



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 10:07 am BST

PDB ID : 9TIC / pdb_00009tic
EMDB ID : EMD-55951
Title : Phage 812 baseplate in the pre-contraction state (C3)
Authors : Binovsky, J.; Plevka, P.
Deposited on : 2025-12-05
Resolution : 5.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

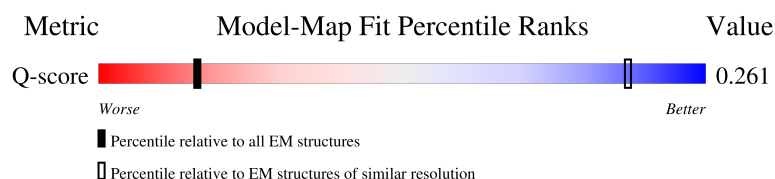
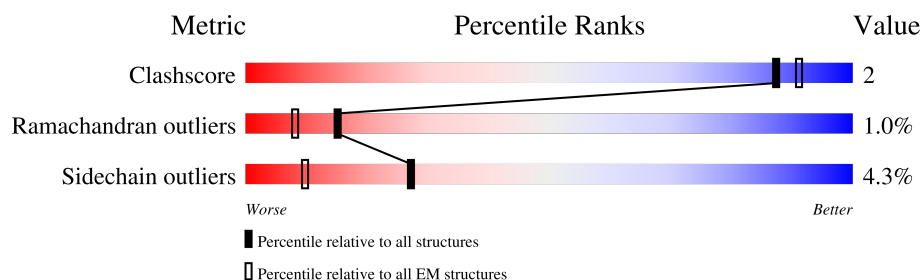
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 5.90 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	501 (5.40 - 6.40)

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	458	32% 94% 6%
1	8	458	30% 91% 9%
1	9	458	28% 95% 5%
1	w	458	29% 92% 7%

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Mol	Chain	Length	Quality of chain
1	x	458	25% 94% 6%
1	y	458	24% 94% 5%
2	l	173	98% 83% 14% ..
2	P	173	83% 9% 7%
2	Q	173	14% 87% 7% 6%
2	R	173	39% 85% 8% 6%
2	S	173	62% 94% ..
2	T	173	83% 83% 16% ..
2	U	173	91% 84% 13% ..
2	V	173	95% 83% 14% ..
2	W	173	99% 86% 11% ..
2	X	173	98% 87% 10% ..
2	Y	173	99% 86% 12% ..
2	Z	173	96% 82% 16% ..
2	e	173	89% 5% 6%
2	f	173	9% 89% .. 6%
2	g	173	16% 94% 6%
2	h	173	43% 94% 5% ..
2	i	173	47% 83% 5% 12%
2	j	173	76% 91% 8% ..
2	k	173	86% 85% 13% ..
2	l	173	94% 88% 10% ..
2	m	173	94% 91% 6% ..
2	n	173	92% 88% 11% .
2	o	173	85% 87% 11% ..

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Mol	Chain	Length	Quality of chain
2	p	173	
3	2	1152	
3	3	1152	
3	4	1152	
3	5	1152	
3	6	1152	
3	7	1152	
3	q	1152	
3	r	1152	
3	s	1152	
3	t	1152	
3	u	1152	
3	v	1152	
4	A	848	
5	AA	640	
5	AB	640	
5	a	640	
5	b	640	
5	c	640	
5	z	640	
6	AC	142	
6	AD	142	
6	AE	142	
6	AF	142	
6	AG	142	

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Mol	Chain	Length	Quality of chain
6	AH	142	
7	AI	587	
7	AJ	587	
7	AK	587	
7	AL	587	
7	AM	587	
7	AN	587	
8	B	295	
9	C	808	
10	D	174	
10	E	174	
11	F	263	
11	G	263	
12	H	234	
12	I	234	
13	J	348	
13	K	348	
13	L	348	
13	M	348	
14	N	1019	
14	O	1019	
15	d	124	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 256934 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 ORF68.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
1	8	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
1	9	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
1	w	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
1	x	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
1	y	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		

- Molecule 2 is a protein called ORF64.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	P	161	Total	C	N	O	S	0	0
			1266	809	207	249	1		
2	Q	163	Total	C	N	O	S	0	0
			1277	817	208	251	1		
2	R	162	Total	C	N	O	S	0	0
			1272	812	208	251	1		
2	S	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	T	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	U	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	V	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	W	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	Y	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	Z	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	e	163	Total	C	N	O	S	0	0
			1280	818	209	252	1		
2	f	162	Total	C	N	O	S	0	0
			1270	811	207	251	1		
2	g	163	Total	C	N	O	S	0	0
			1278	817	208	252	1		
2	h	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	i	152	Total	C	N	O	S	0	0
			1199	769	196	233	1		
2	j	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	k	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	l	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	m	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	n	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	o	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	p	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		

- Molecule 3 is a protein called ORF65.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	3	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	4	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	5	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	7	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	q	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	r	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	s	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	t	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	u	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	v	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		

- Molecule 4 is a protein called ORF58.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	309	Total	C	N	O	S	0	0
			2462	1555	400	501	6		

- Molecule 5 is a protein called CBM-cenC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AA	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		
5	AB	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		
5	a	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		
5	b	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		
5	c	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		
5	z	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		

- Molecule 6 is a protein called ORF50.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AC	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		
6	AD	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		
6	AE	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		
6	AF	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		
6	AG	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		
6	AH	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		

- Molecule 7 is a protein called ORF49.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AI	550	Total	C	N	O	S	0	0
			4284	2698	729	850	7		
7	AJ	550	Total	C	N	O	S	0	0
			4284	2698	729	850	7		
7	AK	549	Total	C	N	O	S	0	0
			4267	2684	724	852	7		
7	AL	549	Total	C	N	O	S	0	0
			4267	2684	724	852	7		
7	AM	342	Total	C	N	O	S	0	0
			2667	1678	459	523	7		
7	AN	342	Total	C	N	O	S	0	0
			2667	1678	459	523	7		

- Molecule 8 is a protein called ORF57.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	292	Total	C	N	O	S	0	0
			2424	1572	369	476	7		

- Molecule 9 is a protein called ORF56.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	725	Total	C	N	O	S	0	0
			5852	3738	984	1110	20		

- Molecule 10 is a protein called ORF60.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	160	Total	C	N	O	S	0	0
			1294	831	206	253	4		
10	E	154	Total	C	N	O	S	0	0
			1248	803	200	241	4		

- Molecule 11 is a protein called ORF59.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	238	Total	C	N	O	S	0	0
			1878	1164	335	375	4		
11	G	237	Total	C	N	O	S	0	0
			1871	1160	334	373	4		

- Molecule 12 is a protein called ORF61.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	212	Total	C	N	O	S	0	0
			1694	1060	290	339	5		
12	I	213	Total	C	N	O	S	0	0
			1701	1065	291	340	5		

- Molecule 13 is a protein called ORF62.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	348	Total	C	N	O	S	0	0
			2760	1734	459	560	7		
13	K	348	Total	C	N	O	S	0	0
			2760	1734	459	560	7		
13	L	348	Total	C	N	O	S	0	0
			2760	1734	459	560	7		
13	M	348	Total	C	N	O	S	0	0
			2760	1734	459	560	7		

- Molecule 14 is a protein called ORF63.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	721	Total	C	N	O	S	0	0
			5845	3728	945	1161	11		
14	O	721	Total	C	N	O	S	0	0
			5845	3728	945	1161	11		

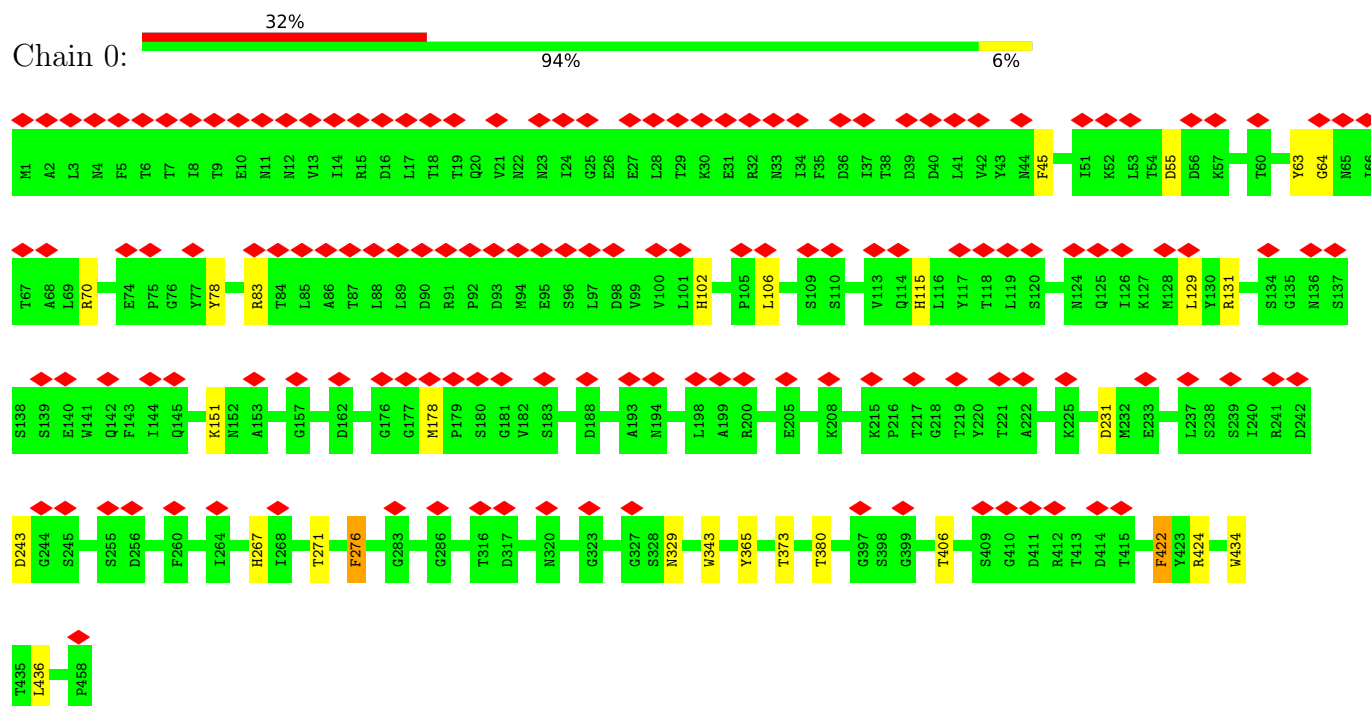
- Molecule 15 is a protein called ORF67.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	d	71	597	390	94	113	0	0

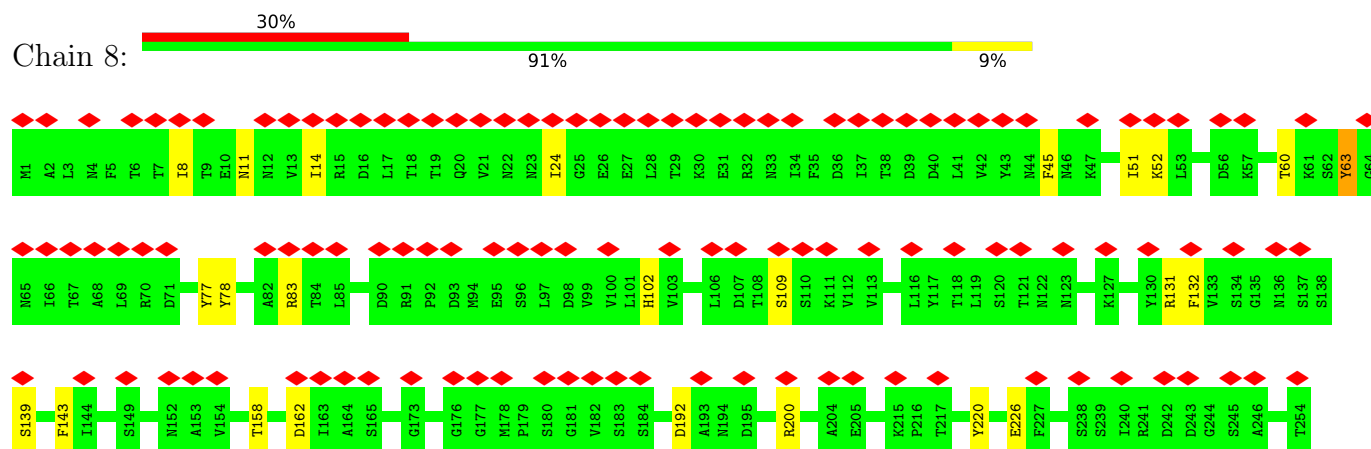
3 Residue-property plots [i](#)

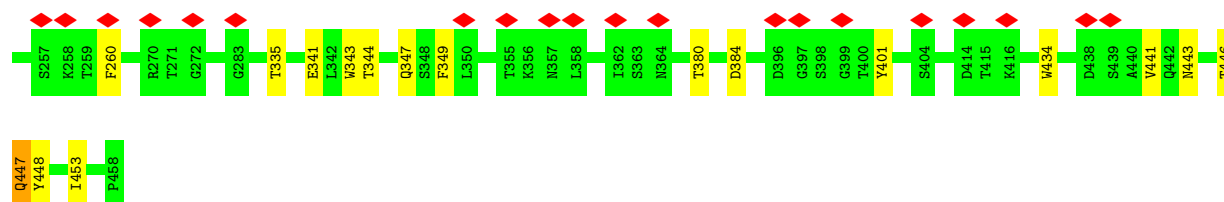
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: ORF68

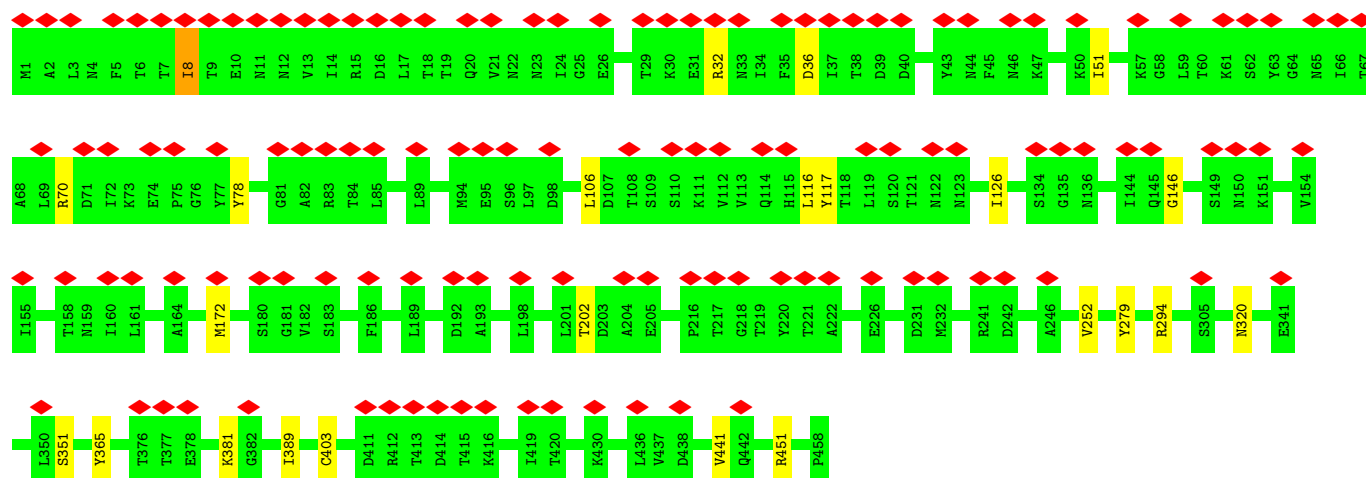


• Molecule 1: ORF68

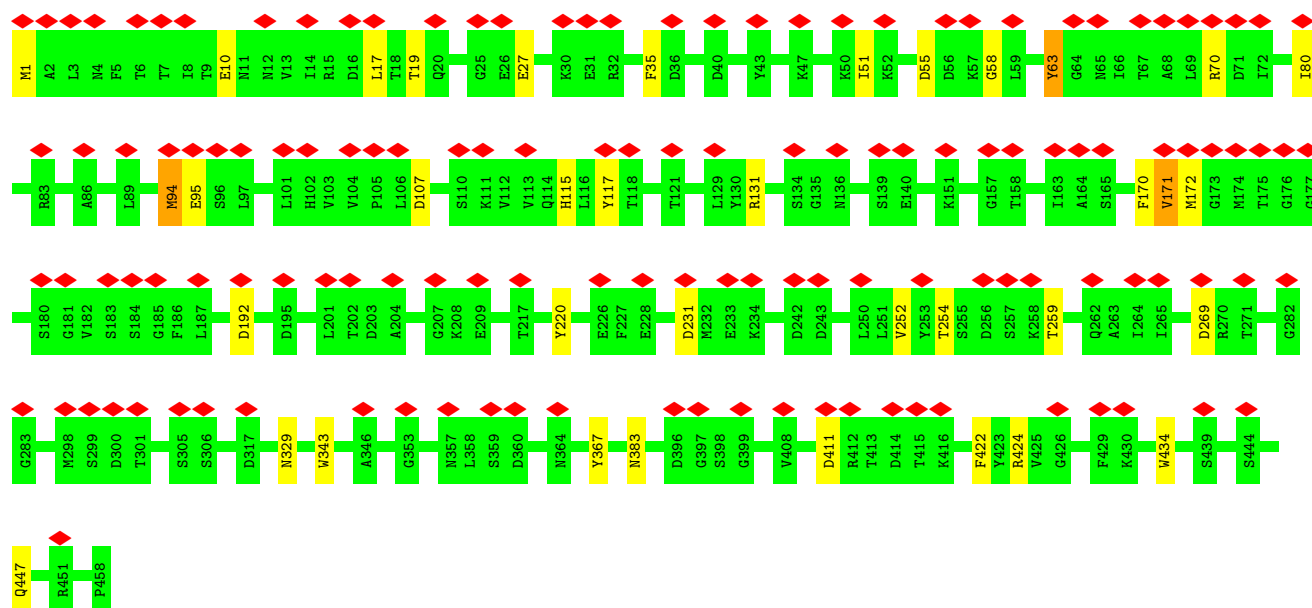
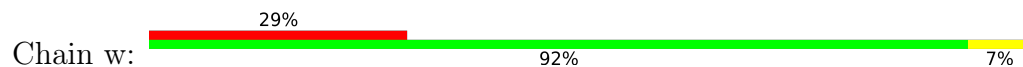




• Molecule 1: ORF68

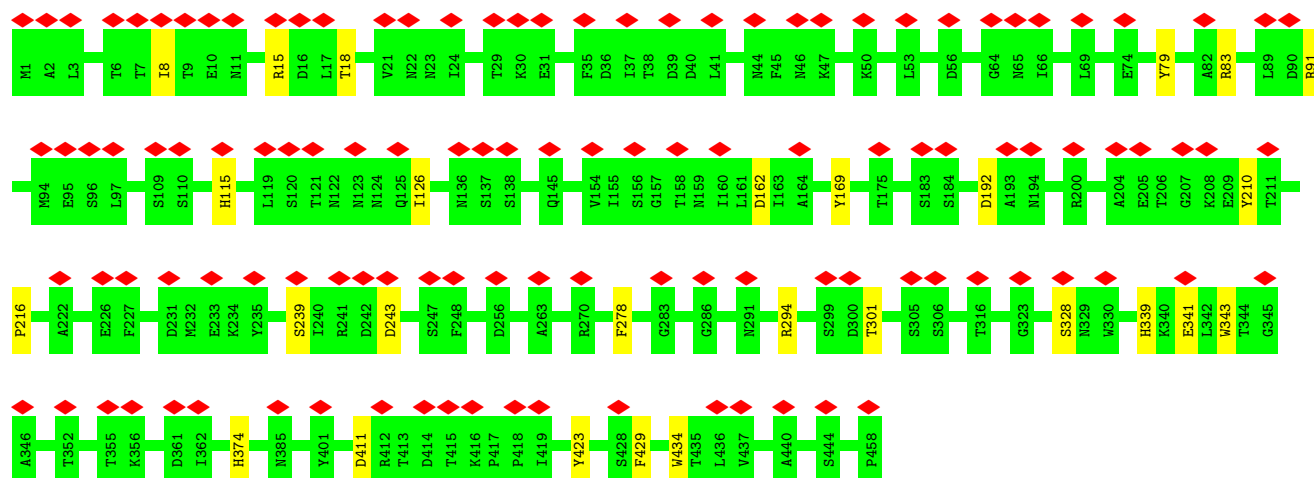


• Molecule 1: ORF68

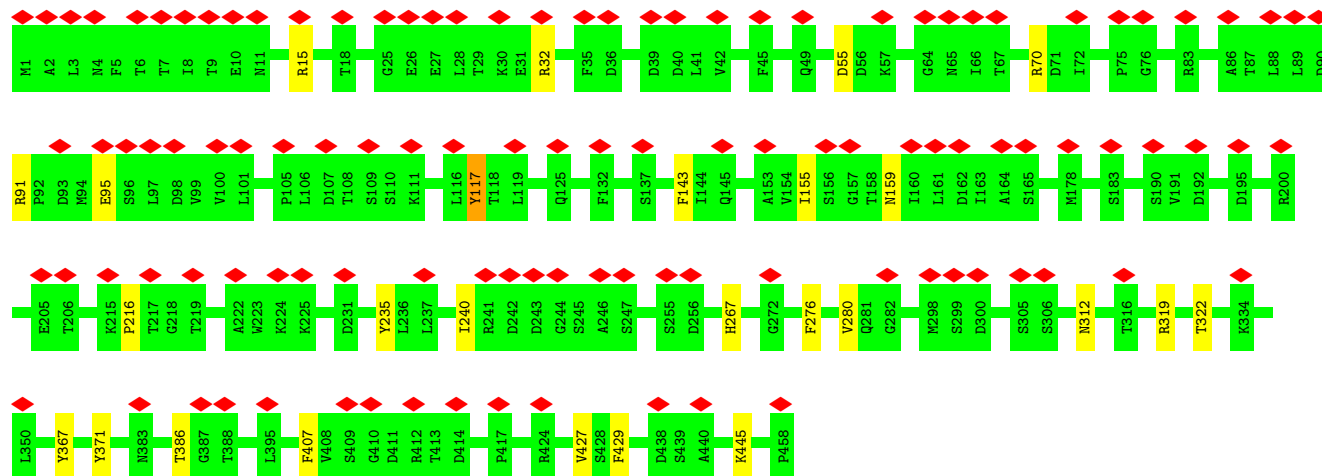


• Molecule 1: ORF68

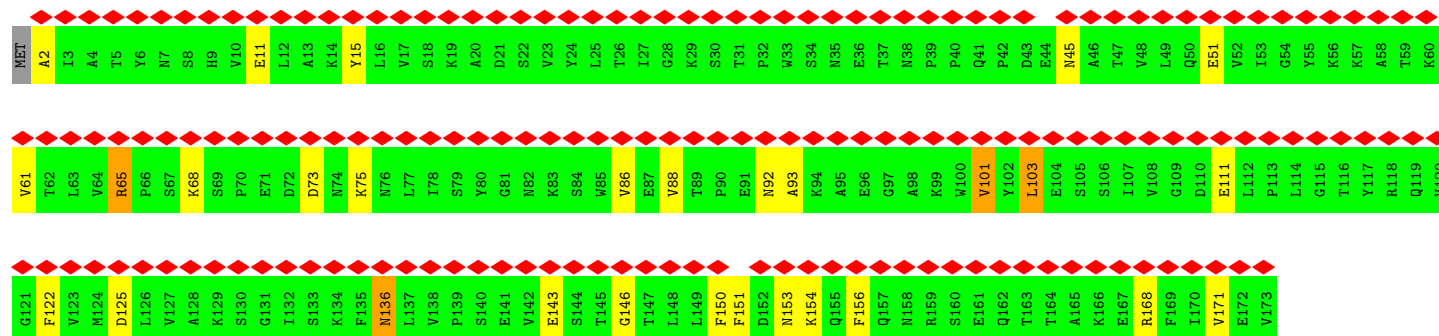
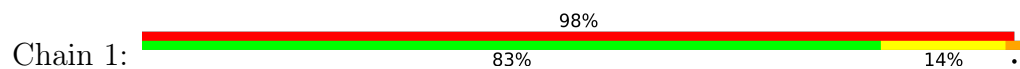




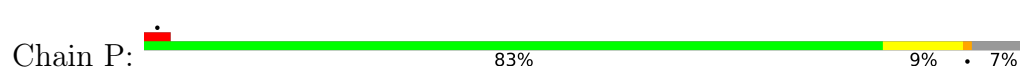
• Molecule 1: ORF68



• Molecule 2: ORF64

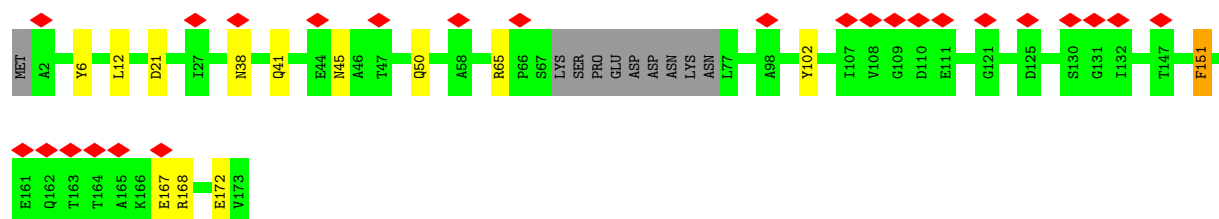
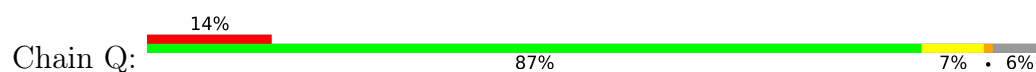


• Molecule 2: ORF64

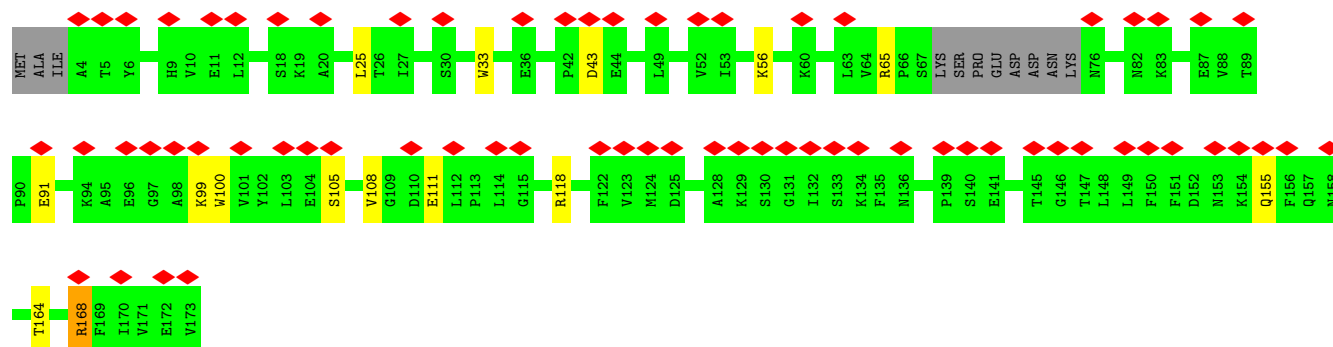
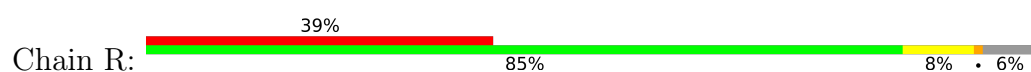




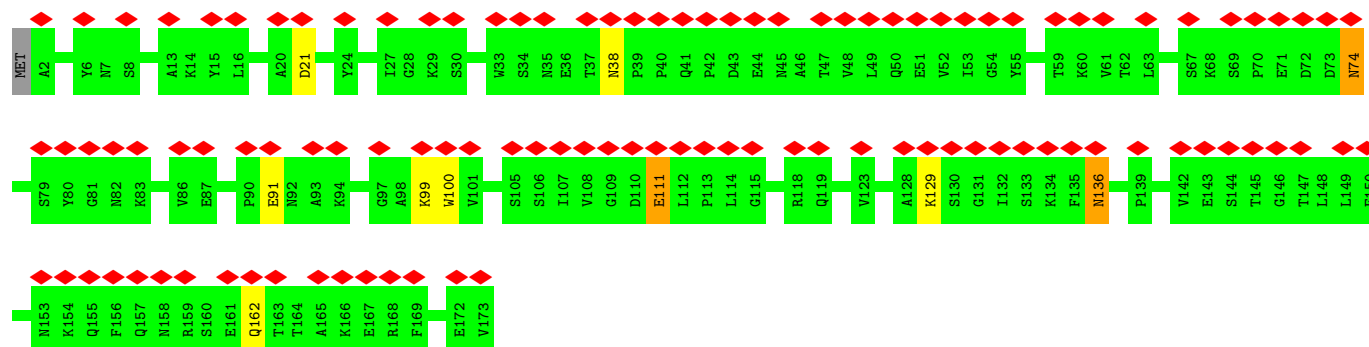
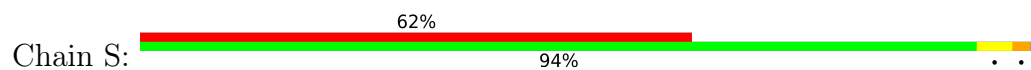
• Molecule 2: ORF64



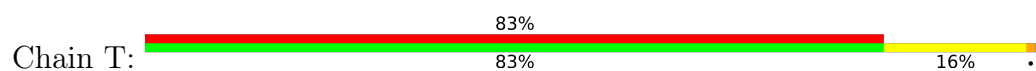
• Molecule 2: ORF64

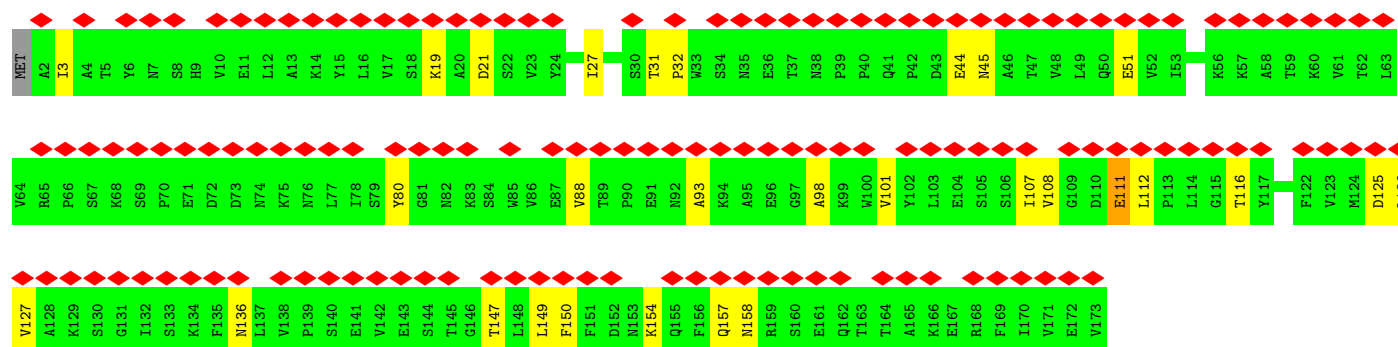


• Molecule 2: ORF64

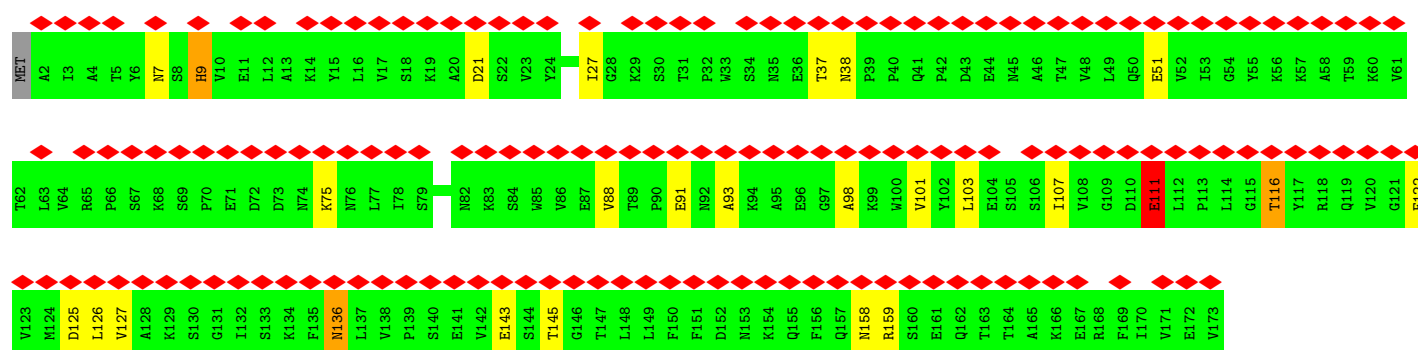
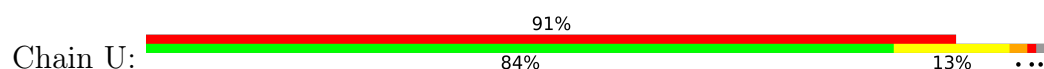


• Molecule 2: ORF64

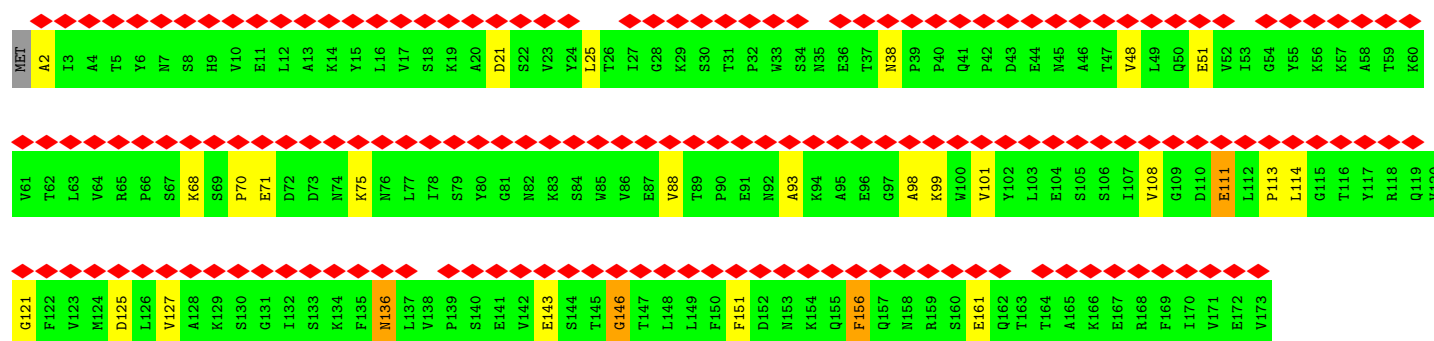
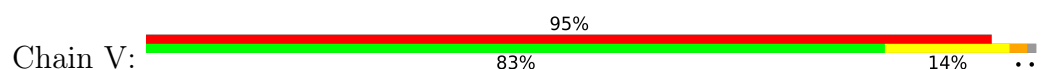




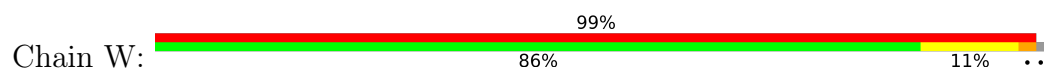
• Molecule 2: ORF64

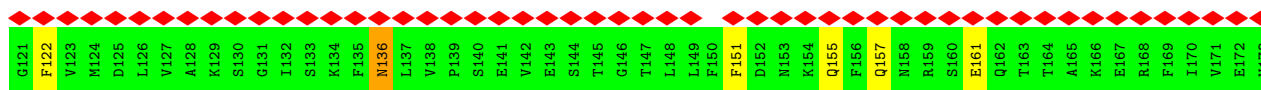


• Molecule 2: ORF64

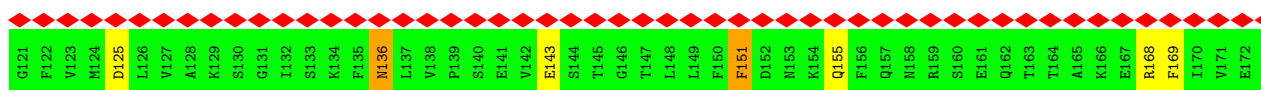
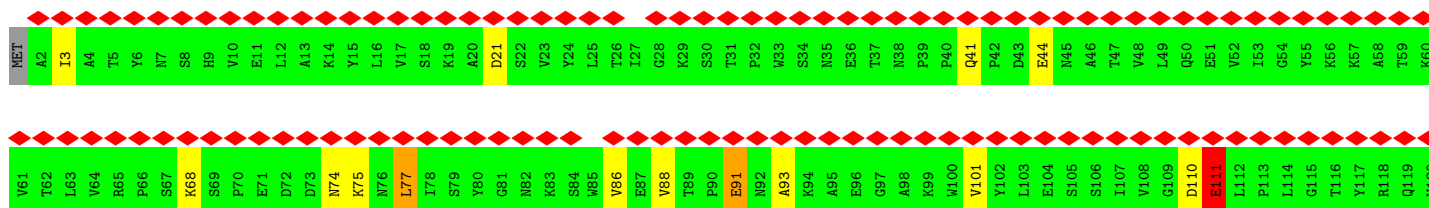
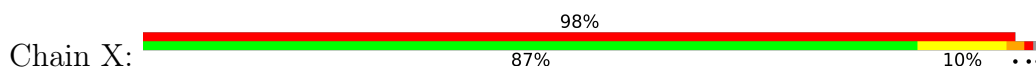


• Molecule 2: ORF64

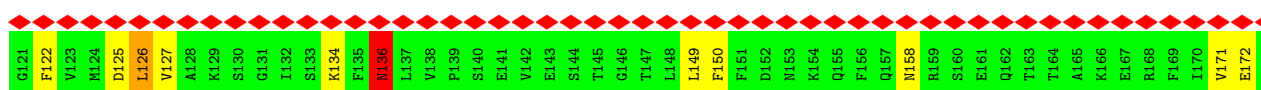
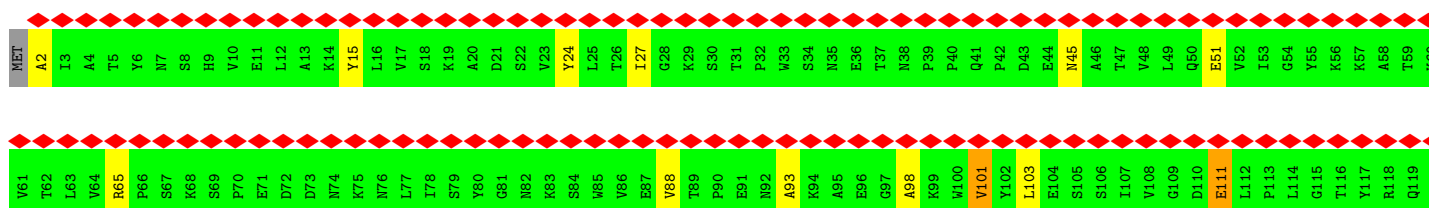
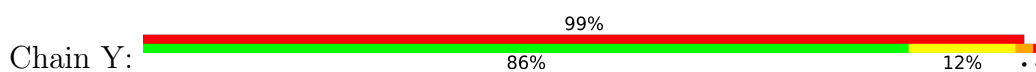




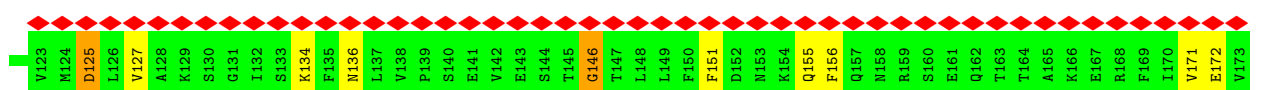
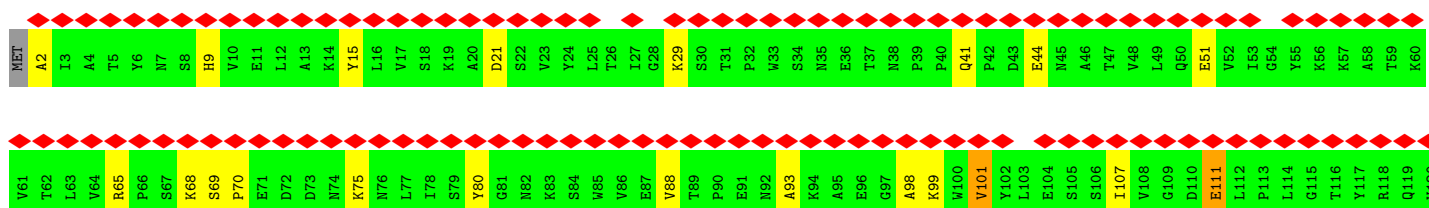
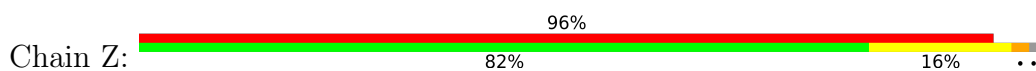
• Molecule 2: ORF64



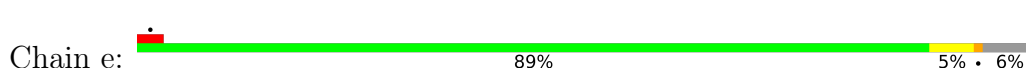
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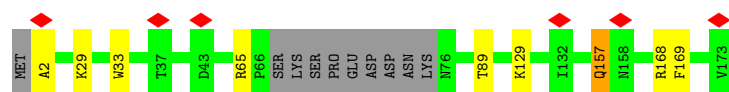


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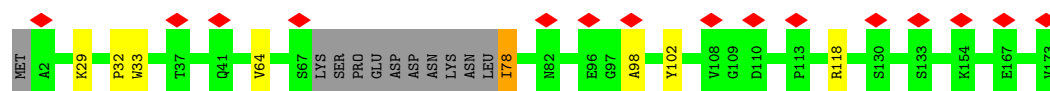
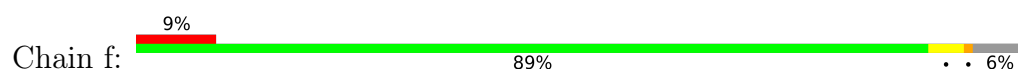


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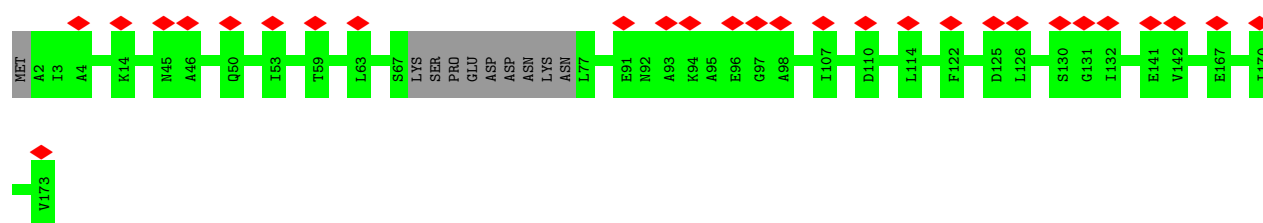




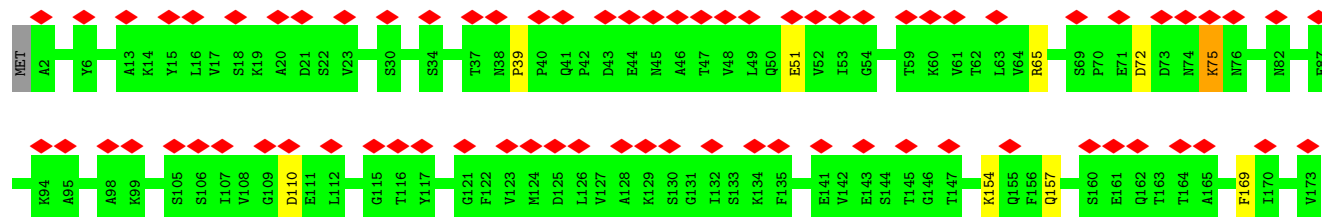
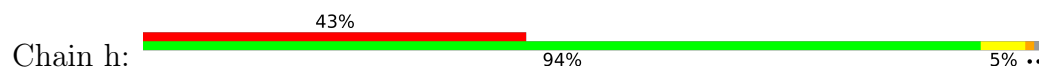
• Molecule 2: ORF64



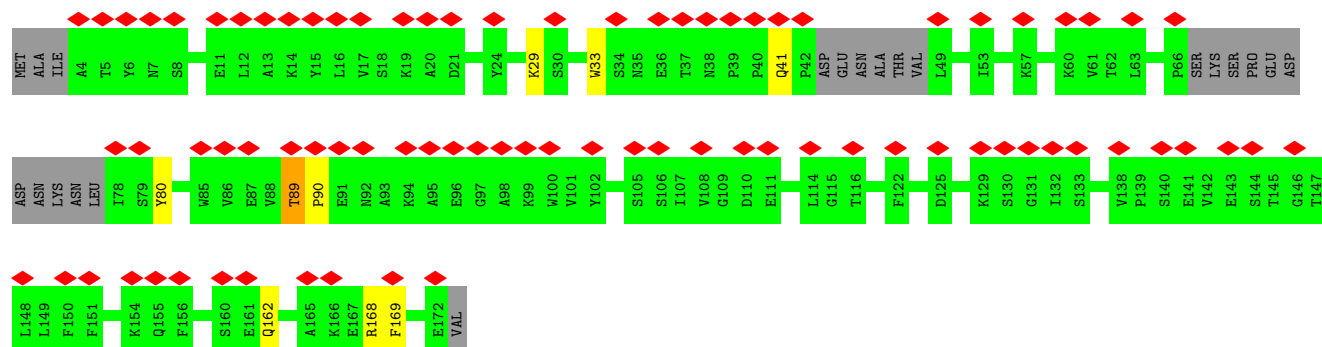
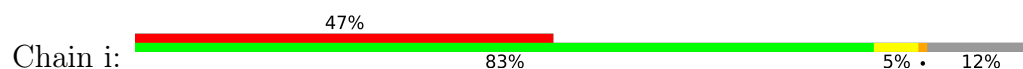
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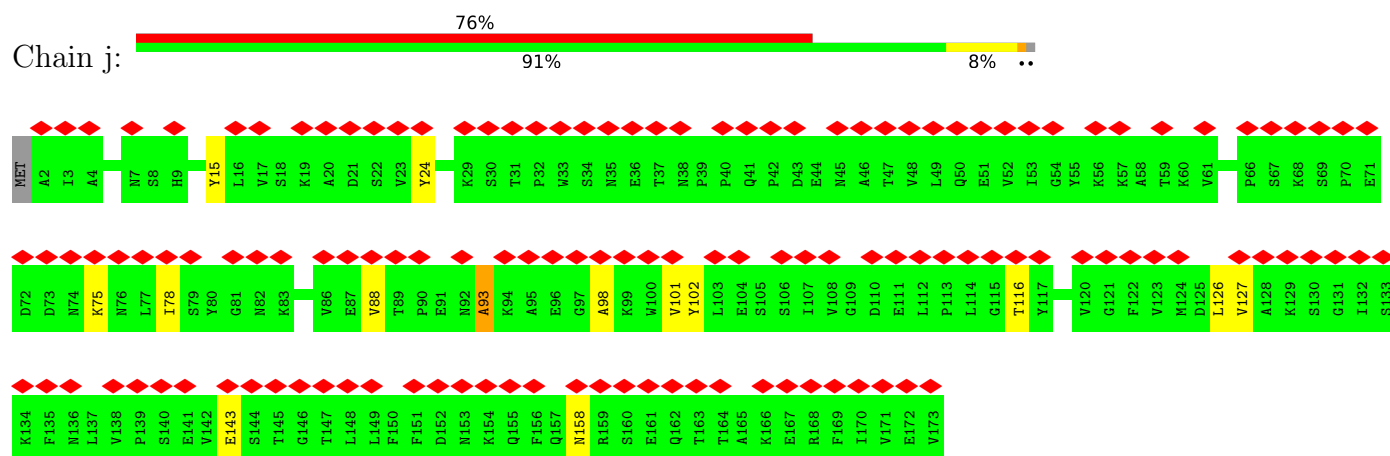
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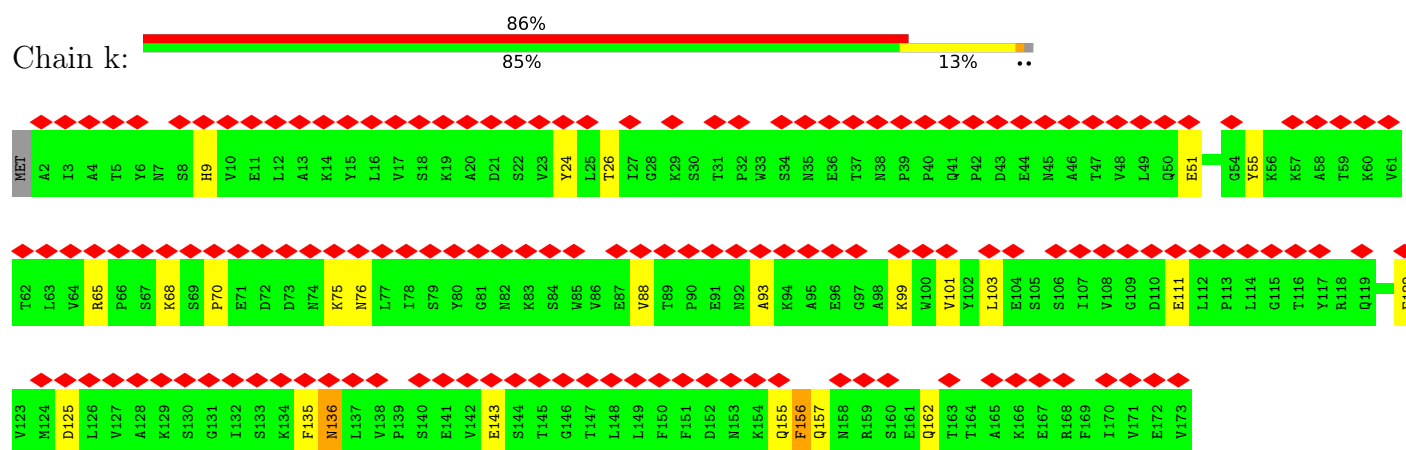
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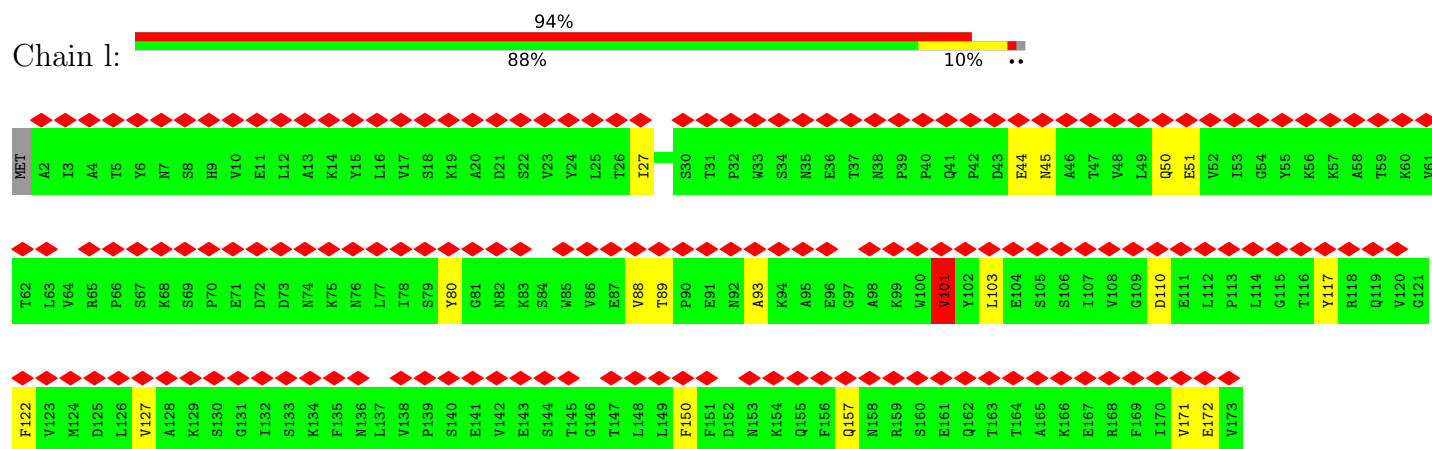
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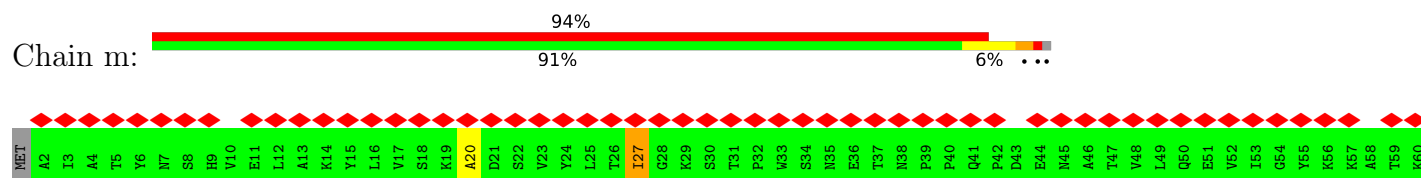
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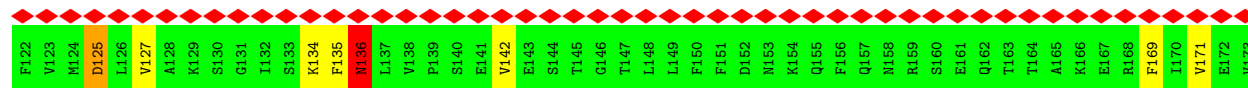
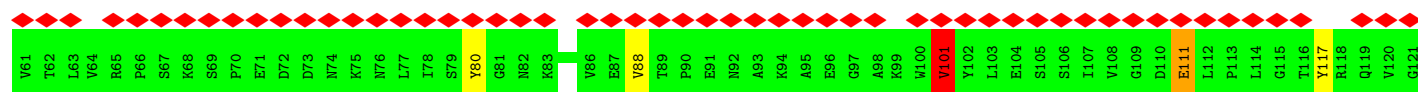


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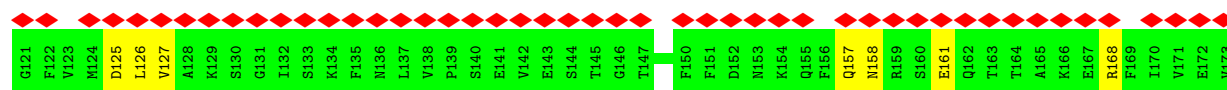
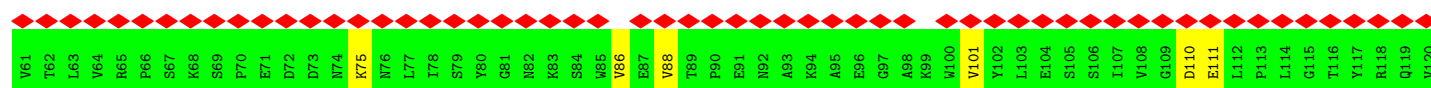
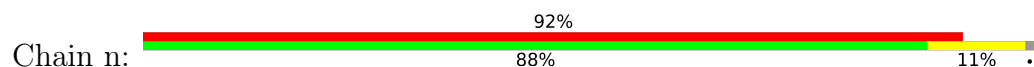


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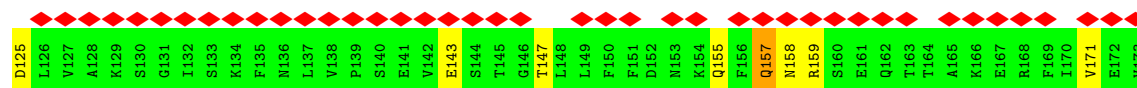
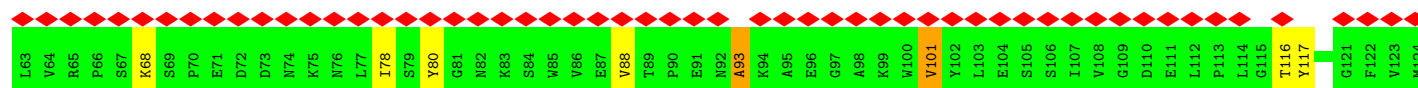
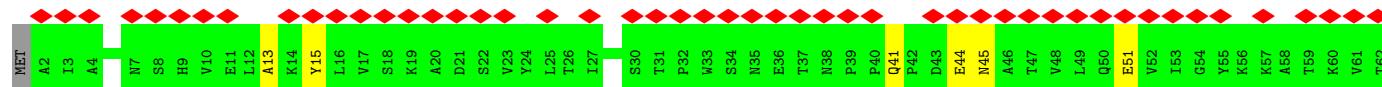
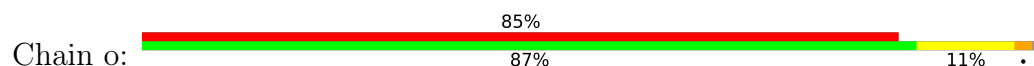




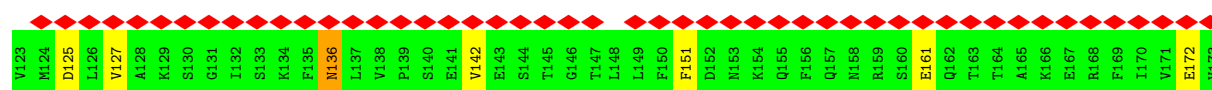
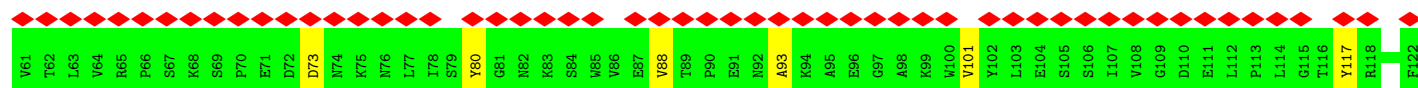
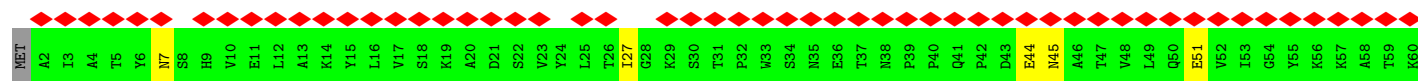
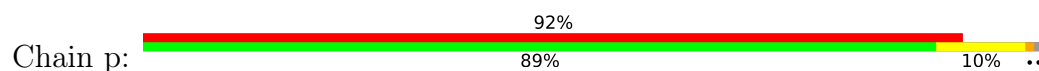
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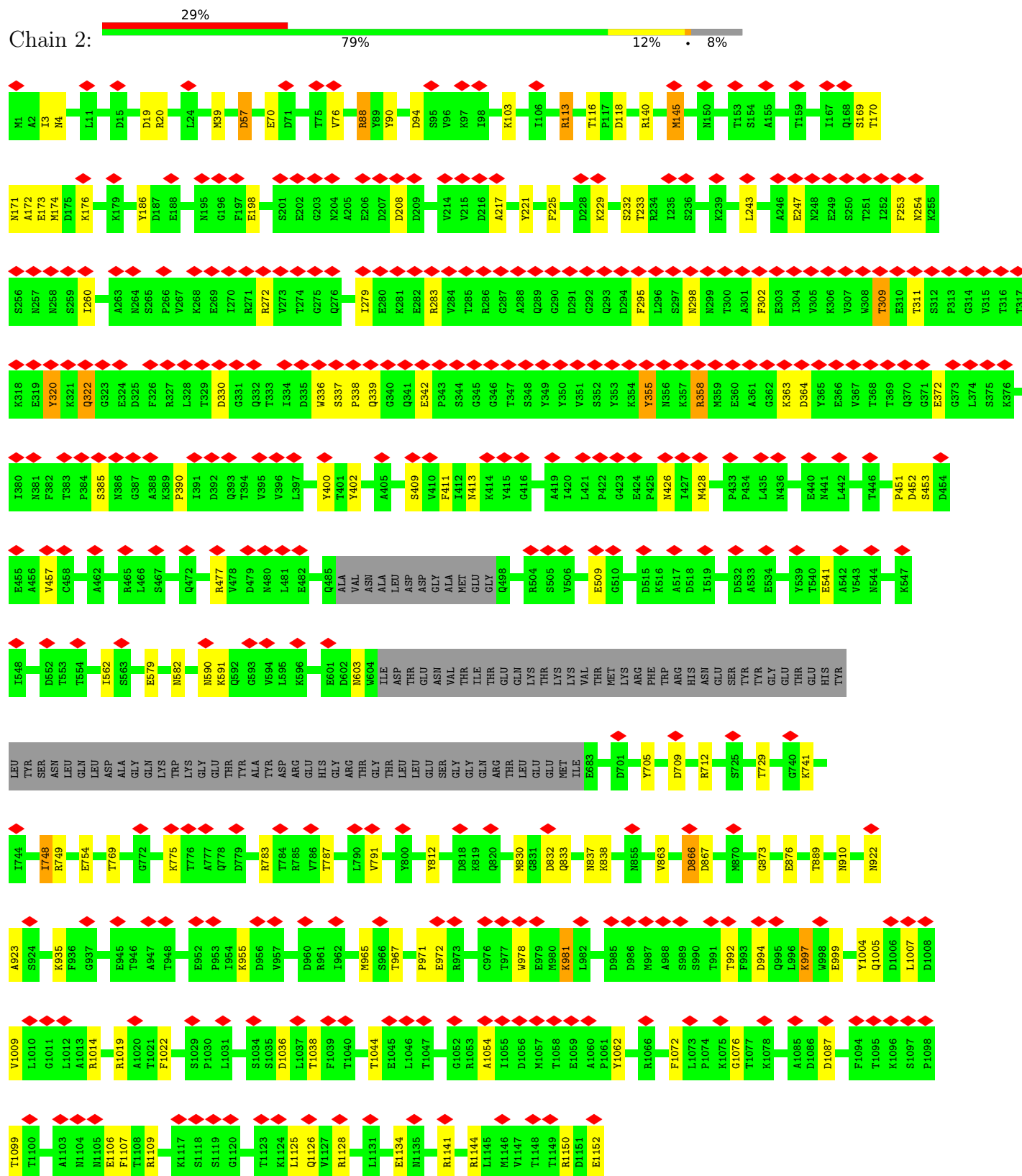
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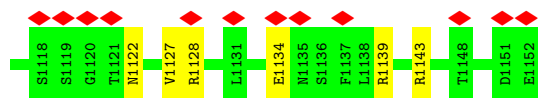
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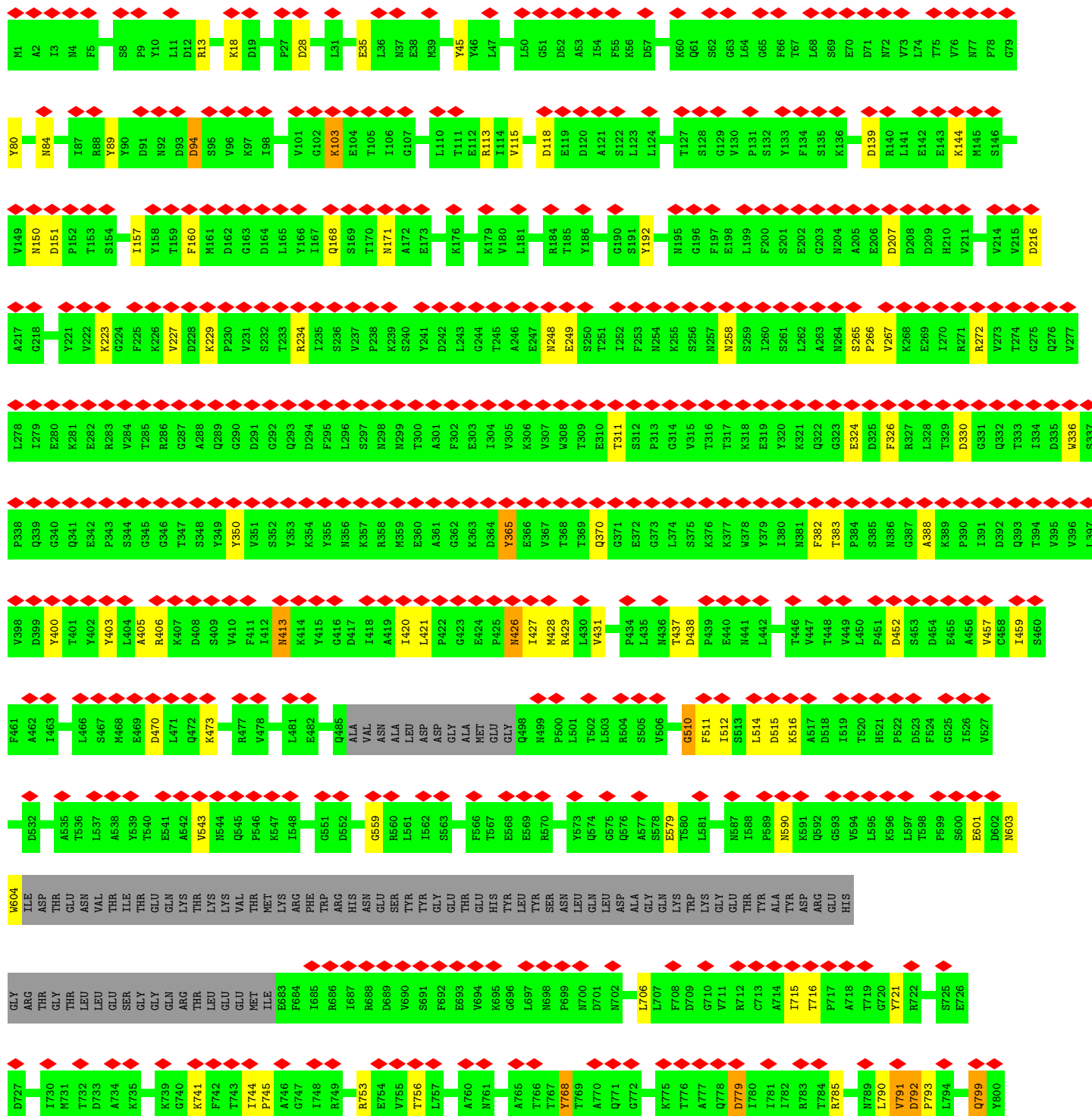
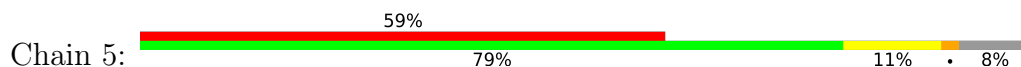
- Molecule 3: ORF65

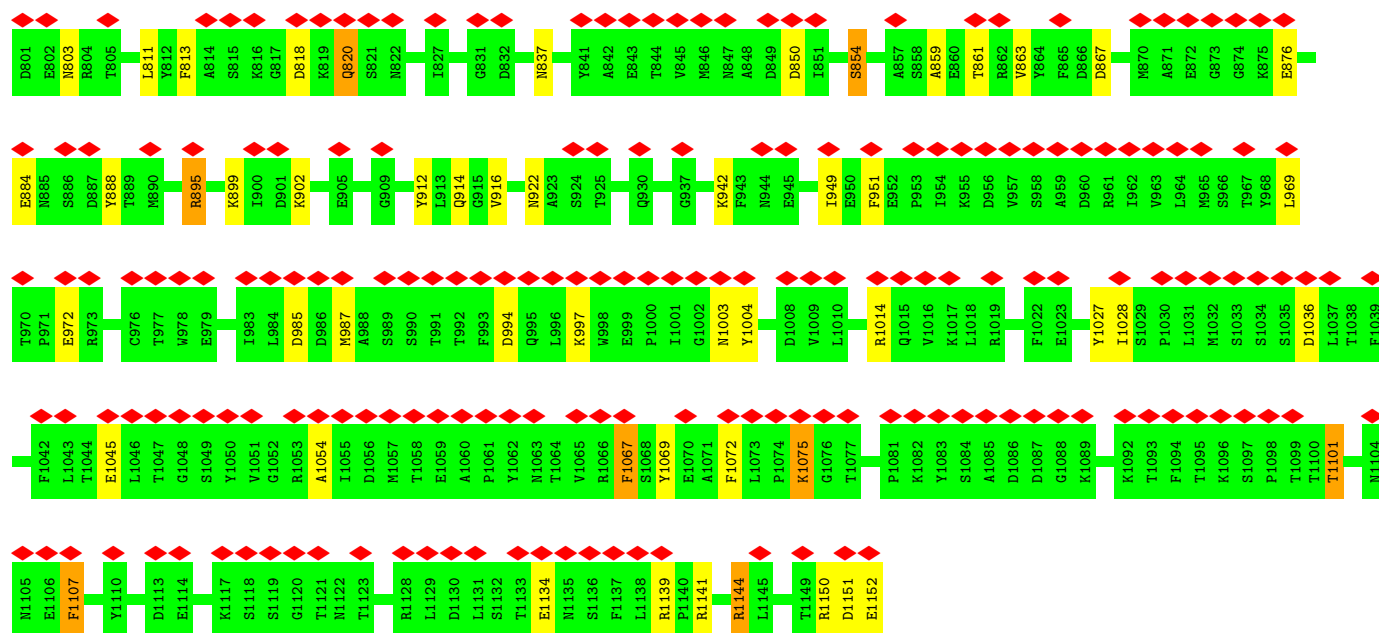


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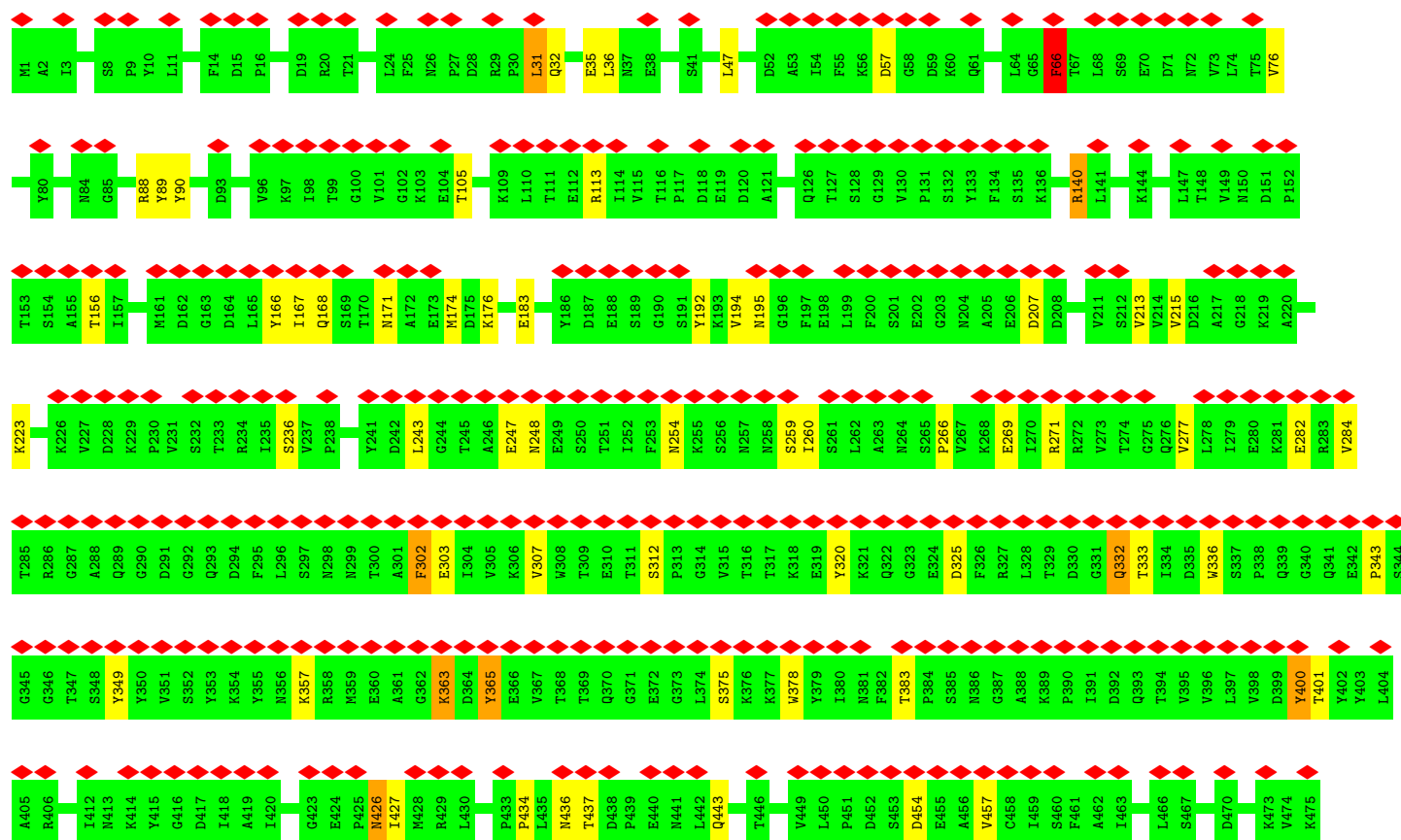
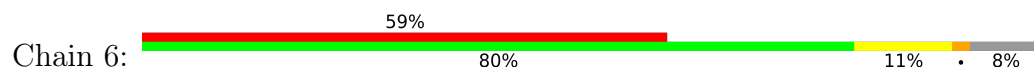


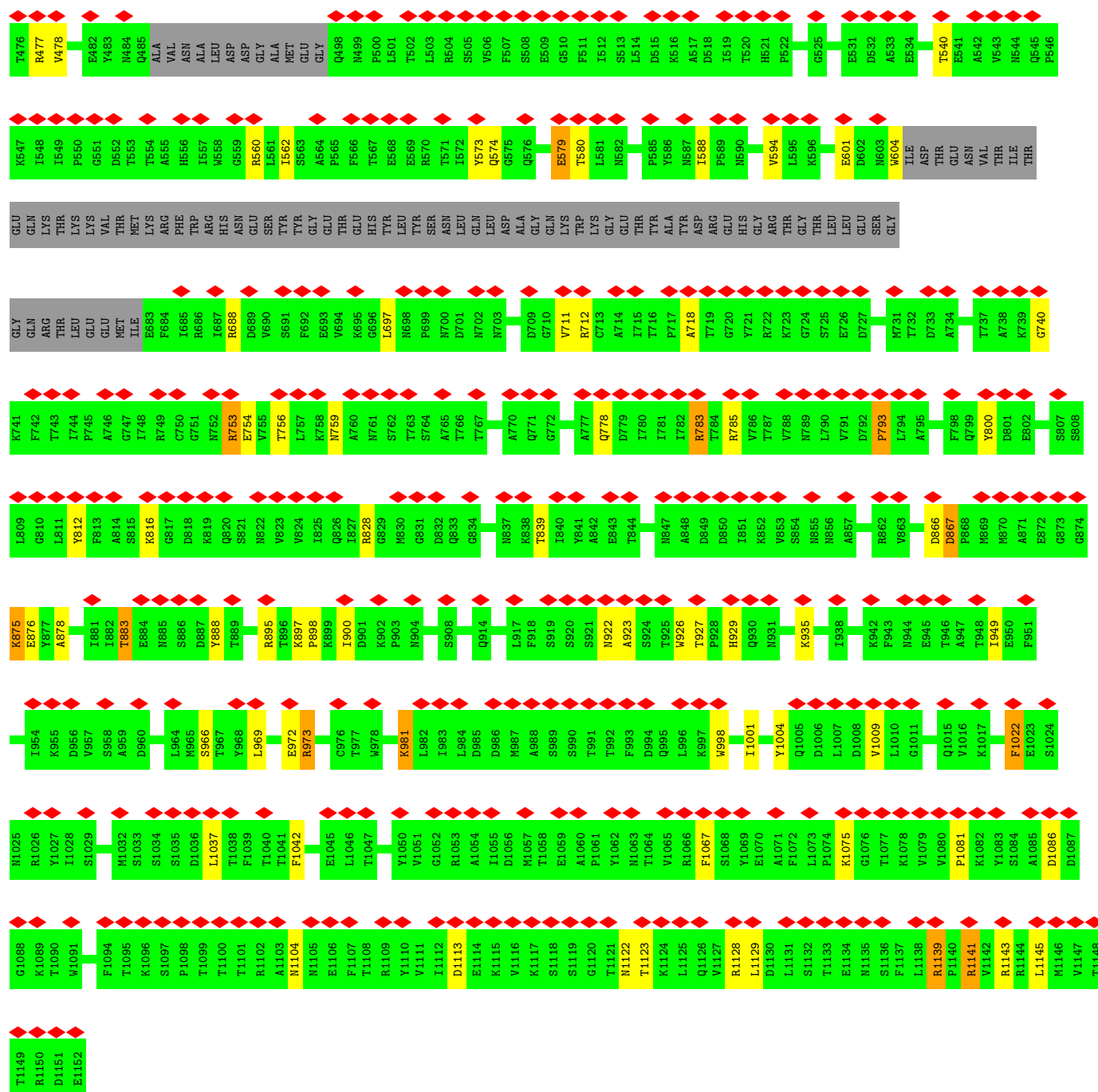
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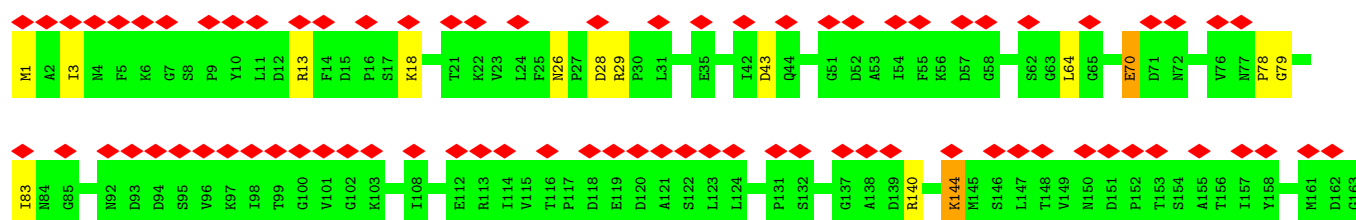
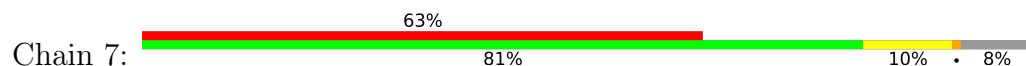


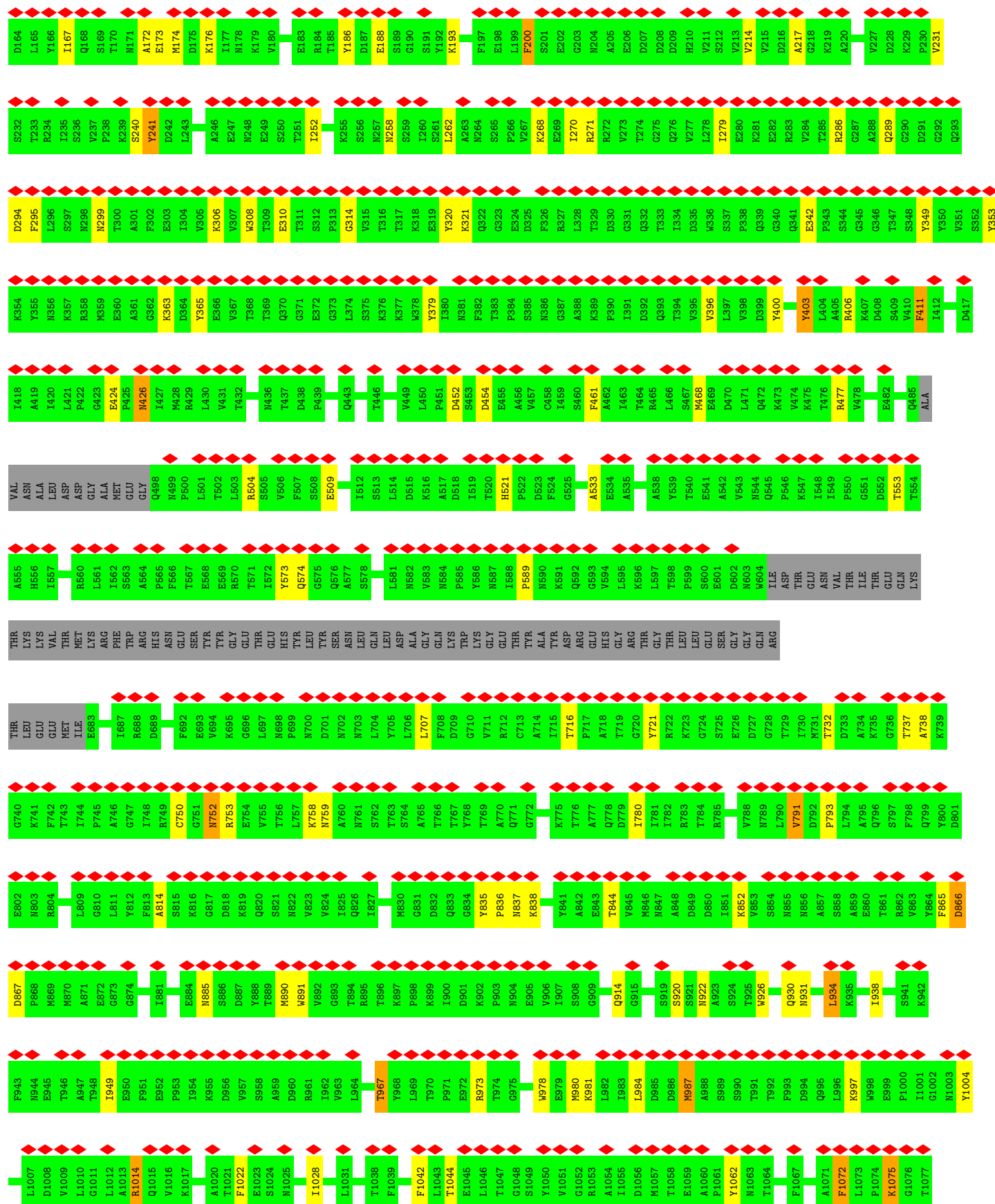
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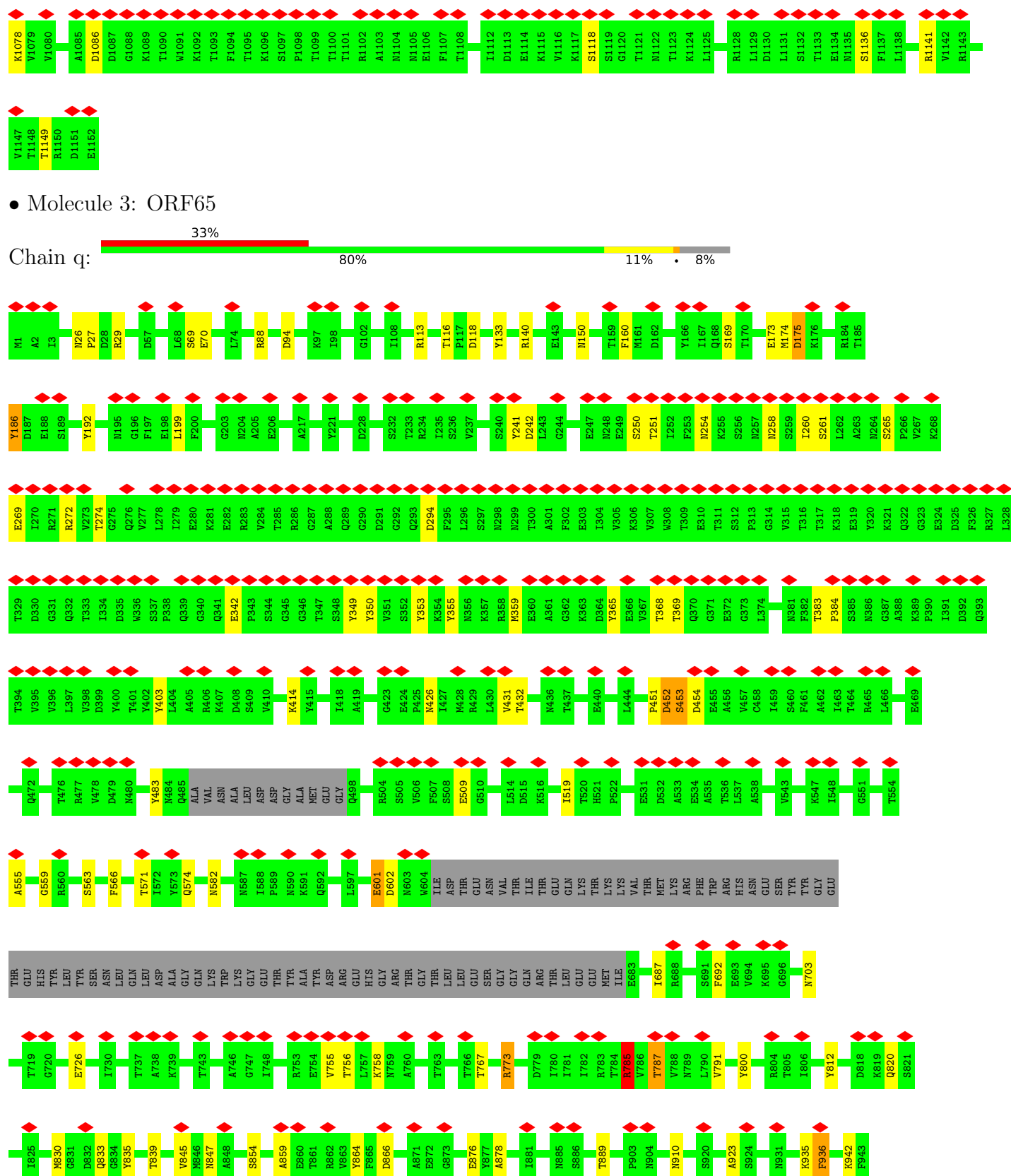


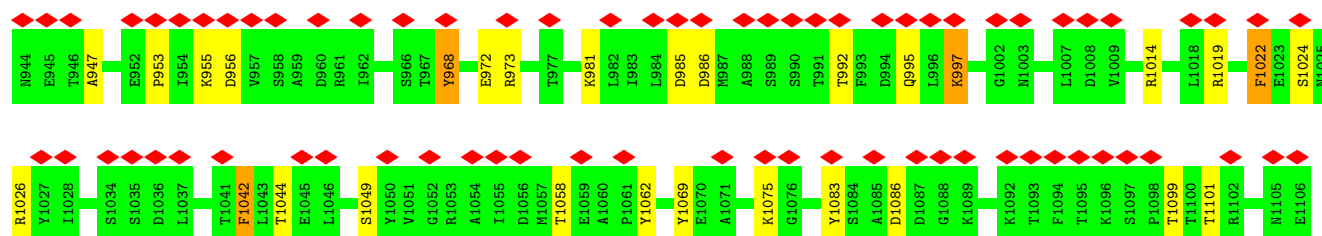


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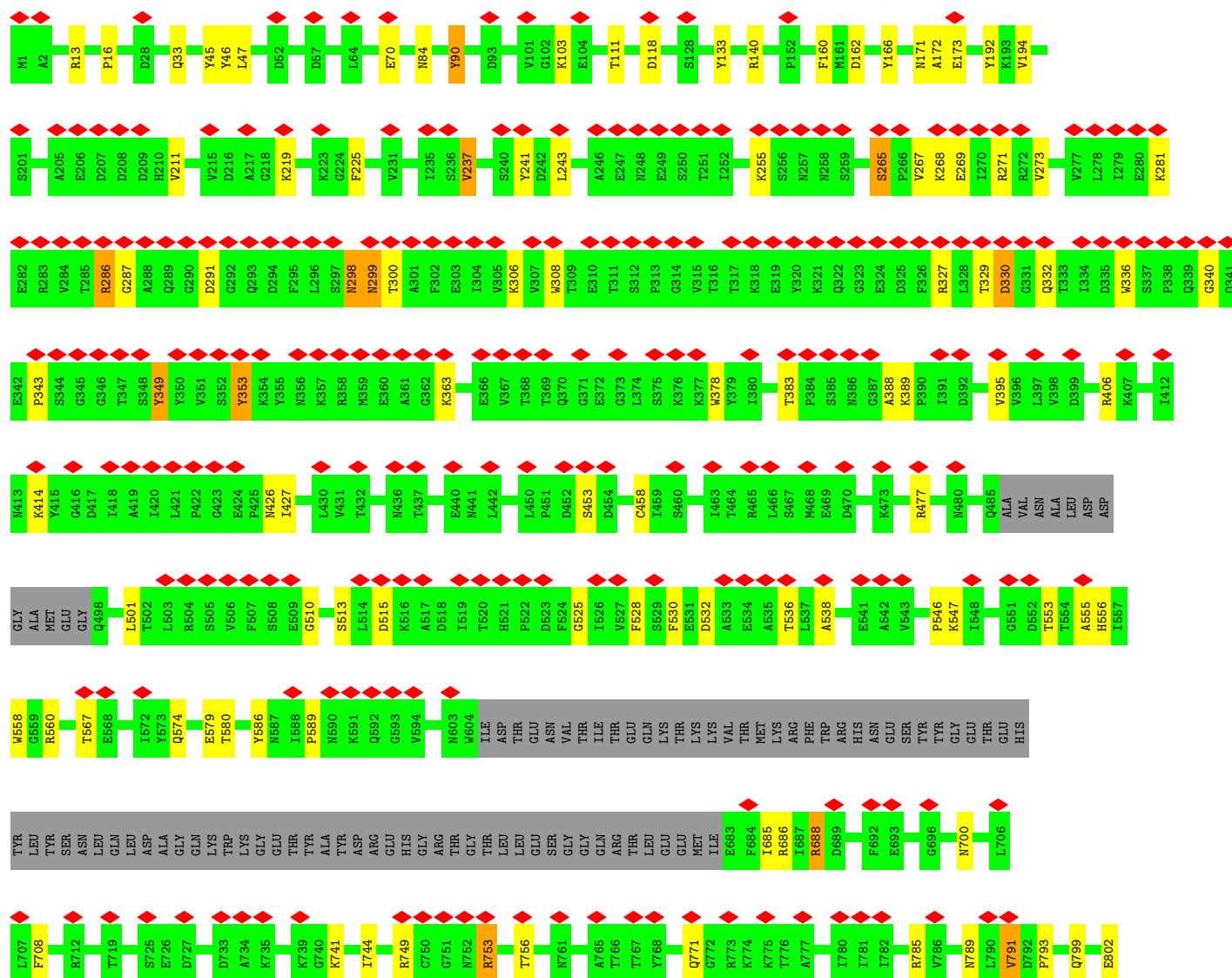
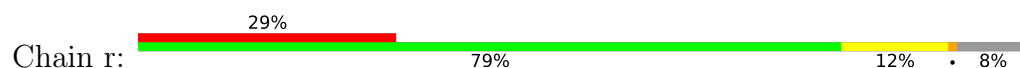


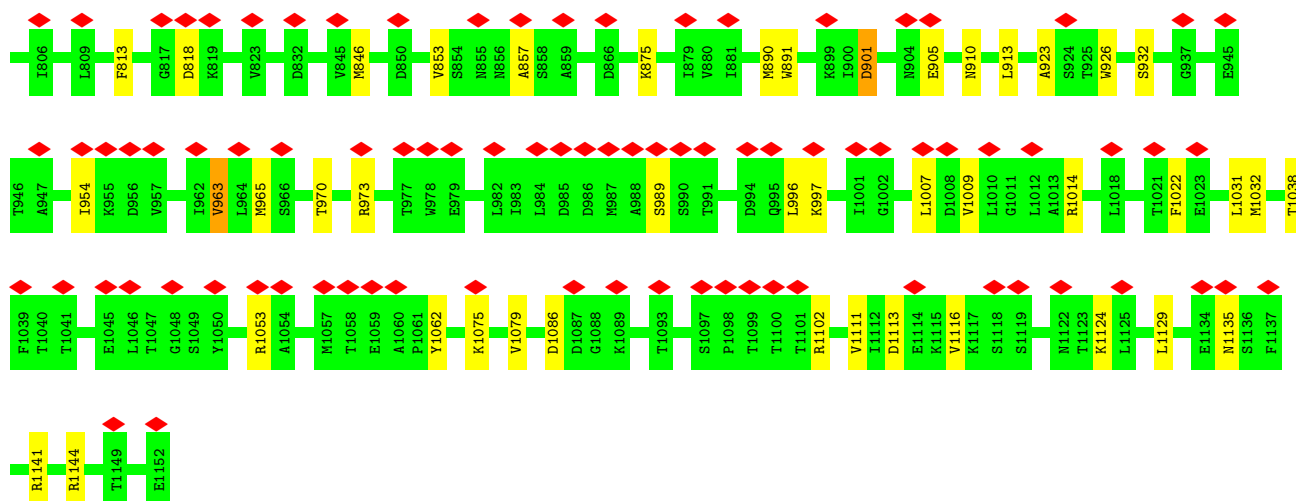




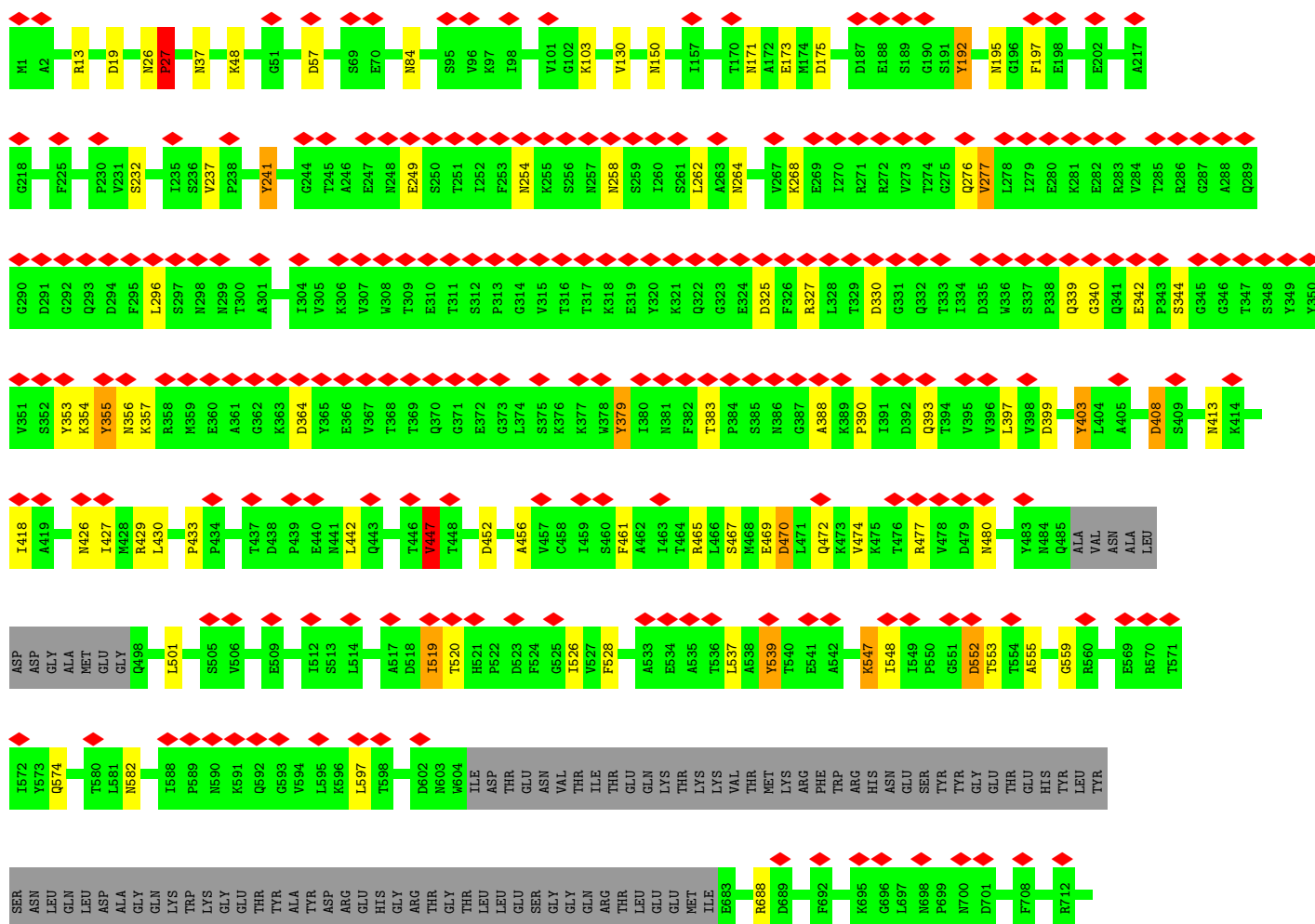
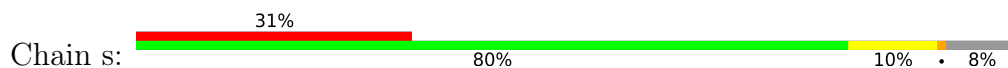


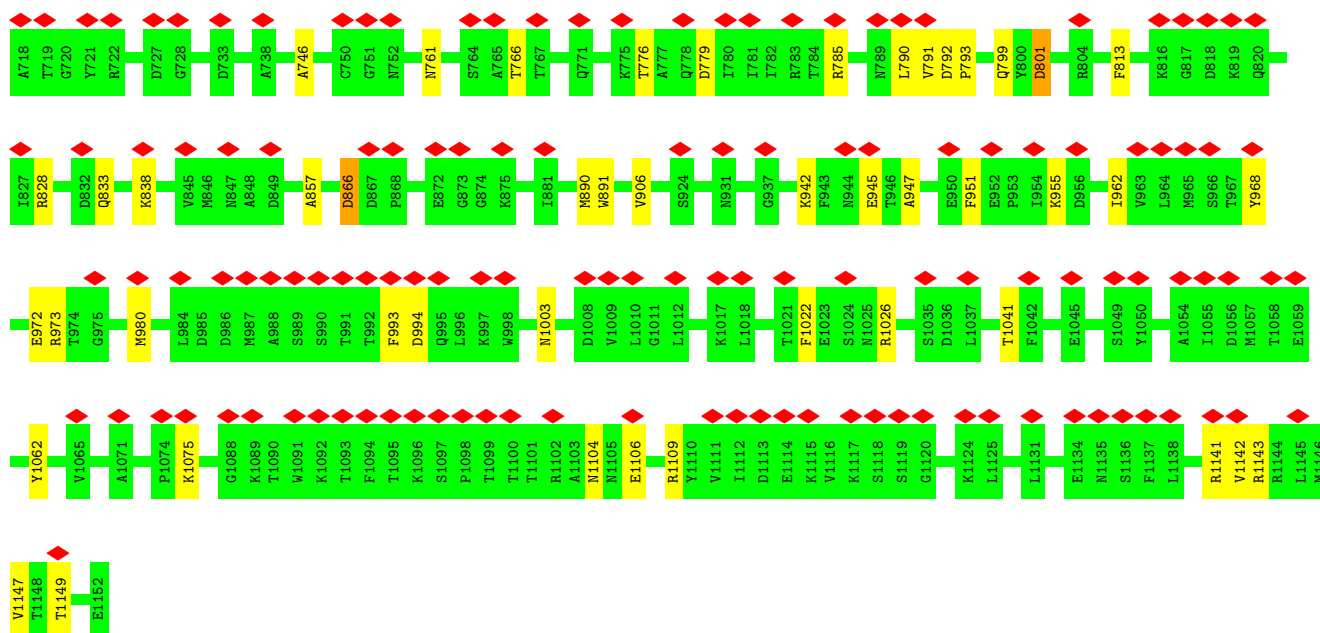
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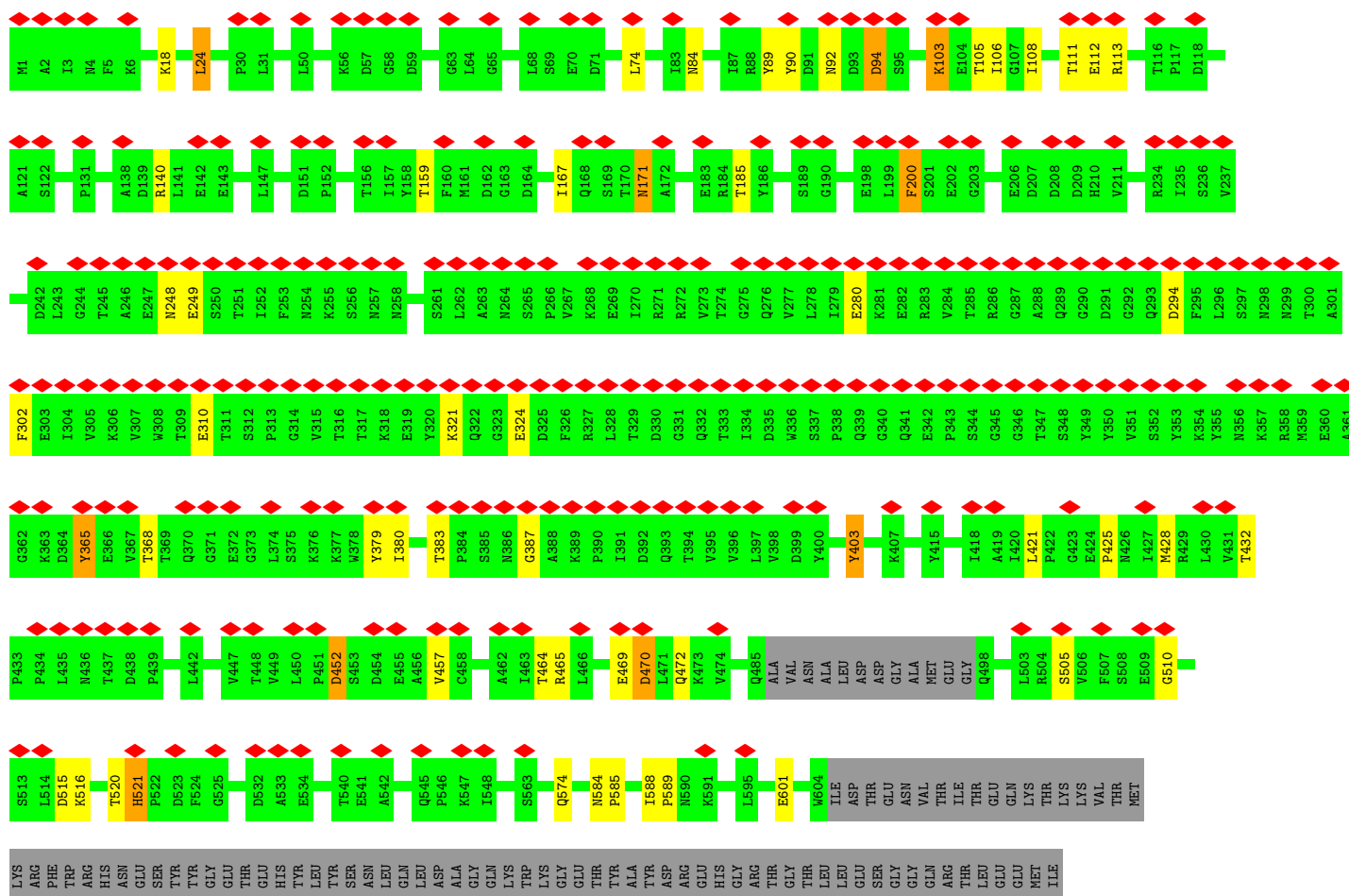
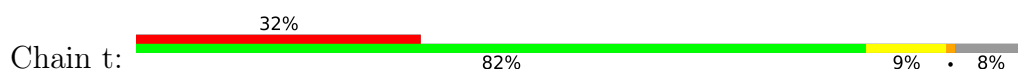


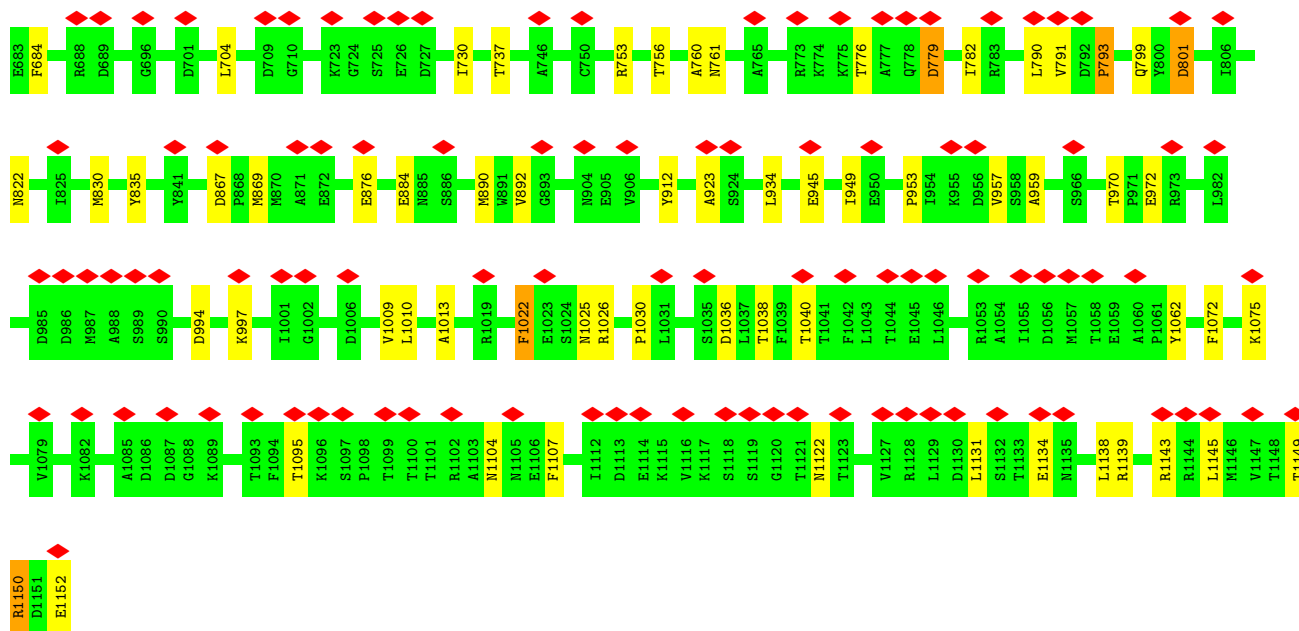
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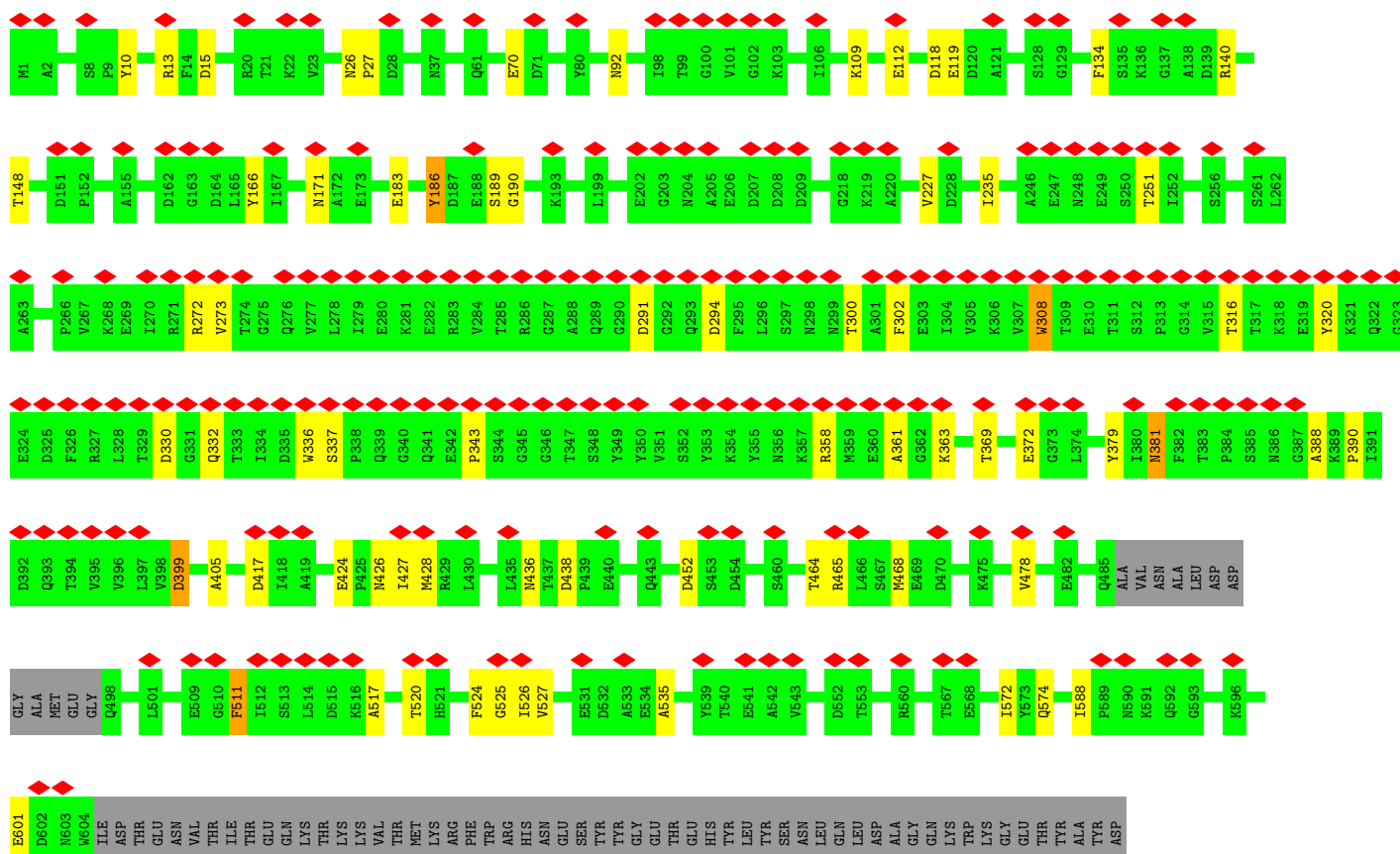
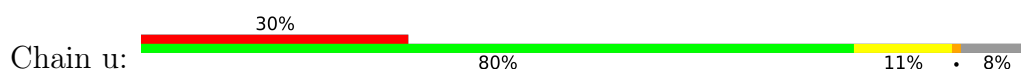


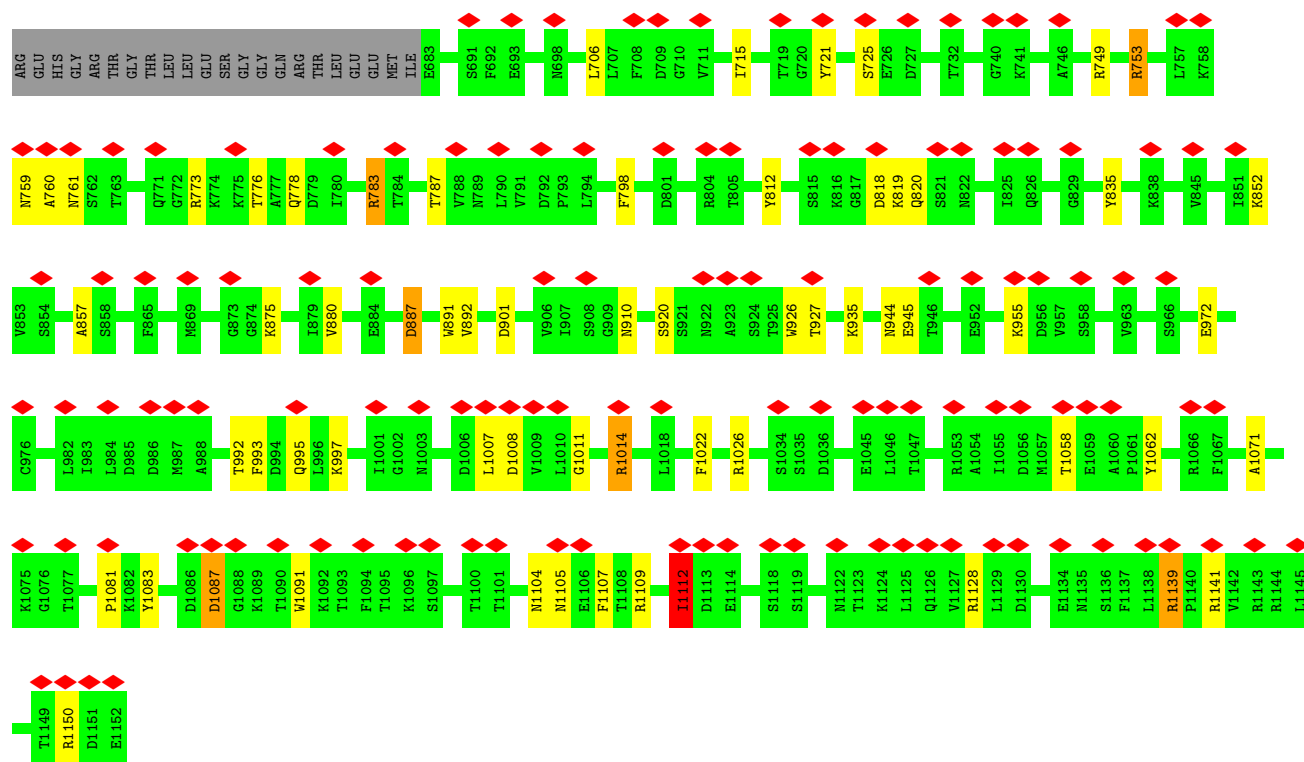
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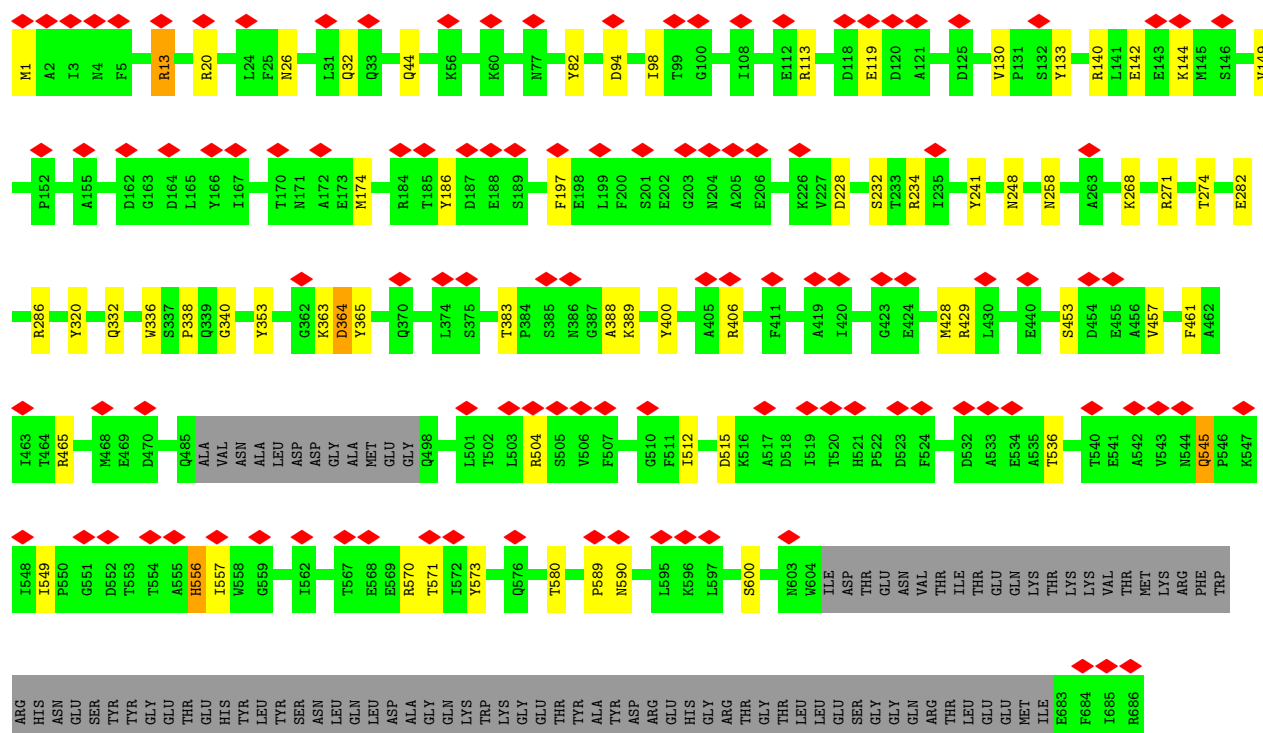
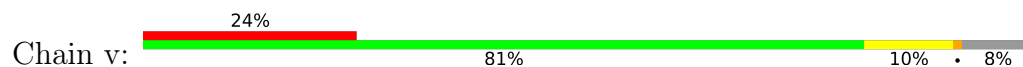


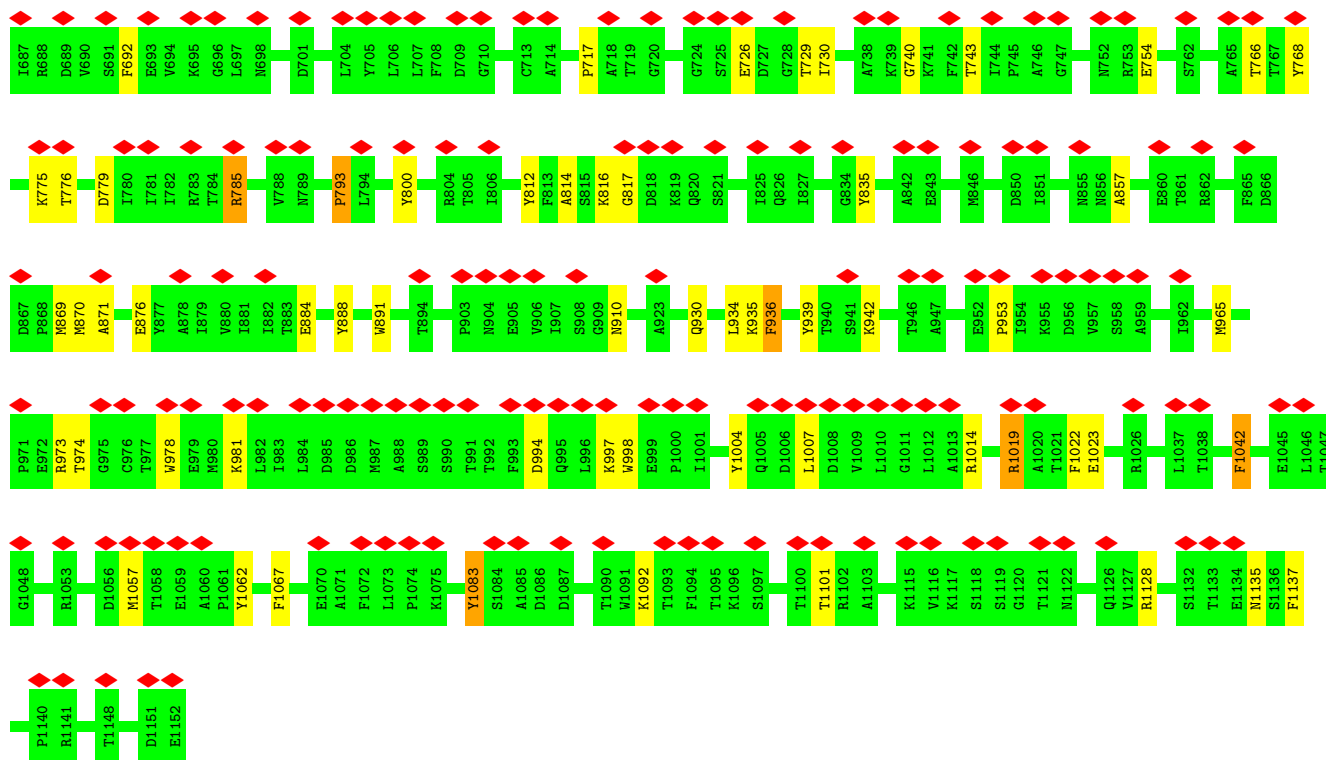
• Molecule 3: ORF65





• Molecule 3: ORF65

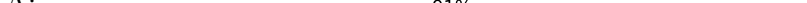


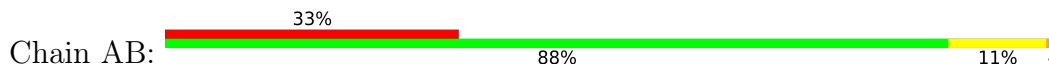


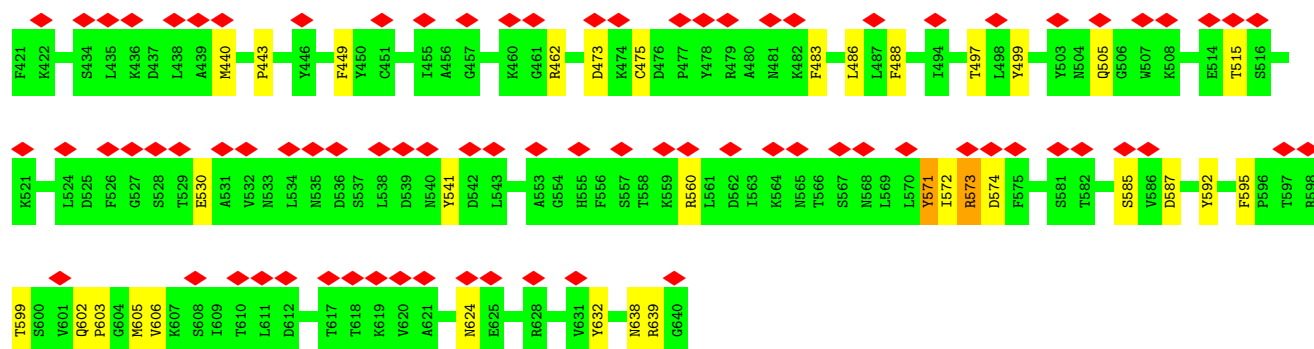
• Molecule 4: ORF58

Chain A: 33% 64%

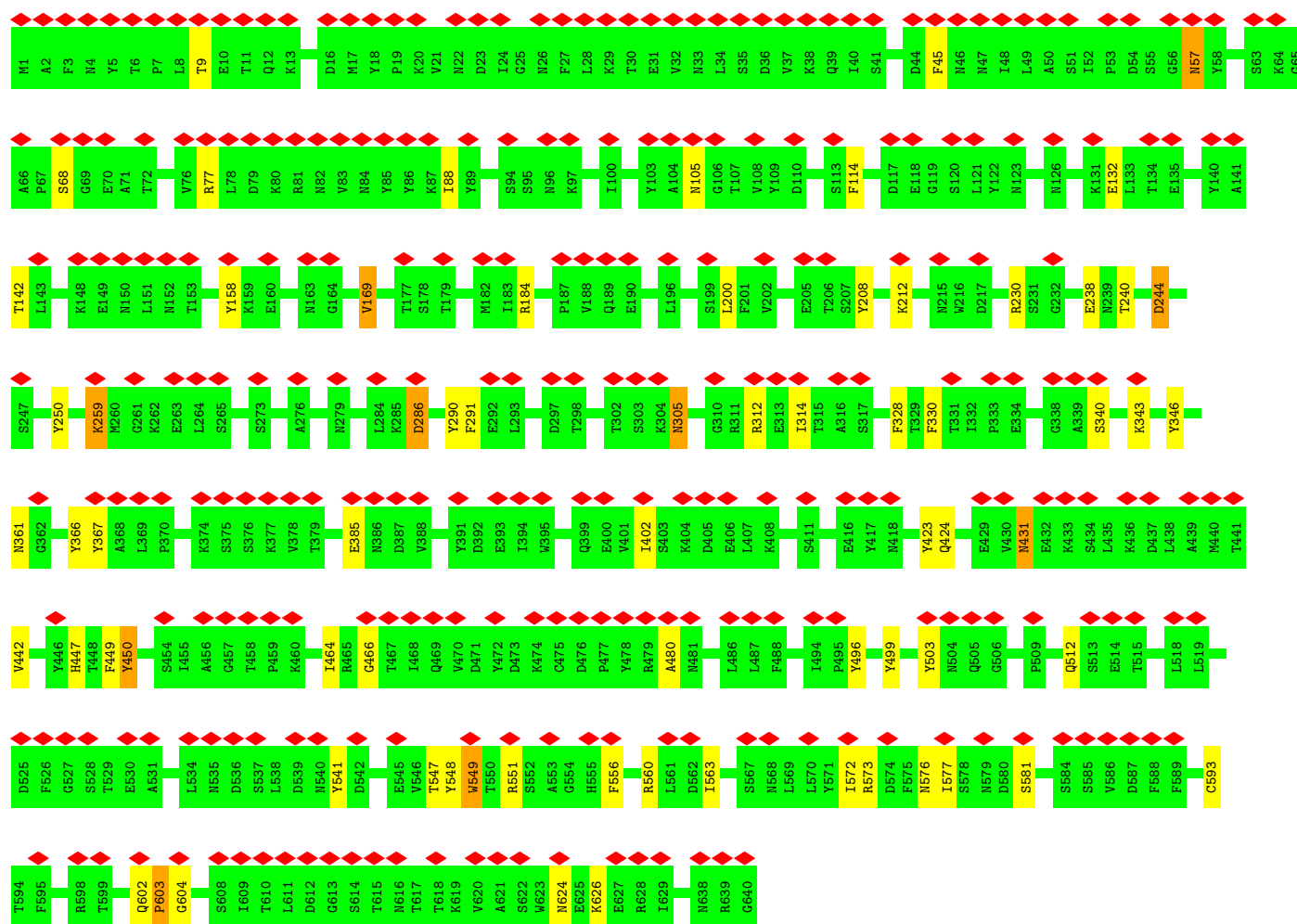
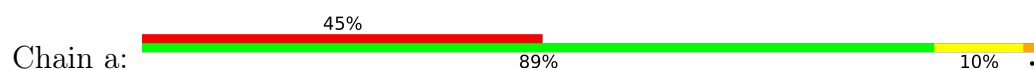
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Chain AA:  33% 91% 8%

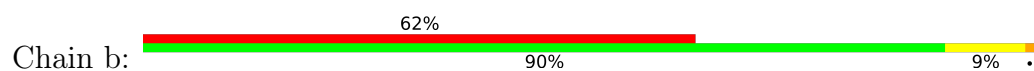


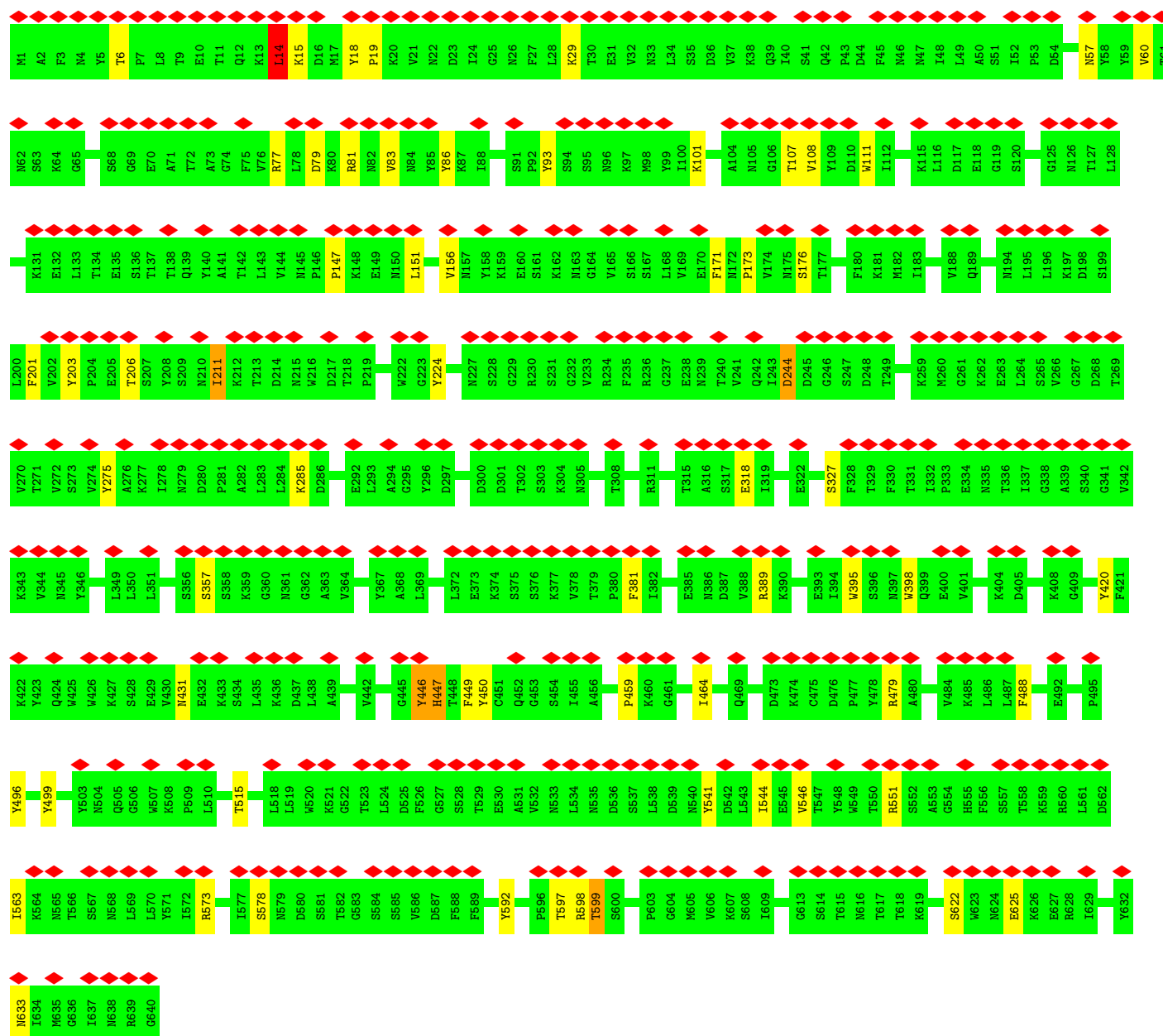


• Molecule 5: CBM-cenC domain-containing protein

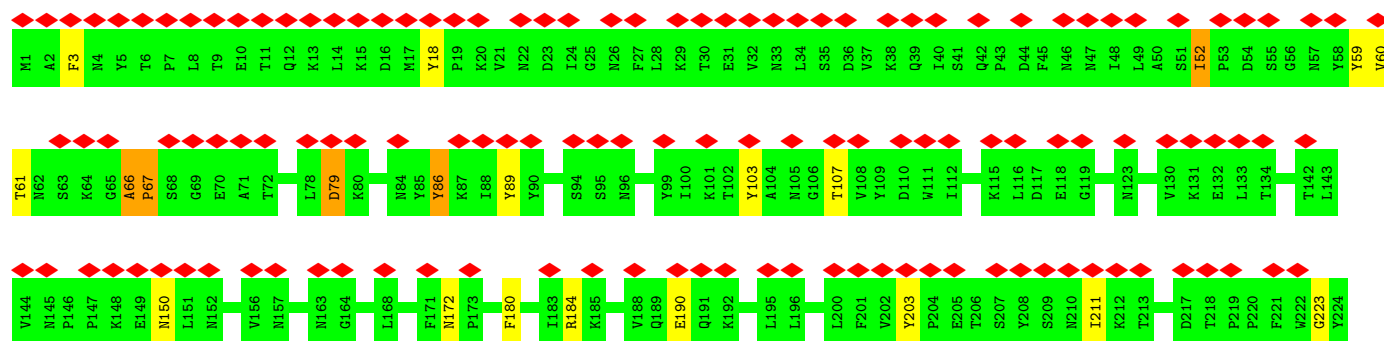
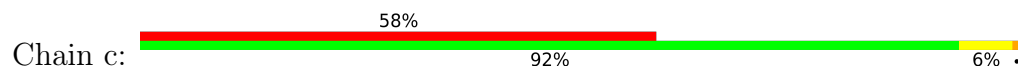


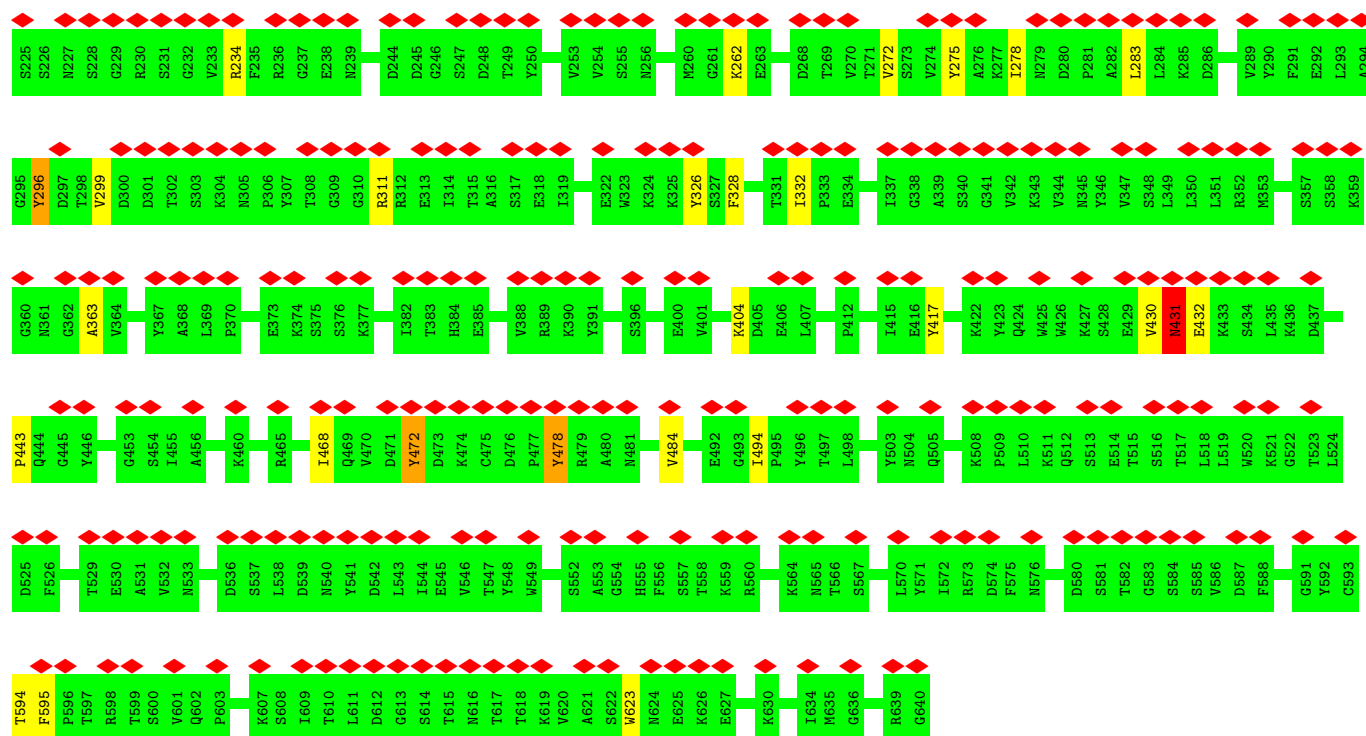
• Molecule 5: CBM-cenC domain-containing protein



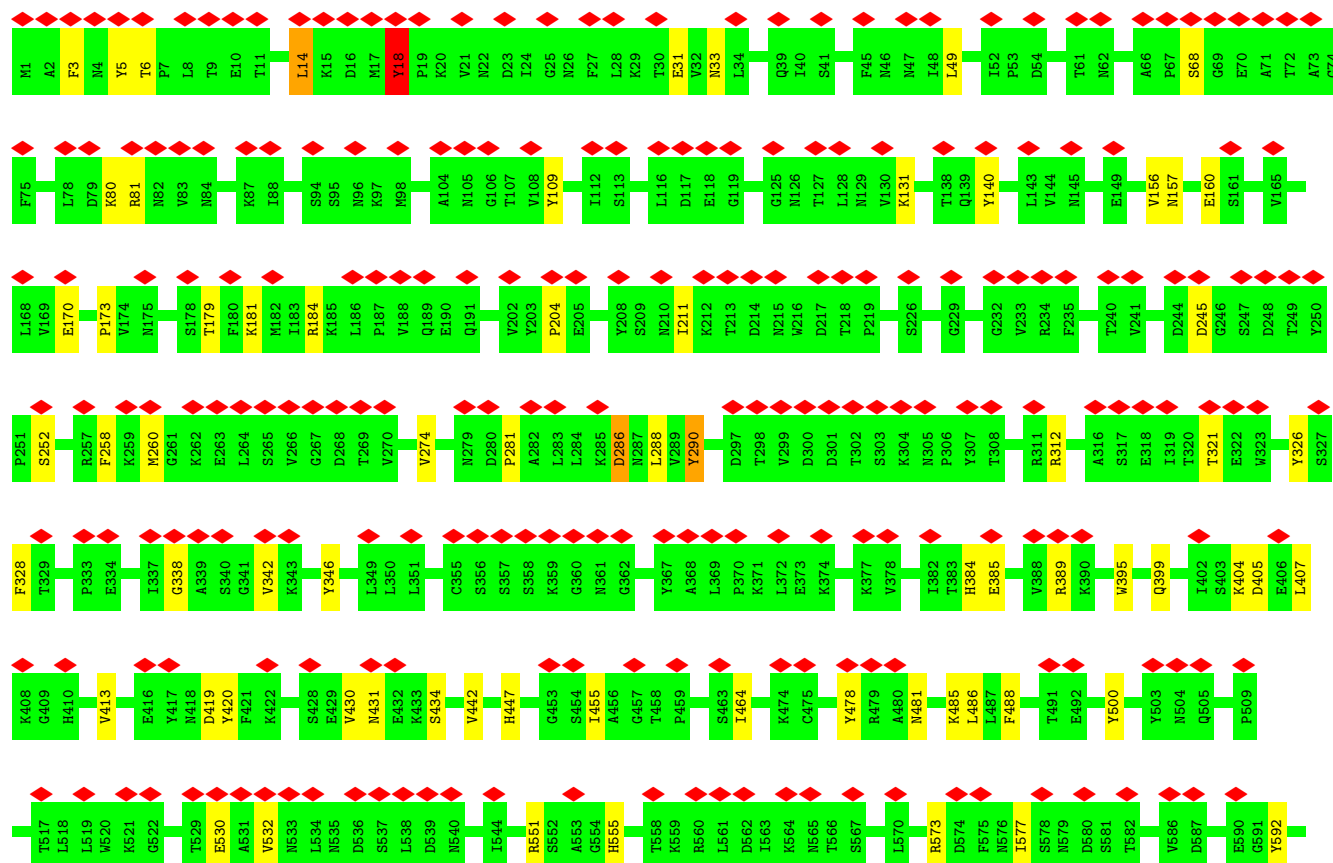
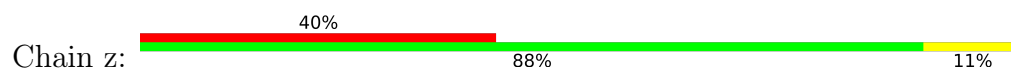


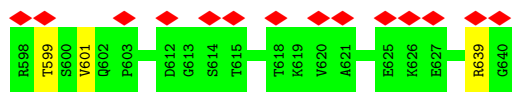
• Molecule 5: CBM-cenC domain-containing protein



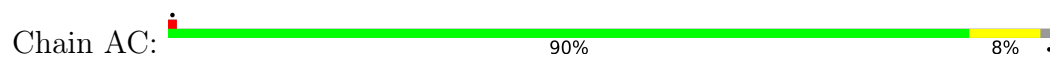


• Molecule 5: CBM-cenC domain-containing protein

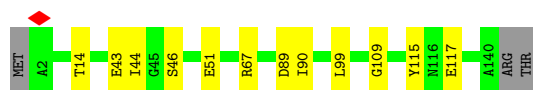




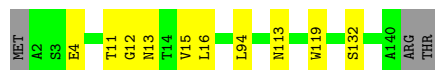
• Molecule 6: ORF50



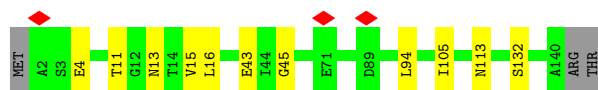
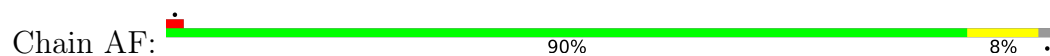
• Molecule 6: ORF50



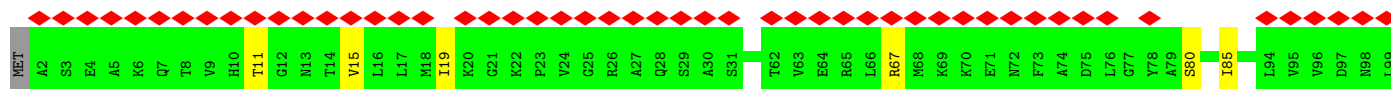
• Molecule 6: ORF50



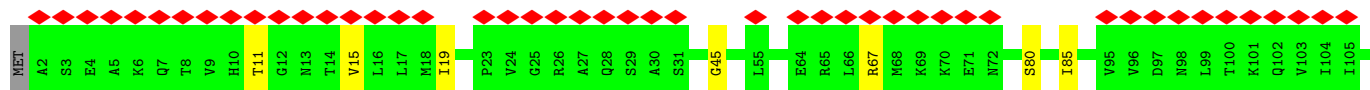
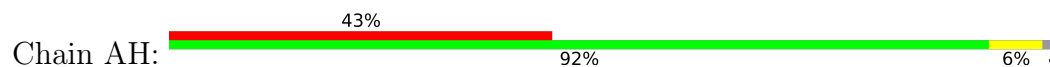
• Molecule 6: ORF50



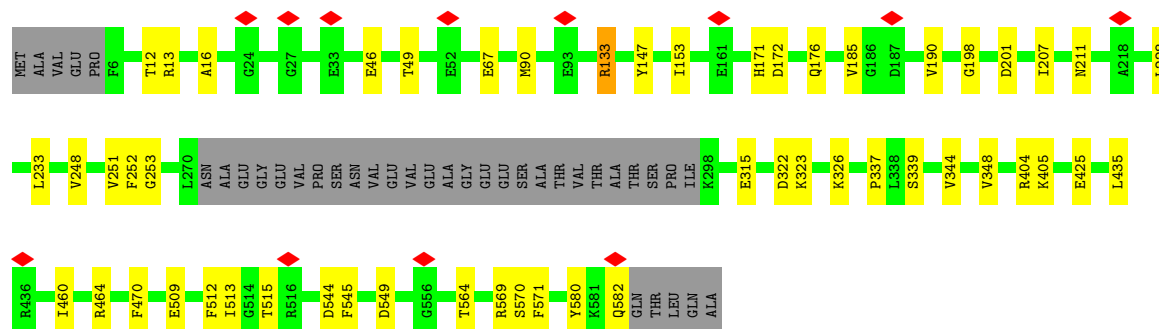
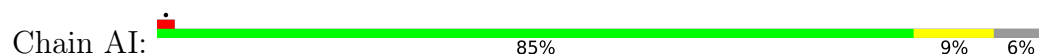
• Molecule 6: ORF50



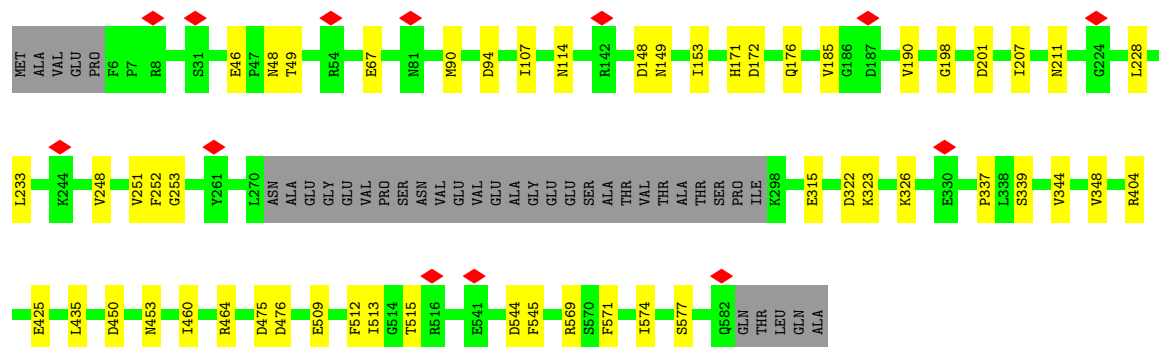
• Molecule 6: ORF50



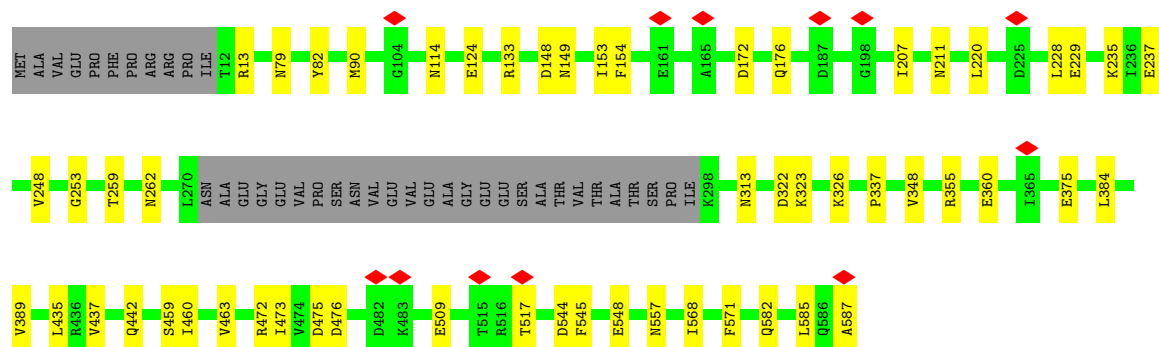
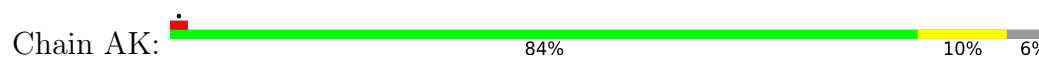
- Molecule 7: ORF49



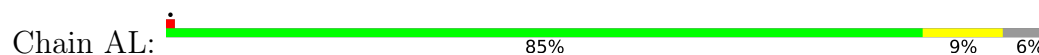
- Molecule 7: ORF49

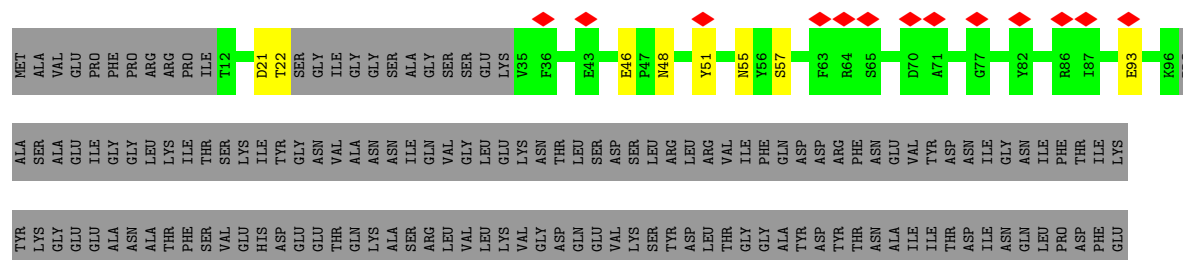


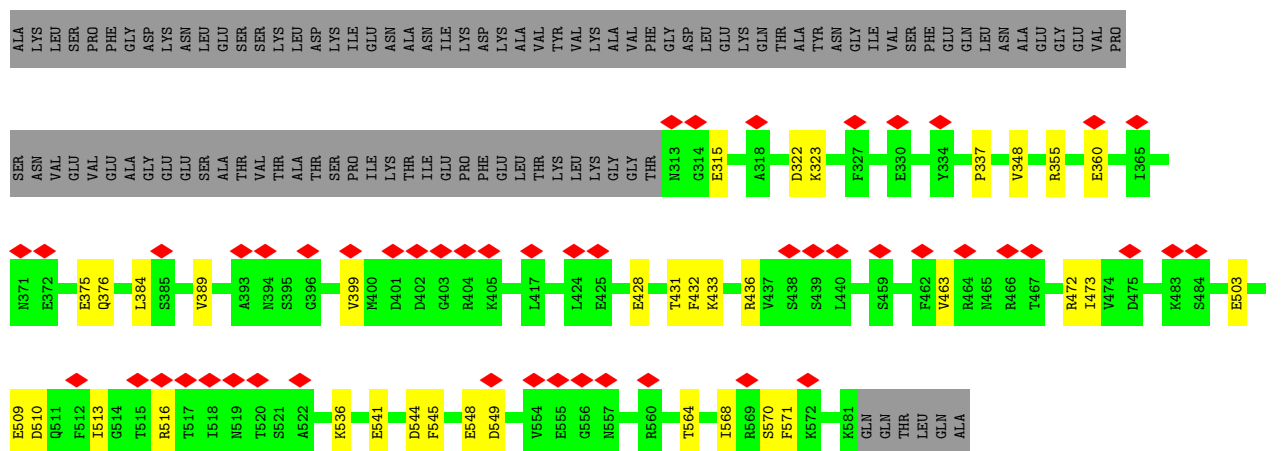
- Molecule 7: ORF49



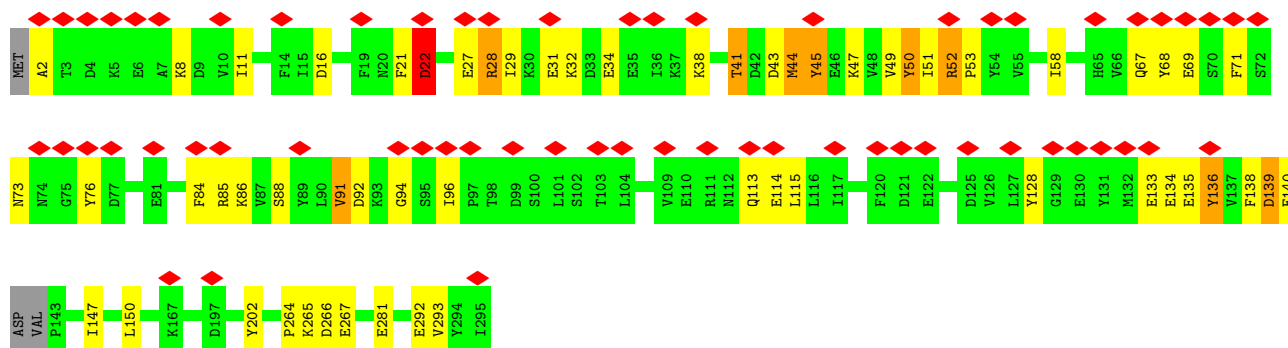
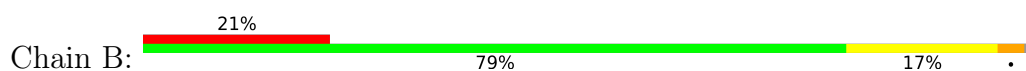
- Molecule 7: ORF49



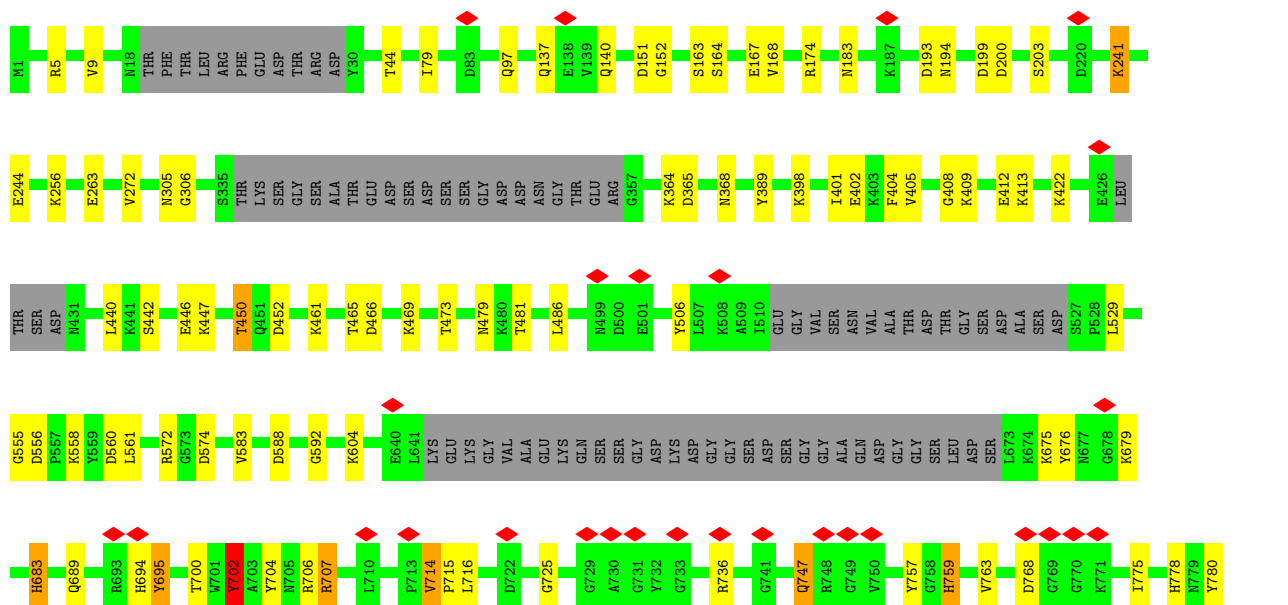
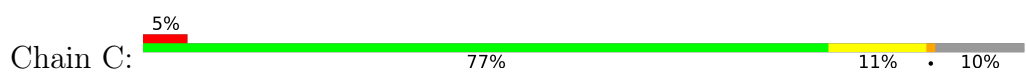


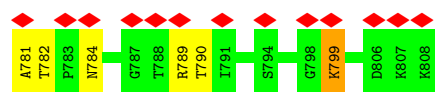


• Molecule 8: ORF57

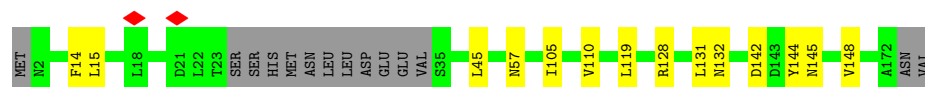
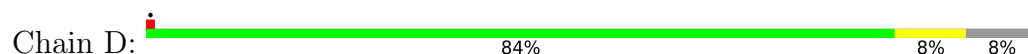


• Molecule 9: ORF56

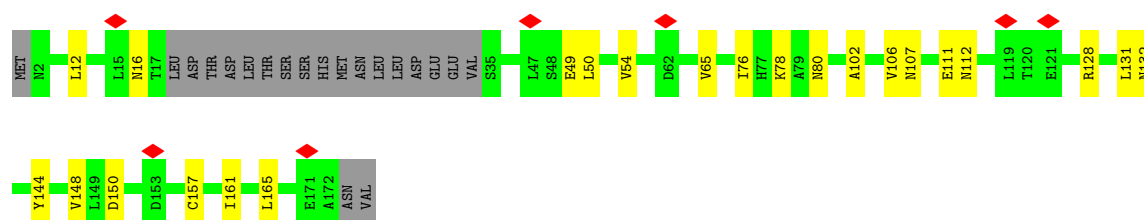
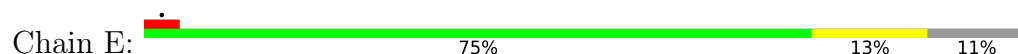




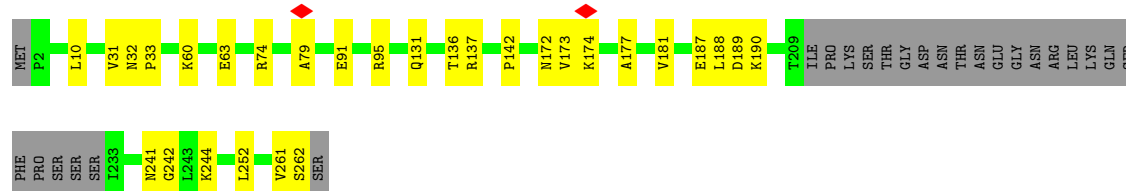
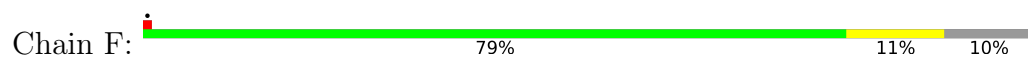
• Molecule 10: ORF60



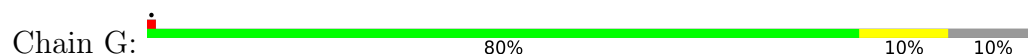
• Molecule 10: ORF60



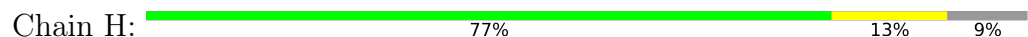
• Molecule 11: ORF59



• Molecule 11: ORF59



• Molecule 12: ORF61



GLU
SER
ILE
ASN
PHE
VAL
LEU
GLY
GLN
ASP
GLU
GLY
ILE
PHE
ALA
LEU
PHE
GLU

• Molecule 12: ORF61

Chain I:  74% 18% 9%

MET R2 Q9 H10 E11 Q15 Q19 E44 T45 D46 E47 E48 K49 M50 K51 D52 R55 L56 D73 V74 S75 V86 D95 L96 N97 H108 G109 T110 S111 D112 D124 L125 L126 D126 R141 H152 F163 M166 I174 E175 V178 S184 L193

I194 D195 W196 K197 I198 Q199 Q206 E210 V214 GLU GLU SER ILE ASN PHE VAL LEU GLY GLN ASP GLU GLY ILE PHE ALA LEU PHE GLU

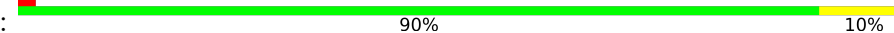
• Molecule 13: ORF62

Chain J:  90% 10%

K1 K16 T28 S31 R76 Q110 C133 K134 E135 D177 R180 T193 N194 V197 R198 I204 P205 D206 V207 V210 I238 L242 D253 V254 E261 V262 N263 I276 R289 D299 D315 V316 D320 V321 D324 N325 L326 D327

V332 I338 G341 E342 I343 L347 K348

• Molecule 13: ORF62

Chain K:  90% 10%

M1 L6 K16 D26 L36 V40 S41 L42 E45 E46 F47 I59 Q84 F85 T86 Q87 D90 A97 Q110 D117 E126 S154 R158 K179 R180 F181 F182 H183 V186 R191 T216 R226 L242 Q243 D244 V245 R246 P247

I250 D253 V254 N294 D299 D320 V321 N325 K348

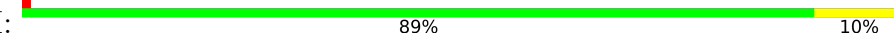
• Molecule 13: ORF62

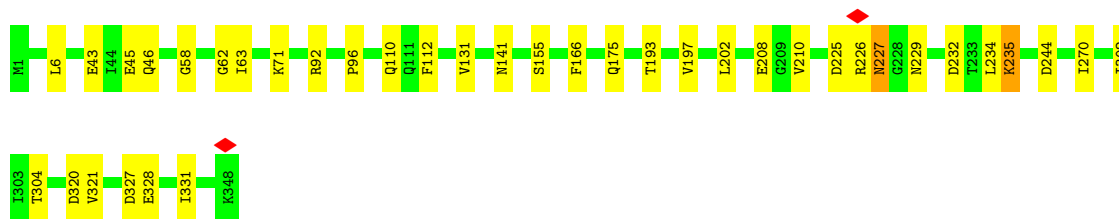
Chain L:  89% 11%

M1 K2 S11 K12 L13 L14 D15 S41 R72 R76 F85 P96 Q106 E107 Y108 L115 C133 R158 E176 R181 T193 V197 D225 R226 N229 K259 E260 E261 V268 R275 I276 G277 L284 L295 K296 T297 S298 D299

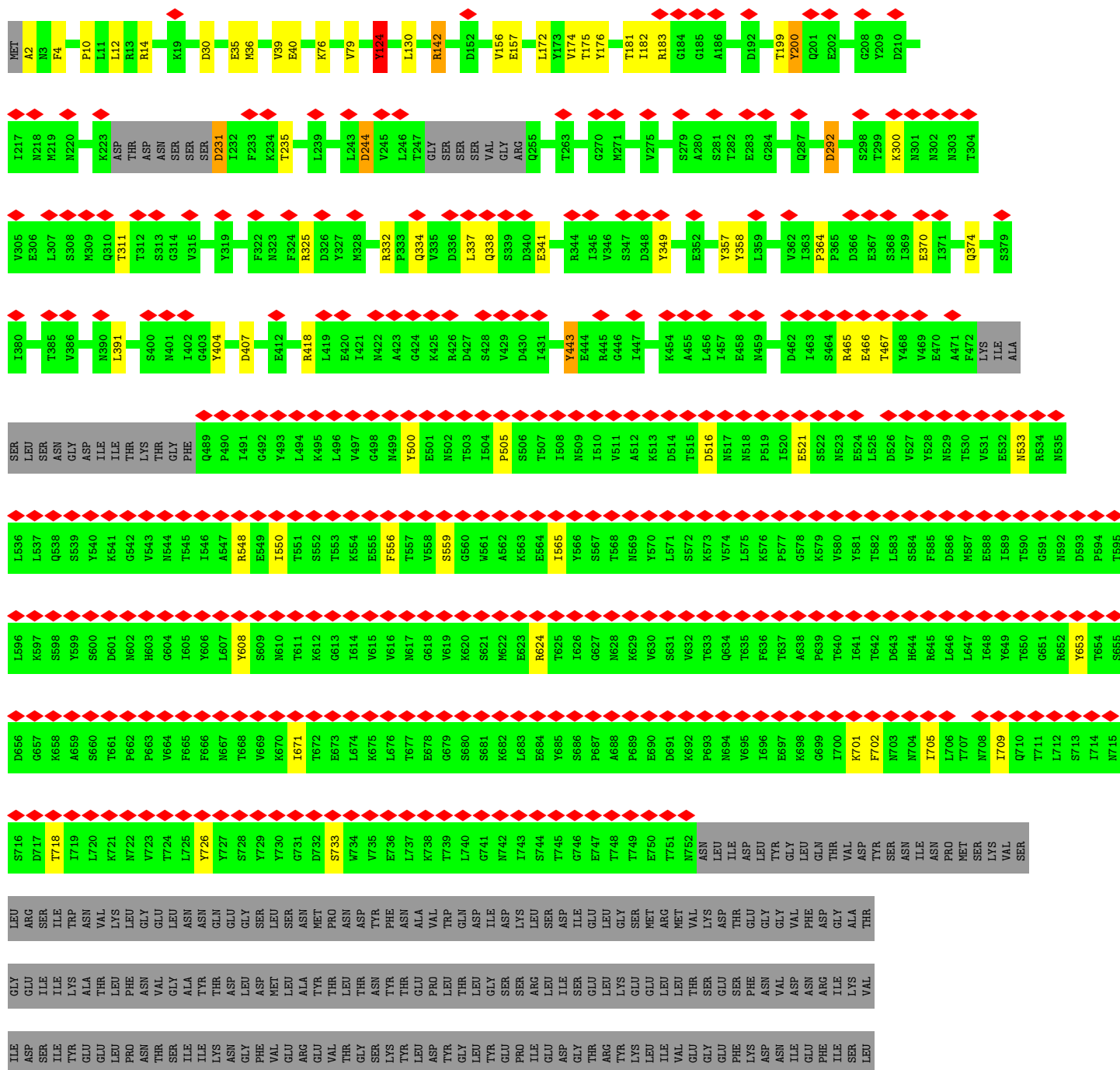
D315 V316 D320 V321 N325 Q335 I338 E342 I343 K344 V345 K348

• Molecule 13: ORF62

Chain M:  89% 10%



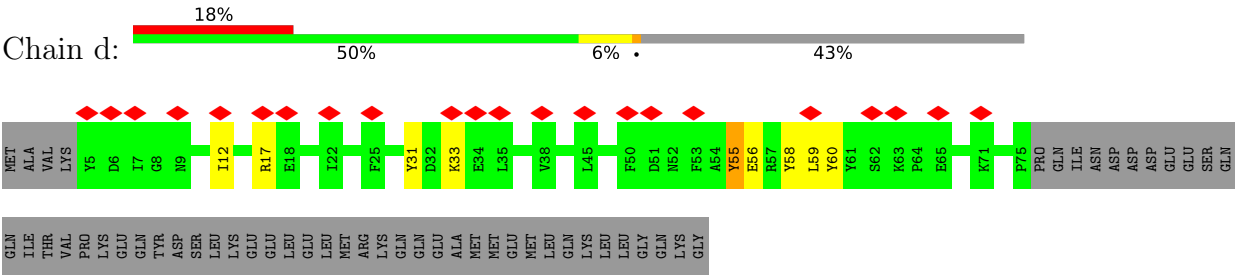
• Molecule 14: ORF63



Chain O: 31% 65% 6% 29%



● Molecule 15: ORF67



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	3586	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.106	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	1067.0079, 1067.0079, 1067.0079	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.6671999, 1.6671999, 1.6671999	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.78	0/3619	1.34	7/4913 (0.1%)
1	8	0.79	0/3619	1.35	11/4913 (0.2%)
1	9	0.80	0/3619	1.37	10/4913 (0.2%)
1	w	0.77	0/3619	1.34	13/4913 (0.3%)
1	x	0.77	0/3619	1.34	7/4913 (0.1%)
1	y	0.75	0/3619	1.33	7/4913 (0.1%)
2	1	0.80	0/1377	1.47	8/1872 (0.4%)
2	P	0.70	0/1292	1.29	1/1756 (0.1%)
2	Q	0.71	0/1303	1.27	5/1771 (0.3%)
2	R	0.74	0/1298	1.23	3/1764 (0.2%)
2	S	0.74	0/1377	1.32	5/1872 (0.3%)
2	T	0.74	0/1377	1.39	7/1872 (0.4%)
2	U	0.70	0/1377	1.41	8/1872 (0.4%)
2	V	0.74	0/1377	1.43	8/1872 (0.4%)
2	W	0.78	0/1377	1.46	11/1872 (0.6%)
2	X	0.80	0/1377	1.51	9/1872 (0.5%)
2	Y	0.75	0/1377	1.46	6/1872 (0.3%)
2	Z	0.75	0/1377	1.48	10/1872 (0.5%)
2	e	0.67	0/1306	1.15	2/1774 (0.1%)
2	f	0.65	0/1296	1.17	0/1760
2	g	0.65	0/1304	1.12	0/1771
2	h	0.67	0/1378	1.20	3/1872 (0.2%)
2	i	0.68	0/1224	1.26	2/1660 (0.1%)
2	j	0.73	0/1378	1.33	2/1872 (0.1%)
2	k	0.74	0/1378	1.38	6/1872 (0.3%)
2	l	0.77	0/1378	1.39	6/1872 (0.3%)
2	m	0.77	0/1378	1.37	6/1872 (0.3%)
2	n	0.76	0/1378	1.39	2/1872 (0.1%)
2	o	0.78	0/1378	1.36	4/1872 (0.2%)
2	p	0.79	0/1378	1.35	4/1872 (0.2%)
3	2	0.84	0/8526	1.46	36/11565 (0.3%)
3	3	0.84	0/8526	1.46	40/11565 (0.3%)
3	4	0.85	0/8526	1.47	43/11565 (0.4%)
3	5	0.89	0/8526	1.48	48/11565 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	6	0.90	0/8526	1.50	45/11565 (0.4%)
3	7	0.89	1/8526 (0.0%)	1.47	39/11565 (0.3%)
3	q	0.85	0/8526	1.45	37/11565 (0.3%)
3	r	0.83	1/8526 (0.0%)	1.42	38/11565 (0.3%)
3	s	0.85	0/8526	1.47	48/11565 (0.4%)
3	t	0.83	0/8526	1.42	35/11565 (0.3%)
3	u	0.82	0/8526	1.41	32/11565 (0.3%)
3	v	0.81	0/8526	1.41	38/11565 (0.3%)
4	A	0.13	0/2511	0.38	0/3394
5	AA	0.80	0/5253	1.39	25/7135 (0.4%)
5	AB	0.81	0/5253	1.44	30/7135 (0.4%)
5	a	0.84	0/5253	1.45	23/7135 (0.3%)
5	b	0.83	0/5253	1.42	17/7135 (0.2%)
5	c	0.83	0/5253	1.42	10/7135 (0.1%)
5	z	0.81	0/5253	1.39	22/7135 (0.3%)
6	AC	0.12	0/1107	0.33	0/1496
6	AD	0.11	0/1107	0.33	0/1496
6	AE	0.12	0/1107	0.33	0/1496
6	AF	0.12	0/1107	0.34	0/1496
6	AG	0.12	0/1107	0.33	0/1496
6	AH	0.12	0/1107	0.33	0/1496
7	AI	0.17	0/4355	0.44	2/5880 (0.0%)
7	AJ	0.11	0/4355	0.36	0/5880
7	AK	0.21	0/4335	0.45	0/5853
7	AL	0.20	0/4335	0.46	0/5853
7	AM	0.15	0/2712	0.40	0/3663
7	AN	0.15	0/2712	0.41	0/3663
8	B	0.62	0/2481	1.18	11/3349 (0.3%)
9	C	0.42	0/5985	0.75	6/8050 (0.1%)
10	D	0.12	0/1315	0.34	0/1788
10	E	0.16	0/1269	0.43	0/1724
11	F	0.12	0/1907	0.40	0/2565
11	G	0.12	0/1900	0.41	0/2555
12	H	0.12	0/1722	0.38	0/2331
12	I	0.12	0/1729	0.37	0/2341
13	J	0.15	0/2803	0.40	0/3794
13	K	0.17	0/2803	0.42	0/3794
13	L	0.31	0/2803	0.64	2/3794 (0.1%)
13	M	0.17	0/2803	0.43	0/3794
14	N	0.70	1/5967 (0.0%)	1.19	13/8098 (0.2%)
14	O	0.67	0/5967	1.11	7/8098 (0.1%)
15	d	0.82	0/613	1.41	0/830
All	All	0.72	3/262008 (0.0%)	1.25	820/355215 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	5
1	8	0	4
1	9	0	3
1	w	0	3
1	x	0	4
1	y	0	2
2	1	0	3
2	P	0	1
2	Q	0	2
2	R	0	1
2	T	0	1
2	U	0	1
2	W	0	1
2	Y	0	1
2	Z	0	2
2	e	0	1
2	i	0	1
2	j	0	2
2	k	0	1
2	l	0	2
2	m	0	1
2	o	0	4
2	p	0	2
3	2	0	10
3	3	0	8
3	4	0	11
3	5	0	14
3	6	0	13
3	7	0	8
3	q	0	15
3	r	0	11
3	s	0	8
3	t	0	7
3	u	0	11
3	v	0	11
5	AA	0	5
5	AB	0	15
5	a	0	12
5	b	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	c	0	11
5	z	0	8
7	AI	0	1
8	B	0	6
9	C	0	8
13	L	0	1
14	N	0	13
14	O	0	8
15	d	0	2
All	All	0	272

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	r	271	ARG	CA-C	7.07	1.55	1.52
14	N	364	PRO	CA-C	6.17	1.55	1.51
3	7	424	GLU	CA-C	5.29	1.57	1.53

All (820) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	134	GLU	N-CA-C	9.13	121.93	108.60
3	s	26	ASN	CA-C-N	9.11	131.23	119.84
3	s	26	ASN	C-N-CA	9.11	131.23	119.84
3	u	381	ASN	CA-CB-CG	8.99	121.59	112.60
3	2	603	ASN	CA-CB-CG	8.90	121.50	112.60
5	AB	595	PHE	CA-CB-CG	8.80	122.60	113.80
3	3	197	PHE	CA-CB-CG	8.67	122.47	113.80
2	P	169	PHE	CA-CB-CG	8.57	122.37	113.80
1	y	143	PHE	CA-CB-CG	8.43	122.23	113.80
2	p	136	ASN	CA-CB-CG	8.40	121.00	112.60
3	3	302	PHE	CA-CB-CG	8.26	122.06	113.80
3	t	801	ASP	CA-CB-CG	8.10	120.70	112.60
2	X	21	ASP	CA-CB-CG	-8.00	104.60	112.60
5	AB	483	PHE	CA-CB-CG	8.00	121.80	113.80
3	6	66	PHE	CA-CB-CG	7.97	121.77	113.80
5	AB	291	PHE	CA-CB-CG	7.97	121.77	113.80
5	b	244	ASP	CA-CB-CG	7.94	120.54	112.60
2	V	136	ASN	CA-CB-CG	7.88	120.48	112.60
3	u	399	ASP	CA-CB-CG	7.86	120.46	112.60
3	v	364	ASP	CA-CB-CG	7.67	120.27	112.60
2	U	21	ASP	CA-CB-CG	-7.56	105.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7	26	ASN	CA-CB-CG	7.54	120.14	112.60
3	t	779	ASP	CA-CB-CG	7.51	120.11	112.60
3	s	197	PHE	CA-CB-CG	7.50	121.30	113.80
3	v	936	PHE	CA-CB-CG	7.48	121.28	113.80
3	6	302	PHE	CA-CB-CG	7.46	121.26	113.80
3	q	265	SER	N-CA-C	7.45	114.84	108.13
3	2	866	ASP	CA-CB-CG	7.44	120.04	112.60
5	a	244	ASP	CA-CB-CG	7.42	120.02	112.60
3	q	26	ASN	CA-C-N	7.39	129.07	119.84
3	q	26	ASN	C-N-CA	7.39	129.07	119.84
3	v	1022	PHE	CA-CB-CG	7.38	121.18	113.80
3	t	200	PHE	CA-CB-CG	7.38	121.18	113.80
3	5	13	ARG	NE-CZ-NH2	7.37	125.83	119.20
3	5	265	SER	N-CA-C	7.34	114.83	108.22
3	4	801	ASP	CA-CB-CG	7.32	119.92	112.60
2	Z	21	ASP	CA-CB-CG	-7.31	105.29	112.60
3	4	26	ASN	CA-C-N	7.26	128.92	119.84
3	4	26	ASN	C-N-CA	7.26	128.92	119.84
8	B	134	GLU	CA-C-N	7.21	135.31	121.54
8	B	134	GLU	C-N-CA	7.21	135.31	121.54
2	W	136	ASN	CA-CB-CG	7.20	119.80	112.60
5	c	404	LYS	N-CA-C	7.20	119.75	111.11
3	4	1107	PHE	CA-CB-CG	7.17	120.97	113.80
3	7	13	ARG	NE-CZ-NH2	7.09	125.58	119.20
3	v	406	ARG	NE-CZ-NH2	7.08	125.57	119.20
2	Z	172	GLU	N-CA-CB	-7.05	99.44	110.44
1	y	32	ARG	NE-CZ-NH2	7.03	125.52	119.20
3	5	94	ASP	CA-CB-CG	7.02	119.62	112.60
2	W	21	ASP	CA-CB-CG	-7.02	105.58	112.60
3	6	1141	ARG	NE-CZ-NH2	6.99	125.49	119.20
5	a	312	ARG	NE-CZ-NH2	6.97	125.47	119.20
3	4	254	ASN	CA-CB-CG	6.96	119.56	112.60
3	v	228	ASP	CA-CB-CG	6.96	119.56	112.60
3	6	1122	ASN	CA-CB-CG	6.96	119.56	112.60
5	b	381	PHE	CA-CB-CG	-6.96	106.84	113.80
1	8	384	ASP	CA-CB-CG	6.96	119.56	112.60
3	7	1042	PHE	CA-CB-CG	6.91	120.70	113.80
3	7	1072	PHE	CA-CB-CG	6.86	120.66	113.80
3	q	454	ASP	CA-CB-CG	6.85	119.45	112.60
3	2	364	ASP	CA-CB-CG	6.83	119.44	112.60
3	3	200	PHE	CA-CB-CG	6.83	120.63	113.80
3	t	470	ASP	CA-CB-CG	6.82	119.42	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	156	PHE	CA-CB-CG	6.81	120.61	113.80
3	6	140	ARG	NE-CZ-NH2	6.81	125.33	119.20
1	w	269	ASP	CA-CB-CG	6.78	119.38	112.60
3	2	298	ASN	CA-CB-CG	6.77	119.37	112.60
8	B	85	ARG	NE-CZ-NH2	6.76	125.28	119.20
2	Q	151	PHE	CA-CB-CG	6.75	120.55	113.80
3	q	985	ASP	CA-CB-CG	6.72	119.32	112.60
3	3	866	ASP	CA-CB-CG	6.70	119.30	112.60
5	c	79	ASP	CA-CB-CG	6.69	119.29	112.60
2	m	169	PHE	CA-CB-CG	6.69	120.49	113.80
3	s	447	VAL	CB-CA-C	6.68	117.98	111.23
3	q	160	PHE	CA-CB-CG	6.67	120.47	113.80
3	4	1067	PHE	CA-CB-CG	6.67	120.47	113.80
5	z	258	PHE	CA-CB-CG	6.66	120.46	113.80
3	4	389	LYS	CA-C-N	6.65	126.68	119.89
3	4	389	LYS	C-N-CA	6.65	126.68	119.89
3	5	311	THR	CA-C-N	6.62	131.66	122.06
3	5	311	THR	C-N-CA	6.62	131.66	122.06
5	AB	279	ASN	CA-CB-CG	6.61	119.21	112.60
3	q	1042	PHE	CA-CB-CG	6.61	120.41	113.80
3	t	793	PRO	CA-N-CD	-6.61	102.75	112.00
3	3	759	ASN	CA-CB-CG	6.59	119.19	112.60
3	5	818	ASP	CA-CB-CG	6.58	119.17	112.60
3	2	225	PHE	CA-CB-CG	6.57	120.37	113.80
5	AB	16	ASP	CA-CB-CG	6.54	119.14	112.60
5	z	33	ASN	CA-CB-CG	6.52	119.12	112.60
5	c	494	ILE	CB-CA-C	6.51	117.92	110.89
2	R	155	GLN	OE1-CD-NE2	-6.50	116.09	122.60
3	7	200	PHE	CA-CB-CG	6.49	120.29	113.80
3	7	193	LYS	CA-C-N	6.49	128.80	120.88
3	7	193	LYS	C-N-CA	6.49	128.80	120.88
8	B	22	ASP	CA-CB-CG	6.49	119.09	112.60
3	u	302	PHE	CA-CB-CG	6.48	120.28	113.80
3	v	1135	ASN	CA-CB-CG	6.48	119.08	112.60
3	4	197	PHE	CA-CB-CG	6.47	120.27	113.80
2	1	65	ARG	NE-CZ-NH2	6.47	125.02	119.20
5	a	602	GLN	CA-C-N	6.45	127.90	119.84
5	a	602	GLN	C-N-CA	6.45	127.90	119.84
2	U	136	ASN	CA-CB-CG	6.44	119.04	112.60
2	1	136	ASN	OD1-CG-ND2	-6.43	116.17	122.60
5	AB	12	GLN	OE1-CD-NE2	-6.43	116.17	122.60
3	v	1019	ARG	NE-CZ-NH2	6.43	124.99	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	408	ASP	CA-CB-CG	6.43	119.03	112.60
1	8	14	ILE	N-CA-C	6.43	117.11	110.36
3	v	994	ASP	CA-CB-CG	6.42	119.02	112.60
3	v	197	PHE	CA-CB-CG	6.42	120.22	113.80
3	r	532	ASP	CA-CB-CG	6.42	119.02	112.60
3	q	692	PHE	N-CA-C	6.41	118.81	109.07
5	b	551	ARG	N-CA-C	6.40	118.25	111.28
3	u	1141	ARG	NE-CZ-NH2	6.39	124.95	119.20
1	y	276	PHE	CA-CB-CG	6.38	120.18	113.80
5	AB	488	PHE	CA-CB-CG	6.36	120.16	113.80
3	5	1067	PHE	CA-CB-CG	6.35	120.15	113.80
2	X	136	ASN	CA-CB-CG	6.33	118.93	112.60
5	z	286	ASP	CA-CB-CG	6.33	118.93	112.60
3	3	431	VAL	CA-CB-CG1	6.32	121.15	110.40
3	4	968	TYR	CA-C-N	6.32	133.19	121.62
3	4	968	TYR	C-N-CA	6.32	133.19	121.62
3	q	1107	PHE	CA-CB-CG	6.32	120.12	113.80
5	AA	296	TYR	CA-C-N	6.31	129.03	120.38
5	AA	296	TYR	C-N-CA	6.31	129.03	120.38
1	8	349	PHE	CA-CB-CG	6.30	120.10	113.80
3	3	760	ALA	CA-C-N	6.30	128.63	120.44
3	3	760	ALA	C-N-CA	6.30	128.63	120.44
5	AA	312	ARG	NE-CZ-NH2	6.30	124.87	119.20
2	1	136	ASN	CA-CB-CG	6.29	118.89	112.60
5	z	573	ARG	NE-CZ-NH2	6.29	124.86	119.20
3	3	295	PHE	CA-CB-CG	6.29	120.09	113.80
3	r	477	ARG	NE-CZ-NH2	6.26	124.84	119.20
3	5	429	ARG	NE-CZ-NH2	6.26	124.83	119.20
2	1	111	GLU	CA-C-N	6.26	137.06	121.80
2	1	111	GLU	C-N-CA	6.26	137.06	121.80
3	6	1022	PHE	CA-CB-CG	6.26	120.06	113.80
3	r	1022	PHE	CA-CB-CG	6.25	120.06	113.80
1	w	35	PHE	CA-CB-CG	6.25	120.05	113.80
5	z	551	ARG	N-CA-C	6.24	118.89	111.71
3	u	381	ASN	OD1-CG-ND2	-6.23	116.37	122.60
3	s	258	ASN	CA-CB-CG	6.21	118.81	112.60
3	6	1042	PHE	CA-CB-CG	6.19	119.99	113.80
3	3	801	ASP	CA-CB-CG	6.19	118.79	112.60
3	u	15	ASP	CA-CB-CG	6.19	118.79	112.60
3	u	1087	ASP	CA-CB-CG	6.19	118.79	112.60
5	AB	473	ASP	CA-CB-CG	6.18	118.78	112.60
14	N	244	ASP	CA-CB-CG	6.18	118.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	x	15	ARG	NE-CZ-NH2	6.18	124.76	119.20
5	a	9	THR	CA-C-N	6.18	128.85	120.38
5	a	9	THR	C-N-CA	6.18	128.85	120.38
3	6	236	SER	CA-C-N	6.17	130.22	123.43
3	6	236	SER	C-N-CA	6.17	130.22	123.43
3	2	1036	ASP	CA-CB-CG	6.17	118.77	112.60
5	AB	443	PRO	CA-C-N	6.16	129.87	120.82
5	AB	443	PRO	C-N-CA	6.16	129.87	120.82
2	W	111	GLU	CA-C-N	6.15	136.81	121.80
2	W	111	GLU	C-N-CA	6.15	136.81	121.80
2	V	146	GLY	N-CA-C	6.15	120.43	112.68
1	w	422	PHE	CA-CB-CG	6.14	119.94	113.80
3	5	421	LEU	CA-C-N	6.13	126.10	120.03
3	5	421	LEU	C-N-CA	6.13	126.10	120.03
2	Q	50	GLN	OE1-CD-NE2	-6.13	116.47	122.60
5	AA	257	ARG	NE-CZ-NH2	6.13	124.72	119.20
2	l	110	ASP	N-CA-C	6.12	117.74	111.14
3	3	1042	PHE	CA-CB-CG	6.11	119.91	113.80
3	r	1144	ARG	NE-CZ-NH2	6.10	124.69	119.20
3	s	801	ASP	CA-CB-CG	6.10	118.70	112.60
7	AI	147	TYR	O-C-N	-6.09	116.10	123.29
5	AB	574	ASP	N-CA-C	6.09	117.40	108.14
3	6	437	THR	CA-C-N	6.09	128.83	120.67
3	6	437	THR	C-N-CA	6.09	128.83	120.67
3	r	1141	ARG	NE-CZ-NH2	6.09	124.68	119.20
3	2	783	ARG	NE-CZ-NH2	6.08	124.68	119.20
1	w	447	GLN	OE1-CD-NE2	-6.08	116.52	122.60
3	2	1126	GLN	OE1-CD-NE2	-6.08	116.52	122.60
3	s	866	ASP	CA-CB-CG	6.08	118.68	112.60
1	8	131	ARG	NE-CZ-NH2	6.08	124.67	119.20
3	2	729	THR	CA-C-N	6.07	128.91	122.11
3	2	729	THR	C-N-CA	6.07	128.91	122.11
3	3	139	ASP	CA-CB-CG	6.07	118.67	112.60
3	t	302	PHE	CA-CB-CG	6.07	119.86	113.80
3	4	389	LYS	N-CA-C	6.06	118.27	109.84
3	r	538	ALA	N-CA-C	6.06	118.53	110.53
2	Y	65	ARG	NE-CZ-NH2	6.06	124.65	119.20
3	3	198	GLU	N-CA-C	6.05	118.58	110.35
3	7	1022	PHE	CA-CB-CG	6.05	119.85	113.80
3	4	574	GLN	OE1-CD-NE2	-6.04	116.56	122.60
3	v	388	ALA	N-CA-C	6.04	117.38	108.86
3	2	867	ASP	CA-CB-CG	6.04	118.64	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	102	HIS	CA-CB-CG	6.03	119.83	113.80
5	AA	389	ARG	NE-CZ-NH2	6.03	124.63	119.20
1	w	131	ARG	NE-CZ-NH2	6.03	124.63	119.20
3	3	712	ARG	NE-CZ-NH2	6.02	124.62	119.20
2	e	169	PHE	CA-CB-CG	6.02	119.82	113.80
3	s	399	ASP	CA-CB-CG	6.02	118.62	112.60
3	5	413	ASN	CA-CB-CG	6.02	118.62	112.60
3	5	382	PHE	CA-CB-CG	6.01	119.81	113.80
5	AB	81	ARG	CA-C-N	6.00	133.00	121.54
5	AB	81	ARG	C-N-CA	6.00	133.00	121.54
2	Z	155	GLN	OE1-CD-NE2	-6.00	116.60	122.60
3	r	688	ARG	NE-CZ-NH2	5.99	124.59	119.20
3	q	1019	ARG	NE-CZ-NH2	5.99	124.59	119.20
3	u	1112	ILE	CA-CB-CG1	5.99	120.58	110.40
3	v	590	ASN	CA-CB-CG	5.98	118.58	112.60
5	AA	287	ASN	CA-CB-CG	5.98	118.58	112.60
5	c	431	ASN	CA-CB-CG	5.98	118.58	112.60
3	3	308	TRP	CA-CB-CG	5.97	124.95	113.60
3	r	13	ARG	NE-CZ-NH2	5.97	124.57	119.20
14	O	121	ASN	O-C-N	-5.97	114.97	122.19
5	AA	379	THR	CA-C-N	5.96	127.30	119.84
5	AA	379	THR	C-N-CA	5.96	127.30	119.84
2	i	169	PHE	CA-CB-CG	5.96	119.77	113.80
3	u	1091	TRP	CA-C-N	5.96	130.03	122.16
3	u	1091	TRP	C-N-CA	5.96	130.03	122.16
3	r	265	SER	N-CA-C	5.96	115.17	108.25
1	x	278	PHE	CA-CB-CG	5.96	119.76	113.80
1	0	131	ARG	NE-CZ-NH2	5.95	124.56	119.20
3	r	771	GLN	N-CA-C	5.95	118.05	110.61
3	5	854	SER	N-CA-C	5.95	117.82	108.96
1	0	422	PHE	CA-CB-CG	5.94	119.74	113.80
3	6	400	TYR	N-CA-C	5.94	118.32	108.99
3	t	185	THR	CA-C-N	5.94	128.52	120.44
3	t	185	THR	C-N-CA	5.94	128.52	120.44
7	AI	133	ARG	NE-CZ-NH2	5.94	124.54	119.20
3	v	365	TYR	N-CA-C	5.93	118.08	109.07
3	5	272	ARG	NE-CZ-NH2	5.92	124.53	119.20
2	n	110	ASP	N-CA-C	5.92	117.82	111.36
3	5	1107	PHE	CA-CB-CG	5.92	119.72	113.80
3	q	1022	PHE	CA-CB-CG	5.91	119.71	113.80
3	4	1128	ARG	NE-CZ-NH2	5.91	124.52	119.20
3	6	259	SER	CA-C-N	5.90	131.07	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6	259	SER	C-N-CA	5.90	131.07	122.69
3	t	588	ILE	N-CA-C	5.90	115.45	108.96
14	O	344	ARG	NE-CZ-NH2	5.89	124.51	119.20
3	5	13	ARG	NE-CZ-NH1	-5.89	115.61	121.50
3	q	1141	ARG	NE-CZ-NH2	5.88	124.50	119.20
3	s	477	ARG	NE-CZ-NH2	5.88	124.49	119.20
3	2	712	ARG	NE-CZ-NH2	5.88	124.49	119.20
14	O	263	THR	O-C-N	-5.88	117.64	123.46
9	C	759	HIS	CA-CB-CG	5.88	119.68	113.80
3	3	308	TRP	CB-CA-C	5.88	119.93	109.65
3	4	765	ALA	N-CA-C	5.87	118.33	109.23
3	t	1150	ARG	NE-CZ-NH2	5.87	124.49	119.20
5	z	312	ARG	NE-CZ-NH2	5.87	124.48	119.20
3	4	1143	ARG	NE-CZ-NH2	5.87	124.48	119.20
3	t	684	PHE	CA-CB-CG	5.87	119.67	113.80
3	s	1003	ASN	CA-C-N	5.86	130.46	122.19
3	s	1003	ASN	C-N-CA	5.86	130.46	122.19
5	a	556	PHE	CA-CB-CG	5.86	119.66	113.80
2	Z	21	ASP	N-CA-C	5.84	117.72	111.36
5	AA	184	ARG	NE-CZ-NH2	5.84	124.45	119.20
2	U	111	GLU	CA-C-N	5.82	135.54	121.68
2	U	111	GLU	C-N-CA	5.82	135.54	121.68
3	u	140	ARG	NE-CZ-NH2	5.82	124.44	119.20
3	4	552	ASP	CA-CB-CG	5.82	118.42	112.60
3	2	208	ASP	CA-CB-CG	5.82	118.42	112.60
2	U	159	ARG	NE-CZ-NH2	5.82	124.44	119.20
3	u	1022	PHE	CA-CB-CG	5.81	119.61	113.80
3	r	140	ARG	NE-CZ-NH2	5.80	124.42	119.20
3	t	1022	PHE	CA-CB-CG	5.80	119.60	113.80
3	3	140	ARG	NE-CZ-NH2	5.80	124.42	119.20
5	AB	389	ARG	NE-CZ-NH2	5.80	124.42	119.20
2	m	101	VAL	CA-CB-CG1	5.79	120.24	110.40
3	6	1143	ARG	NE-CZ-NH2	5.79	124.41	119.20
5	AA	48	ILE	N-CA-C	5.79	116.01	110.74
3	u	588	ILE	N-CA-C	5.79	114.20	107.89
5	c	443	PRO	N-CA-C	5.78	119.71	110.40
3	t	171	ASN	CA-CB-CG	5.78	118.38	112.60
3	u	361	ALA	N-CA-C	5.78	117.27	110.97
3	3	1128	ARG	NE-CZ-NH2	5.78	124.40	119.20
3	7	533	ALA	N-CA-C	5.78	119.40	111.54
2	Z	9	HIS	CA-CB-CG	5.78	119.58	113.80
3	2	295	PHE	CA-CB-CG	5.77	119.57	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AB	184	ARG	NE-CZ-NH2	5.77	124.40	119.20
2	k	156	PHE	CA-CB-CG	5.77	119.57	113.80
3	t	1143	ARG	NE-CZ-NH2	5.77	124.39	119.20
3	2	113	ARG	NE-CZ-NH2	5.76	124.39	119.20
3	7	866	ASP	CA-CB-CG	5.76	118.36	112.60
1	9	36	ASP	CA-CB-CG	5.76	118.36	112.60
1	9	320	ASN	CA-CB-CG	5.76	118.36	112.60
3	2	1014	ARG	NE-CZ-NH2	5.76	124.38	119.20
2	n	111	GLU	N-CA-C	5.76	119.41	112.38
3	q	936	PHE	CA-CB-CG	5.75	119.55	113.80
2	l	101	VAL	CA-CB-CG1	5.75	120.18	110.40
3	t	1143	ARG	NE-CZ-NH1	-5.75	115.75	121.50
3	4	792	ASP	CA-C-N	5.75	126.21	120.52
3	4	792	ASP	C-N-CA	5.75	126.21	120.52
3	u	773	ARG	NE-CZ-NH2	5.74	124.37	119.20
3	4	162	ASP	CA-CB-CG	5.74	118.34	112.60
3	5	1151	ASP	CA-CB-CG	5.74	118.34	112.60
2	Y	111	GLU	N-CA-C	5.74	118.51	109.39
3	t	588	ILE	CA-C-N	5.73	127.01	119.84
3	t	588	ILE	C-N-CA	5.73	127.01	119.84
5	a	442	VAL	N-CA-C	5.73	113.55	107.76
3	5	753	ARG	NE-CZ-NH2	5.73	124.36	119.20
3	7	759	ASN	CA-CB-CG	5.73	118.33	112.60
14	N	418	ARG	NE-CZ-NH2	5.72	124.35	119.20
3	v	113	ARG	NE-CZ-NH2	5.72	124.34	119.20
1	0	55	ASP	CA-CB-CG	5.71	118.31	112.60
3	t	94	ASP	CA-CB-CG	5.71	118.31	112.60
3	q	254	ASN	CA-CB-CG	5.70	118.30	112.60
2	m	136	ASN	CA-CB-CG	5.70	118.30	112.60
3	5	207	ASP	CA-CB-CG	5.70	118.30	112.60
3	2	342	GLU	N-CA-C	5.70	113.35	108.22
2	k	135	PHE	CA-CB-CG	5.70	119.50	113.80
2	1	146	GLY	N-CA-C	5.70	119.22	112.33
2	U	9	HIS	CB-CG-CD2	-5.69	123.80	131.20
3	4	25	PHE	CA-CB-CG	-5.69	108.11	113.80
2	Y	111	GLU	CA-C-N	5.69	132.50	122.08
2	Y	111	GLU	C-N-CA	5.69	132.50	122.08
3	2	910	ASN	CA-CB-CG	-5.69	106.91	112.60
8	B	84	PHE	CA-CB-CG	5.69	119.49	113.80
3	v	1019	ARG	NE-CZ-NH1	-5.69	115.81	121.50
5	AB	311	ARG	NE-CZ-NH2	5.68	124.32	119.20
5	b	573	ARG	NE-CZ-NH2	5.68	124.31	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	172	ALA	CA-C-N	5.68	132.38	121.54
3	3	172	ALA	C-N-CA	5.68	132.38	121.54
3	5	510	GLY	CA-C-N	5.68	132.38	121.54
3	5	510	GLY	C-N-CA	5.68	132.38	121.54
2	T	21	ASP	CA-CB-CG	-5.68	106.92	112.60
5	a	114	PHE	CA-CB-CG	5.67	119.47	113.80
5	a	431	ASN	N-CA-C	5.67	119.78	112.86
3	u	465	ARG	NE-CZ-NH2	5.67	124.31	119.20
2	k	136	ASN	CA-CB-CG	5.67	118.27	112.60
1	x	115	HIS	CA-CB-CG	5.67	119.47	113.80
5	AB	462	ARG	NE-CZ-NH2	5.67	124.30	119.20
3	s	537	LEU	N-CA-C	5.67	117.64	110.33
2	W	82	ASN	CA-CB-CG	5.66	118.26	112.60
1	w	70	ARG	NE-CZ-NH2	5.66	124.29	119.20
3	3	1005	GLN	OE1-CD-NE2	-5.66	116.94	122.60
3	t	112	GLU	N-CA-C	5.66	118.00	110.53
3	s	519	ILE	CA-C-N	5.65	129.64	120.60
3	s	519	ILE	C-N-CA	5.65	129.64	120.60
14	O	472	PHE	CA-CB-CG	5.64	119.44	113.80
3	7	461	PHE	CA-CB-CG	5.64	119.44	113.80
3	3	243	LEU	CA-C-N	5.64	125.46	120.10
3	3	243	LEU	C-N-CA	5.64	125.46	120.10
3	s	150	ASN	CA-CB-CG	5.64	118.24	112.60
5	a	286	ASP	CA-CB-CG	5.63	118.23	112.60
3	s	980	MET	N-CA-C	5.62	117.62	109.07
2	j	93	ALA	CA-C-N	5.62	128.13	120.54
2	j	93	ALA	C-N-CA	5.62	128.13	120.54
3	6	312	SER	N-CA-C	5.62	113.27	108.22
3	5	1144	ARG	NE-CZ-NH2	5.61	124.25	119.20
2	Z	111	GLU	N-CA-C	5.61	118.31	109.39
3	t	472	GLN	OE1-CD-NE2	-5.61	116.99	122.60
3	v	13	ARG	NE-CZ-NH2	5.61	124.25	119.20
2	X	111	GLU	CA-C-N	5.60	135.47	121.80
2	X	111	GLU	C-N-CA	5.60	135.47	121.80
5	b	389	ARG	NE-CZ-NH2	5.60	124.24	119.20
3	7	78	PRO	N-CA-C	5.60	120.01	111.11
3	u	887	ASP	CA-CB-CG	5.60	118.20	112.60
3	4	1086	ASP	CA-CB-CG	5.59	118.19	112.60
3	v	1067	PHE	CA-CB-CG	5.59	119.39	113.80
14	N	341	GLU	CB-CG-CD	-5.59	103.10	112.60
2	T	111	GLU	CA-C-N	5.59	135.43	121.80
2	T	111	GLU	C-N-CA	5.59	135.43	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	292	ASP	CA-CB-CG	5.58	118.18	112.60
2	l	89	THR	CA-C-N	5.58	125.25	119.05
2	l	89	THR	C-N-CA	5.58	125.25	119.05
3	3	1108	THR	CA-CB-CG2	5.58	119.99	110.50
3	4	931	ASN	CA-CB-CG	5.58	118.18	112.60
3	6	929	HIS	CA-C-N	5.58	128.03	120.38
3	6	929	HIS	C-N-CA	5.58	128.03	120.38
2	h	65	ARG	NE-CZ-NH2	5.58	124.22	119.20
3	r	515	ASP	N-CA-C	5.58	119.71	113.01
2	e	65	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	0	115	HIS	CB-CG-CD2	-5.58	123.95	131.20
3	q	773	ARG	NE-CZ-NH2	5.57	124.22	119.20
3	r	160	PHE	CA-CB-CG	5.57	119.37	113.80
2	Z	29	LYS	CB-CA-C	5.57	120.23	112.11
3	r	753	ARG	NE-CZ-NH2	5.57	124.21	119.20
14	N	231	ASP	CA-C-N	5.56	131.98	121.97
14	N	231	ASP	C-N-CA	5.56	131.98	121.97
5	AA	441	THR	CA-C-N	5.56	126.38	122.60
5	AA	441	THR	C-N-CA	5.56	126.38	122.60
5	AB	6	THR	CA-C-N	5.55	126.78	119.84
5	AB	6	THR	C-N-CA	5.55	126.78	119.84
14	N	364	PRO	N-CA-CB	5.55	106.30	103.19
3	s	27	PRO	CA-N-CD	-5.55	104.23	112.00
5	AB	573	ARG	NE-CZ-NH2	5.55	124.19	119.20
2	k	65	ARG	NE-CZ-NH2	5.55	124.19	119.20
2	S	136	ASN	CA-CB-CG	5.55	118.15	112.60
2	Y	136	ASN	CA-CB-CG	5.55	118.15	112.60
3	7	289	GLN	CA-C-N	5.54	125.61	120.34
3	7	289	GLN	C-N-CA	5.54	125.61	120.34
3	4	339	GLN	OE1-CD-NE2	-5.54	117.06	122.60
5	AA	575	PHE	CA-CB-CG	5.54	119.34	113.80
1	9	146	GLY	CA-C-N	5.54	128.73	122.59
1	9	146	GLY	C-N-CA	5.54	128.73	122.59
3	v	234	ARG	NE-CZ-NH2	5.54	124.18	119.20
3	2	20	ARG	NE-CZ-NH2	5.53	124.18	119.20
2	S	111	GLU	CA-C-N	5.53	131.11	122.26
2	S	111	GLU	C-N-CA	5.53	131.11	122.26
2	X	136	ASN	OD1-CG-ND2	-5.53	117.07	122.60
2	l	172	GLU	CA-C-N	5.53	131.65	121.70
2	l	172	GLU	C-N-CA	5.53	131.65	121.70
3	s	364	ASP	CA-CB-CG	5.52	118.12	112.60
3	v	241	TYR	CA-C-N	5.52	128.55	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	v	241	TYR	C-N-CA	5.52	128.55	120.71
3	7	753	ARG	NE-CZ-NH2	5.52	124.17	119.20
3	s	237	VAL	N-CA-C	5.52	114.15	109.02
3	5	779	ASP	CA-CB-CG	5.52	118.12	112.60
3	r	901	ASP	CA-CB-CG	5.51	118.11	112.60
3	s	13	ARG	NE-CZ-NH2	5.51	124.16	119.20
3	7	140	ARG	NE-CZ-NH2	5.51	124.16	119.20
3	5	113	ARG	NE-CZ-NH2	5.51	124.16	119.20
14	O	244	ASP	CA-CB-CG	5.51	118.11	112.60
3	2	302	PHE	CA-CB-CG	5.51	119.31	113.80
5	AB	392	ASP	CA-CB-CG	5.51	118.11	112.60
1	w	411	ASP	CA-CB-CG	5.51	118.11	112.60
3	q	923	ALA	N-CA-C	5.50	119.82	113.38
3	u	294	ASP	CA-CB-CG	5.50	118.10	112.60
2	V	111	GLU	CB-CG-CD	5.50	121.95	112.60
5	b	173	PRO	N-CA-CB	5.50	108.06	103.17
9	C	784	ASN	CA-CB-CG	-5.50	107.10	112.60
2	W	136	ASN	OD1-CG-ND2	-5.50	117.10	122.60
3	4	1022	PHE	CA-CB-CG	5.49	119.29	113.80
3	t	452	ASP	CA-CB-CG	5.49	118.09	112.60
3	3	974	THR	CA-C-N	5.48	125.31	120.10
3	3	974	THR	C-N-CA	5.48	125.31	120.10
3	s	1143	ARG	NE-CZ-NH2	5.48	124.13	119.20
2	1	103	LEU	N-CA-CB	-5.48	101.31	110.57
14	N	124	TYR	CA-CB-CG	5.48	123.76	113.90
3	2	477	ARG	NE-CZ-NH2	5.47	124.13	119.20
3	2	140	ARG	NE-CZ-NH2	5.47	124.12	119.20
3	r	1113	ASP	CA-CB-CG	5.47	118.07	112.60
1	8	200	ARG	NE-CZ-NH2	5.46	124.12	119.20
5	a	480	ALA	N-CA-C	5.46	115.45	108.24
2	X	169	PHE	CA-CB-CG	5.46	119.26	113.80
5	b	81	ARG	CA-C-N	5.46	131.96	121.54
5	b	81	ARG	C-N-CA	5.46	131.96	121.54
3	5	603	ASN	CA-CB-CG	5.45	118.05	112.60
3	q	800	TYR	CA-C-N	5.45	130.32	121.98
3	q	800	TYR	C-N-CA	5.45	130.32	121.98
3	4	330	ASP	CA-CB-CG	5.45	118.05	112.60
3	r	818	ASP	CA-CB-CG	5.45	118.05	112.60
3	4	968	TYR	N-CA-C	5.44	115.74	108.23
2	X	151	PHE	N-CA-C	5.44	116.55	108.60
3	5	267	VAL	CA-CB-CG1	5.44	119.65	110.40
1	0	424	ARG	NE-CZ-NH2	5.44	124.09	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	o	13	ALA	CA-C-N	5.44	127.57	120.28
2	o	13	ALA	C-N-CA	5.44	127.57	120.28
3	t	521	HIS	CB-CG-CD2	-5.44	124.13	131.20
3	7	978	TRP	N-CA-C	5.44	117.66	109.23
2	T	136	ASN	OD1-CG-ND2	-5.44	117.16	122.60
8	B	52	ARG	NE-CZ-NH2	5.44	124.09	119.20
3	7	29	ARG	NE-CZ-NH2	5.43	124.09	119.20
3	u	901	ASP	CA-CB-CG	5.43	118.03	112.60
3	s	408	ASP	CA-CB-CG	5.43	118.03	112.60
3	5	151	ASP	CA-CB-CG	5.43	118.03	112.60
3	s	27	PRO	N-CA-C	5.43	123.65	112.47
3	s	470	ASP	CA-CB-CG	5.42	118.02	112.60
3	3	400	TYR	CA-CB-CG	5.42	123.65	113.90
5	a	573	ARG	NE-CZ-NH2	5.42	124.08	119.20
3	6	867	ASP	CA-CB-CG	5.42	118.02	112.60
3	v	545	GLN	OE1-CD-NE2	-5.42	117.19	122.60
3	s	327	ARG	CA-C-N	5.41	128.53	120.95
3	s	327	ARG	C-N-CA	5.41	128.53	120.95
1	x	374	HIS	N-CA-C	5.41	117.62	109.23
3	7	353	TYR	N-CA-C	5.41	117.48	108.99
2	m	20	ALA	N-CA-C	5.41	118.67	111.75
3	r	271	ARG	N-CA-C	5.41	116.74	108.30
3	t	892	VAL	CA-C-N	5.41	126.23	121.58
3	t	892	VAL	C-N-CA	5.41	126.23	121.58
3	u	749	ARG	NE-CZ-NH2	5.41	124.07	119.20
3	3	783	ARG	CB-CA-C	5.41	117.58	110.06
3	s	433	PRO	CB-CA-C	5.41	117.52	110.92
2	X	168	ARG	NE-CZ-NH2	5.41	124.06	119.20
3	q	1049	SER	N-CA-C	5.41	117.48	108.99
3	3	945	GLU	N-CA-C	5.40	118.33	111.69
2	Q	21	ASP	CA-CB-CG	-5.40	107.20	112.60
3	2	775	LYS	N-CA-C	5.40	117.51	110.43
3	6	1009	VAL	CA-CB-CG1	5.39	119.57	110.40
3	6	1086	ASP	CA-CB-CG	5.39	117.99	112.60
3	q	968	TYR	N-CA-C	5.39	117.04	108.79
3	s	761	ASN	CA-CB-CG	5.39	117.99	112.60
3	q	1150	ARG	NE-CZ-NH2	5.39	124.05	119.20
3	r	286	ARG	NE-CZ-NH2	5.39	124.05	119.20
2	h	39	PRO	N-CA-CB	5.38	106.20	103.19
1	8	143	PHE	CA-CB-CG	5.38	119.18	113.80
3	6	783	ARG	NE-CZ-NH2	5.38	124.04	119.20
2	U	116	THR	CA-CB-OG1	5.38	117.66	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	234	ARG	NE-CZ-NH2	5.37	124.04	119.20
3	s	175	ASP	CA-C-N	5.37	128.23	120.38
3	s	175	ASP	C-N-CA	5.37	128.23	120.38
3	s	1109	ARG	NE-CZ-NH2	5.37	124.04	119.20
8	B	50	TYR	CB-CA-C	5.37	120.32	110.11
3	q	140	ARG	NE-CZ-NH2	5.37	124.03	119.20
3	7	793	PRO	CA-C-N	5.37	131.02	122.59
3	7	793	PRO	C-N-CA	5.37	131.02	122.59
2	W	50	GLN	OE1-CD-NE2	-5.37	117.23	122.60
3	2	57	ASP	CA-CB-CG	5.37	117.97	112.60
5	AA	449	PHE	N-CA-C	5.37	117.23	109.07
3	6	168	GLN	OE1-CD-NE2	-5.36	117.24	122.60
5	AA	36	ASP	CA-C-N	5.36	127.69	120.50
5	AA	36	ASP	C-N-CA	5.36	127.69	120.50
3	v	785	ARG	NE-CZ-NH2	5.36	124.03	119.20
3	5	1003	ASN	CA-C-N	5.35	131.76	121.54
3	5	1003	ASN	C-N-CA	5.35	131.76	121.54
3	t	753	ARG	NE-CZ-NH2	5.35	124.02	119.20
3	u	1014	ARG	NE-CZ-NH2	5.35	124.02	119.20
3	q	758	LYS	N-CA-C	5.35	116.97	108.79
1	9	172	MET	N-CA-C	5.35	117.52	109.23
1	y	91	ARG	NE-CZ-NH2	5.34	124.01	119.20
8	B	58	ILE	CA-C-N	5.34	129.21	122.16
8	B	58	ILE	C-N-CA	5.34	129.21	122.16
3	v	536	THR	CA-C-N	5.34	129.89	120.87
3	v	536	THR	C-N-CA	5.34	129.89	120.87
2	1	101	VAL	CB-CA-C	5.33	118.10	110.84
5	AB	449	PHE	N-CA-C	5.33	117.18	109.07
2	k	76	ASN	CA-CB-CG	5.33	117.94	112.60
3	6	375	SER	CA-C-N	5.33	128.66	120.82
3	6	375	SER	C-N-CA	5.33	128.66	120.82
3	6	759	ASN	CA-CB-CG	5.33	117.93	112.60
1	9	51	ILE	CA-C-N	5.33	129.30	120.94
1	9	51	ILE	C-N-CA	5.33	129.30	120.94
3	r	271	ARG	CA-C-N	5.33	128.79	120.75
3	r	271	ARG	C-N-CA	5.33	128.79	120.75
3	4	957	VAL	CA-CB-CG1	5.33	119.46	110.40
3	4	506	VAL	N-CA-C	5.33	115.38	108.35
3	5	266	PRO	CA-C-N	5.32	128.75	120.34
3	5	266	PRO	C-N-CA	5.32	128.75	120.34
2	V	136	ASN	OD1-CG-ND2	-5.32	117.28	122.60
3	q	986	ASP	CA-CB-CG	5.32	117.92	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	s	480	ASN	CA-CB-CG	5.32	117.92	112.60
3	3	571	THR	N-CA-C	5.32	116.77	110.97
3	s	547	LYS	CA-C-N	5.32	127.74	120.35
3	s	547	LYS	C-N-CA	5.32	127.74	120.35
3	t	167	ILE	CB-CA-C	5.32	117.75	111.32
3	s	237	VAL	CA-C-N	5.31	125.23	119.76
3	s	237	VAL	C-N-CA	5.31	125.23	119.76
14	N	334	GLN	OE1-CD-NE2	-5.31	117.29	122.60
3	v	556	HIS	CB-CG-CD2	-5.31	124.29	131.20
3	5	895	ARG	NE-CZ-NH2	5.31	123.98	119.20
5	AA	471	ASP	CA-CB-CG	5.31	117.91	112.60
2	m	111	GLU	CB-CG-CD	5.31	121.62	112.60
1	x	339	HIS	N-CA-C	5.30	116.90	108.79
3	s	552	ASP	CA-CB-CG	5.30	117.90	112.60
3	s	688	ARG	NE-CZ-NH2	5.30	123.97	119.20
3	4	785	ARG	NE-CZ-NH2	5.29	123.96	119.20
5	a	402	ILE	N-CA-C	5.29	117.49	108.86
1	9	294	ARG	NE-CZ-NH2	5.29	123.96	119.20
5	a	560	ARG	NE-CZ-NH2	5.29	123.96	119.20
3	5	951	PHE	CA-CB-CG	5.29	119.09	113.80
5	AB	560	ARG	NE-CZ-NH2	5.29	123.96	119.20
3	q	601	GLU	N-CA-C	5.29	117.29	108.99
3	7	295	PHE	N-CA-C	5.28	116.87	108.79
3	7	320	TYR	CA-CB-CG	5.28	123.41	113.90
2	T	32	PRO	N-CA-C	5.28	119.51	111.11
3	u	783	ARG	NE-CZ-NH2	5.28	123.95	119.20
5	z	384	HIS	CB-CG-CD2	-5.28	124.33	131.20
3	2	1022	PHE	CA-CB-CG	5.28	119.08	113.80
3	5	234	ARG	NE-CZ-NH2	5.28	123.95	119.20
5	b	14	LEU	CA-C-N	5.28	127.30	120.44
5	b	14	LEU	C-N-CA	5.28	127.30	120.44
3	5	716	THR	CA-C-N	5.27	125.56	119.92
3	5	716	THR	C-N-CA	5.27	125.56	119.92
2	V	21	ASP	CA-CB-CG	-5.27	107.33	112.60
2	Y	101	VAL	CB-CA-C	5.27	118.25	110.77
3	r	1135	ASN	N-CA-CB	-5.27	102.65	110.71
3	6	1128	ARG	NE-CZ-NH2	5.26	123.94	119.20
3	7	716	THR	CA-C-N	5.26	125.26	119.89
3	7	716	THR	C-N-CA	5.26	125.26	119.89
5	a	328	PHE	CA-CB-CG	5.26	119.06	113.80
5	a	447	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	8	162	ASP	CA-CB-CG	5.26	117.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	u	1026	ARG	NE-CZ-NH2	5.26	123.94	119.20
5	z	447	HIS	CA-CB-CG	5.26	119.06	113.80
3	5	1141	ARG	NE-CZ-NH2	5.26	123.93	119.20
3	2	994	ASP	CA-CB-CG	5.26	117.86	112.60
3	6	325	ASP	CA-CB-CG	5.26	117.86	112.60
3	2	1087	ASP	CA-CB-CG	5.25	117.86	112.60
3	5	799	GLN	OE1-CD-NE2	-5.25	117.35	122.60
3	7	271	ARG	NE-CZ-NH2	5.25	123.93	119.20
5	z	555	HIS	CA-CB-CG	5.25	119.05	113.80
1	w	107	ASP	CA-C-N	5.25	130.78	121.80
1	w	107	ASP	C-N-CA	5.25	130.78	121.80
5	AB	352	ARG	N-CA-C	5.25	115.46	108.38
2	p	172	GLU	CA-C-N	5.25	131.14	121.70
2	p	172	GLU	C-N-CA	5.25	131.14	121.70
3	r	332	GLN	OE1-CD-NE2	-5.25	117.35	122.60
3	6	895	ARG	NE-CZ-NH2	5.25	123.92	119.20
3	v	94	ASP	CA-CB-CG	5.25	117.84	112.60
3	2	283	ARG	NE-CZ-NH2	5.24	123.92	119.20
3	r	989	SER	CA-C-N	5.24	128.16	119.35
3	r	989	SER	C-N-CA	5.24	128.16	119.35
5	z	252	SER	N-CA-C	5.24	117.22	108.99
3	t	113	ARG	NE-CZ-NH2	5.24	123.91	119.20
2	W	155	GLN	OE1-CD-NE2	-5.24	117.36	122.60
5	c	3	PHE	CA-CB-CG	5.23	119.03	113.80
3	2	358	ARG	NE-CZ-NH2	5.23	123.91	119.20
3	4	785	ARG	CA-C-N	5.23	127.71	120.49
3	4	785	ARG	C-N-CA	5.23	127.71	120.49
1	w	51	ILE	CA-C-N	5.23	128.77	121.24
1	w	51	ILE	C-N-CA	5.23	128.77	121.24
3	6	207	ASP	CA-CB-CG	5.23	117.83	112.60
3	7	454	ASP	CA-CB-CG	5.23	117.83	112.60
5	b	57	ASN	CA-CB-CG	5.23	117.83	112.60
1	w	115	HIS	CB-CG-CD2	-5.23	124.41	131.20
3	3	477	ARG	NE-CZ-NH2	5.23	123.90	119.20
3	2	1141	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	9	32	ARG	NE-CZ-NH2	5.22	123.90	119.20
5	c	311	ARG	NE-CZ-NH2	5.22	123.90	119.20
3	7	914	GLN	CA-C-N	5.22	127.02	121.48
3	7	914	GLN	C-N-CA	5.22	127.02	121.48
14	N	311	THR	O-C-N	-5.22	117.01	122.18
3	v	779	ASP	CA-CB-CG	5.22	117.82	112.60
3	r	785	ARG	NE-CZ-NH2	5.22	123.90	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AA	324	LYS	CA-C-N	5.22	131.50	121.54
5	AA	324	LYS	C-N-CA	5.22	131.50	121.54
14	O	662	PRO	N-CA-CB	5.22	106.11	103.19
3	v	20	ARG	NE-CZ-NH2	5.22	123.89	119.20
3	v	1042	PHE	CA-CB-CG	5.22	119.02	113.80
3	5	803	ASN	CA-CB-CG	5.21	117.81	112.60
3	5	1003	ASN	N-CA-C	5.21	117.11	109.24
3	6	898	PRO	N-CA-CB	5.21	107.88	103.19
5	a	291	PHE	CA-CB-CG	5.21	119.01	113.80
5	z	431	ASN	CA-CB-CG	5.21	117.81	112.60
3	7	286	ARG	NE-CZ-NH2	5.21	123.89	119.20
3	4	753	ARG	NE-CZ-NH2	5.21	123.89	119.20
2	h	157	GLN	OE1-CD-NE2	-5.21	117.39	122.60
3	u	13	ARG	NE-CZ-NH2	5.21	123.89	119.20
2	W	71	GLU	CB-CG-CD	-5.21	103.75	112.60
5	AB	256	ASN	CA-CB-CG	5.20	117.80	112.60
3	s	264	ASN	CA-CB-CG	5.20	117.80	112.60
3	3	549	ILE	CA-C-N	5.20	124.92	119.82
3	3	549	ILE	C-N-CA	5.20	124.92	119.82
3	u	26	ASN	CA-C-N	5.20	126.34	119.84
3	u	26	ASN	C-N-CA	5.20	126.34	119.84
1	w	424	ARG	NE-CZ-NH2	5.20	123.88	119.20
3	2	832	ASP	CA-CB-CG	5.20	117.80	112.60
5	z	173	PRO	N-CA-CB	5.20	107.79	103.17
3	7	504	ARG	NE-CZ-NH2	5.19	123.87	119.20
13	L	72	ARG	NE-CZ-NH2	5.19	123.87	119.20
5	AA	400	GLU	CA-C-N	5.19	130.26	122.58
5	AA	400	GLU	C-N-CA	5.19	130.26	122.58
2	X	155	GLN	OE1-CD-NE2	-5.18	117.42	122.60
3	r	225	PHE	CA-CB-CG	5.18	118.98	113.80
3	q	602	ASP	CA-CB-CG	-5.18	107.42	112.60
3	5	997	LYS	N-CA-C	5.17	117.05	109.24
1	8	11	ASN	CA-CB-CG	5.17	117.77	112.60
5	a	576	ASN	OD1-CG-ND2	-5.17	117.42	122.60
5	b	479	ARG	NE-CZ-NH2	5.17	123.86	119.20
5	a	212	LYS	CA-C-N	5.17	131.71	122.09
5	a	212	LYS	C-N-CA	5.17	131.71	122.09
3	r	255	LYS	N-CA-C	5.17	118.05	111.69
3	4	532	ASP	CA-CB-CG	5.17	117.77	112.60
3	6	579	GLU	N-CA-C	5.17	117.11	108.99
3	6	753	ARG	NE-CZ-NH2	5.17	123.85	119.20
2	i	168	ARG	NE-CZ-NH2	5.17	123.85	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	1128	ARG	NE-CZ-NH2	5.17	123.85	119.20
3	7	406	ARG	NE-CZ-NH2	5.17	123.85	119.20
2	T	31	THR	CA-C-N	5.17	125.16	119.89
2	T	31	THR	C-N-CA	5.17	125.16	119.89
2	Z	65	ARG	NE-CZ-NH2	5.17	123.85	119.20
5	a	57	ASN	CA-CB-CG	5.16	117.76	112.60
3	4	684	PHE	CA-CB-CG	5.16	118.96	113.80
3	6	113	ARG	NE-CZ-NH2	5.16	123.84	119.20
3	s	828	ARG	NE-CZ-NH2	5.16	123.84	119.20
3	3	944	ASN	CA-CB-CG	5.16	117.76	112.60
5	c	332	ILE	N-CA-C	5.16	113.82	109.02
3	6	793	PRO	N-CA-C	5.15	119.40	111.57
13	L	181	ARG	NE-CZ-NH2	5.15	123.84	119.20
5	a	466	GLY	N-CA-C	5.15	119.00	110.55
3	t	140	ARG	NE-CZ-NH2	5.15	123.84	119.20
3	6	195	ASN	CA-CB-CG	5.15	117.75	112.60
2	V	71	GLU	CB-CG-CD	-5.15	103.84	112.60
2	o	93	ALA	CA-C-N	5.15	127.49	120.54
2	o	93	ALA	C-N-CA	5.15	127.49	120.54
3	q	820	GLN	OE1-CD-NE2	-5.15	117.45	122.60
3	u	1150	ARG	NE-CZ-NH2	5.15	123.83	119.20
3	r	1102	ARG	NE-CZ-NH2	5.14	123.83	119.20
2	Z	41	GLN	OE1-CD-NE2	-5.14	117.46	122.60
3	t	171	ASN	OD1-CG-ND2	-5.14	117.46	122.60
3	4	27	PRO	N-CA-C	5.14	123.05	112.47
5	b	327	SER	N-CA-C	5.14	116.65	108.79
3	r	237	VAL	N-CA-C	-5.14	104.98	109.19
3	q	353	TYR	N-CA-C	5.14	116.10	108.60
3	3	234	ARG	NE-CZ-NH2	5.13	123.82	119.20
2	R	168	ARG	NE-CZ-NH2	5.13	123.82	119.20
3	v	26	ASN	CA-C-N	5.13	124.75	119.05
3	v	26	ASN	C-N-CA	5.13	124.75	119.05
14	N	505	PRO	N-CA-CB	5.13	107.82	103.35
3	6	365	TYR	CA-CB-CG	5.13	123.14	113.90
2	U	111	GLU	CB-CG-CD	5.13	121.32	112.60
2	W	93	ALA	CA-C-N	5.13	127.46	120.54
2	W	93	ALA	C-N-CA	5.13	127.46	120.54
3	t	505	SER	N-CA-C	5.13	116.60	108.96
1	y	70	ARG	NE-CZ-NH2	5.13	123.81	119.20
3	5	837	ASN	N-CA-C	5.12	114.80	108.19
3	q	785	ARG	NE-CZ-NH2	5.12	123.81	119.20
3	s	37	ASN	CA-C-N	5.12	127.15	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	s	37	ASN	C-N-CA	5.12	127.15	120.28
1	0	231	ASP	CA-CB-CG	5.12	117.72	112.60
3	3	339	GLN	OE1-CD-NE2	-5.12	117.48	122.60
3	s	539	TYR	N-CA-C	5.12	117.03	108.99
3	t	972	GLU	CA-C-N	5.12	129.57	121.44
3	t	972	GLU	C-N-CA	5.12	129.57	121.44
1	x	162	ASP	CA-CB-CG	5.12	117.72	112.60
3	v	429	ARG	CB-CA-C	5.11	117.56	111.22
3	5	28	ASP	CA-CB-CG	5.11	117.71	112.60
5	z	290	TYR	N-CA-C	5.11	116.84	109.07
3	3	225	PHE	CA-CB-CG	5.11	118.91	113.80
3	6	900	ILE	CB-CA-C	5.11	115.43	110.63
5	AB	23	ASP	CA-C-N	5.11	127.08	120.70
5	AB	23	ASP	C-N-CA	5.11	127.08	120.70
5	b	201	PHE	N-CA-C	5.11	116.89	110.91
3	u	759	ASN	CA-CB-CG	5.11	117.71	112.60
3	4	32	GLN	OE1-CD-NE2	-5.11	117.50	122.60
9	C	683	HIS	CA-CB-CG	5.11	118.91	113.80
2	S	162	GLN	OE1-CD-NE2	-5.11	117.49	122.60
3	t	867	ASP	CA-CB-CG	5.11	117.71	112.60
1	y	319	ARG	NE-CZ-NH2	5.11	123.79	119.20
1	8	447	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	8	51	ILE	CA-C-N	5.10	128.45	120.75
1	8	51	ILE	C-N-CA	5.10	128.45	120.75
3	v	1137	PHE	CA-CB-CG	5.10	118.90	113.80
3	2	254	ASN	CA-CB-CG	5.09	117.69	112.60
3	4	454	ASP	CA-C-N	5.09	130.46	122.21
3	4	454	ASP	C-N-CA	5.09	130.46	122.21
3	v	461	PHE	CA-CB-CG	5.09	118.89	113.80
5	b	6	THR	CA-C-N	5.09	125.09	119.90
5	b	6	THR	C-N-CA	5.09	125.09	119.90
3	6	878	ALA	N-CA-C	5.09	117.12	109.23
3	3	251	THR	CA-CB-CG2	5.09	119.15	110.50
2	S	21	ASP	CA-CB-CG	-5.09	107.51	112.60
3	q	118	ASP	CA-CB-CG	5.09	117.69	112.60
3	r	749	ARG	NE-CZ-NH2	5.09	123.78	119.20
3	r	1086	ASP	CA-CB-CG	5.09	117.69	112.60
5	z	328	PHE	CA-CB-CG	5.09	118.89	113.80
3	u	721	TYR	CA-C-N	5.09	127.93	120.71
3	u	721	TYR	C-N-CA	5.09	127.93	120.71
3	7	1014	ARG	NE-CZ-NH2	5.08	123.78	119.20
1	9	451	ARG	NE-CZ-NH2	5.08	123.78	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	374	GLN	OE1-CD-NE2	-5.08	117.52	122.60
3	7	411	PHE	CA-CB-CG	5.08	118.88	113.80
3	2	1109	ARG	NE-CZ-NH2	5.08	123.77	119.20
3	6	828	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	y	267	HIS	CB-CG-CD2	-5.08	124.60	131.20
5	b	449	PHE	N-CA-C	5.07	116.01	108.60
5	z	6	THR	CA-C-N	5.07	125.31	119.83
5	z	6	THR	C-N-CA	5.07	125.31	119.83
3	5	514	LEU	CA-C-N	5.07	131.23	121.54
3	5	514	LEU	C-N-CA	5.07	131.23	121.54
3	r	327	ARG	N-CA-C	5.07	117.71	109.24
2	Z	146	GLY	N-CA-C	5.07	120.72	112.61
3	r	1053	ARG	NE-CZ-NH2	5.07	123.76	119.20
5	AA	14	LEU	CA-C-N	5.07	127.07	120.28
5	AA	14	LEU	C-N-CA	5.07	127.07	120.28
5	c	3	PHE	N-CA-C	5.07	116.47	110.19
2	p	151	PHE	N-CA-C	5.07	116.00	108.60
3	v	465	ARG	NE-CZ-NH2	5.07	123.76	119.20
3	v	504	ARG	NE-CZ-NH2	5.07	123.76	119.20
3	q	294	ASP	CA-CB-CG	5.07	117.67	112.60
3	q	113	ARG	NE-CZ-NH2	5.06	123.75	119.20
5	z	639	ARG	NE-CZ-NH2	5.06	123.75	119.20
3	4	381	ASN	CA-CB-CG	5.06	117.66	112.60
3	v	1128	ARG	NE-CZ-NH2	5.06	123.75	119.20
3	s	1141	ARG	NE-CZ-NH2	5.05	123.75	119.20
3	7	477	ARG	NE-CZ-NH2	5.05	123.75	119.20
3	r	406	ARG	NE-CZ-NH2	5.05	123.74	119.20
3	s	776	THR	CA-CB-CG2	5.05	119.08	110.50
5	z	389	ARG	NE-CZ-NH2	5.05	123.74	119.20
3	6	1139	ARG	NE-CZ-NH2	5.05	123.74	119.20
3	q	384	PRO	CA-C-N	5.05	131.18	121.54
3	q	384	PRO	C-N-CA	5.05	131.18	121.54
5	z	442	VAL	CA-C-N	5.05	126.15	119.84
5	z	442	VAL	C-N-CA	5.05	126.15	119.84
3	6	866	ASP	CA-CB-CG	5.04	117.64	112.60
3	t	822	ASN	CA-CB-CG	5.04	117.64	112.60
2	V	151	PHE	N-CA-C	5.04	115.19	108.38
3	2	94	ASP	CA-CB-CG	5.04	117.64	112.60
5	AB	602	GLN	CA-C-N	5.04	126.14	119.84
5	AB	602	GLN	C-N-CA	5.04	126.14	119.84
3	u	1104	ASN	CA-CB-CG	5.04	117.64	112.60
8	B	113	GLN	OE1-CD-NE2	-5.04	117.56	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	533	ASN	CA-CB-CG	5.04	117.64	112.60
3	r	299	ASN	CA-C-N	5.04	129.37	121.76
3	r	299	ASN	C-N-CA	5.04	129.37	121.76
3	2	1005	GLN	OE1-CD-NE2	-5.04	117.56	122.60
3	r	556	HIS	CB-CG-CD2	-5.04	124.66	131.20
2	Q	38	ASN	CA-C-N	5.03	125.56	120.38
2	Q	38	ASN	C-N-CA	5.03	125.56	120.38
1	x	294	ARG	NE-CZ-NH2	5.03	123.73	119.20
5	AA	152	ASN	N-CA-C	5.03	120.31	113.37
9	C	725	GLY	CA-C-N	5.03	125.56	119.98
9	C	725	GLY	C-N-CA	5.03	125.56	119.98
3	5	139	ASP	CA-CB-CG	5.03	117.63	112.60
2	R	65	ARG	NE-CZ-NH2	5.03	123.72	119.20
3	s	254	ASN	CA-CB-CG	5.03	117.63	112.60
3	s	792	ASP	CA-CB-CG	5.03	117.63	112.60
3	4	588	ILE	N-CA-C	5.03	113.69	109.02
3	5	785	ARG	NE-CZ-NH2	5.03	123.72	119.20
3	u	511	PHE	CA-CB-CG	5.03	118.83	113.80
5	AB	191	GLN	OE1-CD-NE2	-5.02	117.58	122.60
3	v	271	ARG	NE-CZ-NH2	5.02	123.72	119.20
5	AA	628	ARG	NE-CZ-NH2	5.02	123.72	119.20
3	7	750	CYS	N-CA-C	5.02	117.38	110.35
9	C	747	GLN	OE1-CD-NE2	-5.02	117.58	122.60
3	s	1143	ARG	NE-CZ-NH1	-5.02	116.48	121.50
3	v	44	GLN	OE1-CD-NE2	-5.02	117.58	122.60
3	4	773	ARG	CA-C-N	5.01	128.78	121.31
3	4	773	ARG	C-N-CA	5.01	128.78	121.31
3	7	403	TYR	CA-CB-CG	5.01	122.92	113.90
14	N	332	ARG	NE-CZ-NH2	5.01	123.71	119.20
3	q	175	ASP	N-CA-C	5.01	118.50	112.38
3	6	426	ASN	N-CA-C	5.01	114.85	108.24
3	7	752	ASN	CA-CB-CG	5.01	117.61	112.60
2	m	125	ASP	CA-CB-CG	5.01	117.61	112.60
2	k	9	HIS	CB-CG-CD2	-5.01	124.69	131.20
3	t	521	HIS	CA-CB-CG	-5.01	108.79	113.80
3	3	172	ALA	N-CA-C	-5.00	106.39	113.20
3	6	243	LEU	CA-C-N	5.00	125.88	121.58
3	6	243	LEU	C-N-CA	5.00	125.88	121.58
5	z	81	ARG	CA-C-N	5.00	130.36	121.80
5	z	81	ARG	C-N-CA	5.00	130.36	121.80
3	5	820	GLN	OE1-CD-NE2	-5.00	117.60	122.60
3	q	452	ASP	CA-C-N	5.00	131.09	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	q	452	ASP	C-N-CA	5.00	131.09	121.54

There are no chirality outliers.

All (272) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	276	PHE	Sidechain
1	0	365	TYR	Sidechain
1	0	45	PHE	Sidechain
1	0	63	TYR	Sidechain
1	0	78	TYR	Sidechain
2	1	15	TYR	Sidechain
2	1	156	PHE	Sidechain
2	1	65	ARG	Sidechain
3	2	1004	TYR	Sidechain
3	2	1019	ARG	Sidechain
3	2	1062	TYR	Sidechain
3	2	113	ARG	Sidechain
3	2	1144	ARG	Sidechain
3	2	186	TYR	Sidechain
3	2	221	TYR	Sidechain
3	2	320	TYR	Sidechain
3	2	400	TYR	Sidechain
3	2	88	ARG	Sidechain
3	3	1083	TYR	Sidechain
3	3	166	TYR	Sidechain
3	3	192	TYR	Sidechain
3	3	29	ARG	Sidechain
3	3	400	TYR	Sidechain
3	3	402	TYR	Sidechain
3	3	403	TYR	Sidechain
3	3	835	TYR	Sidechain
3	4	1004	TYR	Sidechain
3	4	1050	TYR	Sidechain
3	4	1062	TYR	Sidechain
3	4	1139	ARG	Sidechain
3	4	133	TYR	Sidechain
3	4	166	TYR	Sidechain
3	4	46	TYR	Sidechain
3	4	804	ARG	Sidechain
3	4	888	TYR	Sidechain
3	4	89	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	4	973	ARG	Sidechain
3	5	1004	TYR	Sidechain
3	5	1027	TYR	Sidechain
3	5	1069	TYR	Sidechain
3	5	192	TYR	Sidechain
3	5	350	TYR	Sidechain
3	5	365	TYR	Sidechain
3	5	403	TYR	Sidechain
3	5	45	TYR	Sidechain
3	5	721	TYR	Sidechain
3	5	768	TYR	Sidechain
3	5	80	TYR	Sidechain
3	5	888	TYR	Sidechain
3	5	89	TYR	Sidechain
3	5	895	ARG	Sidechain
3	6	1004	TYR	Sidechain
3	6	1141	ARG	Sidechain
3	6	140	ARG	Sidechain
3	6	271	ARG	Sidechain
3	6	400	TYR	Sidechain
3	6	477	ARG	Sidechain
3	6	560	ARG	Sidechain
3	6	573	TYR	Sidechain
3	6	66	PHE	Sidechain
3	6	712	ARG	Sidechain
3	6	800	TYR	Sidechain
3	6	89	TYR	Sidechain
3	6	90	TYR	Sidechain
3	7	1004	TYR	Sidechain
3	7	1062	TYR	Sidechain
3	7	1141	ARG	Sidechain
3	7	241	TYR	Sidechain
3	7	365	TYR	Sidechain
3	7	379	TYR	Sidechain
3	7	573	TYR	Sidechain
3	7	721	TYR	Sidechain
1	8	401	TYR	Sidechain
1	8	448	TYR	Sidechain
1	8	63	TYR	Sidechain
1	8	78	TYR	Sidechain
1	9	117	TYR	Sidechain
1	9	365	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	9	78	TYR	Sidechain
5	AA	158	TYR	Sidechain
5	AA	250	TYR	Sidechain
5	AA	296	TYR	Sidechain
5	AA	499	TYR	Sidechain
5	AA	86	TYR	Sidechain
5	AB	18	TYR	Sidechain
5	AB	208	TYR	Sidechain
5	AB	224	TYR	Sidechain
5	AB	366	TYR	Sidechain
5	AB	420	TYR	Sidechain
5	AB	499	TYR	Sidechain
5	AB	541	TYR	Sidechain
5	AB	571	TYR	Sidechain
5	AB	573	ARG	Sidechain
5	AB	58	TYR	Sidechain
5	AB	592	TYR	Sidechain
5	AB	632	TYR	Sidechain
5	AB	639	ARG	Sidechain
5	AB	90	TYR	Sidechain
5	AB	93	TYR	Sidechain
7	AI	133	ARG	Sidechain
8	B	128	TYR	Sidechain
8	B	136	TYR	Sidechain
8	B	202	TYR	Sidechain
8	B	22	ASP	Sidechain
8	B	50	TYR	Sidechain
8	B	76	TYR	Sidechain
9	C	695	TYR	Sidechain
9	C	702	TYR	Sidechain
9	C	704	TYR	Sidechain
9	C	707	ARG	Sidechain
9	C	736	ARG	Sidechain
9	C	757	TYR	Sidechain
9	C	768	ASP	Sidechain
9	C	789	ARG	Sidechain
13	L	108	TYR	Sidechain
14	N	124	TYR	Sidechain
14	N	142	ARG	Sidechain
14	N	200	TYR	Sidechain
14	N	325	ARG	Sidechain
14	N	349	TYR	Sidechain

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Mol	Chain	Res	Type	Group
14	N	357	TYR	Sidechain
14	N	358	TYR	Sidechain
14	N	404	TYR	Sidechain
14	N	407	ASP	Sidechain
14	N	443	TYR	Sidechain
14	N	500	TYR	Sidechain
14	N	608	TYR	Sidechain
14	N	726	TYR	Sidechain
14	O	140	TYR	Sidechain
14	O	205	ARG	Sidechain
14	O	293	TYR	Sidechain
14	O	453	TYR	Sidechain
14	O	468	TYR	Sidechain
14	O	471	ALA	Mainchain
14	O	599	TYR	Sidechain
14	O	608	TYR	Sidechain
2	P	125	ASP	Sidechain
2	Q	6	TYR	Sidechain
2	Q	65	ARG	Sidechain
2	R	168	ARG	Sidechain
2	T	80	TYR	Sidechain
2	U	9	HIS	Sidechain
2	W	117	TYR	Sidechain
2	Y	15	TYR	Sidechain
2	Z	15	TYR	Sidechain
2	Z	80	TYR	Sidechain
5	a	184	ARG	Sidechain
5	a	230	ARG	Sidechain
5	a	250	TYR	Sidechain
5	a	366	TYR	Sidechain
5	a	367	TYR	Sidechain
5	a	423	TYR	Sidechain
5	a	450	TYR	Sidechain
5	a	496	TYR	Sidechain
5	a	503	TYR	Sidechain
5	a	541	TYR	Sidechain
5	a	548	TYR	Sidechain
5	a	77	ARG	Sidechain
5	b	203	TYR	Sidechain
5	b	224	TYR	Sidechain
5	b	275	TYR	Sidechain
5	b	420	TYR	Sidechain

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Mol	Chain	Res	Type	Group
5	b	446	TYR	Sidechain
5	b	499	TYR	Sidechain
5	b	541	TYR	Sidechain
5	c	18	TYR	Sidechain
5	c	184	ARG	Sidechain
5	c	203	TYR	Sidechain
5	c	275	TYR	Sidechain
5	c	296	TYR	Sidechain
5	c	326	TYR	Sidechain
5	c	417	TYR	Sidechain
5	c	472	TYR	Sidechain
5	c	478	TYR	Sidechain
5	c	86	TYR	Sidechain
5	c	89	TYR	Sidechain
15	d	17	ARG	Sidechain
15	d	55	TYR	Sidechain
2	e	168	ARG	Sidechain
2	i	80	TYR	Sidechain
2	j	102	TYR	Sidechain
2	j	15	TYR	Sidechain
2	k	24	TYR	Sidechain
2	l	117	TYR	Sidechain
2	l	80	TYR	Sidechain
2	m	80	TYR	Sidechain
2	o	117	TYR	Sidechain
2	o	15	TYR	Sidechain
2	o	159	ARG	Sidechain
2	o	80	TYR	Sidechain
2	p	117	TYR	Sidechain
2	p	80	TYR	Sidechain
3	q	1069	TYR	Sidechain
3	q	1083	TYR	Sidechain
3	q	1141	ARG	Sidechain
3	q	1150	ARG	Sidechain
3	q	133	TYR	Sidechain
3	q	186	TYR	Sidechain
3	q	241	TYR	Sidechain
3	q	272	ARG	Sidechain
3	q	29	ARG	Sidechain
3	q	349	TYR	Sidechain
3	q	403	TYR	Sidechain
3	q	785	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	q	835	TYR	Sidechain
3	q	864	TYR	Sidechain
3	q	968	TYR	Sidechain
3	r	1062	TYR	Sidechain
3	r	133	TYR	Sidechain
3	r	166	TYR	Sidechain
3	r	241	TYR	Sidechain
3	r	349	TYR	Sidechain
3	r	353	TYR	Sidechain
3	r	46	TYR	Sidechain
3	r	560	ARG	Sidechain
3	r	586	TYR	Sidechain
3	r	753	ARG	Sidechain
3	r	90	TYR	Sidechain
3	s	1062	TYR	Sidechain
3	s	192	TYR	Sidechain
3	s	241	TYR	Sidechain
3	s	355	TYR	Sidechain
3	s	379	TYR	Sidechain
3	s	403	TYR	Sidechain
3	s	539	TYR	Sidechain
3	s	968	TYR	Sidechain
3	t	379	TYR	Sidechain
3	t	403	TYR	Sidechain
3	t	521	HIS	Sidechain
3	t	835	TYR	Sidechain
3	t	89	TYR	Sidechain
3	t	90	TYR	Sidechain
3	t	912	TYR	Sidechain
3	u	1014	ARG	Sidechain
3	u	1062	TYR	Sidechain
3	u	1083	TYR	Sidechain
3	u	1109	ARG	Sidechain
3	u	1128	ARG	Sidechain
3	u	166	TYR	Sidechain
3	u	186	TYR	Sidechain
3	u	272	ARG	Sidechain
3	u	320	TYR	Sidechain
3	u	753	ARG	Sidechain
3	u	835	TYR	Sidechain
3	v	1004	TYR	Sidechain
3	v	1083	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	v	13	ARG	Sidechain
3	v	140	ARG	Sidechain
3	v	286	ARG	Sidechain
3	v	320	TYR	Sidechain
3	v	353	TYR	Sidechain
3	v	400	TYR	Sidechain
3	v	573	TYR	Sidechain
3	v	82	TYR	Sidechain
3	v	835	TYR	Sidechain
1	w	117	TYR	Sidechain
1	w	220	TYR	Sidechain
1	w	63	TYR	Sidechain
1	x	169	TYR	Sidechain
1	x	210	TYR	Sidechain
1	x	423	TYR	Sidechain
1	x	91	ARG	Sidechain
1	y	367	TYR	Sidechain
1	y	371	TYR	Sidechain
5	z	109	TYR	Sidechain
5	z	140	TYR	Sidechain
5	z	18	TYR	Sidechain
5	z	290	TYR	Sidechain
5	z	326	TYR	Sidechain
5	z	346	TYR	Sidechain
5	z	420	TYR	Sidechain
5	z	478	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	3548	0	3468	4	0
1	8	3548	0	3468	7	0
1	9	3548	0	3468	3	0
1	w	3548	0	3468	5	0
1	x	3548	0	3468	2	0
1	y	3548	0	3468	2	0
2	1	1349	0	1339	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1266	0	1258	15	0
2	Q	1277	0	1274	4	0
2	R	1272	0	1264	8	0
2	S	1349	0	1339	5	0
2	T	1349	0	1339	7	0
2	U	1349	0	1339	6	0
2	V	1349	0	1339	5	0
2	W	1349	0	1339	6	0
2	X	1349	0	1339	7	0
2	Y	1349	0	1339	6	0
2	Z	1349	0	1339	8	0
2	e	1280	0	1275	11	0
2	f	1270	0	1263	4	0
2	g	1278	0	1274	0	0
2	h	1350	0	1339	3	0
2	i	1199	0	1195	4	0
2	j	1350	0	1339	2	0
2	k	1350	0	1339	2	0
2	l	1350	0	1339	3	0
2	m	1350	0	1339	4	0
2	n	1350	0	1339	5	0
2	o	1350	0	1339	6	0
2	p	1350	0	1339	1	0
3	2	8364	0	8206	25	0
3	3	8364	0	8206	20	0
3	4	8364	0	8206	19	0
3	5	8364	0	8206	14	0
3	6	8364	0	8206	19	0
3	7	8364	0	8206	24	0
3	q	8364	0	8206	14	0
3	r	8364	0	8206	23	0
3	s	8364	0	8206	19	0
3	t	8364	0	8206	12	0
3	u	8364	0	8206	21	0
3	v	8364	0	8206	18	0
4	A	2462	0	2382	17	0
5	AA	5127	0	4969	12	0
5	AB	5127	0	4969	5	0
5	a	5127	0	4969	7	0
5	b	5127	0	4969	15	0
5	c	5127	0	4969	8	0
5	z	5127	0	4969	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AC	1091	0	1081	7	0
6	AD	1091	0	1079	26	0
6	AE	1091	0	1081	7	0
6	AF	1091	0	1081	8	0
6	AG	1091	0	1081	7	0
6	AH	1091	0	1081	6	0
7	AI	4284	0	4241	57	0
7	AJ	4284	0	4241	42	0
7	AK	4267	0	4220	44	0
7	AL	4267	0	4220	39	0
7	AM	2667	0	2631	24	0
7	AN	2667	0	2631	27	0
8	B	2424	0	2330	43	0
9	C	5852	0	5760	76	0
10	D	1294	0	1301	8	0
10	E	1248	0	1257	15	0
11	F	1878	0	1841	38	0
11	G	1871	0	1837	19	0
12	H	1694	0	1663	34	0
12	I	1701	0	1672	45	0
13	J	2760	0	2729	23	0
13	K	2760	0	2729	22	0
13	L	2760	0	2729	29	0
13	M	2760	0	2729	29	0
14	N	5845	0	5710	33	0
14	O	5845	0	5710	30	0
15	d	597	0	570	1	0
All	All	256934	0	252277	992	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 2.

All (992) 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)
8:B:150:LEU:HD12	9:C:679:LYS:CE	1.36	1.52
8:B:150:LEU:HD12	9:C:679:LYS:NZ	1.09	1.40
8:B:150:LEU:CD1	9:C:679:LYS:HD2	1.62	1.28
8:B:150:LEU:CD1	9:C:679:LYS:CE	2.14	1.25
14:O:176:TYR:CE2	2:e:157:GLN:NE2	2.04	1.25
8:B:150:LEU:CD1	9:C:679:LYS:NZ	1.99	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:150:LEU:CD1	9:C:679:LYS:CD	2.18	1.21
8:B:150:LEU:HD13	9:C:679:LYS:CD	1.78	1.14
7:AI:580:TYR:OH	12:H:138:LEU:HD12	1.47	1.12
6:AD:44:ILE:N	11:F:32:ASN:ND2	1.98	1.11
7:AJ:404:ARG:HD2	13:M:96:PRO:HG2	1.33	1.10
6:AD:43:GLU:CD	11:F:32:ASN:H	1.65	1.04
6:AD:43:GLU:OE2	11:F:31:VAL:HA	1.59	1.01
14:O:176:TYR:CZ	2:e:157:GLN:NE2	2.21	1.00
8:B:150:LEU:HD13	9:C:679:LYS:HD2	0.99	0.98
8:B:150:LEU:HD12	9:C:679:LYS:HZ1	1.25	0.95
6:AD:44:ILE:H	11:F:32:ASN:HD22	1.15	0.95
7:AJ:404:ARG:HD2	13:M:96:PRO:CG	1.97	0.95
6:AD:46:SER:HB2	11:F:10:LEU:HD22	1.49	0.94
6:AD:51:GLU:OE1	11:F:74:ARG:HB2	1.71	0.91
14:O:176:TYR:OH	2:e:157:GLN:OE1	1.89	0.90
7:AK:587:ALA:HA	12:H:196:TRP:CZ2	1.74	0.90
8:B:150:LEU:HD12	9:C:679:LYS:HZ2	1.19	0.89
7:AI:404:ARG:HD2	13:L:96:PRO:HG2	1.56	0.87
7:AJ:571:PHE:CE2	12:I:166:ASN:HA	2.10	0.87
6:AD:44:ILE:H	11:F:32:ASN:ND2	1.65	0.87
8:B:150:LEU:HD12	9:C:679:LYS:CD	1.98	0.87
7:AI:470:PHE:CZ	12:I:9:GLN:OE1	2.29	0.85
7:AJ:404:ARG:CD	13:M:96:PRO:HG2	2.06	0.85
6:AD:43:GLU:OE2	11:F:31:VAL:HG13	1.78	0.83
6:AD:43:GLU:OE1	11:F:32:ASN:OD1	1.68	0.83
14:O:176:TYR:CE2	2:e:157:GLN:CD	2.57	0.83
14:N:176:TYR:OH	2:P:157:GLN:OE1	1.97	0.82
7:AM:55:ASN:ND2	7:AM:57:SER:OG	2.13	0.81
8:B:150:LEU:HD12	9:C:679:LYS:HE3	1.60	0.81
7:AI:470:PHE:CE1	12:I:9:GLN:OE1	2.33	0.81
7:AI:580:TYR:CZ	12:H:138:LEU:HD12	2.15	0.81
8:B:147:ILE:HD13	9:C:679:LYS:HE2	1.63	0.81
7:AN:55:ASN:ND2	7:AN:57:SER:OG	2.13	0.81
7:AI:404:ARG:HD2	13:L:96:PRO:CG	2.10	0.81
11:G:49:THR:OG1	11:G:52:ASP:O	1.99	0.80
8:B:150:LEU:CD1	9:C:679:LYS:HZ2	1.74	0.80
8:B:147:ILE:HA	9:C:679:LYS:HZ3	1.46	0.80
8:B:150:LEU:HB2	9:C:679:LYS:HZ2	1.48	0.78
7:AI:464:ARG:NH1	12:I:11:GLU:OE1	2.15	0.78
6:AD:51:GLU:OE1	11:F:74:ARG:CG	2.32	0.78
13:M:6:LEU:N	13:M:45:GLU:OE1	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AD:43:GLU:OE2	11:F:31:VAL:CA	2.31	0.77
13:J:177:ASP:OD1	13:J:180:ARG:NH1	2.18	0.76
7:AI:425:GLU:OE2	11:F:79:ALA:O	2.04	0.76
5:b:544:ILE:HG23	5:b:563:ILE:HD11	1.66	0.76
6:AD:51:GLU:OE1	11:F:74:ARG:CB	2.34	0.75
7:AI:404:ARG:CD	13:L:96:PRO:HG2	2.16	0.75
7:AI:12:THR:O	7:AJ:453:ASN:ND2	2.20	0.75
8:B:53:PRO:HB3	9:C:782:THR:HG23	1.70	0.73
7:AI:470:PHE:CE2	12:I:9:GLN:HB2	2.24	0.73
10:D:142:ASP:O	10:D:145:ASN:ND2	2.21	0.73
6:AH:67:ARG:NH2	6:AH:117:GLU:OE2	2.22	0.72
6:AG:67:ARG:NH2	6:AG:117:GLU:OE2	2.22	0.72
14:O:176:TYR:CZ	2:e:157:GLN:OE1	2.42	0.72
14:O:176:TYR:CZ	2:e:157:GLN:CD	2.67	0.71
8:B:150:LEU:CB	9:C:679:LYS:HZ2	2.03	0.71
14:O:176:TYR:CE2	2:e:157:GLN:OE1	2.43	0.71
13:M:43:GLU:OE1	14:O:2:ALA:N	2.22	0.71
10:E:107:ASN:ND2	10:E:111:GLU:OE2	2.24	0.70
7:AI:464:ARG:HG2	14:N:10:PRO:HG3	1.73	0.70
13:M:141:ASN:ND2	13:M:166:PHE:O	2.25	0.70
7:AI:13:ARG:HH22	12:I:108:HIS:HD2	1.38	0.69
11:G:167:THR:HG23	11:G:169:GLU:HG3	1.74	0.69
7:AI:580:TYR:OH	12:H:138:LEU:CD1	2.36	0.69
11:F:137:ARG:NH1	11:F:142:PRO:O	2.26	0.69
4:A:240:ASP:OD1	4:A:260:SER:N	2.25	0.69
6:AD:43:GLU:CD	11:F:32:ASN:N	2.46	0.69
7:AJ:569:ARG:O	12:I:166:ASN:OD1	2.12	0.68
13:L:85:PHE:O	13:L:158:ARG:NH2	2.27	0.68
8:B:150:LEU:CD1	9:C:679:LYS:HE3	2.19	0.68
2:P:12:LEU:HD22	2:Q:12:LEU:HD21	1.76	0.67
7:AI:470:PHE:CE2	12:I:9:GLN:CB	2.77	0.67
6:AE:4:GLU:OE2	6:AE:13:ASN:ND2	2.27	0.67
14:N:176:TYR:CZ	2:P:157:GLN:OE1	2.12	0.67
7:AJ:571:PHE:CZ	12:I:166:ASN:HA	2.28	0.67
13:K:191:ARG:NH2	13:K:244:ASP:OD2	2.27	0.67
6:AF:4:GLU:OE2	6:AF:13:ASN:ND2	2.28	0.67
2:U:116:THR:HG22	2:U:158:ASN:HA	1.76	0.67
3:v:580:THR:HG21	3:v:814:ALA:HB2	1.77	0.67
7:AI:571:PHE:CE2	12:H:166:ASN:HA	2.30	0.66
13:L:76:ARG:NH2	13:L:133:CYS:O	2.28	0.65
7:AK:587:ALA:CA	12:H:196:TRP:CZ2	2.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:147:ILE:HD13	9:C:679:LYS:CE	2.27	0.65
13:K:85:PHE:O	13:K:158:ARG:NH1	2.29	0.65
9:C:461:LYS:O	9:C:465:THR:HG23	1.97	0.65
7:AM:544:ASP:OD1	7:AM:545:PHE:N	2.30	0.64
3:q:582:ASN:HA	3:q:889:THR:HG22	1.78	0.64
4:A:287:SER:OG	4:A:289:ASP:OD1	2.07	0.64
10:E:12:LEU:O	10:E:16:ASN:ND2	2.29	0.64
12:H:44:GLU:OE1	12:H:44:GLU:N	2.30	0.64
7:AN:337:PRO:HG3	7:AN:348:VAL:HG21	1.80	0.64
12:H:137:GLN:OE1	12:H:187:ARG:NH1	2.29	0.64
3:v:580:THR:HG21	3:v:814:ALA:CB	2.27	0.64
7:AJ:90:MET:HE1	7:AJ:326:LYS:HB2	1.79	0.64
11:F:189:ASP:OD1	11:F:190:LYS:N	2.30	0.64
13:K:242:LEU:O	13:K:246:ARG:N	2.31	0.64
7:AI:90:MET:HE1	7:AI:326:LYS:HB2	1.80	0.64
8:B:147:ILE:HA	9:C:679:LYS:NZ	2.12	0.64
1:8:132:PHE:H	1:9:126:ILE:HD12	1.62	0.64
5:AA:240:THR:HG21	5:AA:323:TRP:CH2	2.33	0.64
12:I:47:GLU:OE1	12:I:47:GLU:N	2.31	0.64
13:J:261:GLU:OE2	13:J:263:ASN:ND2	2.30	0.64
7:AN:544:ASP:OD1	7:AN:545:PHE:N	2.30	0.63
13:J:242:LEU:HD23	13:J:242:LEU:O	1.98	0.63
13:J:324:ASP:OD1	13:J:325:ASN:ND2	2.31	0.63
7:AI:470:PHE:CD2	12:I:9:GLN:HB3	2.33	0.63
14:N:156:VAL:HG22	2:P:158:ASN:HB3	1.81	0.63
3:s:555:ALA:HB2	3:s:947:ALA:HB1	1.80	0.63
8:B:150:LEU:HB2	9:C:679:LYS:NZ	2.12	0.63
9:C:9:VAL:HG22	9:C:79:ILE:HG12	1.81	0.63
9:C:763:VAL:HA	9:C:775:ILE:HG22	1.81	0.63
2:R:108:VAL:HA	2:R:164:THR:HG22	1.80	0.63
6:AD:43:GLU:OE2	11:F:31:VAL:CG1	2.46	0.63
7:AI:569:ARG:O	12:H:166:ASN:HB3	1.99	0.63
9:C:469:LYS:O	9:C:473:THR:OG1	2.14	0.63
9:C:305:ASN:OD1	9:C:306:GLY:N	2.32	0.62
13:K:179:LYS:O	13:K:183:HIS:ND1	2.32	0.62
3:s:447:VAL:HG13	3:s:456:ALA:HB1	1.80	0.62
10:E:49:GLU:N	10:E:49:GLU:OE1	2.33	0.62
10:E:76:ILE:O	10:E:80:ASN:ND2	2.32	0.62
7:AI:405:LYS:NZ	12:I:46:ASP:OD2	2.30	0.62
14:N:172:LEU:HB3	2:P:162:GLN:HE22	1.64	0.62
7:AM:337:PRO:HG3	7:AM:348:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:150:LEU:CG	9:C:679:LYS:NZ	2.62	0.62
3:3:267:VAL:HG12	3:3:268:LYS:H	1.63	0.62
7:AN:428:GLU:OE2	7:AN:433:LYS:NZ	2.32	0.62
10:D:144:TYR:O	10:D:148:VAL:HG23	1.99	0.61
13:M:46:GLN:OE1	14:O:2:ALA:N	2.32	0.61
7:AK:259:THR:O	7:AK:262:ASN:ND2	2.33	0.61
9:C:365:ASP:OD2	9:C:389:TYR:OH	2.09	0.61
7:AJ:337:PRO:HG3	7:AJ:348:VAL:HG21	1.83	0.61
14:O:197:ILE:HD11	2:e:2:ALA:HA	1.81	0.61
7:AL:153:ILE:HG22	7:AL:248:VAL:O	2.01	0.61
7:AJ:464:ARG:N	12:I:112:ASP:OD2	2.30	0.61
7:AM:428:GLU:OE2	7:AM:433:LYS:NZ	2.34	0.61
9:C:193:ASP:OD1	9:C:194:ASN:N	2.34	0.60
7:AK:90:MET:HE1	7:AK:326:LYS:HB2	1.82	0.60
7:AK:153:ILE:HG22	7:AK:248:VAL:O	2.01	0.60
8:B:292:GLU:OE1	8:B:293:VAL:HG12	2.02	0.60
7:AL:259:THR:O	7:AL:262:ASN:ND2	2.33	0.60
7:AK:337:PRO:HG3	7:AK:348:VAL:HG21	1.84	0.60
7:AL:90:MET:HE1	7:AL:326:LYS:HB2	1.82	0.60
9:C:163:SER:N	9:C:167:GLU:OE2	2.32	0.60
7:AI:337:PRO:HG3	7:AI:348:VAL:HG21	1.84	0.59
7:AM:376:GLN:OE1	7:AM:376:GLN:N	2.35	0.59
14:N:172:LEU:HB3	2:P:162:GLN:NE2	2.17	0.59
3:v:998:TRP:CG	3:v:1019:ARG:HH12	2.20	0.59
9:C:683:HIS:CD2	9:C:706:ARG:HH22	2.21	0.59
9:C:572:ARG:NE	9:C:574:ASP:OD2	2.33	0.59
3:q:1044:THR:HG21	3:q:1139:ARG:HG2	1.84	0.59
12:I:73:ASP:OD2	12:I:75:SER:OG	2.17	0.59
14:N:705:ILE:O	2:V:113:PRO:HB3	2.03	0.59
7:AI:13:ARG:HH22	12:I:108:HIS:CD2	2.20	0.59
7:AL:337:PRO:HG3	7:AL:348:VAL:HG21	1.84	0.59
13:K:6:LEU:N	13:K:45:GLU:OE1	2.36	0.59
7:AN:376:GLN:N	7:AN:376:GLN:OE1	2.35	0.58
4:A:23:VAL:HG11	4:A:94:PHE:CE1	2.38	0.58
13:J:320:ASP:OD1	13:J:321:VAL:N	2.36	0.58
2:Y:158:ASN:ND2	2:Z:156:PHE:CE1	2.70	0.58
13:M:225:ASP:OD1	13:M:229:ASN:N	2.37	0.58
2:S:91:GLU:CD	2:S:91:GLU:H	2.09	0.58
2:n:157:GLN:OE1	2:o:157:GLN:HG2	2.03	0.58
8:B:51:ILE:HB	9:C:781:ALA:O	2.03	0.58
9:C:174:ARG:NH1	11:G:208:ASN:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:147:ILE:CD1	9:C:679:LYS:HE2	2.31	0.58
14:O:460:TYR:CE1	2:i:162:GLN:HA	2.38	0.58
2:n:157:GLN:OE1	2:o:157:GLN:CG	2.50	0.58
7:AI:569:ARG:O	12:H:166:ASN:CB	2.51	0.58
7:AI:582:GLN:C	12:H:213:SER:O	2.46	0.58
7:AL:463:VAL:HG21	7:AL:472:ARG:NE	2.19	0.58
11:F:177:ALA:O	11:F:181:VAL:HG23	2.03	0.58
11:G:177:ALA:O	11:G:181:VAL:HG23	2.04	0.58
7:AI:13:ARG:NH2	7:AJ:450:ASP:OD1	2.37	0.58
7:AK:463:VAL:HG21	7:AK:472:ARG:NE	2.18	0.58
11:F:60:LYS:NZ	11:F:63:GLU:OE2	2.30	0.57
13:J:207:VAL:HG21	13:J:238:ILE:HD11	1.85	0.57
7:AJ:315:GLU:OE1	7:AJ:315:GLU:N	2.38	0.57
7:AJ:544:ASP:OD1	7:AJ:545:PHE:N	2.36	0.57
7:AI:315:GLU:OE1	7:AI:315:GLU:N	2.38	0.57
3:s:857:ALA:HB2	3:s:891:TRP:CD2	2.39	0.57
7:AI:571:PHE:CZ	12:H:166:ASN:HA	2.39	0.57
4:A:240:ASP:OD1	4:A:260:SER:OG	2.19	0.57
7:AJ:198:GLY:N	7:AJ:201:ASP:OD1	2.38	0.57
7:AN:399:VAL:O	7:AN:436:ARG:NH2	2.36	0.57
4:A:56:ASP:OD1	4:A:59:SER:OG	2.22	0.57
13:J:28:THR:HG1	13:J:31:SER:HG	1.53	0.57
12:H:124:ASP:OD1	12:H:125:LEU:N	2.38	0.57
13:K:180:ARG:NH1	13:L:316:VAL:HG21	2.20	0.57
7:AI:198:GLY:N	7:AI:201:ASP:OD1	2.38	0.57
7:AK:568:ILE:HG23	7:AK:568:ILE:O	2.04	0.57
2:1:75:LYS:HE2	2:1:86:VAL:HG22	1.87	0.56
7:AJ:574:ILE:HD12	12:I:163:PHE:CZ	2.40	0.56
7:AM:399:VAL:O	7:AM:436:ARG:NH2	2.35	0.56
3:t:365:TYR:CD1	3:t:380:ILE:HG23	2.40	0.56
3:7:814:ALA:HB2	3:7:891:TRP:CZ2	2.40	0.56
4:A:230:ILE:O	4:A:246:LEU:N	2.36	0.56
7:AI:172:ASP:O	7:AI:176:GLN:N	2.38	0.56
7:AJ:114:ASN:HB2	13:M:155:SER:HB3	1.88	0.56
3:s:192:TYR:HA	3:s:442:LEU:HD13	1.87	0.56
7:AI:544:ASP:OD1	7:AI:545:PHE:N	2.36	0.56
13:L:335:GLN:N	13:L:335:GLN:OE1	2.36	0.56
14:N:157:GLU:N	14:N:157:GLU:OE1	2.38	0.56
11:F:187:GLU:OE2	13:L:2:LYS:NZ	2.38	0.56
7:AN:510:ASP:O	7:AN:516:ARG:NH1	2.36	0.56
13:K:97:ALA:N	13:K:117:ASP:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:78:ASP:OD1	14:O:79:VAL:N	2.39	0.56
6:AD:44:ILE:HG23	11:F:33:PRO:O	2.06	0.56
7:AL:568:ILE:HG23	7:AL:568:ILE:O	2.04	0.56
2:W:38:ASN:ND2	2:X:77:LEU:HD13	2.21	0.56
5:b:14:LEU:HD12	5:b:14:LEU:H	1.70	0.56
3:q:854:SER:HB3	3:q:859:ALA:HB3	1.88	0.56
3:t:959:ALA:HB3	3:t:1013:ALA:HB3	1.87	0.56
3:u:857:ALA:HB2	3:u:891:TRP:CG	2.40	0.56
7:AI:13:ARG:NH2	12:I:108:HIS:HD2	2.03	0.55
7:AL:229:GLU:OE1	7:AL:229:GLU:N	2.39	0.55
12:I:193:LEU:HD21	12:I:196:TRP:CD1	2.41	0.55
3:v:775:LYS:HE3	3:v:965:MET:SD	2.45	0.55
9:C:364:LYS:NZ	9:C:368:ASN:OD1	2.40	0.55
7:AI:470:PHE:CE2	12:I:9:GLN:HB3	2.42	0.55
13:M:227:ASN:O	13:M:227:ASN:ND2	2.36	0.55
14:N:176:TYR:OH	2:P:157:GLN:CD	2.39	0.55
2:e:29:LYS:HE3	2:e:33:TRP:CZ3	2.42	0.55
12:I:95:ASP:OD1	12:I:96:LEU:N	2.40	0.55
13:J:253:ASP:OD1	13:J:254:VAL:N	2.38	0.55
7:AK:148:ASP:OD1	7:AK:149:ASN:N	2.39	0.55
7:AL:207:ILE:O	7:AL:211:ASN:ND2	2.40	0.55
3:s:501:LEU:HD12	3:s:501:LEU:H	1.72	0.55
3:3:791:VAL:HG23	3:3:792:ASP:H	1.72	0.55
8:B:266:ASP:OD1	8:B:267:GLU:N	2.40	0.55
3:4:814:ALA:HB2	3:4:891:TRP:CE2	2.41	0.55
7:AI:16:ALA:O	12:I:109:GLY:HA3	2.06	0.55
7:AK:544:ASP:OD1	7:AK:545:PHE:N	2.40	0.55
12:H:15:GLN:OE1	12:H:15:GLN:N	2.37	0.55
14:N:174:VAL:O	2:P:164:THR:N	2.35	0.55
3:u:308:TRP:CD1	3:u:316:THR:HG1	2.24	0.55
7:AK:207:ILE:O	7:AK:211:ASN:ND2	2.40	0.55
3:s:813:PHE:CE2	3:s:890:MET:HE3	2.42	0.55
9:C:706:ARG:HH11	9:C:778:HIS:CG	2.25	0.54
7:AM:510:ASP:O	7:AM:516:ARG:NH1	2.36	0.54
13:K:253:ASP:OD1	13:K:254:VAL:N	2.40	0.54
13:M:234:LEU:O	13:M:234:LEU:HD23	2.07	0.54
6:AD:67:ARG:NH2	6:AD:117:GLU:OE2	2.41	0.54
12:H:73:ASP:OD2	12:H:75:SER:OG	2.20	0.54
12:I:210:GLU:OE1	12:I:210:GLU:N	2.40	0.54
13:M:225:ASP:N	13:M:229:ASN:O	2.35	0.54
6:AC:12:GLY:O	6:AF:45:GLY:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:15:ASP:OD1	14:O:16:ARG:N	2.41	0.54
5:a:626:LYS:HE2	15:d:55:TYR:CD1	2.42	0.54
5:c:283:LEU:HB2	5:c:363:ALA:HB2	1.90	0.54
7:AL:148:ASP:OD1	7:AL:149:ASN:N	2.39	0.54
8:B:150:LEU:CG	9:C:679:LYS:HZ2	2.18	0.54
12:H:95:ASP:OD1	12:H:96:LEU:N	2.41	0.54
13:L:295:LEU:HD22	13:L:338:ILE:CG2	2.38	0.54
4:A:245:VAL:C	4:A:246:LEU:HD12	2.33	0.54
5:AA:37:VAL:HG21	5:AA:59:TYR:HB2	1.89	0.54
7:AL:557:ASN:ND2	7:AN:570:SER:O	2.38	0.54
11:F:190:LYS:NZ	13:J:135:GLU:OE2	2.35	0.54
13:M:244:ASP:OD1	14:O:96:ASN:ND2	2.39	0.54
2:l:101:VAL:HB	2:l:171:VAL:CG2	2.38	0.54
2:n:158:ASN:ND2	2:o:155:GLN:HB3	2.23	0.54
9:C:199:ASP:OD1	9:C:200:ASP:N	2.41	0.54
9:C:241:LYS:NZ	9:C:560:ASP:OD2	2.41	0.54
13:K:87:GLN:N	13:K:87:GLN:OE1	2.41	0.54
4:A:152:ASP:OD1	4:A:153:GLY:N	2.40	0.54
7:AK:587:ALA:N	12:H:196:TRP:CE2	2.68	0.54
13:J:16:LYS:NZ	14:N:30:ASP:OD2	2.41	0.54
14:N:2:ALA:N	14:N:40:GLU:OE1	2.40	0.54
13:L:193:THR:O	13:L:197:VAL:HG23	2.06	0.53
9:C:401:ILE:O	9:C:405:VAL:HG23	2.07	0.53
7:AI:404:ARG:HD2	13:L:96:PRO:HG3	1.87	0.53
7:AK:229:GLU:OE1	7:AK:229:GLU:N	2.40	0.53
10:E:144:TYR:O	10:E:148:VAL:HG23	2.09	0.53
12:I:109:GLY:O	12:I:110:THR:OG1	2.23	0.53
5:c:59:TYR:CE2	5:c:61:THR:HG22	2.43	0.53
7:AK:582:GLN:NE2	12:H:199:GLN:HG2	2.23	0.53
9:C:193:ASP:OD1	9:C:194:ASN:ND2	2.41	0.53
7:AI:67:GLU:N	7:AI:67:GLU:OE1	2.39	0.53
7:AJ:172:ASP:O	7:AJ:176:GLN:N	2.39	0.53
7:AN:548:GLU:N	7:AN:548:GLU:OE1	2.41	0.53
7:AL:544:ASP:OD1	7:AL:545:PHE:N	2.41	0.53
13:K:320:ASP:OD1	13:K:321:VAL:N	2.42	0.53
7:AJ:67:GLU:N	7:AJ:67:GLU:OE1	2.38	0.53
7:AJ:577:SER:O	12:I:206:GLN:HA	2.09	0.53
7:AM:548:GLU:OE1	7:AM:548:GLU:N	2.42	0.53
3:2:217:ALA:HB1	3:2:229:LYS:O	2.09	0.53
3:s:857:ALA:HB2	3:s:891:TRP:CE3	2.44	0.53
3:6:875:LYS:HD3	3:6:876:GLU:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:260:MET:HE2	5:AA:260:MET:HA	1.91	0.52
12:I:15:GLN:OE1	12:I:15:GLN:N	2.40	0.52
12:I:97:ASN:ND2	12:I:126:ASP:OD2	2.42	0.52
13:K:16:LYS:NZ	14:O:30:ASP:OD2	2.32	0.52
3:v:998:TRP:CD1	3:v:1019:ARG:HH12	2.26	0.52
9:C:561:LEU:CD1	9:C:583:VAL:HG22	2.38	0.52
13:L:320:ASP:OD1	13:L:321:VAL:N	2.41	0.52
2:W:35:ASN:HD22	2:X:74:ASN:HA	1.74	0.52
7:AM:375:GLU:N	7:AM:375:GLU:OE1	2.41	0.52
14:O:96:ASN:OD1	14:O:97:ALA:N	2.42	0.52
3:2:171:ASN:C	3:2:173:GLU:H	2.18	0.52
14:O:86:LYS:NZ	14:O:104:ASP:OD2	2.36	0.52
2:f:64:VAL:HG21	2:f:102:TYR:CD1	2.45	0.52
3:t:1131:LEU:HD12	3:t:1131:LEU:H	1.74	0.52
3:s:833:GLN:H	3:s:833:GLN:CD	2.17	0.52
6:AC:67:ARG:NH2	6:AC:117:GLU:OE2	2.42	0.52
7:AK:384:LEU:HD21	7:AK:389:VAL:HG11	1.92	0.52
11:F:174:LYS:O	13:L:11:SER:OG	2.16	0.52
2:Q:102:TYR:CD1	2:Q:168:ARG:HD3	2.45	0.52
3:6:266:PRO:HA	3:6:378:TRP:CH2	2.45	0.52
3:6:1129:LEU:HD11	3:6:1145:LEU:HD22	1.91	0.52
7:AJ:404:ARG:HD2	13:M:96:PRO:HG3	1.89	0.52
7:AM:503:GLU:OE1	7:AM:536:LYS:NZ	2.42	0.52
9:C:486:LEU:HD11	9:C:506:TYR:HB2	1.90	0.52
12:I:175:GLU:CD	12:I:193:LEU:HD22	2.35	0.52
1:x:343:TRP:CG	1:x:434:TRP:HE1	2.28	0.52
2:Z:134:LYS:HE2	2:Z:136:ASN:O	2.09	0.52
3:v:869:MET:HE2	3:v:871:ALA:HB2	1.92	0.52
9:C:556:ASP:OD2	9:C:558:LYS:NZ	2.38	0.52
11:F:241:ASN:OD1	11:F:242:GLY:N	2.43	0.52
3:q:812:TYR:CZ	3:q:935:LYS:HE2	2.45	0.52
7:AL:384:LEU:HD21	7:AL:389:VAL:HG11	1.92	0.51
5:c:211:ILE:HG21	5:c:223:GLY:HA3	1.92	0.51
5:z:14:LEU:HD12	5:z:14:LEU:H	1.74	0.51
7:AK:587:ALA:HA	12:H:196:TRP:HZ2	1.60	0.51
13:M:327:ASP:OD1	13:M:328:GLU:N	2.43	0.51
14:N:4:PHE:CD1	14:N:36:MET:HE1	2.45	0.51
2:o:116:THR:HG22	2:o:158:ASN:HA	1.91	0.51
3:v:600:SER:HA	3:v:768:TYR:CD2	2.44	0.51
13:M:71:LYS:NZ	13:M:175:GLN:OE1	2.32	0.51
13:M:320:ASP:OD1	13:M:321:VAL:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:176:TYR:CD2	2:e:157:GLN:NE2	2.69	0.51
2:W:38:ASN:OD1	2:X:77:LEU:HB2	2.11	0.51
3:u:1112:ILE:HD12	3:u:1112:ILE:H	1.76	0.51
7:AK:557:ASN:ND2	7:AM:570:SER:O	2.38	0.51
3:7:835:TYR:CD1	3:7:926:TRP:HB2	2.46	0.51
12:I:124:ASP:OD1	12:I:125:LEU:N	2.43	0.51
6:AE:113:ASN:ND2	6:AE:132:SER:OG	2.39	0.51
7:AN:375:GLU:OE1	7:AN:375:GLU:N	2.42	0.51
13:M:208:GLU:OE2	13:M:226:ARG:NH2	2.42	0.51
2:U:91:GLU:CD	2:U:91:GLU:H	2.19	0.51
2:W:35:ASN:ND2	2:X:74:ASN:HA	2.26	0.51
3:6:883:THR:HG21	3:6:888:TYR:CD2	2.45	0.51
4:A:99:ILE:HG23	4:A:100:ASN:ND2	2.26	0.51
13:M:193:THR:O	13:M:197:VAL:HG23	2.11	0.51
5:c:86:TYR:CE2	5:c:103:TYR:CD1	2.98	0.51
3:u:706:LEU:H	3:u:715:ILE:HD11	1.76	0.51
3:v:816:LYS:HA	3:v:888:TYR:CD2	2.46	0.51
9:C:151:ASP:OD1	9:C:152:GLY:N	2.44	0.50
3:7:144:LYS:HE3	3:7:144:LYS:HA	1.91	0.50
6:AE:12:GLY:O	6:AH:45:GLY:N	2.41	0.50
7:AK:114:ASN:N	7:AK:313:ASN:OD1	2.43	0.50
2:P:155:GLN:HA	2:P:155:GLN:HE21	1.75	0.50
9:C:263:GLU:OE1	9:C:263:GLU:N	2.44	0.50
12:I:141:ARG:NH1	12:I:184:SER:OG	2.45	0.50
14:N:175:THR:HA	2:P:164:THR:O	2.12	0.50
6:AF:113:ASN:ND2	6:AF:132:SER:OG	2.39	0.50
2:1:153:ASN:O	2:1:154:LYS:HE3	2.12	0.50
7:AL:587:ALA:HB2	12:I:196:TRP:CE2	2.47	0.50
2:R:56:LYS:HZ2	2:R:111:GLU:CD	2.19	0.50
2:X:91:GLU:CD	2:X:91:GLU:H	2.19	0.50
3:s:947:ALA:HB3	3:s:1022:PHE:HB2	1.93	0.50
5:z:18:TYR:CD1	5:z:18:TYR:C	2.89	0.50
3:5:813:PHE:CE1	3:5:861:THR:HB	2.47	0.50
7:AN:549:ASP:OD2	7:AN:564:THR:OG1	2.20	0.50
11:F:172:ASN:ND2	13:L:15:ASP:OD1	2.43	0.50
13:J:289:ARG:HG2	13:J:343:ILE:HD13	1.93	0.50
4:A:170:THR:HG21	4:A:175:GLU:O	2.11	0.50
6:AE:119:TRP:CH2	6:AF:105:ILE:HD11	2.47	0.50
6:AG:80:SER:OG	6:AG:85:ILE:N	2.45	0.50
11:G:86:LYS:NZ	11:G:90:GLU:OE2	2.44	0.50
13:L:261:GLU:N	13:L:261:GLU:OE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:110:GLN:OE1	13:M:110:GLN:N	2.42	0.50
5:c:278:ILE:HD11	5:c:363:ALA:HB1	1.93	0.50
5:AA:25:GLY:HA3	5:z:5:TYR:CD1	2.46	0.50
7:AN:503:GLU:OE1	7:AN:536:LYS:NZ	2.42	0.50
3:2:791:VAL:H	3:2:923:ALA:HB3	1.77	0.49
8:B:150:LEU:CD1	9:C:679:LYS:HZ1	1.98	0.49
9:C:560:ASP:OD1	9:C:561:LEU:N	2.45	0.49
10:E:78:LYS:NZ	10:E:150:ASP:OD2	2.40	0.49
2:j:116:THR:HG22	2:j:158:ASN:HA	1.94	0.49
3:2:812:TYR:CE2	3:2:935:LYS:HE2	2.47	0.49
7:AI:171:HIS:NE2	7:AI:233:LEU:O	2.42	0.49
9:C:707:ARG:NE	9:C:714:VAL:H	2.10	0.49
10:E:161:ILE:O	10:E:165:LEU:N	2.43	0.49
14:N:200:TYR:CE1	2:R:164:THR:HG23	2.46	0.49
5:b:459:PRO:HD2	5:b:464:ILE:HG21	1.94	0.49
9:C:137:GLN:N	9:C:137:GLN:OE1	2.42	0.49
12:H:166:ASN:ND2	12:H:200:GLY:O	2.45	0.49
3:q:555:ALA:HB1	3:q:563:SER:O	2.12	0.49
2:1:151:PHE:O	2:Z:2:ALA:HA	2.13	0.49
9:C:588:ASP:O	9:C:592:GLY:N	2.46	0.49
13:J:315:ASP:OD1	13:J:316:VAL:N	2.46	0.49
3:5:103:LYS:HE3	3:5:103:LYS:HA	1.94	0.49
3:6:31:LEU:HD23	3:6:32:GLN:H	1.78	0.49
6:AH:115:TYR:OH	6:AH:117:GLU:OE2	2.31	0.49
7:AI:322:ASP:OD1	7:AI:323:LYS:N	2.45	0.49
7:AL:114:ASN:N	7:AL:313:ASN:OD1	2.43	0.49
2:Y:24:TYR:HB2	2:Y:126:LEU:HD21	1.94	0.49
6:AH:80:SER:OG	6:AH:85:ILE:N	2.45	0.49
7:AK:475:ASP:OD1	7:AK:476:ASP:N	2.45	0.49
13:L:107:GLU:OE1	13:L:107:GLU:N	2.44	0.49
2:T:107:ILE:HD12	2:T:107:ILE:H	1.78	0.49
3:r:1031:LEU:HD23	3:r:1032:MET:H	1.78	0.49
2:k:103:LEU:HD11	2:k:122:PHE:CD2	2.47	0.49
3:s:296:LEU:HD22	3:s:353:TYR:CE1	2.48	0.49
3:u:1112:ILE:H	3:u:1112:ILE:CD1	2.25	0.49
2:1:2:ALA:HA	2:Z:151:PHE:O	2.13	0.49
3:2:1150:ARG:HE	3:2:1152:GLU:CD	2.20	0.49
7:AJ:512:PHE:O	7:AJ:515:THR:HG22	2.12	0.49
12:H:68:GLU:OE1	12:H:68:GLU:N	2.42	0.49
2:R:99:LYS:HE3	2:R:100:TRP:CZ2	2.48	0.49
3:4:553:THR:HG22	3:4:555:ALA:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:718:ALA:H	3:6:740:GLY:HA2	1.76	0.49
6:AD:43:GLU:CG	11:F:31:VAL:HG13	2.43	0.49
7:AI:512:PHE:O	7:AI:515:THR:HG22	2.12	0.49
7:AJ:425:GLU:OE2	11:G:80:ASP:HB2	2.12	0.49
2:m:134:LYS:HE2	2:m:136:ASN:O	2.13	0.49
3:r:791:VAL:H	3:r:923:ALA:HB3	1.78	0.49
3:4:969:LEU:HD23	3:4:970:THR:N	2.28	0.48
6:AD:51:GLU:OE1	11:F:74:ARG:HG2	2.09	0.48
8:B:2:ALA:N	8:B:73:ASN:HD22	2.11	0.48
12:H:102:GLU:O	12:H:106:ASN:ND2	2.41	0.48
5:c:66:ALA:HB1	5:c:67:PRO:HD2	1.95	0.48
7:AJ:171:HIS:NE2	7:AJ:233:LEU:O	2.42	0.48
7:AL:475:ASP:OD1	7:AL:476:ASP:N	2.44	0.48
12:I:52:ASP:HB3	12:I:56:LEU:HD13	1.94	0.48
7:AK:153:ILE:HG23	7:AK:154:PHE:CD1	2.48	0.48
12:I:193:LEU:HD21	12:I:196:TRP:HD1	1.78	0.48
2:X:75:LYS:HE2	2:X:86:VAL:HG21	1.94	0.48
1:0:267:HIS:CE1	1:0:271:THR:HG21	2.48	0.48
3:5:985:ASP:HA	3:5:1014:ARG:HE	1.79	0.48
5:AA:121:LEU:HD22	5:z:160:GLU:HB3	1.95	0.48
7:AL:153:ILE:HG23	7:AL:154:PHE:CD1	2.48	0.48
11:G:168:GLU:OE1	11:G:168:GLU:N	2.42	0.48
13:J:332:VAL:HG22	13:J:338:ILE:HD13	1.95	0.48
2:i:89:THR:HG22	2:i:90:PRO:HD2	1.95	0.48
7:AN:509:GLU:HA	7:AN:513:ILE:HD12	1.95	0.48
3:v:692:PHE:CE2	3:v:740:GLY:HA3	2.48	0.48
3:v:717:PRO:HB3	3:v:730:ILE:HD12	1.95	0.48
9:C:479:ASN:ND2	9:C:481:THR:OG1	2.46	0.48
11:G:43:ARG:NH1	11:G:58:TYR:O	2.44	0.48
11:G:52:ASP:OD1	11:G:53:ILE:N	2.44	0.48
14:N:156:VAL:HG13	2:P:160:SER:OG	2.14	0.48
2:S:74:ASN:C	2:S:74:ASN:HD22	2.22	0.48
3:r:16:PRO:HB3	3:r:45:TYR:CZ	2.49	0.48
6:AE:119:TRP:HH2	6:AF:105:ILE:HD11	1.79	0.48
3:3:171:ASN:C	3:3:173:GLU:H	2.21	0.48
3:3:407:LYS:HD2	3:3:431:VAL:HG13	1.94	0.48
4:A:23:VAL:HG11	4:A:94:PHE:CD1	2.49	0.48
5:b:14:LEU:H	5:b:14:LEU:CD1	2.27	0.48
3:7:890:MET:HE2	3:7:934:LEU:HD21	1.95	0.48
7:AJ:322:ASP:OD1	7:AJ:323:LYS:N	2.45	0.48
7:AK:79:ASN:OD1	7:AK:82:TYR:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AM:473:ILE:N	7:AM:473:ILE:HD12	2.29	0.48
9:C:5:ARG:NH1	9:C:555:GLY:O	2.40	0.48
10:E:12:LEU:CD1	10:E:65:VAL:HG12	2.43	0.48
12:H:24:ASP:OD1	12:H:25:VAL:N	2.47	0.48
2:f:29:LYS:HE3	2:f:33:TRP:CE3	2.49	0.48
3:7:1044:THR:HB	3:7:1136:SER:HB2	1.95	0.47
6:AC:26:ARG:NE	6:AF:43:GLU:OE2	2.47	0.47
7:AI:580:TYR:CZ	12:H:138:LEU:CD1	2.93	0.47
13:M:202:LEU:HD21	13:M:210:VAL:HG12	1.95	0.47
7:AJ:148:ASP:OD1	7:AJ:149:ASN:N	2.44	0.47
7:AL:509:GLU:OE1	7:AN:472:ARG:NH2	2.45	0.47
1:w:17:LEU:HD22	1:x:18:THR:HG23	1.96	0.47
3:2:90:TYR:CD2	3:2:145:MET:SD	3.07	0.47
9:C:706:ARG:HH11	9:C:778:HIS:CD2	2.32	0.47
11:G:77:ARG:NE	11:G:78:GLU:O	2.46	0.47
13:J:110:GLN:OE1	13:J:110:GLN:N	2.44	0.47
5:a:158:TYR:CD2	5:a:169:VAL:HG22	2.49	0.47
5:b:147:PRO:HA	5:b:398:TRP:CD1	2.50	0.47
7:AN:473:ILE:N	7:AN:473:ILE:HD12	2.30	0.47
12:I:195:ASP:OD2	12:I:197:LYS:NZ	2.47	0.47
9:C:140:GLN:NE2	13:K:154:SER:O	2.41	0.47
9:C:272:VAL:HG13	9:C:272:VAL:O	2.15	0.47
10:E:102:ALA:O	10:E:106:VAL:HG23	2.15	0.47
5:a:259:LYS:HE3	5:a:346:TYR:CE1	2.49	0.47
2:m:101:VAL:HB	2:m:171:VAL:CG2	2.44	0.47
5:z:430:VAL:HG11	5:z:455:ILE:HD13	1.96	0.47
13:K:36:LEU:O	13:K:40:VAL:HG23	2.15	0.47
13:L:176:GLU:OE1	13:L:176:GLU:N	2.42	0.47
14:N:443:TYR:CD2	14:N:443:TYR:C	2.93	0.47
3:2:582:ASN:HA	3:2:889:THR:HG22	1.97	0.47
4:A:13:LEU:HD23	4:A:13:LEU:H	1.80	0.47
7:AI:228:LEU:HD21	7:AI:253:GLY:HA3	1.96	0.47
7:AK:322:ASP:OD1	7:AK:323:LYS:N	2.47	0.47
7:AL:153:ILE:HG23	7:AL:154:PHE:HD1	1.79	0.47
7:AL:587:ALA:HA	12:I:196:TRP:CZ2	2.49	0.47
7:AN:322:ASP:OD1	7:AN:323:LYS:N	2.48	0.47
8:B:281:GLU:OE1	8:B:281:GLU:N	2.43	0.47
14:O:508:ILE:HD12	14:O:696:ILE:HD13	1.96	0.47
5:a:593:CYS:HA	5:a:603:PRO:HA	1.96	0.47
3:q:1044:THR:HG21	3:q:1139:ARG:CG	2.45	0.47
3:u:857:ALA:HB2	3:u:891:TRP:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:981:LYS:HE2	3:2:981:LYS:HA	1.97	0.47
3:3:812:TYR:CE2	3:3:935:LYS:HE2	2.49	0.47
3:7:252:ILE:H	3:7:252:ILE:HD12	1.80	0.47
3:7:732:THR:HG22	3:7:738:ALA:HB2	1.97	0.47
13:J:276:ILE:HG22	13:J:276:ILE:O	2.14	0.47
13:J:289:ARG:NH2	13:J:341:GLY:O	2.47	0.47
4:A:256:GLN:HG3	4:A:266:VAL:HG22	1.97	0.47
7:AL:442:GLN:N	7:AL:442:GLN:OE1	2.48	0.47
11:G:189:ASP:OD1	11:G:190:LYS:N	2.44	0.47
13:K:180:ARG:HH11	13:L:316:VAL:HG21	1.80	0.47
2:1:75:LYS:HE2	2:1:86:VAL:CG2	2.45	0.47
3:5:706:LEU:HB2	3:5:715:ILE:HD11	1.96	0.47
3:6:812:TYR:CZ	3:6:935:LYS:HE2	2.50	0.47
7:AK:442:GLN:OE1	7:AK:442:GLN:N	2.48	0.47
7:AM:509:GLU:HA	7:AM:513:ILE:HD12	1.97	0.47
14:N:624:ARG:HD2	14:N:653:TYR:CE1	2.50	0.47
3:5:792:ASP:N	3:5:793:PRO:HD3	2.30	0.46
7:AN:463:VAL:HG21	7:AN:472:ARG:NE	2.30	0.46
2:m:27:ILE:HD11	2:m:117:TYR:CE2	2.51	0.46
3:q:787:THR:HG23	3:q:839:THR:HA	1.96	0.46
3:s:268:LYS:HD2	3:s:403:TYR:CZ	2.50	0.46
1:w:343:TRP:CG	1:w:434:TRP:HE1	2.33	0.46
3:3:326:PHE:CD2	3:3:334:ILE:HG23	2.49	0.46
7:AJ:207:ILE:O	7:AJ:211:ASN:ND2	2.42	0.46
13:J:193:THR:HG22	13:J:194:ASN:N	2.29	0.46
13:K:182:PHE:O	13:K:186:VAL:HG23	2.16	0.46
13:K:247:PRO:HB2	13:K:250:ILE:HD12	1.97	0.46
13:M:112:PHE:HB3	13:M:131:VAL:HG12	1.98	0.46
14:N:76:LYS:HE3	14:N:79:VAL:HG23	1.96	0.46
2:S:99:LYS:HE3	2:S:100:TRP:CZ2	2.51	0.46
3:t:704:LEU:HB2	3:t:730:ILE:HG23	1.97	0.46
3:3:600:SER:HA	3:3:768:TYR:CE1	2.50	0.46
7:AK:235:LYS:NZ	7:AK:237:GLU:OE2	2.38	0.46
10:E:111:GLU:OE2	11:G:256:TYR:OH	2.33	0.46
11:G:83:LYS:NZ	11:G:91:GLU:OE1	2.48	0.46
12:H:211:ILE:O	12:H:211:ILE:HG22	2.14	0.46
14:O:460:TYR:CZ	2:i:162:GLN:C	2.93	0.46
7:AJ:435:LEU:CD2	7:AJ:460:ILE:HD13	2.46	0.46
7:AJ:577:SER:HB2	12:I:206:GLN:HB3	1.96	0.46
7:AL:90:MET:HE1	7:AL:326:LYS:CB	2.46	0.46
7:AM:322:ASP:OD1	7:AM:323:LYS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:799:LYS:HE3	9:C:799:LYS:HA	1.97	0.46
2:l:103:LEU:HD11	2:l:122:PHE:CD2	2.51	0.46
2:o:147:THR:HG23	2:p:7:ASN:HB3	1.96	0.46
8:B:51:ILE:HG22	9:C:781:ALA:HA	1.97	0.46
5:b:151:LEU:HD22	5:b:176:SER:HB2	1.96	0.46
3:5:470:ASP:HA	3:5:473:LYS:HE2	1.98	0.46
7:AI:207:ILE:O	7:AI:211:ASN:ND2	2.41	0.46
7:AJ:228:LEU:HD21	7:AJ:253:GLY:HA3	1.95	0.46
3:u:1071:ALA:HA	3:u:1107:PHE:CE2	2.51	0.46
3:v:857:ALA:HB2	3:v:891:TRP:CD2	2.51	0.46
7:AJ:574:ILE:HD12	12:I:163:PHE:CE2	2.51	0.46
7:AK:153:ILE:HG23	7:AK:154:PHE:HD1	1.80	0.46
9:C:164:SER:O	9:C:168:VAL:HG23	2.15	0.46
1:w:171:VAL:C	1:w:172:MET:HE2	2.41	0.46
6:AD:43:GLU:HG2	11:F:31:VAL:CG1	2.46	0.46
7:AI:46:GLU:O	7:AI:49:THR:OG1	2.34	0.46
7:AM:463:VAL:HG21	7:AM:472:ARG:NE	2.30	0.46
3:6:1067:PHE:CE1	3:6:1081:PRO:HB3	2.51	0.46
7:AL:548:GLU:OE1	7:AL:548:GLU:N	2.47	0.46
12:H:150:MET:O	12:I:19:GLN:NE2	2.44	0.46
3:2:971:PRO:HA	3:4:438:ASP:CG	2.41	0.46
7:AI:464:ARG:N	12:H:112:ASP:OD2	2.45	0.46
7:AI:509:GLU:OE1	7:AK:472:ARG:NH2	2.47	0.46
7:AN:48:ASN:OD1	7:AN:323:LYS:NZ	2.49	0.46
9:C:174:ARG:NH2	11:G:208:ASN:OD1	2.47	0.46
3:3:357:LYS:HE3	3:3:357:LYS:HA	1.97	0.45
7:AK:124:GLU:O	7:AK:133:ARG:N	2.45	0.45
7:AK:548:GLU:OE1	7:AK:548:GLU:N	2.47	0.45
9:C:442:SER:O	9:C:446:GLU:N	2.45	0.45
13:J:28:THR:OG1	13:J:31:SER:OG	2.27	0.45
2:S:111:GLU:CG	2:S:136:ASN:HD21	2.28	0.45
5:b:18:TYR:CD2	5:b:19:PRO:HD3	2.51	0.45
6:AG:115:TYR:OH	6:AG:117:GLU:OE2	2.30	0.45
10:D:131:LEU:C	10:D:131:LEU:HD23	2.41	0.45
3:v:336:TRP:C	3:v:338:PRO:HD2	2.42	0.45
3:3:894:THR:HG21	3:3:897:LYS:HE3	1.99	0.45
3:6:793:PRO:HG2	3:6:926:TRP:CH2	2.51	0.45
6:AE:11:THR:O	6:AE:15:VAL:HG23	2.17	0.45
7:AI:435:LEU:CD2	7:AI:460:ILE:HD13	2.46	0.45
7:AL:322:ASP:OD1	7:AL:323:LYS:N	2.48	0.45
11:F:136:THR:HG22	11:G:37:THR:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:172:LEU:O	2:P:162:GLN:NE2	2.43	0.45
3:2:217:ALA:HB2	3:2:232:SER:HA	1.99	0.45
3:7:1075:LYS:HE2	3:7:1075:LYS:C	2.41	0.45
7:AL:517:THR:HA	7:AN:568:ILE:HG23	1.99	0.45
11:F:91:GLU:OE2	11:F:95:ARG:NH2	2.49	0.45
12:H:89:GLU:O	12:H:93:GLY:N	2.49	0.45
13:L:299:ASP:OD1	13:L:299:ASP:N	2.49	0.45
3:r:171:ASN:C	3:r:173:GLU:H	2.24	0.45
3:3:981:LYS:HE3	3:3:998:TRP:CZ2	2.51	0.45
7:AK:375:GLU:OE1	7:AK:375:GLU:N	2.44	0.45
2:Z:101:VAL:HB	2:Z:171:VAL:CG2	2.47	0.45
3:s:356:ASN:ND2	3:s:397:LEU:H	2.15	0.45
3:t:970:THR:HG22	3:t:1030:PRO:HA	1.98	0.45
3:7:310:GLU:CD	3:7:314:GLY:H	2.25	0.45
4:A:41:VAL:HG11	4:A:84:ILE:HG21	1.98	0.45
9:C:694:HIS:CG	9:C:716:LEU:HB3	2.52	0.45
13:L:297:THR:HG22	13:L:297:THR:O	2.16	0.45
2:V:2:ALA:HA	2:W:151:PHE:O	2.16	0.45
3:t:103:LYS:HE3	3:t:103:LYS:HA	1.96	0.45
7:AK:585:LEU:HB2	12:H:198:ILE:HB	1.98	0.45
7:AL:473:ILE:HD12	7:AL:473:ILE:N	2.32	0.45
12:H:4:LYS:O	12:H:65:ILE:N	2.41	0.45
3:v:570:ARG:HD3	3:v:939:TYR:CZ	2.52	0.45
3:5:1150:ARG:HE	3:5:1152:GLU:CD	2.25	0.45
3:7:984:LEU:H	3:7:987:MET:HG3	1.81	0.45
5:AA:473:ASP:HB3	5:AA:480:ALA:HB1	1.97	0.45
7:AL:375:GLU:OE1	7:AL:375:GLU:N	2.43	0.45
7:AL:460:ILE:HD12	7:AL:460:ILE:N	2.32	0.45
9:C:244:GLU:N	9:C:244:GLU:OE1	2.49	0.45
3:r:194:VAL:HG11	3:r:219:LYS:HD2	1.99	0.45
3:2:279:ILE:HD11	3:2:355:TYR:CZ	2.51	0.45
3:6:816:LYS:HA	3:6:888:TYR:CD1	2.52	0.45
10:E:157:CYS:SG	11:G:249:ASN:ND2	2.89	0.45
13:M:302:ILE:HG22	13:M:304:THR:HG22	1.97	0.45
2:l:150:PHE:CZ	2:l:171:VAL:HG11	2.52	0.45
7:AJ:339:SER:OG	7:AJ:344:VAL:HG11	2.17	0.45
13:M:331:ILE:N	13:M:331:ILE:HD12	2.32	0.45
5:b:446:TYR:C	5:b:447:HIS:CG	2.94	0.45
3:2:812:TYR:CZ	3:2:935:LYS:HE2	2.53	0.44
1:8:77:TYR:CE2	1:8:102:HIS:CD2	3.06	0.44
3:r:857:ALA:HB2	3:r:891:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:z:260:MET:HE2	5:z:260:MET:HA	1.98	0.44
6:AF:11:THR:O	6:AF:15:VAL:HG23	2.17	0.44
7:AJ:509:GLU:OE1	7:AL:472:ARG:NH2	2.47	0.44
7:AK:473:ILE:HD12	7:AK:473:ILE:N	2.32	0.44
7:AL:124:GLU:O	7:AL:133:ARG:N	2.46	0.44
7:AM:48:ASN:OD1	7:AM:323:LYS:NZ	2.50	0.44
8:B:43:ASP:CG	8:B:47:LYS:HZ2	2.25	0.44
13:L:342:GLU:C	13:L:343:ILE:HD12	2.43	0.44
3:u:812:TYR:CE1	3:u:935:LYS:HE2	2.52	0.44
6:AC:14:THR:OG1	6:AC:99:LEU:HD13	2.18	0.44
7:AI:404:ARG:CG	13:L:96:PRO:HG2	2.47	0.44
7:AI:509:GLU:HG2	7:AI:513:ILE:HD12	2.00	0.44
7:AK:460:ILE:HD12	7:AK:460:ILE:N	2.32	0.44
9:C:398:LYS:NZ	9:C:402:GLU:OE2	2.43	0.44
12:I:48:GLU:OE1	12:I:51:LYS:NZ	2.25	0.44
13:K:59:ILE:HD12	14:O:63:PHE:CZ	2.51	0.44
13:M:63:ILE:N	13:M:63:ILE:HD12	2.33	0.44
13:M:270:ILE:N	13:M:270:ILE:HD12	2.32	0.44
14:O:459:ASN:HB2	2:h:169:PHE:CE2	2.53	0.44
2:T:112:LEU:HD23	2:T:112:LEU:HA	1.92	0.44
3:r:791:VAL:HG23	3:r:793:PRO:CD	2.47	0.44
3:2:176:LYS:CD	3:2:176:LYS:H	2.30	0.44
3:4:945:GLU:CD	3:4:945:GLU:H	2.25	0.44
7:AK:517:THR:HG22	7:AK:517:THR:O	2.17	0.44
7:AL:517:THR:O	7:AL:517:THR:HG22	2.17	0.44
9:C:702:TYR:CD1	9:C:702:TYR:N	2.86	0.44
2:Y:134:LYS:HE2	2:Y:136:ASN:O	2.17	0.44
5:b:597:THR:C	5:b:599:THR:H	2.25	0.44
3:r:267:VAL:HB	3:r:378:TRP:CD1	2.53	0.44
2:1:103:LEU:HD11	2:1:122:PHE:CD2	2.52	0.44
6:AC:89:ASP:OD1	6:AC:90:ILE:N	2.48	0.44
9:C:44:THR:HG23	9:C:97:GLN:NE2	2.32	0.44
3:7:200:PHE:CE1	3:7:214:VAL:HG11	2.52	0.44
3:7:780:ILE:HD12	3:7:967:THR:HG21	1.99	0.44
10:E:107:ASN:OD1	10:E:112:ASN:ND2	2.48	0.44
3:r:90:TYR:CD2	3:r:90:TYR:C	2.95	0.44
3:u:405:ALA:HB2	3:u:428:MET:SD	2.58	0.44
1:0:343:TRP:CD1	1:0:434:TRP:HE1	2.36	0.44
3:4:511:PHE:CG	3:4:535:ALA:HB3	2.53	0.44
11:G:162:ARG:O	11:G:165:VAL:HG12	2.17	0.44
3:2:1072:PHE:N	3:2:1107:PHE:CD1	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AJ:509:GLU:HG2	7:AJ:513:ILE:HD12	2.00	0.44
2:k:26:THR:HB	2:k:55:TYR:CD2	2.53	0.44
3:3:265:SER:HB2	3:3:266:PRO:HA	2.00	0.44
3:7:865:PHE:C	3:7:867:ASP:H	2.26	0.44
7:AK:509:GLU:OE1	7:AM:472:ARG:NH2	2.45	0.44
9:C:404:PHE:O	9:C:408:GLY:N	2.48	0.44
14:N:556:PHE:CE1	14:N:671:ILE:HG21	2.52	0.44
2:T:19:LYS:HE2	2:T:19:LYS:HA	1.99	0.44
5:c:272:VAL:HG21	5:c:328:PHE:CE1	2.53	0.44
3:r:47:LEU:C	3:r:47:LEU:HD23	2.43	0.44
9:C:412:GLU:OE1	9:C:412:GLU:N	2.44	0.43
13:K:84:GLN:NE2	13:K:126:GLU:OE1	2.50	0.43
2:T:147:THR:HG23	2:U:7:ASN:HB3	1.99	0.43
2:U:91:GLU:CD	2:U:91:GLU:N	2.76	0.43
3:4:201:SER:HB3	3:4:456:ALA:H	1.82	0.43
1:8:343:TRP:CD1	1:8:434:TRP:HE1	2.36	0.43
1:9:8:ILE:HD12	1:9:8:ILE:H	1.84	0.43
7:AN:536:LYS:NZ	7:AN:541:GLU:OE1	2.48	0.43
9:C:486:LEU:HD11	9:C:506:TYR:CG	2.53	0.43
2:Y:150:PHE:CE2	2:Y:171:VAL:HG11	2.54	0.43
3:r:553:THR:HG22	3:r:555:ALA:H	1.83	0.43
5:z:131:LYS:HE2	5:z:395:TRP:CG	2.53	0.43
3:2:176:LYS:H	3:2:176:LYS:HD2	1.83	0.43
1:8:341:GLU:HA	1:8:453:ILE:HD13	2.01	0.43
5:AA:216:TRP:CD1	5:AA:258:PHE:CE2	3.06	0.43
7:AI:571:PHE:CE1	12:H:203:TYR:HB2	2.53	0.43
7:AJ:46:GLU:O	7:AJ:49:THR:OG1	2.36	0.43
14:O:177:ASP:C	14:O:179:ALA:H	2.26	0.43
1:0:106:LEU:C	1:8:60:THR:HG23	2.43	0.43
3:4:201:SER:CB	3:4:456:ALA:H	2.31	0.43
7:AK:517:THR:HA	7:AM:568:ILE:HG23	1.99	0.43
8:B:21:PHE:CE1	8:B:32:LYS:HD2	2.54	0.43
14:O:61:ASP:OD1	14:O:71:ARG:NH1	2.45	0.43
3:u:517:ALA:HB1	3:u:524:PHE:CE1	2.53	0.43
3:7:186:TYR:CD1	3:7:186:TYR:C	2.96	0.43
7:AI:339:SER:OG	7:AI:344:VAL:HG11	2.18	0.43
7:AL:93:GLU:OE1	7:AL:93:GLU:N	2.48	0.43
13:K:42:LEU:C	13:K:42:LEU:HD13	2.43	0.43
5:a:549:TRP:CH2	5:a:551:ARG:HA	2.53	0.43
3:4:857:ALA:HA	3:4:891:TRP:CD1	2.53	0.43
6:AD:43:GLU:CD	11:F:31:VAL:HG13	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AK:172:ASP:O	7:AK:176:GLN:N	2.44	0.43
7:AL:172:ASP:O	7:AL:176:GLN:N	2.45	0.43
9:C:203:SER:O	9:C:256:LYS:HE2	2.19	0.43
14:O:103:LYS:NZ	14:O:111:ILE:O	2.44	0.43
3:q:947:ALA:HB3	3:q:1022:PHE:CB	2.48	0.43
3:s:813:PHE:CZ	3:s:890:MET:HE3	2.53	0.43
3:u:526:ILE:HD13	3:u:535:ALA:HB1	2.00	0.43
2:T:107:ILE:HD12	2:T:107:ILE:N	2.34	0.43
2:T:116:THR:HG22	2:T:158:ASN:HA	2.00	0.43
5:c:66:ALA:HB1	5:c:67:PRO:CD	2.48	0.43
3:r:963:VAL:HG13	3:r:965:MET:HE2	2.01	0.43
3:3:981:LYS:HE3	3:3:998:TRP:CE2	2.54	0.43
3:4:957:VAL:HG12	3:4:958:SER:N	2.33	0.43
4:A:29:ALA:HB3	4:A:92:ILE:HD13	2.01	0.43
5:AB:101:LYS:HE2	5:AB:103:TYR:CZ	2.53	0.43
14:N:156:VAL:CG2	2:P:158:ASN:HB3	2.49	0.43
3:r:286:ARG:CZ	3:r:336:TRP:CD1	3.01	0.43
3:3:507:PHE:CE2	3:3:1055:ILE:HD11	2.54	0.43
5:AA:177:THR:HG22	5:z:399:GLN:HE22	1.84	0.43
7:AM:431:THR:HG23	7:AM:432:PHE:N	2.34	0.43
12:I:55:ARG:C	12:I:56:LEU:HD12	2.43	0.43
12:I:174:ILE:O	12:I:178:VAL:HG23	2.18	0.43
13:J:198:ARG:NH2	13:J:210:VAL:O	2.52	0.43
13:L:13:LEU:HD12	13:L:41:SER:OG	2.19	0.43
2:X:151:PHE:O	2:Y:2:ALA:HA	2.19	0.43
3:7:186:TYR:C	3:7:188:GLU:H	2.27	0.43
3:7:262:LEU:HD22	3:7:400:TYR:CE1	2.54	0.43
6:AD:89:ASP:OD1	6:AD:90:ILE:N	2.48	0.43
6:AF:94:LEU:N	6:AF:94:LEU:HD12	2.34	0.43
10:E:128:ARG:O	10:E:132:ASN:ND2	2.48	0.43
2:j:24:TYR:CE1	2:j:126:LEU:HD11	2.54	0.43
3:u:812:TYR:CD1	3:u:935:LYS:HE2	2.54	0.43
3:v:726:GLU:HB2	3:v:729:THR:HG21	2.00	0.43
3:6:793:PRO:CG	3:6:926:TRP:CH2	3.02	0.42
3:7:70:GLU:H	3:7:70:GLU:CD	2.27	0.42
6:AE:94:LEU:N	6:AE:94:LEU:HD12	2.34	0.42
7:AI:470:PHE:CE2	12:I:9:GLN:OE1	2.71	0.42
7:AM:93:GLU:OE1	7:AM:93:GLU:N	2.47	0.42
13:J:347:LEU:N	13:J:347:LEU:HD22	2.34	0.42
2:R:25:LEU:HD22	2:R:105:SER:HB3	1.99	0.42
2:n:24:TYR:HB2	2:n:126:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:r:965:MET:HE3	3:r:1038:THR:O	2.19	0.42
7:AK:13:ARG:NH2	7:AL:461:GLU:OE1	2.44	0.42
2:T:149:LEU:HD23	2:T:150:PHE:CE2	2.55	0.42
2:Z:125:ASP:O	2:Z:146:GLY:HA3	2.19	0.42
7:AK:435:LEU:HG	7:AK:437:VAL:HG23	2.01	0.42
8:B:8:LYS:HA	8:B:11:ILE:HB	2.01	0.42
10:E:50:LEU:O	10:E:54:VAL:HG23	2.19	0.42
13:J:76:ARG:NE	13:J:133:CYS:O	2.47	0.42
14:N:174:VAL:O	2:P:163:THR:HA	2.19	0.42
14:O:459:ASN:OD1	2:h:154:LYS:HE2	2.19	0.42
2:Z:101:VAL:HB	2:Z:171:VAL:HG22	2.00	0.42
3:r:265:SER:HB2	3:r:378:TRP:CZ3	2.55	0.42
3:t:1072:PHE:HB2	3:t:1107:PHE:CD1	2.54	0.42
3:6:812:TYR:CE2	3:6:935:LYS:HE2	2.54	0.42
3:7:64:LEU:H	3:7:79:GLY:CA	2.33	0.42
5:AA:324:LYS:HE2	5:AA:326:TYR:CE1	2.55	0.42
6:AG:11:THR:O	6:AG:15:VAL:HG23	2.19	0.42
7:AK:459:SER:C	7:AK:460:ILE:HD12	2.44	0.42
3:u:511:PHE:CE1	3:u:535:ALA:HB2	2.54	0.42
3:2:1076:GLY:HA2	3:2:1134:GLU:CD	2.45	0.42
6:AD:14:THR:OG1	6:AD:99:LEU:HD13	2.18	0.42
7:AI:185:VAL:HG23	7:AI:190:VAL:HG21	2.02	0.42
7:AJ:251:VAL:HG23	7:AJ:252:PHE:N	2.35	0.42
7:AK:90:MET:HE1	7:AK:326:LYS:CB	2.47	0.42
7:AN:384:LEU:HD21	7:AN:389:VAL:CG1	2.50	0.42
13:L:225:ASP:N	13:L:229:ASN:O	2.44	0.42
14:N:12:LEU:O	14:N:14:ARG:NH2	2.53	0.42
3:t:24:LEU:HB3	3:u:10:TYR:CE1	2.55	0.42
3:2:748:ILE:HD13	3:2:749:ARG:H	1.83	0.42
3:5:405:ALA:HB3	3:5:426:ASN:O	2.20	0.42
3:5:744:ILE:HG23	3:5:745:PRO:HD2	2.01	0.42
8:B:45:TYR:CD1	8:B:45:TYR:C	2.97	0.42
10:D:128:ARG:O	10:D:132:ASN:ND2	2.45	0.42
13:K:1:MET:HE1	13:K:47:PHE:CE2	2.55	0.42
14:N:548:ARG:H	14:N:548:ARG:HD3	1.85	0.42
2:S:91:GLU:CD	2:S:91:GLU:N	2.74	0.42
3:r:306:LYS:HE3	3:r:308:TRP:CG	2.55	0.42
3:u:109:LYS:HE3	3:u:148:THR:HG21	2.01	0.42
3:2:981:LYS:HD3	3:2:981:LYS:C	2.45	0.42
3:7:707:LEU:HD12	3:7:758:LYS:HE2	2.02	0.42
7:AK:207:ILE:HD13	7:AK:220:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:28:ARG:HG3	8:B:28:ARG:HH21	1.85	0.42
12:I:50:MET:HE1	13:L:115:LEU:HB3	2.01	0.42
5:b:77:ARG:HH22	5:b:79:ASP:CG	2.28	0.42
3:r:501:LEU:CD1	3:s:501:LEU:HD11	2.50	0.42
3:t:1150:ARG:HE	3:t:1152:GLU:CD	2.28	0.42
5:z:14:LEU:H	5:z:14:LEU:CD1	2.32	0.42
3:4:594:VAL:HG22	3:4:843:GLU:CD	2.45	0.42
3:5:1072:PHE:HB2	3:5:1107:PHE:CE1	2.54	0.42
3:6:363:LYS:HA	3:6:363:LYS:HE3	2.01	0.42
7:AI:251:VAL:HG23	7:AI:252:PHE:N	2.35	0.42
8:B:49:VAL:HA	8:B:52:ARG:CG	2.50	0.42
14:N:35:GLU:O	14:N:39:VAL:HG23	2.19	0.42
5:b:18:TYR:CD1	5:b:18:TYR:C	2.98	0.42
3:s:171:ASN:C	3:s:173:GLU:H	2.28	0.42
3:u:992:THR:H	3:u:995:GLN:NE2	2.18	0.42
3:3:603:ASN:HD21	3:3:769:THR:HG22	1.84	0.42
6:AD:43:GLU:HG2	11:F:31:VAL:HG12	2.01	0.42
7:AI:549:ASP:OD2	7:AI:564:THR:OG1	2.25	0.42
7:AK:355:ARG:NH1	7:AK:360:GLU:OE1	2.53	0.42
7:AL:207:ILE:HD13	7:AL:220:LEU:HD23	2.02	0.42
7:AN:315:GLU:OE1	7:AN:315:GLU:N	2.53	0.42
8:B:16:ASP:OD2	8:B:32:LYS:HE2	2.19	0.42
13:M:202:LEU:CD2	13:M:210:VAL:HG12	2.50	0.42
14:N:550:ILE:HD11	14:N:565:ILE:HB	2.00	0.42
2:V:125:ASP:O	2:V:146:GLY:HA3	2.20	0.42
2:f:32:PRO:HA	2:f:118:ARG:NE	2.34	0.42
3:2:247:GLU:CD	3:2:272:ARG:HH12	2.28	0.42
3:3:31:LEU:HB2	14:N:130:LEU:HD21	2.01	0.42
3:7:306:LYS:HE3	3:7:308:TRP:CG	2.54	0.42
5:AA:449:PHE:CD1	5:AA:451:CYS:SG	3.13	0.42
14:N:733:SER:HB2	2:U:37:THR:HG23	2.02	0.42
3:v:1057:MET:HE2	3:v:1062:TYR:CD1	2.55	0.42
5:z:184:ARG:HD3	5:z:395:TRP:CZ2	2.55	0.42
3:5:326:PHE:HB3	3:5:336:TRP:CE3	2.55	0.41
7:AJ:153:ILE:HG22	7:AJ:248:VAL:O	2.20	0.41
7:AL:79:ASN:OD1	7:AL:82:TYR:N	2.49	0.41
7:AL:584:THR:HG23	12:I:199:GLN:HG2	2.02	0.41
7:AM:315:GLU:OE1	7:AM:315:GLU:N	2.53	0.41
3:q:947:ALA:HB3	3:q:1022:PHE:HB3	2.02	0.41
3:q:1062:TYR:CZ	3:q:1125:LEU:HB2	2.55	0.41
3:s:548:ILE:CG1	3:s:553:THR:HG21	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:u:300:THR:HG21	3:u:358:ARG:HD2	2.01	0.41
3:3:66:PHE:HB2	3:3:74:LEU:HD11	2.02	0.41
3:5:406:ARG:HA	3:5:431:VAL:HG21	2.02	0.41
5:AB:52:ILE:HG23	5:AB:58:TYR:CE1	2.55	0.41
7:AJ:48:ASN:OD1	7:AJ:323:LYS:NZ	2.49	0.41
7:AN:431:THR:HG23	7:AN:432:PHE:N	2.35	0.41
11:G:131:GLN:OE1	11:G:131:GLN:N	2.48	0.41
12:I:86:VAL:HG22	12:I:86:VAL:O	2.20	0.41
13:M:58:GLY:O	13:M:62:GLY:N	2.50	0.41
3:r:813:PHE:CZ	3:r:890:MET:SD	3.14	0.41
3:s:597:LEU:HG	3:s:766:THR:HG21	2.02	0.41
3:s:955:LYS:HE2	3:s:993:PHE:CE2	2.55	0.41
3:u:336:TRP:CH2	3:u:343:PRO:HD3	2.55	0.41
3:2:336:TRP:C	3:2:338:PRO:HD2	2.45	0.41
6:AD:90:ILE:HG23	6:AD:109:GLY:HA2	2.02	0.41
6:AH:19:ILE:HG23	6:AH:19:ILE:O	2.20	0.41
7:AJ:185:VAL:HG23	7:AJ:190:VAL:HG21	2.02	0.41
7:AL:228:LEU:HD21	7:AL:253:GLY:HA3	2.01	0.41
7:AL:459:SER:C	7:AL:460:ILE:HD12	2.44	0.41
10:D:110:VAL:HG21	11:F:261:VAL:HG11	2.02	0.41
13:L:106:GLN:OE1	13:L:106:GLN:N	2.43	0.41
13:L:284:ILE:HG22	13:L:345:VAL:HG21	2.01	0.41
2:Q:167:GLU:N	2:Q:167:GLU:CD	2.78	0.41
3:r:336:TRP:CH2	3:r:343:PRO:HD3	2.55	0.41
2:1:150:PHE:CE1	2:1:171:VAL:HG11	2.55	0.41
3:4:421:LEU:HD12	3:4:422:PRO:HD2	2.03	0.41
3:4:981:LYS:HE2	3:4:998:TRP:CD2	2.56	0.41
6:AG:113:ASN:ND2	6:AG:132:SER:OG	2.46	0.41
7:AK:228:LEU:HD21	7:AK:253:GLY:HA3	2.01	0.41
8:B:51:ILE:HD12	8:B:51:ILE:C	2.46	0.41
2:f:78:ILE:N	2:f:78:ILE:HD12	2.36	0.41
3:v:549:ILE:HD11	3:v:953:PRO:HD3	2.01	0.41
3:2:409:SER:HB3	3:2:411:PHE:CZ	2.56	0.41
3:4:90:TYR:CD1	3:4:90:TYR:C	2.98	0.41
3:6:949:ILE:HD11	3:6:1022:PHE:CG	2.55	0.41
4:A:304:THR:HG22	4:A:305:ASP:N	2.36	0.41
5:AB:45:PHE:HA	5:AB:48:ILE:HD12	2.02	0.41
6:AD:43:GLU:OE2	11:F:32:ASN:N	2.52	0.41
7:AM:384:LEU:HD21	7:AM:389:VAL:CG1	2.50	0.41
7:AN:355:ARG:NH1	7:AN:360:GLU:OE1	2.53	0.41
10:D:14:PHE:C	10:D:15:LEU:HD12	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:173:VAL:O	11:F:173:VAL:HG22	2.21	0.41
13:M:232:ASP:OD1	13:M:235:LYS:NZ	2.51	0.41
2:P:91:GLU:N	2:P:91:GLU:CD	2.78	0.41
2:V:25:LEU:HD12	2:V:121:GLY:O	2.20	0.41
2:Z:69:SER:HB2	2:Z:70:PRO:HD3	2.03	0.41
1:y:386:THR:HG21	1:y:407:PHE:CE2	2.56	0.41
3:2:39:MET:SD	3:2:39:MET:C	3.03	0.41
3:3:1071:ALA:HA	3:3:1107:PHE:CZ	2.55	0.41
7:AL:435:LEU:HG	7:AL:437:VAL:HG23	2.01	0.41
7:AM:21:ASP:OD1	7:AM:22:THR:N	2.53	0.41
9:C:450:THR:HG23	9:C:452:ASP:OD1	2.21	0.41
10:E:131:LEU:C	10:E:131:LEU:HD23	2.46	0.41
14:N:200:TYR:HE1	2:R:164:THR:HG23	1.85	0.41
14:O:72:LYS:NZ	14:O:74:ASP:OD1	2.54	0.41
14:O:495:LYS:HB2	14:O:734:TRP:CH2	2.54	0.41
5:b:488:PHE:CE2	5:b:496:TYR:HB2	2.56	0.41
1:w:1:MET:HA	1:w:27:GLU:OE2	2.21	0.41
3:2:1054:ALA:HA	3:2:1125:LEU:O	2.20	0.41
3:3:543:VAL:HG22	3:3:1040:THR:HG23	2.02	0.41
3:4:1062:TYR:CE1	3:4:1122:ASN:HB3	2.56	0.41
7:AM:46:GLU:N	7:AM:51:TYR:OH	2.53	0.41
5:a:200:LEU:HD22	5:a:238:GLU:HB3	2.03	0.41
5:b:622:SER:HB2	5:b:625:GLU:CD	2.46	0.41
5:z:170:GLU:CD	5:z:181:LYS:HE2	2.45	0.41
3:4:539:TYR:CE1	3:4:961:ARG:NH2	2.88	0.41
3:6:66:PHE:CZ	3:7:922:ASN:ND2	2.89	0.41
7:AN:46:GLU:N	7:AN:51:TYR:OH	2.53	0.41
8:B:264:PRO:O	8:B:265:LYS:C	2.63	0.41
10:D:45:LEU:HD12	10:D:45:LEU:N	2.36	0.41
10:D:105:ILE:HG22	10:D:119:LEU:HD22	2.02	0.41
2:n:75:LYS:HE3	2:n:86:VAL:HG21	2.02	0.41
3:r:33:GLN:HG3	3:s:27:PRO:HA	2.03	0.41
3:u:186:TYR:CD2	3:u:190:GLY:HA3	2.56	0.41
5:z:281:PRO:HD3	5:z:321:THR:HG23	2.03	0.41
1:0:406:THR:HG22	1:0:422:PHE:CD2	2.55	0.41
3:5:405:ALA:HB3	3:5:427:ILE:HA	2.03	0.41
3:7:64:LEU:H	3:7:79:GLY:HA3	1.86	0.41
4:A:189:GLN:OE1	4:A:189:GLN:N	2.49	0.41
5:AA:416:GLU:C	5:AA:418:ASN:H	2.29	0.41
5:AB:216:TRP:CH2	5:AB:258:PHE:CZ	3.09	0.41
6:AC:72:ASN:O	6:AC:76:LEU:N	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AJ:475:ASP:OD1	7:AJ:476:ASP:N	2.50	0.41
7:AN:21:ASP:OD1	7:AN:22:THR:N	2.53	0.41
7:AN:93:GLU:OE1	7:AN:93:GLU:N	2.47	0.41
8:B:27:GLU:H	8:B:27:GLU:CD	2.28	0.41
9:C:675:LYS:HE3	9:C:676:TYR:CZ	2.56	0.41
11:F:131:GLN:OE1	11:F:131:GLN:N	2.49	0.41
13:L:315:ASP:OD1	13:L:316:VAL:HG23	2.21	0.41
14:N:702:PHE:CE2	14:N:709:ILE:HD11	2.56	0.41
2:Q:12:LEU:C	2:Q:12:LEU:HD23	2.45	0.41
2:U:103:LEU:HD11	2:U:122:PHE:CD2	2.56	0.41
3:r:298:ASN:C	3:r:300:THR:H	2.28	0.41
3:r:1031:LEU:HD23	3:r:1032:MET:N	2.34	0.41
1:w:170:PHE:CD2	1:w:172:MET:CE	3.04	0.41
3:3:1125:LEU:CD2	3:3:1149:THR:HG21	2.51	0.41
3:5:854:SER:HB3	3:5:859:ALA:CB	2.51	0.41
5:AA:165:VAL:C	5:AA:184:ARG:HH11	2.29	0.41
7:AI:569:ARG:O	12:H:166:ASN:HB2	2.20	0.41
7:AJ:435:LEU:HD22	7:AJ:460:ILE:HD13	2.03	0.41
9:C:447:LYS:NZ	9:C:466:ASP:OD2	2.46	0.41
13:J:197:VAL:HG13	13:J:242:LEU:HD21	2.03	0.41
13:K:226:ARG:NH2	13:K:294:ASN:OD1	2.47	0.41
14:O:176:TYR:OH	2:e:157:GLN:CD	2.55	0.41
2:i:29:LYS:HE3	2:i:33:TRP:CE3	2.55	0.41
2:o:101:VAL:HB	2:o:171:VAL:HG22	2.03	0.41
3:t:890:MET:SD	3:t:934:LEU:HD11	2.60	0.41
3:t:1062:TYR:CE1	3:t:1122:ASN:HB2	2.56	0.41
3:2:769:THR:HG22	3:2:769:THR:O	2.22	0.40
3:4:336:TRP:CZ3	3:4:343:PRO:HD3	2.55	0.40
3:6:966:SER:HB3	3:6:1037:LEU:HD13	2.03	0.40
1:8:443:ASN:HD21	1:8:447:GLN:NE2	2.19	0.40
6:AG:67:ARG:NH2	6:AG:115:TYR:HH	2.18	0.40
6:AH:11:THR:O	6:AH:15:VAL:HG23	2.21	0.40
7:AJ:94:ASP:OD1	7:AJ:323:LYS:NZ	2.46	0.40
11:F:188:LEU:HD21	11:F:252:LEU:HD11	2.04	0.40
2:m:101:VAL:HB	2:m:171:VAL:HG22	2.03	0.40
3:4:1069:TYR:CZ	3:4:1110:TYR:HB2	2.56	0.40
5:AB:606:VAL:HG12	5:AB:624:ASN:HA	2.03	0.40
11:F:261:VAL:HG22	11:F:262:SER:N	2.36	0.40
2:R:91:GLU:N	2:R:91:GLU:CD	2.79	0.40
2:W:103:LEU:HD11	2:W:122:PHE:CD2	2.57	0.40
2:Y:103:LEU:HD11	2:Y:122:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:a:385:GLU:CD	5:a:385:GLU:H	2.28	0.40
3:u:920:SER:HB2	3:u:926:TRP:CD2	2.56	0.40
6:AC:90:ILE:HG23	6:AC:109:GLY:HA2	2.03	0.40
7:AJ:107:ILE:N	7:AJ:107:ILE:HD12	2.37	0.40
14:N:705:ILE:O	2:V:113:PRO:CB	2.69	0.40
5:b:156:VAL:HG22	5:b:171:PHE:CD1	2.56	0.40
3:q:992:THR:H	3:q:995:GLN:NE2	2.18	0.40
3:r:708:PHE:CZ	3:r:744:ILE:HG23	2.57	0.40
3:v:556:HIS:C	3:v:557:ILE:HD12	2.47	0.40
3:2:309:THR:HB	3:2:311:THR:HG23	2.03	0.40
3:3:1125:LEU:HD22	3:3:1149:THR:HG21	2.04	0.40
3:4:969:LEU:HD23	3:4:970:THR:C	2.45	0.40
3:7:920:SER:HB2	3:7:926:TRP:CE3	2.56	0.40
1:8:139:SER:CB	1:9:126:ILE:HG21	2.50	0.40
6:AG:19:ILE:O	6:AG:19:ILE:HG23	2.21	0.40
7:AI:153:ILE:HG22	7:AI:248:VAL:O	2.21	0.40
7:AI:570:SER:HA	12:H:164:GLY:O	2.21	0.40
7:AK:582:GLN:HE21	12:H:199:GLN:HG2	1.85	0.40
8:B:44:MET:SD	8:B:47:LYS:HD2	2.61	0.40
11:G:240:THR:HG22	11:G:240:THR:O	2.21	0.40
13:J:204:ILE:HG13	13:J:238:ILE:HD13	2.03	0.40
14:N:337:LEU:H	14:N:338:GLN:NE2	2.19	0.40
14:O:162:ILE:HG21	14:O:172:LEU:HD13	2.03	0.40
2:R:33:TRP:CD1	2:R:118:ARG:HD3	2.57	0.40
2:h:72:ASP:HA	2:h:75:LYS:HD3	2.04	0.40
3:q:251:THR:HG21	3:q:261:SER:H	1.86	0.40
3:q:755:VAL:HG23	3:q:767:THR:HA	2.02	0.40
3:q:830:MET:SD	3:q:878:ALA:HB2	2.61	0.40
3:t:1139:ARG:HG3	3:t:1139:ARG:HH21	1.85	0.40
3:u:1008:ASP:CG	3:u:1139:ARG:HH22	2.28	0.40
3:v:812:TYR:CZ	3:v:935:LYS:HE2	2.57	0.40
1:y:117:TYR:CD1	1:y:117:TYR:N	2.90	0.40
5:z:3:PHE:CE2	5:z:5:TYR:HB2	2.56	0.40
3:6:192:TYR:CG	3:7:468:MET:HE1	2.56	0.40
3:6:336:TRP:CZ3	3:6:343:PRO:HD3	2.57	0.40
3:6:981:LYS:HE2	3:6:998:TRP:CD1	2.56	0.40
6:AD:67:ARG:NH2	6:AD:115:TYR:OH	2.55	0.40
7:AI:464:ARG:NH1	12:I:11:GLU:CB	2.85	0.40
9:C:440:LEU:O	9:C:440:LEU:HD23	2.22	0.40
13:K:110:GLN:OE1	13:K:110:GLN:N	2.55	0.40
13:L:268:VAL:HG22	13:L:321:VAL:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:101:LYS:HB2	5:b:111:TRP:CD2	2.57	0.40
5:z:485:LYS:C	5:z:486:LEU:HD12	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	456/458 (100%)	412 (90%)	43 (9%)	1 (0%)	43	77
1	8	456/458 (100%)	419 (92%)	34 (8%)	3 (1%)	18	56
1	9	456/458 (100%)	419 (92%)	35 (8%)	2 (0%)	30	67
1	w	456/458 (100%)	419 (92%)	35 (8%)	2 (0%)	30	67
1	x	456/458 (100%)	416 (91%)	37 (8%)	3 (1%)	18	56
1	y	456/458 (100%)	421 (92%)	34 (8%)	1 (0%)	43	77
2	1	170/173 (98%)	149 (88%)	18 (11%)	3 (2%)	6	34
2	P	157/173 (91%)	151 (96%)	6 (4%)	0	100	100
2	Q	159/173 (92%)	152 (96%)	7 (4%)	0	100	100
2	R	158/173 (91%)	150 (95%)	8 (5%)	0	100	100
2	S	170/173 (98%)	154 (91%)	16 (9%)	0	100	100
2	T	170/173 (98%)	156 (92%)	12 (7%)	2 (1%)	10	43
2	U	170/173 (98%)	153 (90%)	14 (8%)	3 (2%)	6	34
2	V	170/173 (98%)	148 (87%)	17 (10%)	5 (3%)	3	23
2	W	170/173 (98%)	154 (91%)	14 (8%)	2 (1%)	10	43
2	X	170/173 (98%)	150 (88%)	16 (9%)	4 (2%)	4	27
2	Y	170/173 (98%)	153 (90%)	15 (9%)	2 (1%)	10	43
2	Z	170/173 (98%)	149 (88%)	19 (11%)	2 (1%)	10	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	e	159/173 (92%)	155 (98%)	4 (2%)	0	100	100
2	f	158/173 (91%)	153 (97%)	4 (2%)	1 (1%)	21	59
2	g	159/173 (92%)	152 (96%)	7 (4%)	0	100	100
2	h	170/173 (98%)	161 (95%)	8 (5%)	1 (1%)	21	59
2	i	146/173 (84%)	138 (94%)	8 (6%)	0	100	100
2	j	170/173 (98%)	157 (92%)	11 (6%)	2 (1%)	10	43
2	k	170/173 (98%)	152 (89%)	16 (9%)	2 (1%)	10	43
2	l	170/173 (98%)	161 (95%)	8 (5%)	1 (1%)	21	59
2	m	170/173 (98%)	161 (95%)	9 (5%)	0	100	100
2	n	170/173 (98%)	162 (95%)	8 (5%)	0	100	100
2	o	170/173 (98%)	159 (94%)	10 (6%)	1 (1%)	21	59
2	p	170/173 (98%)	161 (95%)	7 (4%)	2 (1%)	10	43
3	2	1056/1152 (92%)	920 (87%)	113 (11%)	23 (2%)	5	29
3	3	1056/1152 (92%)	910 (86%)	118 (11%)	28 (3%)	4	25
3	4	1056/1152 (92%)	910 (86%)	126 (12%)	20 (2%)	6	31
3	5	1056/1152 (92%)	908 (86%)	131 (12%)	17 (2%)	7	37
3	6	1056/1152 (92%)	934 (88%)	107 (10%)	15 (1%)	9	40
3	7	1056/1152 (92%)	889 (84%)	152 (14%)	15 (1%)	9	40
3	q	1056/1152 (92%)	898 (85%)	136 (13%)	22 (2%)	5	29
3	r	1056/1152 (92%)	923 (87%)	111 (10%)	22 (2%)	5	29
3	s	1056/1152 (92%)	907 (86%)	123 (12%)	26 (2%)	4	26
3	t	1056/1152 (92%)	931 (88%)	107 (10%)	18 (2%)	7	36
3	u	1056/1152 (92%)	930 (88%)	109 (10%)	17 (2%)	7	37
3	v	1056/1152 (92%)	931 (88%)	112 (11%)	13 (1%)	10	43
4	A	307/848 (36%)	300 (98%)	7 (2%)	0	100	100
5	AA	638/640 (100%)	582 (91%)	53 (8%)	3 (0%)	24	63
5	AB	638/640 (100%)	574 (90%)	57 (9%)	7 (1%)	11	46
5	a	638/640 (100%)	564 (88%)	68 (11%)	6 (1%)	14	50
5	b	638/640 (100%)	574 (90%)	58 (9%)	6 (1%)	14	50
5	c	638/640 (100%)	566 (89%)	66 (10%)	6 (1%)	14	50
5	z	638/640 (100%)	580 (91%)	49 (8%)	9 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AC	137/142 (96%)	137 (100%)	0	0	100	100
6	AD	137/142 (96%)	137 (100%)	0	0	100	100
6	AE	137/142 (96%)	136 (99%)	1 (1%)	0	100	100
6	AF	137/142 (96%)	136 (99%)	1 (1%)	0	100	100
6	AG	137/142 (96%)	136 (99%)	1 (1%)	0	100	100
6	AH	137/142 (96%)	136 (99%)	1 (1%)	0	100	100
7	AI	546/587 (93%)	534 (98%)	12 (2%)	0	100	100
7	AJ	546/587 (93%)	536 (98%)	10 (2%)	0	100	100
7	AK	545/587 (93%)	531 (97%)	14 (3%)	0	100	100
7	AL	545/587 (93%)	531 (97%)	14 (3%)	0	100	100
7	AM	336/587 (57%)	329 (98%)	7 (2%)	0	100	100
7	AN	336/587 (57%)	329 (98%)	7 (2%)	0	100	100
8	B	288/295 (98%)	252 (88%)	28 (10%)	8 (3%)	4	24
9	C	713/808 (88%)	685 (96%)	27 (4%)	1 (0%)	48	83
10	D	156/174 (90%)	154 (99%)	2 (1%)	0	100	100
10	E	150/174 (86%)	150 (100%)	0	0	100	100
11	F	234/263 (89%)	231 (99%)	3 (1%)	0	100	100
11	G	233/263 (89%)	232 (100%)	1 (0%)	0	100	100
12	H	210/234 (90%)	205 (98%)	5 (2%)	0	100	100
12	I	211/234 (90%)	207 (98%)	4 (2%)	0	100	100
13	J	346/348 (99%)	342 (99%)	4 (1%)	0	100	100
13	K	346/348 (99%)	342 (99%)	3 (1%)	1 (0%)	36	72
13	L	346/348 (99%)	338 (98%)	8 (2%)	0	100	100
13	M	346/348 (99%)	343 (99%)	3 (1%)	0	100	100
14	N	713/1019 (70%)	667 (94%)	44 (6%)	2 (0%)	36	72
14	O	713/1019 (70%)	672 (94%)	37 (5%)	4 (1%)	21	59
15	d	69/124 (56%)	60 (87%)	8 (12%)	1 (1%)	9	40
All	All	32279/35785 (90%)	29416 (91%)	2528 (8%)	335 (1%)	15	48

All (335) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	93	ALA

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Mol	Chain	Res	Type
3	2	453	SER
3	2	590	ASN
3	2	997	LYS
3	3	356	ASN
3	4	173	GLU
3	4	453	SER
3	4	791	VAL
3	4	1105	ASN
3	5	150	ASN
3	5	791	VAL
3	6	176	LYS
3	6	973	ARG
3	7	589	PRO
3	7	930	GLN
5	AB	530	GLU
14	O	237	HIS
2	T	93	ALA
2	U	93	ALA
2	V	93	ALA
2	V	114	LEU
2	W	93	ALA
5	a	68	SER
5	a	581	SER
5	b	357	SER
5	c	431	ASN
2	j	93	ALA
2	k	93	ALA
2	l	93	ALA
2	o	93	ALA
3	q	94	ASP
3	q	242	ASP
3	q	453	SER
3	q	1026	ARG
3	s	27	PRO
3	s	84	ASN
3	s	746	ALA
3	t	515	ASP
3	t	589	PRO
3	t	793	PRO
3	u	171	ASN
3	v	793	PRO
5	z	49	LEU

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Mol	Chain	Res	Type
5	z	204	PRO
3	2	3	ILE
3	2	243	LEU
3	2	428	MET
3	2	452	ASP
3	3	171	ASN
3	3	173	GLU
3	3	207	ASP
3	3	297	SER
3	3	781	ILE
3	4	4	ASN
3	4	452	ASP
3	4	760	ALA
3	5	84	ASN
3	5	216	ASP
3	5	452	ASP
3	5	515	ASP
3	5	922	ASN
3	6	57	ASP
3	6	171	ASN
3	6	333	THR
3	6	436	ASN
3	6	697	LEU
3	6	972	GLU
3	6	1001	ILE
3	7	217	ALA
3	7	838	LYS
8	B	135	GLU
13	K	216	THR
14	O	694	ASN
2	U	98	ALA
2	U	111	GLU
2	X	111	GLU
2	Y	93	ALA
2	Z	93	ALA
5	a	624	ASN
5	b	83	VAL
15	d	56	GLU
2	p	93	ALA
3	q	785	ARG
3	q	997	LYS
3	r	84	ASN

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Mol	Chain	Res	Type
3	r	426	ASN
3	r	789	ASN
3	r	791	VAL
3	s	262	LEU
3	s	339	GLN
3	s	426	ASN
3	s	452	ASP
3	s	559	GLY
3	s	791	VAL
3	t	791	VAL
3	t	1075	LYS
3	u	189	SER
3	u	819	LYS
3	u	972	GLU
3	v	512	ILE
3	v	930	GLN
3	v	973	ARG
2	1	92	ASN
3	2	4	ASN
3	2	339	GLN
3	2	390	PRO
3	2	402	TYR
3	2	426	ASN
3	2	709	ASP
3	2	972	GLU
3	3	189	SER
3	3	361	ALA
3	3	426	ASN
3	3	697	LEU
3	4	256	SER
3	4	276	GLN
3	4	339	GLN
3	4	376	LYS
3	4	428	MET
3	4	960	ASP
3	5	1075	LYS
3	5	1101	THR
3	5	1144	ARG
3	6	248	ASN
3	6	454	ASP
3	7	172	ALA
3	7	173	GLU

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Mol	Chain	Res	Type
3	7	240	SER
3	7	426	ASN
3	7	997	LYS
1	9	106	LEU
5	AB	603	PRO
8	B	38	LYS
8	B	91	VAL
8	B	139	ASP
2	T	98	ALA
5	a	340	SER
5	c	190	GLU
2	f	98	ALA
3	q	27	PRO
3	q	383	THR
3	q	953	PRO
3	q	973	ARG
3	r	172	ALA
3	r	388	ALA
3	r	389	LYS
3	r	513	SER
3	r	926	TRP
3	s	241	TYR
3	s	357	LYS
3	s	379	TYR
3	s	1149	THR
3	t	425	PRO
3	t	428	MET
3	t	760	ALA
3	u	332	GLN
3	u	337	SER
3	u	388	ALA
3	u	725	SER
3	v	32	GLN
3	v	515	ASP
1	x	328	SER
5	z	14	LEU
5	z	68	SER
5	z	245	ASP
5	z	405	ASP
2	1	73	ASP
3	2	57	ASP
3	2	172	ALA

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Mol	Chain	Res	Type
3	2	322	GLN
3	2	330	ASP
3	2	385	SER
3	2	922	ASN
3	3	84	ASN
3	3	197	PHE
3	3	226	LYS
3	3	243	LEU
3	3	339	GLN
3	3	388	ALA
3	3	760	ALA
3	3	1118	SER
3	4	188	GLU
3	4	777	ALA
3	5	559	GLY
3	5	972	GLU
3	5	1054	ALA
3	6	434	PRO
3	6	922	ASN
3	6	923	ALA
3	7	241	TYR
3	7	931	ASN
3	7	1118	SER
5	AA	247	SER
5	AA	510	LEU
5	AB	82	ASN
5	AB	323	TRP
8	B	41	THR
8	B	133	GLU
14	N	300	LYS
14	N	533	ASN
2	V	98	ALA
2	X	93	ALA
2	X	110	ASP
2	Y	98	ALA
5	a	305	ASN
5	b	598	ARG
5	c	67	PRO
2	p	73	ASP
3	q	169	SER
3	q	250	SER
3	q	452	ASP

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Mol	Chain	Res	Type
3	q	559	GLY
3	r	287	GLY
3	r	299	ASN
3	r	330	ASP
3	r	546	PRO
3	s	19	ASP
3	s	344	SER
3	s	429	ARG
3	s	461	PHE
3	s	1104	ASN
3	t	84	ASN
3	t	310	GLU
3	t	452	ASP
3	t	923	ALA
3	t	953	PRO
3	t	1104	ASN
3	t	1145	LEU
3	u	452	ASP
3	v	389	LYS
1	w	94	MET
1	y	445	LYS
3	3	227	VAL
3	3	268	LYS
3	3	589	PRO
3	3	1104	ASN
3	4	957	VAL
3	4	1004	TYR
3	4	1106	GLU
3	5	426	ASN
3	6	332	GLN
1	8	109	SER
1	8	226	GLU
1	9	381	LYS
5	AB	53	PRO
5	AB	106	GLY
5	AB	256	ASN
8	B	22	ASP
9	C	715	PRO
2	W	71	GLU
2	Z	98	ALA
5	a	604	GLY
5	b	211	ILE

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Mol	Chain	Res	Type
5	b	285	LYS
5	b	578	SER
5	c	66	ALA
5	c	262	LYS
2	h	110	ASP
2	j	98	ALA
3	q	150	ASN
3	q	414	LYS
3	q	426	ASN
3	q	451	PRO
3	q	791	VAL
3	q	866	ASP
3	q	956	ASP
3	r	162	ASP
3	r	291	ASP
3	r	340	GLY
3	r	510	GLY
3	r	589	PRO
3	s	276	GLN
3	s	354	LYS
3	s	388	ALA
3	s	838	LYS
3	s	972	GLU
3	t	387	GLY
3	t	585	PRO
3	u	291	ASP
3	u	1105	ASN
3	v	428	MET
3	v	453	SER
3	v	974	THR
5	z	404	LYS
1	0	64	GLY
3	2	337	SER
3	2	451	PRO
3	4	291	ASP
3	5	388	ALA
3	7	837	ASN
1	8	24	ILE
5	AA	211	ILE
8	B	94	GLY
2	X	143	GLU
2	k	70	PRO

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Mol	Chain	Res	Type
3	q	972	GLU
3	u	27	PRO
3	u	760	ALA
3	v	589	PRO
1	w	58	GLY
1	x	341	GLU
5	z	211	ILE
3	3	791	VAL
3	4	313	PRO
3	7	791	VAL
14	O	362	VAL
3	r	970	THR
3	u	390	PRO
3	v	340	GLY
5	z	338	GLY
3	3	267	VAL
3	3	1088	GLY
3	5	510	GLY
5	c	52	ILE
3	r	1111	VAL
3	s	277	VAL
3	u	1081	PRO
3	v	817	GLY
3	3	215	VAL
3	3	287	GLY
3	5	792	ASP
3	7	836	PRO
14	O	550	ILE
2	V	108	VAL
3	r	1116	VAL
3	s	340	GLY
3	t	510	GLY
3	u	525	GLY
3	u	1011	GLY
3	2	873	GLY
2	V	70	PRO
3	r	525	GLY
3	s	793	PRO
1	x	216	PRO
3	3	340	GLY

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	405/405 (100%)	394 (97%)	11 (3%)	39	60
1	8	405/405 (100%)	390 (96%)	15 (4%)	30	51
1	9	405/405 (100%)	395 (98%)	10 (2%)	42	62
1	w	405/405 (100%)	389 (96%)	16 (4%)	28	49
1	x	405/405 (100%)	395 (98%)	10 (2%)	42	62
1	y	405/405 (100%)	391 (96%)	14 (4%)	32	53
2	1	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	P	142/153 (93%)	134 (94%)	8 (6%)	19	40
2	Q	143/153 (94%)	139 (97%)	4 (3%)	38	59
2	R	143/153 (94%)	142 (99%)	1 (1%)	76	81
2	S	152/153 (99%)	149 (98%)	3 (2%)	48	66
2	T	152/153 (99%)	138 (91%)	14 (9%)	8	27
2	U	152/153 (99%)	138 (91%)	14 (9%)	8	27
2	V	152/153 (99%)	138 (91%)	14 (9%)	8	27
2	W	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	X	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	Y	152/153 (99%)	140 (92%)	12 (8%)	11	31
2	Z	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	e	143/153 (94%)	140 (98%)	3 (2%)	47	65
2	f	142/153 (93%)	141 (99%)	1 (1%)	76	81
2	g	143/153 (94%)	143 (100%)	0	100	100
2	h	152/153 (99%)	150 (99%)	2 (1%)	61	73
2	i	134/153 (88%)	132 (98%)	2 (2%)	57	71
2	j	152/153 (99%)	146 (96%)	6 (4%)	28	49
2	k	152/153 (99%)	138 (91%)	14 (9%)	8	27
2	l	152/153 (99%)	143 (94%)	9 (6%)	18	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	m	152/153 (99%)	143 (94%)	9 (6%)	18	39
2	n	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	o	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	p	152/153 (99%)	141 (93%)	11 (7%)	13	34
3	2	934/1010 (92%)	879 (94%)	55 (6%)	18	39
3	3	934/1010 (92%)	874 (94%)	60 (6%)	16	37
3	4	934/1010 (92%)	868 (93%)	66 (7%)	13	35
3	5	934/1010 (92%)	864 (92%)	70 (8%)	12	33
3	6	934/1010 (92%)	864 (92%)	70 (8%)	12	33
3	7	934/1010 (92%)	881 (94%)	53 (6%)	18	40
3	q	934/1010 (92%)	876 (94%)	58 (6%)	16	38
3	r	934/1010 (92%)	873 (94%)	61 (6%)	15	37
3	s	934/1010 (92%)	879 (94%)	55 (6%)	18	39
3	t	934/1010 (92%)	869 (93%)	65 (7%)	14	35
3	u	934/1010 (92%)	875 (94%)	59 (6%)	16	37
3	v	934/1010 (92%)	887 (95%)	47 (5%)	22	42
4	A	278/758 (37%)	277 (100%)	1 (0%)	84	84
5	AA	577/577 (100%)	562 (97%)	15 (3%)	40	61
5	AB	577/577 (100%)	551 (96%)	26 (4%)	24	46
5	a	577/577 (100%)	546 (95%)	31 (5%)	20	41
5	b	577/577 (100%)	556 (96%)	21 (4%)	31	52
5	c	577/577 (100%)	558 (97%)	19 (3%)	33	55
5	z	577/577 (100%)	552 (96%)	25 (4%)	26	47
6	AC	119/122 (98%)	119 (100%)	0	100	100
6	AD	119/122 (98%)	119 (100%)	0	100	100
6	AE	119/122 (98%)	118 (99%)	1 (1%)	73	79
6	AF	119/122 (98%)	118 (99%)	1 (1%)	73	79
6	AG	119/122 (98%)	119 (100%)	0	100	100
6	AH	119/122 (98%)	119 (100%)	0	100	100
7	AI	466/495 (94%)	466 (100%)	0	100	100
7	AJ	466/495 (94%)	466 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AK	464/495 (94%)	463 (100%)	1 (0%)	87	86
7	AL	464/495 (94%)	463 (100%)	1 (0%)	87	86
7	AM	290/495 (59%)	289 (100%)	1 (0%)	86	85
7	AN	290/495 (59%)	289 (100%)	1 (0%)	86	85
8	B	268/271 (99%)	245 (91%)	23 (9%)	10	29
9	C	630/695 (91%)	612 (97%)	18 (3%)	37	58
10	D	150/164 (92%)	149 (99%)	1 (1%)	76	81
10	E	144/164 (88%)	144 (100%)	0	100	100
11	F	205/228 (90%)	204 (100%)	1 (0%)	81	83
11	G	204/228 (90%)	203 (100%)	1 (0%)	81	83
12	H	190/209 (91%)	190 (100%)	0	100	100
12	I	191/209 (91%)	189 (99%)	2 (1%)	68	77
13	J	311/311 (100%)	311 (100%)	0	100	100
13	K	311/311 (100%)	311 (100%)	0	100	100
13	L	311/311 (100%)	310 (100%)	1 (0%)	86	85
13	M	311/311 (100%)	308 (99%)	3 (1%)	68	77
14	N	658/928 (71%)	638 (97%)	20 (3%)	36	57
14	O	658/928 (71%)	645 (98%)	13 (2%)	48	66
15	d	63/112 (56%)	57 (90%)	6 (10%)	8	25
All	All	28711/31524 (91%)	27490 (96%)	1221 (4%)	27	47

All (1221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	70	ARG
1	0	83	ARG
1	0	129	LEU
1	0	151	LYS
1	0	178	MET
1	0	243	ASP
1	0	276	PHE
1	0	329	ASN
1	0	373	THR
1	0	380	THR
1	0	436	LEU

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Mol	Chain	Res	Type
2	1	11	GLU
2	1	45	ASN
2	1	51	GLU
2	1	61	VAL
2	1	68	LYS
2	1	88	VAL
2	1	101	VAL
2	1	125	ASP
2	1	136	ASN
2	1	143	GLU
2	1	168	ARG
3	2	19	ASP
3	2	70	GLU
3	2	76	VAL
3	2	88	ARG
3	2	103	LYS
3	2	116	THR
3	2	118	ASP
3	2	145	MET
3	2	169	SER
3	2	170	THR
3	2	174	MET
3	2	198	GLU
3	2	233	THR
3	2	253	PHE
3	2	260	ILE
3	2	309	THR
3	2	320	TYR
3	2	322	GLN
3	2	355	TYR
3	2	358	ARG
3	2	363	LYS
3	2	372	GLU
3	2	413	ASN
3	2	457	VAL
3	2	509	GLU
3	2	541	GLU
3	2	562	ILE
3	2	579	GLU
3	2	591	LYS
3	2	705	TYR
3	2	741	LYS

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Mol	Chain	Res	Type
3	2	748	ILE
3	2	754	GLU
3	2	787	THR
3	2	830	MET
3	2	833	GLN
3	2	837	ASN
3	2	838	LYS
3	2	863	VAL
3	2	866	ASP
3	2	876	GLU
3	2	955	LYS
3	2	965	MET
3	2	967	THR
3	2	978	TRP
3	2	981	LYS
3	2	992	THR
3	2	997	LYS
3	2	999	GLU
3	2	1007	LEU
3	2	1009	VAL
3	2	1038	THR
3	2	1044	THR
3	2	1099	THR
3	2	1106	GLU
3	3	19	ASP
3	3	36	LEU
3	3	92	ASN
3	3	103	LYS
3	3	111	THR
3	3	128	SER
3	3	130	VAL
3	3	139	ASP
3	3	200	PHE
3	3	213	VAL
3	3	251	THR
3	3	260	ILE
3	3	269	GLU
3	3	270	ILE
3	3	273	VAL
3	3	281	LYS
3	3	289	GLN
3	3	302	PHE

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Mol	Chain	Res	Type
3	3	308	TRP
3	3	321	LYS
3	3	332	GLN
3	3	357	LYS
3	3	359	MET
3	3	363	LYS
3	3	365	TYR
3	3	380	ILE
3	3	397	LEU
3	3	400	TYR
3	3	401	THR
3	3	408	ASP
3	3	412	ILE
3	3	413	ASN
3	3	414	LYS
3	3	428	MET
3	3	571	THR
3	3	574	GLN
3	3	579	GLU
3	3	586	TYR
3	3	592	GLN
3	3	768	TYR
3	3	769	THR
3	3	783	ARG
3	3	785	ARG
3	3	786	VAL
3	3	787	THR
3	3	802	GLU
3	3	845	VAL
3	3	852	LYS
3	3	866	ASP
3	3	872	GLU
3	3	875	LYS
3	3	910	ASN
3	3	954	ILE
3	3	960	ASP
3	3	970	THR
3	3	973	ARG
3	3	1028	ILE
3	3	1050	TYR
3	3	1139	ARG
3	3	1146	MET

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Mol	Chain	Res	Type
3	4	27	PRO
3	4	57	ASP
3	4	90	TYR
3	4	92	ASN
3	4	112	GLU
3	4	115	VAL
3	4	183	GLU
3	4	188	GLU
3	4	237	VAL
3	4	248	ASN
3	4	251	THR
3	4	258	ASN
3	4	274	THR
3	4	308	TRP
3	4	322	GLN
3	4	350	TYR
3	4	368	THR
3	4	383	THR
3	4	391	ILE
3	4	403	TYR
3	4	409	SER
3	4	413	ASN
3	4	427	ILE
3	4	430	LEU
3	4	432	THR
3	4	443	GLN
3	4	465	ARG
3	4	467	SER
3	4	471	LEU
3	4	475	LYS
3	4	518	ASP
3	4	528	PHE
3	4	547	LYS
3	4	556	HIS
3	4	566	PHE
3	4	568	GLU
3	4	586	TYR
3	4	588	ILE
3	4	601	GLU
3	4	687	ILE
3	4	695	LYS
3	4	722	ARG

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Mol	Chain	Res	Type
3	4	729	THR
3	4	755	VAL
3	4	756	THR
3	4	779	ASP
3	4	790	LEU
3	4	801	ASP
3	4	833	GLN
3	4	845	VAL
3	4	847	ASN
3	4	879	ILE
3	4	884	GLU
3	4	906	VAL
3	4	913	LEU
3	4	945	GLU
3	4	968	TYR
3	4	973	ARG
3	4	1007	LEU
3	4	1026	ARG
3	4	1038	THR
3	4	1045	GLU
3	4	1067	PHE
3	4	1087	ASP
3	4	1127	VAL
3	4	1134	GLU
3	5	18	LYS
3	5	35	GLU
3	5	94	ASP
3	5	103	LYS
3	5	115	VAL
3	5	118	ASP
3	5	144	LYS
3	5	157	ILE
3	5	160	PHE
3	5	168	GLN
3	5	171	ASN
3	5	223	LYS
3	5	227	VAL
3	5	229	LYS
3	5	248	ASN
3	5	249	GLU
3	5	258	ASN
3	5	324	GLU

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Mol	Chain	Res	Type
3	5	330	ASP
3	5	365	TYR
3	5	370	GLN
3	5	383	THR
3	5	400	TYR
3	5	413	ASN
3	5	420	ILE
3	5	428	MET
3	5	437	THR
3	5	438	ASP
3	5	457	VAL
3	5	459	ILE
3	5	511	PHE
3	5	512	ILE
3	5	516	LYS
3	5	543	VAL
3	5	579	GLU
3	5	590	ASN
3	5	601	GLU
3	5	604	TRP
3	5	741	LYS
3	5	756	THR
3	5	768	TYR
3	5	779	ASP
3	5	790	LEU
3	5	791	VAL
3	5	799	GLN
3	5	811	LEU
3	5	820	GLN
3	5	850	ASP
3	5	863	VAL
3	5	867	ASP
3	5	876	GLU
3	5	884	GLU
3	5	899	LYS
3	5	902	LYS
3	5	912	TYR
3	5	914	GLN
3	5	916	VAL
3	5	942	LYS
3	5	949	ILE
3	5	969	LEU

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Mol	Chain	Res	Type
3	5	987	MET
3	5	994	ASP
3	5	1028	ILE
3	5	1036	ASP
3	5	1045	GLU
3	5	1067	PHE
3	5	1075	LYS
3	5	1101	THR
3	5	1134	GLU
3	5	1139	ARG
3	6	31	LEU
3	6	35	GLU
3	6	36	LEU
3	6	47	LEU
3	6	76	VAL
3	6	88	ARG
3	6	105	THR
3	6	156	THR
3	6	166	TYR
3	6	167	ILE
3	6	174	MET
3	6	183	GLU
3	6	194	VAL
3	6	213	VAL
3	6	215	VAL
3	6	223	LYS
3	6	247	GLU
3	6	254	ASN
3	6	260	ILE
3	6	269	GLU
3	6	277	VAL
3	6	282	GLU
3	6	284	VAL
3	6	302	PHE
3	6	303	GLU
3	6	307	VAL
3	6	320	TYR
3	6	332	GLN
3	6	349	TYR
3	6	357	LYS
3	6	363	LYS
3	6	365	TYR

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Mol	Chain	Res	Type
3	6	383	THR
3	6	401	THR
3	6	426	ASN
3	6	427	ILE
3	6	443	GLN
3	6	457	VAL
3	6	478	VAL
3	6	540	THR
3	6	562	ILE
3	6	574	GLN
3	6	579	GLU
3	6	580	THR
3	6	588	ILE
3	6	594	VAL
3	6	601	GLU
3	6	604	TRP
3	6	688	ARG
3	6	711	VAL
3	6	753	ARG
3	6	754	GLU
3	6	756	THR
3	6	778	GLN
3	6	783	ARG
3	6	785	ARG
3	6	839	THR
3	6	867	ASP
3	6	875	LYS
3	6	883	THR
3	6	897	LYS
3	6	927	THR
3	6	969	LEU
3	6	973	ARG
3	6	981	LYS
3	6	1075	LYS
3	6	1104	ASN
3	6	1113	ASP
3	6	1123	THR
3	6	1139	ARG
3	7	1	MET
3	7	3	ILE
3	7	18	LYS
3	7	28	ASP

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Mol	Chain	Res	Type
3	7	43	ASP
3	7	70	GLU
3	7	83	ILE
3	7	144	LYS
3	7	167	ILE
3	7	174	MET
3	7	176	LYS
3	7	231	VAL
3	7	258	ASN
3	7	268	LYS
3	7	270	ILE
3	7	279	ILE
3	7	294	ASP
3	7	299	ASN
3	7	321	LYS
3	7	342	GLU
3	7	349	TYR
3	7	363	LYS
3	7	396	VAL
3	7	403	TYR
3	7	411	PHE
3	7	426	ASN
3	7	452	ASP
3	7	509	GLU
3	7	521	HIS
3	7	553	THR
3	7	574	GLN
3	7	737	THR
3	7	752	ASN
3	7	791	VAL
3	7	844	THR
3	7	852	LYS
3	7	866	ASP
3	7	885	ASN
3	7	934	LEU
3	7	938	ILE
3	7	949	ILE
3	7	967	THR
3	7	973	ARG
3	7	980	MET
3	7	981	LYS
3	7	987	MET

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Mol	Chain	Res	Type
3	7	1014	ARG
3	7	1028	ILE
3	7	1072	PHE
3	7	1075	LYS
3	7	1078	LYS
3	7	1086	ASP
3	7	1149	THR
1	8	8	ILE
1	8	45	PHE
1	8	52	LYS
1	8	63	TYR
1	8	83	ARG
1	8	158	THR
1	8	192	ASP
1	8	220	TYR
1	8	260	PHE
1	8	335	THR
1	8	344	THR
1	8	347	GLN
1	8	380	THR
1	8	441	VAL
1	8	446	THR
1	9	8	ILE
1	9	70	ARG
1	9	116	LEU
1	9	202	THR
1	9	252	VAL
1	9	279	TYR
1	9	351	SER
1	9	389	ILE
1	9	403	CYS
1	9	441	VAL
4	A	300	LYS
5	AA	21	VAL
5	AA	88	ILE
5	AA	161	SER
5	AA	170	GLU
5	AA	208	TYR
5	AA	211	ILE
5	AA	216	TRP
5	AA	233	VAL
5	AA	277	LYS

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Mol	Chain	Res	Type
5	AA	355	CYS
5	AA	374	LYS
5	AA	380	PRO
5	AA	452	GLN
5	AA	563	ILE
5	AA	587	ASP
5	AB	7	PRO
5	AB	9	THR
5	AB	36	ASP
5	AB	47	ASN
5	AB	70	GLU
5	AB	113	SER
5	AB	183	ILE
5	AB	256	ASN
5	AB	288	LEU
5	AB	290	TYR
5	AB	291	PHE
5	AB	299	VAL
5	AB	345	ASN
5	AB	440	MET
5	AB	475	CYS
5	AB	486	LEU
5	AB	497	THR
5	AB	505	GLN
5	AB	515	THR
5	AB	571	TYR
5	AB	572	ILE
5	AB	585	SER
5	AB	587	ASP
5	AB	599	THR
5	AB	605	MET
5	AB	638	ASN
6	AE	16	LEU
6	AF	16	LEU
7	AK	571	PHE
7	AL	571	PHE
7	AM	571	PHE
7	AN	571	PHE
8	B	22	ASP
8	B	28	ARG
8	B	29	ILE
8	B	31	GLU

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Mol	Chain	Res	Type
8	B	34	GLU
8	B	41	THR
8	B	44	MET
8	B	45	TYR
8	B	67	GLN
8	B	68	TYR
8	B	69	GLU
8	B	71	PHE
8	B	86	LYS
8	B	88	SER
8	B	91	VAL
8	B	92	ASP
8	B	96	ILE
8	B	114	GLU
8	B	115	LEU
8	B	136	TYR
8	B	138	PHE
8	B	139	ASP
8	B	140	GLU
9	C	183	ASN
9	C	241	LYS
9	C	409	LYS
9	C	413	LYS
9	C	422	LYS
9	C	450	THR
9	C	529	LEU
9	C	604	LYS
9	C	689	GLN
9	C	695	TYR
9	C	700	THR
9	C	702	TYR
9	C	714	VAL
9	C	747	GLN
9	C	759	HIS
9	C	780	TYR
9	C	790	THR
9	C	799	LYS
10	D	57	ASN
11	F	244	LYS
11	G	77	ARG
12	I	44	GLU
12	I	152	HIS

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Mol	Chain	Res	Type
13	L	259	LYS
13	M	92	ARG
13	M	227	ASN
13	M	235	LYS
14	N	124	TYR
14	N	142	ARG
14	N	181	THR
14	N	182	ILE
14	N	183	ARG
14	N	199	THR
14	N	231	ASP
14	N	235	THR
14	N	244	ASP
14	N	292	ASP
14	N	370	GLU
14	N	391	LEU
14	N	465	ARG
14	N	466	GLU
14	N	467	THR
14	N	516	ASP
14	N	521	GLU
14	N	559	SER
14	N	701	LYS
14	N	718	THR
14	O	137	MET
14	O	152	ASP
14	O	180	SER
14	O	181	THR
14	O	183	ARG
14	O	201	GLN
14	O	247	THR
14	O	255	GLN
14	O	366	ASP
14	O	425	LYS
14	O	469	VAL
14	O	506	SER
14	O	718	THR
2	P	38	ASN
2	P	60	LYS
2	P	82	ASN
2	P	89	THR
2	P	129	LYS

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Mol	Chain	Res	Type
2	P	150	PHE
2	P	155	GLN
2	P	157	GLN
2	Q	41	GLN
2	Q	45	ASN
2	Q	151	PHE
2	Q	172	GLU
2	R	43	ASP
2	S	38	ASN
2	S	74	ASN
2	S	129	LYS
2	T	3	ILE
2	T	27	ILE
2	T	44	GLU
2	T	45	ASN
2	T	51	GLU
2	T	88	VAL
2	T	101	VAL
2	T	108	VAL
2	T	111	GLU
2	T	125	ASP
2	T	126	LEU
2	T	127	VAL
2	T	154	LYS
2	T	157	GLN
2	U	27	ILE
2	U	38	ASN
2	U	51	GLU
2	U	75	LYS
2	U	88	VAL
2	U	101	VAL
2	U	107	ILE
2	U	111	GLU
2	U	125	ASP
2	U	126	LEU
2	U	127	VAL
2	U	136	ASN
2	U	143	GLU
2	U	145	THR
2	V	38	ASN
2	V	48	VAL
2	V	51	GLU

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Mol	Chain	Res	Type
2	V	68	LYS
2	V	75	LYS
2	V	88	VAL
2	V	99	LYS
2	V	101	VAL
2	V	111	GLU
2	V	127	VAL
2	V	136	ASN
2	V	143	GLU
2	V	156	PHE
2	V	161	GLU
2	W	19	LYS
2	W	51	GLU
2	W	68	LYS
2	W	83	LYS
2	W	88	VAL
2	W	101	VAL
2	W	107	ILE
2	W	111	GLU
2	W	136	ASN
2	W	157	GLN
2	W	161	GLU
2	X	3	ILE
2	X	41	GLN
2	X	44	GLU
2	X	68	LYS
2	X	77	LEU
2	X	88	VAL
2	X	91	GLU
2	X	101	VAL
2	X	111	GLU
2	X	125	ASP
2	X	136	ASN
2	Y	27	ILE
2	Y	45	ASN
2	Y	51	GLU
2	Y	88	VAL
2	Y	101	VAL
2	Y	111	GLU
2	Y	125	ASP
2	Y	126	LEU
2	Y	127	VAL

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Mol	Chain	Res	Type
2	Y	136	ASN
2	Y	149	LEU
2	Y	172	GLU
2	Z	44	GLU
2	Z	51	GLU
2	Z	68	LYS
2	Z	75	LYS
2	Z	88	VAL
2	Z	99	LYS
2	Z	101	VAL
2	Z	107	ILE
2	Z	111	GLU
2	Z	125	ASP
2	Z	127	VAL
5	a	45	PHE
5	a	57	ASN
5	a	88	ILE
5	a	105	ASN
5	a	132	GLU
5	a	142	THR
5	a	169	VAL
5	a	208	TYR
5	a	240	THR
5	a	244	ASP
5	a	259	LYS
5	a	286	ASP
5	a	290	TYR
5	a	305	ASN
5	a	314	ILE
5	a	330	PHE
5	a	343	LYS
5	a	361	ASN
5	a	424	GLN
5	a	431	ASN
5	a	449	PHE
5	a	450	TYR
5	a	464	ILE
5	a	499	TYR
5	a	512	GLN
5	a	547	THR
5	a	549	TRP
5	a	563	ILE

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Mol	Chain	Res	Type
5	a	572	ILE
5	a	577	ILE
5	a	603	PRO
5	b	14	LEU
5	b	15	LYS
5	b	29	LYS
5	b	60	VAL
5	b	86	TYR
5	b	93	TYR
5	b	107	THR
5	b	108	VAL
5	b	206	THR
5	b	211	ILE
5	b	244	ASP
5	b	318	GLU
5	b	395	TRP
5	b	431	ASN
5	b	447	HIS
5	b	450	TYR
5	b	515	THR
5	b	546	VAL
5	b	592	TYR
5	b	599	THR
5	b	633	ASN
5	c	52	ILE
5	c	60	VAL
5	c	79	ASP
5	c	107	THR
5	c	150	ASN
5	c	172	ASN
5	c	180	PHE
5	c	296	TYR
5	c	299	VAL
5	c	430	VAL
5	c	431	ASN
5	c	432	GLU
5	c	468	ILE
5	c	472	TYR
5	c	478	TYR
5	c	484	VAL
5	c	594	THR
5	c	595	PHE

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Mol	Chain	Res	Type
5	c	623	TRP
15	d	12	ILE
15	d	31	TYR
15	d	33	LYS
15	d	58	TYR
15	d	59	LEU
15	d	60	TYR
2	e	89	THR
2	e	129	LYS
2	e	157	GLN
2	f	78	ILE
2	h	51	GLU
2	h	75	LYS
2	i	41	GLN
2	i	89	THR
2	j	75	LYS
2	j	78	ILE
2	j	88	VAL
2	j	101	VAL
2	j	127	VAL
2	j	143	GLU
2	k	51	GLU
2	k	68	LYS
2	k	75	LYS
2	k	88	VAL
2	k	99	LYS
2	k	101	VAL
2	k	111	GLU
2	k	125	ASP
2	k	136	ASN
2	k	143	GLU
2	k	155	GLN
2	k	156	PHE
2	k	157	GLN
2	k	162	GLN
2	l	27	ILE
2	l	44	GLU
2	l	45	ASN
2	l	50	GLN
2	l	51	GLU
2	l	88	VAL
2	l	101	VAL

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Mol	Chain	Res	Type
2	l	127	VAL
2	l	157	GLN
2	m	27	ILE
2	m	88	VAL
2	m	101	VAL
2	m	111	GLU
2	m	125	ASP
2	m	127	VAL
2	m	135	PHE
2	m	136	ASN
2	m	142	VAL
2	n	7	ASN
2	n	27	ILE
2	n	44	GLU
2	n	45	ASN
2	n	51	GLU
2	n	88	VAL
2	n	101	VAL
2	n	125	ASP
2	n	127	VAL
2	n	161	GLU
2	n	168	ARG
2	o	41	GLN
2	o	44	GLU
2	o	45	ASN
2	o	51	GLU
2	o	68	LYS
2	o	78	ILE
2	o	88	VAL
2	o	101	VAL
2	o	125	ASP
2	o	143	GLU
2	o	157	GLN
2	p	27	ILE
2	p	44	GLU
2	p	45	ASN
2	p	51	GLU
2	p	88	VAL
2	p	101	VAL
2	p	125	ASP
2	p	127	VAL
2	p	136	ASN

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Mol	Chain	Res	Type
2	p	142	VAL
2	p	161	GLU
3	q	69	SER
3	q	70	GLU
3	q	88	ARG
3	q	116	THR
3	q	173	GLU
3	q	174	MET
3	q	175	ASP
3	q	186	TYR
3	q	192	TYR
3	q	199	LEU
3	q	258	ASN
3	q	260	ILE
3	q	269	GLU
3	q	274	THR
3	q	342	GLU
3	q	350	TYR
3	q	355	TYR
3	q	359	MET
3	q	365	TYR
3	q	368	THR
3	q	369	THR
3	q	431	VAL
3	q	432	THR
3	q	453	SER
3	q	483	TYR
3	q	509	GLU
3	q	519	ILE
3	q	566	PHE
3	q	571	THR
3	q	574	GLN
3	q	601	GLU
3	q	687	ILE
3	q	703	ASN
3	q	726	GLU
3	q	756	THR
3	q	773	ARG
3	q	787	THR
3	q	833	GLN
3	q	845	VAL
3	q	847	ASN

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Mol	Chain	Res	Type
3	q	876	GLU
3	q	910	ASN
3	q	936	PHE
3	q	942	LYS
3	q	955	LYS
3	q	981	LYS
3	q	997	LYS
3	q	1014	ARG
3	q	1024	SER
3	q	1042	PHE
3	q	1058	THR
3	q	1075	LYS
3	q	1086	ASP
3	q	1099	THR
3	q	1101	THR
3	q	1127	VAL
3	q	1144	ARG
3	q	1149	THR
3	r	70	GLU
3	r	103	LYS
3	r	111	THR
3	r	118	ASP
3	r	192	TYR
3	r	211	VAL
3	r	237	VAL
3	r	243	LEU
3	r	268	LYS
3	r	269	GLU
3	r	273	VAL
3	r	281	LYS
3	r	298	ASN
3	r	329	THR
3	r	330	ASP
3	r	349	TYR
3	r	353	TYR
3	r	363	LYS
3	r	383	THR
3	r	395	VAL
3	r	414	LYS
3	r	427	ILE
3	r	453	SER
3	r	458	CYS

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Mol	Chain	Res	Type
3	r	528	PHE
3	r	530	PHE
3	r	536	THR
3	r	547	LYS
3	r	558	TRP
3	r	567	THR
3	r	574	GLN
3	r	579	GLU
3	r	580	THR
3	r	685	ILE
3	r	686	ARG
3	r	688	ARG
3	r	700	ASN
3	r	741	LYS
3	r	756	THR
3	r	799	GLN
3	r	802	GLU
3	r	846	MET
3	r	853	VAL
3	r	875	LYS
3	r	901	ASP
3	r	905	GLU
3	r	910	ASN
3	r	913	LEU
3	r	932	SER
3	r	954	ILE
3	r	963	VAL
3	r	973	ARG
3	r	996	LEU
3	r	997	LYS
3	r	1007	LEU
3	r	1009	VAL
3	r	1014	ARG
3	r	1075	LYS
3	r	1079	VAL
3	r	1124	LYS
3	r	1129	LEU
3	s	27	PRO
3	s	48	LYS
3	s	57	ASP
3	s	103	LYS
3	s	130	VAL

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Mol	Chain	Res	Type
3	s	195	ASN
3	s	232	SER
3	s	249	GLU
3	s	277	VAL
3	s	325	ASP
3	s	330	ASP
3	s	342	GLU
3	s	355	TYR
3	s	383	THR
3	s	390	PRO
3	s	393	GLN
3	s	408	ASP
3	s	413	ASN
3	s	418	ILE
3	s	427	ILE
3	s	430	LEU
3	s	447	VAL
3	s	465	ARG
3	s	467	SER
3	s	469	GLU
3	s	470	ASP
3	s	472	GLN
3	s	474	VAL
3	s	519	ILE
3	s	520	THR
3	s	526	ILE
3	s	528	PHE
3	s	547	LYS
3	s	552	ASP
3	s	574	GLN
3	s	582	ASN
3	s	779	ASP
3	s	785	ARG
3	s	790	LEU
3	s	799	GLN
3	s	801	ASP
3	s	866	ASP
3	s	906	VAL
3	s	942	LYS
3	s	945	GLU
3	s	951	PHE
3	s	962	ILE

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Mol	Chain	Res	Type
3	s	973	ARG
3	s	994	ASP
3	s	1026	ARG
3	s	1041	THR
3	s	1075	LYS
3	s	1106	GLU
3	s	1142	VAL
3	s	1147	VAL
3	t	18	LYS
3	t	24	LEU
3	t	74	LEU
3	t	92	ASN
3	t	94	ASP
3	t	103	LYS
3	t	105	THR
3	t	106	ILE
3	t	108	ILE
3	t	111	THR
3	t	159	THR
3	t	171	ASN
3	t	200	PHE
3	t	248	ASN
3	t	249	GLU
3	t	280	GLU
3	t	294	ASP
3	t	321	LYS
3	t	324	GLU
3	t	365	TYR
3	t	368	THR
3	t	383	THR
3	t	403	TYR
3	t	421	LEU
3	t	432	THR
3	t	457	VAL
3	t	464	THR
3	t	465	ARG
3	t	469	GLU
3	t	470	ASP
3	t	516	LYS
3	t	520	THR
3	t	574	GLN
3	t	584	ASN

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Mol	Chain	Res	Type
3	t	601	GLU
3	t	737	THR
3	t	756	THR
3	t	761	ASN
3	t	776	THR
3	t	779	ASP
3	t	782	ILE
3	t	790	LEU
3	t	799	GLN
3	t	801	ASP
3	t	830	MET
3	t	869	MET
3	t	876	GLU
3	t	884	GLU
3	t	945	GLU
3	t	949	ILE
3	t	957	VAL
3	t	994	ASP
3	t	997	LYS
3	t	1009	VAL
3	t	1010	LEU
3	t	1022	PHE
3	t	1025	ASN
3	t	1026	ARG
3	t	1036	ASP
3	t	1038	THR
3	t	1040	THR
3	t	1095	THR
3	t	1134	GLU
3	t	1138	LEU
3	t	1149	THR
3	u	70	GLU
3	u	92	ASN
3	u	112	GLU
3	u	118	ASP
3	u	119	GLU
3	u	134	PHE
3	u	183	GLU
3	u	227	VAL
3	u	235	ILE
3	u	251	THR
3	u	273	VAL

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Mol	Chain	Res	Type
3	u	308	TRP
3	u	330	ASP
3	u	363	LYS
3	u	369	THR
3	u	372	GLU
3	u	379	TYR
3	u	381	ASN
3	u	399	ASP
3	u	417	ASP
3	u	424	GLU
3	u	426	ASN
3	u	427	ILE
3	u	436	ASN
3	u	438	ASP
3	u	464	THR
3	u	468	MET
3	u	478	VAL
3	u	520	THR
3	u	527	VAL
3	u	572	ILE
3	u	574	GLN
3	u	601	GLU
3	u	753	ARG
3	u	761	ASN
3	u	776	THR
3	u	778	GLN
3	u	783	ARG
3	u	787	THR
3	u	798	PHE
3	u	818	ASP
3	u	820	GLN
3	u	852	LYS
3	u	875	LYS
3	u	880	VAL
3	u	887	ASP
3	u	892	VAL
3	u	910	ASN
3	u	927	THR
3	u	944	ASN
3	u	945	GLU
3	u	955	LYS
3	u	993	PHE

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Mol	Chain	Res	Type
3	u	997	LYS
3	u	1007	LEU
3	u	1058	THR
3	u	1087	ASP
3	u	1112	ILE
3	u	1139	ARG
3	v	1	MET
3	v	98	ILE
3	v	119	GLU
3	v	130	VAL
3	v	133	TYR
3	v	142	GLU
3	v	144	LYS
3	v	149	VAL
3	v	174	MET
3	v	186	TYR
3	v	232	SER
3	v	248	ASN
3	v	258	ASN
3	v	268	LYS
3	v	274	THR
3	v	282	GLU
3	v	332	GLN
3	v	363	LYS
3	v	364	ASP
3	v	383	THR
3	v	457	VAL
3	v	545	GLN
3	v	571	THR
3	v	743	THR
3	v	754	GLU
3	v	766	THR
3	v	776	THR
3	v	785	ARG
3	v	793	PRO
3	v	800	TYR
3	v	870	MET
3	v	876	GLU
3	v	884	GLU
3	v	910	ASN
3	v	934	LEU
3	v	936	PHE

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Mol	Chain	Res	Type
3	v	942	LYS
3	v	978	TRP
3	v	981	LYS
3	v	997	LYS
3	v	1007	LEU
3	v	1014	ARG
3	v	1023	GLU
3	v	1042	PHE
3	v	1083	TYR
3	v	1092	LYS
3	v	1101	THR
1	w	10	GLU
1	w	19	THR
1	w	55	ASP
1	w	63	TYR
1	w	80	ILE
1	w	94	MET
1	w	95	GLU
1	w	171	VAL
1	w	192	ASP
1	w	231	ASP
1	w	252	VAL
1	w	254	THR
1	w	259	THR
1	w	329	ASN
1	w	367	TYR
1	w	383	ASN
1	x	8	ILE
1	x	79	TYR
1	x	83	ARG
1	x	126	ILE
1	x	192	ASP
1	x	239	SER
1	x	243	ASP
1	x	301	THR
1	x	411	ASP
1	x	429	PHE
1	y	15	ARG
1	y	55	ASP
1	y	95	GLU
1	y	117	TYR
1	y	155	ILE

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Mol	Chain	Res	Type
1	y	159	ASN
1	y	216	PRO
1	y	235	TYR
1	y	240	ILE
1	y	280	VAL
1	y	312	ASN
1	y	322	THR
1	y	427	VAL
1	y	429	PHE
5	z	18	TYR
5	z	31	GLU
5	z	80	LYS
5	z	156	VAL
5	z	157	ASN
5	z	179	THR
5	z	274	VAL
5	z	286	ASP
5	z	288	LEU
5	z	342	VAL
5	z	385	GLU
5	z	407	LEU
5	z	413	VAL
5	z	419	ASP
5	z	434	SER
5	z	464	ILE
5	z	481	ASN
5	z	488	PHE
5	z	500	TYR
5	z	530	GLU
5	z	532	VAL
5	z	577	ILE
5	z	592	TYR
5	z	599	THR
5	z	601	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (329) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	12	ASN
1	0	65	ASN
1	0	123	ASN
1	0	142	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	0	291	ASN
1	0	303	ASN
1	0	391	HIS
2	1	119	GLN
3	2	32	GLN
3	2	92	ASN
3	2	178	ASN
3	2	254	ASN
3	2	257	ASN
3	2	332	GLN
3	2	441	ASN
3	2	944	ASN
3	2	1025	ASN
3	3	44	GLN
3	3	61	GLN
3	3	92	ASN
3	3	248	ASN
3	3	298	ASN
3	3	700	ASN
3	3	1025	ASN
3	4	4	ASN
3	4	293	GLN
3	4	426	ASN
3	4	484	ASN
3	4	576	GLN
3	4	778	GLN
3	4	820	GLN
3	4	822	ASN
3	4	944	ASN
3	4	1003	ASN
3	4	1005	GLN
3	4	1126	GLN
3	5	26	ASN
3	5	37	ASN
3	5	61	GLN
3	5	77	ASN
3	5	322	GLN
3	5	436	ASN
3	5	485	GLN
3	5	498	GLN
3	5	556	HIS
3	5	590	ASN

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Mol	Chain	Res	Type
3	5	799	GLN
3	5	847	ASN
3	5	910	ASN
3	5	914	GLN
3	5	1015	GLN
3	5	1135	ASN
3	6	126	GLN
3	6	168	GLN
3	6	248	ASN
3	6	254	ASN
3	6	257	ASN
3	6	299	ASN
3	6	381	ASN
3	6	576	GLN
3	6	587	ASN
3	6	590	ASN
3	6	698	ASN
3	6	820	GLN
3	6	930	GLN
3	6	1015	GLN
3	6	1126	GLN
3	7	322	GLN
3	7	356	ASN
3	7	393	GLN
3	7	833	GLN
3	7	855	ASN
3	7	1015	GLN
3	7	1104	ASN
1	8	102	HIS
1	8	115	HIS
1	8	123	ASN
1	8	150	ASN
1	8	273	GLN
1	8	320	ASN
1	9	20	GLN
1	9	142	GLN
1	9	145	GLN
1	9	347	GLN
4	A	22	ASN
4	A	100	ASN
4	A	162	ASN
5	AA	145	ASN

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Mol	Chain	Res	Type
5	AA	157	ASN
5	AA	194	ASN
5	AA	444	GLN
5	AA	533	ASN
5	AA	633	ASN
5	AB	152	ASN
5	AB	397	ASN
5	AB	504	ASN
5	AB	616	ASN
6	AE	113	ASN
6	AF	113	ASN
6	AG	50	GLN
6	AG	120	GLN
6	AH	50	GLN
6	AH	120	GLN
7	AI	41	GLN
7	AI	120	GLN
7	AI	204	ASN
7	AI	442	GLN
7	AI	543	GLN
7	AJ	41	GLN
7	AJ	120	GLN
7	AJ	204	ASN
7	AJ	442	GLN
7	AJ	543	GLN
7	AK	55	ASN
7	AK	329	HIS
7	AK	407	HIS
7	AK	511	GLN
7	AK	519	ASN
7	AK	582	GLN
7	AK	583	GLN
7	AL	407	HIS
7	AL	511	GLN
7	AL	519	ASN
7	AL	583	GLN
7	AM	41	GLN
7	AM	55	ASN
7	AN	41	GLN
7	AN	55	ASN
7	AN	557	ASN
8	B	187	ASN

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Mol	Chain	Res	Type
9	C	97	GLN
9	C	183	ASN
9	C	194	ASN
9	C	431	ASN
9	C	479	ASN
9	C	571	GLN
9	C	747	GLN
9	C	802	GLN
10	D	46	GLN
10	D	57	ASN
10	D	77	HIS
10	E	46	GLN
10	E	71	ASN
10	E	96	GLN
10	E	107	ASN
10	E	112	ASN
11	F	42	GLN
11	F	179	GLN
11	G	107	ASN
11	G	179	GLN
12	H	139	GLN
12	H	152	HIS
12	I	9	GLN
12	I	108	HIS
12	I	192	ASN
12	I	206	GLN
13	J	8	ASN
13	J	167	ASN
13	J	175	GLN
13	J	281	GLN
13	J	308	GLN
13	K	60	GLN
13	K	161	ASN
13	K	218	HIS
13	K	283	HIS
13	L	46	GLN
13	L	54	ASN
13	L	111	GLN
13	L	229	ASN
13	M	8	ASN
13	M	141	ASN
13	M	283	HIS

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Mol	Chain	Res	Type
14	N	9	HIS
14	N	38	GLN
14	N	135	HIS
14	N	268	ASN
14	N	303	ASN
14	N	320	ASN
14	N	338	GLN
14	N	389	ASN
14	N	523	ASN
14	N	533	ASN
14	N	569	ASN
14	N	710	GLN
14	O	129	HIS
14	O	320	ASN
14	O	710	GLN
2	P	155	GLN
2	Q	119	GLN
2	Q	157	GLN
2	Q	158	ASN
2	S	7	ASN
2	S	38	ASN
2	S	74	ASN
2	T	7	ASN
2	T	9	HIS
2	T	38	ASN
2	T	162	GLN
2	U	7	ASN
2	U	119	GLN
2	U	153	ASN
2	U	158	ASN
2	V	38	ASN
2	V	45	ASN
2	V	92	ASN
2	W	119	GLN
2	W	153	ASN
2	X	38	ASN
2	X	157	GLN
2	Y	38	ASN
2	Y	50	GLN
2	Y	74	ASN
2	Y	162	GLN
5	a	12	GLN

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Mol	Chain	Res	Type
5	a	384	HIS
5	a	533	ASN
5	a	579	ASN
5	b	42	GLN
5	b	84	ASN
5	b	126	ASN
5	b	150	ASN
5	b	256	ASN
5	b	481	ASN
5	b	504	ASN
5	c	26	ASN
5	c	145	ASN
5	c	444	GLN
5	c	540	ASN
5	c	565	ASN
5	c	576	ASN
5	c	638	ASN
15	d	37	GLN
15	d	72	ASN
2	e	9	HIS
2	f	7	ASN
2	g	7	ASN
2	h	82	ASN
2	i	41	GLN
2	j	7	ASN
2	j	158	ASN
2	k	7	ASN
2	k	153	ASN
2	l	9	HIS
2	l	119	GLN
2	l	153	ASN
2	m	9	HIS
2	m	119	GLN
2	m	153	ASN
2	m	158	ASN
2	o	7	ASN
2	o	119	GLN
2	o	153	ASN
2	p	7	ASN
2	p	92	ASN
2	p	162	GLN
3	q	178	ASN

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Mol	Chain	Res	Type
3	q	195	ASN
3	q	204	ASN
3	q	386	ASN
3	q	441	ASN
3	q	590	ASN
3	q	700	ASN
3	q	799	GLN
3	q	822	ASN
3	q	914	GLN
3	q	944	ASN
3	q	995	GLN
3	q	1135	ASN
3	r	254	ASN
3	r	257	ASN
3	r	299	ASN
3	r	332	GLN
3	r	393	GLN
3	r	426	ASN
3	r	480	ASN
3	r	545	GLN
3	r	799	GLN
3	r	820	GLN
3	r	944	ASN
3	r	995	GLN
3	r	1025	ASN
3	s	61	GLN
3	s	356	ASN
3	s	480	ASN
3	s	498	GLN
3	s	789	ASN
3	t	37	ASN
3	t	61	GLN
3	t	92	ASN
3	t	195	ASN
3	t	910	ASN
3	t	1015	GLN
3	u	32	GLN
3	u	204	ASN
3	u	248	ASN
3	u	254	ASN
3	u	276	GLN
3	u	356	ASN

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Mol	Chain	Res	Type
3	u	386	ASN
3	u	393	GLN
3	u	480	ASN
3	u	484	ASN
3	u	556	HIS
3	u	576	GLN
3	u	592	GLN
3	u	789	ASN
3	u	822	ASN
3	u	995	GLN
3	v	441	ASN
3	v	752	ASN
3	v	799	GLN
3	v	914	GLN
3	v	1003	ASN
1	w	12	ASN
1	w	20	GLN
1	w	312	ASN
1	w	320	ASN
1	w	391	HIS
1	x	11	ASN
1	x	102	HIS
1	x	150	ASN
1	y	65	ASN
1	y	262	GLN
5	z	126	ASN
5	z	139	GLN
5	z	145	ASN
5	z	335	ASN
5	z	452	GLN
5	z	533	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

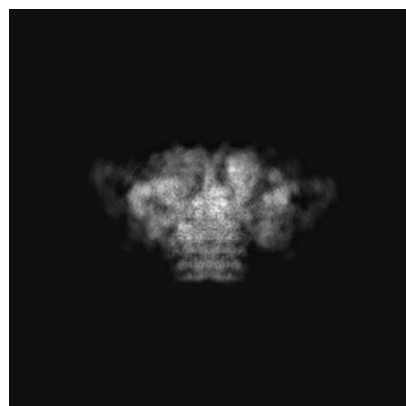
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55951. These allow visual inspection of the internal detail of the map and identification of artifacts.

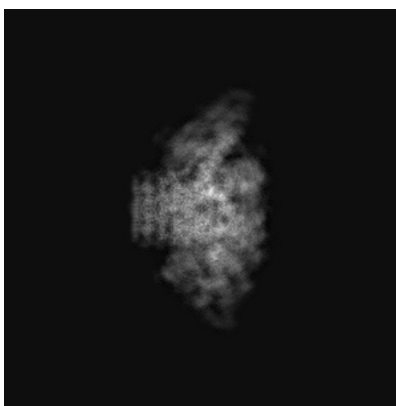
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

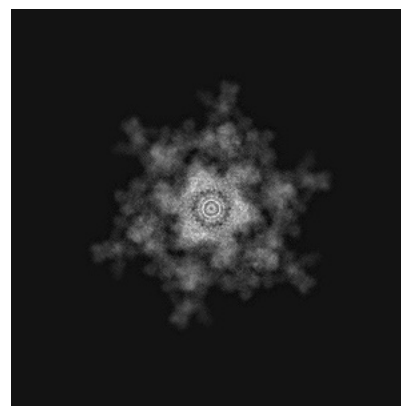
6.1.1 Primary map



X

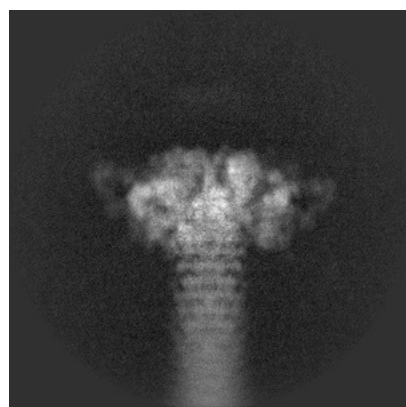


Y

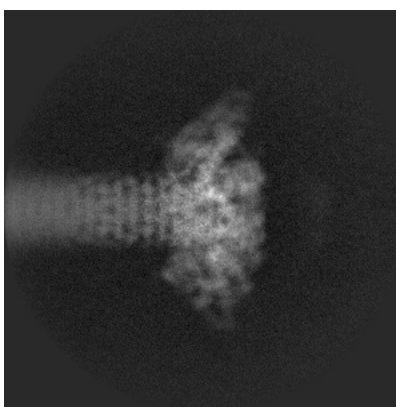


Z

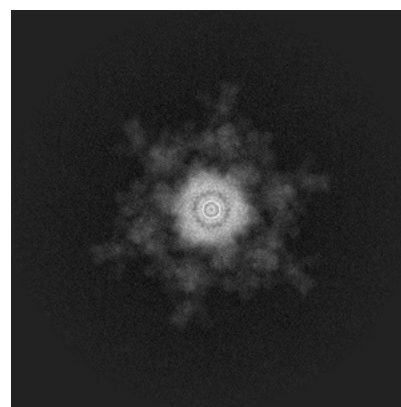
6.1.2 Raw map



X



Y

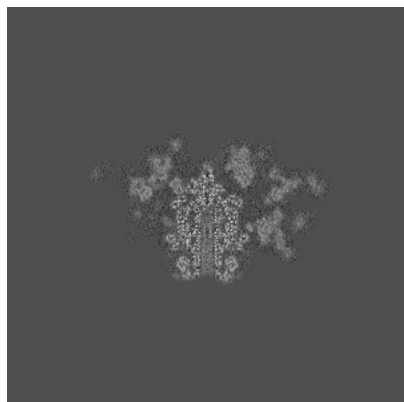


Z

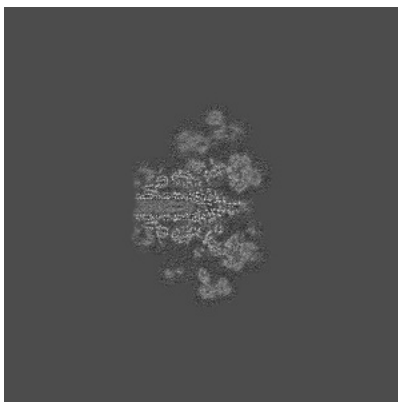
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

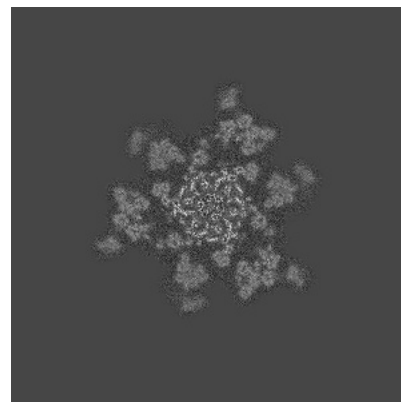
6.2.1 Primary map



X Index: 320

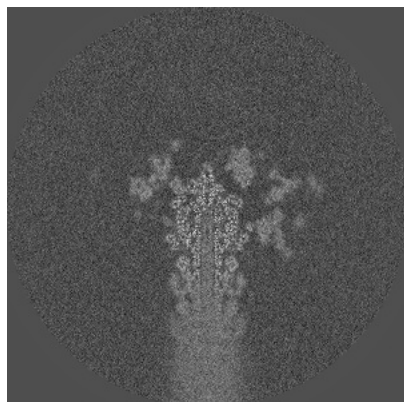


Y Index: 320

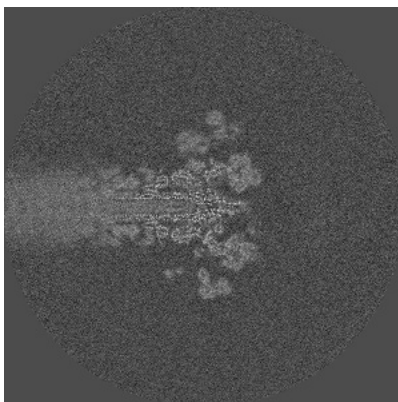


Z Index: 320

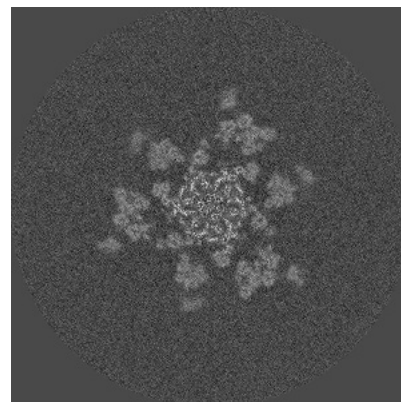
6.2.2 Raw map



X Index: 320



Y Index: 320

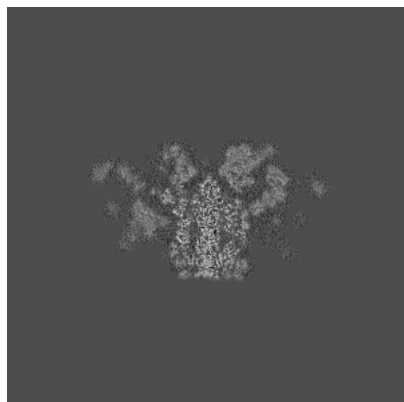


Z Index: 320

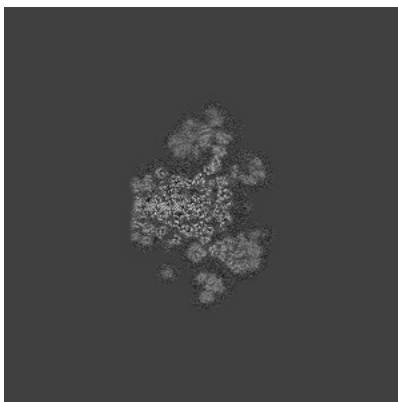
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

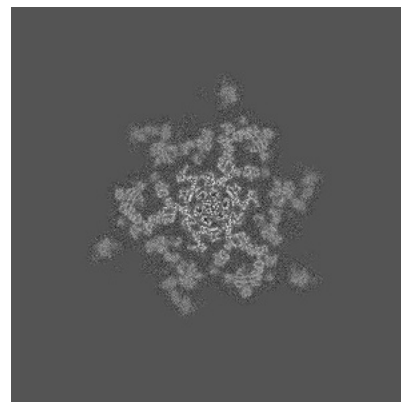
6.3.1 Primary map



X Index: 307

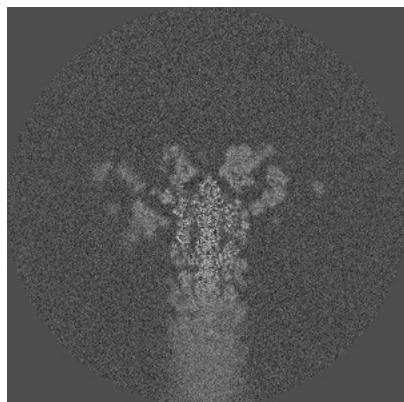


Y Index: 333

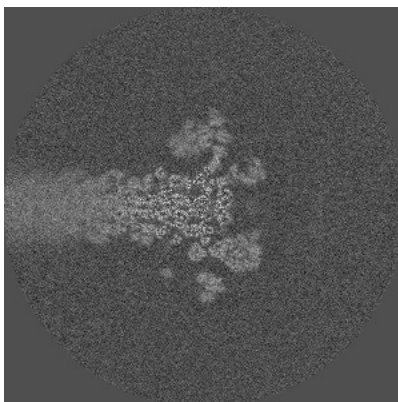


Z Index: 330

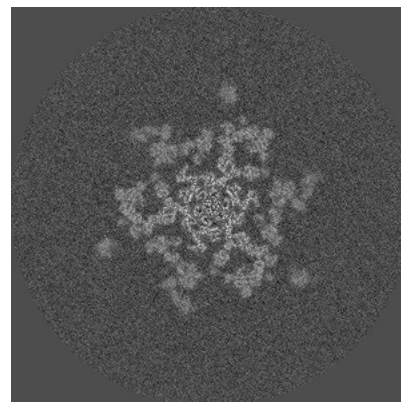
6.3.2 Raw map



X Index: 307



Y Index: 332

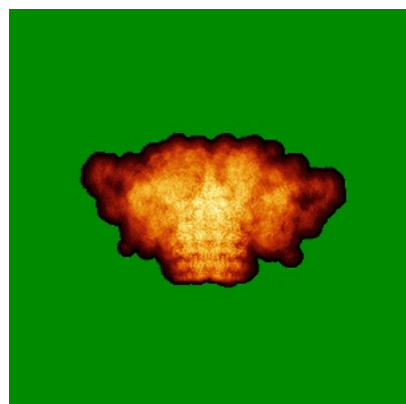


Z Index: 330

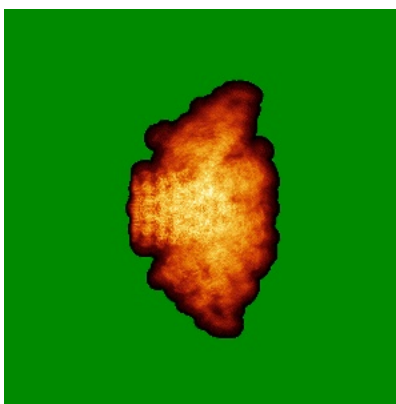
The images above show the largest variance slices of the map in three orthogonal directions.

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

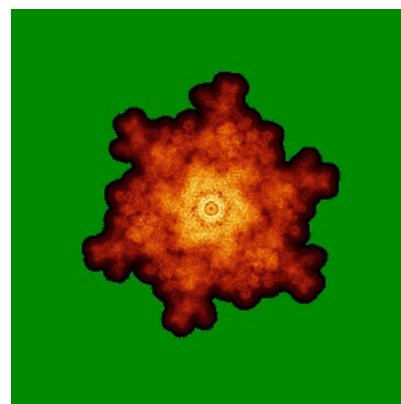
6.4.1 Primary map



X

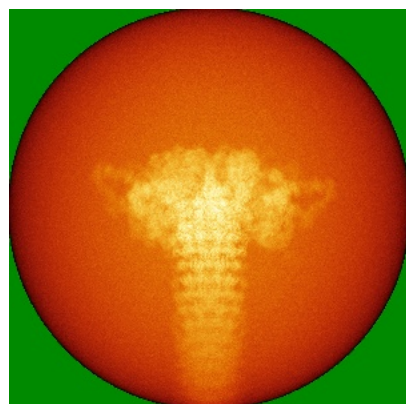


Y

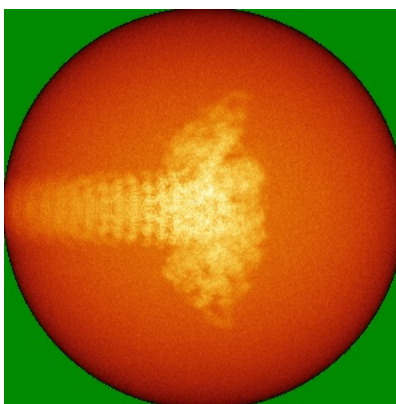


Z

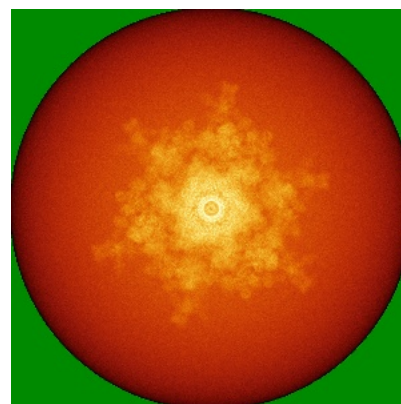
6.4.2 Raw map



X



Y

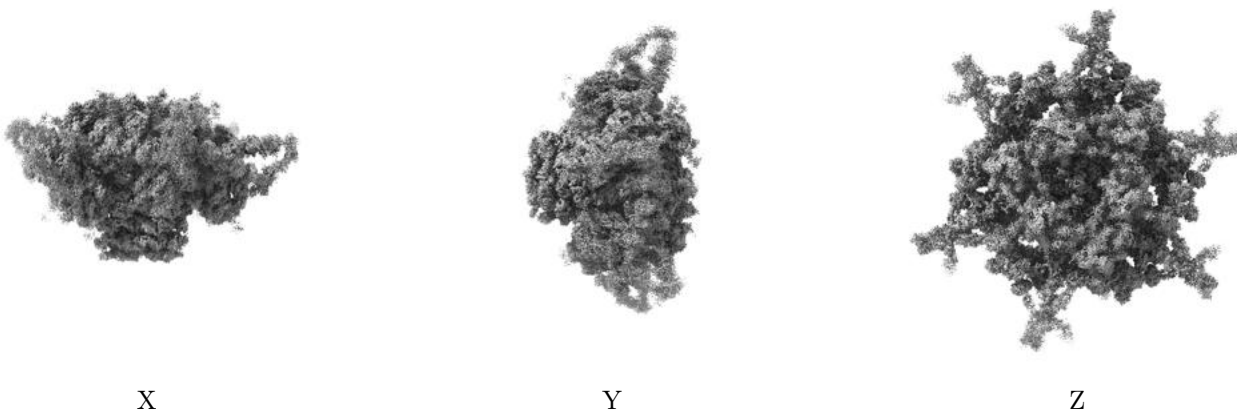


Z

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

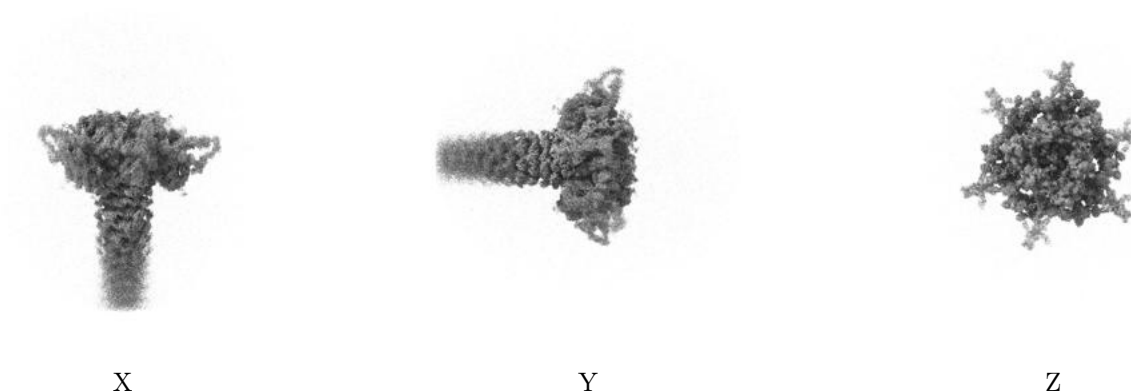
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

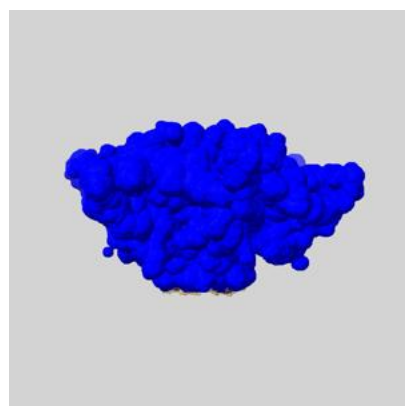
6.6 Mask visualisation [i](#)

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

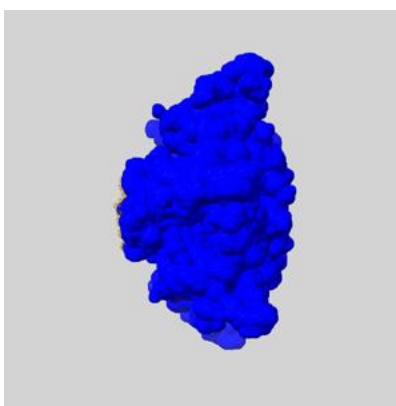
A mask typically either:

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

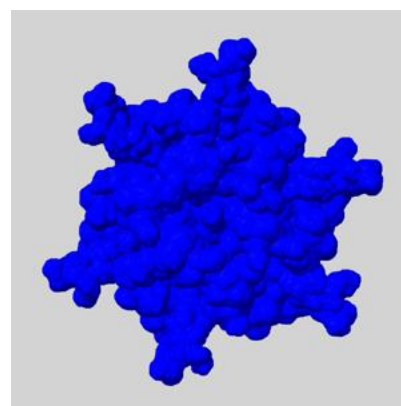
6.6.1 emd_55951_msk_1.map [i](#)



X



Y

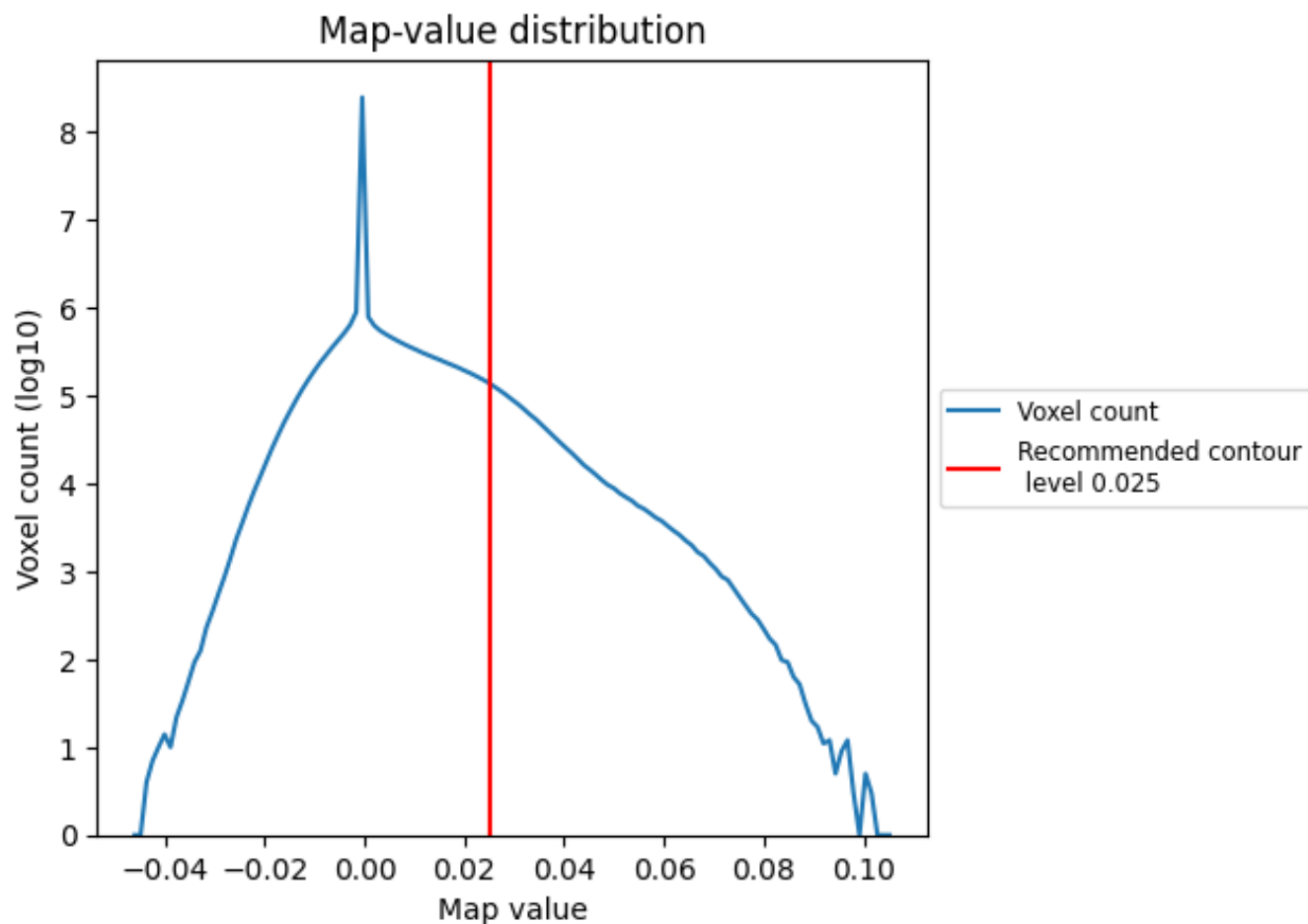


Z

7 Map analysis [i](#)

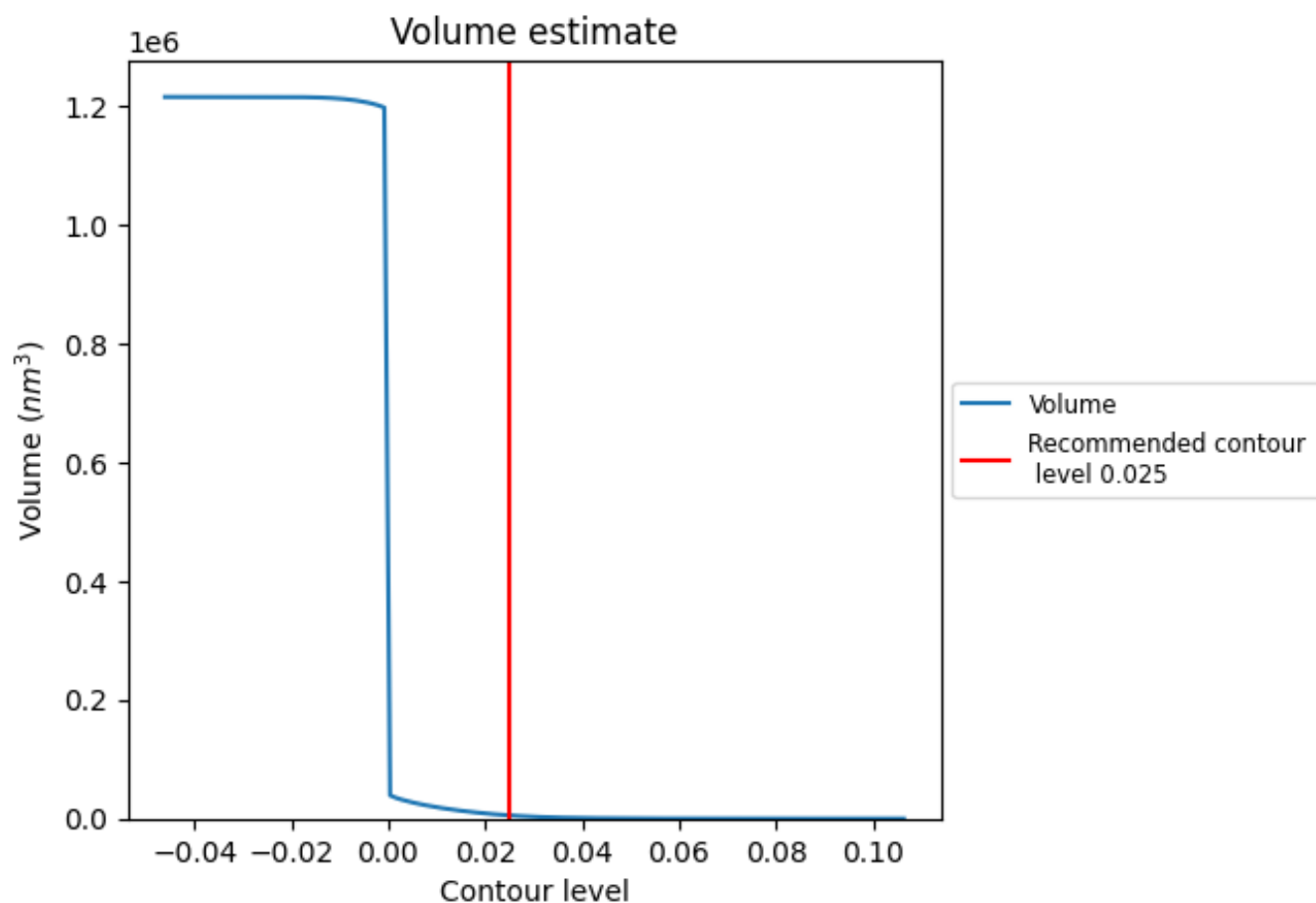
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

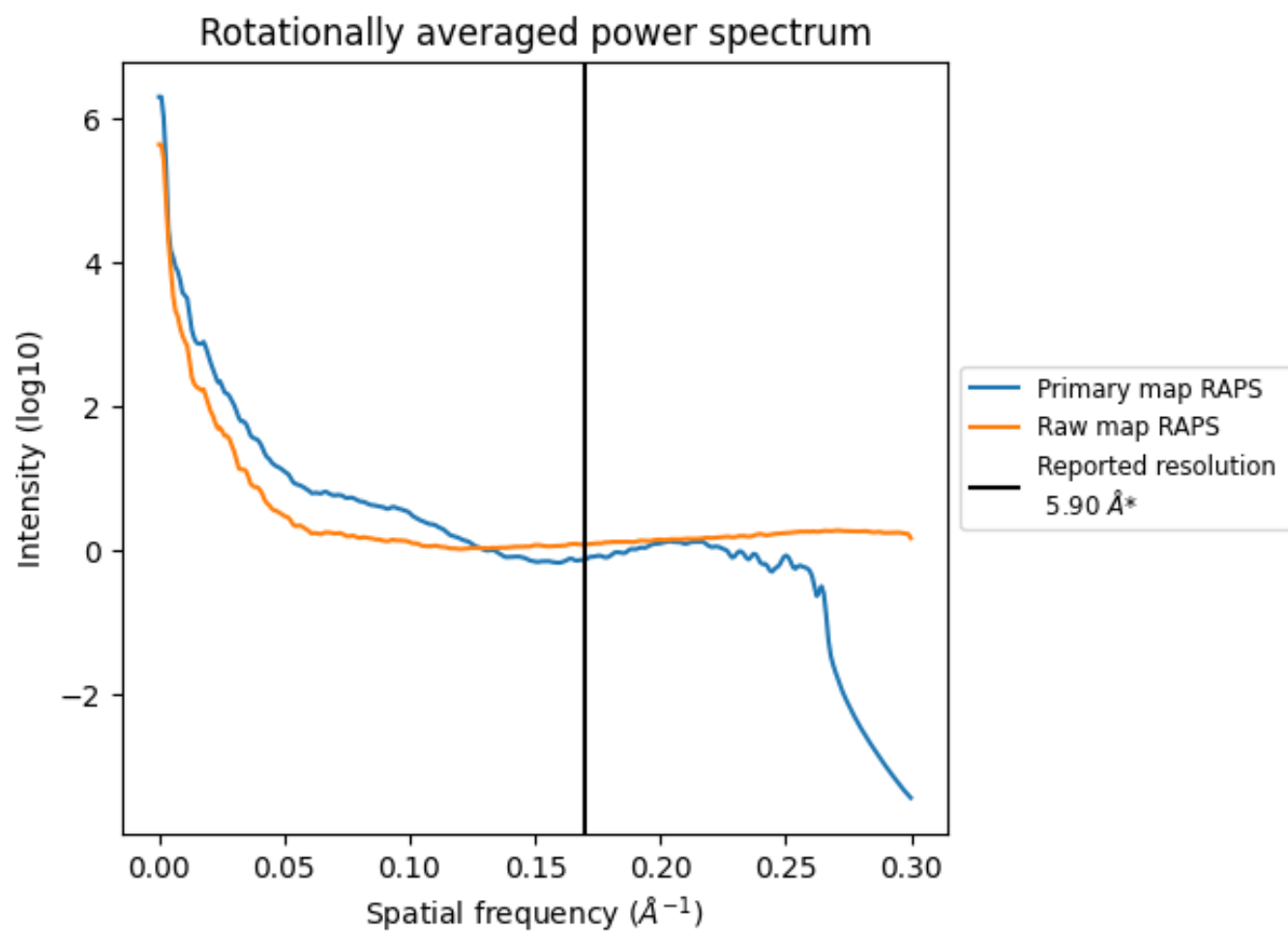
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5425 nm^3 ; this corresponds to an approximate mass of 4901 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 ⓘ

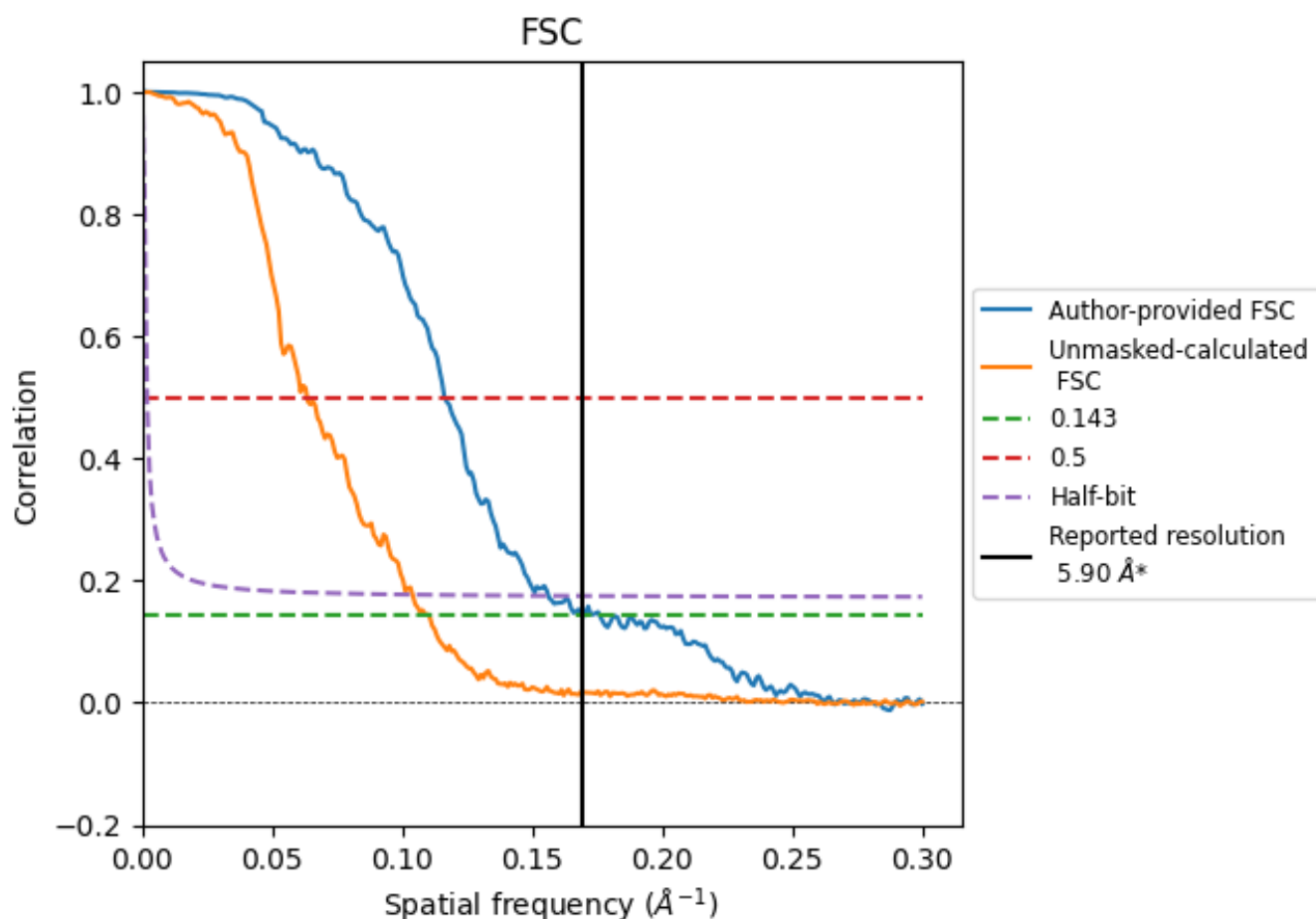


*Reported resolution corresponds to spatial frequency of 0.169 Å⁻¹

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 0.169 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.90	-	-
Author-provided FSC curve	5.90	8.61	6.40
Unmasked-calculated*	9.09	15.77	9.62

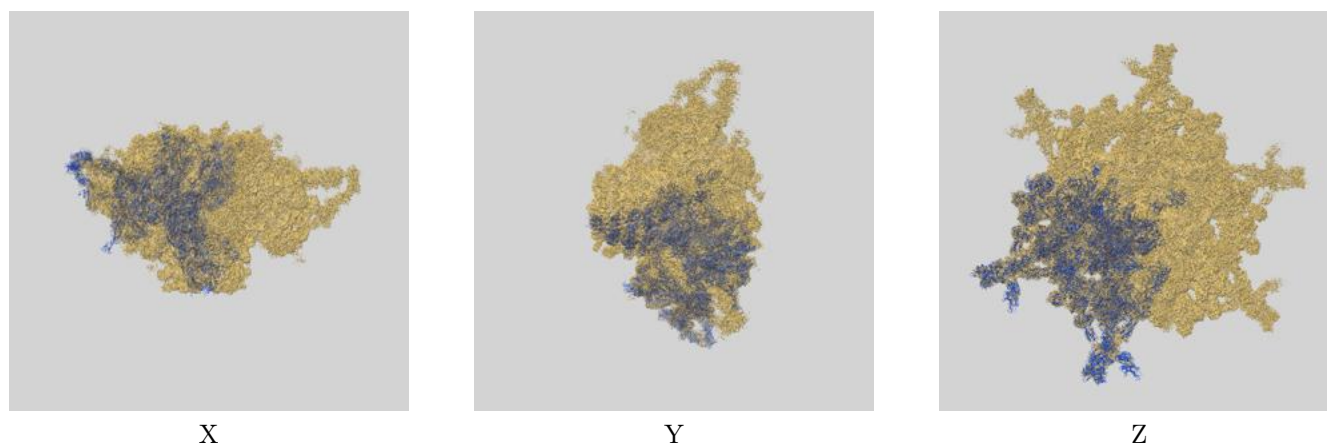
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.09 differs from the reported value 5.9 by more than 10 %

9 Map-model fit [i](#)

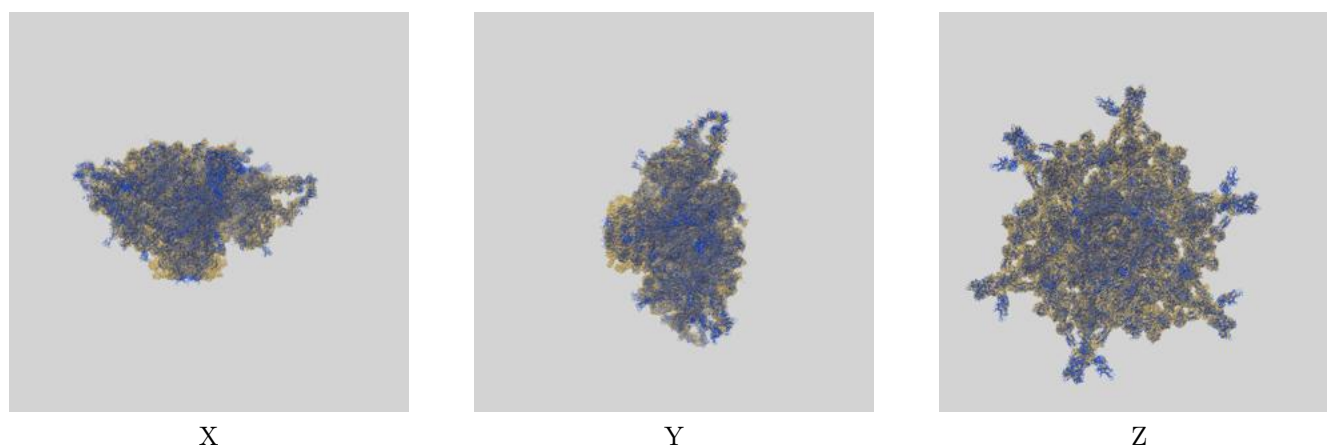
This section contains information regarding the fit between EMDB map EMD-55951 and PDB model 9TIC. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

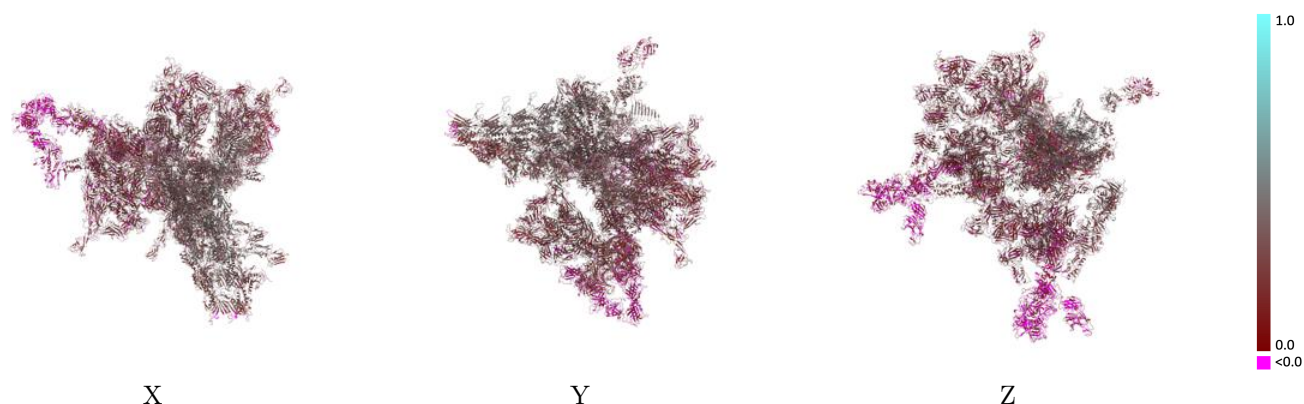


9.1.2 Map-model assembly overlay [i](#)



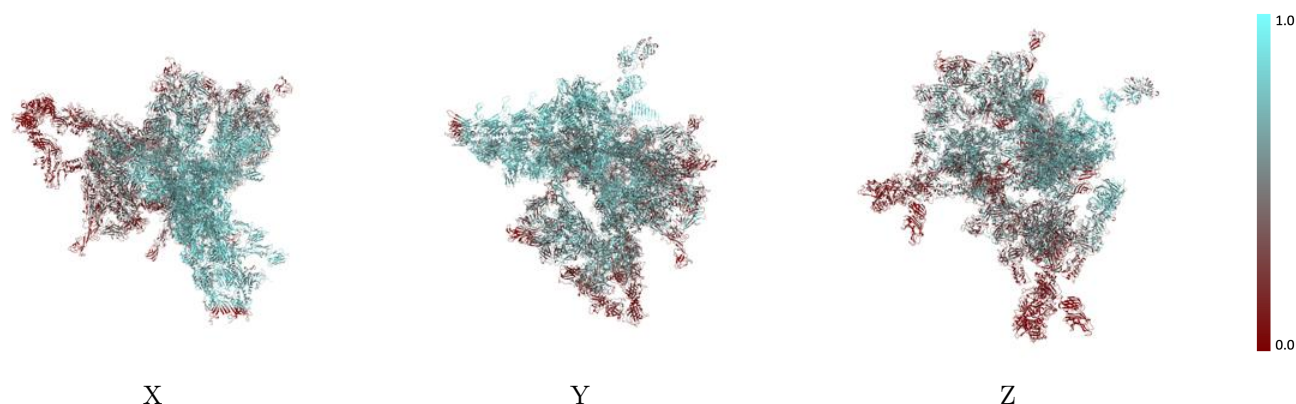
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



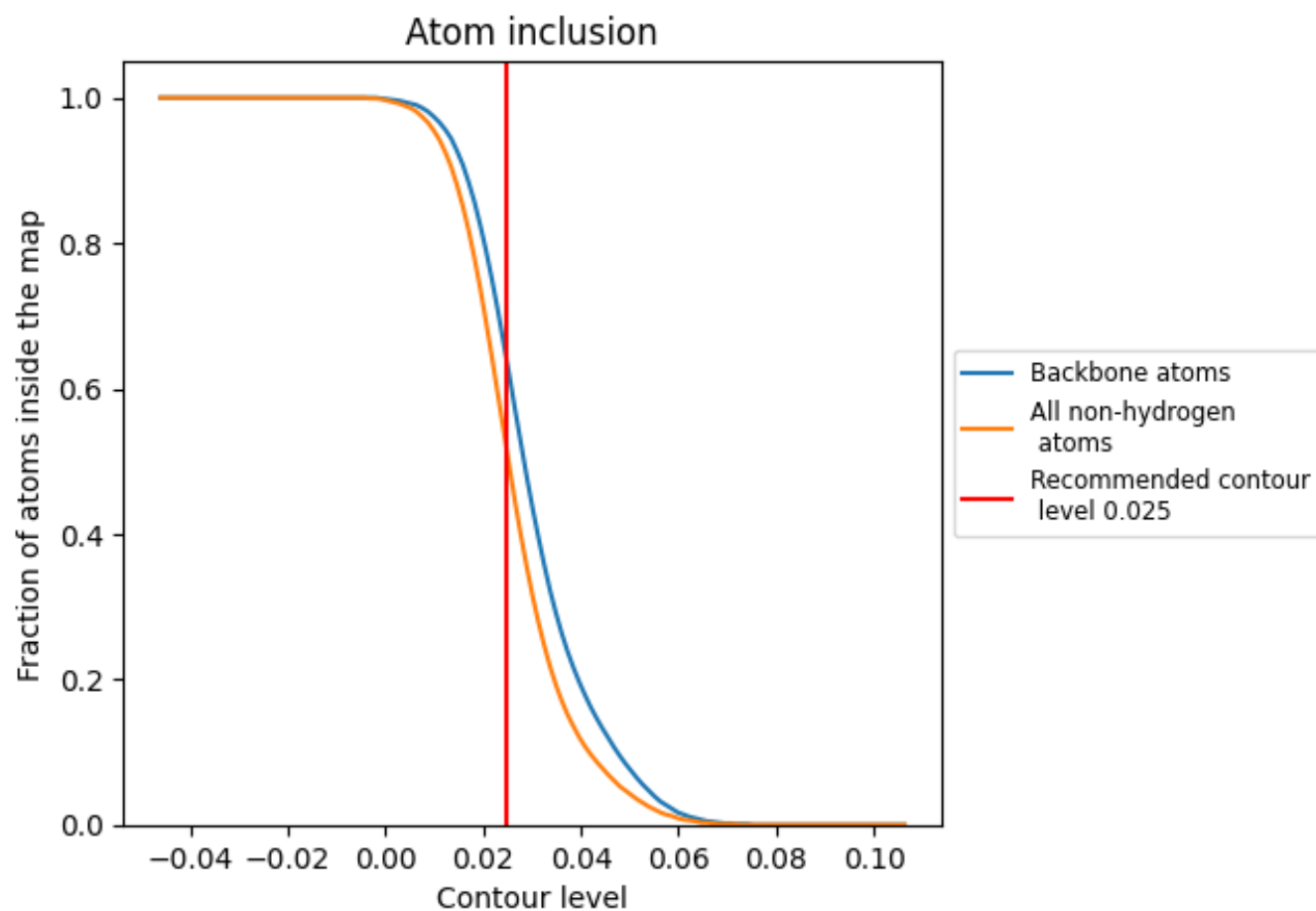
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 51% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5090	 0.2610
0	 0.5570	 0.2920
1	 0.0500	 0.0060
2	 0.5310	 0.2760
3	 0.5190	 0.2780
4	 0.5130	 0.2700
5	 0.3150	 0.2460
6	 0.3190	 0.2390
7	 0.2990	 0.2380
8	 0.5570	 0.2680
9	 0.5740	 0.2960
A	 0.7770	 0.3890
AA	 0.5150	 0.2590
AB	 0.5380	 0.2680
AC	 0.7680	 0.3970
AD	 0.7650	 0.4030
AE	 0.7580	 0.3830
AF	 0.7490	 0.3770
AG	 0.3760	 0.2410
AH	 0.4210	 0.2580
AI	 0.7540	 0.3540
AJ	 0.7510	 0.3580
AK	 0.7320	 0.3480
AL	 0.7370	 0.3420
AM	 0.6250	 0.2600
AN	 0.6200	 0.2590
B	 0.6120	 0.2620
C	 0.7180	 0.3380
D	 0.7400	 0.3590
E	 0.7340	 0.3550
F	 0.7700	 0.3970
G	 0.7710	 0.3900
H	 0.7520	 0.3700
I	 0.7600	 0.3710
J	 0.7550	 0.3680



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Chain	Atom inclusion	Q-score
K	 0.7540	 0.3680
L	 0.7440	 0.3510
M	 0.7620	 0.3520
N	 0.4010	 0.1610
O	 0.4640	 0.1870
P	 0.7080	 0.3200
Q	 0.5970	 0.2150
R	 0.4430	 0.1390
S	 0.3210	 0.0900
T	 0.1940	 0.0790
U	 0.1350	 0.0370
V	 0.0660	 0.0290
W	 0.0540	 0.0210
X	 0.0490	 0.0160
Y	 0.0400	 0.0130
Z	 0.0680	 0.0250
a	 0.4440	 0.2480
b	 0.3440	 0.2360
c	 0.3770	 0.2460
d	 0.4910	 0.2700
e	 0.7270	 0.3170
f	 0.6690	 0.2650
g	 0.6200	 0.2290
h	 0.4710	 0.1450
i	 0.4150	 0.1110
j	 0.2530	 0.0900
k	 0.1510	 0.0490
l	 0.0890	 0.0370
m	 0.1070	 0.0230
n	 0.1010	 0.0420
o	 0.1670	 0.0280
p	 0.1130	 0.0340
q	 0.5160	 0.2770
r	 0.5390	 0.2820
s	 0.5230	 0.2730
t	 0.5170	 0.2780
u	 0.5180	 0.2710
v	 0.5820	 0.2910
w	 0.5640	 0.3090
x	 0.5700	 0.3120
y	 0.5790	 0.3190
z	 0.4870	 0.2460