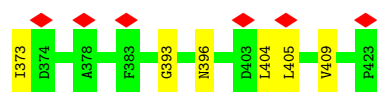


• Molecule 3: Gene 5 protein

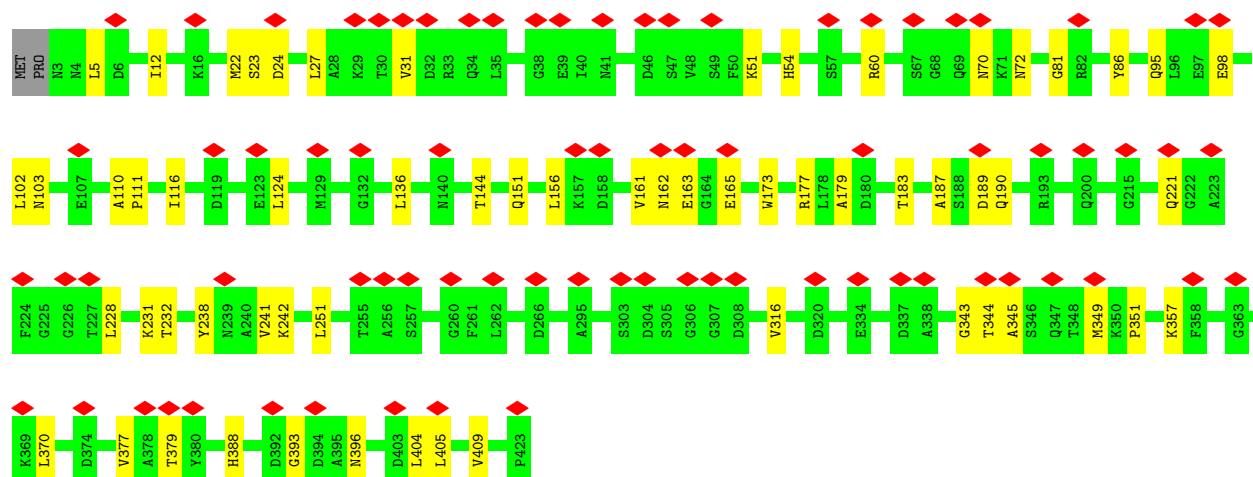
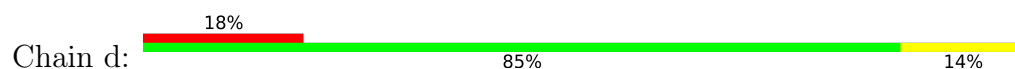


• Molecule 3: Gene 5 protein

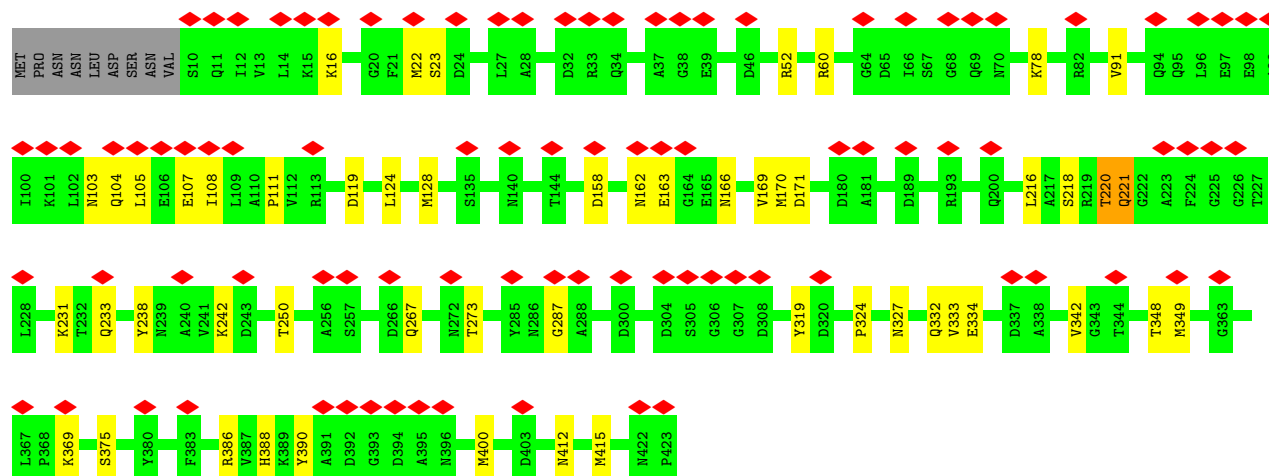
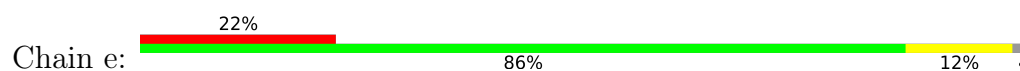




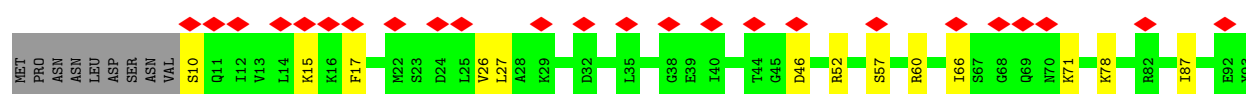
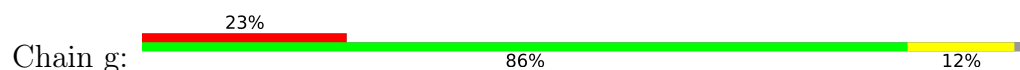
• Molecule 3: Gene 5 protein

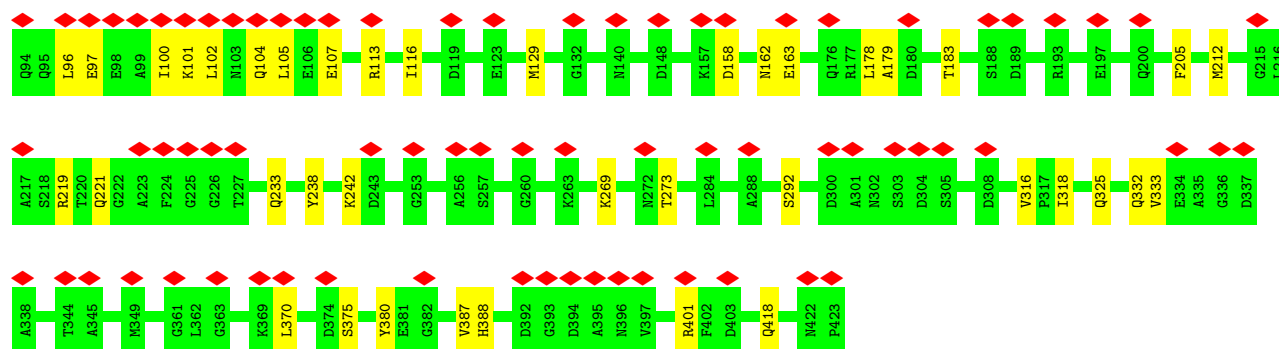


• Molecule 3: Gene 5 protein

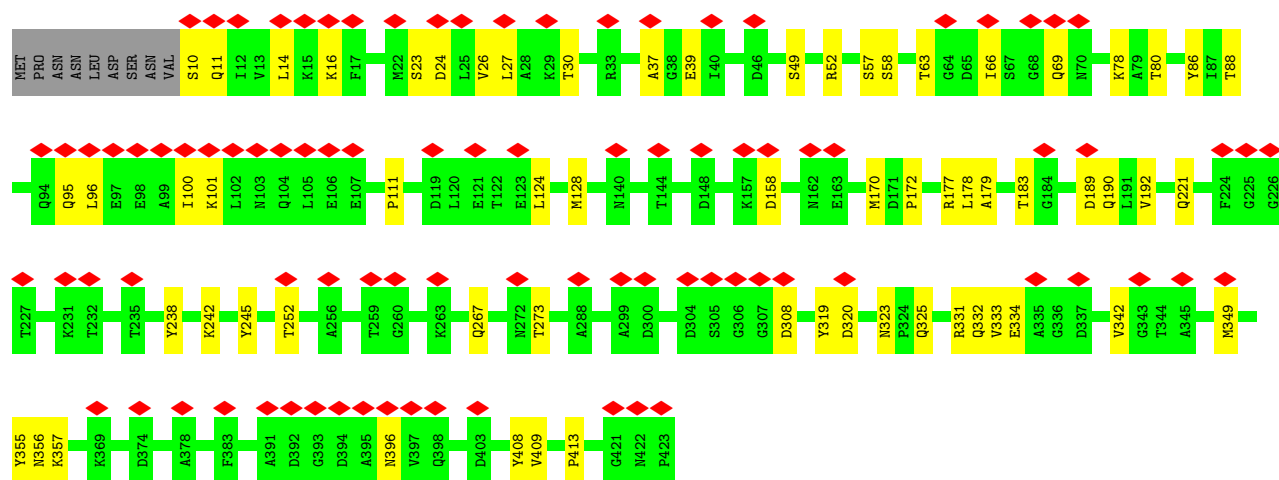
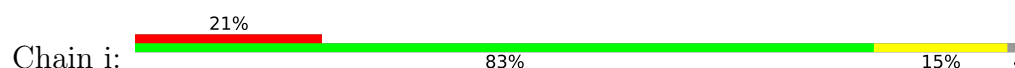


• Molecule 3: Gene 5 protein

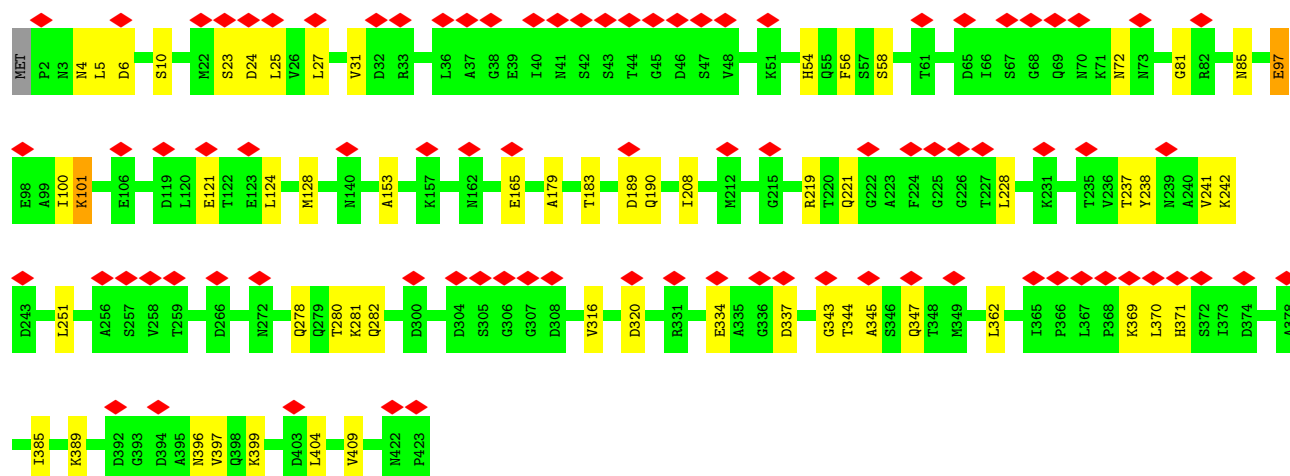
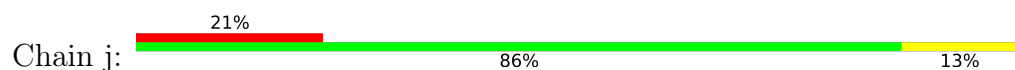




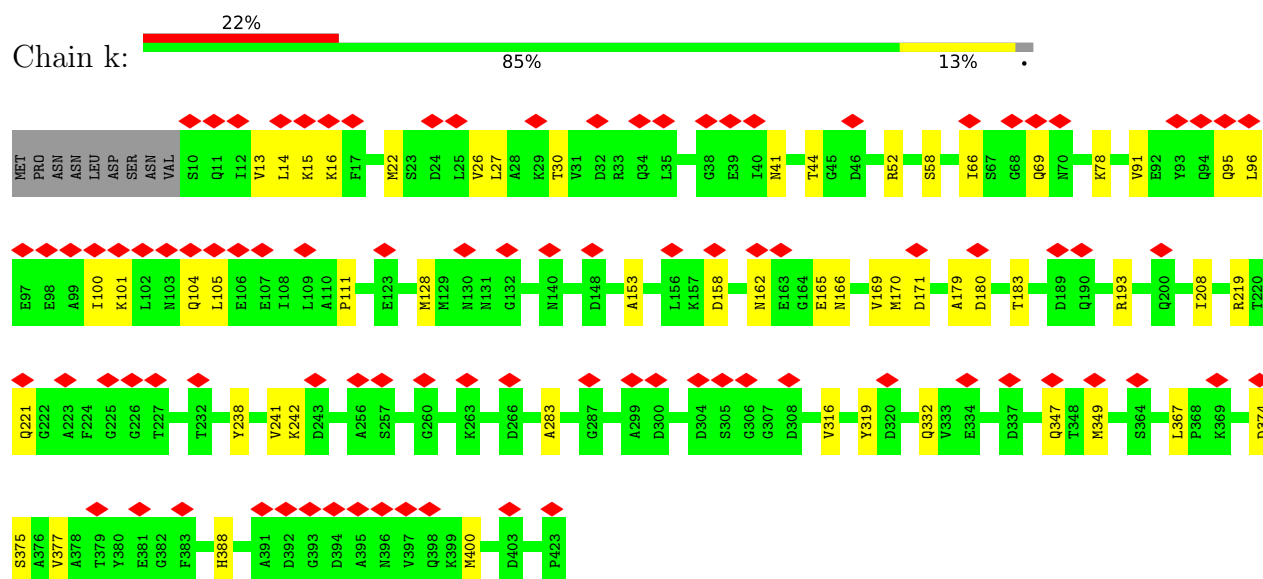
• Molecule 3: Gene 5 protein



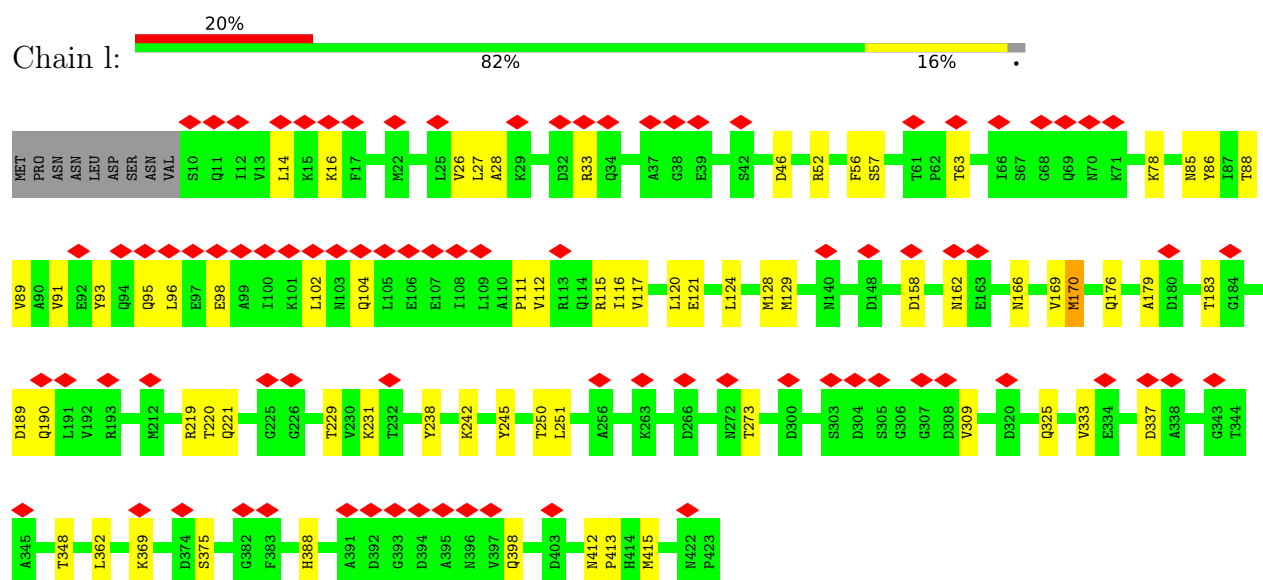
• Molecule 3: Gene 5 protein



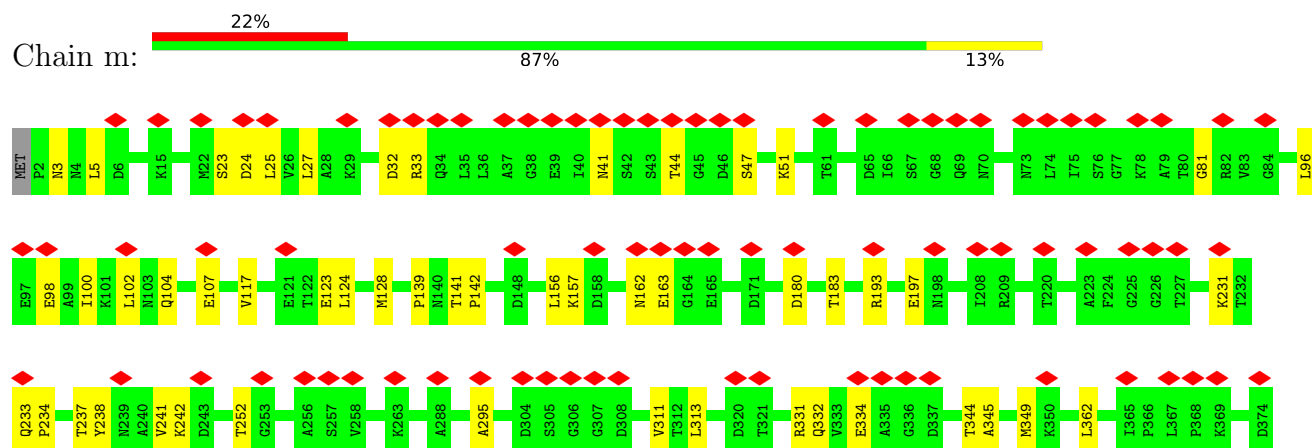
• Molecule 3: Gene 5 protein

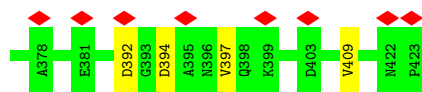


• Molecule 3: Gene 5 protein

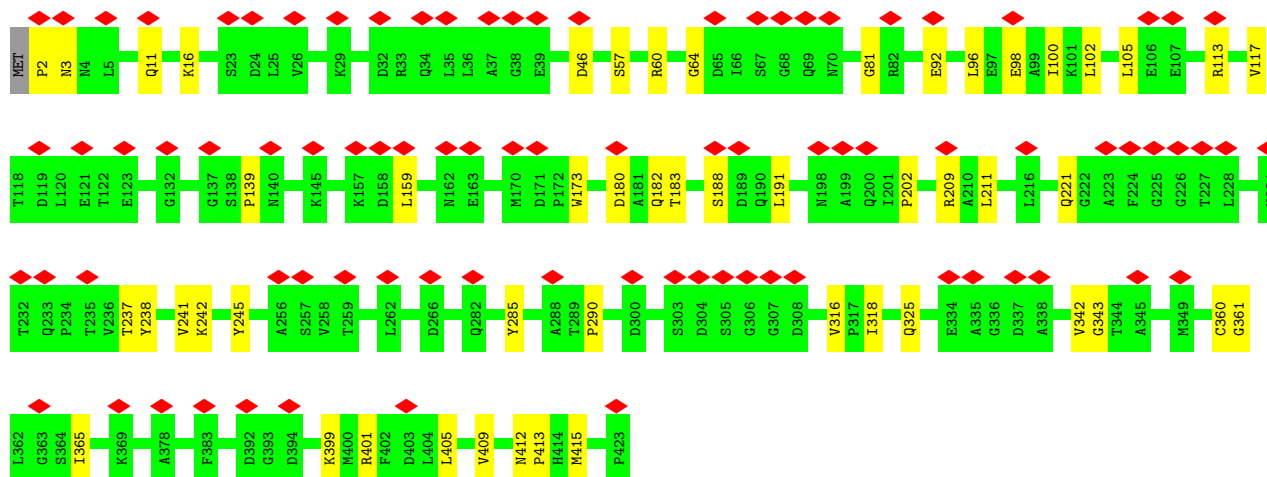
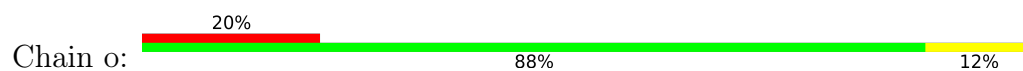


• Molecule 3: Gene 5 protein

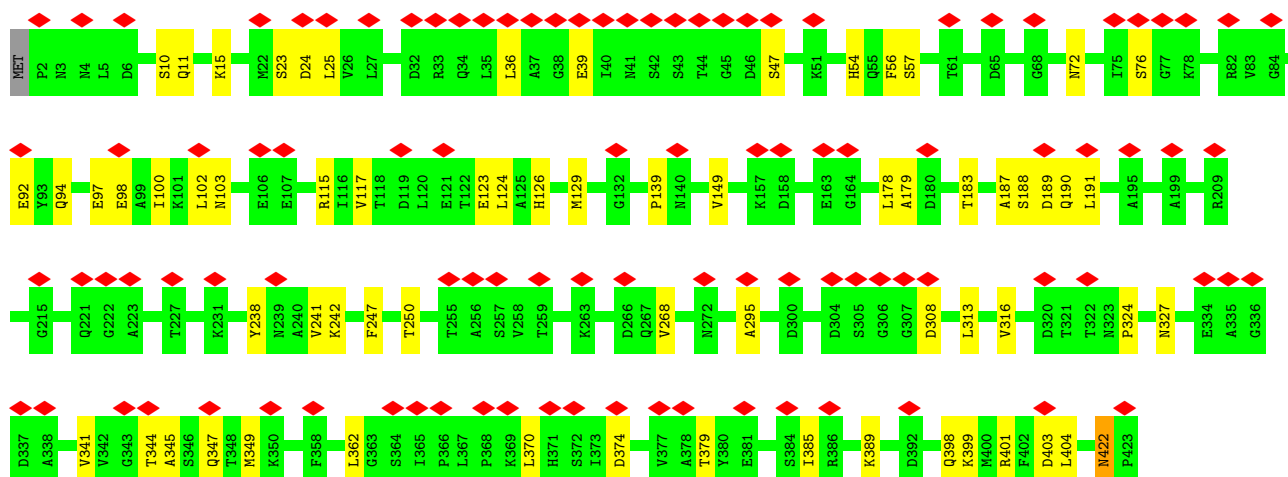
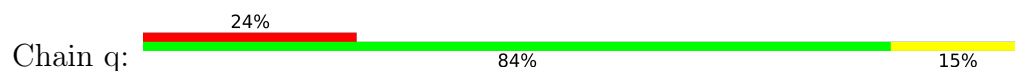




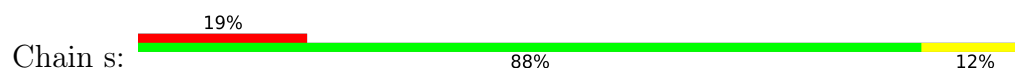
• Molecule 3: Gene 5 protein

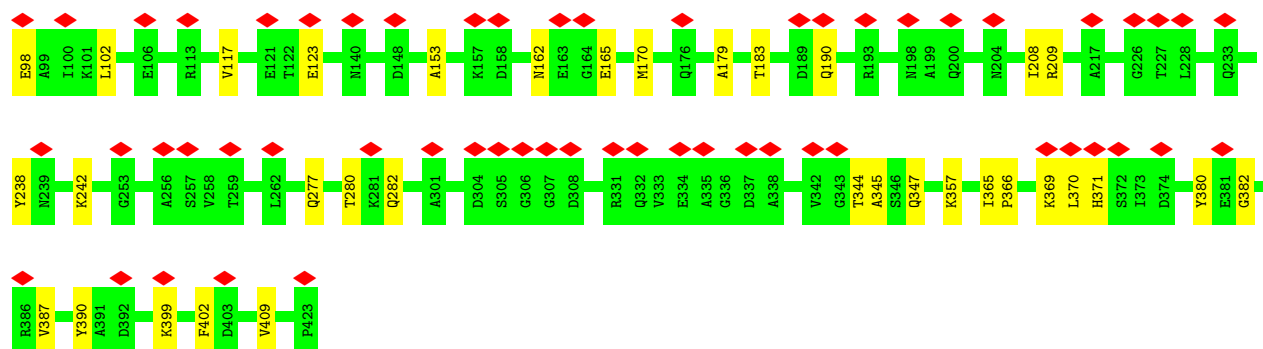


• Molecule 3: Gene 5 protein

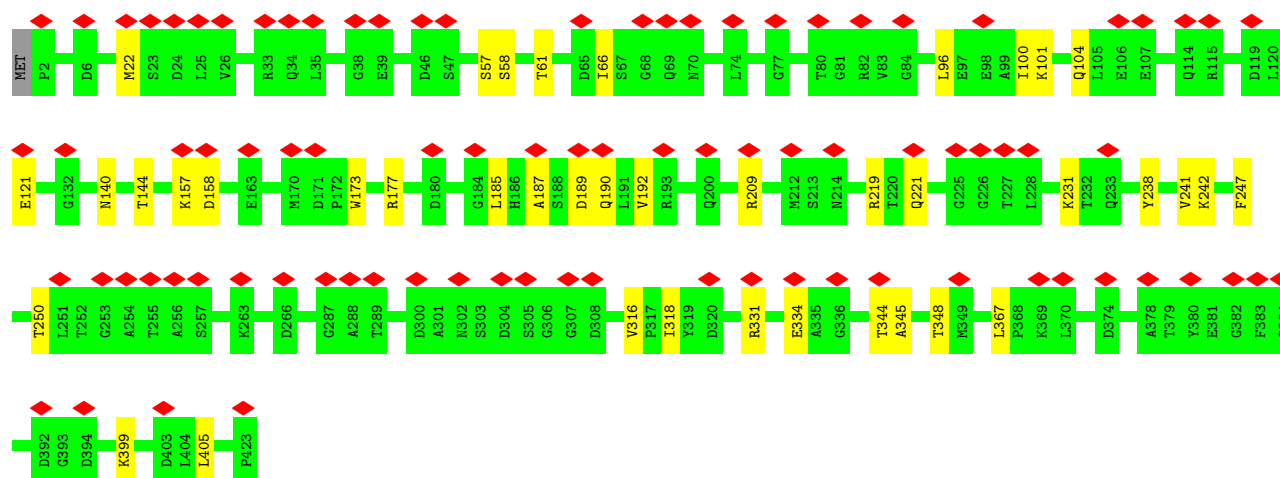
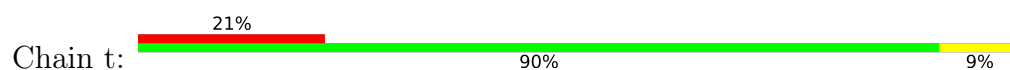


• Molecule 3: Gene 5 protein

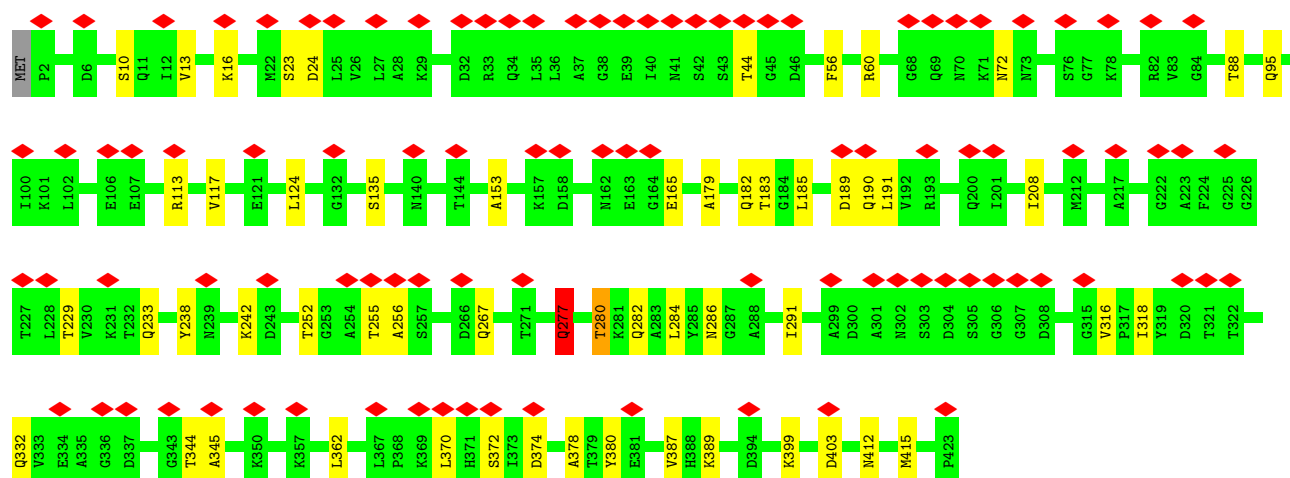
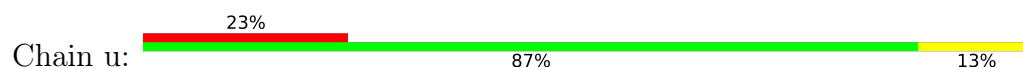




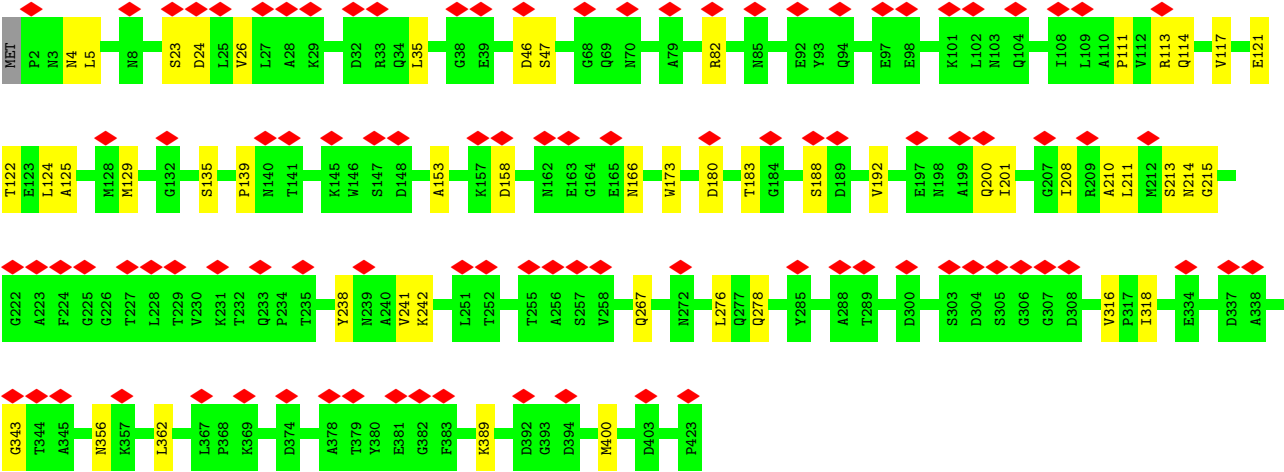
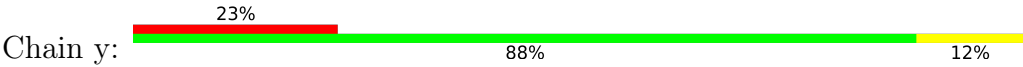
• Molecule 3: Gene 5 protein



• Molecule 3: Gene 5 protein



• Molecule 3: Gene 5 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39000	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	14.559	Depositor
Minimum map value	-8.202	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.62	Depositor
Map size (Å)	574.464, 574.464, 574.464	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.122, 1.122, 1.122	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.43	0/1186	0.66	0/1611
1	1	0.39	0/1259	0.63	0/1713
1	Y	0.63	0/1188	0.92	0/1614
1	f	0.26	0/1259	0.48	0/1713
1	h	0.36	0/1186	0.59	0/1611
1	n	0.26	0/1186	0.51	0/1611
1	p	0.37	0/1259	0.60	1/1713 (0.1%)
1	r	0.13	0/1186	0.31	0/1611
1	v	0.13	0/1186	0.35	0/1611
1	w	0.14	0/1186	0.34	0/1611
1	x	0.31	0/1259	0.54	0/1713
1	z	0.15	0/1256	0.36	0/1709
2	A	0.29	0/5064	0.51	1/6846 (0.0%)
2	B	0.13	0/5064	0.34	0/6846
2	C	0.25	0/5064	0.48	0/6846
2	D	0.13	0/5064	0.35	0/6846
2	E	0.22	0/5064	0.44	1/6846 (0.0%)
2	F	0.18	0/5064	0.38	0/6846
2	G	0.13	0/5064	0.34	0/6846
2	H	0.19	0/5064	0.42	1/6846 (0.0%)
2	I	0.31	0/5064	0.53	2/6846 (0.0%)
2	J	0.22	0/5064	0.43	0/6846
2	K	0.20	0/5064	0.39	0/6846
2	L	0.13	0/5064	0.35	0/6846
3	M	0.32	0/3274	0.52	0/4455
3	N	0.14	0/3274	0.33	0/4455
3	O	0.13	0/3274	0.35	0/4455
3	P	0.14	0/3274	0.35	0/4455
3	Q	0.13	0/3274	0.33	0/4455
3	R	0.23	0/3274	0.43	0/4455
3	S	0.14	0/3274	0.33	0/4455
3	T	0.19	0/3274	0.39	1/4455 (0.0%)
3	U	0.13	0/3274	0.32	0/4455
3	V	0.13	0/3274	0.33	0/4455

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	W	0.13	0/3274	0.33	0/4455
3	X	0.29	0/3274	0.51	3/4455 (0.1%)
3	Z	0.13	0/3266	0.33	0/4444
3	a	0.19	0/3266	0.37	0/4444
3	b	0.25	0/3266	0.43	0/4444
3	c	0.13	0/3266	0.33	0/4444
3	d	0.36	0/3266	0.55	0/4444
3	e	0.29	0/3213	0.49	0/4371
3	g	0.20	0/3213	0.39	0/4371
3	i	0.28	0/3213	0.44	1/4371 (0.0%)
3	j	0.27	0/3274	0.46	0/4455
3	k	0.22	0/3213	0.41	0/4371
3	l	0.27	0/3213	0.49	0/4371
3	m	0.13	0/3274	0.34	0/4455
3	o	0.13	0/3274	0.35	0/4455
3	q	0.19	0/3274	0.38	0/4455
3	s	0.14	0/3274	0.34	0/4455
3	t	0.24	0/3274	0.39	0/4455
3	u	0.27	0/3274	0.48	1/4455 (0.0%)
3	y	0.19	0/3274	0.41	0/4455
All	All	0.22	0/173239	0.42	12/235168 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	p	156	ASP	N-CA-C	-7.94	98.71	110.46
2	E	218	ASN	N-CA-C	-7.26	103.51	112.88
3	X	120	LEU	CA-C-N	-6.52	111.03	120.29
3	X	120	LEU	C-N-CA	-6.52	111.03	120.29
3	T	222	GLY	CA-C-O	-6.12	117.11	121.88
2	H	46	GLY	N-CA-C	-5.98	106.79	113.79
2	I	199	TYR	CB-CA-C	-5.94	109.71	116.54
3	X	120	LEU	N-CA-C	-5.63	105.14	111.28
2	I	204	PRO	N-CA-C	-5.56	102.46	111.03
3	u	277	GLN	N-CA-C	-5.53	101.67	109.96
3	i	172	PRO	CB-CA-C	-5.06	104.27	112.62
2	A	630	ALA	N-CA-C	-5.03	105.80	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1161	0	1122	23	0
1	1	1232	0	1191	26	0
1	Y	1162	0	1124	16	0
1	f	1232	0	1191	20	0
1	h	1161	0	1122	24	0
1	n	1161	0	1122	13	0
1	p	1232	0	1191	19	0
1	r	1161	0	1122	22	0
1	v	1161	0	1122	17	0
1	w	1161	0	1122	20	0
1	x	1232	0	1191	18	0
1	z	1229	0	1182	31	0
2	A	4973	0	4895	84	0
2	B	4973	0	4895	83	0
2	C	4973	0	4895	76	0
2	D	4973	0	4895	74	0
2	E	4973	0	4895	84	0
2	F	4973	0	4895	101	0
2	G	4973	0	4895	88	0
2	H	4973	0	4895	70	0
2	I	4973	0	4895	85	0
2	J	4973	0	4895	80	0
2	K	4973	0	4895	74	0
2	L	4973	0	4895	84	0
3	M	3209	0	3149	34	0
3	N	3209	0	3149	31	0
3	O	3209	0	3149	40	0
3	P	3209	0	3149	31	0
3	Q	3209	0	3149	39	0
3	R	3209	0	3149	35	0
3	S	3209	0	3149	35	0
3	T	3209	0	3149	35	0
3	U	3209	0	3149	30	0
3	V	3209	0	3149	27	0
3	W	3209	0	3149	27	0
3	X	3209	0	3149	20	0
3	Z	3202	0	3141	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	a	3202	0	3141	47	0
3	b	3202	0	3141	37	0
3	c	3202	0	3141	33	0
3	d	3202	0	3141	46	0
3	e	3149	0	3094	37	0
3	g	3149	0	3094	36	0
3	i	3149	0	3094	41	0
3	j	3209	0	3149	41	0
3	k	3149	0	3094	38	0
3	l	3149	0	3094	41	0
3	m	3209	0	3149	36	0
3	o	3209	0	3149	31	0
3	q	3209	0	3149	48	0
3	s	3209	0	3149	37	0
3	t	3209	0	3149	26	0
3	u	3209	0	3149	34	0
3	y	3209	0	3149	27	0
All	All	169896	0	166697	1936	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 6.

All (1936) 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:V:238:TYR:O	3:V:242:LYS:HB3	1.60	1.00
2:B:621:VAL:O	2:B:625:ALA:HB2	1.64	0.96
2:C:58:PHE:HB3	3:l:96:LEU:HB3	1.46	0.96
2:L:621:VAL:O	2:L:625:ALA:HB2	1.68	0.94
3:U:238:TYR:O	3:U:242:LYS:HB3	1.68	0.93
2:C:621:VAL:O	2:C:625:ALA:HB2	1.69	0.92
2:J:621:VAL:O	2:J:625:ALA:HB2	1.68	0.91
3:y:238:TYR:O	3:y:242:LYS:HB3	1.69	0.90
2:G:621:VAL:O	2:G:625:ALA:HB2	1.72	0.87
3:X:238:TYR:O	3:X:242:LYS:HB3	1.74	0.86
3:o:238:TYR:O	3:o:242:LYS:HB3	1.75	0.86
2:K:621:VAL:O	2:K:625:ALA:HB2	1.74	0.86
2:D:621:VAL:O	2:D:625:ALA:HB2	1.75	0.86
3:O:238:TYR:O	3:O:242:LYS:HB3	1.77	0.84
2:D:606:GLN:HA	2:D:609:GLN:HE21	1.43	0.83
3:j:81:GLY:HA3	3:j:409:VAL:HG12	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:81:GLY:HA3	3:T:409:VAL:HG22	1.58	0.83
3:W:81:GLY:HA3	3:W:409:VAL:HG22	1.61	0.82
3:l:238:TYR:O	3:l:242:LYS:HB3	1.79	0.82
2:L:596:PRO:HB3	2:L:601:GLU:HG3	1.62	0.82
3:e:238:TYR:O	3:e:242:LYS:HB3	1.80	0.82
2:D:596:PRO:HB3	2:D:601:GLU:HG3	1.61	0.81
3:g:238:TYR:O	3:g:242:LYS:HB3	1.81	0.81
3:i:238:TYR:O	3:i:242:LYS:HB3	1.81	0.80
2:G:596:PRO:HB3	2:G:601:GLU:HG3	1.63	0.80
3:N:238:TYR:O	3:N:242:LYS:HB3	1.81	0.79
2:J:596:PRO:HB3	2:J:601:GLU:HG3	1.65	0.79
2:G:636:LYS:HD2	2:H:638:THR:HA	1.64	0.79
2:K:596:PRO:HB3	2:K:601:GLU:HG3	1.64	0.78
2:L:490:ARG:HG3	2:L:509:ASP:HB3	1.66	0.78
2:L:653:GLN:HA	2:L:656:MET:HE3	1.66	0.78
2:B:115:THR:HG22	2:B:116:ASP:H	1.49	0.77
2:H:596:PRO:HB3	2:H:601:GLU:HG3	1.63	0.77
3:W:238:TYR:O	3:W:242:LYS:HB3	1.84	0.77
1:f:86:LEU:HG	1:f:90:MET:HE2	1.66	0.77
1:l:44:MET:HE1	1:l:86:LEU:HA	1.66	0.77
2:H:115:THR:HG22	2:H:116:ASP:H	1.49	0.77
3:c:98:GLU:HA	3:c:102:LEU:HB2	1.65	0.77
2:E:115:THR:HG22	2:E:116:ASP:H	1.50	0.76
2:F:115:THR:HG22	2:F:116:ASP:H	1.51	0.76
3:l:220:THR:HG22	3:l:348:THR:HG22	1.68	0.76
2:G:115:THR:HG22	2:G:116:ASP:H	1.51	0.76
2:H:621:VAL:O	2:H:625:ALA:HB2	1.85	0.76
2:I:636:LYS:HD2	2:J:638:THR:HA	1.68	0.76
3:P:238:TYR:O	3:P:242:LYS:HB3	1.86	0.76
2:B:621:VAL:O	2:B:625:ALA:CB	2.33	0.75
2:D:115:THR:HG22	2:D:116:ASP:H	1.51	0.75
2:E:356:ILE:H	2:E:404:THR:HG22	1.51	0.75
2:I:233:VAL:HG12	2:I:284:VAL:HG22	1.67	0.75
2:L:115:THR:HG22	2:L:116:ASP:H	1.50	0.75
2:F:621:VAL:O	2:F:625:ALA:HB2	1.86	0.75
2:G:346:ALA:HA	2:H:416:LEU:HD11	1.69	0.75
3:M:40:ILE:HA	3:M:44:THR:HG21	1.69	0.75
2:B:346:ALA:HA	2:C:416:LEU:HD11	1.69	0.75
3:b:389:LYS:HG2	3:b:400:MET:HG2	1.69	0.74
3:o:221:GLN:HE22	3:o:343:GLY:HA3	1.51	0.74
2:F:636:LYS:HD2	2:G:638:THR:HA	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:98:GLU:HA	3:Z:102:LEU:HB2	1.69	0.74
3:m:81:GLY:HA3	3:m:409:VAL:HG12	1.69	0.74
3:a:98:GLU:HA	3:a:102:LEU:HB2	1.68	0.74
2:C:547:LEU:HD12	2:C:564:ILE:HG23	1.69	0.74
2:I:115:THR:HG22	2:I:116:ASP:H	1.53	0.74
3:R:25:LEU:HD21	3:R:28:ALA:HB3	1.70	0.74
1:p:30:GLU:HG3	1:p:33:SER:H	1.51	0.74
1:z:44:MET:HE1	1:z:86:LEU:HA	1.68	0.74
2:I:621:VAL:O	2:I:625:ALA:HB2	1.88	0.74
1:h:35:GLU:O	1:h:39:ASN:ND2	2.21	0.74
3:s:238:TYR:O	3:s:242:LYS:HB3	1.88	0.74
2:E:596:PRO:HB3	2:E:601:GLU:HG2	1.70	0.73
2:H:531:ASP:OD1	2:H:532:VAL:N	2.21	0.73
3:R:98:GLU:HA	3:R:102:LEU:HB2	1.70	0.73
2:K:115:THR:HG22	2:K:116:ASP:H	1.53	0.73
3:o:81:GLY:HA3	3:o:409:VAL:HG22	1.69	0.73
2:A:416:LEU:HD11	2:L:346:ALA:HA	1.70	0.73
2:A:115:THR:HG22	2:A:116:ASP:H	1.54	0.72
2:D:111:ASP:HA	2:D:154:ARG:HH21	1.54	0.72
2:I:361:MET:HE1	1:x:115:THR:HA	1.70	0.72
1:w:77:LYS:HD3	1:z:50:ILE:HD11	1.70	0.72
2:B:596:PRO:HB3	2:B:601:GLU:HG3	1.71	0.72
2:F:233:VAL:HG12	2:F:284:VAL:HG22	1.71	0.72
2:H:346:ALA:HA	2:I:416:LEU:HD11	1.71	0.72
2:D:346:ALA:HA	2:E:416:LEU:HD11	1.72	0.72
3:R:238:TYR:O	3:R:242:LYS:HB3	1.90	0.72
3:q:238:TYR:O	3:q:242:LYS:HB3	1.90	0.72
3:S:98:GLU:HA	3:S:102:LEU:HB2	1.71	0.71
3:T:344:THR:HG22	3:T:345:ALA:H	1.54	0.71
2:J:346:ALA:HA	2:K:416:LEU:HD11	1.71	0.71
2:J:636:LYS:HD2	2:K:638:THR:HA	1.71	0.71
3:N:81:GLY:HA3	3:N:409:VAL:HG22	1.71	0.71
3:b:81:GLY:HA3	3:b:409:VAL:HG22	1.72	0.71
3:c:86:TYR:HB3	3:c:405:LEU:HD23	1.73	0.71
3:i:10:SER:N	3:q:47:SER:HG	1.88	0.71
3:M:221:GLN:HE22	3:M:344:THR:H	1.37	0.70
2:H:556:PRO:HB3	2:I:555:LEU:HD21	1.73	0.70
2:E:346:ALA:HA	2:F:416:LEU:HD11	1.72	0.70
3:d:344:THR:HG22	3:d:345:ALA:H	1.55	0.70
1:Y:107:GLN:NE2	1:Y:111:ASP:OD2	2.24	0.70
2:E:218:ASN:HA	3:e:16:LYS:HD3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:238:TYR:O	3:S:242:LYS:HB3	1.92	0.70
3:d:102:LEU:HD21	3:j:5:LEU:CD1	2.21	0.70
2:C:247:ILE:HG22	2:C:248:THR:HG23	1.74	0.69
3:i:27:LEU:HD12	3:i:128:MET:HE1	1.74	0.69
2:E:561:ARG:HH12	2:F:555:LEU:HD23	1.57	0.69
2:L:602:GLN:O	2:L:606:GLN:NE2	2.25	0.69
3:P:98:GLU:HA	3:P:102:LEU:HB2	1.72	0.69
2:D:489:VAL:O	2:D:511:GLN:NE2	2.24	0.69
3:Q:344:THR:HG22	3:Q:345:ALA:H	1.58	0.69
2:G:353:PRO:HD3	1:h:126:ARG:HH22	1.57	0.69
1:p:150:LEU:HD12	1:p:151:PRO:HD2	1.72	0.69
3:M:60:ARG:NH2	3:m:123:GLU:OE1	2.26	0.69
3:b:233:GLN:NE2	3:b:332:GLN:OE1	2.26	0.69
2:C:115:THR:HG22	2:C:116:ASP:H	1.58	0.69
3:T:389:LYS:HG2	3:T:400:MET:HG2	1.75	0.69
1:h:86:LEU:O	1:h:90:MET:HG2	1.93	0.69
3:c:22:MET:HE2	3:k:162:ASN:HD22	1.58	0.68
1:0:32:GLN:HG2	1:r:24:ALA:HB2	1.75	0.68
3:M:238:TYR:O	3:M:242:LYS:HB3	1.92	0.68
1:f:158:PRO:HA	3:q:370:LEU:HD21	1.75	0.68
2:K:636:LYS:HD2	2:L:638:THR:HA	1.74	0.68
3:d:349:MET:HE2	3:d:351:PRO:HG3	1.76	0.68
2:H:636:LYS:HD2	2:I:638:THR:HA	1.75	0.68
3:R:111:PRO:HG2	3:b:56:PHE:HE2	1.57	0.67
3:d:86:TYR:HB3	3:d:405:LEU:HD23	1.75	0.67
3:O:81:GLY:HA3	3:O:409:VAL:HG22	1.76	0.67
3:S:344:THR:HG22	3:S:345:ALA:H	1.59	0.67
2:A:368:GLU:HG2	1:Y:119:VAL:HG21	1.77	0.67
3:N:365:ILE:HD11	3:N:405:LEU:HD23	1.75	0.67
2:A:642:ALA:H	2:L:636:LYS:HZ1	1.41	0.67
2:B:259:VAL:HG12	2:B:261:ASP:H	1.58	0.67
3:a:276:LEU:O	3:a:278:GLN:NE2	2.28	0.67
3:m:193:ARG:NH1	3:m:197:GLU:OE2	2.27	0.67
2:B:57:GLN:HG3	1:Y:124:ARG:HH21	1.59	0.67
3:l:412:ASN:HB3	3:l:415:MET:HE2	1.76	0.67
1:z:51:ASN:HB3	1:z:52:PRO:HD3	1.76	0.67
2:E:657:GLU:HG2	2:E:661:ASN:HD21	1.58	0.67
3:q:247:PHE:HD1	3:q:316:VAL:HG12	1.59	0.67
3:j:344:THR:HB	3:j:347:GLN:HB2	1.75	0.66
2:C:1:MET:HE1	2:C:3:GLU:HB2	1.77	0.66
2:C:346:ALA:HA	2:D:416:LEU:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:636:LYS:HD2	2:E:638:THR:HA	1.77	0.66
2:I:24:LYS:NZ	2:I:28:GLU:OE2	2.28	0.66
3:R:344:THR:HG22	3:R:345:ALA:H	1.58	0.66
1:f:51:ASN:HB3	1:f:52:PRO:HD3	1.77	0.66
2:I:42:GLY:HA2	2:I:45:GLU:HG3	1.78	0.66
2:I:589:LEU:HD22	2:I:596:PRO:HG3	1.78	0.66
2:J:174:LYS:O	2:J:315:ARG:NH2	2.29	0.66
3:a:268:VAL:HG22	3:a:341:VAL:HG12	1.76	0.66
3:j:27:LEU:HD22	3:j:128:MET:HE1	1.78	0.66
3:a:389:LYS:HG2	3:a:400:MET:HE3	1.78	0.66
2:K:103:LYS:HE2	2:K:510:ARG:HG3	1.78	0.66
3:P:247:PHE:HD1	3:P:316:VAL:HG12	1.61	0.66
2:H:245:HIS:HB3	2:H:270:GLY:HA2	1.78	0.66
2:D:193:GLU:OE1	2:E:18:ARG:NH2	2.29	0.66
3:M:12:ILE:HD13	3:U:44:THR:HG23	1.78	0.66
3:c:115:ARG:NH2	3:c:119:ASP:OD1	2.29	0.66
1:l:136:LYS:NZ	2:A:41:GLY:O	2.29	0.65
3:k:52:ARG:NH1	3:k:78:LYS:O	2.29	0.65
3:q:344:THR:HB	3:q:347:GLN:HB2	1.78	0.65
3:X:344:THR:HG22	3:X:345:ALA:H	1.59	0.65
3:y:124:LEU:HD12	3:y:362:LEU:HD13	1.78	0.65
2:F:346:ALA:HA	2:G:416:LEU:HD11	1.79	0.65
1:Y:51:ASN:HB3	1:Y:52:PRO:HD3	1.78	0.65
2:I:589:LEU:HD23	2:I:594:ALA:HB3	1.79	0.65
2:D:114:GLU:HB2	2:D:154:ARG:HH22	1.62	0.65
3:O:267:GLN:NE2	3:O:418:GLN:OE1	2.29	0.65
3:P:25:LEU:HD22	3:P:121:GLU:HG2	1.77	0.65
1:r:141:THR:HG22	1:r:143:ASP:H	1.62	0.65
2:J:643:GLN:OE1	2:J:647:LYS:NZ	2.30	0.65
2:G:94:ARG:NH2	2:G:527:ASP:OD2	2.29	0.64
3:j:241:VAL:HG21	3:j:316:VAL:HG11	1.79	0.64
2:J:115:THR:HG21	2:J:156:ALA:HB1	1.78	0.64
3:g:57:SER:HB3	3:g:325:GLN:HB3	1.78	0.64
2:A:661:ASN:HA	2:B:666:LEU:HD21	1.80	0.64
2:C:621:VAL:O	2:C:625:ALA:CB	2.44	0.64
3:a:81:GLY:HA3	3:a:409:VAL:HG22	1.79	0.64
3:T:187:ALA:HB3	3:X:192:VAL:HG21	1.79	0.64
3:t:241:VAL:HG21	3:t:316:VAL:HG11	1.80	0.64
3:k:221:GLN:HG2	3:k:349:MET:HE1	1.79	0.64
2:C:58:PHE:HB3	3:l:96:LEU:CB	2.26	0.64
2:J:569:LEU:HD23	2:J:580:PHE:HZ	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:52:ARG:NH1	3:g:78:LYS:O	2.31	0.63
2:J:636:LYS:NZ	2:K:637:ALA:O	2.25	0.63
2:J:621:VAL:O	2:J:625:ALA:CB	2.44	0.63
3:j:228:LEU:HD23	3:j:251:LEU:HD13	1.81	0.63
3:t:344:THR:HG22	3:t:345:ALA:H	1.63	0.63
1:v:51:ASN:HB3	1:v:52:PRO:HD3	1.79	0.63
2:E:488:GLU:OE1	2:E:510:ARG:NH1	2.31	0.63
3:l:14:LEU:HG	3:l:16:LYS:H	1.63	0.63
3:o:92:GLU:HG2	3:o:399:LYS:HG2	1.81	0.63
1:0:51:ASN:HB3	1:0:52:PRO:HD3	1.81	0.63
2:C:92:GLY:H	2:C:97:SER:HB2	1.62	0.63
3:N:182:GLN:HE22	3:N:202:PRO:HD3	1.63	0.63
3:a:95:GLN:OE1	3:a:396:ASN:ND2	2.31	0.63
3:b:238:TYR:O	3:b:242:LYS:HB3	1.98	0.63
2:F:636:LYS:NZ	2:G:637:ALA:O	2.28	0.63
3:S:170:MET:HE1	3:S:178:LEU:HD12	1.80	0.63
3:a:399:LYS:HE3	3:g:71:LYS:HZ1	1.62	0.63
2:E:220:PHE:CD1	2:E:224:VAL:HG21	2.34	0.63
2:I:120:ALA:HA	2:I:159:PRO:HB3	1.81	0.63
2:I:636:LYS:NZ	2:J:637:ALA:O	2.24	0.63
3:T:28:ALA:O	3:T:33:ARG:NH2	2.31	0.63
3:a:123:GLU:OE2	3:g:60:ARG:NH1	2.32	0.63
2:L:652:GLN:HG3	2:L:656:MET:HE2	1.80	0.63
3:Z:187:ALA:HB3	3:t:192:VAL:HG11	1.80	0.62
2:B:657:GLU:HG2	2:B:661:ASN:HD21	1.63	0.62
3:P:81:GLY:HA3	3:P:409:VAL:HG22	1.81	0.62
3:d:81:GLY:HA3	3:d:409:VAL:HG22	1.81	0.62
3:j:124:LEU:HG	3:j:128:MET:HE2	1.81	0.62
3:R:187:ALA:HB3	3:V:192:VAL:HG21	1.81	0.62
3:S:158:ASP:OD2	3:W:173:TRP:NE1	2.32	0.62
1:n:49:MET:HE1	1:n:54:ASP:HB3	1.79	0.62
3:q:76:SER:O	3:q:242:LYS:NZ	2.32	0.62
2:A:174:LYS:O	2:A:315:ARG:NH2	2.33	0.62
2:C:218:ASN:HD21	3:l:104:GLN:HG2	1.64	0.62
2:E:246:PRO:HA	2:E:250:GLU:HG3	1.81	0.62
2:E:640:GLU:HG2	2:F:641:THR:HG22	1.81	0.62
3:W:166:ASN:OD1	3:W:356:ASN:ND2	2.32	0.62
2:K:465:ALA:HB1	2:K:532:VAL:HG21	1.81	0.62
3:k:193:ARG:NH2	3:s:190:GLN:OE1	2.33	0.62
1:0:147:PRO:HB3	3:s:43:SER:HB3	1.82	0.62
2:I:510:ARG:NH2	2:I:511:GLN:O	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:300:ARG:NH2	2:L:481:GLU:OE2	2.30	0.62
2:G:365:ARG:O	2:G:385:ARG:NH1	2.33	0.61
3:Z:144:THR:HG22	3:Z:177:ARG:HD2	1.81	0.61
3:q:54:HIS:HE2	3:q:76:SER:HG	1.45	0.61
2:D:636:LYS:NZ	2:E:638:THR:O	2.29	0.61
2:E:636:LYS:HD2	2:F:638:THR:HA	1.81	0.61
3:m:344:THR:HG22	3:m:345:ALA:H	1.65	0.61
2:J:618:PRO:HA	2:J:621:VAL:HG12	1.82	0.61
3:T:61:THR:HG21	3:T:65:ASP:H	1.65	0.61
2:B:62:PRO:HD3	1:Y:125:ARG:HH21	1.65	0.61
2:D:347:ASP:OD1	2:D:348:THR:N	2.33	0.61
2:G:668:GLN:OE1	2:H:670:ARG:NH1	2.34	0.61
3:O:221:GLN:HE22	3:O:344:THR:H	1.46	0.61
3:b:36:LEU:HD13	3:b:409:VAL:HG21	1.82	0.61
1:1:117:THR:O	2:L:365:ARG:NH2	2.33	0.61
1:z:101:GLN:NE2	1:z:105:ASN:OD1	2.33	0.61
1:1:51:ASN:HB3	1:1:52:PRO:HD3	1.82	0.61
2:G:580:PHE:HB2	2:H:567:ILE:HD13	1.83	0.61
3:S:399:LYS:HD3	3:c:71:LYS:HE2	1.82	0.61
3:Z:139:PRO:HG2	3:Z:343:GLY:HA2	1.83	0.61
3:c:81:GLY:HA3	3:c:409:VAL:HG22	1.83	0.61
3:q:98:GLU:HA	3:q:102:LEU:HB2	1.82	0.61
1:w:41:LEU:HD12	1:w:86:LEU:HD22	1.83	0.61
3:P:123:GLU:OE1	3:X:60:ARG:NH1	2.29	0.61
3:k:91:VAL:HG12	3:s:72:ASN:HB2	1.82	0.61
3:t:238:TYR:O	3:t:242:LYS:HB3	2.01	0.61
2:G:120:ALA:HA	2:G:159:PRO:HB3	1.83	0.60
3:Z:81:GLY:HA3	3:Z:409:VAL:HG22	1.82	0.60
3:k:96:LEU:HB3	1:r:150:LEU:HD13	1.83	0.60
3:m:98:GLU:HA	3:m:102:LEU:HB2	1.83	0.60
2:F:378:ARG:NH2	2:H:347:ASP:OD1	2.34	0.60
2:G:540:ARG:NH2	2:H:98:GLU:OE2	2.34	0.60
2:I:661:ASN:HA	2:J:666:LEU:HD11	1.82	0.60
2:A:319:ASP:OD1	2:L:165:ARG:NH1	2.33	0.60
2:A:464:MET:HE3	2:A:468:LEU:HD21	1.83	0.60
1:f:57:TYR:HD1	1:f:74:LEU:HD11	1.65	0.60
2:C:578:ASP:OD1	2:C:579:ASP:N	2.34	0.60
2:D:599:GLU:HG2	2:D:600:LYS:N	2.15	0.60
2:H:244:ARG:NH1	2:H:250:GLU:OE1	2.33	0.60
2:E:57:GLN:HG3	1:z:124:ARG:HH22	1.67	0.60
3:S:350:LYS:NZ	3:c:283:ALA:O	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:276:LEU:O	3:c:278:GLN:NE2	2.34	0.60
2:A:318:ILE:HB	2:A:323:ARG:HE	1.66	0.60
3:c:136:LEU:HD13	3:c:151:GLN:HG3	1.83	0.60
3:M:300:ASP:OD1	3:M:301:ALA:N	2.35	0.60
3:P:278:GLN:O	3:P:281:LYS:NZ	2.33	0.60
1:r:18:PHE:HE2	1:r:96:LEU:HD13	1.65	0.60
2:A:207:LEU:HB3	2:A:225:ILE:HG23	1.82	0.60
2:A:599:GLU:HG2	2:A:600:LYS:H	1.67	0.60
2:B:218:ASN:OD1	2:B:219:TRP:N	2.35	0.60
2:E:362:GLU:HA	1:w:114:MET:HE1	1.84	0.60
3:P:139:PRO:HG2	3:P:343:GLY:HA2	1.83	0.60
3:S:192:VAL:HG11	3:c:187:ALA:HB3	1.83	0.60
3:X:273:THR:OG1	3:X:331:ARG:NH1	2.35	0.60
3:s:344:THR:HG22	3:s:345:ALA:H	1.66	0.60
2:E:37:ALA:HB2	2:E:328:ILE:HG21	1.83	0.59
2:E:220:PHE:HD1	2:E:224:VAL:HG21	1.66	0.59
3:P:22:MET:SD	3:X:162:ASN:ND2	2.74	0.59
3:a:144:THR:HG22	3:a:177:ARG:HD2	1.84	0.59
1:h:51:ASN:HB3	1:h:52:PRO:HD3	1.83	0.59
3:i:124:LEU:HG	3:i:128:MET:HE2	1.85	0.59
1:v:32:GLN:HG3	1:x:24:ALA:HB2	1.85	0.59
1:v:18:PHE:HE2	1:v:96:LEU:HD13	1.68	0.59
3:g:370:LEU:HD12	3:q:398:GLN:HE21	1.66	0.59
2:F:636:LYS:HZ3	2:G:641:THR:HB	1.67	0.59
1:p:51:ASN:HB3	1:p:52:PRO:HD3	1.83	0.59
3:V:140:ASN:OD1	3:V:141:THR:N	2.36	0.59
3:b:144:THR:HG22	3:b:177:ARG:HD2	1.85	0.59
3:i:26:VAL:HG23	3:i:27:LEU:HD22	1.85	0.59
1:0:139:VAL:HG12	2:L:215:TRP:NE1	2.18	0.59
2:E:486:GLU:HB3	2:E:510:ARG:HD2	1.84	0.59
2:G:152:ARG:HH22	2:G:516:VAL:HA	1.68	0.59
3:t:140:ASN:OD1	3:t:344:THR:OG1	2.20	0.59
2:D:668:GLN:OE1	2:E:670:ARG:NH1	2.36	0.59
2:I:657:GLU:HG2	2:I:661:ASN:HD21	1.66	0.59
3:R:381:GLU:N	3:R:381:GLU:OE2	2.36	0.59
3:W:98:GLU:HA	3:W:102:LEU:HB2	1.84	0.59
3:Z:37:ALA:N	3:Z:39:GLU:OE1	2.35	0.59
3:c:95:GLN:OE1	3:c:396:ASN:ND2	2.35	0.59
2:A:636:LYS:HE3	2:B:638:THR:HA	1.83	0.59
1:f:139:VAL:HG23	1:f:140:PHE:HD1	1.68	0.59
2:G:347:ASP:OD2	1:h:125:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:y:276:LEU:O	3:y:278:GLN:NE2	2.36	0.58
3:O:189:ASP:OD1	3:O:190:GLN:N	2.36	0.58
1:x:3:THR:OG1	1:x:4:VAL:N	2.34	0.58
2:E:378:ARG:NH2	2:G:347:ASP:OD1	2.36	0.58
3:S:189:ASP:OD1	3:S:190:GLN:N	2.36	0.58
2:A:196:GLU:HG3	2:A:201:LYS:HB3	1.85	0.58
2:A:666:LEU:HD22	2:L:664:TYR:CD2	2.39	0.58
3:a:399:LYS:HE3	3:g:71:LYS:NZ	2.16	0.58
3:d:136:LEU:HD13	3:d:151:GLN:HG3	1.86	0.58
3:u:182:GLN:HE21	3:u:191:LEU:HD21	1.68	0.58
1:O:118:LEU:HD21	2:J:361:MET:HG2	1.86	0.58
3:Q:192:VAL:HG11	3:a:187:ALA:HB3	1.86	0.58
3:T:192:VAL:HG11	3:d:187:ALA:HB3	1.86	0.58
3:u:238:TYR:O	3:u:242:LYS:HB3	2.03	0.58
3:T:91:VAL:HG12	3:d:72:ASN:HB2	1.85	0.58
3:i:52:ARG:NH1	3:i:78:LYS:O	2.35	0.58
3:j:85:ASN:HB2	3:o:60:ARG:HH11	1.68	0.58
1:v:48:TRP:HZ2	1:v:85:GLN:HG3	1.68	0.58
2:B:365:ARG:NH2	1:p:117:THR:O	2.35	0.58
3:U:221:GLN:HE22	3:U:343:GLY:HA3	1.68	0.58
3:a:375:SER:OG	3:a:386:ARG:NH1	2.37	0.58
3:S:187:ALA:HB3	3:W:192:VAL:HG21	1.86	0.58
3:q:94:GLN:HB2	3:q:97:GLU:HG3	1.85	0.58
3:u:189:ASP:OD1	3:u:190:GLN:N	2.37	0.58
2:D:599:GLU:HG2	2:D:600:LYS:H	1.69	0.58
3:O:221:GLN:NE2	3:O:344:THR:H	2.02	0.58
3:P:401:ARG:NH1	3:c:393:GLY:O	2.37	0.58
3:V:344:THR:HG22	3:V:345:ALA:H	1.67	0.58
2:A:338:TYR:HB2	2:A:420:THR:HG21	1.86	0.58
3:X:153:ALA:HB2	3:X:208:ILE:HB	1.85	0.58
3:e:105:LEU:HA	3:e:108:ILE:HB	1.86	0.58
1:O:45:MET:HA	1:O:45:MET:HE3	1.85	0.57
3:P:96:LEU:O	3:P:100:ILE:HG12	2.03	0.57
3:a:247:PHE:HD1	3:a:316:VAL:HG12	1.68	0.57
3:M:189:ASP:OD1	3:M:190:GLN:N	2.36	0.57
3:S:144:THR:HG22	3:S:177:ARG:HD2	1.86	0.57
1:f:36:ASP:OD2	1:v:23:ASN:ND2	2.36	0.57
3:i:10:SER:N	3:q:47:SER:OG	2.36	0.57
2:C:661:ASN:HA	2:D:666:LEU:HD11	1.85	0.57
3:R:192:VAL:HG21	3:b:187:ALA:HB3	1.87	0.57
3:Z:238:TYR:O	3:Z:242:LYS:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:356:ASN:OD1	3:i:357:LYS:N	2.37	0.57
2:A:629:ALA:HB2	2:B:631:GLN:OE1	2.04	0.57
3:U:344:THR:HB	3:U:347:GLN:HG2	1.87	0.57
3:Z:86:TYR:HB3	3:Z:405:LEU:HD23	1.87	0.57
3:d:102:LEU:CD2	3:j:5:LEU:CD1	2.82	0.57
3:e:220:THR:HG23	3:e:348:THR:HB	1.87	0.57
3:k:15:LYS:HD2	1:r:142:SER:HB2	1.84	0.57
2:J:215:TRP:HE1	1:v:141:THR:HA	1.70	0.57
2:K:5:LEU:HA	2:K:8:LYS:HE2	1.87	0.57
3:M:51:LYS:NZ	3:Z:8:ASN:OD1	2.30	0.57
3:Z:106:GLU:N	3:Z:106:GLU:OE1	2.37	0.57
2:L:387:VAL:HB	2:L:396:ALA:HB3	1.86	0.57
1:r:51:ASN:HB3	1:r:52:PRO:HD3	1.86	0.57
3:R:61:THR:HG21	3:R:65:ASP:H	1.69	0.57
1:r:45:MET:HG2	1:r:57:TYR:CG	2.38	0.57
3:u:113:ARG:HD3	3:u:378:ALA:HB1	1.86	0.57
2:B:636:LYS:HZ3	2:C:642:ALA:H	1.51	0.57
2:J:53:LYS:HZ2	2:J:56:GLU:HA	1.70	0.57
3:c:119:ASP:OD2	3:k:58:SER:OG	2.21	0.57
1:n:51:ASN:HB3	1:n:52:PRO:HD3	1.85	0.57
2:J:255:ASP:OD1	2:J:256:SER:N	2.37	0.57
2:L:12:ILE:HD12	2:L:230:TYR:CE2	2.39	0.57
2:L:313:GLY:O	2:L:463:ASN:ND2	2.38	0.57
3:t:331:ARG:NH2	3:t:334:GLU:OE2	2.37	0.57
2:D:229:LYS:HG2	2:D:288:VAL:HG22	1.87	0.57
3:O:60:ARG:NH1	3:s:123:GLU:OE2	2.33	0.57
1:h:16:ARG:NH2	1:w:40:ASP:OD2	2.38	0.57
3:i:11:GLN:HG3	1:v:150:LEU:HD13	1.85	0.57
2:E:255:ASP:OD1	2:E:256:SER:N	2.36	0.56
2:A:254:TYR:CZ	2:A:518:LEU:HD23	2.39	0.56
3:d:98:GLU:HA	3:d:102:LEU:HB2	1.87	0.56
3:q:92:GLU:HB3	3:q:399:LYS:HB3	1.86	0.56
3:y:389:LYS:HG2	3:y:400:MET:HG2	1.86	0.56
1:0:125:ARG:HH12	2:K:62:PRO:HD3	1.70	0.56
2:A:346:ALA:HA	2:B:416:LEU:HD11	1.88	0.56
2:A:410:ASN:HB3	2:L:406:PRO:HB2	1.86	0.56
2:B:362:GLU:OE2	1:n:108:ARG:NH2	2.38	0.56
2:C:233:VAL:HG12	2:C:284:VAL:HG22	1.86	0.56
2:G:510:ARG:H	2:G:510:ARG:HD3	1.71	0.56
2:I:668:GLN:OE1	2:J:670:ARG:NH1	2.38	0.56
1:w:75:PRO:HB2	1:w:77:LYS:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:TYR:CE1	2:B:232:GLU:HG3	2.40	0.56
2:F:586:ASN:HA	2:F:589:LEU:HD12	1.88	0.56
2:K:114:GLU:OE2	2:K:154:ARG:NH2	2.38	0.56
3:Q:98:GLU:HA	3:Q:102:LEU:HB2	1.87	0.56
3:Z:367:LEU:HD21	3:Z:405:LEU:HD12	1.87	0.56
3:i:331:ARG:NH2	3:i:334:GLU:OE2	2.37	0.56
1:x:51:ASN:HB3	1:x:52:PRO:HD3	1.86	0.56
1:z:42:GLU:HG3	1:z:66:PRO:HG2	1.88	0.56
2:L:488:GLU:HA	2:L:510:ARG:HD3	1.87	0.56
3:T:90:ALA:O	3:d:72:ASN:ND2	2.35	0.56
3:a:112:VAL:HG23	3:a:113:ARG:HD2	1.88	0.56
2:H:657:GLU:HG2	2:H:661:ASN:HD21	1.70	0.56
2:K:486:GLU:HB3	2:K:510:ARG:CZ	2.36	0.56
3:O:98:GLU:HA	3:O:102:LEU:HB2	1.88	0.56
3:e:324:PRO:O	3:e:327:ASN:ND2	2.39	0.56
3:m:124:LEU:HG	3:m:128:MET:HE2	1.86	0.56
2:B:599:GLU:HG2	2:B:600:LYS:N	2.21	0.56
2:E:115:THR:HG21	2:E:156:ALA:HB1	1.88	0.56
2:E:589:LEU:HD23	2:E:594:ALA:HB3	1.88	0.56
2:E:603:GLN:HG3	2:E:604:ILE:HG12	1.88	0.56
2:I:365:ARG:O	2:I:385:ARG:NH1	2.35	0.56
2:J:407:ALA:HB3	2:K:410:ASN:HD22	1.71	0.56
2:K:661:ASN:HA	2:L:666:LEU:HD11	1.87	0.56
3:P:267:GLN:HG2	3:P:342:VAL:HB	1.88	0.56
3:a:124:LEU:HG	3:a:128:MET:HE2	1.86	0.56
3:e:107:GLU:OE1	3:j:54:HIS:ND1	2.28	0.56
2:A:247:ILE:HG22	2:A:248:THR:HG23	1.88	0.56
2:A:347:ASP:OD1	2:K:378:ARG:NH2	2.39	0.56
2:E:218:ASN:O	2:E:219:TRP:HB2	2.06	0.56
1:f:141:THR:HG22	1:f:143:ASP:H	1.71	0.56
3:l:52:ARG:NH1	3:l:78:LYS:O	2.40	0.56
1:z:5:LEU:HD11	1:z:10:ILE:HG13	1.88	0.56
2:F:241:ILE:HG22	2:F:275:ALA:HB1	1.88	0.55
3:l:86:TYR:HB3	3:l:88:THR:HG23	1.88	0.55
1:p:3:THR:OG1	1:p:4:VAL:N	2.34	0.55
3:g:96:LEU:O	3:g:100:ILE:HG13	2.07	0.55
1:0:101:GLN:NE2	1:0:105:ASN:OD1	2.40	0.55
2:E:255:ASP:OD2	2:E:283:ARG:NH2	2.38	0.55
2:J:589:LEU:HD23	2:J:594:ALA:HB3	1.88	0.55
2:K:636:LYS:NZ	2:L:637:ALA:O	2.32	0.55
3:e:105:LEU:HA	3:e:108:ILE:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:120:ALA:HA	2:H:159:PRO:HB3	1.88	0.55
3:U:344:THR:HG22	3:U:345:ALA:H	1.71	0.55
3:W:140:ASN:OD1	3:W:347:GLN:NE2	2.39	0.55
3:j:189:ASP:OD1	3:j:190:GLN:N	2.39	0.55
2:F:120:ALA:HA	2:F:159:PRO:HB3	1.87	0.55
3:P:100:ILE:HG13	3:P:101:LYS:HG3	1.88	0.55
3:T:238:TYR:O	3:T:242:LYS:HB3	2.06	0.55
3:s:277:GLN:HB3	3:s:280:THR:HG22	1.89	0.55
2:B:27:ARG:O	2:B:31:ILE:HG13	2.07	0.55
2:C:378:ARG:NH1	1:z:124:ARG:O	2.40	0.55
2:J:54:LEU:HD23	2:J:59:GLU:HG3	1.89	0.55
2:L:111:ASP:HA	2:L:154:ARG:HH12	1.72	0.55
3:M:96:LEU:O	3:M:100:ILE:HG12	2.07	0.55
3:O:401:ARG:NH1	3:b:396:ASN:OD1	2.36	0.55
1:l:118:LEU:HD23	2:L:365:ARG:HH21	1.71	0.55
2:G:643:GLN:HA	2:G:646:ILE:HD12	1.89	0.55
2:J:628:VAL:HA	2:J:631:GLN:HG2	1.87	0.55
3:R:140:ASN:OD1	3:R:344:THR:OG1	2.24	0.55
3:Z:123:GLU:OE2	3:e:60:ARG:NH2	2.40	0.55
3:d:103:ASN:OD1	3:d:103:ASN:N	2.39	0.55
2:B:174:LYS:O	2:B:315:ARG:NH2	2.40	0.55
3:e:52:ARG:NH1	3:e:78:LYS:O	2.39	0.55
2:D:35:ARG:NH2	2:E:319:ASP:OD2	2.40	0.54
2:I:336:ARG:NH1	1:f:145:TYR:OH	2.39	0.54
3:N:209:ARG:NH1	3:N:209:ARG:HB3	2.23	0.54
3:Q:317:PRO:HA	3:Q:329:VAL:HG21	1.90	0.54
3:T:104:GLN:OE1	3:d:51:LYS:NZ	2.40	0.54
3:a:238:TYR:O	3:a:242:LYS:HB3	2.07	0.54
3:c:173:TRP:NE1	3:k:158:ASP:OD2	2.37	0.54
2:F:10:GLU:O	2:F:14:LEU:HG	2.08	0.54
2:L:120:ALA:HA	2:L:159:PRO:HB3	1.89	0.54
3:g:10:SER:N	3:m:47:SER:HG	2.05	0.54
3:g:316:VAL:HG23	3:g:318:ILE:HG13	1.88	0.54
1:O:139:VAL:HG12	2:L:215:TRP:HE1	1.73	0.54
2:E:86:THR:HG22	2:E:87:VAL:H	1.72	0.54
2:L:57:GLN:HG3	1:r:124:ARG:HH12	1.72	0.54
2:L:621:VAL:O	2:L:625:ALA:CB	2.50	0.54
3:V:153:ALA:HB2	3:V:208:ILE:HB	1.89	0.54
2:A:642:ALA:N	2:L:636:LYS:HZ1	2.05	0.54
2:B:94:ARG:NH1	2:B:95:GLU:OE2	2.41	0.54
2:K:657:GLU:HG2	2:K:661:ASN:HD21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:316:VAL:HG23	3:M:318:ILE:HG13	1.89	0.54
3:s:81:GLY:HA3	3:s:409:VAL:HG22	1.89	0.54
2:D:120:ALA:HA	2:D:159:PRO:HB3	1.89	0.54
2:E:57:GLN:HG3	1:z:124:ARG:NH2	2.22	0.54
3:W:316:VAL:HG23	3:W:318:ILE:HG13	1.90	0.54
2:A:625:ALA:HB3	2:B:627:MET:CE	2.37	0.54
2:C:212:MET:HA	2:C:212:MET:HE3	1.90	0.54
3:U:278:GLN:O	3:U:281:LYS:NZ	2.41	0.54
3:X:129:MET:HB2	3:X:418:GLN:HE21	1.72	0.54
3:c:238:TYR:O	3:c:242:LYS:HB3	2.07	0.54
3:d:144:THR:HG22	3:d:177:ARG:HD2	1.89	0.54
3:o:96:LEU:O	3:o:100:ILE:HG12	2.08	0.54
1:w:100:PRO:HA	1:w:103:LEU:HD12	1.90	0.54
2:A:53:LYS:NZ	2:A:56:GLU:HA	2.23	0.54
2:A:222:ALA:HB2	3:k:377:VAL:HG21	1.89	0.54
2:A:599:GLU:HG2	2:A:600:LYS:N	2.22	0.54
2:B:114:GLU:OE1	2:B:154:ARG:NH1	2.36	0.54
3:e:111:PRO:HG2	3:j:56:PHE:HE2	1.73	0.54
3:i:189:ASP:OD1	3:i:190:GLN:N	2.40	0.54
3:l:189:ASP:OD1	3:l:190:GLN:N	2.40	0.54
3:s:98:GLU:HA	3:s:102:LEU:HB2	1.89	0.54
3:O:182:GLN:HE22	3:O:202:PRO:HD3	1.72	0.54
3:e:233:GLN:HG3	3:e:334:GLU:HA	1.89	0.54
2:F:596:PRO:HB2	2:F:602:GLN:HG2	1.89	0.54
3:N:96:LEU:O	3:N:100:ILE:HG12	2.07	0.54
3:m:238:TYR:O	3:m:242:LYS:HB3	2.08	0.54
1:w:45:MET:HE1	1:w:55:ILE:HG21	1.90	0.54
2:C:244:ARG:NH1	2:C:250:GLU:OE1	2.41	0.54
2:F:579:ASP:OD1	2:F:580:PHE:N	2.40	0.54
2:D:551:LEU:HD11	2:D:561:ARG:HG3	1.90	0.53
2:E:193:GLU:OE2	2:F:18:ARG:NH2	2.41	0.53
2:K:215:TRP:CG	1:x:139:VAL:HG23	2.43	0.53
3:M:180:ASP:O	3:M:183:THR:OG1	2.26	0.53
3:j:280:THR:HG22	3:j:282:GLN:HG2	1.89	0.53
2:F:229:LYS:HG2	2:F:288:VAL:HG22	1.90	0.53
3:S:96:LEU:O	3:S:100:ILE:HG12	2.08	0.53
1:h:113:LEU:O	1:h:117:THR:HG22	2.08	0.53
3:i:95:GLN:HG2	3:i:96:LEU:HD22	1.91	0.53
3:Q:412:ASN:HB3	3:Q:415:MET:HE3	1.90	0.53
2:E:507:VAL:HG13	2:E:508:VAL:HG13	1.90	0.53
2:J:247:ILE:HG22	2:J:248:THR:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:140:ASN:OD1	3:S:344:THR:OG1	2.26	0.53
3:V:337:ASP:OD1	3:V:338:ALA:N	2.41	0.53
3:g:46:ASP:HB3	3:q:100:ILE:HD12	1.91	0.53
3:l:111:PRO:HG2	3:u:56:PHE:HE2	1.74	0.53
2:C:75:ARG:O	2:C:79:GLU:HG2	2.09	0.53
2:E:75:ARG:NH2	2:E:79:GLU:OE1	2.42	0.53
2:I:241:ILE:N	2:I:254:TYR:O	2.35	0.53
2:K:53:LYS:HD2	2:K:56:GLU:HA	1.91	0.53
2:K:174:LYS:O	2:K:315:ARG:NH2	2.41	0.53
3:O:63:THR:O	1:x:159:ASN:ND2	2.41	0.53
3:Q:22:MET:SD	3:a:162:ASN:ND2	2.82	0.53
3:Q:104:GLN:O	3:Q:108:ILE:HD12	2.08	0.53
3:R:221:GLN:NE2	3:R:343:GLY:HA3	2.24	0.53
2:A:259:VAL:HG12	2:A:261:ASP:H	1.73	0.53
2:A:489:VAL:O	2:A:511:GLN:NE2	2.38	0.53
2:B:5:LEU:HA	2:B:8:LYS:HE2	1.91	0.53
2:K:46:GLY:HA2	2:K:216:GLU:HG2	1.89	0.53
3:S:66:ILE:HD11	3:W:88:THR:HG21	1.90	0.53
2:E:120:ALA:HA	2:E:159:PRO:HB3	1.90	0.53
2:I:210:THR:O	2:I:211:SER:C	2.51	0.53
2:K:618:PRO:HA	2:K:621:VAL:HG12	1.89	0.53
2:L:247:ILE:HG22	2:L:248:THR:HG23	1.91	0.53
3:R:111:PRO:HG2	3:b:56:PHE:CE2	2.40	0.53
3:d:31:VAL:HG11	3:d:124:LEU:HD21	1.91	0.53
3:d:238:TYR:O	3:d:242:LYS:HB3	2.08	0.53
3:o:64:GLY:O	1:p:158:PRO:HD2	2.09	0.53
3:y:111:PRO:HA	3:y:114:GLN:HG3	1.91	0.53
3:Q:238:TYR:O	3:Q:242:LYS:HB3	2.09	0.53
3:l:91:VAL:HG12	3:u:72:ASN:HB2	1.91	0.53
1:r:50:ILE:HG13	1:r:51:ASN:N	2.23	0.53
3:u:412:ASN:HD22	3:u:415:MET:HE3	1.73	0.53
3:y:241:VAL:HG11	3:y:316:VAL:HG21	1.89	0.53
2:B:115:THR:HG21	2:B:156:ALA:HB1	1.91	0.53
2:B:313:GLY:O	2:B:463:ASN:ND2	2.40	0.53
2:F:539:ARG:NE	2:G:93:ASP:OD2	2.41	0.53
2:H:217:TYR:N	3:g:104:GLN:OE1	2.40	0.53
3:Q:173:TRP:NE1	3:a:158:ASP:OD2	2.42	0.53
3:e:267:GLN:HB2	3:e:342:VAL:HG22	1.90	0.53
3:k:219:ARG:NH1	3:k:221:GLN:OE1	2.41	0.53
3:u:124:LEU:HD22	3:u:362:LEU:HD22	1.91	0.53
1:l:44:MET:HE1	1:l:86:LEU:CA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:71:THR:OG1	2:E:72:GLU:OE2	2.26	0.53
2:I:599:GLU:HG2	2:I:600:LYS:N	2.23	0.53
3:O:180:ASP:O	3:O:183:THR:OG1	2.26	0.53
3:i:273:THR:HG21	3:i:333:VAL:HG22	1.91	0.53
3:l:95:GLN:HG2	3:l:96:LEU:HD22	1.90	0.53
3:m:233:GLN:NE2	3:m:234:PRO:O	2.42	0.53
1:0:89:ARG:O	1:r:17:LYS:NZ	2.42	0.52
2:A:634:ALA:HA	2:L:633:GLU:OE2	2.09	0.52
1:0:48:TRP:CZ2	1:0:85:GLN:HG3	2.44	0.52
2:E:407:ALA:HB3	2:F:410:ASN:HD22	1.74	0.52
2:F:599:GLU:HG2	2:F:600:LYS:N	2.24	0.52
2:H:81:ARG:HD3	2:I:462:ASP:OD2	2.09	0.52
2:J:53:LYS:NZ	2:J:56:GLU:HA	2.24	0.52
3:i:78:LYS:HG3	3:s:7:SER:HB3	1.90	0.52
3:t:209:ARG:NH1	3:t:209:ARG:HB2	2.23	0.52
3:u:153:ALA:HB2	3:u:208:ILE:HB	1.90	0.52
2:G:114:GLU:HB2	2:G:154:ARG:HH21	1.73	0.52
2:I:115:THR:HG21	2:I:157:ILE:H	1.72	0.52
2:L:137:ARG:NH2	2:L:158:GLU:OE2	2.42	0.52
1:h:50:ILE:HG13	1:h:51:ASN:N	2.24	0.52
2:E:618:PRO:HA	2:E:621:VAL:HG12	1.91	0.52
2:F:247:ILE:HG22	2:F:248:THR:HG23	1.92	0.52
2:G:187:MET:HG2	2:G:228:ALA:HB2	1.91	0.52
2:K:599:GLU:HG2	2:K:600:LYS:N	2.24	0.52
3:N:209:ARG:HB3	3:N:209:ARG:HH11	1.74	0.52
3:O:113:ARG:HH12	3:O:378:ALA:HB3	1.74	0.52
3:Z:369:LYS:NZ	3:Z:373:ILE:O	2.36	0.52
1:0:48:TRP:HZ2	1:0:85:GLN:HG3	1.74	0.52
2:F:586:ASN:O	2:F:590:ILE:HG12	2.09	0.52
3:c:124:LEU:HD12	3:c:362:LEU:HD13	1.92	0.52
3:o:209:ARG:NH1	3:o:211:LEU:HD21	2.24	0.52
2:A:35:ARG:HG3	2:A:39:VAL:HG21	1.92	0.52
2:B:241:ILE:HD12	2:B:275:ALA:HB1	1.91	0.52
2:E:254:TYR:CZ	2:E:518:LEU:HD23	2.45	0.52
2:F:313:GLY:O	2:F:463:ASN:ND2	2.42	0.52
2:G:365:ARG:HG2	1:f:114:MET:HE1	1.91	0.52
2:I:618:PRO:HA	2:I:621:VAL:HG12	1.90	0.52
2:K:578:ASP:O	2:K:582:GLU:HG2	2.09	0.52
2:K:613:GLN:NE2	2:K:613:GLN:O	2.42	0.52
2:L:244:ARG:HA	2:L:250:GLU:O	2.10	0.52
3:M:136:LEU:HD11	3:M:155:PHE:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:10:SER:N	3:m:47:SER:OG	2.42	0.52
3:k:22:MET:SD	3:s:162:ASN:ND2	2.74	0.52
3:u:344:THR:HG22	3:u:345:ALA:H	1.75	0.52
2:B:423:ASP:HA	2:B:426:GLU:HG2	1.91	0.52
2:E:668:GLN:OE1	2:F:670:ARG:NH1	2.41	0.52
2:J:56:GLU:O	2:J:57:GLN:NE2	2.43	0.52
2:K:247:ILE:HG22	2:K:248:THR:HG23	1.92	0.52
2:L:618:PRO:HA	2:L:621:VAL:HG12	1.92	0.52
3:i:221:GLN:HG2	3:i:349:MET:HE1	1.92	0.52
2:A:120:ALA:HA	2:A:159:PRO:HB3	1.92	0.52
2:A:606:GLN:O	2:A:610:MET:HG2	2.09	0.52
2:C:254:TYR:CZ	2:C:518:LEU:HD23	2.45	0.52
2:C:318:ILE:HB	2:C:323:ARG:HE	1.74	0.52
3:b:156:LEU:HD12	3:b:161:VAL:HG21	1.91	0.52
3:b:231:LYS:HB2	3:b:252:THR:HG23	1.92	0.52
3:i:14:LEU:HD21	3:i:16:LYS:HE3	1.92	0.52
1:n:18:PHE:HB2	1:n:87:LEU:HD11	1.92	0.52
1:1:100:PRO:HA	1:1:103:LEU:HD12	1.92	0.52
2:A:114:GLU:HB2	2:A:154:ARG:NH2	2.25	0.52
2:G:618:PRO:HA	2:G:621:VAL:HG12	1.91	0.52
2:J:239:ASP:O	2:J:256:SER:OG	2.21	0.52
2:J:613:GLN:O	2:J:613:GLN:NE2	2.43	0.52
3:N:57:SER:HB3	3:N:325:GLN:HG3	1.90	0.52
3:P:231:LYS:HB2	3:P:250:THR:HG23	1.90	0.52
3:R:219:ARG:NH2	3:R:221:GLN:OE1	2.43	0.52
3:Z:165:GLU:H	3:Z:357:LYS:HB2	1.75	0.52
1:h:41:LEU:HD12	1:h:86:LEU:HD22	1.91	0.52
3:j:153:ALA:HB2	3:j:208:ILE:HB	1.90	0.52
3:s:344:THR:HB	3:s:347:GLN:HB2	1.92	0.52
1:w:51:ASN:HB3	1:w:52:PRO:HD3	1.91	0.52
1:1:22:SER:OG	1:1:23:ASN:N	2.43	0.52
2:A:332:MET:HE3	2:A:336:ARG:HH21	1.73	0.52
2:C:187:MET:HG2	2:C:228:ALA:HB2	1.92	0.52
2:D:386:GLU:OE2	2:D:388:ARG:NH1	2.43	0.52
2:H:488:GLU:OE1	2:H:488:GLU:N	2.42	0.52
3:W:189:ASP:OD1	3:W:190:GLN:N	2.43	0.52
3:j:221:GLN:HE21	3:j:343:GLY:HA3	1.75	0.52
2:C:618:PRO:HA	2:C:621:VAL:HG12	1.92	0.51
3:a:180:ASP:O	3:a:183:THR:OG1	2.28	0.51
3:e:319:TYR:CD1	3:e:332:GLN:HB2	2.44	0.51
3:j:278:GLN:O	3:j:281:LYS:NZ	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:661:ASN:HA	2:C:666:LEU:HD11	1.91	0.51
2:D:628:VAL:HA	2:D:631:GLN:HG2	1.92	0.51
2:L:365:ARG:O	2:L:385:ARG:NH1	2.41	0.51
2:L:551:LEU:HD13	2:L:564:ILE:HG21	1.91	0.51
3:O:57:SER:HB3	3:O:325:GLN:HG3	1.92	0.51
3:Q:219:ARG:O	3:Q:348:THR:OG1	2.23	0.51
3:l:219:ARG:NH1	3:l:221:GLN:OE1	2.43	0.51
3:m:27:LEU:HD22	3:m:128:MET:HE1	1.92	0.51
2:E:657:GLU:OE2	2:F:659:GLN:HA	2.11	0.51
2:G:662:THR:O	2:G:666:LEU:HG	2.10	0.51
2:H:618:PRO:HA	2:H:621:VAL:HG12	1.93	0.51
2:I:313:GLY:O	2:I:463:ASN:ND2	2.44	0.51
2:K:73:LEU:HD22	2:K:328:ILE:HD11	1.93	0.51
3:Z:170:MET:HE3	3:Z:210:ALA:HB1	1.92	0.51
3:d:156:LEU:HD12	3:d:161:VAL:HG21	1.92	0.51
3:k:238:TYR:O	3:k:242:LYS:HB3	2.10	0.51
3:m:231:LYS:HB2	3:m:252:THR:HG23	1.92	0.51
3:t:231:LYS:HB3	3:t:250:THR:HG23	1.92	0.51
2:H:622:LEU:HD23	2:I:627:MET:HE3	1.91	0.51
2:K:58:PHE:CE1	1:x:151:PRO:HG3	2.45	0.51
2:K:172:ASP:OD2	2:K:173:ALA:N	2.44	0.51
3:S:219:ARG:O	3:S:348:THR:OG1	2.21	0.51
3:c:349:MET:HE2	3:c:351:PRO:HG3	1.91	0.51
1:l:48:TRP:O	1:l:52:PRO:HD2	2.10	0.51
2:E:68:LYS:HE3	2:F:426:GLU:OE2	2.11	0.51
2:F:218:ASN:HB2	1:w:140:PHE:HE1	1.75	0.51
2:F:589:LEU:HD22	2:F:596:PRO:HG3	1.92	0.51
2:I:487:ARG:O	2:I:510:ARG:NH2	2.42	0.51
2:J:72:GLU:HG3	2:J:428:THR:HB	1.91	0.51
3:X:23:SER:OG	3:X:24:ASP:N	2.44	0.51
3:m:124:LEU:HD22	3:m:362:LEU:HD22	1.93	0.51
3:o:16:LYS:HE3	3:y:35:LEU:HD21	1.92	0.51
3:o:180:ASP:O	3:o:183:THR:OG1	2.28	0.51
2:C:640:GLU:O	2:C:643:GLN:HB3	2.10	0.51
2:D:187:MET:HG2	2:D:228:ALA:HB2	1.92	0.51
2:L:53:LYS:HD2	2:L:56:GLU:HA	1.91	0.51
3:Q:91:VAL:HG12	3:a:72:ASN:HB2	1.91	0.51
3:Q:135:SER:HB3	3:Q:294:THR:HG21	1.91	0.51
3:T:108:ILE:HD12	3:d:54:HIS:CE1	2.46	0.51
3:u:185:LEU:HD12	3:u:191:LEU:HD22	1.92	0.51
2:A:587:GLN:HA	2:A:590:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:565:GLN:O	2:D:569:LEU:HG	2.09	0.51
2:H:9:HIS:O	2:H:13:MET:HG2	2.10	0.51
2:J:115:THR:HG22	2:J:116:ASP:H	1.76	0.51
2:J:216:GLU:OE1	1:v:144:ARG:NH2	2.44	0.51
1:p:50:ILE:HG13	1:p:51:ASN:N	2.26	0.51
2:F:190:LEU:HD22	2:F:194:LYS:HD3	1.92	0.51
2:H:115:THR:HG21	2:H:156:ALA:HB1	1.93	0.51
2:J:137:ARG:HG2	2:J:139:THR:HG23	1.91	0.51
2:J:537:THR:HG21	2:K:531:ASP:HB2	1.92	0.51
2:F:207:LEU:HB3	2:F:225:ILE:HG23	1.93	0.51
2:J:60:LYS:O	1:x:146:TYR:OH	2.20	0.51
2:L:599:GLU:HG2	2:L:600:LYS:N	2.24	0.51
3:O:102:LEU:HD13	3:O:105:LEU:HD13	1.92	0.51
3:Q:96:LEU:O	3:Q:100:ILE:HG12	2.11	0.51
3:U:329:VAL:HG12	3:U:331:ARG:H	1.75	0.51
3:V:170:MET:HE2	3:V:210:ALA:HB1	1.92	0.51
3:e:162:ASN:OD1	3:e:163:GLU:N	2.44	0.51
1:l:125:ARG:HH21	2:A:62:PRO:HD3	1.76	0.51
3:S:104:GLN:OE1	3:c:51:LYS:NZ	2.41	0.51
2:D:313:GLY:O	2:D:463:ASN:ND2	2.42	0.50
2:G:67:ASN:HB3	2:H:330:LYS:HD2	1.92	0.50
2:L:337:LEU:O	2:L:341:GLN:HG2	2.11	0.50
3:R:173:TRP:NE1	3:b:158:ASP:OD2	2.43	0.50
3:T:367:LEU:HD21	3:T:405:LEU:HD12	1.93	0.50
3:y:23:SER:OG	3:y:24:ASP:N	2.43	0.50
2:G:239:ASP:O	2:G:256:SER:OG	2.26	0.50
3:R:139:PRO:HB3	3:R:349:MET:SD	2.52	0.50
3:b:173:TRP:NE1	3:i:158:ASP:OD2	2.44	0.50
1:h:87:LEU:O	1:h:91:LEU:HG	2.11	0.50
3:j:27:LEU:O	3:j:31:VAL:HG23	2.11	0.50
3:t:187:ALA:HB3	3:y:192:VAL:HG21	1.93	0.50
1:w:13:PHE:HE2	1:w:83:GLY:HA3	1.76	0.50
2:B:625:ALA:HB1	2:B:628:VAL:HG23	1.93	0.50
2:C:625:ALA:HB3	2:D:627:MET:HE3	1.92	0.50
2:F:607:GLN:HA	2:F:610:MET:HG3	1.92	0.50
2:G:75:ARG:HH22	2:H:450:MET:HE3	1.77	0.50
2:J:661:ASN:HA	2:K:666:LEU:HD11	1.93	0.50
3:O:162:ASN:HD21	3:s:22:MET:HE3	1.76	0.50
3:P:49:SER:HB2	3:u:13:VAL:HG22	1.94	0.50
3:Z:173:TRP:NE1	3:e:158:ASP:OD2	2.44	0.50
3:i:37:ALA:N	3:i:39:GLU:OE1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:l:26:VAL:HG23	3:l:27:LEU:HD22	1.93	0.50
3:m:162:ASN:OD1	3:m:163:GLU:N	2.42	0.50
2:B:265:GLU:HG3	2:B:267:ALA:H	1.76	0.50
2:D:586:ASN:O	2:D:590:ILE:HG12	2.11	0.50
2:E:516:VAL:O	2:E:518:LEU:HD12	2.10	0.50
2:F:365:ARG:HH12	1:h:117:THR:HG23	1.76	0.50
2:I:531:ASP:OD1	2:I:532:VAL:N	2.39	0.50
3:X:91:VAL:HG23	3:X:400:MET:HB2	1.92	0.50
3:s:369:LYS:HE2	3:s:370:LEU:O	2.11	0.50
2:A:490:ARG:HG3	2:A:509:ASP:HB2	1.93	0.50
2:E:35:ARG:HG3	2:E:39:VAL:HG21	1.92	0.50
3:O:63:THR:OG1	1:x:159:ASN:ND2	2.45	0.50
1:r:100:PRO:HA	1:r:103:LEU:HD12	1.93	0.50
2:C:27:ARG:NH1	2:C:164:SER:O	2.40	0.50
2:I:292:ASP:OD1	2:I:293:GLY:N	2.44	0.50
3:T:96:LEU:O	3:T:100:ILE:HG12	2.11	0.50
2:B:636:LYS:HZ3	2:C:642:ALA:N	2.10	0.50
2:C:637:ALA:HA	2:C:640:GLU:HB3	1.92	0.50
2:J:509:ASP:OD2	2:J:510:ARG:N	2.44	0.50
2:L:35:ARG:HG3	2:L:39:VAL:HG21	1.94	0.50
2:L:125:PHE:HB2	2:L:464:MET:HE2	1.94	0.50
3:e:267:GLN:HB2	3:e:342:VAL:CG2	2.42	0.50
1:p:157:ILE:N	1:p:158:PRO:HD3	2.26	0.50
1:r:138:ASP:OD1	1:r:139:VAL:N	2.45	0.50
1:l:50:ILE:HG13	1:l:51:ASN:N	2.27	0.50
2:I:628:VAL:HA	2:I:631:GLN:HG2	1.94	0.50
2:K:115:THR:HG21	2:K:157:ILE:H	1.77	0.50
3:O:41:ASN:H	3:O:44:THR:HG22	1.76	0.50
3:S:180:ASP:O	3:S:183:THR:HG22	2.12	0.50
3:S:316:VAL:HG23	3:S:318:ILE:HG13	1.94	0.50
3:T:344:THR:HG22	3:T:345:ALA:N	2.22	0.50
3:V:102:LEU:HB3	3:V:105:LEU:HD21	1.94	0.50
3:d:241:VAL:HG21	3:d:316:VAL:HG21	1.94	0.50
2:A:2:ALA:O	2:A:8:LYS:NZ	2.33	0.50
2:B:622:LEU:HG	2:C:627:MET:HE3	1.94	0.50
2:F:347:ASP:OD2	1:w:125:ARG:NH2	2.45	0.50
2:G:263:GLU:HG3	2:G:516:VAL:HB	1.94	0.50
2:I:239:ASP:O	2:I:256:SER:OG	2.25	0.50
3:g:370:LEU:HA	3:q:398:GLN:HE21	1.77	0.50
3:q:344:THR:HG22	3:q:345:ALA:H	1.76	0.50
1:z:45:MET:HA	1:z:48:TRP:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:385:ARG:NH2	1:p:115:THR:OG1	2.44	0.49
2:C:622:LEU:HG	2:D:627:MET:SD	2.52	0.49
2:D:92:GLY:H	2:D:97:SER:HB2	1.77	0.49
2:I:209:VAL:HG22	2:I:290:ASP:HA	1.94	0.49
3:N:113:ARG:H	3:N:113:ARG:HD2	1.77	0.49
3:j:100:ILE:HD12	3:l:46:ASP:HB3	1.94	0.49
3:q:324:PRO:O	3:q:327:ASN:ND2	2.45	0.49
2:D:600:LYS:HA	2:D:603:GLN:HE22	1.77	0.49
2:I:94:ARG:HG3	2:I:527:ASP:OD2	2.12	0.49
2:L:238:VAL:HG11	2:L:281:ARG:HD3	1.94	0.49
3:N:180:ASP:O	3:N:183:THR:OG1	2.29	0.49
3:N:401:ARG:NH1	3:a:393:GLY:O	2.46	0.49
3:O:96:LEU:O	3:O:100:ILE:HG12	2.12	0.49
3:Z:231:LYS:HB3	3:Z:250:THR:HG23	1.94	0.49
3:j:238:TYR:O	3:j:242:LYS:HB3	2.12	0.49
1:z:44:MET:HE2	1:z:89:ARG:HG3	1.94	0.49
2:A:100:LEU:O	2:A:104:LEU:HD23	2.12	0.49
2:A:488:GLU:HG2	2:A:488:GLU:O	2.11	0.49
2:C:387:VAL:HB	2:C:396:ALA:HB3	1.93	0.49
2:F:115:THR:HG21	2:F:156:ALA:HB1	1.95	0.49
2:F:375:ASN:O	1:h:126:ARG:NH1	2.46	0.49
2:J:599:GLU:HG2	2:J:600:LYS:N	2.27	0.49
3:Z:22:MET:SD	3:e:162:ASN:ND2	2.85	0.49
3:Z:123:GLU:OE1	3:Z:408:TYR:OH	2.27	0.49
1:f:139:VAL:HG23	1:f:140:PHE:CD1	2.47	0.49
1:h:18:PHE:HB2	1:h:87:LEU:HD11	1.93	0.49
3:k:96:LEU:O	3:k:100:ILE:HG13	2.12	0.49
3:m:295:ALA:HB3	3:m:313:LEU:HD23	1.94	0.49
2:A:273:GLU:OE1	2:A:274:VAL:HG12	2.12	0.49
2:B:73:LEU:O	2:B:77:ILE:HG12	2.12	0.49
2:B:556:PRO:HB3	2:C:555:LEU:HD11	1.93	0.49
2:C:551:LEU:HD21	2:C:564:ILE:HG21	1.95	0.49
2:G:661:ASN:HA	2:H:666:LEU:HD21	1.93	0.49
2:J:198:GLU:HG2	2:J:199:TYR:H	1.77	0.49
2:K:254:TYR:HE1	2:K:518:LEU:HB3	1.76	0.49
3:M:102:LEU:HD13	3:M:105:LEU:HD13	1.93	0.49
3:N:60:ARG:NH2	3:q:123:GLU:OE2	2.36	0.49
3:R:144:THR:HG22	3:R:177:ARG:HD2	1.94	0.49
3:U:277:GLN:HB3	3:U:280:THR:HG22	1.94	0.49
3:d:86:TYR:OH	3:l:63:THR:O	2.21	0.49
1:l:115:THR:HG21	2:K:385:ARG:HH21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:114:GLU:HB2	2:A:154:ARG:HH22	1.78	0.49
2:C:58:PHE:O	3:l:96:LEU:HD12	2.12	0.49
2:G:15:ARG:NH1	2:G:230:TYR:OH	2.45	0.49
2:L:652:GLN:HE21	2:L:656:MET:HE2	1.76	0.49
3:U:182:GLN:NE2	3:U:195:ALA:HB2	2.28	0.49
1:Y:45:MET:HG3	1:Y:57:TYR:CD1	2.47	0.49
3:a:401:ARG:HH12	3:g:66:ILE:HG13	1.78	0.49
3:e:119:ASP:OD2	3:j:58:SER:OG	2.23	0.49
3:i:23:SER:OG	3:i:24:ASP:N	2.45	0.49
3:j:369:LYS:HD3	3:j:370:LEU:O	2.12	0.49
3:m:23:SER:OG	3:m:24:ASP:N	2.45	0.49
1:n:136:LYS:O	1:n:136:LYS:HG2	2.12	0.49
3:y:153:ALA:HB2	3:y:208:ILE:HB	1.95	0.49
3:y:166:ASN:OD1	3:y:356:ASN:ND2	2.46	0.49
2:A:615:GLN:O	2:A:618:PRO:HD2	2.12	0.49
2:K:652:GLN:O	2:K:656:MET:HG2	2.12	0.49
3:Z:51:LYS:NZ	3:t:104:GLN:OE1	2.37	0.49
3:Z:221:GLN:NE2	3:Z:343:GLY:HA3	2.28	0.49
2:A:621:VAL:HA	2:A:624:GLN:HG2	1.94	0.49
2:E:653:GLN:O	2:E:656:MET:HG3	2.13	0.49
2:J:58:PHE:CD2	3:i:100:ILE:HA	2.47	0.49
2:K:49:ALA:HB2	3:s:371:HIS:HB3	1.95	0.49
2:K:621:VAL:HA	2:K:624:GLN:HE21	1.78	0.49
3:Z:162:ASN:HD22	3:t:22:MET:HE2	1.77	0.49
3:d:231:LYS:HG2	3:d:232:THR:HG23	1.93	0.49
3:i:111:PRO:HG2	3:q:56:PHE:HE2	1.77	0.49
3:o:98:GLU:HA	3:o:102:LEU:HB2	1.95	0.49
3:q:385:ILE:HG12	3:q:404:LEU:HD12	1.94	0.49
2:E:241:ILE:HG23	2:E:275:ALA:HB2	1.95	0.49
2:I:240:VAL:HA	2:I:255:ASP:HA	1.93	0.49
2:J:96:ALA:HB1	2:J:510:ARG:NH2	2.27	0.49
3:N:278:GLN:O	3:N:281:LYS:NZ	2.39	0.49
3:R:96:LEU:O	3:R:100:ILE:HG12	2.12	0.49
3:b:98:GLU:HA	3:b:102:LEU:HD12	1.94	0.49
1:f:24:ALA:HB2	1:h:32:GLN:HG2	1.95	0.49
2:G:115:THR:HG21	2:G:157:ILE:H	1.78	0.49
3:e:91:VAL:HG12	3:j:72:ASN:HB2	1.93	0.49
3:i:49:SER:HB3	3:i:80:THR:HG22	1.94	0.49
3:i:192:VAL:HG11	3:q:187:ALA:HB3	1.94	0.49
2:A:11:ARG:O	2:A:15:ARG:HG2	2.13	0.49
2:D:621:VAL:O	2:D:625:ALA:CB	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:595:LYS:O	2:F:595:LYS:HG2	2.12	0.49
2:F:598:ASN:HA	2:F:602:GLN:HG3	1.94	0.49
2:J:387:VAL:HB	2:J:396:ALA:HB3	1.94	0.49
3:e:231:LYS:HB3	3:e:250:THR:HG23	1.94	0.49
3:g:97:GLU:HA	3:g:100:ILE:HD12	1.95	0.49
3:m:311:VAL:HG13	3:m:313:LEU:HD11	1.95	0.49
2:C:378:ARG:HD2	1:z:125:ARG:NH1	2.28	0.48
2:D:180:ASP:OD1	2:D:180:ASP:N	2.42	0.48
2:E:531:ASP:OD1	2:E:532:VAL:N	2.41	0.48
2:G:573:ASP:OD1	2:H:90:ARG:NH2	2.46	0.48
2:J:617:ASN:HA	2:J:620:MET:HE3	1.95	0.48
2:K:2:ALA:O	2:K:8:LYS:NZ	2.46	0.48
3:i:319:TYR:CD1	3:i:332:GLN:HB2	2.47	0.48
3:t:96:LEU:O	3:t:100:ILE:HG12	2.12	0.48
2:B:58:PHE:HB3	3:u:44:THR:HG23	1.95	0.48
2:B:239:ASP:O	2:B:256:SER:OG	2.23	0.48
2:B:406:PRO:HB2	2:C:410:ASN:HB3	1.95	0.48
2:G:340:LEU:HD22	1:w:130:PRO:HD3	1.95	0.48
3:U:23:SER:OG	3:U:24:ASP:N	2.42	0.48
3:U:182:GLN:HE21	3:U:195:ALA:HB2	1.78	0.48
3:V:316:VAL:HG13	3:V:318:ILE:HG13	1.95	0.48
3:Z:177:ARG:HH22	3:e:287:GLY:HA3	1.78	0.48
3:i:57:SER:HB3	3:i:325:GLN:HB3	1.93	0.48
3:j:101:LYS:HB2	3:j:101:LYS:HE2	1.60	0.48
3:o:46:ASP:OD1	3:o:46:ASP:N	2.44	0.48
2:B:207:LEU:HD12	2:B:226:TYR:HD2	1.78	0.48
2:F:60:LYS:O	1:w:146:TYR:OH	2.25	0.48
2:I:603:GLN:HG3	2:I:604:ILE:HG12	1.93	0.48
3:M:250:THR:OG1	3:M:308:ASP:OD2	2.30	0.48
3:O:153:ALA:HB2	3:O:208:ILE:HB	1.94	0.48
3:R:94:GLN:HB3	3:R:96:LEU:HD23	1.95	0.48
3:T:129:MET:HG3	3:T:418:GLN:HE21	1.78	0.48
1:Y:101:GLN:NE2	1:Y:101:GLN:O	2.46	0.48
3:a:27:LEU:HD13	3:a:128:MET:HE1	1.96	0.48
3:b:241:VAL:HG11	3:b:316:VAL:HG21	1.95	0.48
3:k:153:ALA:HB2	3:k:208:ILE:HB	1.94	0.48
2:C:636:LYS:HD3	2:D:638:THR:HA	1.94	0.48
2:I:387:VAL:HB	2:I:396:ALA:HB3	1.95	0.48
3:N:229:THR:HG22	3:N:338:ALA:HA	1.94	0.48
3:V:165:GLU:OE2	3:V:167:TYR:OH	2.31	0.48
3:W:276:LEU:O	3:W:278:GLN:NE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:u:117:VAL:HG21	3:u:380:TYR:HD2	1.78	0.48
1:z:45:MET:HE2	1:z:57:TYR:HB2	1.94	0.48
2:B:77:ILE:HG22	2:B:81:ARG:HD2	1.95	0.48
2:D:622:LEU:HA	2:D:625:ALA:HB3	1.95	0.48
2:H:67:ASN:HB3	2:I:330:LYS:HD2	1.95	0.48
2:J:647:LYS:HE3	2:K:648:ALA:HA	1.96	0.48
3:a:86:TYR:HB2	3:a:404:LEU:O	2.14	0.48
3:c:179:ALA:O	3:c:183:THR:HG23	2.12	0.48
3:j:237:THR:OG1	3:j:320:ASP:OD1	2.23	0.48
1:p:87:LEU:O	1:p:91:LEU:HG	2.13	0.48
1:v:47:GLU:OE2	1:x:80:HIS:HB2	2.13	0.48
2:G:599:GLU:HG2	2:G:600:LYS:H	1.77	0.48
3:O:262:LEU:HD12	3:O:311:VAL:HG11	1.95	0.48
3:V:273:THR:OG1	3:V:331:ARG:NH1	2.47	0.48
1:1:124:ARG:NH1	2:A:57:GLN:HG3	2.28	0.48
2:B:329:ALA:HA	2:B:332:MET:HE3	1.95	0.48
2:C:162:ASP:O	2:C:166:SER:HB2	2.13	0.48
2:H:207:LEU:HB3	2:H:225:ILE:HG23	1.96	0.48
2:L:8:LYS:O	2:L:12:ILE:HG12	2.13	0.48
3:R:158:ASP:OD2	3:V:173:TRP:NE1	2.46	0.48
3:V:143:ILE:HD11	3:V:174:SER:HB3	1.96	0.48
3:d:173:TRP:NE1	3:l:158:ASP:OD2	2.46	0.48
3:l:229:THR:OG1	3:l:337:ASP:O	2.21	0.48
3:m:41:ASN:HB2	3:m:44:THR:HG22	1.95	0.48
2:B:2:ALA:HA	2:B:7:LYS:HE2	1.96	0.48
2:E:626:GLN:HA	2:F:627:MET:HG2	1.95	0.48
2:F:182:LEU:O	2:F:233:VAL:HG22	2.14	0.48
2:H:313:GLY:O	2:H:463:ASN:ND2	2.46	0.48
2:L:598:ASN:OD1	2:L:602:GLN:NE2	2.42	0.48
3:V:23:SER:OG	3:V:24:ASP:N	2.43	0.48
3:g:113:ARG:HD3	3:g:380:TYR:CD2	2.48	0.48
3:s:179:ALA:O	3:s:183:THR:HG23	2.14	0.48
2:A:217:TYR:O	3:k:104:GLN:NE2	2.47	0.48
2:E:487:ARG:HG3	2:E:489:VAL:HG23	1.94	0.48
2:J:604:ILE:HG13	2:J:605:VAL:N	2.28	0.48
3:O:316:VAL:HG13	3:O:318:ILE:HG13	1.96	0.48
3:R:389:LYS:HG2	3:R:400:MET:HG2	1.96	0.48
3:g:179:ALA:O	3:g:183:THR:HG23	2.14	0.48
3:q:124:LEU:HD22	3:q:362:LEU:HD22	1.95	0.48
1:x:28:ASP:OD1	1:x:29:VAL:N	2.47	0.48
1:1:158:PRO:HD2	3:P:64:GLY:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:490:ARG:HD2	2:B:509:ASP:HB2	1.94	0.48
2:D:664:TYR:CD2	2:E:666:LEU:HD22	2.48	0.48
2:E:597:ARG:HG3	2:E:599:GLU:OE1	2.13	0.48
3:O:51:LYS:NZ	3:b:8:ASN:OD1	2.33	0.48
3:W:106:GLU:HG2	3:W:107:GLU:OE1	2.13	0.48
3:c:86:TYR:HB2	3:c:404:LEU:O	2.14	0.48
3:d:86:TYR:HB2	3:d:404:LEU:O	2.14	0.48
3:m:25:LEU:HD21	3:m:117:VAL:HG11	1.96	0.48
3:m:180:ASP:O	3:m:183:THR:OG1	2.32	0.48
1:r:86:LEU:HG	1:r:90:MET:HE2	1.96	0.48
1:z:45:MET:HE1	1:z:55:ILE:HD11	1.96	0.48
2:A:621:VAL:O	2:A:625:ALA:N	2.47	0.47
2:F:309:ILE:HG21	2:F:471:ALA:HB2	1.95	0.47
3:O:365:ILE:HD11	3:O:405:LEU:HD23	1.96	0.47
3:O:370:LEU:HA	3:b:398:GLN:HE21	1.79	0.47
3:Q:188:SER:OG	3:Q:191:LEU:HB3	2.14	0.47
3:m:3:ASN:HB3	3:m:5:LEU:HD22	1.96	0.47
2:K:628:VAL:HA	2:K:631:GLN:HG2	1.96	0.47
3:O:40:ILE:HA	3:O:44:THR:HG21	1.95	0.47
3:d:102:LEU:CD2	3:j:5:LEU:HD12	2.44	0.47
1:f:158:PRO:CA	3:q:370:LEU:HD21	2.43	0.47
1:p:29:VAL:HG13	1:p:30:GLU:N	2.29	0.47
1:v:86:LEU:O	1:v:90:MET:HG2	2.14	0.47
1:z:57:TYR:HD2	1:z:74:LEU:HD11	1.77	0.47
2:F:207:LEU:H	2:F:207:LEU:HD23	1.79	0.47
2:I:35:ARG:HG3	2:I:39:VAL:HG21	1.95	0.47
3:P:153:ALA:HB2	3:P:208:ILE:HB	1.95	0.47
3:Q:36:LEU:HD23	3:Q:36:LEU:O	2.14	0.47
3:Q:179:ALA:O	3:Q:183:THR:HG23	2.14	0.47
3:S:247:PHE:CD1	3:S:316:VAL:HG12	2.50	0.47
3:T:22:MET:HG2	3:d:162:ASN:HD22	1.78	0.47
3:k:14:LEU:HG	3:k:16:LYS:H	1.79	0.47
3:k:27:LEU:HD22	3:k:128:MET:HE1	1.95	0.47
1:n:40:ASP:OD2	1:z:17:LYS:NZ	2.41	0.47
3:o:57:SER:HB3	3:o:325:GLN:HG3	1.95	0.47
3:q:422:ASN:C	3:q:422:ASN:HD22	2.20	0.47
3:s:26:VAL:O	3:s:30:THR:HG23	2.14	0.47
2:C:35:ARG:HG3	2:C:39:VAL:HG21	1.96	0.47
2:D:241:ILE:HG23	2:D:275:ALA:HB2	1.96	0.47
2:D:423:ASP:HA	2:D:426:GLU:HG2	1.94	0.47
2:F:567:ILE:HD13	2:F:588:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:162:ASN:OD1	3:O:163:GLU:N	2.47	0.47
3:U:303:SER:HA	3:U:309:VAL:HG12	1.96	0.47
3:a:356:ASN:OD1	3:a:357:LYS:N	2.42	0.47
3:g:26:VAL:HG23	3:g:27:LEU:HD22	1.96	0.47
2:C:599:GLU:HG2	2:C:600:LYS:N	2.30	0.47
2:G:66:ILE:HD11	2:G:342:VAL:HG11	1.95	0.47
2:H:75:ARG:NH1	2:H:79:GLU:HB2	2.29	0.47
2:K:318:ILE:HB	2:K:323:ARG:HE	1.79	0.47
3:M:182:GLN:HE22	3:M:202:PRO:HD3	1.79	0.47
3:S:169:VAL:HG22	3:S:211:LEU:HD12	1.96	0.47
3:T:95:GLN:OE1	3:T:396:ASN:ND2	2.37	0.47
3:b:86:TYR:HB3	3:b:405:LEU:HD12	1.96	0.47
3:u:316:VAL:HG23	3:u:318:ILE:HG13	1.96	0.47
1:l:146:TYR:OH	2:A:60:LYS:O	2.28	0.47
2:A:621:VAL:HG23	2:A:624:GLN:HE21	1.79	0.47
2:B:636:LYS:NZ	2:C:638:THR:HA	2.29	0.47
2:C:487:ARG:HG3	2:C:487:ARG:HH11	1.79	0.47
2:F:302:PRO:O	2:F:478:MET:HG3	2.15	0.47
2:F:425:GLN:NE2	2:F:425:GLN:O	2.46	0.47
2:F:662:THR:O	2:F:666:LEU:HG	2.14	0.47
2:G:187:MET:HE1	2:G:210:THR:HB	1.97	0.47
3:d:111:PRO:HG2	3:l:56:PHE:HE1	1.79	0.47
1:h:77:LYS:H	1:h:77:LYS:HG3	1.43	0.47
1:p:29:VAL:HG13	1:p:30:GLU:H	1.79	0.47
3:q:247:PHE:CD1	3:q:316:VAL:HG12	2.44	0.47
2:G:589:LEU:HD22	2:G:596:PRO:HG3	1.97	0.47
2:I:244:ARG:HA	2:I:250:GLU:O	2.15	0.47
2:I:254:TYR:HB3	2:I:258:GLN:NE2	2.29	0.47
2:I:407:ALA:HB3	2:J:410:ASN:HD22	1.80	0.47
2:K:615:GLN:O	2:K:618:PRO:HD2	2.14	0.47
3:Q:86:TYR:CD1	3:Q:405:LEU:HD21	2.49	0.47
3:Q:104:GLN:OE1	3:a:51:LYS:NZ	2.46	0.47
3:Q:129:MET:HG3	3:Q:418:GLN:NE2	2.29	0.47
3:d:102:LEU:HD21	3:j:5:LEU:HD13	1.96	0.47
3:u:277:GLN:HG2	3:u:280:THR:H	1.80	0.47
3:y:26:VAL:HG21	3:y:213:SER:HB2	1.97	0.47
1:l:125:ARG:NH2	2:A:62:PRO:HD3	2.29	0.47
2:A:220:PHE:HE2	2:B:22:PRO:HA	1.79	0.47
2:D:260:GLU:OE2	2:D:267:ALA:N	2.47	0.47
2:D:615:GLN:HG3	2:D:616:PRO:HD3	1.96	0.47
2:E:643:GLN:HA	2:E:646:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:209:VAL:HG21	3:s:382:GLY:H	1.79	0.47
3:S:162:ASN:C	3:S:162:ASN:HD22	2.23	0.47
1:n:17:LYS:NZ	1:p:40:ASP:OD2	2.39	0.47
2:A:632:ALA:O	2:A:636:LYS:HB2	2.15	0.47
2:B:618:PRO:HA	2:B:621:VAL:HG12	1.97	0.47
2:E:551:LEU:HD11	2:E:561:ARG:HG3	1.97	0.47
2:F:589:LEU:HD23	2:F:594:ALA:HB3	1.96	0.47
2:G:244:ARG:HA	2:G:250:GLU:O	2.14	0.47
2:H:73:LEU:HD22	2:H:328:ILE:HD11	1.97	0.47
2:L:190:LEU:HD11	2:L:194:LYS:HD3	1.96	0.47
3:S:27:LEU:HD22	3:S:128:MET:HE1	1.97	0.47
3:X:277:GLN:HB3	3:X:280:THR:HG22	1.97	0.47
3:Z:276:LEU:O	3:Z:278:GLN:NE2	2.47	0.47
3:g:87:ILE:HG21	3:g:116:ILE:HG23	1.97	0.47
3:g:219:ARG:NH1	3:g:221:GLN:OE1	2.46	0.47
3:y:316:VAL:HG13	3:y:318:ILE:HG13	1.97	0.47
2:A:577:LEU:O	2:A:581:LYS:HG3	2.15	0.47
2:C:120:ALA:HA	2:C:159:PRO:HB3	1.97	0.47
2:D:600:LYS:HA	2:D:603:GLN:NE2	2.29	0.47
2:F:215:TRP:NE1	1:z:139:VAL:HA	2.30	0.47
2:H:569:LEU:HD13	2:H:580:PHE:HZ	1.78	0.47
2:K:9:HIS:CE1	2:K:13:MET:HE3	2.50	0.47
2:L:5:LEU:HD13	2:L:8:LYS:HE2	1.97	0.47
3:V:106:GLU:H	3:V:106:GLU:CD	2.23	0.47
3:Z:229:THR:HG22	3:Z:338:ALA:HA	1.96	0.47
3:d:221:GLN:HG2	3:d:344:THR:O	2.15	0.47
3:i:267:GLN:HB2	3:i:342:VAL:HG22	1.97	0.47
3:k:241:VAL:HG11	3:k:316:VAL:HG21	1.97	0.47
3:y:125:ALA:O	3:y:129:MET:HG2	2.15	0.47
2:B:520:ASP:HB3	2:B:523:VAL:HG23	1.97	0.46
2:L:137:ARG:HB2	2:L:160:ILE:HD11	1.96	0.46
3:Q:165:GLU:HG3	3:Q:209:ARG:HH22	1.80	0.46
3:Q:187:ALA:HB1	3:U:189:ASP:HA	1.97	0.46
3:U:387:VAL:HG22	3:U:402:PHE:CD1	2.50	0.46
3:s:23:SER:OG	3:s:24:ASP:N	2.47	0.46
2:G:599:GLU:HG2	2:G:600:LYS:N	2.31	0.46
2:G:664:TYR:HE2	2:H:669:ALA:HB3	1.80	0.46
2:H:664:TYR:CD2	2:I:666:LEU:HD22	2.49	0.46
2:I:203:PRO:O	2:I:205:THR:HG23	2.15	0.46
2:I:229:LYS:HB2	2:I:229:LYS:HE2	1.63	0.46
2:L:57:GLN:HG3	1:r:124:ARG:HH22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:114:GLN:HE21	3:M:114:GLN:HB2	1.56	0.46
3:O:209:ARG:NH1	3:O:211:LEU:HD21	2.30	0.46
3:S:367:LEU:HD21	3:S:405:LEU:HD12	1.97	0.46
3:T:389:LYS:HE3	3:T:389:LYS:HB2	1.74	0.46
3:Z:346:SER:O	3:Z:346:SER:OG	2.31	0.46
3:c:298:THR:HB	3:c:312:THR:HG23	1.97	0.46
3:k:180:ASP:O	3:k:183:THR:OG1	2.28	0.46
1:v:57:TYR:HD1	1:v:74:LEU:HD21	1.80	0.46
2:A:15:ARG:HH21	2:A:183:TRP:CD1	2.34	0.46
2:D:246:PRO:HA	2:D:250:GLU:HG3	1.98	0.46
2:I:114:GLU:OE2	2:J:525:ARG:NH2	2.49	0.46
3:V:15:LYS:O	3:V:16:LYS:HD3	2.14	0.46
3:W:237:THR:HG23	3:W:240:ALA:H	1.80	0.46
1:n:142:SER:OG	1:n:143:ASP:N	2.48	0.46
3:o:412:ASN:HB3	3:o:415:MET:HE3	1.97	0.46
2:B:162:ASP:O	2:B:166:SER:HB2	2.15	0.46
2:C:597:ARG:HG2	2:C:597:ARG:O	2.16	0.46
3:T:180:ASP:O	3:T:183:THR:OG1	2.33	0.46
3:V:98:GLU:HA	3:V:102:LEU:HB2	1.98	0.46
3:g:233:GLN:OE1	3:g:332:GLN:NE2	2.48	0.46
3:k:111:PRO:HG2	3:s:56:PHE:HE2	1.81	0.46
3:l:251:LEU:HB2	3:l:309:VAL:HG23	1.97	0.46
3:o:245:TYR:HD2	3:o:413:PRO:HD2	1.80	0.46
3:s:390:TYR:CE2	1:x:155:GLY:HA3	2.51	0.46
1:0:44:MET:HG3	1:0:89:ARG:NH1	2.31	0.46
1:0:50:ILE:HG23	1:0:51:ASN:N	2.31	0.46
2:B:103:LYS:NZ	2:B:510:ARG:O	2.32	0.46
2:D:46:GLY:HA2	2:D:216:GLU:HG2	1.98	0.46
2:E:229:LYS:HB2	2:E:229:LYS:HE2	1.47	0.46
2:F:100:LEU:HB2	2:F:510:ARG:NH1	2.30	0.46
2:F:244:ARG:HH22	2:F:246:PRO:HG3	1.81	0.46
2:F:365:ARG:O	2:F:385:ARG:NH1	2.38	0.46
2:G:351:GLN:NE2	1:h:123:MET:SD	2.88	0.46
2:H:42:GLY:HA2	2:H:45:GLU:HG3	1.98	0.46
2:I:254:TYR:HB3	2:I:258:GLN:HE21	1.81	0.46
2:J:302:PRO:O	2:J:478:MET:HG3	2.15	0.46
3:a:41:ASN:OD1	3:a:42:SER:N	2.49	0.46
3:b:104:GLN:HB3	3:b:107:GLU:CD	2.39	0.46
1:z:138:ASP:OD2	1:z:139:VAL:N	2.43	0.46
2:F:637:ALA:HA	2:F:640:GLU:HB2	1.97	0.46
2:I:9:HIS:O	2:I:13:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:113:ARG:O	3:Q:117:VAL:HG23	2.16	0.46
3:V:86:TYR:CE1	3:V:405:LEU:HD21	2.51	0.46
3:W:351:PRO:HA	3:W:420:PHE:HE1	1.80	0.46
3:q:241:VAL:HG21	3:q:316:VAL:HG11	1.98	0.46
2:D:247:ILE:HG22	2:D:248:THR:HG23	1.96	0.46
2:K:19:ALA:HA	2:K:171:PRO:HG3	1.97	0.46
3:R:108:ILE:HD12	3:b:54:HIS:CE1	2.51	0.46
3:X:344:THR:HG22	3:X:345:ALA:N	2.28	0.46
3:Z:158:ASP:OD2	3:t:173:TRP:NE1	2.49	0.46
3:b:87:ILE:HG23	3:i:58:SER:HB2	1.98	0.46
3:e:104:GLN:HB3	1:z:141:THR:HA	1.98	0.46
2:B:589:LEU:HD11	2:B:596:PRO:HG3	1.97	0.46
2:G:196:GLU:HG2	2:G:201:LYS:HB3	1.98	0.46
3:P:365:ILE:HD11	3:P:405:LEU:HD23	1.97	0.46
3:Z:86:TYR:HB2	3:Z:404:LEU:O	2.16	0.46
3:i:267:GLN:HB2	3:i:342:VAL:CG2	2.45	0.46
3:q:126:HIS:HA	3:q:129:MET:HE2	1.98	0.46
3:s:153:ALA:HB2	3:s:208:ILE:HB	1.98	0.46
3:y:135:SER:HB2	3:y:267:GLN:NE2	2.31	0.46
1:0:118:LEU:HD23	2:J:365:ARG:HH21	1.81	0.46
2:A:217:TYR:H	3:k:104:GLN:NE2	2.14	0.46
2:B:214:SER:CB	2:B:219:TRP:HE1	2.28	0.46
2:D:616:PRO:O	2:D:620:MET:HG2	2.16	0.46
2:E:622:LEU:HA	2:E:625:ALA:HB2	1.98	0.46
2:I:657:GLU:OE2	2:J:659:GLN:HA	2.14	0.46
2:L:657:GLU:HG2	2:L:661:ASN:HD21	1.81	0.46
3:S:389:LYS:HD3	3:S:389:LYS:C	2.41	0.46
3:U:126:HIS:HA	3:U:129:MET:HG2	1.98	0.46
3:U:388:HIS:HB2	3:U:401:ARG:HG2	1.97	0.46
3:b:276:LEU:O	3:b:278:GLN:NE2	2.48	0.46
3:k:105:LEU:HD22	3:k:400:MET:SD	2.56	0.46
2:F:220:PHE:CE1	2:G:22:PRO:HA	2.51	0.46
2:K:487:ARG:C	2:K:510:ARG:HH22	2.24	0.46
2:L:111:ASP:OD1	2:L:154:ARG:NH1	2.49	0.46
3:N:276:LEU:O	3:N:278:GLN:NE2	2.49	0.46
3:R:369:LYS:NZ	3:R:373:ILE:O	2.35	0.46
3:W:180:ASP:O	3:W:183:THR:HG22	2.16	0.46
3:d:179:ALA:O	3:d:183:THR:HG23	2.16	0.46
3:k:95:GLN:HG2	3:k:96:LEU:HD22	1.98	0.46
3:m:96:LEU:O	3:m:100:ILE:HG12	2.16	0.46
2:A:162:ASP:HB3	2:A:165:ARG:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:244:ARG:NH1	2:I:250:GLU:OE1	2.47	0.45
2:J:92:GLY:H	2:J:97:SER:HB3	1.81	0.45
2:J:245:HIS:HB2	2:J:270:GLY:HA2	1.98	0.45
2:J:361:MET:HE3	2:J:361:MET:HB2	1.88	0.45
2:L:183:TRP:HB2	2:L:230:TYR:HE1	1.81	0.45
2:L:207:LEU:HB3	2:L:225:ILE:HG23	1.98	0.45
3:O:238:TYR:HD1	3:O:318:ILE:HD13	1.80	0.45
3:b:162:ASN:HB3	3:b:163:GLU:OE1	2.16	0.45
3:g:17:PHE:CE2	3:g:107:GLU:HG2	2.51	0.45
2:C:452:ARG:HA	2:C:455:MET:HE2	1.98	0.45
2:E:10:GLU:O	2:E:14:LEU:HG	2.16	0.45
2:F:254:TYR:HE1	2:F:518:LEU:HB3	1.80	0.45
2:H:661:ASN:HA	2:I:666:LEU:HD11	1.98	0.45
3:S:23:SER:HB2	3:c:277:GLN:HE22	1.81	0.45
3:T:107:GLU:OE2	3:T:107:GLU:N	2.48	0.45
3:V:344:THR:HB	3:V:347:GLN:HG2	1.97	0.45
3:a:221:GLN:NE2	3:a:266:ASP:OD1	2.49	0.45
1:h:17:LYS:O	1:w:92:SER:OG	2.20	0.45
3:q:23:SER:OG	3:q:24:ASP:N	2.49	0.45
3:q:139:PRO:HB3	3:q:349:MET:HE2	1.98	0.45
2:E:220:PHE:CD1	2:E:224:VAL:CG2	3.00	0.45
2:F:244:ARG:HA	2:F:250:GLU:O	2.16	0.45
2:G:490:ARG:HB3	2:G:507:VAL:N	2.31	0.45
2:I:318:ILE:HB	2:I:323:ARG:HE	1.82	0.45
2:K:302:PRO:O	2:K:478:MET:HG3	2.17	0.45
3:M:331:ARG:NH1	3:M:337:ASP:OD2	2.32	0.45
3:R:188:SER:O	3:R:192:VAL:HG13	2.17	0.45
3:a:262:LEU:HD12	3:a:311:VAL:HG11	1.99	0.45
3:d:221:GLN:NE2	3:d:343:GLY:HA3	2.32	0.45
1:f:45:MET:HG3	1:f:57:TYR:CE1	2.51	0.45
3:j:23:SER:OG	3:j:24:ASP:N	2.50	0.45
3:k:100:ILE:HD11	1:r:150:LEU:HD11	1.98	0.45
3:t:144:THR:HG22	3:t:177:ARG:HD2	1.99	0.45
2:B:42:GLY:HA2	2:B:45:GLU:HG2	1.97	0.45
2:C:244:ARG:HA	2:C:250:GLU:O	2.16	0.45
2:H:457:SER:HA	2:H:460:TYR:HD2	1.82	0.45
2:L:99:GLU:H	2:L:99:GLU:CD	2.22	0.45
3:e:105:LEU:HA	3:e:108:ILE:CD1	2.46	0.45
3:l:98:GLU:HG2	3:l:102:LEU:HD12	1.97	0.45
2:A:384:LEU:HD12	2:A:385:ARG:H	1.82	0.45
2:J:161:TYR:HB3	2:K:317:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:325:GLN:HG3	3:M:326:TYR:CD1	2.52	0.45
3:N:71:LYS:HD3	3:q:92:GLU:OE2	2.17	0.45
3:a:106:GLU:HG2	3:a:107:GLU:N	2.31	0.45
3:c:25:LEU:HA	3:c:121:GLU:OE1	2.16	0.45
3:d:70:ASN:OD1	3:d:70:ASN:N	2.49	0.45
3:l:95:GLN:HB3	3:l:398:GLN:HB2	1.97	0.45
2:B:490:ARG:HB3	2:B:507:VAL:N	2.32	0.45
2:D:488:GLU:O	2:D:488:GLU:HG2	2.17	0.45
2:F:273:GLU:OE1	2:F:274:VAL:N	2.47	0.45
2:G:99:GLU:HB3	2:G:510:ARG:HD2	1.98	0.45
2:J:207:LEU:HD23	2:J:207:LEU:H	1.81	0.45
2:K:657:GLU:HG2	2:K:661:ASN:ND2	2.32	0.45
3:d:27:LEU:O	3:d:31:VAL:HG13	2.16	0.45
3:k:41:ASN:OD1	3:k:44:THR:N	2.48	0.45
3:q:295:ALA:HB3	3:q:313:LEU:HD23	1.99	0.45
1:w:80:HIS:HB2	1:z:47:GLU:OE2	2.17	0.45
3:y:46:ASP:OD1	3:y:46:ASP:N	2.47	0.45
1:z:57:TYR:CD2	1:z:74:LEU:HD11	2.52	0.45
2:D:103:LYS:HG3	2:D:510:ARG:NH1	2.32	0.45
2:E:100:LEU:O	2:E:104:LEU:HD23	2.16	0.45
2:F:563:ALA:O	2:F:567:ILE:HG12	2.16	0.45
2:G:207:LEU:HB3	2:G:225:ILE:HG23	1.99	0.45
2:G:575:GLU:N	2:G:575:GLU:OE2	2.50	0.45
2:J:520:ASP:HB3	2:J:523:VAL:HG23	1.98	0.45
3:O:163:GLU:OE2	3:s:19:PRO:HB3	2.17	0.45
3:Q:389:LYS:HG2	3:Q:400:MET:HE3	1.98	0.45
3:T:190:GLN:HE21	3:X:193:ARG:HE	1.64	0.45
3:m:344:THR:HG22	3:m:345:ALA:N	2.30	0.45
3:q:188:SER:OG	3:q:191:LEU:HD13	2.16	0.45
3:t:100:ILE:HG13	3:t:101:LYS:HG3	1.98	0.45
3:u:135:SER:HB2	3:u:267:GLN:NE2	2.31	0.45
2:B:599:GLU:HG2	2:B:600:LYS:H	1.81	0.45
2:G:337:LEU:O	2:G:341:GLN:HG2	2.17	0.45
2:I:382:LEU:HG	2:J:356:ILE:HG21	1.98	0.45
3:R:104:GLN:O	3:R:108:ILE:HG12	2.16	0.45
3:R:110:ALA:N	3:R:111:PRO:HD2	2.32	0.45
3:a:61:THR:HG21	3:a:66:ILE:HG22	1.99	0.45
3:b:86:TYR:OH	3:i:63:THR:O	2.28	0.45
3:g:375:SER:HA	3:g:387:VAL:O	2.15	0.45
3:i:66:ILE:HB	3:i:69:GLN:CD	2.42	0.45
3:o:11:GLN:O	3:o:11:GLN:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:487:ARG:NH2	2:C:520:ASP:OD2	2.44	0.45
2:C:657:GLU:HG2	2:C:661:ASN:HD21	1.81	0.45
2:D:365:ARG:O	2:D:385:ARG:NH1	2.50	0.45
2:F:476:LEU:HD12	2:F:476:LEU:HA	1.87	0.45
2:G:103:LYS:HB3	2:G:103:LYS:HE3	1.60	0.45
2:K:207:LEU:HD23	2:K:207:LEU:H	1.82	0.45
3:P:136:LEU:HB2	3:P:419:PHE:HB2	1.99	0.45
3:Q:356:ASN:OD1	3:Q:357:LYS:N	2.48	0.45
3:S:95:GLN:O	3:S:98:GLU:HG3	2.16	0.45
3:X:112:VAL:HG11	3:X:402:PHE:CE1	2.52	0.45
3:j:4:ASN:ND2	3:j:6:ASP:OD1	2.50	0.45
3:l:273:THR:HG21	3:l:333:VAL:HG22	1.99	0.45
3:o:316:VAL:HG23	3:o:318:ILE:HG13	1.98	0.45
3:q:149:VAL:HG21	3:q:178:LEU:HD11	1.97	0.45
3:t:158:ASP:OD2	3:y:173:TRP:NE1	2.46	0.45
2:A:516:VAL:O	2:A:518:LEU:HD12	2.17	0.45
2:D:114:GLU:HB2	2:D:154:ARG:NH2	2.30	0.45
2:D:199:TYR:CG	2:D:295:LEU:HD12	2.51	0.45
2:G:361:MET:HE3	2:G:361:MET:HB2	1.83	0.45
2:H:190:LEU:HG	2:H:194:LYS:HE3	1.98	0.45
2:J:664:TYR:HE2	2:K:669:ALA:HB3	1.82	0.45
3:P:57:SER:HB3	3:P:325:GLN:HG3	1.99	0.45
3:T:104:GLN:O	3:T:108:ILE:HG12	2.17	0.45
3:T:189:ASP:OD2	3:T:190:GLN:N	2.50	0.45
3:a:26:VAL:HG23	3:a:27:LEU:HD23	1.99	0.45
3:c:369:LYS:NZ	3:c:373:ILE:O	2.44	0.45
3:d:22:MET:SD	3:l:162:ASN:ND2	2.78	0.45
3:i:179:ALA:O	3:i:183:THR:HG23	2.16	0.45
3:m:104:GLN:NE2	3:m:107:GLU:OE1	2.50	0.45
3:o:285:TYR:CE1	3:o:290:PRO:HG3	2.52	0.45
1:p:48:TRP:O	1:p:52:PRO:HD2	2.17	0.45
3:q:57:SER:O	3:q:72:ASN:ND2	2.43	0.45
3:s:165:GLU:OE2	3:s:209:ARG:NH2	2.51	0.45
2:F:198:GLU:HG2	2:F:199:TYR:H	1.82	0.44
2:G:14:LEU:O	2:G:18:ARG:HG3	2.16	0.44
2:L:115:THR:HG21	2:L:156:ALA:HB1	1.99	0.44
3:M:136:LEU:HD11	3:M:155:PHE:CD2	2.52	0.44
3:N:56:PHE:O	3:q:115:ARG:NH1	2.49	0.44
3:Q:333:VAL:HG13	3:Q:333:VAL:O	2.17	0.44
3:V:273:THR:HG23	3:V:331:ARG:HG3	1.98	0.44
1:Y:17:LYS:HD3	1:Y:17:LYS:HA	1.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:350:LYS:NZ	3:k:283:ALA:O	2.42	0.44
3:e:103:ASN:HA	1:z:141:THR:HG23	1.99	0.44
3:l:27:LEU:HB3	3:l:124:LEU:HD23	1.99	0.44
3:u:374:ASP:HB2	3:u:389:LYS:HB2	1.99	0.44
2:A:539:ARG:NH1	2:A:543:THR:OG1	2.50	0.44
2:F:570:ASP:O	2:F:581:LYS:NZ	2.42	0.44
2:G:244:ARG:HG3	2:G:251:ILE:HD13	1.99	0.44
2:J:137:ARG:HB2	2:J:160:ILE:HD11	1.99	0.44
3:O:285:TYR:CE1	3:O:290:PRO:HB3	2.53	0.44
3:R:95:GLN:O	3:R:98:GLU:HG3	2.17	0.44
3:d:165:GLU:H	3:d:357:LYS:HB2	1.82	0.44
1:h:6:THR:HA	1:h:71:GLU:HA	1.99	0.44
1:h:13:PHE:CE1	1:h:17:LYS:HE2	2.52	0.44
3:s:117:VAL:HG21	3:s:380:TYR:HD2	1.81	0.44
1:1:6:THR:O	1:1:10:ILE:HG13	2.18	0.44
2:G:516:VAL:O	2:G:518:LEU:HD22	2.16	0.44
2:I:207:LEU:HG	2:I:292:ASP:HB3	1.99	0.44
2:I:490:ARG:HB2	2:I:509:ASP:OD2	2.17	0.44
2:J:600:LYS:O	2:J:604:ILE:HG12	2.18	0.44
2:L:12:ILE:HD12	2:L:230:TYR:HE2	1.80	0.44
2:L:617:ASN:HB3	2:L:618:PRO:HD3	1.98	0.44
3:N:139:PRO:HG2	3:N:343:GLY:HA2	2.00	0.44
3:Q:106:GLU:H	3:Q:106:GLU:CD	2.25	0.44
3:T:231:LYS:HB3	3:T:250:THR:HG23	1.99	0.44
1:f:18:PHE:HB2	1:f:87:LEU:HD11	1.98	0.44
3:l:93:TYR:CE2	3:l:95:GLN:HA	2.52	0.44
2:B:32:GLU:HB2	2:B:215:TRP:CH2	2.53	0.44
2:C:466:LYS:HB3	2:C:466:LYS:HE2	1.74	0.44
2:C:636:LYS:HA	2:C:636:LYS:HD2	1.29	0.44
2:D:364:ILE:O	2:D:364:ILE:HG12	2.17	0.44
3:R:189:ASP:OD1	3:R:190:GLN:N	2.49	0.44
3:a:329:VAL:HG12	3:a:331:ARG:H	1.83	0.44
3:k:374:ASP:OD1	3:k:374:ASP:N	2.51	0.44
1:p:124:ARG:HH11	1:p:124:ARG:HG3	1.82	0.44
3:s:280:THR:HG23	3:s:282:GLN:HG3	1.99	0.44
1:v:44:MET:HE2	1:v:44:MET:HB3	1.84	0.44
1:1:91:LEU:HD23	1:1:91:LEU:HA	1.78	0.44
2:B:207:LEU:HD23	2:B:207:LEU:H	1.83	0.44
2:E:19:ALA:HB2	2:E:183:TRP:CH2	2.52	0.44
2:F:37:ALA:HB2	2:F:328:ILE:HG21	1.98	0.44
2:F:162:ASP:O	2:F:166:SER:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:598:ASN:ND2	2:G:602:GLN:OE1	2.42	0.44
3:d:162:ASN:OD1	3:d:163:GLU:N	2.50	0.44
3:g:102:LEU:HD21	3:g:105:LEU:HA	2.00	0.44
3:j:25:LEU:HD23	3:j:121:GLU:OE1	2.18	0.44
2:A:288:VAL:HB	2:A:296:GLU:HB2	1.98	0.44
2:B:617:ASN:HA	2:B:620:MET:HG2	2.00	0.44
2:C:334:PRO:HB2	2:C:424:ILE:HG13	1.99	0.44
2:C:365:ARG:O	2:C:385:ARG:NH1	2.38	0.44
2:E:220:PHE:HD1	2:E:224:VAL:CG2	2.31	0.44
2:F:2:ALA:O	2:F:8:LYS:NZ	2.36	0.44
2:F:604:ILE:O	2:F:607:GLN:HG3	2.17	0.44
2:G:626:GLN:HA	2:H:627:MET:SD	2.57	0.44
2:H:345:LEU:HB2	2:H:413:LEU:HD21	2.00	0.44
2:J:196:GLU:HG2	2:J:201:LYS:HB3	2.00	0.44
2:J:245:HIS:CE1	2:J:247:ILE:HB	2.52	0.44
2:L:237:SER:HB3	2:L:280:LYS:HE3	1.99	0.44
3:M:139:PRO:HG2	3:M:343:GLY:HA2	1.99	0.44
3:O:188:SER:O	3:O:192:VAL:HG23	2.18	0.44
3:Q:36:LEU:HD22	3:Q:363:GLY:HA3	2.00	0.44
3:T:98:GLU:HA	3:T:102:LEU:HB2	2.00	0.44
3:b:365:ILE:HB	3:b:405:LEU:HD23	1.98	0.44
3:m:233:GLN:NE2	3:m:332:GLN:HE21	2.15	0.44
3:q:15:LYS:HE2	3:q:103:ASN:ND2	2.33	0.44
3:s:344:THR:HG22	3:s:345:ALA:N	2.30	0.44
2:A:606:GLN:OE1	2:A:606:GLN:HA	2.17	0.44
2:D:450:MET:N	2:D:450:MET:SD	2.90	0.44
2:G:610:MET:O	2:G:613:GLN:HG3	2.18	0.44
2:H:27:ARG:NH1	2:H:164:SER:O	2.41	0.44
2:H:595:LYS:HD2	2:H:595:LYS:HA	1.72	0.44
2:I:223:ASP:CB	3:q:379:THR:HG21	2.48	0.44
2:I:657:GLU:HG2	2:I:661:ASN:ND2	2.31	0.44
2:J:27:ARG:HB2	2:J:212:MET:HE2	1.99	0.44
3:N:231:LYS:HB3	3:N:250:THR:HG23	2.00	0.44
3:U:27:LEU:O	3:U:31:VAL:HG13	2.18	0.44
1:Y:126:ARG:NH1	1:Y:128:ASP:OD1	2.51	0.44
3:a:173:TRP:NE1	3:g:158:ASP:OD2	2.48	0.44
3:d:5:LEU:HD12	3:j:97:GLU:HG2	2.00	0.44
3:e:221:GLN:HG3	3:e:349:MET:HE1	1.99	0.44
3:i:100:ILE:HG22	3:i:101:LYS:HG3	2.00	0.44
1:w:7:LYS:HD3	1:w:57:TYR:OH	2.18	0.44
1:l:28:ASP:OD1	1:l:29:VAL:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:333:ASP:HA	2:A:336:ARG:HG2	2.00	0.44
2:D:318:ILE:HB	2:D:323:ARG:HE	1.83	0.44
2:H:207:LEU:HD23	2:H:207:LEU:H	1.82	0.44
2:I:345:LEU:HG	2:J:416:LEU:HD21	2.00	0.44
2:K:47:ALA:O	2:K:63:LYS:HE2	2.18	0.44
1:Y:119:VAL:HG23	1:Y:120:VAL:H	1.82	0.44
3:q:102:LEU:HD23	3:q:102:LEU:HA	1.89	0.44
1:l:17:LYS:HD3	1:l:17:LYS:HA	1.71	0.44
2:A:625:ALA:HB3	2:B:627:MET:HE3	2.00	0.44
2:B:334:PRO:HB2	2:B:424:ILE:HG13	1.99	0.44
2:F:361:MET:HB2	2:F:361:MET:HE3	1.86	0.44
2:K:115:THR:HG22	2:K:116:ASP:N	2.29	0.44
3:M:135:SER:O	3:M:136:LEU:HD12	2.17	0.44
3:O:237:THR:O	3:O:241:VAL:HG22	2.18	0.44
3:S:135:SER:HB2	3:S:267:GLN:OE1	2.18	0.44
3:W:36:LEU:HD21	3:W:409:VAL:HG21	1.99	0.44
3:a:29:LYS:N	3:a:29:LYS:HD3	2.33	0.44
3:b:32:ASP:OD1	3:b:33:ARG:N	2.51	0.44
1:r:35:GLU:HA	1:r:38:VAL:HG12	2.00	0.44
3:u:286:ASN:HB2	3:u:291:ILE:HD11	2.00	0.44
2:B:625:ALA:HB1	2:B:628:VAL:CG2	2.48	0.43
2:C:55:ASP:O	2:C:56:GLU:HB2	2.17	0.43
2:C:647:LYS:HA	2:C:647:LYS:HD2	1.80	0.43
2:G:657:GLU:HG2	2:G:661:ASN:HD21	1.83	0.43
2:H:615:GLN:O	2:H:618:PRO:HD2	2.18	0.43
2:K:95:GLU:OE2	2:K:95:GLU:N	2.45	0.43
2:L:217:TYR:HD2	2:L:219:TRP:CD1	2.36	0.43
3:P:2:PRO:HB2	3:P:3:ASN:H	1.69	0.43
3:P:360:CYS:SG	3:P:361:GLY:N	2.91	0.43
3:R:370:LEU:H	3:R:388:HIS:CE1	2.36	0.43
3:Z:389:LYS:HG2	3:Z:400:MET:HG2	2.00	0.43
3:e:412:ASN:HB3	3:e:415:MET:HE3	2.00	0.43
3:m:392:ASP:HB3	3:m:397:VAL:HG22	1.99	0.43
3:o:360:CYS:SG	3:o:361:GLY:N	2.92	0.43
3:q:374:ASP:HB2	3:q:389:LYS:HG3	2.00	0.43
2:A:187:MET:HG2	2:A:228:ALA:HB2	2.00	0.43
2:G:152:ARG:NH2	2:G:516:VAL:HG22	2.33	0.43
2:G:643:GLN:HG2	2:H:644:THR:HG22	1.99	0.43
2:I:653:GLN:HA	2:I:656:MET:HE3	1.99	0.43
2:J:241:ILE:HG23	2:J:275:ALA:HB2	2.00	0.43
3:Q:400:MET:HE2	3:Q:400:MET:HB3	1.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:180:ASP:O	3:U:183:THR:HG22	2.18	0.43
3:V:31:VAL:HG11	3:V:128:MET:HE1	2.00	0.43
3:g:17:PHE:CE2	3:m:51:LYS:HD2	2.53	0.43
3:q:268:VAL:HG12	3:q:341:VAL:HG22	2.00	0.43
3:q:344:THR:HG22	3:q:345:ALA:N	2.34	0.43
3:u:370:LEU:O	3:u:372:SER:N	2.52	0.43
1:w:48:TRP:O	1:w:52:PRO:HD2	2.17	0.43
2:B:53:LYS:HD3	2:B:53:LYS:HA	1.86	0.43
2:C:615:GLN:O	2:C:618:PRO:HD2	2.18	0.43
2:G:20:TYR:HE1	2:G:212:MET:HE3	1.84	0.43
2:K:510:ARG:NH2	2:K:511:GLN:O	2.26	0.43
2:L:137:ARG:NH1	2:L:139:THR:HB	2.33	0.43
3:N:64:GLY:O	1:f:158:PRO:HD2	2.19	0.43
3:R:180:ASP:O	3:R:183:THR:OG1	2.33	0.43
3:S:145:LYS:HE3	3:S:145:LYS:HB2	1.91	0.43
3:b:117:VAL:HG21	3:b:380:TYR:HD1	1.83	0.43
3:e:221:GLN:HE21	3:e:221:GLN:HB3	1.52	0.43
3:i:320:ASP:OD2	3:i:323:ASN:N	2.51	0.43
3:j:179:ALA:O	3:j:183:THR:HG23	2.19	0.43
3:l:16:LYS:HB3	3:l:16:LYS:HE2	1.86	0.43
3:q:189:ASP:OD2	3:q:190:GLN:N	2.51	0.43
2:C:96:ALA:HB2	2:C:488:GLU:HG2	2.00	0.43
2:C:162:ASP:O	2:C:166:SER:CB	2.66	0.43
2:F:243:TYR:HA	2:F:271:PHE:O	2.19	0.43
2:G:309:ILE:HG21	2:G:471:ALA:HB2	2.00	0.43
2:K:641:THR:O	2:K:644:THR:OG1	2.35	0.43
2:L:486:GLU:HA	2:L:486:GLU:OE2	2.18	0.43
3:P:180:ASP:O	3:P:183:THR:OG1	2.37	0.43
3:T:57:SER:H	3:T:72:ASN:HD21	1.66	0.43
3:W:16:LYS:HE3	3:W:16:LYS:HB3	1.77	0.43
3:W:86:TYR:CE2	3:W:405:LEU:HD21	2.54	0.43
3:W:365:ILE:HD11	3:W:407:ALA:HB2	2.00	0.43
3:e:375:SER:HB3	3:e:388:HIS:CD2	2.53	0.43
3:g:388:HIS:HB2	3:g:401:ARG:HG2	2.01	0.43
3:m:331:ARG:NH2	3:m:334:GLU:OE1	2.50	0.43
2:A:664:TYR:OH	2:B:670:ARG:HG2	2.18	0.43
2:A:670:ARG:NH1	2:L:668:GLN:OE1	2.48	0.43
2:C:623:ALA:HA	2:D:624:GLN:OE1	2.17	0.43
2:D:618:PRO:HA	2:D:621:VAL:HG12	1.99	0.43
2:E:640:GLU:OE1	2:F:644:THR:HB	2.18	0.43
2:E:657:GLU:HG2	2:E:661:ASN:ND2	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:621:VAL:O	2:F:625:ALA:CB	2.60	0.43
2:F:622:LEU:HA	2:F:625:ALA:HB3	2.00	0.43
2:H:142:LEU:HD23	2:H:142:LEU:H	1.83	0.43
2:H:486:GLU:HB3	2:H:510:ARG:HD2	2.00	0.43
2:J:540:ARG:NH2	2:K:98:GLU:OE2	2.51	0.43
2:K:487:ARG:C	2:K:510:ARG:HH12	2.26	0.43
3:R:86:TYR:CE1	3:R:405:LEU:HD21	2.53	0.43
3:S:25:LEU:HD21	3:S:117:VAL:HG12	2.00	0.43
3:W:23:SER:OG	3:W:24:ASP:N	2.51	0.43
3:d:12:ILE:HA	3:j:10:SER:HB2	2.01	0.43
3:g:15:LYS:HE3	3:g:15:LYS:HB2	1.72	0.43
3:g:162:ASN:OD1	3:g:163:GLU:N	2.51	0.43
3:j:385:ILE:HG12	3:j:404:LEU:HD12	2.00	0.43
3:l:231:LYS:HB3	3:l:250:THR:HG23	2.00	0.43
3:l:245:TYR:HD2	3:l:413:PRO:HD2	1.82	0.43
1:p:28:ASP:OD1	1:p:29:VAL:N	2.48	0.43
1:r:48:TRP:O	1:r:52:PRO:HD2	2.18	0.43
1:1:119:VAL:HG23	1:1:121:PRO:HD3	2.00	0.43
2:B:25:GLU:OE1	2:B:25:GLU:N	2.52	0.43
2:D:192:PRO:HD3	2:D:223:ASP:O	2.18	0.43
2:F:5:LEU:HD12	2:F:294:PHE:CD2	2.54	0.43
2:G:292:ASP:OD1	2:G:293:GLY:N	2.50	0.43
2:G:587:GLN:HA	2:G:590:ILE:HG12	2.00	0.43
2:I:210:THR:O	2:I:212:MET:N	2.52	0.43
2:K:104:LEU:HD23	2:K:104:LEU:HA	1.85	0.43
2:L:170:ASP:OD1	2:L:171:PRO:HD2	2.19	0.43
3:M:86:TYR:HE2	3:M:367:LEU:HD21	1.84	0.43
3:W:324:PRO:HA	3:W:327:ASN:ND2	2.34	0.43
3:i:30:THR:OG1	3:i:355:TYR:OH	2.29	0.43
3:o:113:ARG:O	3:o:117:VAL:HG23	2.19	0.43
3:u:255:THR:HG22	3:u:256:ALA:H	1.83	0.43
3:u:277:GLN:HG2	3:u:280:THR:OG1	2.18	0.43
1:v:50:ILE:HG13	1:v:51:ASN:N	2.33	0.43
1:1:137:TYR:O	1:1:138:ASP:HB2	2.18	0.43
2:A:84:ARG:NH2	2:A:122:ASP:OD2	2.50	0.43
2:E:72:GLU:OE2	2:E:72:GLU:N	2.49	0.43
2:F:215:TRP:CD2	1:z:139:VAL:HG12	2.53	0.43
2:H:27:ARG:HB2	2:H:212:MET:HE1	1.99	0.43
2:I:302:PRO:O	2:I:478:MET:HG3	2.19	0.43
2:K:664:TYR:HB3	2:L:666:LEU:HD13	1.99	0.43
3:M:26:VAL:HG21	3:M:213:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:221:GLN:OE1	3:M:343:GLY:HA3	2.19	0.43
3:N:193:ARG:HG2	3:N:193:ARG:HH11	1.82	0.43
3:O:23:SER:OG	3:O:24:ASP:N	2.51	0.43
3:O:35:LEU:HD23	3:O:35:LEU:HA	1.90	0.43
3:P:35:LEU:HD23	3:P:411:PHE:CZ	2.53	0.43
3:i:86:TYR:HB3	3:i:88:THR:HG23	2.01	0.43
3:j:371:HIS:HB3	1:p:153:ILE:HG13	2.01	0.43
3:l:85:ASN:HB2	3:u:60:ARG:HH21	1.84	0.43
3:s:25:LEU:HD11	3:s:117:VAL:HG11	2.01	0.43
1:x:112:ALA:O	1:x:115:THR:HG22	2.19	0.43
1:1:144:ARG:H	1:1:144:ARG:HD2	1.83	0.43
2:A:18:ARG:CZ	2:L:193:GLU:HG3	2.49	0.43
2:J:120:ALA:HA	2:J:159:PRO:HB3	2.00	0.43
3:N:216:LEU:HG	3:N:217:ALA:H	1.84	0.43
3:P:159:LEU:HD23	3:P:159:LEU:HA	1.90	0.43
3:P:319:TYR:CD2	3:P:332:GLN:HB2	2.54	0.43
3:Q:344:THR:HB	3:Q:347:GLN:OE1	2.19	0.43
3:T:123:GLU:OE1	3:d:60:ARG:NH1	2.48	0.43
3:U:143:ILE:HD11	3:U:174:SER:HB3	2.00	0.43
3:a:39:GLU:HA	3:a:39:GLU:OE2	2.19	0.43
3:b:401:ARG:HH12	3:i:66:ILE:HG13	1.84	0.43
1:f:17:LYS:NZ	1:h:89:ARG:O	2.48	0.43
3:i:95:GLN:NE2	3:i:396:ASN:OD1	2.51	0.43
1:r:45:MET:HE2	1:r:45:MET:HB2	1.81	0.43
3:t:247:PHE:CD1	3:t:316:VAL:HG12	2.52	0.43
3:t:367:LEU:HD21	3:t:405:LEU:HD12	2.01	0.43
3:u:344:THR:HG22	3:u:345:ALA:N	2.34	0.43
1:v:48:TRP:O	1:v:52:PRO:HD2	2.19	0.43
2:A:2:ALA:HB2	2:A:11:ARG:HH12	1.84	0.43
2:B:244:ARG:NH1	2:B:250:GLU:OE1	2.50	0.43
2:J:3:GLU:O	2:J:8:LYS:NZ	2.52	0.43
2:J:345:LEU:HB2	2:J:413:LEU:HD21	2.01	0.43
3:O:100:ILE:HG13	3:O:101:LYS:N	2.33	0.43
3:Q:153:ALA:HB2	3:Q:208:ILE:HB	2.01	0.43
3:S:91:VAL:HG12	3:c:72:ASN:HB2	2.01	0.43
3:b:25:LEU:HA	3:b:121:GLU:OE2	2.18	0.43
3:t:157:LYS:HA	3:t:157:LYS:HD2	1.85	0.43
2:A:464:MET:O	2:A:468:LEU:HD23	2.19	0.43
2:A:602:GLN:HG3	2:A:603:GLN:CD	2.44	0.43
2:C:664:TYR:HD2	2:D:666:LEU:HD22	1.84	0.43
2:D:531:ASP:OD1	2:D:532:VAL:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:47:ALA:O	2:E:63:LYS:HE2	2.19	0.43
2:E:589:LEU:HD13	2:E:601:GLU:HB2	2.01	0.43
2:E:640:GLU:OE1	2:F:645:GLN:HG2	2.19	0.43
2:F:7:LYS:HD2	2:F:10:GLU:OE2	2.19	0.43
2:F:20:TYR:CZ	2:F:24:LYS:HE2	2.54	0.43
2:F:355:GLN:HG2	2:F:404:THR:O	2.19	0.43
2:H:386:GLU:N	2:H:386:GLU:OE2	2.52	0.43
2:J:488:GLU:N	2:J:488:GLU:OE1	2.52	0.43
3:M:270:PHE:O	3:M:292:SER:HB3	2.19	0.43
3:P:354:PHE:CE1	3:P:419:PHE:HB3	2.54	0.43
3:T:129:MET:HG3	3:T:418:GLN:NE2	2.34	0.43
3:Z:71:LYS:NZ	3:t:399:LYS:HD3	2.33	0.43
3:o:139:PRO:HG2	3:o:343:GLY:HA2	2.01	0.43
2:A:641:THR:HB	2:L:636:LYS:HD3	2.01	0.42
2:C:244:ARG:HD3	2:C:273:GLU:HG3	2.00	0.42
2:F:384:LEU:HD12	2:F:384:LEU:HA	1.86	0.42
2:I:187:MET:HA	2:I:228:ALA:HA	2.00	0.42
2:J:72:GLU:H	2:J:72:GLU:HG2	1.43	0.42
2:J:599:GLU:HG2	2:J:600:LYS:H	1.84	0.42
2:L:615:GLN:O	2:L:618:PRO:HD2	2.19	0.42
3:R:106:GLU:HG2	3:R:107:GLU:N	2.34	0.42
3:U:89:VAL:HG11	3:U:112:VAL:HG13	2.00	0.42
3:W:125:ALA:O	3:W:129:MET:HG3	2.18	0.42
1:n:18:PHE:CD2	1:n:96:LEU:HD13	2.54	0.42
3:s:390:TYR:CE2	3:s:399:LYS:HD2	2.54	0.42
1:0:48:TRP:O	1:0:52:PRO:HD2	2.19	0.42
2:B:47:ALA:O	2:B:63:LYS:HE2	2.19	0.42
2:B:657:GLU:HG2	2:B:661:ASN:ND2	2.32	0.42
2:D:53:LYS:HD3	2:D:57:GLN:O	2.19	0.42
2:F:254:TYR:CE1	2:F:518:LEU:HB3	2.55	0.42
2:F:661:ASN:HA	2:G:666:LEU:HD21	2.01	0.42
2:G:313:GLY:O	2:G:463:ASN:ND2	2.52	0.42
2:G:602:GLN:HA	2:G:606:GLN:NE2	2.34	0.42
2:K:35:ARG:HG3	2:K:39:VAL:HG21	2.01	0.42
2:K:604:ILE:O	2:K:607:GLN:HG3	2.19	0.42
3:P:197:GLU:OE2	3:P:197:GLU:HA	2.18	0.42
3:T:344:THR:HB	3:T:347:GLN:HG3	2.01	0.42
3:U:121:GLU:HA	3:U:121:GLU:OE2	2.19	0.42
3:U:189:ASP:OD1	3:U:190:GLN:N	2.52	0.42
3:W:237:THR:O	3:W:241:VAL:HG22	2.20	0.42
3:Z:70:ASN:OD1	3:Z:70:ASN:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:189:ASP:OD1	3:d:190:GLN:N	2.52	0.42
3:d:370:LEU:H	3:d:388:HIS:HE1	1.66	0.42
3:j:344:THR:HG22	3:j:345:ALA:H	1.84	0.42
3:m:139:PRO:HB3	3:m:349:MET:HE2	2.01	0.42
3:o:182:GLN:HE22	3:o:202:PRO:HD3	1.84	0.42
3:s:387:VAL:HG22	3:s:402:PHE:HD1	1.84	0.42
1:0:141:THR:HG22	3:s:366:PRO:HB2	2.02	0.42
2:B:575:GLU:OE1	2:C:109:ARG:NH2	2.37	0.42
2:D:653:GLN:O	2:D:656:MET:HG3	2.19	0.42
2:H:662:THR:O	2:H:666:LEU:HG	2.20	0.42
2:I:250:GLU:HG3	2:I:251:ILE:HG12	2.01	0.42
2:J:658:SER:HA	2:J:661:ASN:HD22	1.84	0.42
2:L:75:ARG:NH2	2:L:79:GLU:OE2	2.53	0.42
2:L:99:GLU:HG2	2:L:510:ARG:NH2	2.34	0.42
3:R:109:LEU:O	3:R:112:VAL:HG22	2.19	0.42
3:T:229:THR:OG1	3:T:337:ASP:O	2.34	0.42
3:V:214:ASN:OD1	3:V:215:GLY:N	2.52	0.42
1:Y:151:PRO:O	1:Y:152:LEU:C	2.62	0.42
3:c:12:ILE:HA	3:u:10:SER:HB2	2.01	0.42
3:l:179:ALA:O	3:l:183:THR:HG23	2.19	0.42
3:q:36:LEU:HA	3:q:39:GLU:HG3	2.01	0.42
1:v:45:MET:HA	1:v:45:MET:HE3	2.01	0.42
1:w:16:ARG:NH1	1:w:16:ARG:HG2	2.34	0.42
3:y:4:ASN:OD1	3:y:5:LEU:N	2.50	0.42
3:y:214:ASN:OD1	3:y:215:GLY:N	2.53	0.42
1:z:48:TRP:HZ2	1:z:85:GLN:HG3	1.84	0.42
1:0:122:SER:HA	2:I:379:PRO:HA	2.01	0.42
2:A:613:GLN:O	2:A:613:GLN:NE2	2.51	0.42
2:A:627:MET:HE2	2:L:622:LEU:HA	2.01	0.42
2:C:245:HIS:HD2	2:C:246:PRO:HD2	1.85	0.42
2:G:165:ARG:HH21	2:G:210:THR:HG21	1.84	0.42
2:G:207:LEU:HD23	2:G:207:LEU:H	1.85	0.42
2:G:664:TYR:CE2	2:H:669:ALA:HB3	2.55	0.42
2:H:613:GLN:C	2:H:616:PRO:HD2	2.44	0.42
3:M:267:GLN:NE2	3:M:418:GLN:OE1	2.53	0.42
3:X:214:ASN:OD1	3:X:215:GLY:N	2.53	0.42
3:j:334:GLU:N	3:j:337:ASP:OD2	2.52	0.42
3:l:128:MET:HE3	3:l:128:MET:HB2	1.74	0.42
3:m:163:GLU:HA	3:m:163:GLU:OE2	2.19	0.42
3:q:179:ALA:O	3:q:183:THR:HG23	2.20	0.42
3:u:23:SER:OG	3:u:24:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:111:ASP:O	1:1:115:THR:HG23	2.19	0.42
2:B:636:LYS:NZ	2:C:638:THR:O	2.51	0.42
2:E:450:MET:N	2:E:450:MET:SD	2.92	0.42
2:G:615:GLN:O	2:G:618:PRO:HD2	2.19	0.42
2:H:19:ALA:HA	2:H:171:PRO:HG3	2.01	0.42
2:I:182:LEU:HA	2:I:233:VAL:HG22	2.02	0.42
2:J:653:GLN:HA	2:J:656:MET:HE2	2.02	0.42
2:K:337:LEU:HD12	2:K:337:LEU:HA	1.91	0.42
3:T:156:LEU:HD23	3:T:156:LEU:HA	1.91	0.42
3:U:344:THR:HG22	3:U:345:ALA:N	2.35	0.42
3:X:115:ARG:HA	3:X:115:ARG:HD3	1.72	0.42
3:i:252:THR:HG22	3:i:308:ASP:OD2	2.20	0.42
3:q:25:LEU:HD11	3:q:117:VAL:CG1	2.50	0.42
1:r:50:ILE:HG13	1:r:51:ASN:H	1.85	0.42
2:F:618:PRO:HA	2:F:621:VAL:HG12	2.00	0.42
2:H:53:LYS:HE2	2:H:53:LYS:HB2	1.32	0.42
3:N:237:THR:O	3:N:241:VAL:HG22	2.19	0.42
3:Q:35:LEU:HD23	3:Q:411:PHE:CE1	2.54	0.42
3:e:108:ILE:HG23	3:j:56:PHE:CZ	2.55	0.42
3:l:28:ALA:O	3:l:33:ARG:HD2	2.20	0.42
3:o:221:GLN:NE2	3:o:342:VAL:O	2.53	0.42
1:w:150:LEU:HD23	1:w:150:LEU:H	1.84	0.42
1:x:45:MET:HG2	1:x:57:TYR:CG	2.54	0.42
1:0:3:THR:HG23	1:x:63:ASP:HA	2.02	0.42
2:D:603:GLN:HG2	2:D:604:ILE:HG12	2.01	0.42
2:E:190:LEU:HD11	2:E:194:LYS:HD3	2.01	0.42
2:F:114:GLU:OE1	2:F:154:ARG:NH2	2.51	0.42
2:I:369:LYS:HB2	2:I:369:LYS:HE2	1.86	0.42
3:R:245:TYR:HD2	3:R:413:PRO:HD2	1.85	0.42
3:y:200:GLN:NE2	3:y:201:ILE:O	2.52	0.42
2:B:589:LEU:HD13	2:B:594:ALA:HB3	2.02	0.42
2:C:565:GLN:HE22	2:D:554:MET:HG2	1.85	0.42
2:F:162:ASP:O	2:F:166:SER:CB	2.68	0.42
3:O:276:LEU:O	3:O:278:GLN:NE2	2.53	0.42
3:W:222:GLY:HA3	3:W:263:LYS:HG3	2.01	0.42
3:X:140:ASN:OD1	3:X:141:THR:N	2.52	0.42
3:X:188:SER:O	3:X:192:VAL:HG13	2.20	0.42
3:a:245:TYR:HD2	3:a:413:PRO:HD2	1.84	0.42
3:c:30:THR:HG21	3:c:211:LEU:HD11	2.02	0.42
3:c:96:LEU:O	3:c:100:ILE:HG12	2.20	0.42
3:i:245:TYR:HD2	3:i:413:PRO:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j:124:LEU:HD22	3:j:362:LEU:HD22	2.02	0.42
3:j:165:GLU:OE1	3:j:165:GLU:HA	2.20	0.42
1:w:16:ARG:HG2	1:w:16:ARG:HH11	1.83	0.42
3:y:180:ASP:O	3:y:183:THR:HG22	2.20	0.42
2:A:596:PRO:HB3	2:A:601:GLU:HG2	2.02	0.42
2:B:1:MET:HE2	2:B:1:MET:HB3	1.86	0.42
2:C:239:ASP:HA	2:C:278:SER:HA	2.01	0.42
2:D:360:GLY:O	2:D:364:ILE:HG22	2.19	0.42
2:E:31:ILE:HD11	2:E:165:ARG:HB3	2.01	0.42
2:E:100:LEU:HB2	2:E:510:ARG:HH21	1.84	0.42
2:E:115:THR:HG22	2:E:116:ASP:N	2.28	0.42
2:I:47:ALA:O	2:I:63:LYS:HE2	2.20	0.42
2:I:203:PRO:O	2:I:204:PRO:C	2.61	0.42
2:I:288:VAL:HG12	2:I:295:LEU:HD12	2.01	0.42
2:I:622:LEU:HA	2:I:625:ALA:HB3	2.02	0.42
2:J:487:ARG:HG3	2:J:489:VAL:HG23	2.01	0.42
2:K:45:GLU:OE1	2:K:216:GLU:HB3	2.20	0.42
2:K:617:ASN:HB3	2:K:618:PRO:HD3	2.01	0.42
2:L:142:LEU:HD12	2:L:142:LEU:O	2.20	0.42
3:U:247:PHE:CD1	3:U:316:VAL:HG12	2.55	0.42
3:d:23:SER:OG	3:d:24:ASP:N	2.53	0.42
3:g:212:MET:SD	3:m:157:LYS:HE2	2.59	0.42
3:k:375:SER:HB3	3:k:388:HIS:CD2	2.54	0.42
3:l:124:LEU:HD22	3:l:362:LEU:HD22	2.02	0.42
3:t:316:VAL:HG23	3:t:318:ILE:HG13	2.02	0.42
2:E:640:GLU:O	2:F:645:GLN:NE2	2.46	0.42
2:G:211:SER:O	2:G:212:MET:HE2	2.19	0.42
2:I:487:ARG:H	2:I:510:ARG:HH22	1.66	0.42
3:N:22:MET:HE2	3:N:22:MET:HB3	1.89	0.42
3:T:185:LEU:HD23	3:T:185:LEU:HA	1.92	0.42
3:U:153:ALA:HB2	3:U:208:ILE:HB	2.02	0.42
1:Y:77:LYS:HE3	1:Y:77:LYS:HB2	1.82	0.42
3:a:316:VAL:HG23	3:a:318:ILE:HG13	2.02	0.42
3:b:86:TYR:HB2	3:b:404:LEU:O	2.20	0.42
3:b:375:SER:OG	3:b:386:ARG:NH1	2.53	0.42
3:l:369:LYS:HG3	3:l:375:SER:OG	2.20	0.42
3:t:189:ASP:OD1	3:t:190:GLN:N	2.53	0.42
3:u:88:THR:HG22	3:u:403:ASP:OD2	2.20	0.42
1:v:47:GLU:CD	1:x:80:HIS:HB2	2.45	0.42
3:y:35:LEU:HD23	3:y:35:LEU:HA	1.93	0.42
3:y:47:SER:OG	3:y:82:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:z:17:LYS:HD3	1:z:17:LYS:HA	1.68	0.42
2:B:457:SER:HA	2:B:460:TYR:HD2	1.85	0.41
2:D:103:LYS:HG3	2:D:510:ARG:CZ	2.50	0.41
2:D:103:LYS:HD2	2:D:510:ARG:HD2	2.02	0.41
2:D:196:GLU:HG3	2:D:201:LYS:HD2	2.01	0.41
2:H:365:ARG:O	2:H:385:ARG:NH1	2.52	0.41
2:I:59:GLU:OE1	1:v:124:ARG:HD2	2.19	0.41
2:J:58:PHE:C	3:i:96:LEU:HD12	2.45	0.41
2:J:599:GLU:HG2	2:J:600:LYS:HG2	2.01	0.41
2:L:620:MET:SD	2:L:621:VAL:N	2.93	0.41
3:U:284:LEU:HB3	3:U:291:ILE:HD12	2.01	0.41
1:Y:131:VAL:HG13	1:Y:135:ASN:HD22	1.85	0.41
3:a:389:LYS:HB2	3:a:389:LYS:HE2	1.92	0.41
3:d:95:GLN:OE1	3:d:396:ASN:ND2	2.53	0.41
3:e:105:LEU:HD22	3:e:400:MET:SD	2.60	0.41
3:e:124:LEU:O	3:e:128:MET:HG3	2.20	0.41
3:e:216:LEU:HD12	3:e:216:LEU:HA	1.80	0.41
3:g:129:MET:HB2	3:g:418:GLN:HE21	1.84	0.41
3:o:2:PRO:HB2	3:o:3:ASN:H	1.57	0.41
3:u:16:LYS:HE3	3:u:16:LYS:HB3	1.77	0.41
3:y:139:PRO:HG2	3:y:343:GLY:HA2	2.01	0.41
2:G:642:ALA:O	2:G:645:GLN:HG2	2.21	0.41
2:G:664:TYR:OH	2:H:670:ARG:HG2	2.20	0.41
2:I:25:GLU:HG2	1:f:139:VAL:CG1	2.51	0.41
2:I:162:ASP:HB3	2:I:165:ARG:CG	2.50	0.41
2:L:196:GLU:OE2	2:L:201:LYS:HA	2.20	0.41
3:M:192:VAL:HG21	3:U:187:ALA:HB3	2.01	0.41
3:Q:190:GLN:HE21	3:Q:190:GLN:HB2	1.70	0.41
3:Q:365:ILE:HD11	3:Q:407:ALA:HB2	2.02	0.41
3:b:231:LYS:HB3	3:b:250:THR:HG23	2.02	0.41
1:f:110:TYR:O	1:f:114:MET:HG2	2.20	0.41
3:k:170:MET:HE2	3:k:170:MET:HB3	1.66	0.41
3:u:179:ALA:O	3:u:183:THR:HG23	2.20	0.41
3:u:182:GLN:HE21	3:u:191:LEU:CD2	2.31	0.41
2:D:152:ARG:HD3	2:D:152:ARG:HA	1.82	0.41
2:D:567:ILE:HD13	2:D:588:LEU:HD21	2.01	0.41
2:G:636:LYS:NZ	2:H:637:ALA:O	2.40	0.41
3:M:159:LEU:HD23	3:M:159:LEU:HA	1.91	0.41
3:O:245:TYR:HD2	3:O:413:PRO:HD2	1.85	0.41
3:U:221:GLN:NE2	3:U:342:VAL:O	2.53	0.41
3:e:22:MET:HE3	3:e:23:SER:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:48:TRP:O	1:f:52:PRO:HD2	2.20	0.41
3:l:170:MET:HE3	3:l:170:MET:HB2	1.70	0.41
1:n:17:LYS:HD3	1:n:17:LYS:HA	1.82	0.41
3:t:121:GLU:OE1	3:t:121:GLU:HA	2.20	0.41
3:t:219:ARG:O	3:t:348:THR:OG1	2.30	0.41
2:B:115:THR:HG22	2:B:116:ASP:N	2.27	0.41
2:E:645:GLN:HE21	2:E:645:GLN:HB3	1.71	0.41
2:F:215:TRP:CE2	1:z:139:VAL:HG12	2.56	0.41
2:I:636:LYS:HZ3	2:J:641:THR:N	2.18	0.41
2:K:244:ARG:HA	2:K:250:GLU:O	2.20	0.41
2:L:198:GLU:HG3	2:L:199:TYR:N	2.35	0.41
3:O:229:THR:HG22	3:O:338:ALA:HA	2.02	0.41
3:T:140:ASN:OD1	3:T:344:THR:OG1	2.36	0.41
3:m:156:LEU:HD23	3:m:156:LEU:HA	1.90	0.41
1:n:48:TRP:O	1:n:52:PRO:HD2	2.20	0.41
3:o:105:LEU:HD12	3:o:105:LEU:HA	1.87	0.41
3:s:40:ILE:O	3:s:365:ILE:HD12	2.21	0.41
3:t:247:PHE:HD1	3:t:316:VAL:HG12	1.85	0.41
1:z:45:MET:HE2	1:z:57:TYR:CD2	2.56	0.41
2:B:10:GLU:OE1	2:B:10:GLU:N	2.52	0.41
2:B:32:GLU:HB2	2:B:215:TRP:CZ3	2.56	0.41
2:F:599:GLU:HG2	2:F:600:LYS:H	1.86	0.41
2:F:622:LEU:O	2:G:627:MET:HE2	2.21	0.41
2:G:46:GLY:HA2	2:G:216:GLU:HG2	2.03	0.41
2:G:137:ARG:HB2	2:G:160:ILE:HD11	2.02	0.41
2:H:643:GLN:HB3	2:I:645:GLN:NE2	2.36	0.41
2:K:120:ALA:HA	2:K:159:PRO:HB3	2.02	0.41
3:P:370:LEU:HD11	3:c:396:ASN:HD22	1.86	0.41
3:W:388:HIS:HB2	3:W:401:ARG:HG2	2.03	0.41
3:Z:95:GLN:OE1	3:Z:396:ASN:ND2	2.53	0.41
3:Z:230:VAL:HG23	3:Z:336:GLY:H	1.86	0.41
3:a:309:VAL:HG12	3:a:311:VAL:HG13	2.01	0.41
3:b:284:LEU:HD23	3:b:284:LEU:HA	1.92	0.41
3:d:228:LEU:HD23	3:d:251:LEU:HD23	2.03	0.41
3:g:269:LYS:HZ2	3:g:292:SER:HB2	1.84	0.41
3:k:347:GLN:HE21	3:k:349:MET:HE3	1.86	0.41
3:k:367:LEU:HB3	3:u:95:GLN:NE2	2.36	0.41
3:m:32:ASP:OD1	3:m:33:ARG:N	2.53	0.41
1:r:87:LEU:O	1:r:91:LEU:HG	2.20	0.41
2:A:73:LEU:HD22	2:A:328:ILE:HD11	2.03	0.41
2:A:115:THR:HG21	2:A:156:ALA:HB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:LEU:HD23	2:B:54:LEU:O	2.21	0.41
2:D:334:PRO:HB2	2:D:424:ILE:HG13	2.02	0.41
2:E:615:GLN:O	2:E:618:PRO:HD2	2.21	0.41
2:F:47:ALA:O	2:F:63:LYS:HE2	2.21	0.41
2:H:650:THR:HG22	2:I:652:GLN:HE21	1.85	0.41
2:J:604:ILE:HG13	2:J:605:VAL:HG23	2.01	0.41
2:K:67:ASN:HB3	2:L:330:LYS:HD2	2.02	0.41
3:Q:389:LYS:CG	3:Q:400:MET:HE3	2.51	0.41
3:Q:411:PHE:HB3	3:U:18:LEU:HD13	2.02	0.41
3:U:166:ASN:OD1	3:U:356:ASN:ND2	2.53	0.41
3:V:241:VAL:HG11	3:V:316:VAL:HG21	2.03	0.41
3:W:247:PHE:CD1	3:W:316:VAL:HG12	2.55	0.41
3:k:26:VAL:O	3:k:30:THR:HG23	2.21	0.41
3:o:237:THR:O	3:o:241:VAL:HG22	2.20	0.41
3:s:165:GLU:H	3:s:357:LYS:HB2	1.86	0.41
1:x:91:LEU:HA	1:x:91:LEU:HD23	1.75	0.41
1:1:78:TYR:OH	1:1:116:ASP:OD2	2.28	0.41
2:F:259:VAL:HG12	2:F:261:ASP:H	1.85	0.41
2:H:229:LYS:HG2	2:H:288:VAL:HG22	2.03	0.41
3:M:15:LYS:HB3	3:M:104:GLN:NE2	2.35	0.41
3:N:61:THR:HG21	3:N:65:ASP:O	2.21	0.41
3:N:316:VAL:HG23	3:N:318:ILE:HG13	2.03	0.41
3:P:401:ARG:NH2	3:c:396:ASN:OD1	2.54	0.41
3:S:370:LEU:H	3:S:388:HIS:HE1	1.68	0.41
1:Y:30:GLU:H	1:Y:30:GLU:HG2	1.45	0.41
3:d:110:ALA:N	3:d:111:PRO:HD2	2.36	0.41
3:o:365:ILE:HD12	3:o:405:LEU:HG	2.02	0.41
1:p:7:LYS:O	1:p:11:VAL:HG23	2.21	0.41
1:0:86:LEU:O	1:0:90:MET:HB2	2.20	0.41
2:A:18:ARG:NH1	2:L:193:GLU:HG3	2.36	0.41
2:B:2:ALA:O	2:B:8:LYS:NZ	2.51	0.41
2:B:302:PRO:O	2:B:478:MET:HG3	2.21	0.41
2:B:362:GLU:HG3	1:p:114:MET:HE2	2.03	0.41
2:C:192:PRO:O	2:C:196:GLU:OE1	2.39	0.41
2:C:664:TYR:CD2	2:D:666:LEU:HD22	2.55	0.41
2:D:244:ARG:HB2	2:D:273:GLU:HG3	2.02	0.41
2:F:119:GLU:OE1	2:F:119:GLU:N	2.52	0.41
2:F:207:LEU:HB2	2:F:226:TYR:H	1.86	0.41
2:F:615:GLN:O	2:F:618:PRO:HD2	2.21	0.41
2:G:624:GLN:OE1	2:G:624:GLN:N	2.54	0.41
2:H:90:ARG:HA	2:H:91:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:384:LEU:HD12	2:H:384:LEU:HA	1.94	0.41
2:L:53:LYS:HD3	2:L:53:LYS:HA	1.84	0.41
3:P:350:LYS:HD2	3:X:283:ALA:O	2.21	0.41
3:c:46:ASP:OD2	3:c:83:VAL:HG22	2.21	0.41
3:d:102:LEU:HD23	3:j:5:LEU:HD12	2.01	0.41
3:e:390:TYR:OH	3:m:394:ASP:OD1	2.33	0.41
3:g:100:ILE:HG22	3:g:101:LYS:HG3	2.02	0.41
3:s:170:MET:HE2	3:s:170:MET:HB3	1.82	0.41
3:t:185:LEU:HD23	3:t:185:LEU:HA	1.91	0.41
3:y:188:SER:O	3:y:192:VAL:HG13	2.20	0.41
1:0:81:ALA:O	1:0:85:GLN:HG2	2.21	0.41
2:D:302:PRO:O	2:D:478:MET:HG3	2.21	0.41
2:E:457:SER:O	2:E:461:LEU:HD13	2.21	0.41
2:E:551:LEU:HD13	2:E:564:ILE:HG21	2.03	0.41
2:E:569:LEU:O	2:E:572:ILE:HG22	2.21	0.41
2:F:628:VAL:O	2:F:631:GLN:HG2	2.21	0.41
2:F:643:GLN:HA	2:F:646:ILE:HD12	2.02	0.41
2:G:177:ASP:OD1	2:G:177:ASP:N	2.43	0.41
2:G:353:PRO:HD3	1:h:126:ARG:NH2	2.32	0.41
2:G:569:LEU:O	2:G:572:ILE:HG22	2.21	0.41
2:G:599:GLU:N	2:G:599:GLU:OE2	2.54	0.41
2:H:551:LEU:HD23	2:H:551:LEU:HA	1.86	0.41
2:I:384:LEU:HD23	2:I:398:ALA:O	2.21	0.41
2:I:615:GLN:O	2:I:618:PRO:HD2	2.21	0.41
2:K:214:SER:H	2:K:219:TRP:HE1	1.69	0.41
2:L:595:LYS:HD3	2:L:595:LYS:HA	1.80	0.41
3:M:165:GLU:OE2	3:M:165:GLU:N	2.48	0.41
3:M:170:MET:HE3	3:M:170:MET:HB2	1.92	0.41
3:M:317:PRO:HB2	3:M:329:VAL:HG11	2.03	0.41
3:N:98:GLU:HA	3:N:102:LEU:HB2	2.01	0.41
3:Q:108:ILE:HG23	3:a:54:HIS:ND1	2.36	0.41
3:V:123:GLU:OE1	3:V:123:GLU:HA	2.20	0.41
3:V:344:THR:HG22	3:V:345:ALA:N	2.35	0.41
3:Z:209:ARG:HB3	3:Z:209:ARG:NH1	2.36	0.41
3:d:393:GLY:O	3:o:401:ARG:NH1	2.54	0.41
3:e:319:TYR:HD1	3:e:332:GLN:HB2	1.85	0.41
3:e:369:LYS:HB2	3:e:386:ARG:NH2	2.36	0.41
3:g:273:THR:HG21	3:g:333:VAL:HG22	2.01	0.41
1:h:31:PRO:HA	1:h:34:ILE:HD13	2.03	0.41
3:k:66:ILE:HD12	3:k:69:GLN:HE22	1.86	0.41
3:q:401:ARG:HH21	3:q:403:ASP:CG	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:r:138:ASP:OD1	1:r:139:VAL:HG22	2.21	0.41
1:z:48:TRP:O	1:z:52:PRO:HD2	2.21	0.41
1:0:140:PHE:HA	2:L:215:TRP:CD1	2.56	0.41
1:0:140:PHE:HD1	2:L:215:TRP:CD1	2.39	0.41
2:A:273:GLU:CD	2:A:274:VAL:H	2.29	0.41
2:C:241:ILE:HG12	2:C:275:ALA:HB1	2.01	0.41
2:E:274:VAL:HG22	2:E:276:ARG:NH2	2.36	0.41
2:E:388:ARG:HH12	1:h:107:GLN:HE22	1.69	0.41
2:F:416:LEU:HD23	2:F:416:LEU:HA	1.90	0.41
2:G:92:GLY:H	2:G:97:SER:HB2	1.86	0.41
2:H:476:LEU:HD12	2:H:476:LEU:HA	1.91	0.41
2:H:646:ILE:O	2:H:650:THR:HG23	2.21	0.41
2:I:19:ALA:HB2	2:I:183:TRP:CH2	2.55	0.41
2:K:180:ASP:OD1	2:K:180:ASP:N	2.53	0.41
3:M:241:VAL:HG21	3:M:316:VAL:HG21	2.03	0.41
3:Q:66:ILE:O	3:Q:66:ILE:HG22	2.20	0.41
3:R:359:PHE:HE1	3:R:413:PRO:HA	1.86	0.41
3:S:11:GLN:OE1	3:S:11:GLN:N	2.54	0.41
1:Y:87:LEU:HG	1:Y:91:LEU:HD12	2.01	0.41
3:a:22:MET:HE2	3:a:22:MET:HB3	1.89	0.41
3:a:230:VAL:HG23	3:a:336:GLY:H	1.86	0.41
3:i:14:LEU:HD13	3:q:39:GLU:OE1	2.21	0.41
3:k:13:VAL:HG21	3:k:101:LYS:HE2	2.02	0.41
3:k:179:ALA:O	3:k:183:THR:HG23	2.21	0.41
3:l:375:SER:HB3	3:l:388:HIS:CD2	2.56	0.41
2:B:244:ARG:HH22	2:B:246:PRO:HG3	1.86	0.40
2:H:114:GLU:HB3	2:H:154:ARG:HH21	1.85	0.40
2:I:546:VAL:O	2:I:550:VAL:HG23	2.21	0.40
2:I:598:ASN:HA	2:I:602:GLN:HG2	2.02	0.40
2:J:115:THR:HG22	2:J:116:ASP:N	2.36	0.40
2:K:510:ARG:HE	2:K:511:GLN:N	2.19	0.40
2:L:111:ASP:HA	2:L:154:ARG:NH1	2.36	0.40
3:N:245:TYR:HD2	3:N:413:PRO:HD2	1.87	0.40
3:R:216:LEU:HB3	3:R:350:LYS:NZ	2.36	0.40
3:X:102:LEU:HD13	3:X:102:LEU:HA	1.77	0.40
3:e:273:THR:HG21	3:e:333:VAL:HG22	2.03	0.40
1:h:124:ARG:NH1	1:h:149:ASP:HA	2.37	0.40
3:q:250:THR:OG1	3:q:308:ASP:OD1	2.38	0.40
3:u:233:GLN:OE1	3:u:332:GLN:NE2	2.53	0.40
1:z:144:ARG:HB3	1:z:145:TYR:CD1	2.56	0.40
2:B:487:ARG:HB3	2:B:487:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:142:LEU:H	2:C:142:LEU:HD23	1.86	0.40
2:E:595:LYS:O	2:E:595:LYS:HG2	2.22	0.40
2:F:42:GLY:HA2	2:F:45:GLU:HG3	2.02	0.40
2:F:90:ARG:HA	2:F:91:PRO:HD3	1.96	0.40
2:L:174:LYS:O	2:L:315:ARG:NH2	2.54	0.40
2:L:288:VAL:HB	2:L:296:GLU:HB2	2.03	0.40
3:V:121:GLU:HA	3:V:121:GLU:OE1	2.22	0.40
3:a:22:MET:HG2	3:a:23:SER:N	2.37	0.40
3:b:182:GLN:HE22	3:b:202:PRO:HD3	1.86	0.40
3:c:247:PHE:HD1	3:c:316:VAL:HG12	1.85	0.40
1:f:75:PRO:HB2	1:f:77:LYS:HG2	2.03	0.40
3:l:57:SER:HB3	3:l:325:GLN:HB3	2.03	0.40
3:l:89:VAL:HG11	3:l:112:VAL:HG13	2.03	0.40
3:m:141:THR:HA	3:m:142:PRO:HD3	1.97	0.40
3:m:237:THR:O	3:m:241:VAL:HG22	2.21	0.40
1:n:5:LEU:HD23	1:n:5:LEU:HA	1.81	0.40
3:o:159:LEU:HD23	3:o:159:LEU:HA	1.92	0.40
3:y:210:ALA:O	3:y:211:LEU:HD23	2.21	0.40
2:A:180:ASP:OD1	2:A:180:ASP:N	2.48	0.40
2:B:664:TYR:CD2	2:C:666:LEU:HD22	2.56	0.40
2:C:516:VAL:O	2:C:518:LEU:HD12	2.21	0.40
2:D:115:THR:HG22	2:D:116:ASP:N	2.28	0.40
2:E:243:TYR:HA	2:E:271:PHE:O	2.21	0.40
2:F:617:ASN:HB3	2:F:618:PRO:HD3	2.03	0.40
2:G:551:LEU:HG	2:G:552:SER:H	1.86	0.40
2:H:53:LYS:HA	2:H:57:GLN:O	2.21	0.40
2:K:245:HIS:HB3	2:K:270:GLY:HA2	2.02	0.40
3:N:218:SER:HB3	3:N:350:LYS:HZ3	1.85	0.40
3:Q:113:ARG:HG3	3:Q:380:TYR:CE2	2.56	0.40
3:S:58:SER:OG	3:W:119:ASP:OD2	2.25	0.40
3:S:111:PRO:HA	3:S:114:GLN:HG3	2.03	0.40
3:S:185:LEU:HD23	3:S:185:LEU:HA	1.94	0.40
3:V:156:LEU:HD23	3:V:156:LEU:HA	1.89	0.40
3:a:167:TYR:CE1	3:a:209:ARG:HD3	2.57	0.40
3:b:35:LEU:HD13	3:b:35:LEU:HA	1.73	0.40
3:g:178:LEU:HD12	3:g:205:PHE:CZ	2.56	0.40
3:o:188:SER:OG	3:o:191:LEU:HD13	2.21	0.40
1:z:150:LEU:HG	1:z:151:PRO:HD2	2.03	0.40
1:1:123:MET:HE2	1:1:123:MET:HB3	1.97	0.40
2:B:137:ARG:HG2	2:B:139:THR:HG23	2.04	0.40
2:D:207:LEU:HB3	2:D:225:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:60:LYS:O	1:z:146:TYR:OH	2.30	0.40
2:F:114:GLU:HB2	2:F:154:ARG:NH2	2.36	0.40
2:F:488:GLU:O	2:F:488:GLU:HG2	2.21	0.40
2:G:114:GLU:OE1	2:G:154:ARG:NH2	2.54	0.40
2:J:509:ASP:OD2	2:J:511:GLN:NE2	2.54	0.40
2:K:340:LEU:HD22	1:x:130:PRO:HD3	2.03	0.40
3:N:51:LYS:HE3	3:q:15:LYS:HA	2.03	0.40
3:N:221:GLN:NE2	3:N:343:GLY:HA3	2.36	0.40
3:O:129:MET:SD	3:O:219:ARG:HD3	2.61	0.40
3:Z:46:ASP:O	3:Z:83:VAL:HG13	2.22	0.40
3:k:319:TYR:CD2	3:k:332:GLN:HB2	2.56	0.40
3:o:173:TRP:NE1	3:y:158:ASP:OD1	2.55	0.40
1:r:63:ASP:OD2	1:r:64:GLU:N	2.54	0.40
3:u:165:GLU:N	3:u:165:GLU:OE2	2.55	0.40
3:u:229:THR:O	3:u:252:THR:N	2.53	0.40
2:A:662:THR:O	2:A:666:LEU:N	2.54	0.40
2:C:196:GLU:HG3	2:C:201:LYS:HA	2.03	0.40
2:C:240:VAL:HG12	2:C:255:ASP:HA	2.02	0.40
2:C:554:MET:HB2	2:C:558:ASP:OD2	2.22	0.40
2:E:344:MET:HE2	1:n:126:ARG:HH11	1.87	0.40
2:H:115:THR:HG22	2:H:116:ASP:N	2.26	0.40
2:I:613:GLN:C	2:I:616:PRO:HD2	2.46	0.40
2:I:613:GLN:O	2:I:616:PRO:HD2	2.21	0.40
2:K:309:ILE:HG21	2:K:471:ALA:HB2	2.03	0.40
3:M:98:GLU:HA	3:M:102:LEU:HD12	2.02	0.40
3:Q:185:LEU:HD23	3:Q:185:LEU:HA	1.94	0.40
3:T:333:VAL:O	3:T:333:VAL:HG13	2.22	0.40
1:Y:45:MET:O	1:Y:49:MET:HG2	2.21	0.40
3:a:276:LEU:HD11	3:a:330:SER:HB3	2.03	0.40
3:a:303:SER:HB2	3:a:309:VAL:HG22	2.04	0.40
3:b:11:GLN:O	3:s:10:SER:HB2	2.20	0.40
3:j:219:ARG:NH1	3:j:221:GLN:OE1	2.55	0.40
3:k:13:VAL:HG12	3:s:49:SER:HB2	2.03	0.40
3:s:61:THR:HG22	3:s:64:GLY:H	1.86	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	0	146/160 (91%)	138 (94%)	8 (6%)	0	100	100
1	1	156/160 (98%)	146 (94%)	10 (6%)	0	100	100
1	Y	146/160 (91%)	135 (92%)	10 (7%)	1 (1%)	18	50
1	f	156/160 (98%)	150 (96%)	6 (4%)	0	100	100
1	h	146/160 (91%)	142 (97%)	4 (3%)	0	100	100
1	n	146/160 (91%)	135 (92%)	11 (8%)	0	100	100
1	p	156/160 (98%)	146 (94%)	10 (6%)	0	100	100
1	r	146/160 (91%)	143 (98%)	3 (2%)	0	100	100
1	v	146/160 (91%)	141 (97%)	5 (3%)	0	100	100
1	w	146/160 (91%)	137 (94%)	9 (6%)	0	100	100
1	x	156/160 (98%)	143 (92%)	13 (8%)	0	100	100
1	z	156/160 (98%)	142 (91%)	14 (9%)	0	100	100
2	A	620/708 (88%)	590 (95%)	30 (5%)	0	100	100
2	B	620/708 (88%)	586 (94%)	34 (6%)	0	100	100
2	C	620/708 (88%)	587 (95%)	33 (5%)	0	100	100
2	D	620/708 (88%)	589 (95%)	31 (5%)	0	100	100
2	E	620/708 (88%)	594 (96%)	26 (4%)	0	100	100
2	F	620/708 (88%)	590 (95%)	30 (5%)	0	100	100
2	G	620/708 (88%)	589 (95%)	31 (5%)	0	100	100
2	H	620/708 (88%)	599 (97%)	20 (3%)	1 (0%)	43	71
2	I	620/708 (88%)	591 (95%)	28 (4%)	1 (0%)	43	71
2	J	620/708 (88%)	587 (95%)	33 (5%)	0	100	100
2	K	620/708 (88%)	582 (94%)	38 (6%)	0	100	100
2	L	620/708 (88%)	594 (96%)	26 (4%)	0	100	100
3	M	420/423 (99%)	402 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	N	420/423 (99%)	405 (96%)	15 (4%)	0	100	100
3	O	420/423 (99%)	404 (96%)	16 (4%)	0	100	100
3	P	420/423 (99%)	405 (96%)	15 (4%)	0	100	100
3	Q	420/423 (99%)	407 (97%)	13 (3%)	0	100	100
3	R	420/423 (99%)	410 (98%)	10 (2%)	0	100	100
3	S	420/423 (99%)	412 (98%)	8 (2%)	0	100	100
3	T	420/423 (99%)	406 (97%)	14 (3%)	0	100	100
3	U	420/423 (99%)	401 (96%)	19 (4%)	0	100	100
3	V	420/423 (99%)	401 (96%)	19 (4%)	0	100	100
3	W	420/423 (99%)	401 (96%)	19 (4%)	0	100	100
3	X	420/423 (99%)	398 (95%)	22 (5%)	0	100	100
3	Z	419/423 (99%)	401 (96%)	18 (4%)	0	100	100
3	a	419/423 (99%)	405 (97%)	14 (3%)	0	100	100
3	b	419/423 (99%)	402 (96%)	17 (4%)	0	100	100
3	c	419/423 (99%)	403 (96%)	16 (4%)	0	100	100
3	d	419/423 (99%)	400 (96%)	19 (4%)	0	100	100
3	e	412/423 (97%)	390 (95%)	22 (5%)	0	100	100
3	g	412/423 (97%)	394 (96%)	18 (4%)	0	100	100
3	i	412/423 (97%)	393 (95%)	19 (5%)	0	100	100
3	j	420/423 (99%)	407 (97%)	13 (3%)	0	100	100
3	k	412/423 (97%)	386 (94%)	26 (6%)	0	100	100
3	l	412/423 (97%)	388 (94%)	24 (6%)	0	100	100
3	m	420/423 (99%)	409 (97%)	11 (3%)	0	100	100
3	o	420/423 (99%)	403 (96%)	17 (4%)	0	100	100
3	q	420/423 (99%)	411 (98%)	9 (2%)	0	100	100
3	s	420/423 (99%)	404 (96%)	16 (4%)	0	100	100
3	t	420/423 (99%)	410 (98%)	10 (2%)	0	100	100
3	u	420/423 (99%)	402 (96%)	18 (4%)	0	100	100
3	y	420/423 (99%)	402 (96%)	18 (4%)	0	100	100
All	All	21797/23106 (94%)	20838 (96%)	956 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	211	SER
1	Y	24	ALA
2	H	55	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	128/137 (93%)	123 (96%)	5 (4%)	28	52
1	1	136/137 (99%)	130 (96%)	6 (4%)	25	50
1	Y	128/137 (93%)	107 (84%)	21 (16%)	2	14
1	f	136/137 (99%)	133 (98%)	3 (2%)	45	63
1	h	128/137 (93%)	124 (97%)	4 (3%)	35	57
1	n	128/137 (93%)	124 (97%)	4 (3%)	35	57
1	p	136/137 (99%)	132 (97%)	4 (3%)	37	57
1	r	128/137 (93%)	128 (100%)	0	100	100
1	v	128/137 (93%)	128 (100%)	0	100	100
1	w	128/137 (93%)	128 (100%)	0	100	100
1	x	136/137 (99%)	134 (98%)	2 (2%)	57	68
1	z	135/137 (98%)	135 (100%)	0	100	100
2	A	522/592 (88%)	513 (98%)	9 (2%)	53	67
2	B	522/592 (88%)	521 (100%)	1 (0%)	87	86
2	C	522/592 (88%)	505 (97%)	17 (3%)	33	55
2	D	522/592 (88%)	522 (100%)	0	100	100
2	E	522/592 (88%)	512 (98%)	10 (2%)	50	65
2	F	522/592 (88%)	519 (99%)	3 (1%)	78	79
2	G	522/592 (88%)	522 (100%)	0	100	100
2	H	522/592 (88%)	519 (99%)	3 (1%)	78	79
2	I	522/592 (88%)	512 (98%)	10 (2%)	50	65
2	J	522/592 (88%)	516 (99%)	6 (1%)	65	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	522/592 (88%)	518 (99%)	4 (1%)	73	76
2	L	522/592 (88%)	521 (100%)	1 (0%)	87	86
3	M	350/351 (100%)	338 (97%)	12 (3%)	32	55
3	N	350/351 (100%)	350 (100%)	0	100	100
3	O	350/351 (100%)	350 (100%)	0	100	100
3	P	350/351 (100%)	350 (100%)	0	100	100
3	Q	350/351 (100%)	349 (100%)	1 (0%)	86	83
3	R	350/351 (100%)	346 (99%)	4 (1%)	65	73
3	S	350/351 (100%)	350 (100%)	0	100	100
3	T	350/351 (100%)	349 (100%)	1 (0%)	86	83
3	U	350/351 (100%)	350 (100%)	0	100	100
3	V	350/351 (100%)	350 (100%)	0	100	100
3	W	350/351 (100%)	350 (100%)	0	100	100
3	X	350/351 (100%)	338 (97%)	12 (3%)	32	55
3	Z	349/351 (99%)	349 (100%)	0	100	100
3	a	349/351 (99%)	347 (99%)	2 (1%)	78	79
3	b	349/351 (99%)	344 (99%)	5 (1%)	59	70
3	c	349/351 (99%)	349 (100%)	0	100	100
3	d	349/351 (99%)	346 (99%)	3 (1%)	70	74
3	e	342/351 (97%)	335 (98%)	7 (2%)	48	64
3	g	342/351 (97%)	342 (100%)	0	100	100
3	i	342/351 (97%)	337 (98%)	5 (2%)	57	68
3	j	350/351 (100%)	344 (98%)	6 (2%)	53	67
3	k	342/351 (97%)	338 (99%)	4 (1%)	63	71
3	l	342/351 (97%)	332 (97%)	10 (3%)	37	57
3	m	350/351 (100%)	350 (100%)	0	100	100
3	o	350/351 (100%)	350 (100%)	0	100	100
3	q	350/351 (100%)	347 (99%)	3 (1%)	70	74
3	s	350/351 (100%)	350 (100%)	0	100	100
3	t	350/351 (100%)	345 (99%)	5 (1%)	59	70
3	u	350/351 (100%)	344 (98%)	6 (2%)	53	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	y	350/351 (100%)	346 (99%)	4 (1%)	65	73
All	All	18294/19278 (95%)	18091 (99%)	203 (1%)	63	73

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	16	ARG
1	0	17	LYS
1	0	27	THR
1	0	29	VAL
1	0	30	GLU
1	1	90	MET
1	1	97	GLU
1	1	150	LEU
1	1	153	ILE
1	1	157	ILE
1	1	159	ASN
2	A	621	VAL
2	A	622	LEU
2	A	626	GLN
2	A	635	GLN
2	A	636	LYS
2	A	643	GLN
2	A	654	ASP
2	A	665	LYS
2	A	668	GLN
2	B	643	GLN
2	C	52	THR
2	C	53	LYS
2	C	54	LEU
2	C	56	GLU
2	C	57	GLN
2	C	60	LYS
2	C	631	GLN
2	C	633	GLU
2	C	635	GLN
2	C	636	LYS
2	C	638	THR
2	C	641	THR
2	C	643	GLN
2	C	645	GLN
2	C	646	ILE

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Mol	Chain	Res	Type
2	C	647	LYS
2	C	652	GLN
2	E	207	LEU
2	E	209	VAL
2	E	210	THR
2	E	211	SER
2	E	212	MET
2	E	213	THR
2	E	218	ASN
2	E	220	PHE
2	E	224	VAL
2	E	229	LYS
2	F	177	ASP
2	F	179	SER
2	F	182	LEU
2	H	53	LYS
2	H	54	LEU
2	H	55	ASP
2	I	177	ASP
2	I	179	SER
2	I	182	LEU
2	I	207	LEU
2	I	209	VAL
2	I	215	TRP
2	I	216	GLU
2	I	219	TRP
2	I	220	PHE
2	I	229	LYS
2	J	71	THR
2	J	72	GLU
2	J	83	ASN
2	J	450	MET
2	J	451	ASN
2	J	452	ARG
2	K	519	ASN
2	K	520	ASP
2	K	521	LEU
2	K	532	VAL
2	L	519	ASN
3	M	22	MET
3	M	25	LEU
3	M	29	LYS

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Mol	Chain	Res	Type
3	M	31	VAL
3	M	32	ASP
3	M	40	ILE
3	M	44	THR
3	M	113	ARG
3	M	114	GLN
3	M	118	THR
3	M	119	ASP
3	M	120	LEU
3	Q	190	GLN
3	R	113	ARG
3	R	116	ILE
3	R	117	VAL
3	R	121	GLU
3	T	216	LEU
3	X	91	VAL
3	X	92	GLU
3	X	94	GLN
3	X	102	LEU
3	X	106	GLU
3	X	107	GLU
3	X	112	VAL
3	X	113	ARG
3	X	115	ARG
3	X	116	ILE
3	X	117	VAL
3	X	118	THR
1	Y	5	LEU
1	Y	6	THR
1	Y	9	GLU
1	Y	10	ILE
1	Y	12	LEU
1	Y	17	LYS
1	Y	20	ILE
1	Y	23	ASN
1	Y	25	SER
1	Y	27	THR
1	Y	28	ASP
1	Y	29	VAL
1	Y	30	GLU
1	Y	76	ARG
1	Y	77	LYS

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Mol	Chain	Res	Type
1	Y	90	MET
1	Y	91	LEU
1	Y	139	VAL
1	Y	143	ASP
1	Y	150	LEU
1	Y	152	LEU
3	a	10	SER
3	a	12	ILE
3	b	35	LEU
3	b	40	ILE
3	b	43	SER
3	b	49	SER
3	b	52	ARG
3	d	116	ILE
3	d	377	VAL
3	d	379	THR
3	e	166	ASN
3	e	169	VAL
3	e	170	MET
3	e	171	ASP
3	e	218	SER
3	e	220	THR
3	e	221	GLN
1	f	154	ASP
1	f	156	ASP
1	f	157	ILE
1	h	77	LYS
1	h	111	ASP
1	h	114	MET
1	h	119	VAL
3	i	170	MET
3	i	177	ARG
3	i	178	LEU
3	i	408	TYR
3	i	409	VAL
3	j	97	GLU
3	j	101	LYS
3	j	389	LYS
3	j	396	ASN
3	j	397	VAL
3	j	399	LYS
3	k	165	GLU

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Mol	Chain	Res	Type
3	k	166	ASN
3	k	169	VAL
3	k	171	ASP
3	l	115	ARG
3	l	116	ILE
3	l	117	VAL
3	l	120	LEU
3	l	121	GLU
3	l	129	MET
3	l	166	ASN
3	l	169	VAL
3	l	170	MET
3	l	176	GLN
1	n	3	THR
1	n	4	VAL
1	n	7	LYS
1	n	15	LEU
1	p	139	VAL
1	p	141	THR
1	p	152	LEU
1	p	157	ILE
3	q	10	SER
3	q	11	GLN
3	q	422	ASN
3	t	57	SER
3	t	58	SER
3	t	61	THR
3	t	66	ILE
3	t	221	GLN
3	u	277	GLN
3	u	280	THR
3	u	282	GLN
3	u	284	LEU
3	u	387	VAL
3	u	399	LYS
1	x	88	LEU
1	x	90	MET
3	y	113	ARG
3	y	117	VAL
3	y	121	GLU
3	y	122	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (206)

such sidechains are listed below:

Mol	Chain	Res	Type
1	0	101	GLN
1	0	105	ASN
1	1	39	ASN
1	1	107	GLN
1	1	133	GLN
1	1	135	ASN
2	A	67	ASN
2	A	355	GLN
2	A	602	GLN
2	A	624	GLN
2	A	635	GLN
2	A	671	ASN
2	B	9	HIS
2	B	57	GLN
2	B	258	GLN
2	B	370	HIS
2	B	606	GLN
2	C	23	GLN
2	C	245	HIS
2	C	351	GLN
2	C	519	ASN
2	C	565	GLN
2	C	643	GLN
2	C	661	ASN
2	D	9	HIS
2	D	370	HIS
2	D	411	GLN
2	D	418	GLN
2	D	425	GLN
2	D	609	GLN
2	E	511	GLN
2	E	607	GLN
2	E	609	GLN
2	E	661	ASN
2	F	23	GLN
2	F	393	ASN
2	F	519	ASN
2	F	584	ASN
2	G	23	GLN
2	G	607	GLN
2	G	609	GLN
2	G	652	GLN

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Mol	Chain	Res	Type
2	H	511	GLN
2	H	519	ASN
2	I	153	GLN
2	I	218	ASN
2	I	393	ASN
2	I	519	ASN
2	J	83	ASN
2	J	245	HIS
2	J	393	ASN
2	J	451	ASN
2	J	631	GLN
2	J	671	ASN
2	K	258	GLN
2	K	645	GLN
2	L	57	GLN
2	L	153	GLN
2	L	393	ASN
3	M	72	ASN
3	M	114	GLN
3	M	182	GLN
3	M	221	GLN
3	M	267	GLN
3	M	332	GLN
3	M	396	ASN
3	M	418	GLN
3	N	176	GLN
3	N	239	ASN
3	N	267	GLN
3	N	282	GLN
3	N	332	GLN
3	N	371	HIS
3	O	239	ASN
3	O	272	ASN
3	O	371	HIS
3	P	55	GLN
3	P	332	GLN
3	P	418	GLN
3	Q	55	GLN
3	R	69	GLN
3	R	239	ASN
3	R	388	HIS
3	S	4	ASN

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Mol	Chain	Res	Type
3	S	69	GLN
3	S	162	ASN
3	S	388	HIS
3	T	85	ASN
3	T	233	GLN
3	T	332	GLN
3	T	418	GLN
3	U	140	ASN
3	U	221	GLN
3	U	278	GLN
3	U	356	ASN
3	V	55	GLN
3	V	352	ASN
3	V	356	ASN
3	W	73	ASN
3	W	186	HIS
3	W	371	HIS
3	X	104	GLN
3	X	186	HIS
3	X	221	GLN
3	X	356	ASN
1	Y	80	HIS
1	Y	101	GLN
1	Y	107	GLN
3	Z	72	ASN
3	Z	73	ASN
3	Z	126	HIS
3	Z	166	ASN
3	Z	186	HIS
3	Z	204	ASN
3	Z	272	ASN
3	Z	277	GLN
3	Z	398	GLN
3	a	151	GLN
3	a	166	ASN
3	b	3	ASN
3	b	233	GLN
3	b	277	GLN
3	b	278	GLN
3	b	286	ASN
3	b	347	GLN
3	b	398	GLN

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Mol	Chain	Res	Type
3	c	166	ASN
3	c	204	ASN
3	c	286	ASN
3	c	327	ASN
3	d	4	ASN
3	d	55	GLN
3	d	190	GLN
3	d	388	HIS
3	d	414	HIS
3	e	166	ASN
3	e	200	GLN
3	e	221	GLN
3	e	356	ASN
1	f	32	GLN
3	g	176	GLN
3	g	182	GLN
3	g	332	GLN
3	g	356	ASN
1	h	39	ASN
3	i	332	GLN
3	j	55	GLN
3	j	104	GLN
3	j	323	ASN
3	j	388	HIS
3	j	396	ASN
3	j	398	GLN
3	k	85	ASN
3	k	356	ASN
3	l	233	GLN
3	l	239	ASN
3	l	356	ASN
3	m	72	ASN
3	m	140	ASN
3	m	182	GLN
3	m	233	GLN
3	m	239	ASN
3	m	347	GLN
1	n	39	ASN
1	n	85	GLN
1	n	101	GLN
3	o	73	ASN
3	o	221	GLN

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Mol	Chain	Res	Type
3	o	267	GLN
3	o	279	GLN
3	o	323	ASN
3	o	332	GLN
1	p	23	ASN
1	p	101	GLN
3	q	104	GLN
3	q	398	GLN
1	r	51	ASN
3	s	104	GLN
3	s	114	GLN
3	s	186	HIS
3	t	55	GLN
3	t	69	GLN
3	t	140	ASN
3	t	162	ASN
3	t	166	ASN
3	t	388	HIS
3	u	126	HIS
3	u	182	GLN
3	u	186	HIS
3	u	204	ASN
3	u	267	GLN
3	u	282	GLN
3	u	332	GLN
3	u	388	HIS
3	u	398	GLN
1	v	32	GLN
1	v	133	GLN
1	w	101	GLN
1	x	101	GLN
3	y	182	GLN
3	y	198	ASN
3	y	200	GLN
3	y	347	GLN
3	y	356	ASN
1	z	23	ASN
1	z	32	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

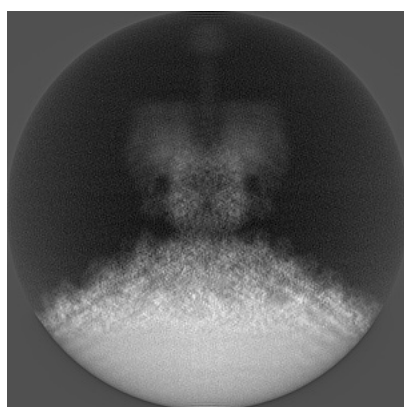
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25372. These allow visual inspection of the internal detail of the map and identification of artifacts.

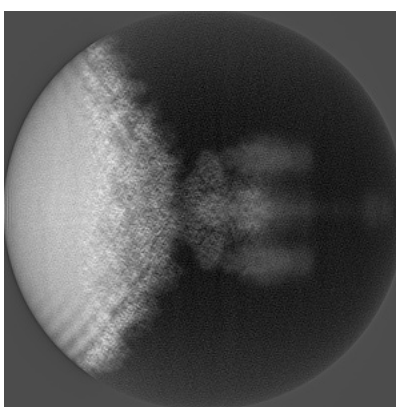
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

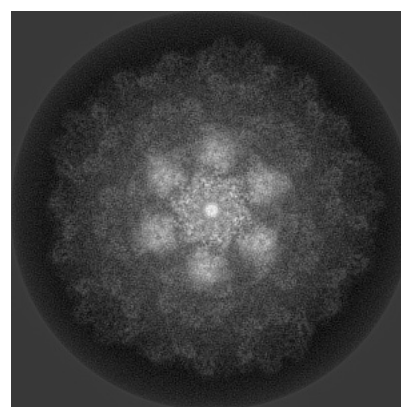
6.1.1 Primary map



X



Y

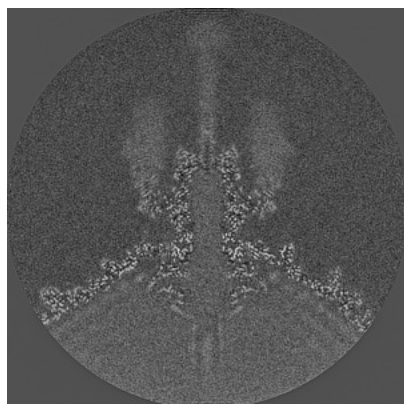


Z

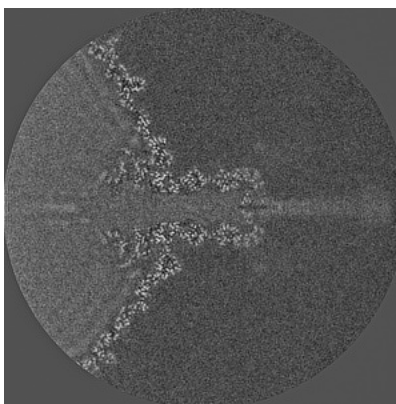
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

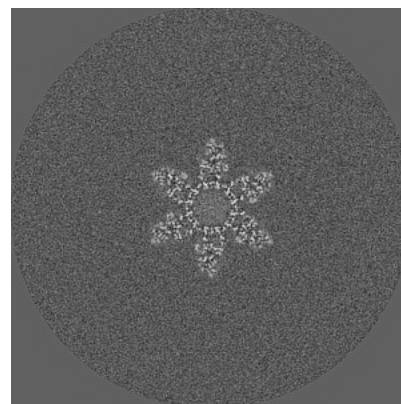
6.2.1 Primary map



X Index: 256



Y Index: 256

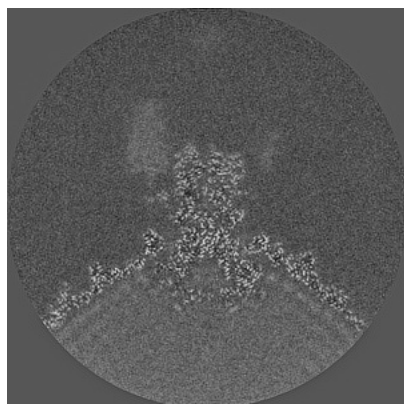


Z Index: 256

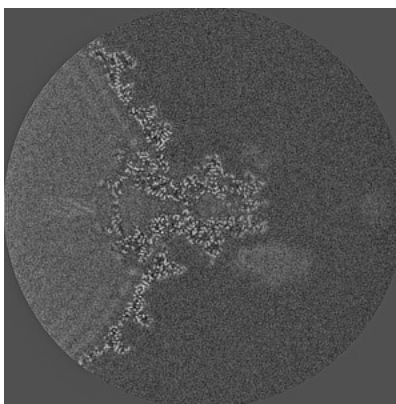
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

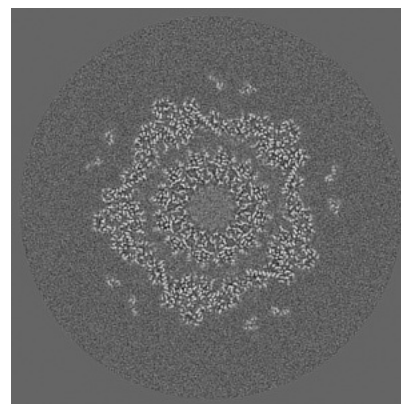
6.3.1 Primary map



X Index: 235



Y Index: 239

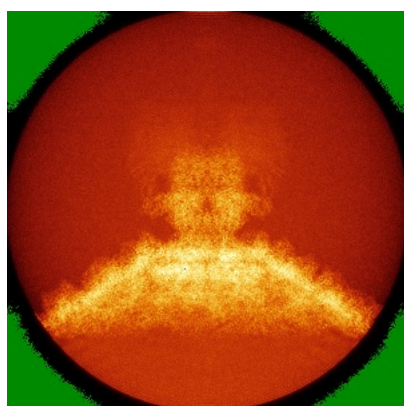


Z Index: 178

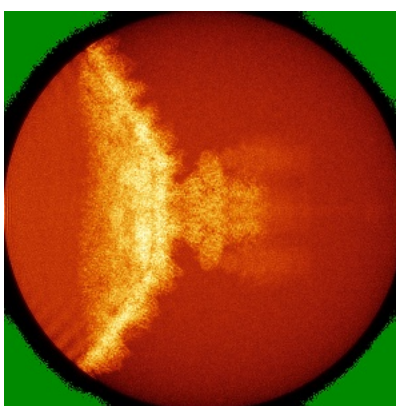
The images above show the largest variance slices of the map in three orthogonal directions.

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

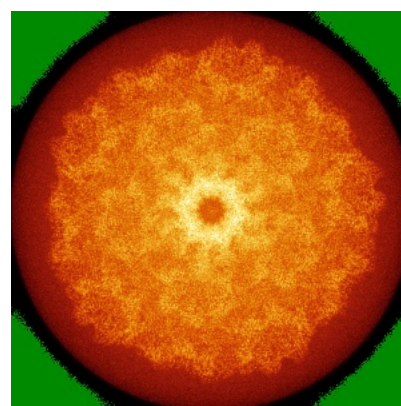
6.4.1 Primary map



X



Y

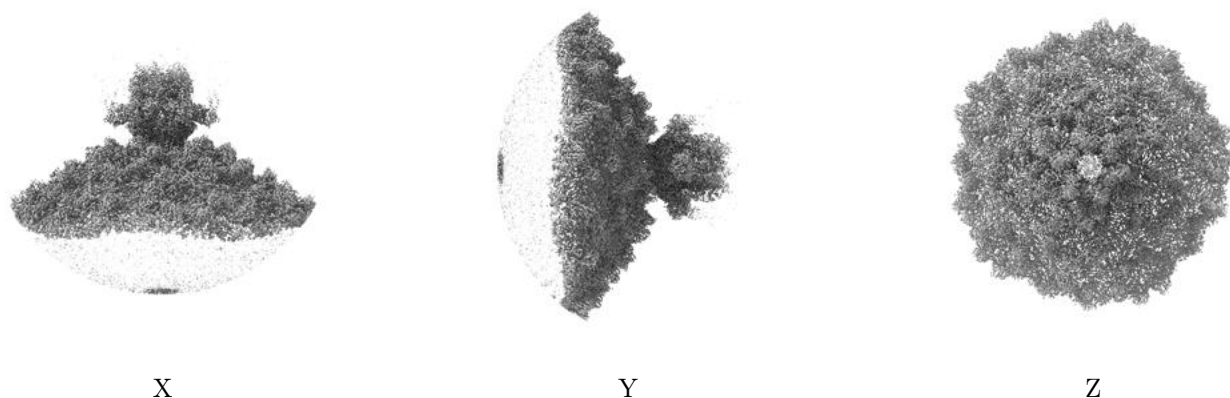


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.62. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

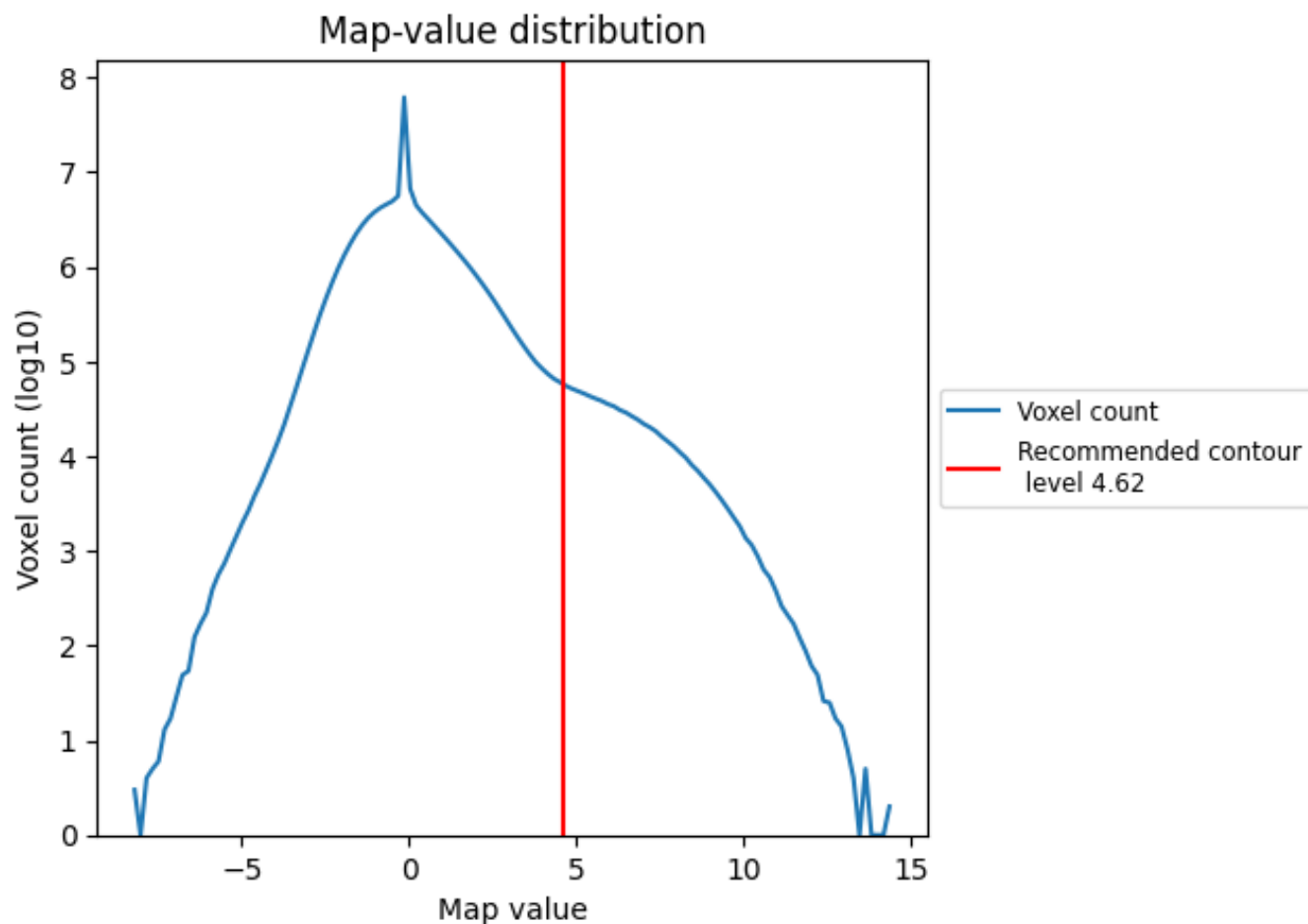
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

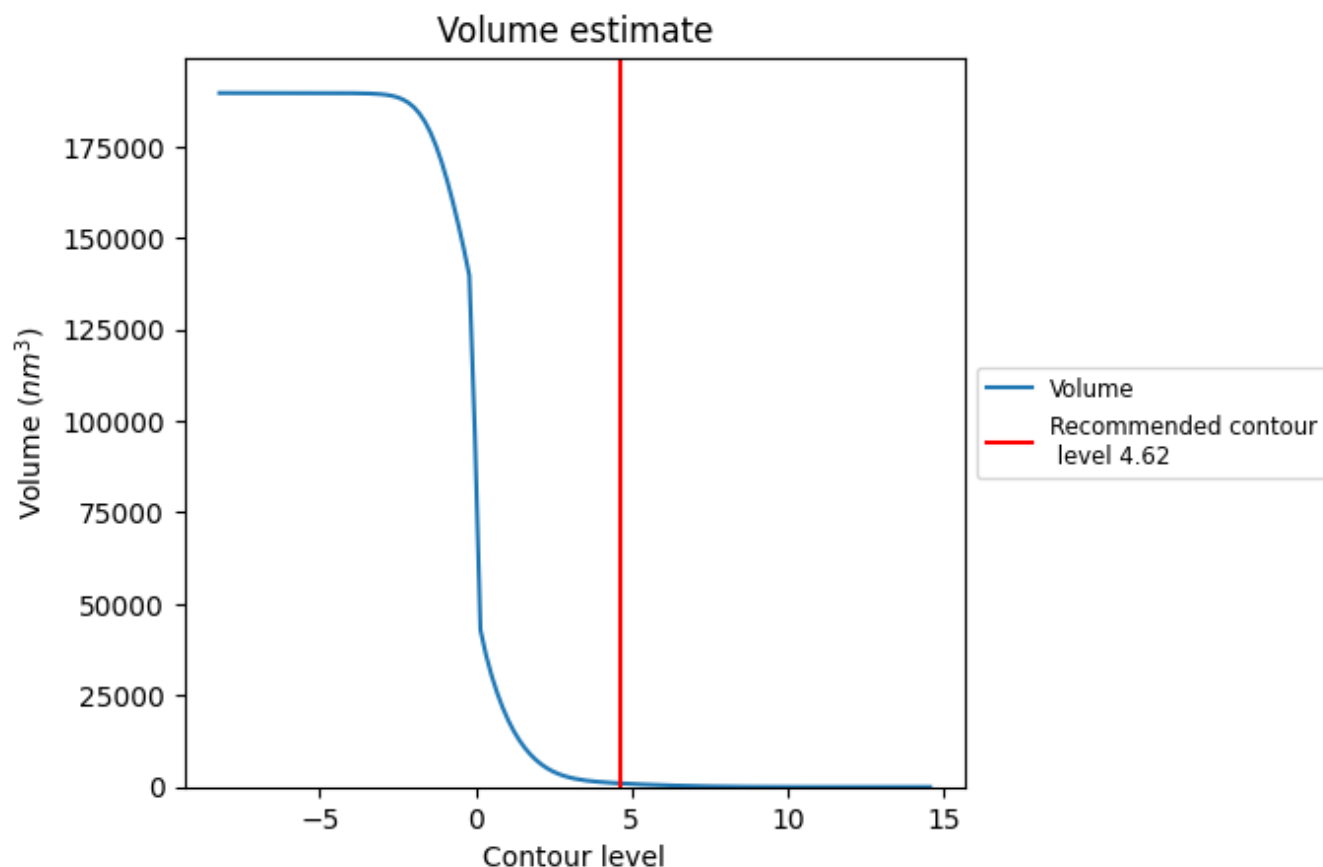
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

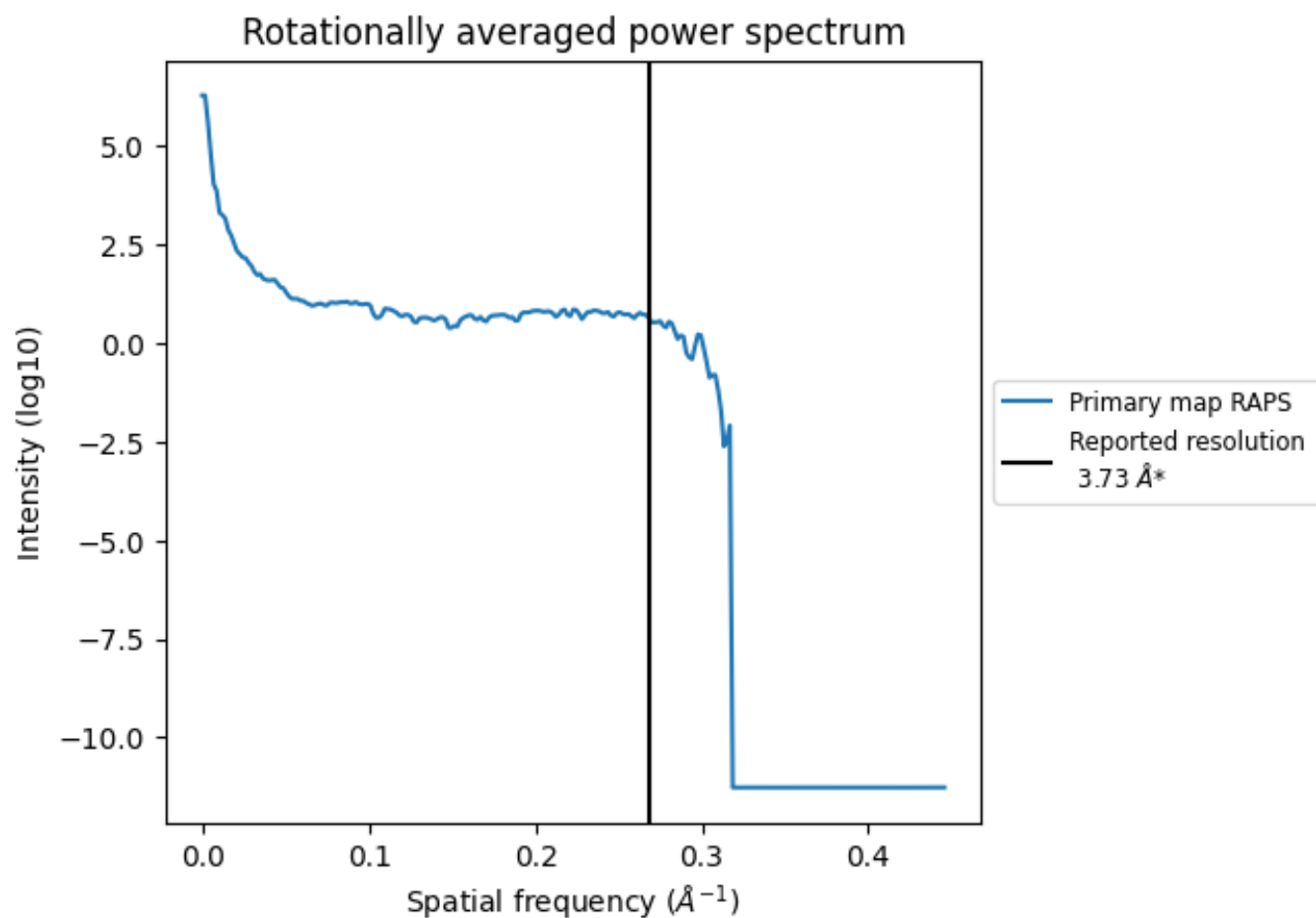
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 990 nm³; this corresponds to an approximate mass of 895 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 ⓘ

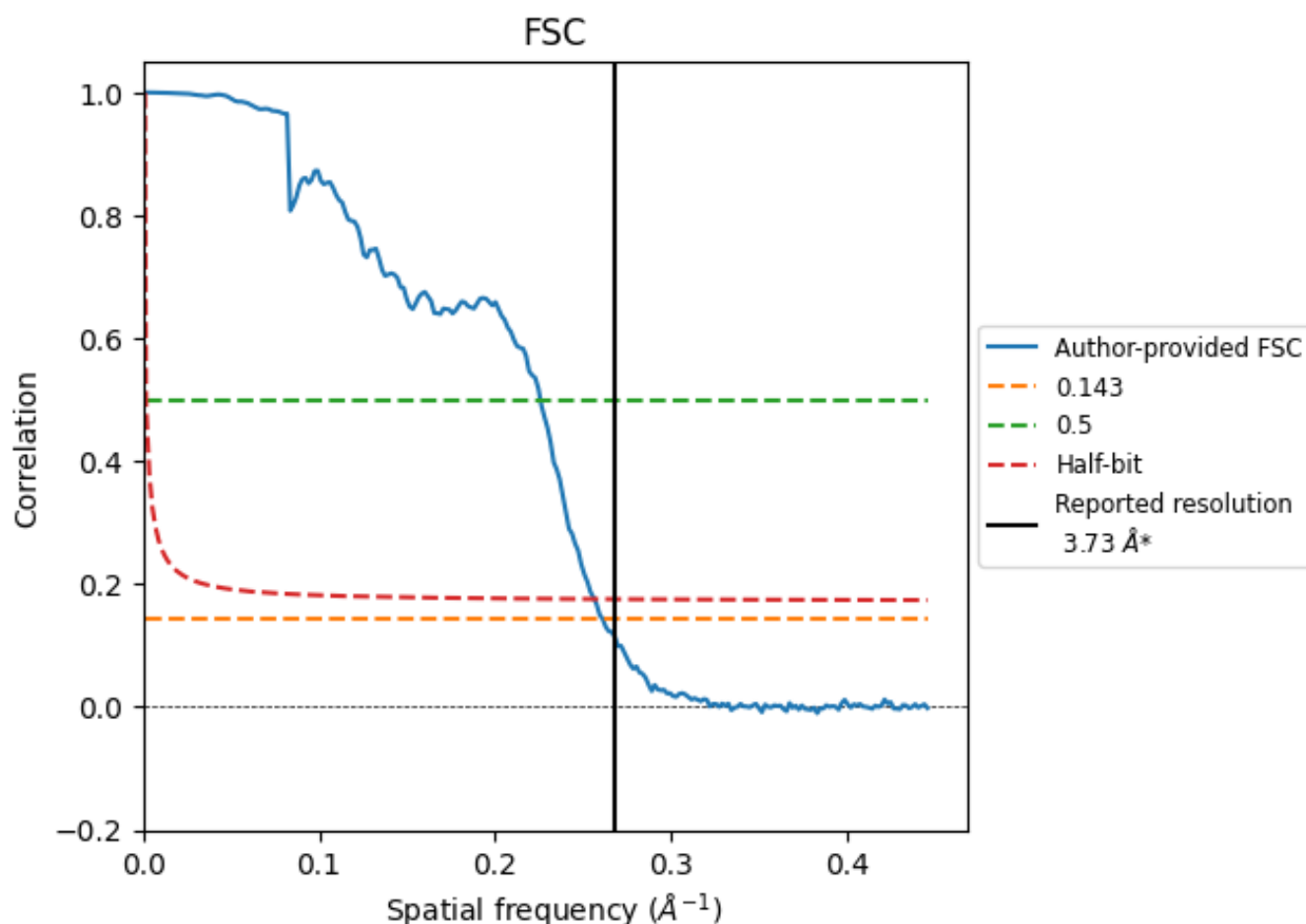


*Reported resolution corresponds to spatial frequency of 0.268 Å⁻¹

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 0.268 Å⁻¹

8.2 Resolution estimates [i](#)

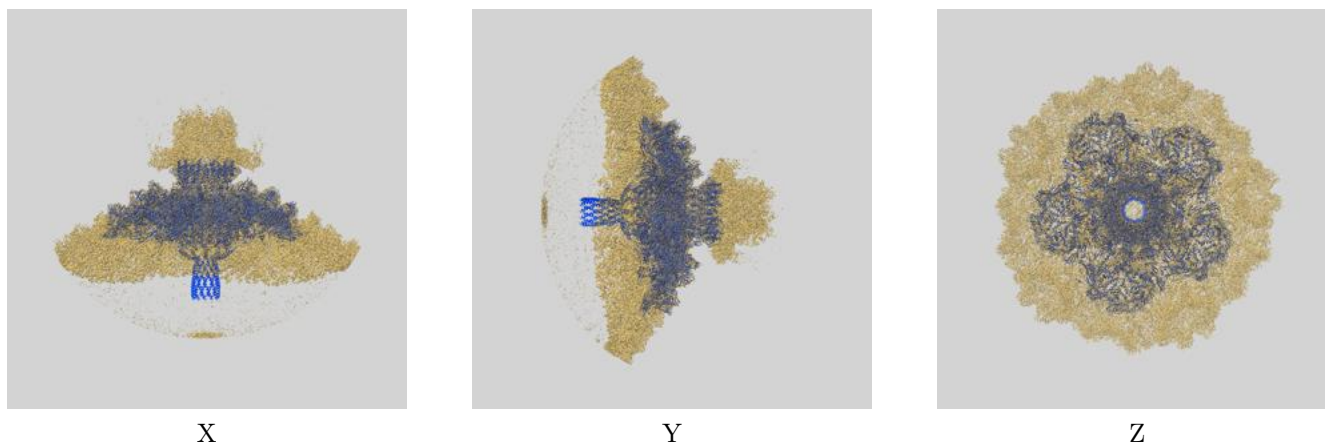
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.73	-	-
Author-provided FSC curve	3.83	4.43	3.90
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

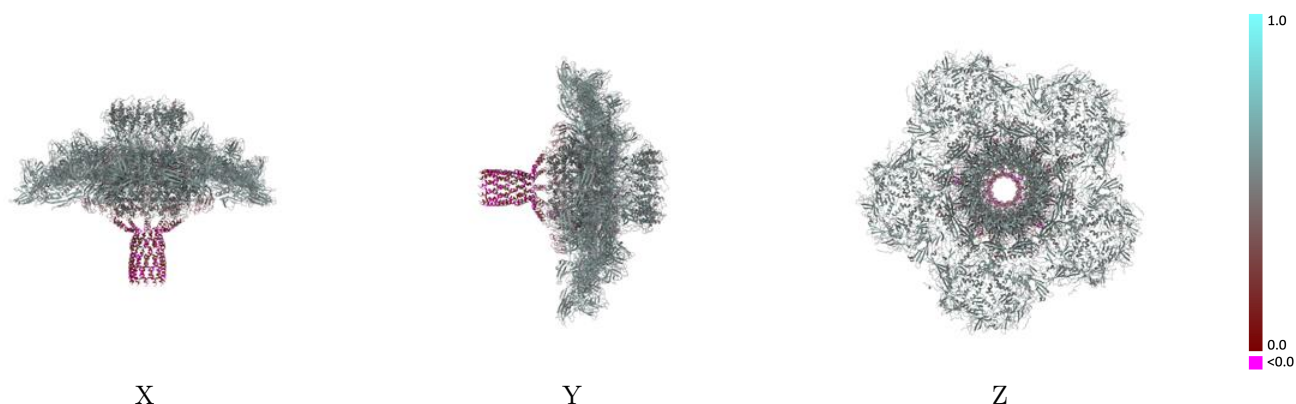
This section contains information regarding the fit between EMDB map EMD-25372 and PDB model 7SPU. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



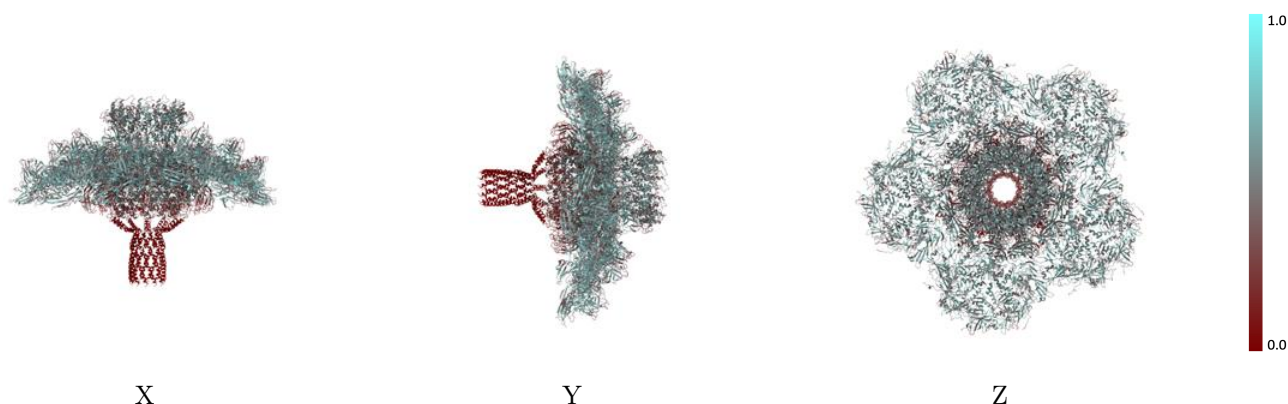
The images above show the 3D surface view of the map at the recommended contour level 4.62 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



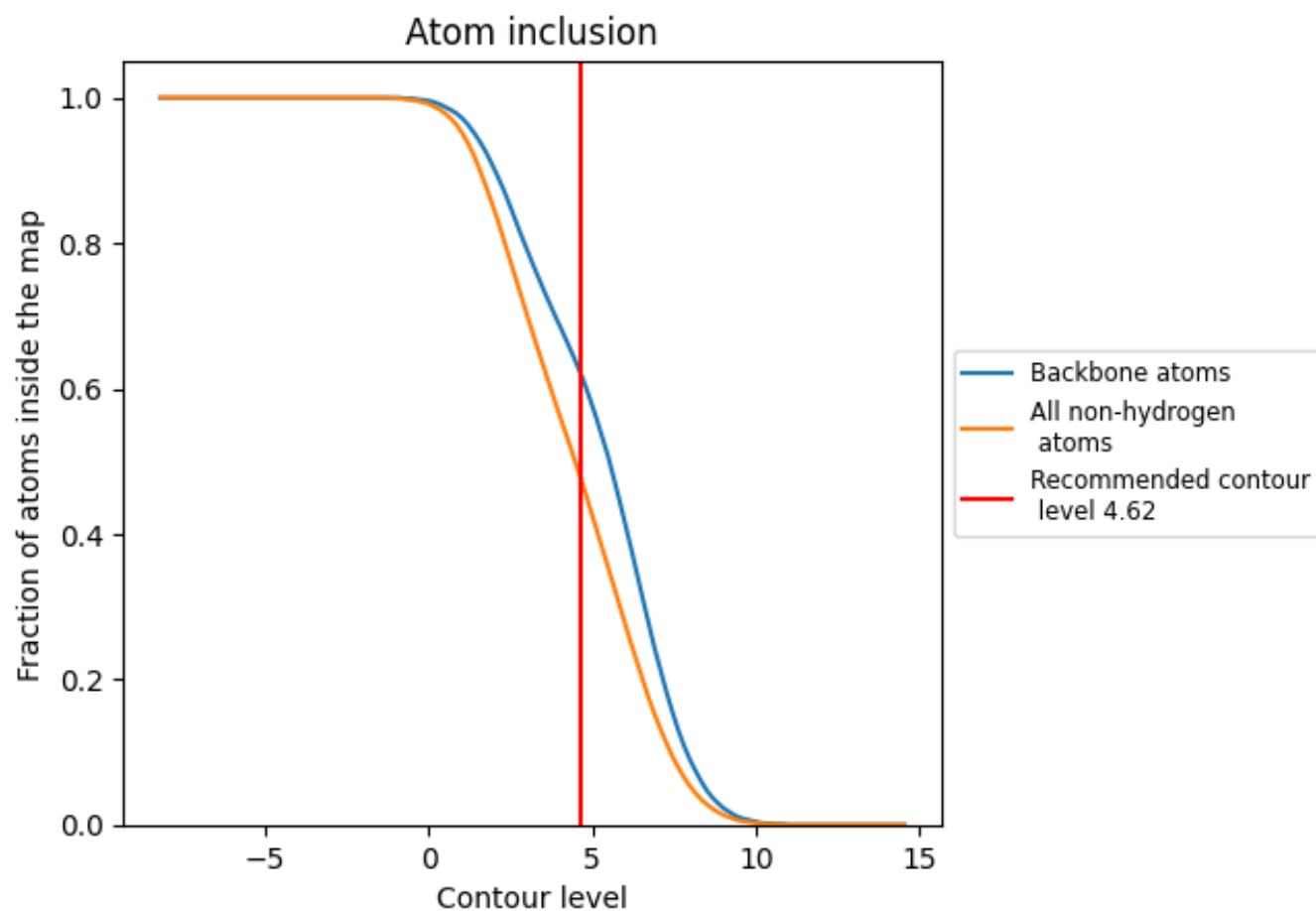
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.62).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 48% 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 (4.62) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4810	 0.4950
0	 0.5000	 0.5130
1	 0.4640	 0.5000
A	 0.3730	 0.4510
B	 0.3720	 0.4420
C	 0.3670	 0.4480
D	 0.3680	 0.4420
E	 0.3750	 0.4510
F	 0.3860	 0.4460
G	 0.3760	 0.4450
H	 0.3680	 0.4450
I	 0.3680	 0.4490
J	 0.3660	 0.4500
K	 0.3730	 0.4430
L	 0.3810	 0.4450
M	 0.5620	 0.5280
N	 0.5600	 0.5270
O	 0.5570	 0.5270
P	 0.5640	 0.5290
Q	 0.5360	 0.5250
R	 0.5460	 0.5300
S	 0.5400	 0.5270
T	 0.5400	 0.5270
U	 0.5470	 0.5220
V	 0.5450	 0.5240
W	 0.5360	 0.5220
X	 0.5350	 0.5220
Y	 0.5000	 0.5160
Z	 0.5580	 0.5300
a	 0.5420	 0.5270
b	 0.5460	 0.5280
c	 0.5600	 0.5320
d	 0.5570	 0.5310
e	 0.5400	 0.4960
f	 0.4820	 0.5160



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Chain	Atom inclusion	Q-score
g	 0.5320	 0.5130
h	 0.4940	 0.5150
i	 0.5390	 0.5090
j	 0.5530	 0.5270
k	 0.5320	 0.5080
l	 0.5360	 0.5070
m	 0.5550	 0.5300
n	 0.4860	 0.5050
o	 0.5640	 0.5290
p	 0.4850	 0.5070
q	 0.5420	 0.5280
r	 0.4820	 0.5110
s	 0.5560	 0.5290
t	 0.5420	 0.5280
u	 0.5420	 0.5270
v	 0.4910	 0.5030
w	 0.4840	 0.5140
x	 0.4870	 0.5110
y	 0.5350	 0.5230
z	 0.4790	 0.5030