Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 10:31 AM EST

PDB ID	:	7TNQ
EMDB ID	:	EMD-26018
Title	:	The symmetry-released subpellicular microtubule map from detergent-extracted Toxoplasma cells
Authors	:	Sun, S.Y.; Pintilie, G.D.; Chen, M.
Deposited on	:	2022-01-21
Resolution	:	8.40 Å(reported)
Based on initial model	:	7MIZ

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:

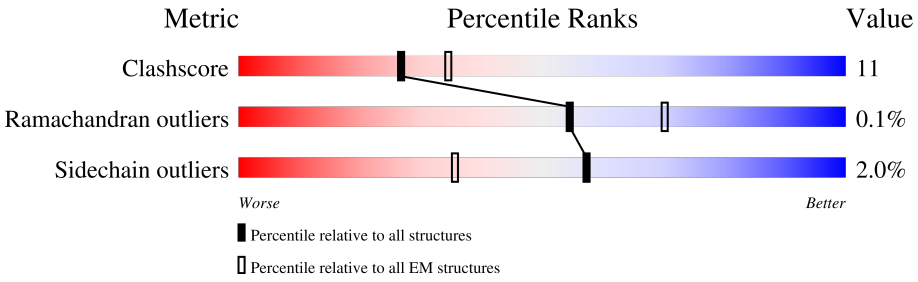
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 8.40 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	351	5% 5% · 94%
1	1	351	6% · · 94%
1	10	351	6% · · 94%
1	11	351	6% · · 94%
1	12	351	5% · ·· 94%
1	13	351	5% · · 94%
1	14	351	6% 6% 94%
1	15	351	5% 5% · 94%

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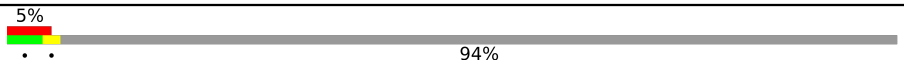
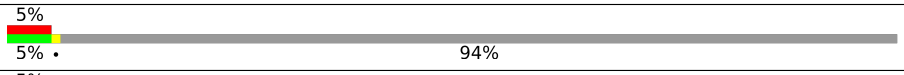
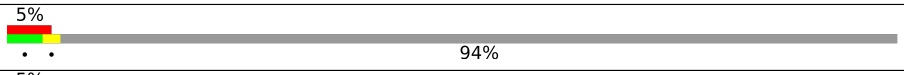
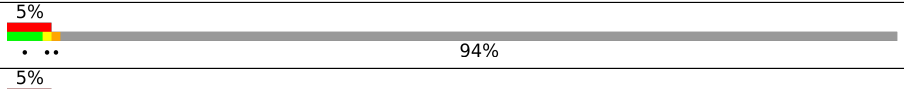
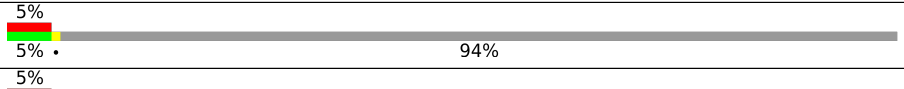
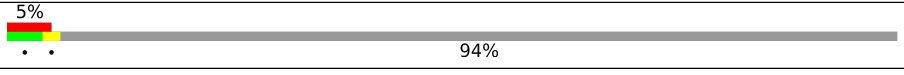
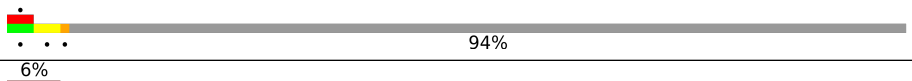
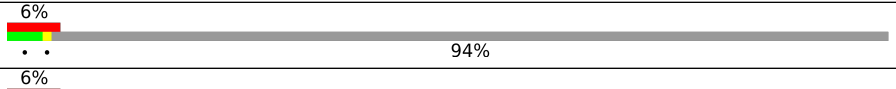
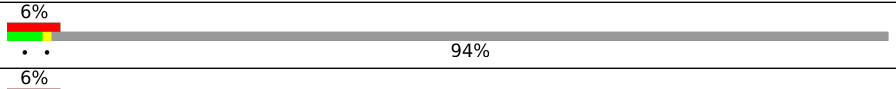
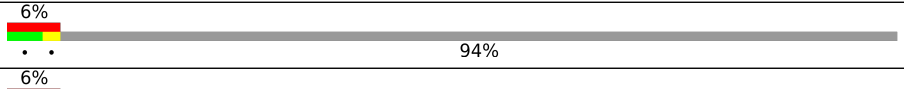
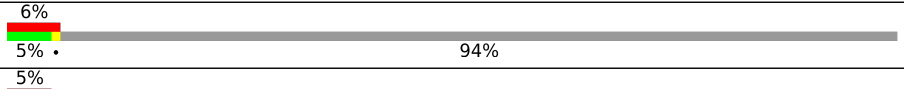
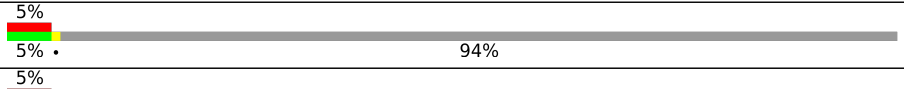
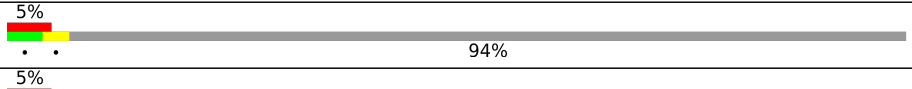
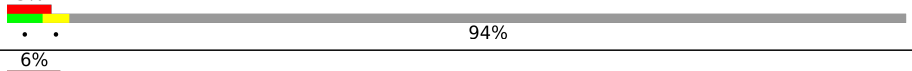
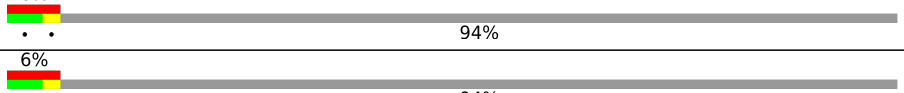
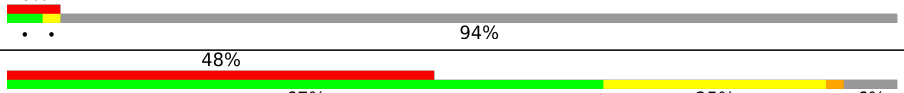
Mol	Chain	Length	Quality of chain
1	16	351	
1	17	351	
1	18	351	
1	19	351	
1	2	351	
1	20	351	
1	21	351	
1	22	351	
1	23	351	
1	3	351	
1	4	351	
1	5	351	
1	6	351	
1	7	351	
1	8	351	
1	9	351	
2	A0	453	
2	A2	453	
2	A4	453	
2	A6	453	
2	A8	453	
2	B0	453	
2	B2	453	
2	B4	453	
2	B6	453	

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Mol	Chain	Length	Quality of chain
2	B8	453	47% 72% 22% • 6%
2	C0	453	53% 71% 23% 6%
2	C2	453	46% 72% 21% • 6%
2	C4	453	54% 67% 26% • 6%
2	C6	453	48% 66% 28% • 6%
2	C8	453	57% 70% 23% • 6%
2	D0	453	51% 73% 20% • 6%
2	D2	453	59% 72% 21% • 6%
2	D4	453	53% 70% 22% • 6%
2	D6	453	60% 76% 17% • 6%
2	D8	453	51% 75% 18% • 6%
2	E0	453	65% 77% 17% 6%
2	E2	453	49% 77% 17% 6%
2	E4	453	76% 76% 18% • 6%
2	E6	453	45% 74% 20% • 6%
2	E8	453	83% 72% 23% 6%
2	F0	453	49% 70% 23% • 6%
3	A1	449	51% 69% 25% • 5%
3	A3	449	67% 76% 18% 5%
3	A5	449	47% 69% 24% • 5%
3	A7	449	60% 77% 17% • 5%
3	A9	449	49% 74% 20% 5%
3	B1	449	56% 78% 16% • 5%
3	B3	449	49% 73% 19% • 5%
3	B5	449	53% 77% 17% • 5%

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Mol	Chain	Length	Quality of chain
3	B7	449	40% 76% 18% • 5%
3	B9	449	51% 76% 18% • 5%
3	C1	449	40% 70% 23% • 5%
3	C3	449	46% 71% 24% 5%
3	C5	449	45% 71% 22% • 5%
3	C7	449	48% 69% 25% • 5%
3	C9	449	51% 69% 24% • 5%
3	D1	449	55% 71% 22% • 5%
3	D3	449	54% 69% 25% • 5%
3	D5	449	55% 66% 25% • 5%
3	D7	449	53% 73% 20% • 5%
3	D9	449	50% 70% 24% • 5%
3	E1	449	46% 74% 20% • 5%
3	E3	449	43% 76% 17% • 5%
3	E5	449	45% 71% 22% • 5%
3	E7	449	40% 73% 21% • 5%
3	E9	449	53% 73% 22% 5%
3	F1	449	43% 68% 26% • 5%
4	a	220	43% 64% 5% 32%
4	b	220	48% 65% • 32%
4	c	220	41% 86% 5% • 9%
4	d	220	55% 85% 6% 9%
4	e	220	36% 85% 6% • 9%
4	f	220	43% 85% 7% 9%
4	g	220	41% 88% • 9%

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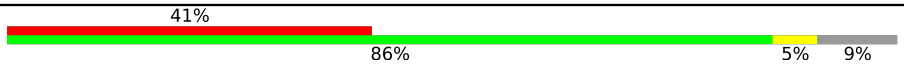
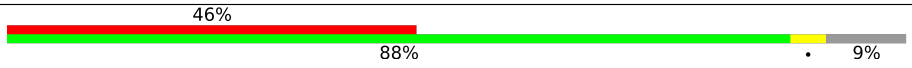
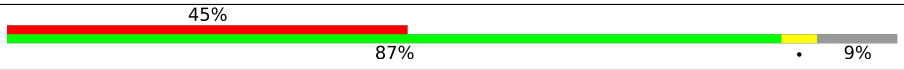
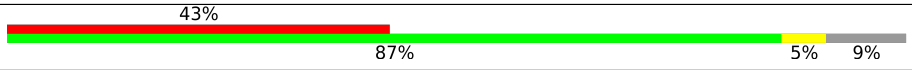
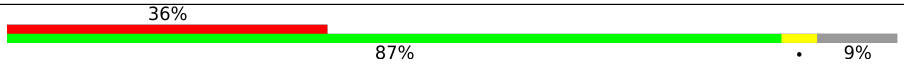
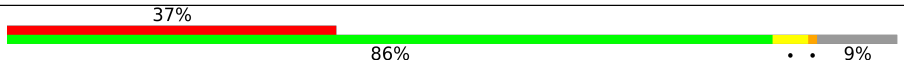
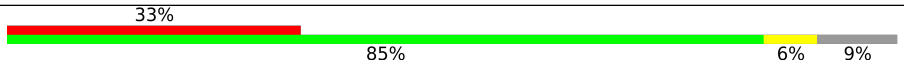
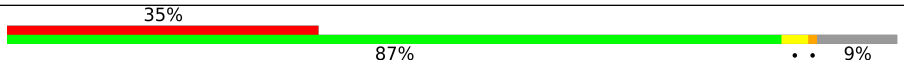
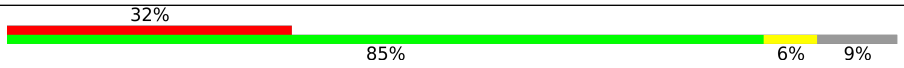
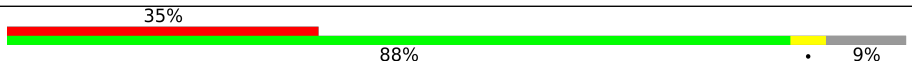
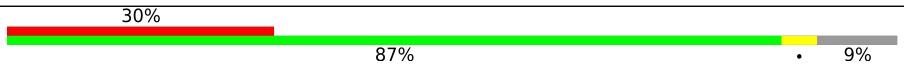
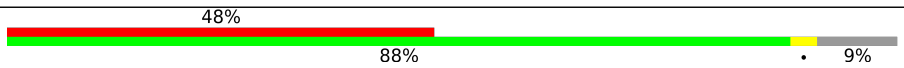
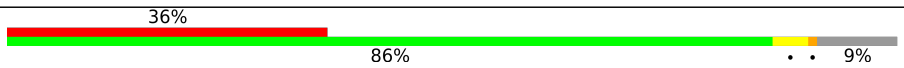
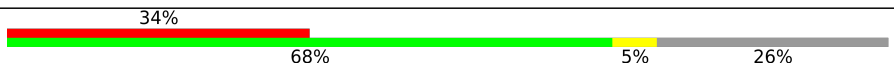
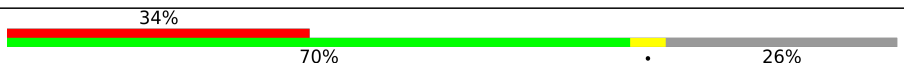
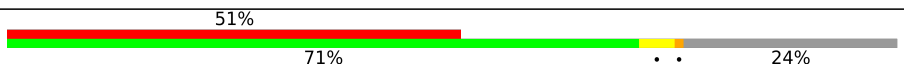
Mol	Chain	Length	Quality of chain
4	h	220	
4	i	220	
4	j	220	
4	m	220	
4	n	220	
4	o	220	
4	p	220	
4	q	220	
4	r	220	
4	s	220	
4	t	220	
4	u	220	
4	v	220	
5	k	189	
5	l	189	
5	w	189	
5	x	189	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 213168 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 Microtubule associated protein SPM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	1	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	10	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	11	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	12	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	13	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	14	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	15	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	16	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	17	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	18	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	19	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	2	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	20	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	21	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	22	20	Total	C	N	O	S	0	0
			160	105	26	28	1		
1	23	20	Total	C	N	O	S	0	0
			160	105	26	28	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	4	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	5	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	6	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	7	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	8	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	9	22	Total	C	N	O	S	0	0
			174	114	28	31	1		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	263	ALA	VAL	conflict	UNP S8F1Y1
1	263	ALA	VAL	conflict	UNP S8F1Y1
10	263	ALA	VAL	conflict	UNP S8F1Y1
11	263	ALA	VAL	conflict	UNP S8F1Y1
12	263	ALA	VAL	conflict	UNP S8F1Y1
13	263	ALA	VAL	conflict	UNP S8F1Y1
14	263	ALA	VAL	conflict	UNP S8F1Y1
15	263	ALA	VAL	conflict	UNP S8F1Y1
16	263	ALA	VAL	conflict	UNP S8F1Y1
17	263	ALA	VAL	conflict	UNP S8F1Y1
18	263	ALA	VAL	conflict	UNP S8F1Y1
19	263	ALA	VAL	conflict	UNP S8F1Y1
2	263	ALA	VAL	conflict	UNP S8F1Y1
20	263	ALA	VAL	conflict	UNP S8F1Y1
21	263	ALA	VAL	conflict	UNP S8F1Y1
22	263	ALA	VAL	conflict	UNP S8F1Y1
23	263	ALA	VAL	conflict	UNP S8F1Y1
3	263	ALA	VAL	conflict	UNP S8F1Y1
4	263	ALA	VAL	conflict	UNP S8F1Y1
5	263	ALA	VAL	conflict	UNP S8F1Y1
6	263	ALA	VAL	conflict	UNP S8F1Y1
7	263	ALA	VAL	conflict	UNP S8F1Y1
8	263	ALA	VAL	conflict	UNP S8F1Y1
9	263	ALA	VAL	conflict	UNP S8F1Y1

- Molecule 2 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	A2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	A4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	A6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	A8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	E2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	F0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		

- Molecule 3 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A9	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B9	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	C9	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	D1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	D3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	D5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	D7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	D9	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	E1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	E3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	E5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	E7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	E9	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	F1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		

- Molecule 4 is a protein called PDI family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	150	Total	C	N	O	S	0	0
			1198	763	213	217	5		
4	b	150	Total	C	N	O	S	0	0
			1198	763	213	217	5		
4	c	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	d	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	e	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	f	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	g	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	h	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	i	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	j	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	m	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	n	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	o	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	p	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	q	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	r	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	s	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	t	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	u	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	v	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		

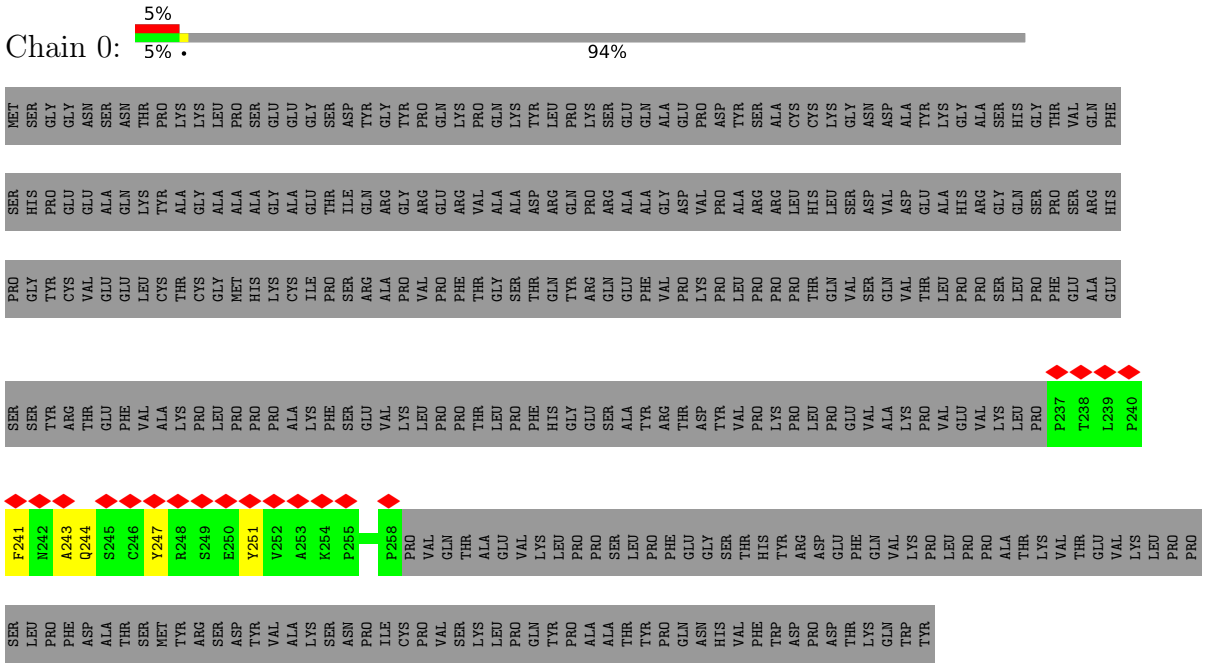
- Molecule 5 is a protein called PDI family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	k	139	Total	C	N	O	S	0	0
			1140	738	203	195	4		
5	l	139	Total	C	N	O	S	0	0
			1140	738	203	195	4		
5	w	143	Total	C	N	O	S	0	0
			1172	755	207	205	5		
5	x	143	Total	C	N	O	S	0	0
			1172	755	207	205	5		

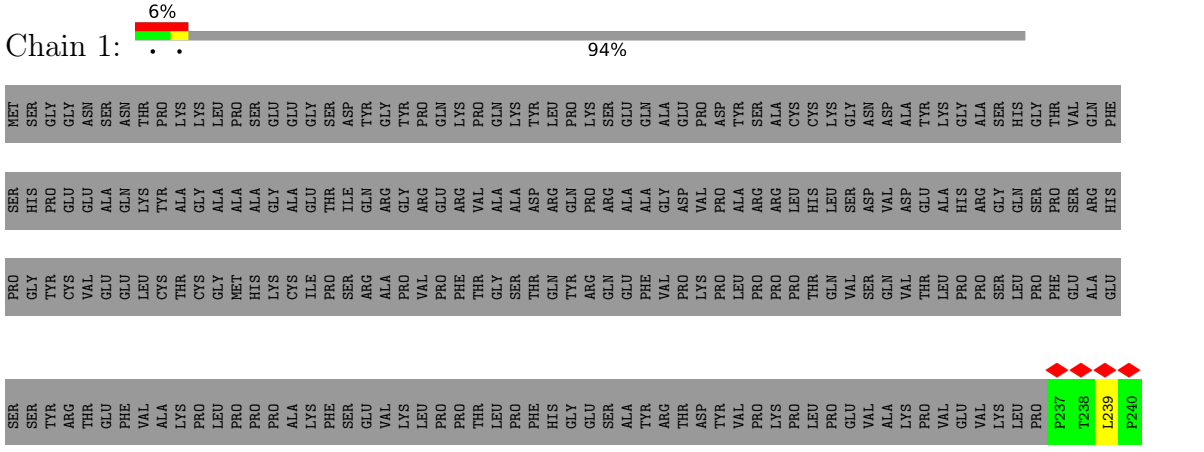
3 Residue-property plots (i)

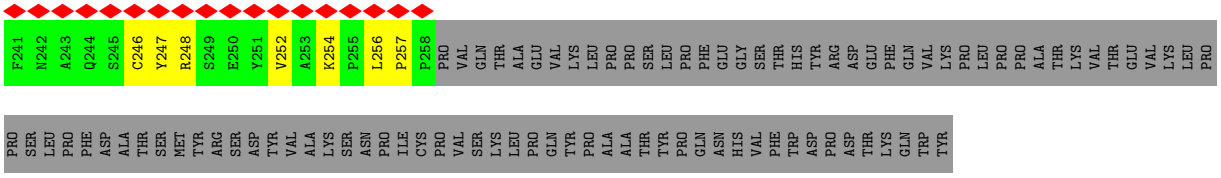
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Microtubule associated protein SPM1

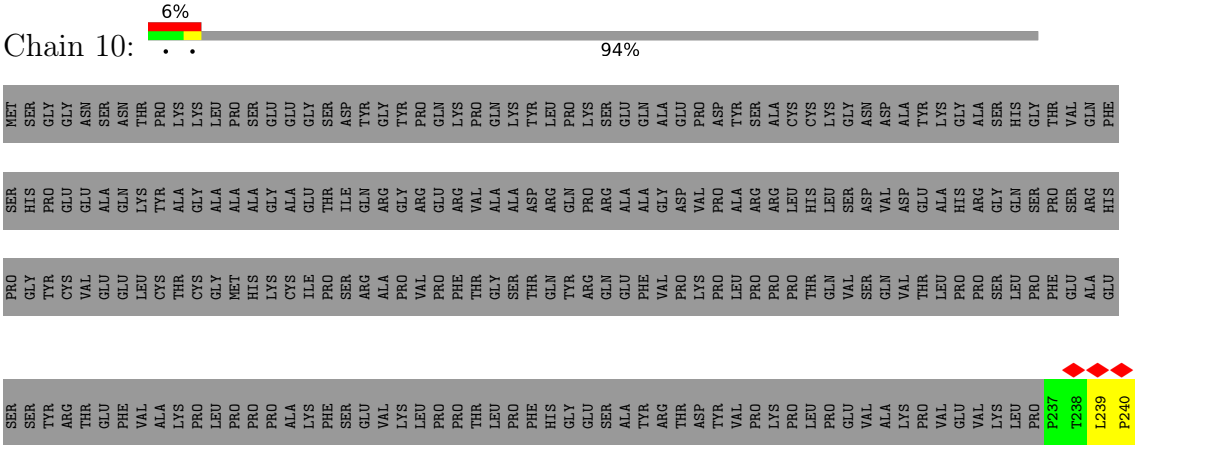


• Molecule 1: Microtubule associated protein SPM1

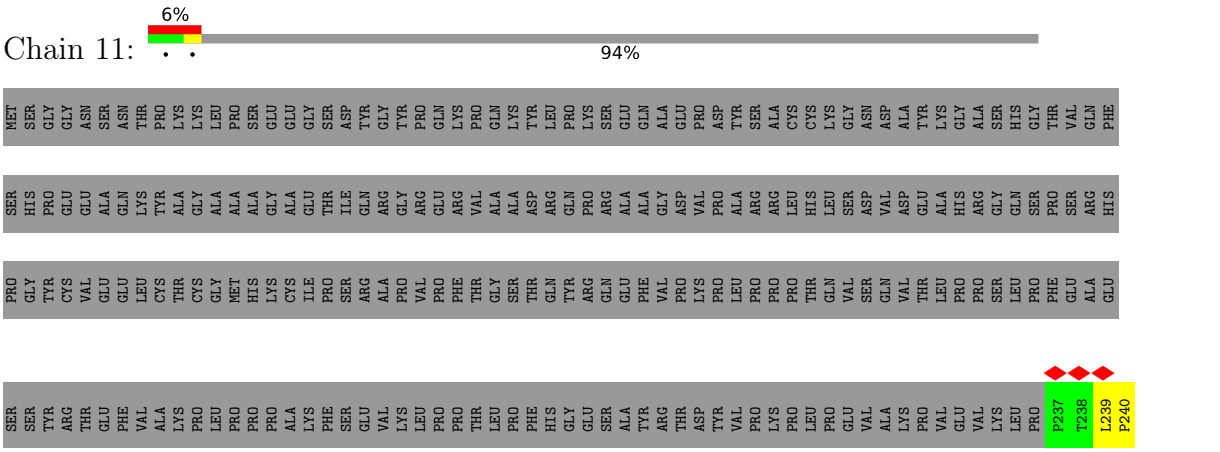




• Molecule 1: Microtubule associated protein SPM1

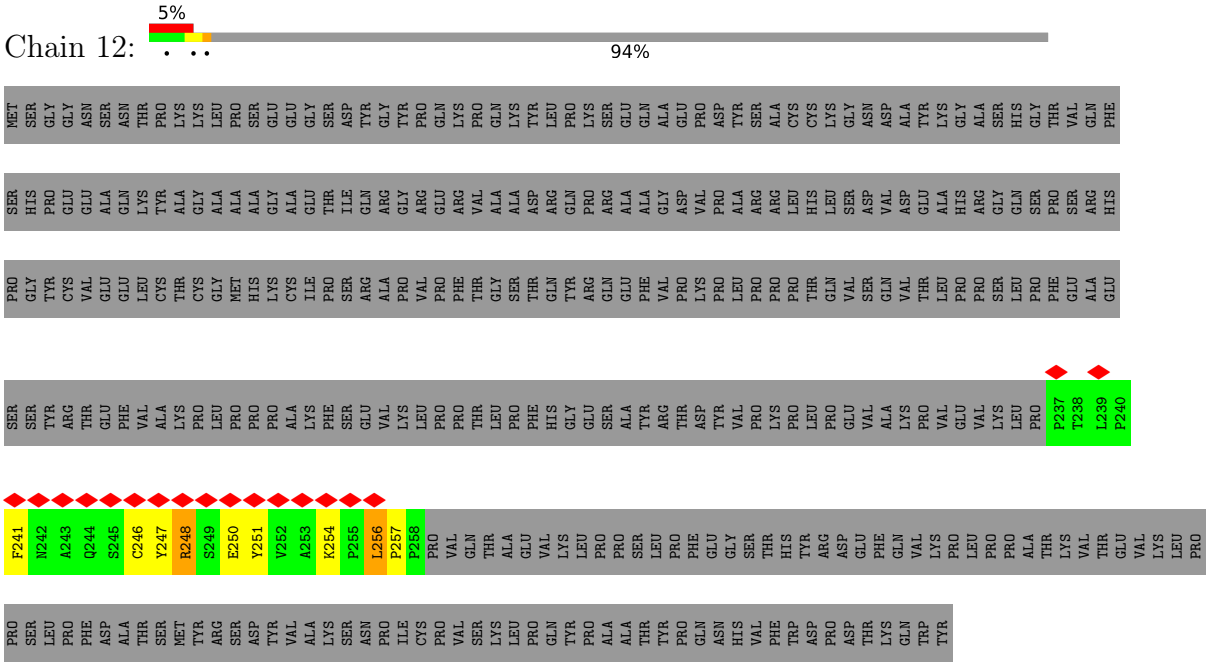


• Molecule 1: Microtubule associated protein SPM1



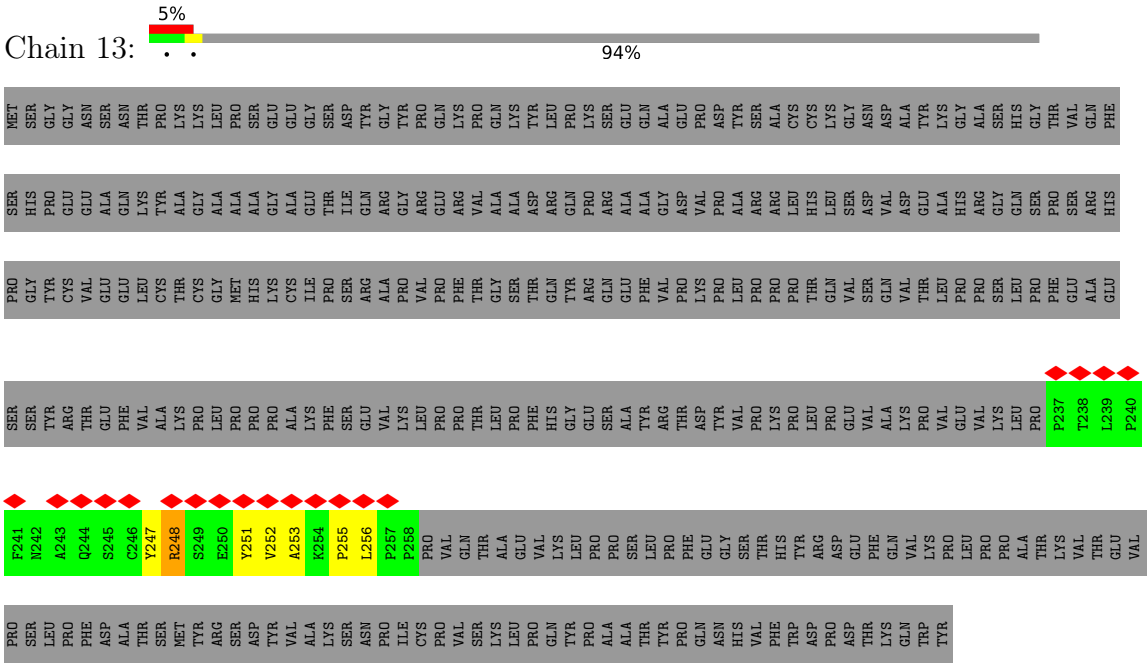
• Molecule 1: Microtubule associated protein SPM1

Chain 12:



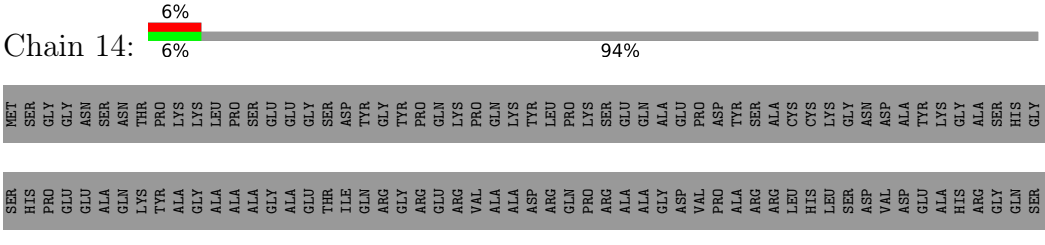
• Molecule 1: Microtubule associated protein SPM1

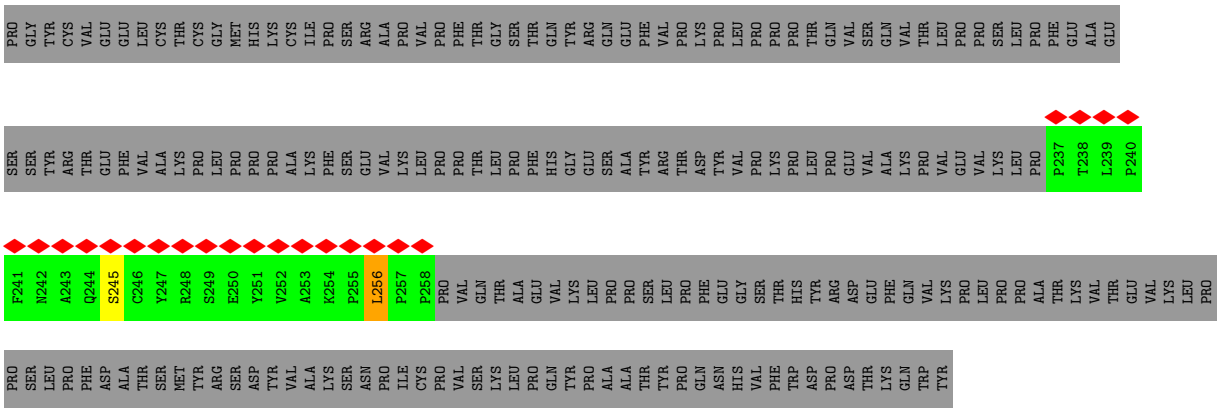
Chain 13:



• Molecule 1: Microtubule associated protein SPM1

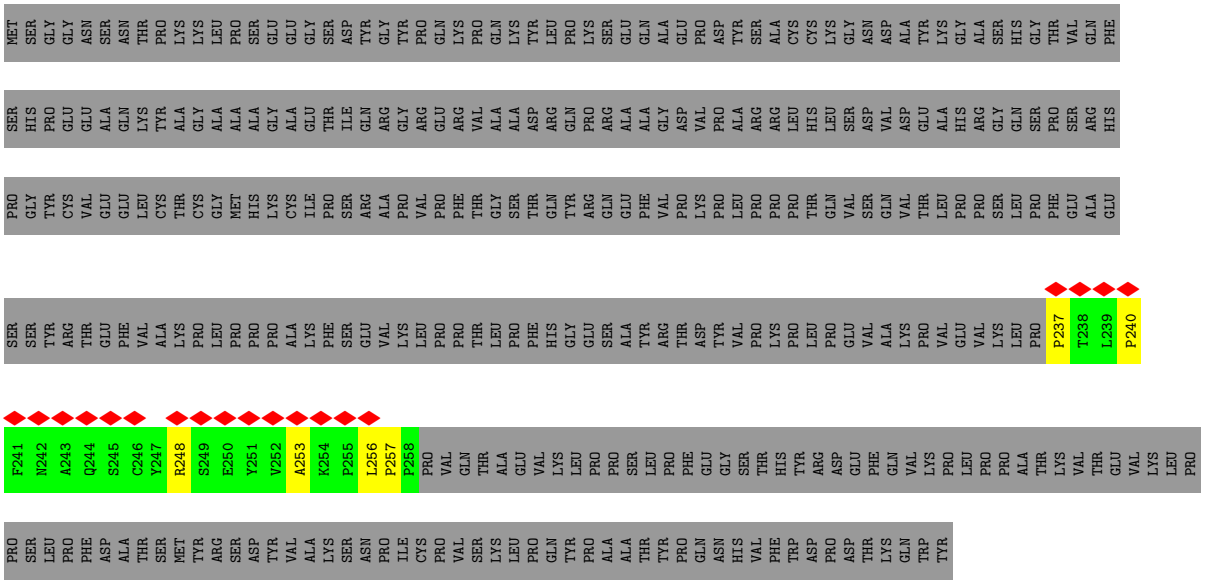
Chain 14:





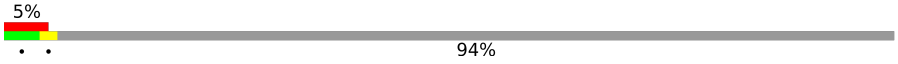
• Molecule 1: Microtubule associated protein SPM1

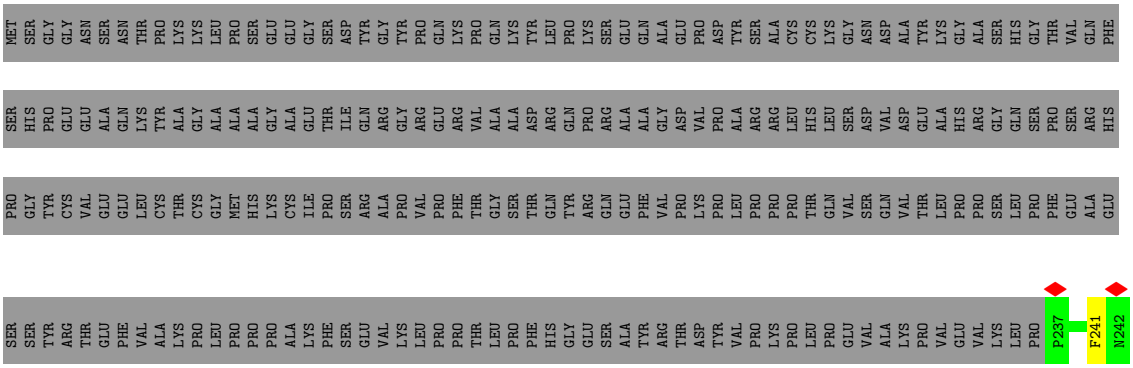
Chain 15:

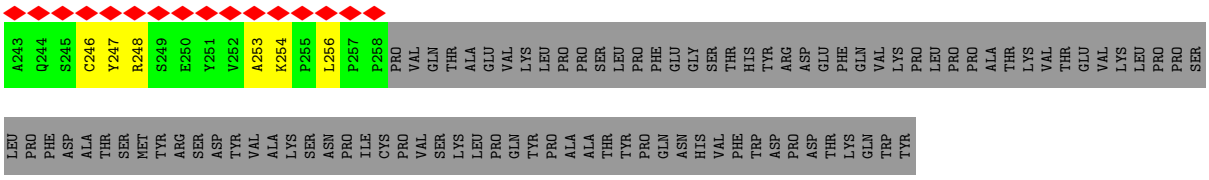


• Molecule 1: Microtubule associated protein SPM1

Chain 16:

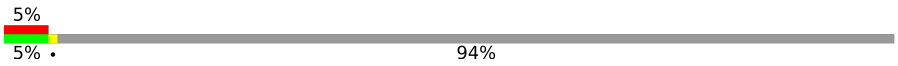


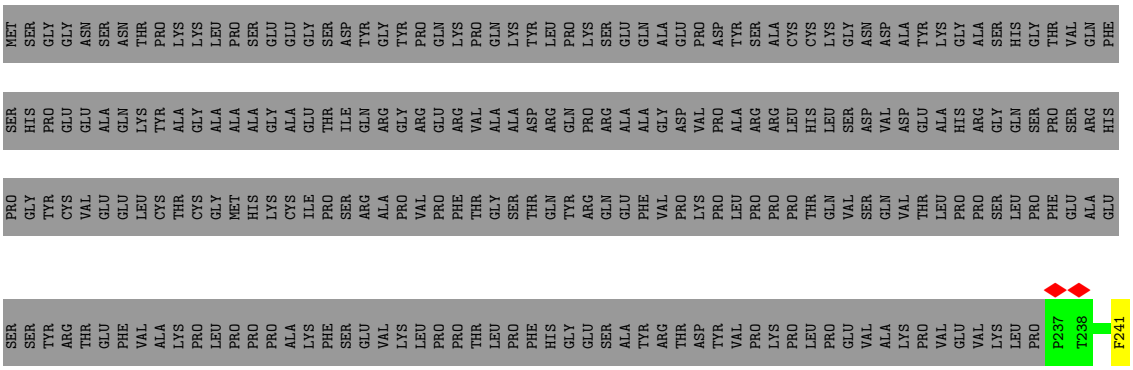


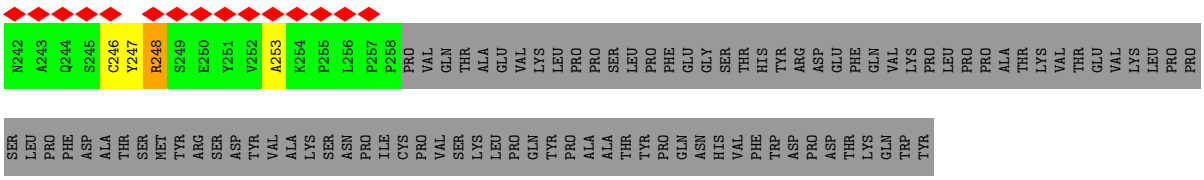


• Molecule 1: Microtubule associated protein SPM1

Chain 17:

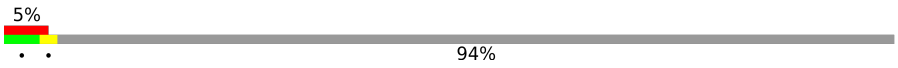


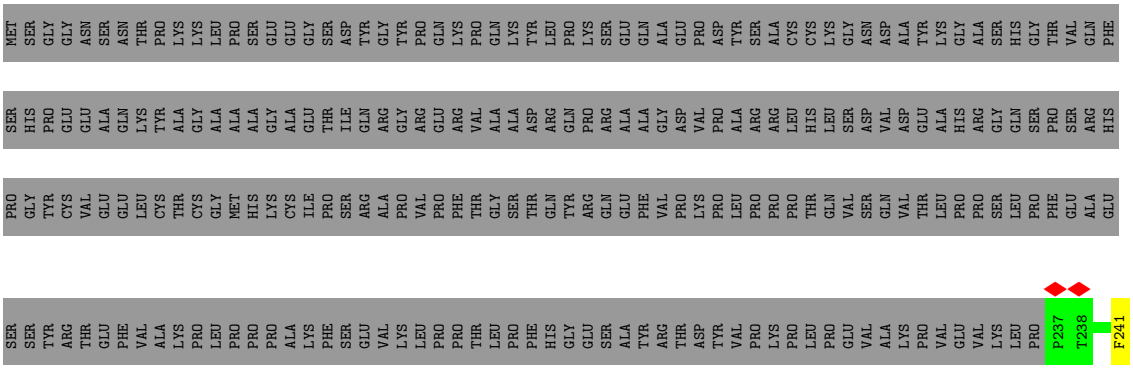


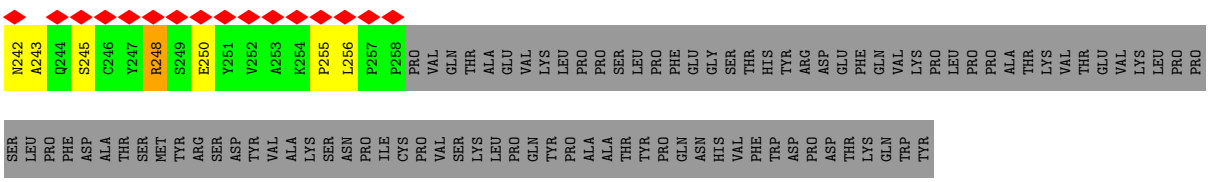


• Molecule 1: Microtubule associated protein SPM1

Chain 18:

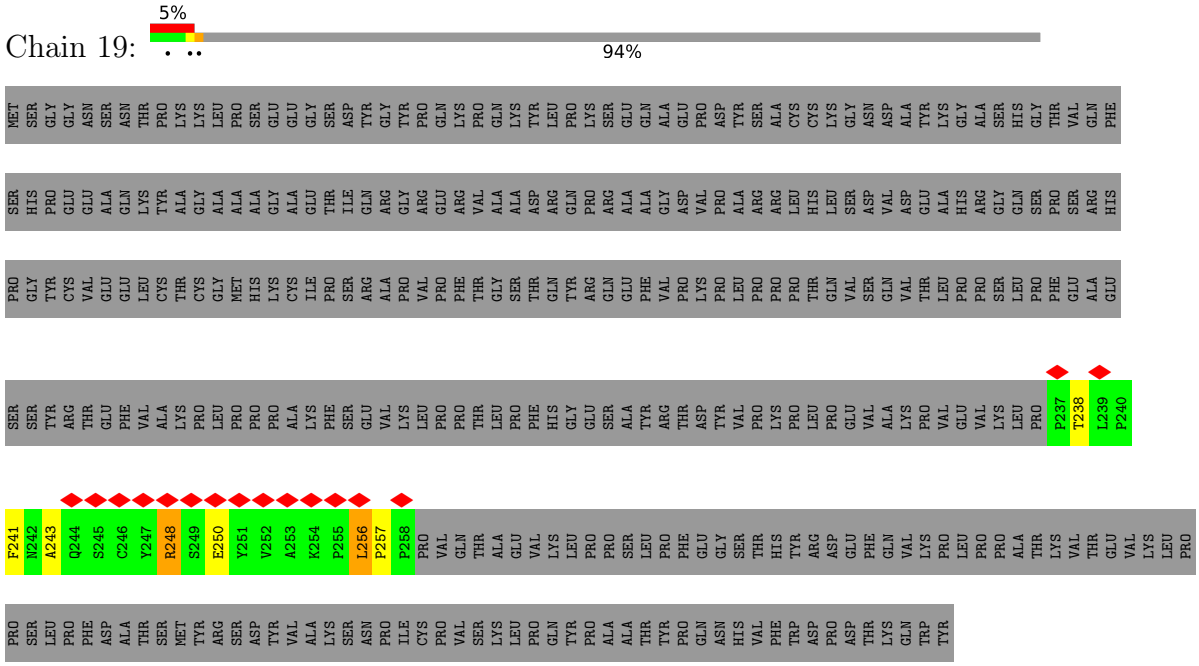






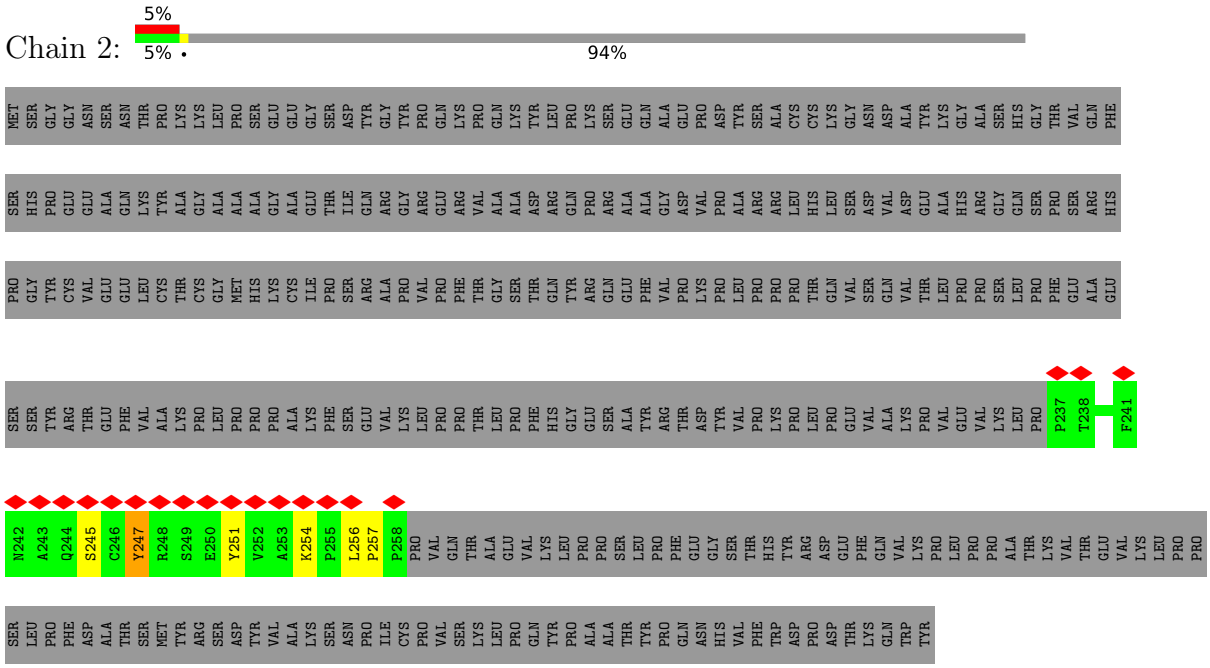
• Molecule 1: Microtubule associated protein SPM1

Chain 19:



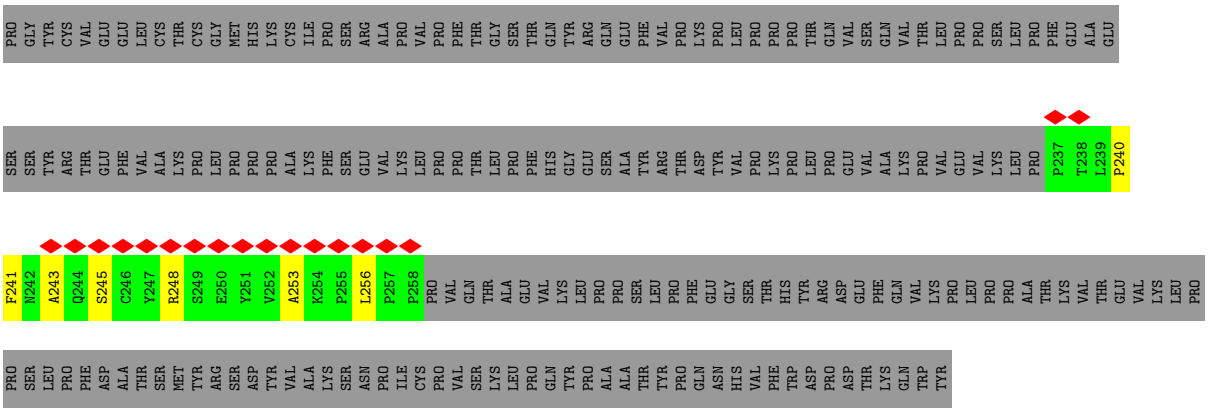
• Molecule 1: Microtubule associated protein SPM1

Chain 2:



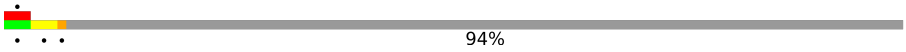
• Molecule 1: Microtubule associated protein SPM1

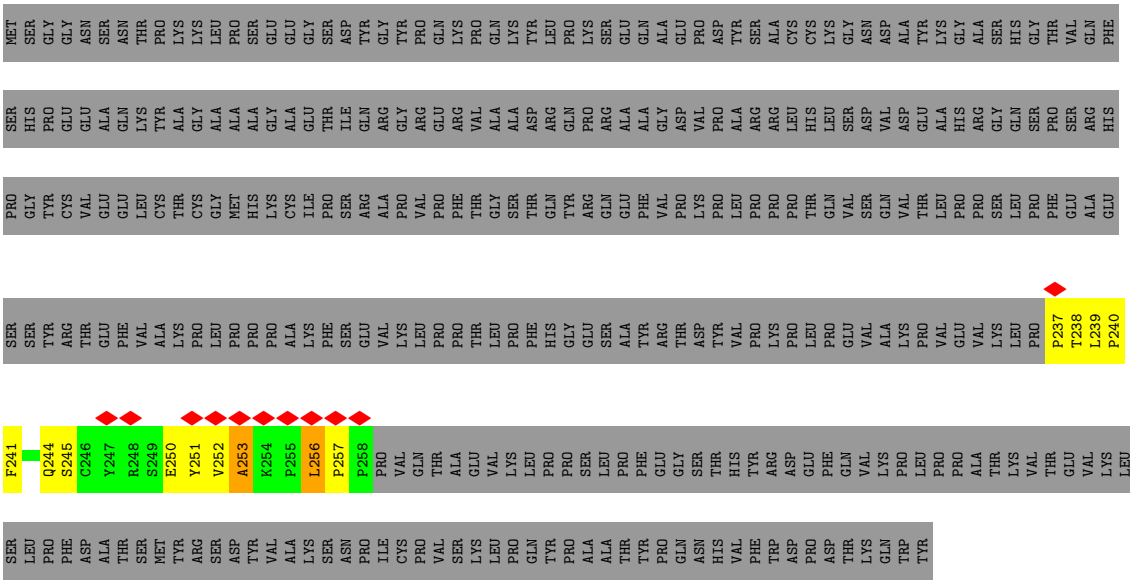
Chain 20:



• Molecule 1: Microtubule associated protein SPM1

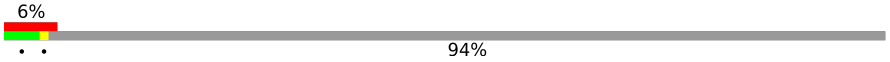
Chain 21:

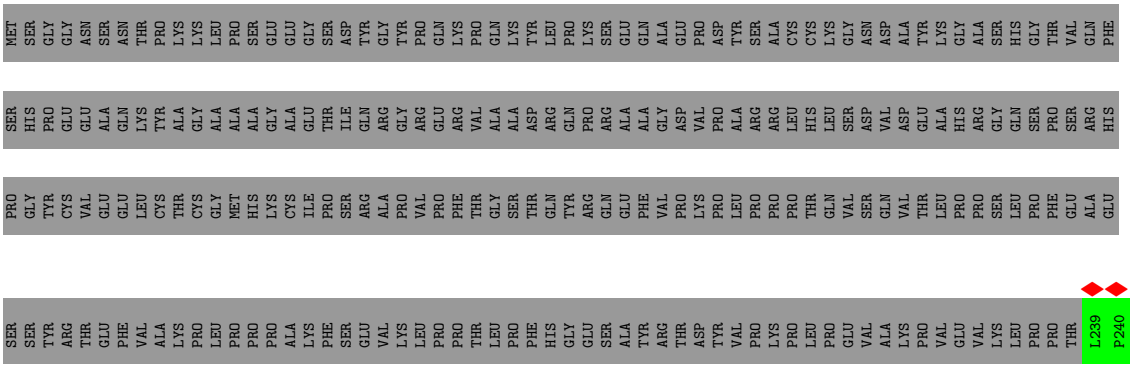


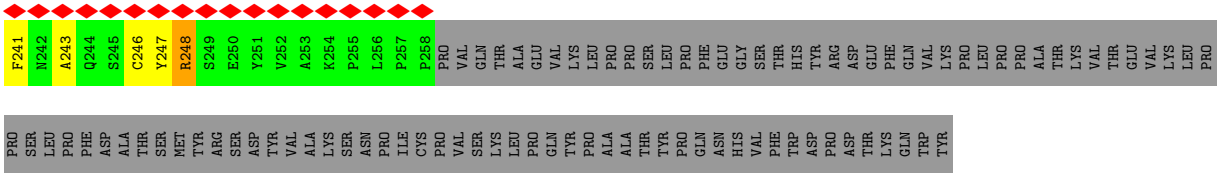


• Molecule 1: Microtubule associated protein SPM1

Chain 22:

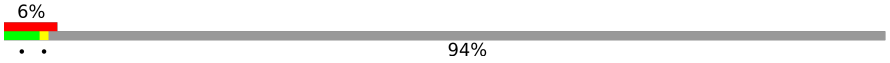


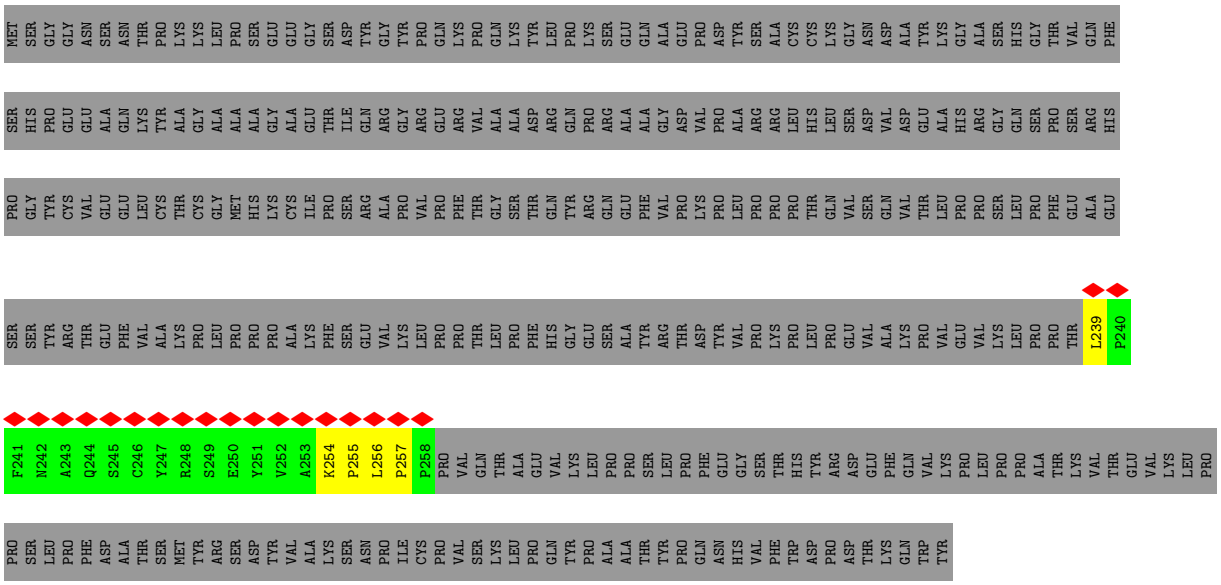




• Molecule 1: Microtubule associated protein SPM1

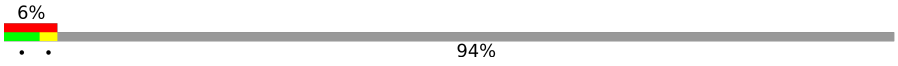
Chain 23:

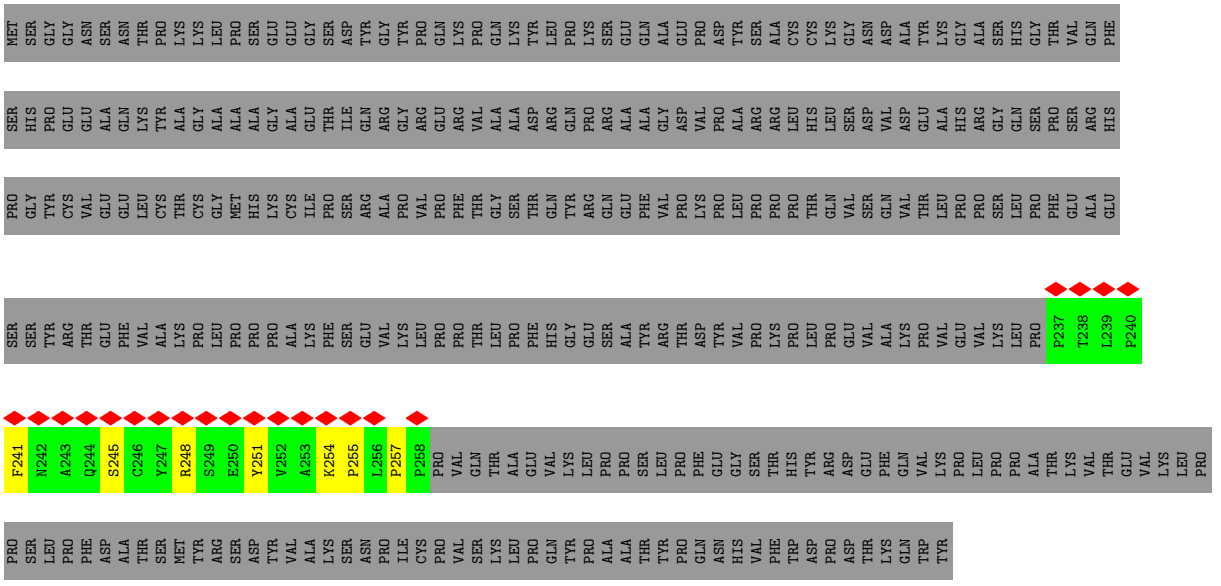




• Molecule 1: Microtubule associated protein SPM1

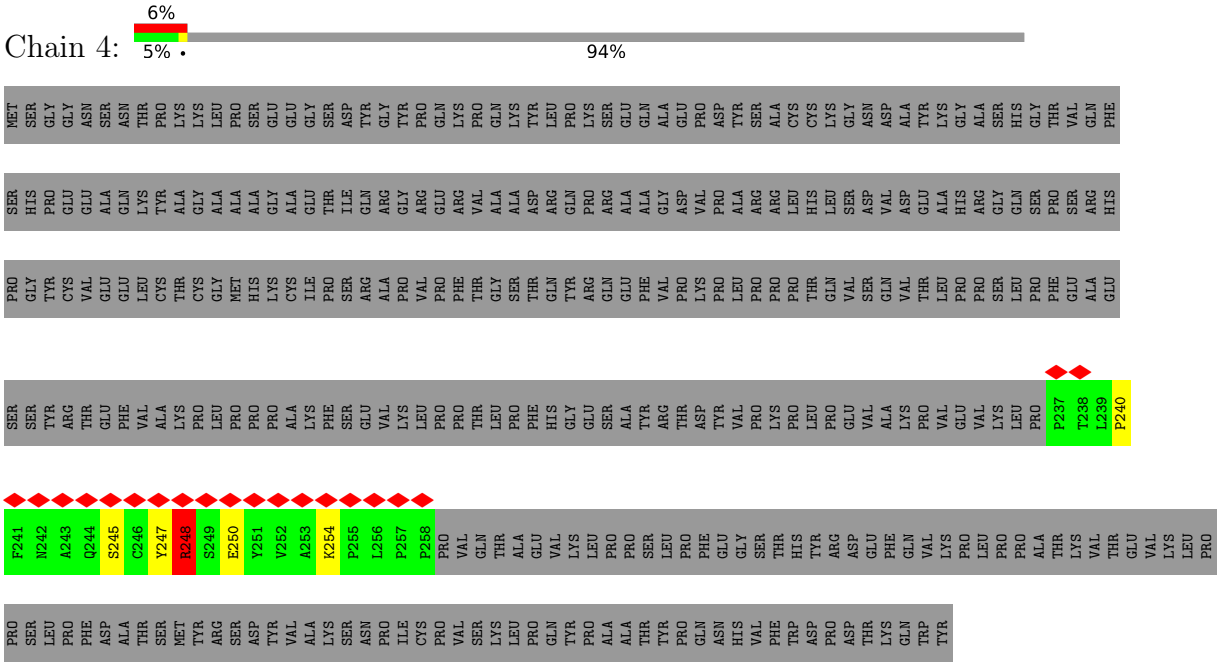
Chain 3:





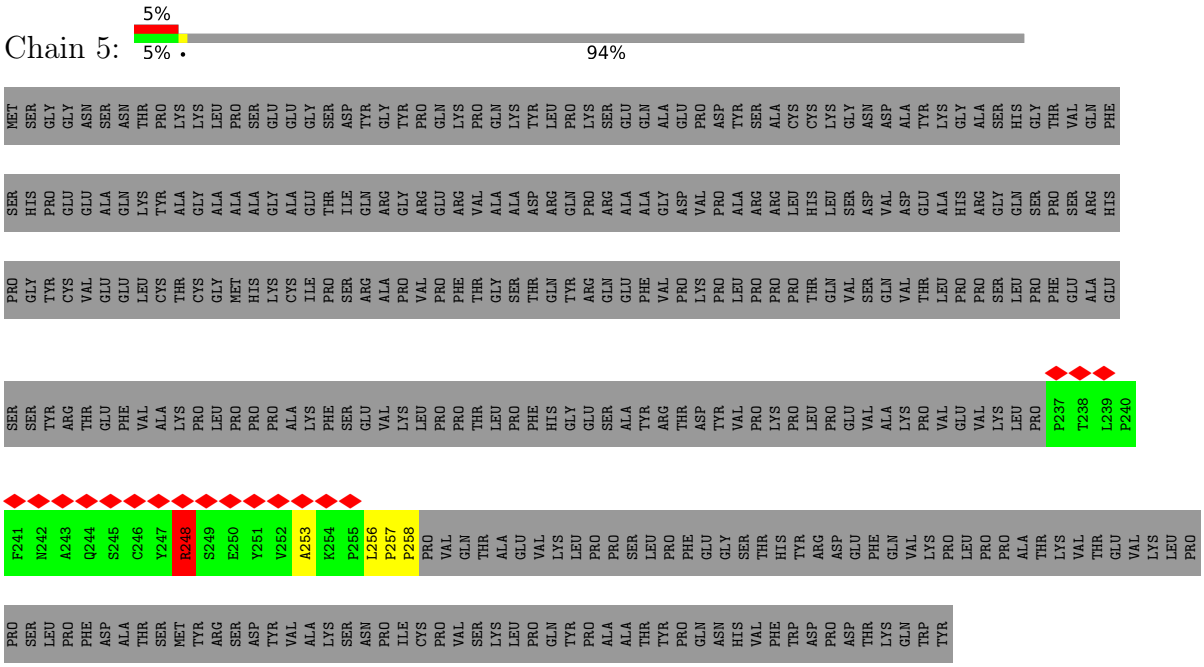
• Molecule 1: Microtubule associated protein SPM1

Chain 4:



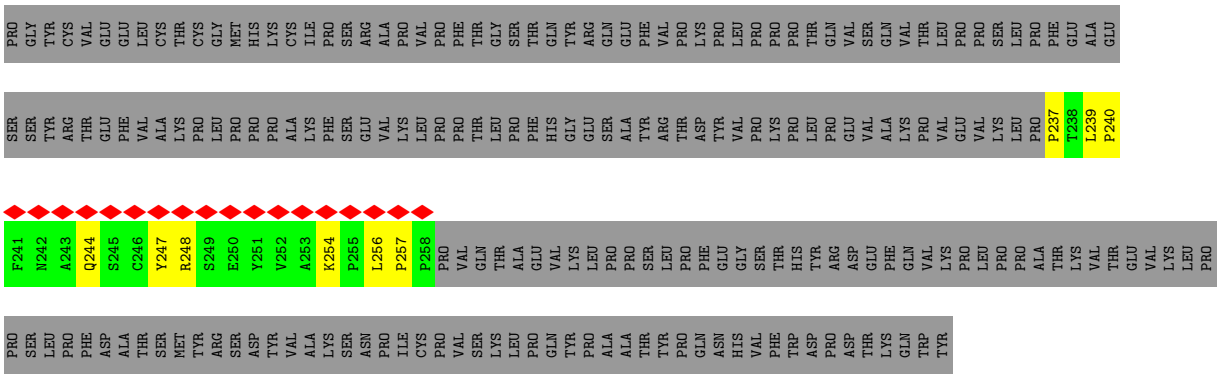
• Molecule 1: Microtubule associated protein SPM1

Chain 5:



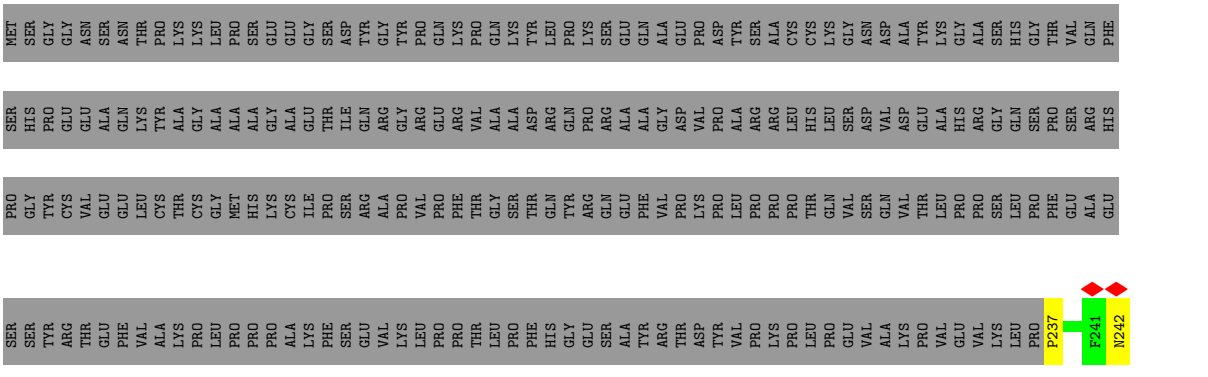
• Molecule 1: Microtubule associated protein SPM1

Chain 6:



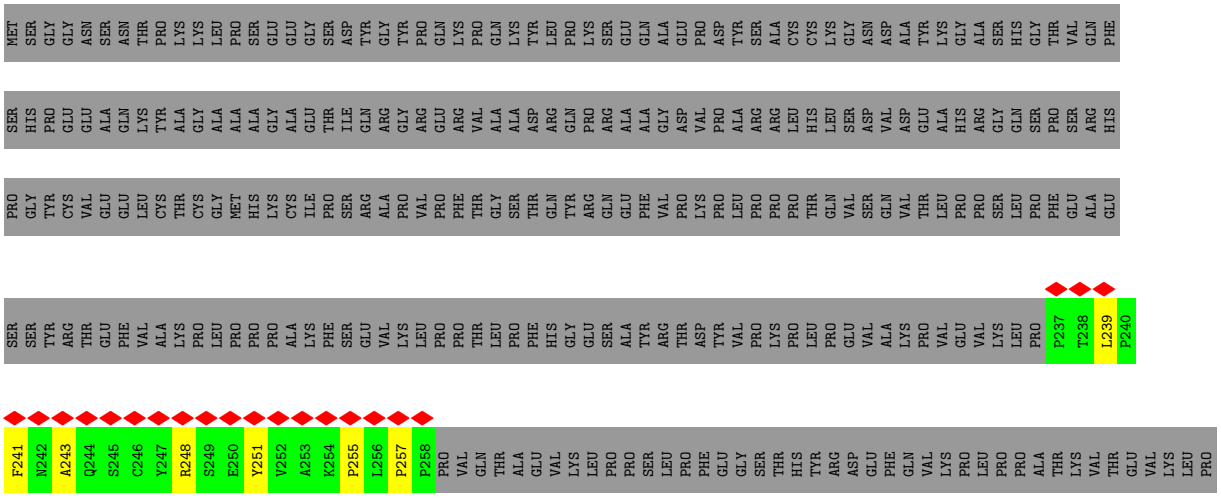
• Molecule 1: Microtubule associated protein SPM1

Chain 7: 5% 94%



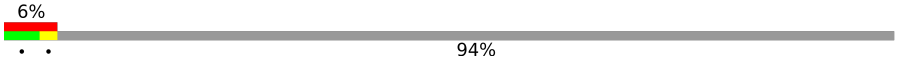
• Molecule 1: Microtubule associated protein SPM1

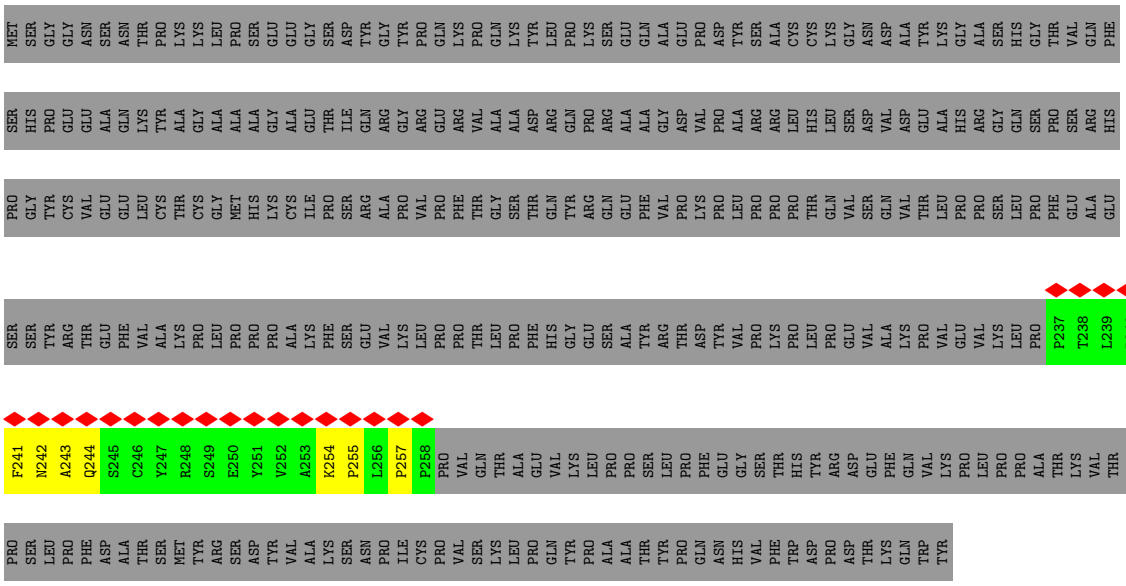
Chain 8: 6% 94%



• Molecule 1: Microtubule associated protein SPM1

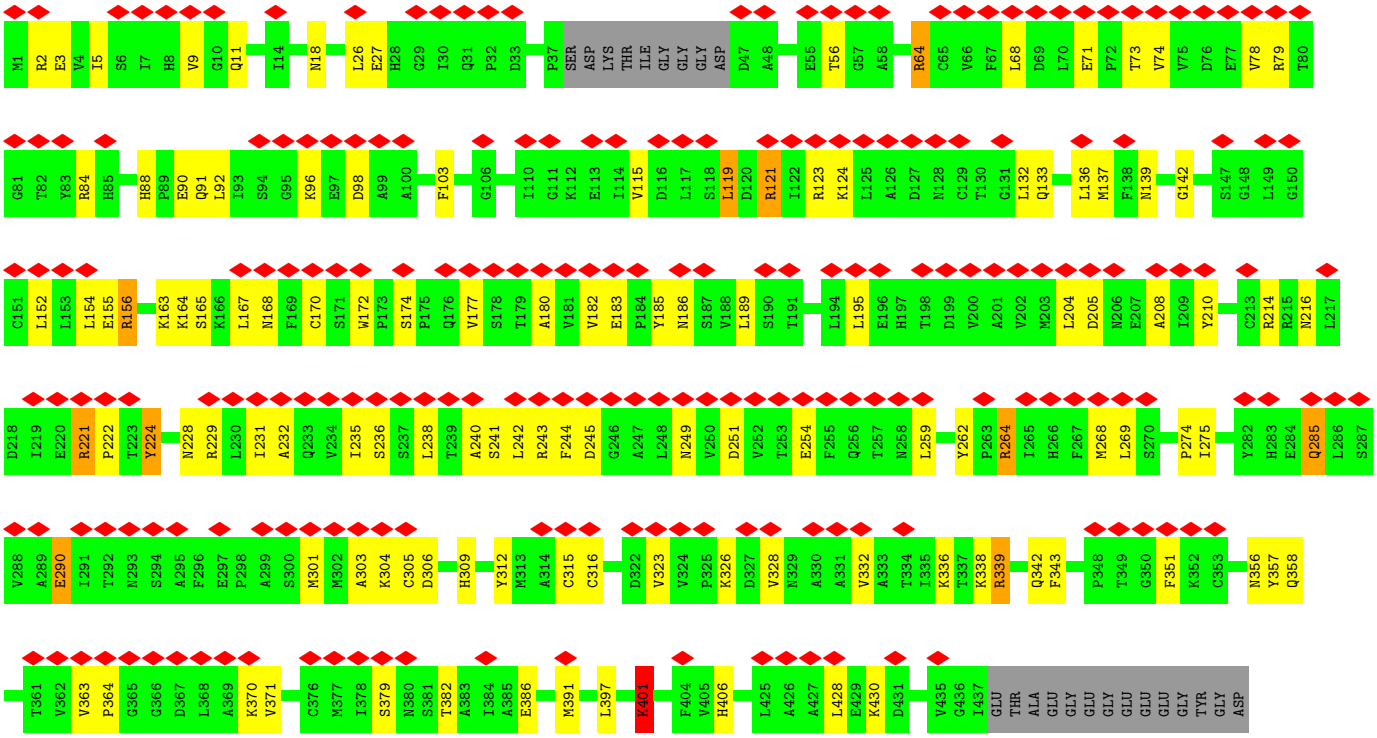
Chain 9:





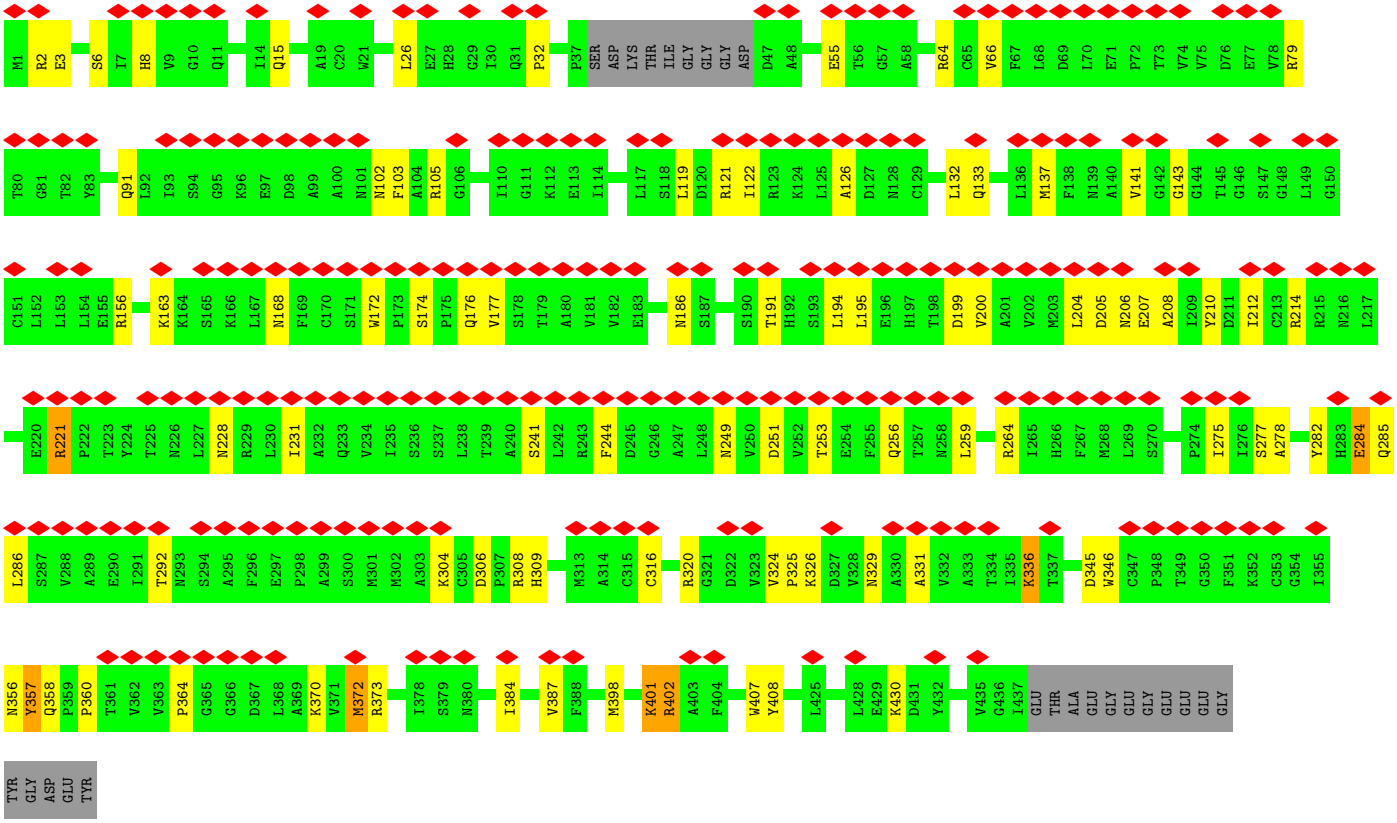
• Molecule 2: Tubulin alpha chain

Chain A0:



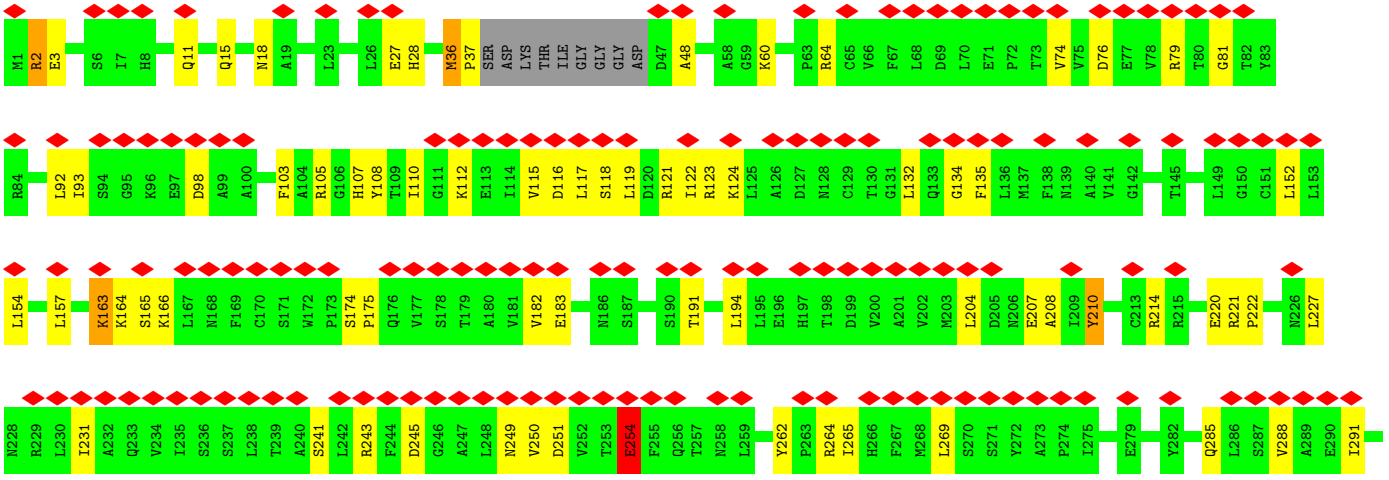
• Molecule 2: Tubulin alpha chain

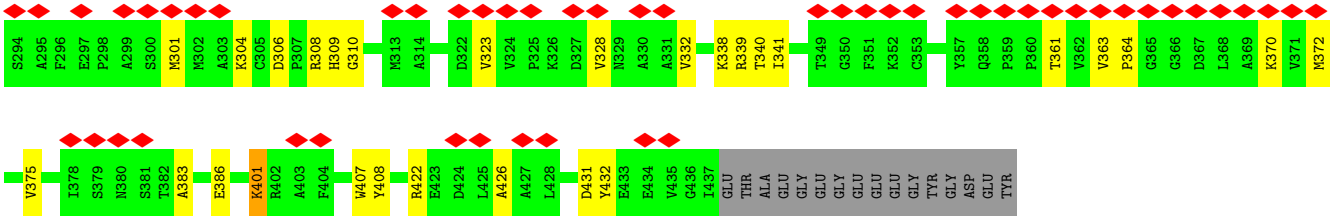
Chain A2:



• Molecule 2: Tubulin alpha chain

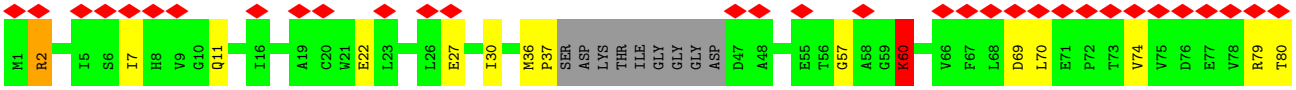
Chain A4:





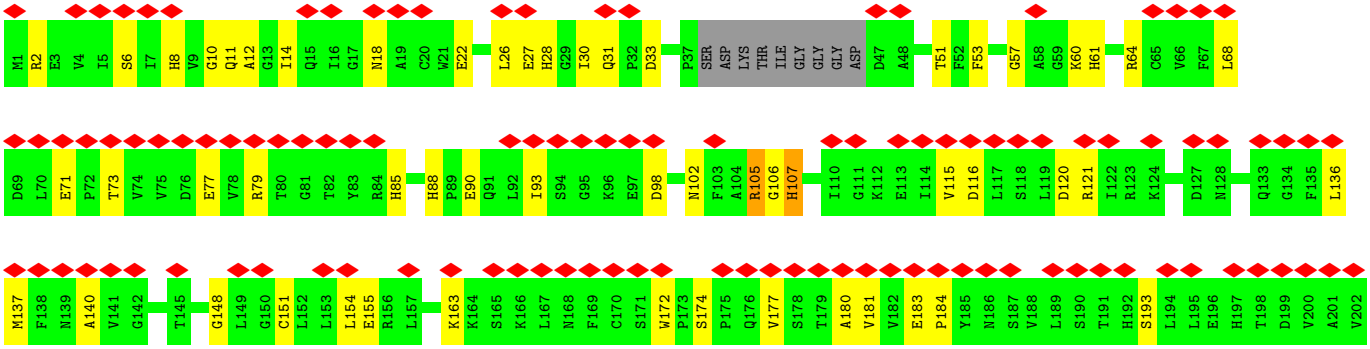
• Molecule 2: Tubulin alpha chain

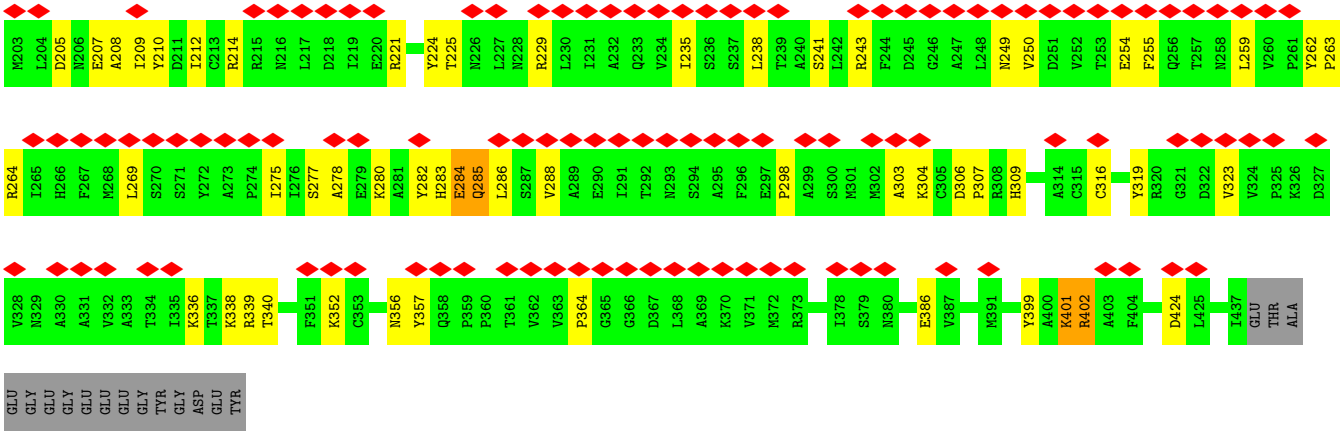
Chain A6:



• Molecule 2: Tubulin alpha chain

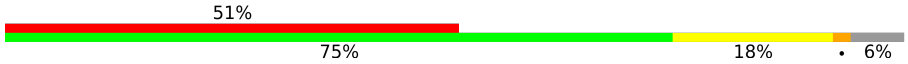
Chain A8:

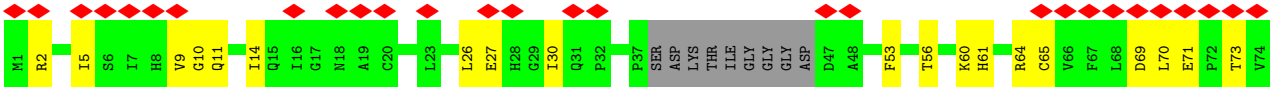


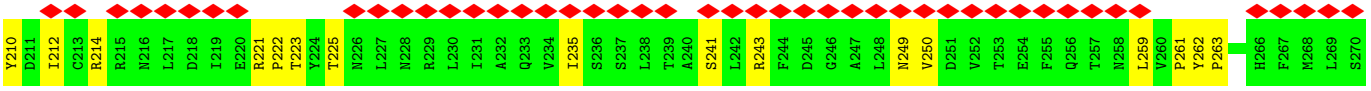


• Molecule 2: Tubulin alpha chain

Chain B0:

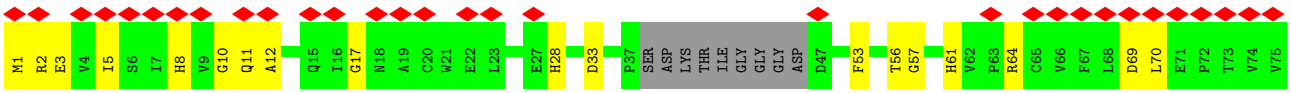


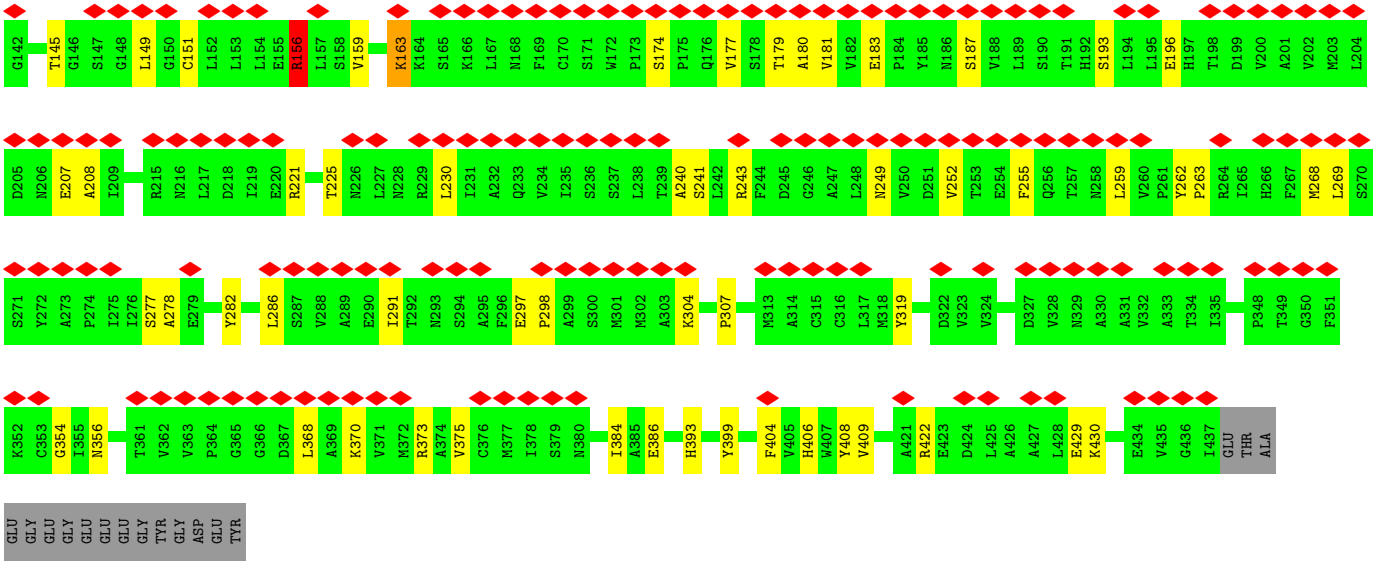




• Molecule 2: Tubulin alpha chain

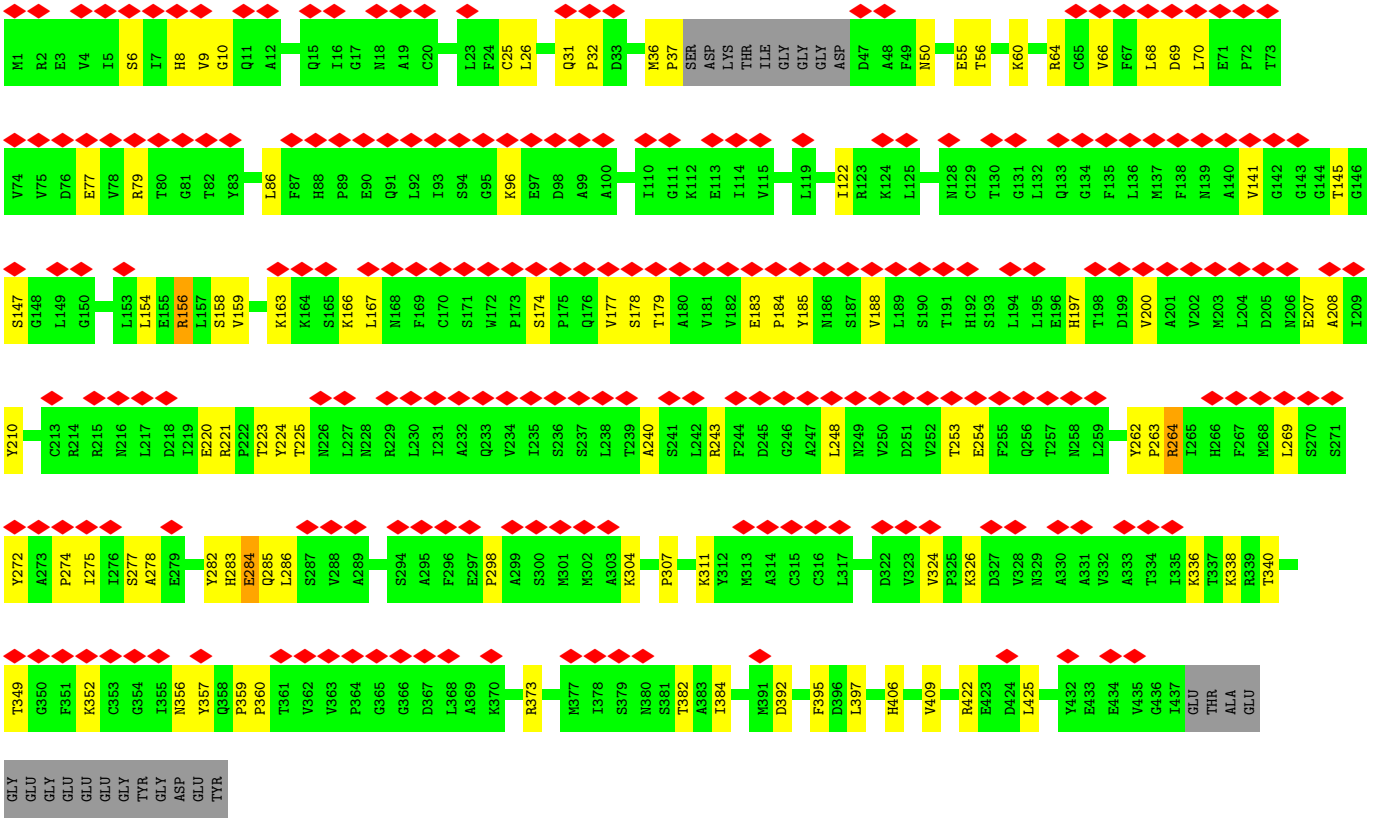
Chain B2:





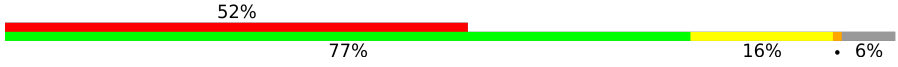
• Molecule 2: Tubulin alpha chain

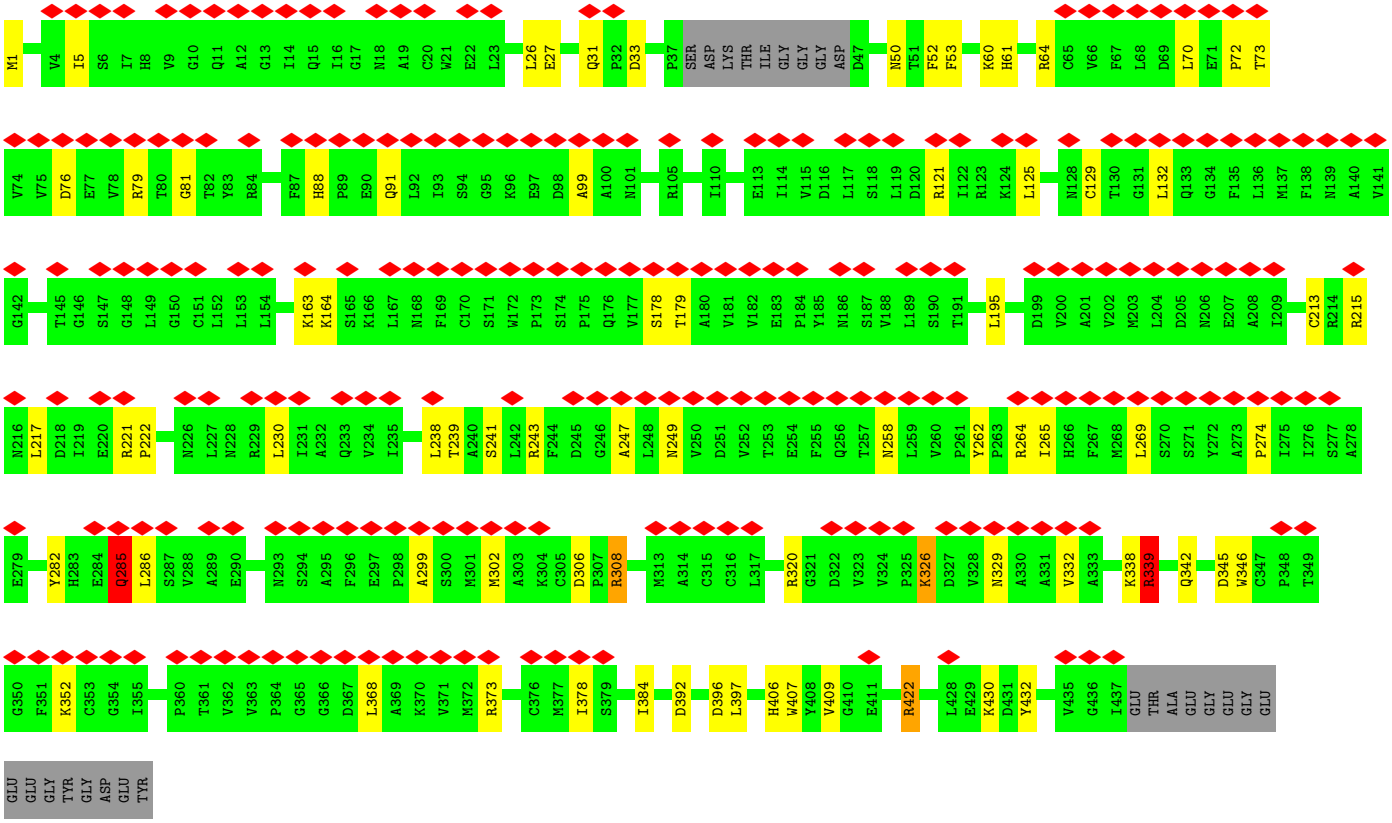
Chain B4:



• Molecule 2: Tubulin alpha chain

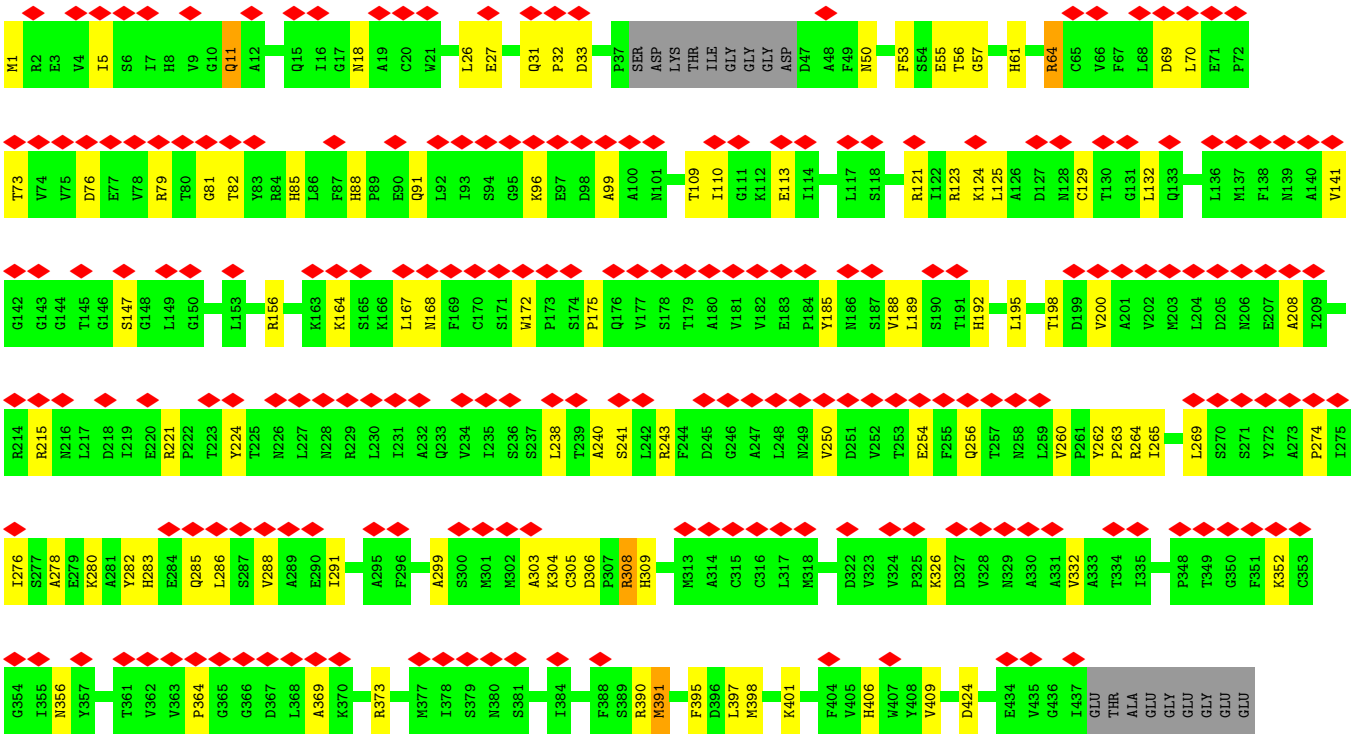
Chain B6:





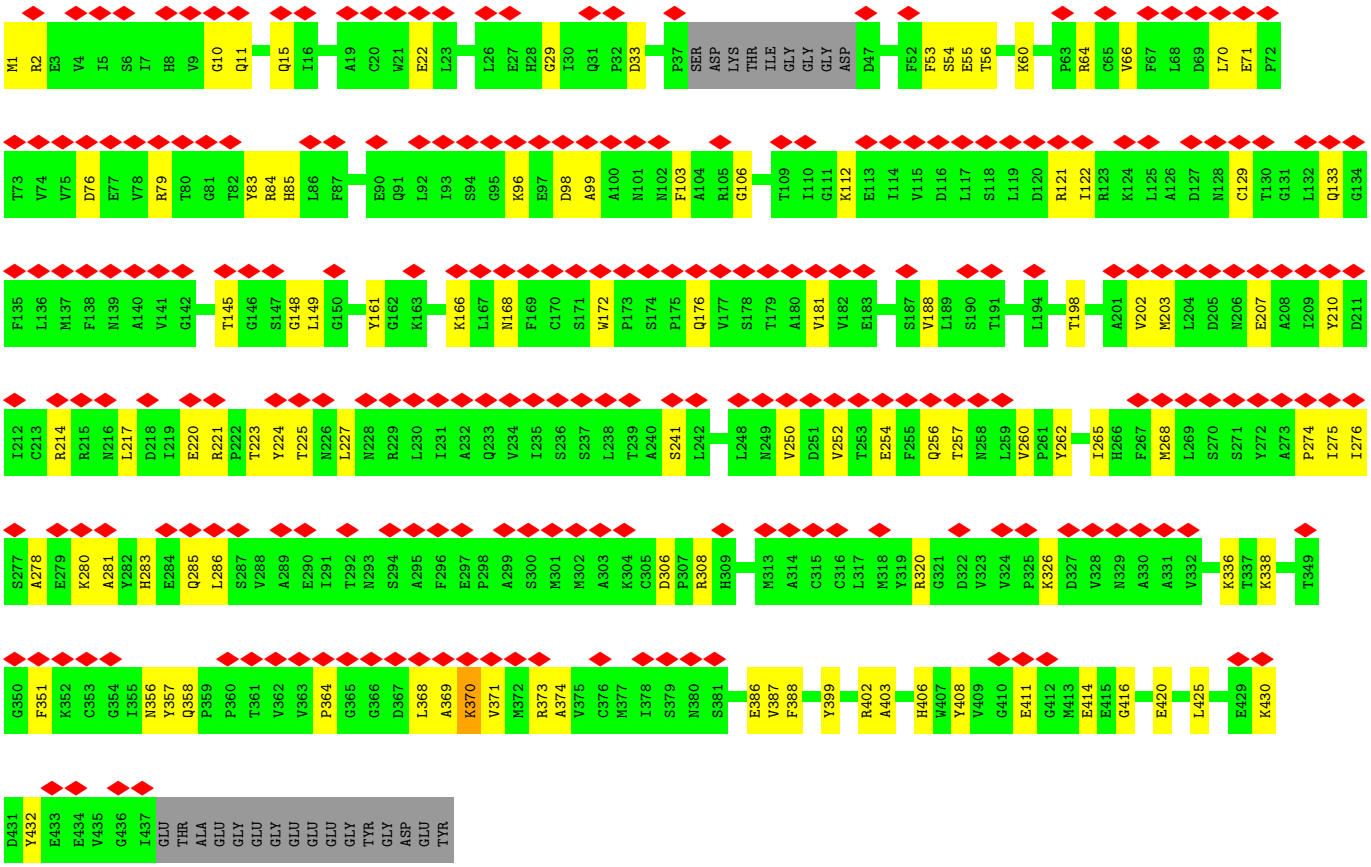
• Molecule 2: Tubulin alpha chain

Chain B8:



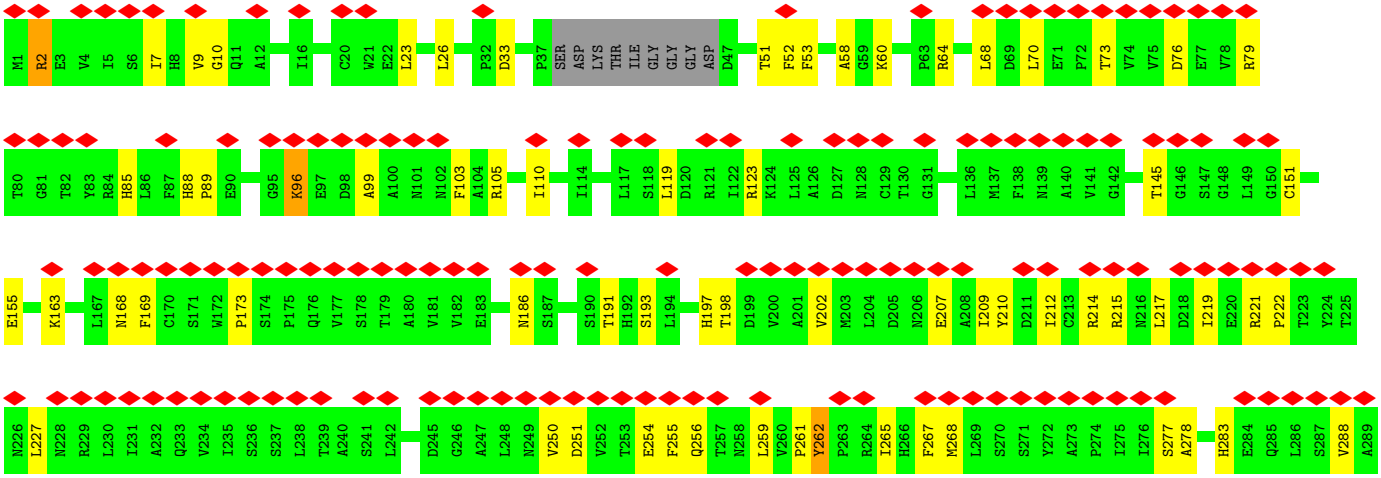
• Molecule 2: Tubulin alpha chain

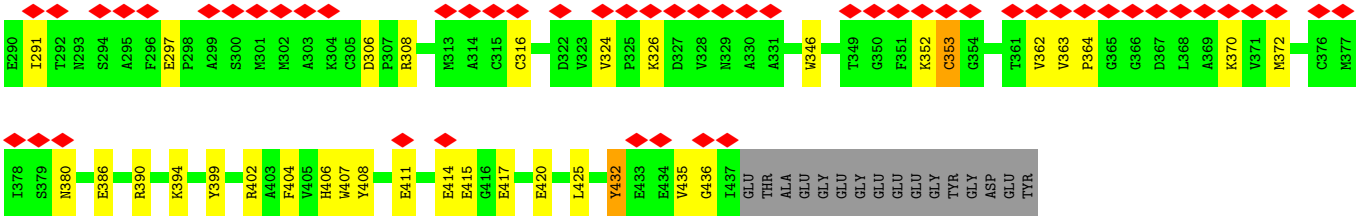
Chain C0:



• Molecule 2: Tubulin alpha chain

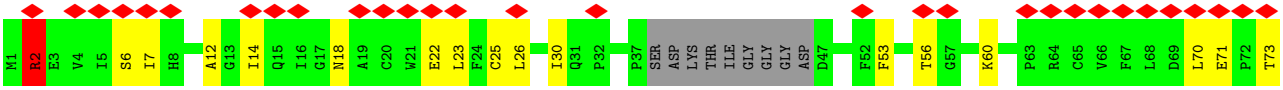
Chain C2:

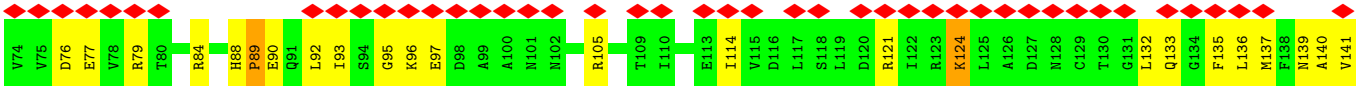


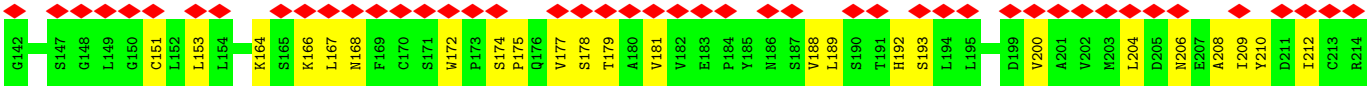


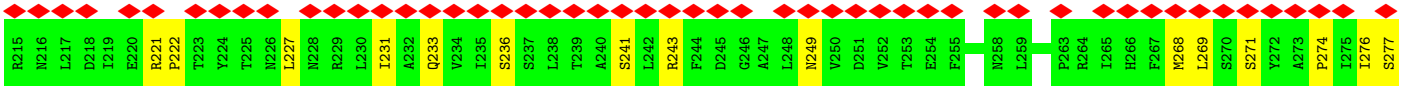
• Molecule 2: Tubulin alpha chain

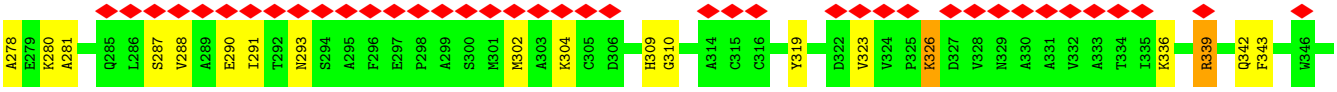
Chain C4:

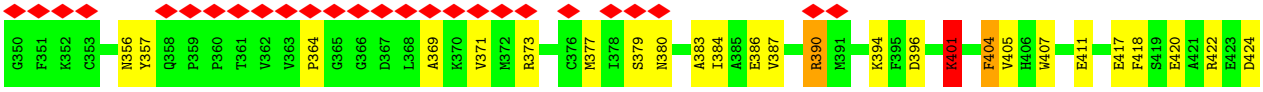


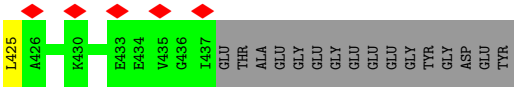






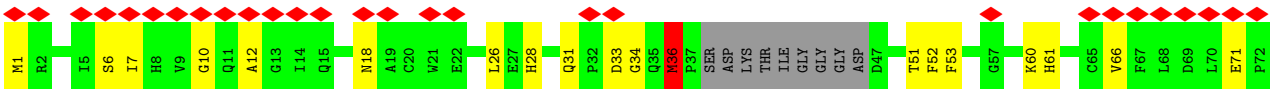


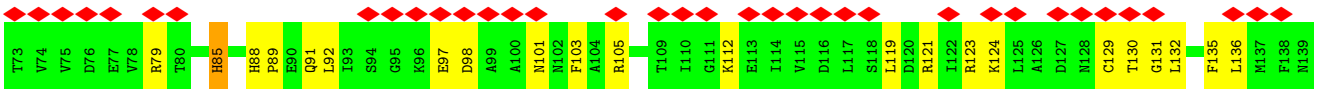


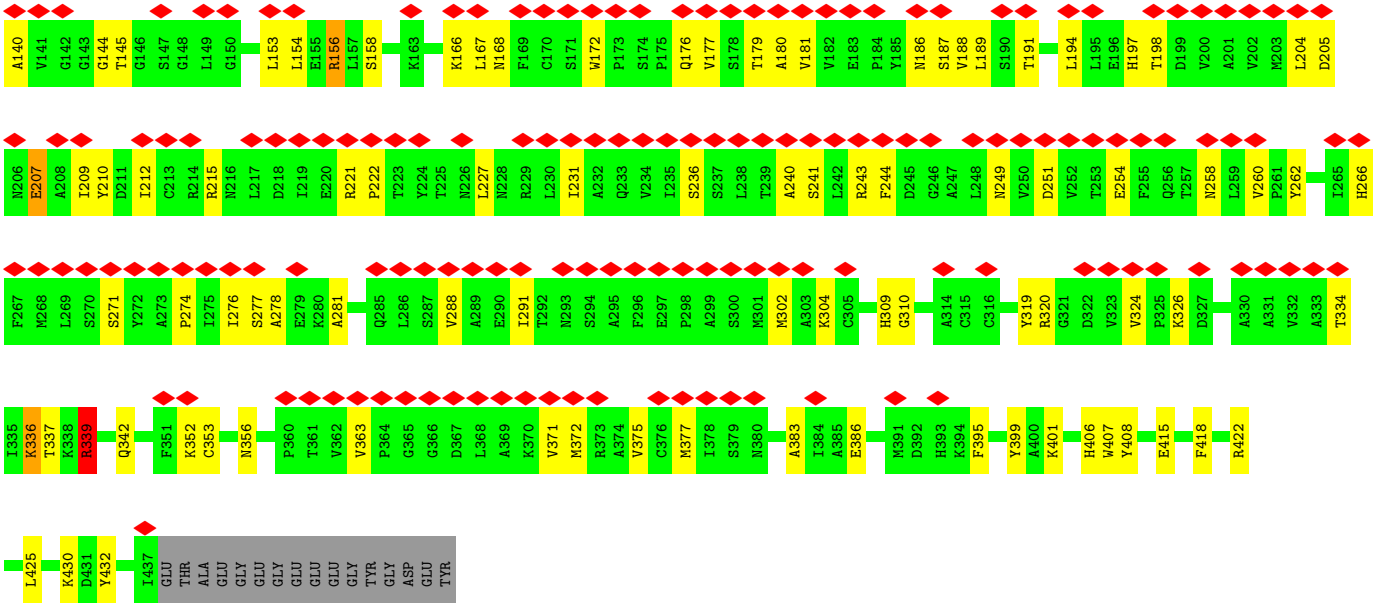


• Molecule 2: Tubulin alpha chain

Chain C6:

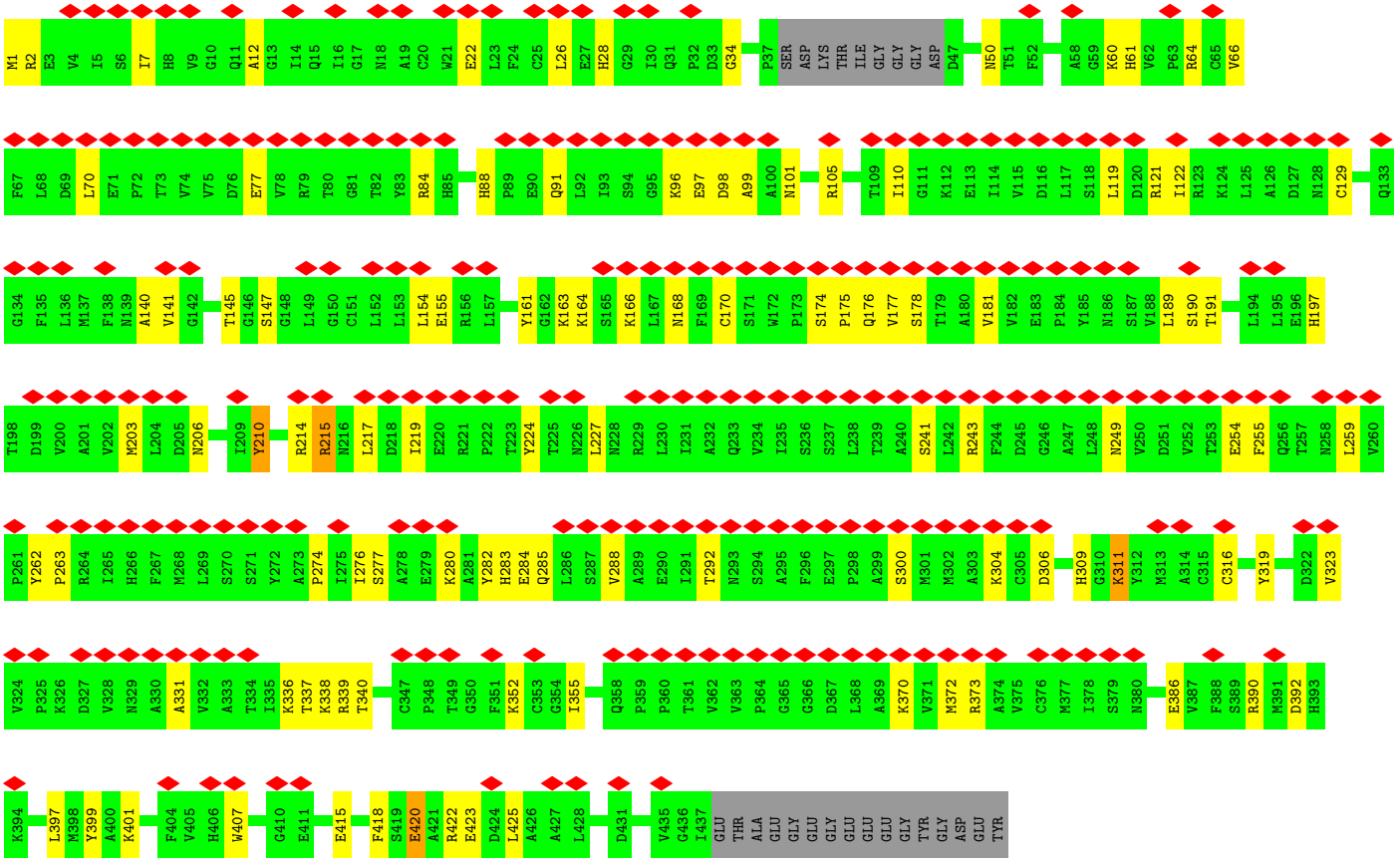






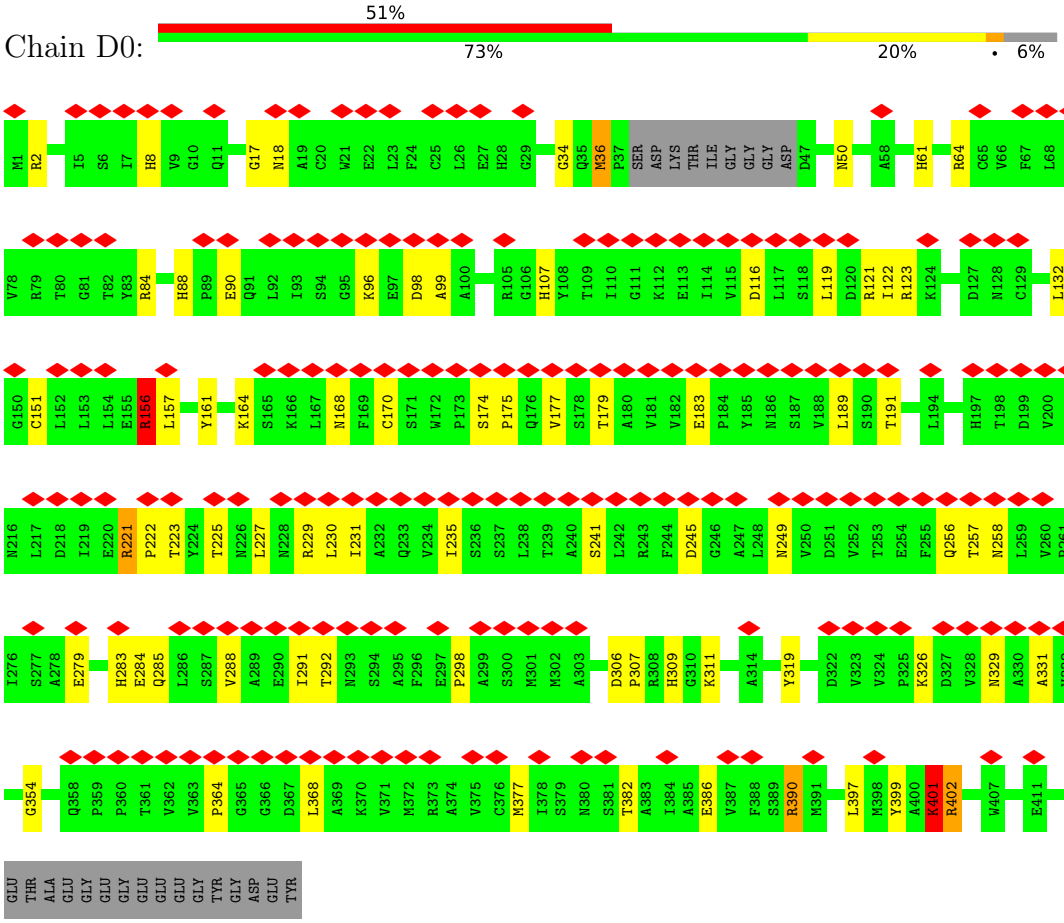
• Molecule 2: Tubulin alpha chain

Chain C8:



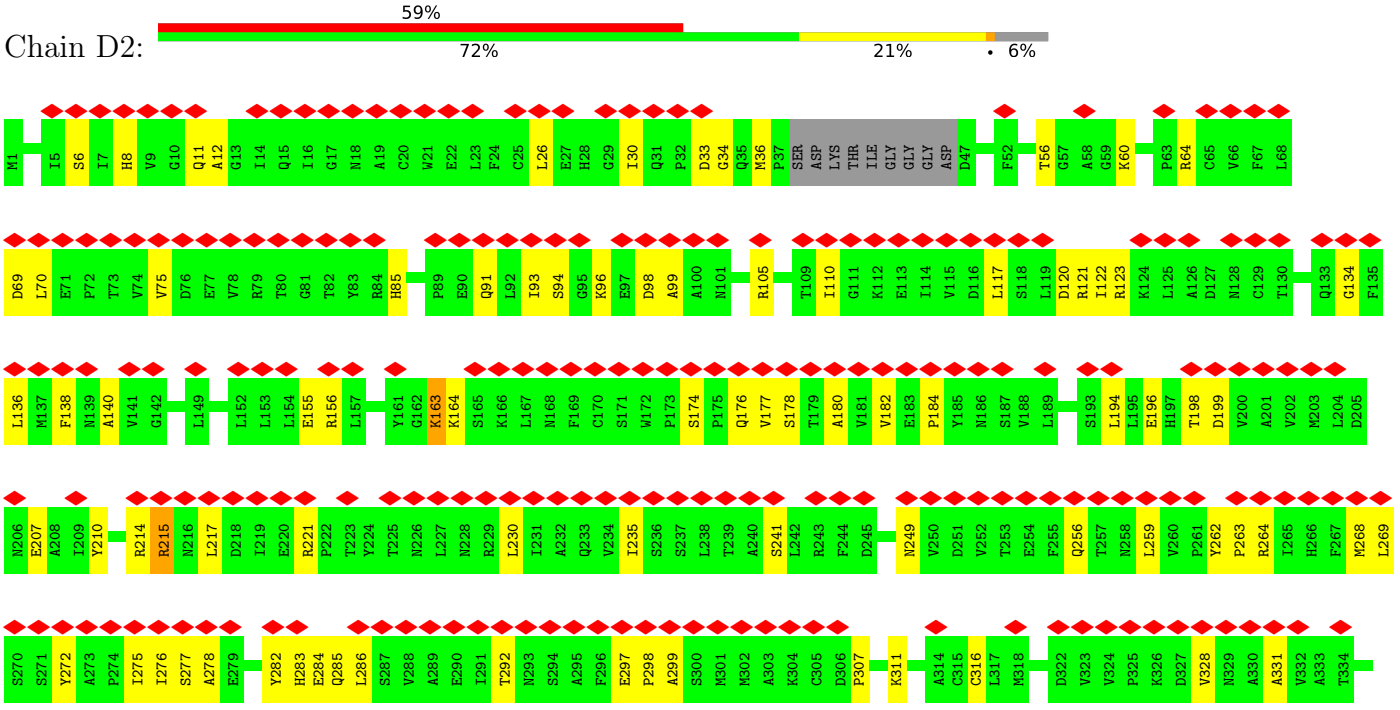
• Molecule 2: Tubulin alpha chain

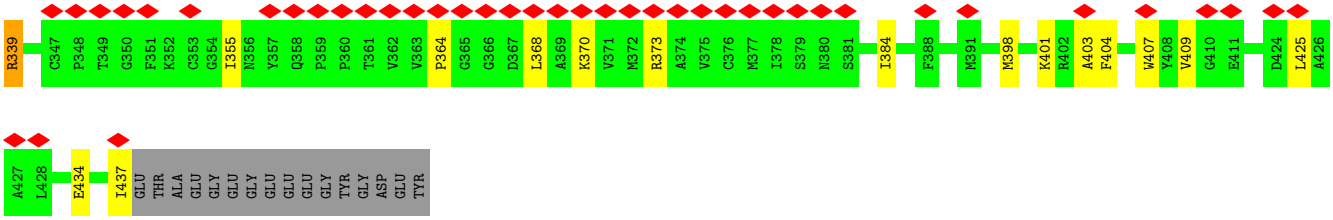
Chain D0:



• Molecule 2: Tubulin alpha chain

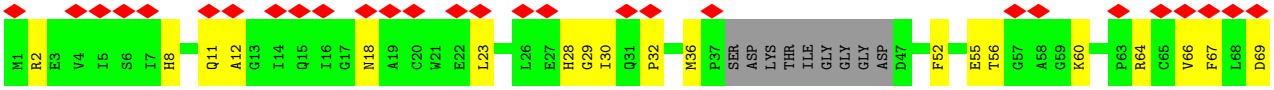
Chain D2:

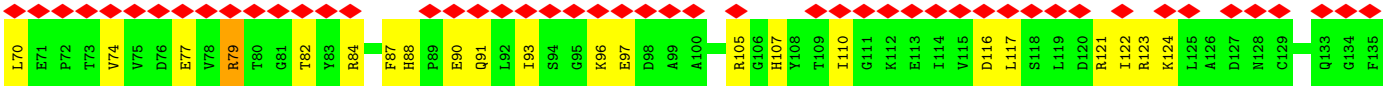


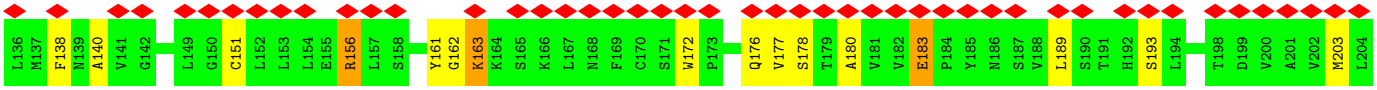


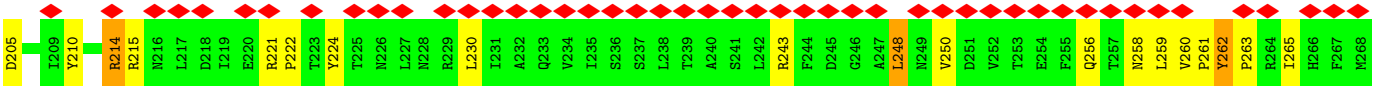
• Molecule 2: Tubulin alpha chain

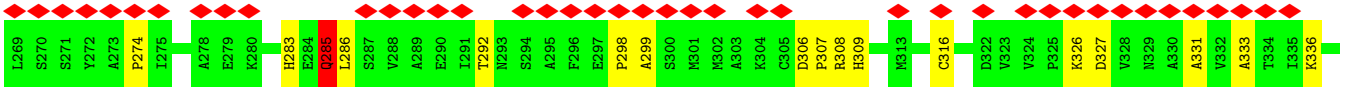
Chain D4:

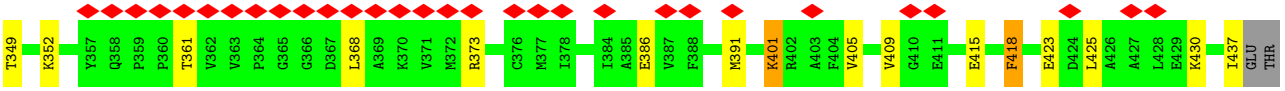


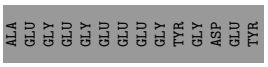






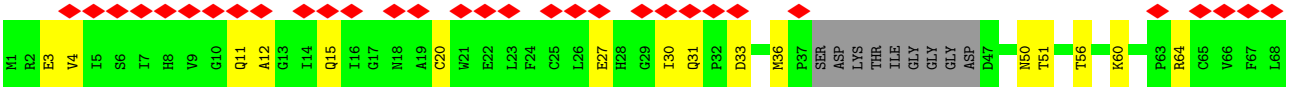


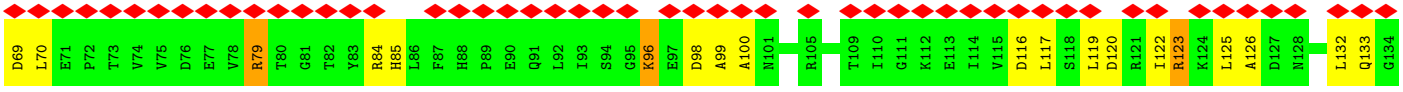


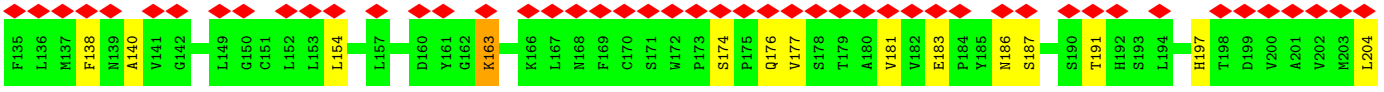


• Molecule 2: Tubulin alpha chain

Chain D6:

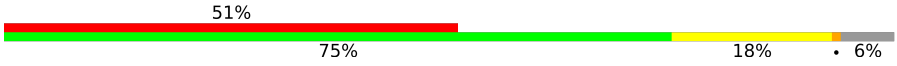


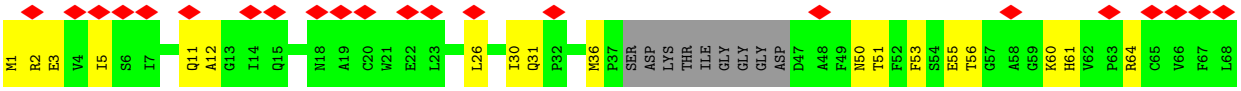




• Molecule 2: Tubulin alpha chain

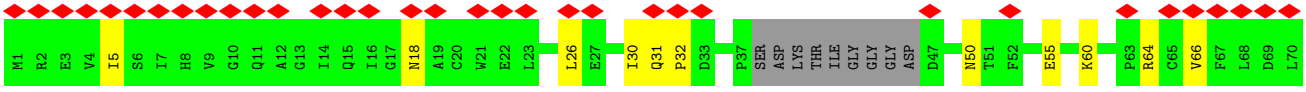
Chain D8:

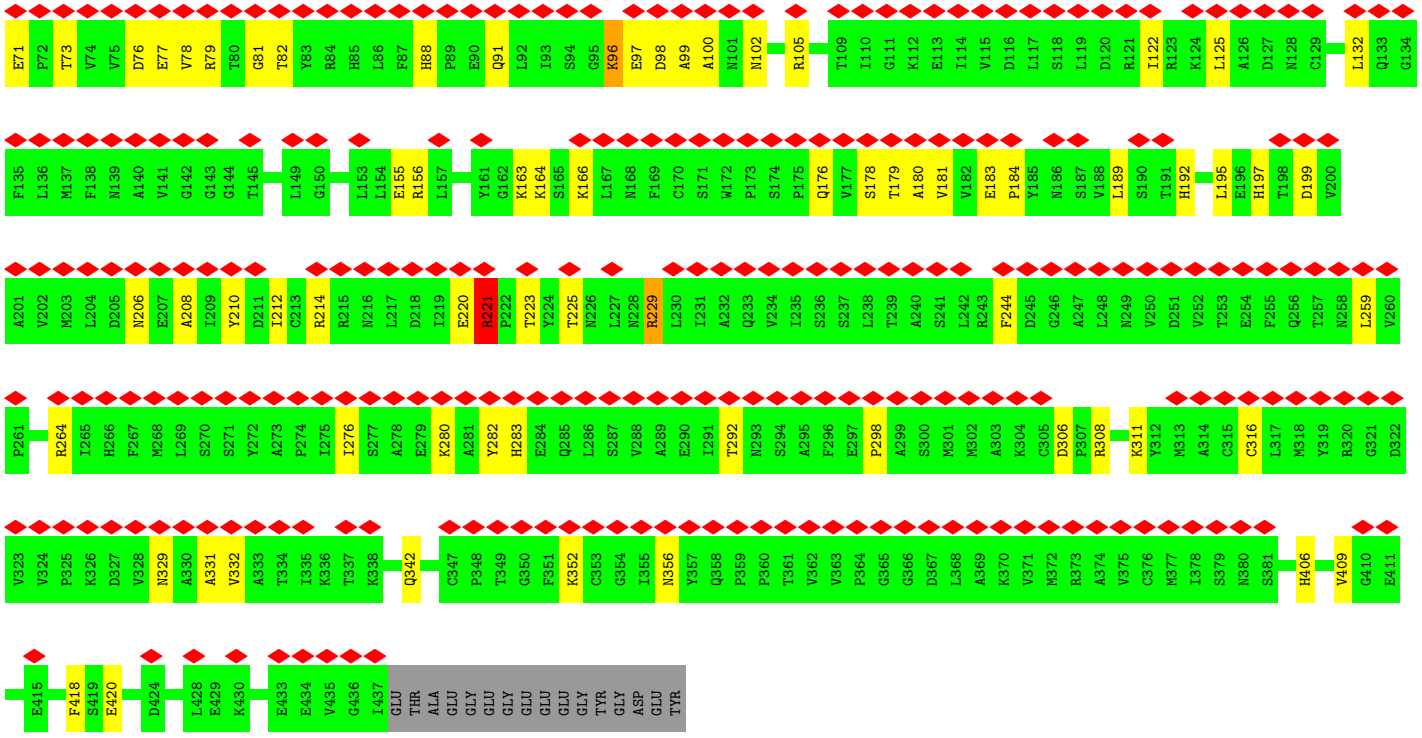




• Molecule 2: Tubulin alpha chain

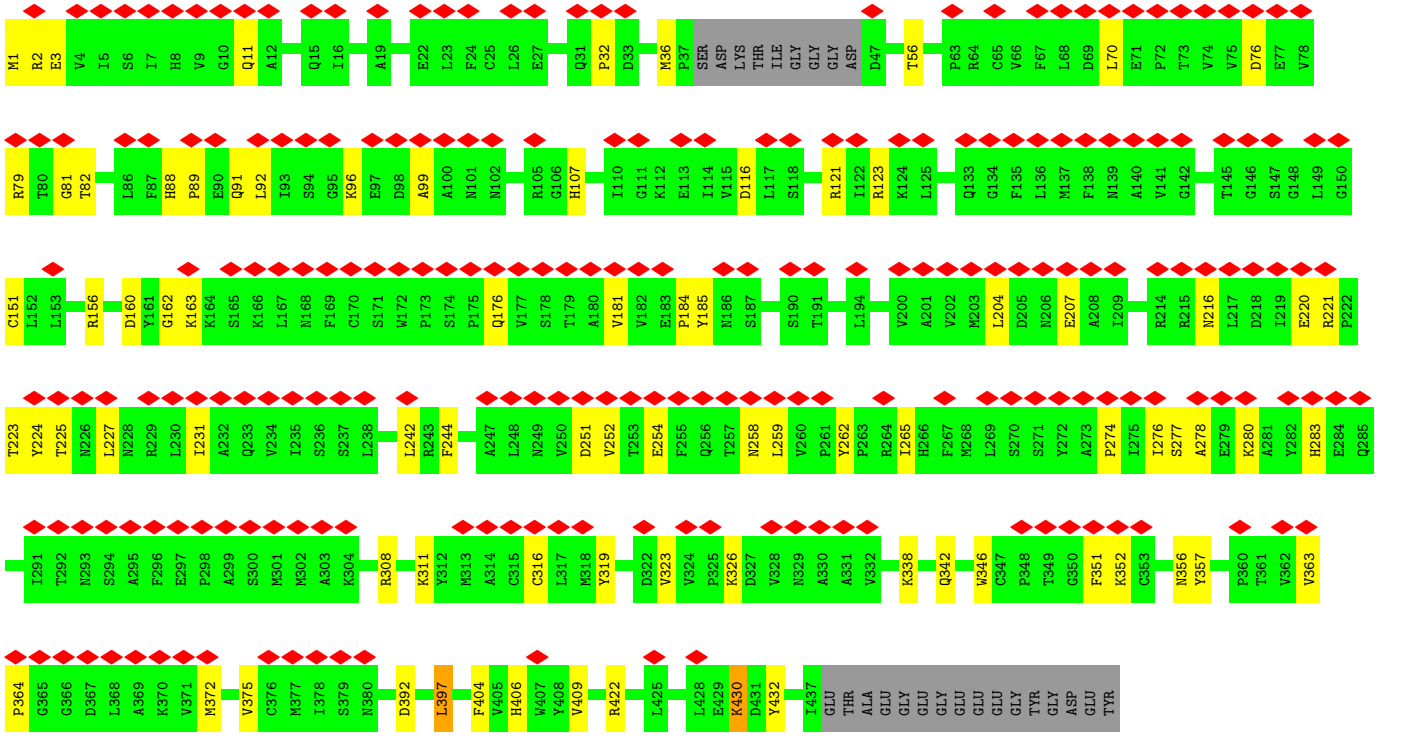
Chain E0:





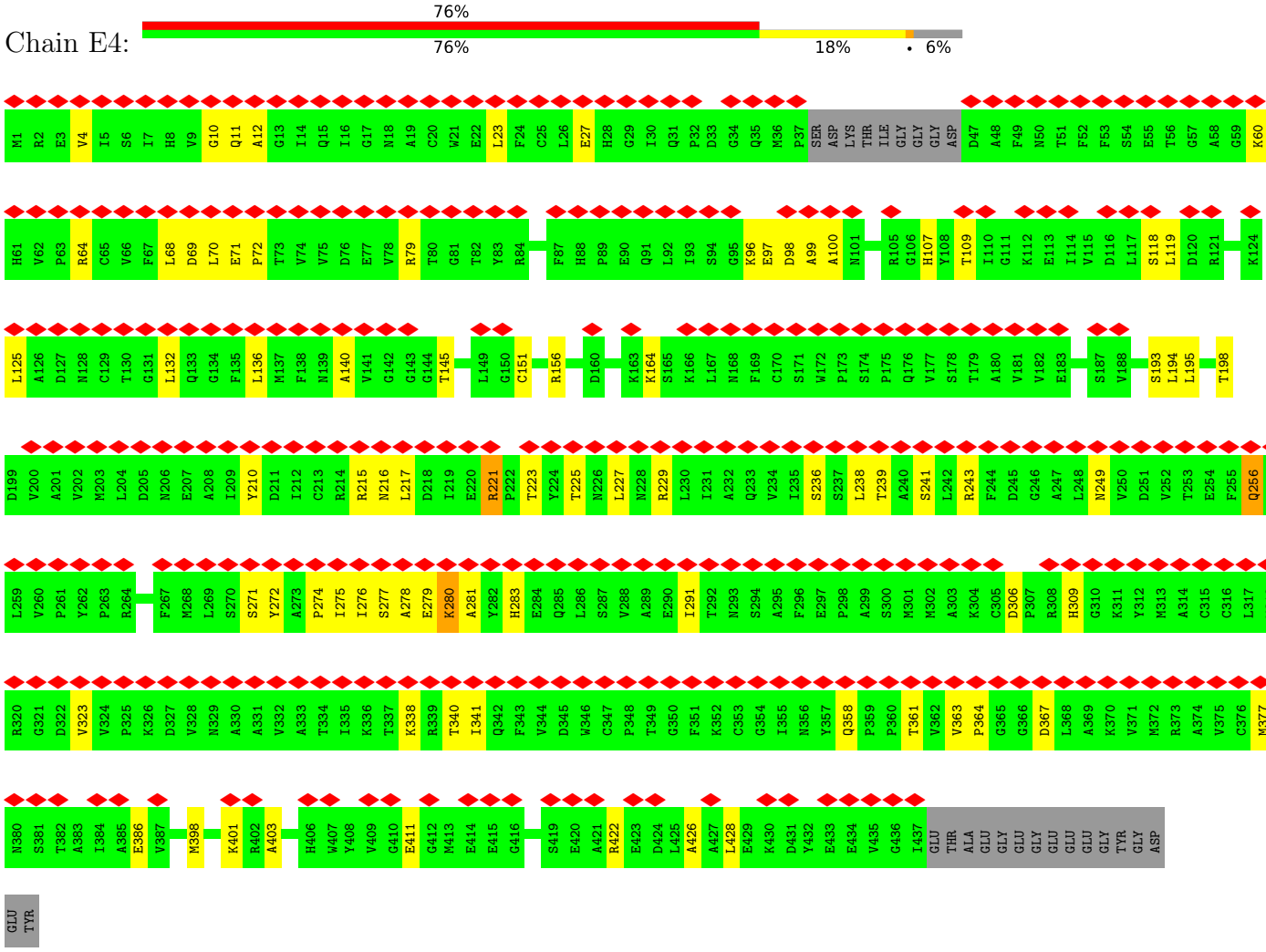
• Molecule 2: Tubulin alpha chain

Chain E2:



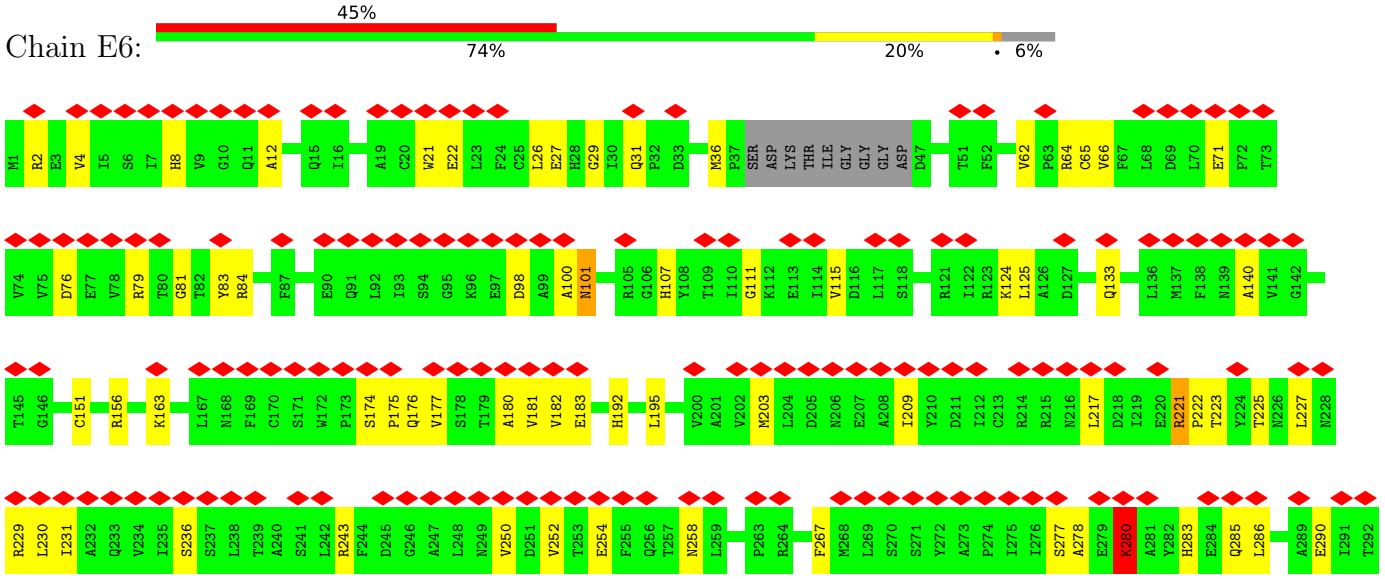
• Molecule 2: Tubulin alpha chain

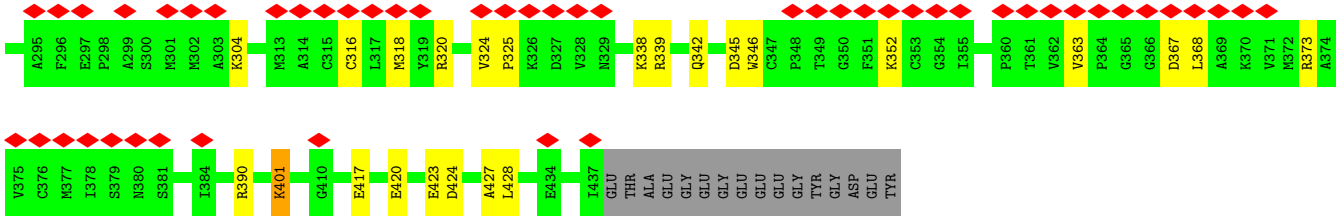
Chain E4:



• Molecule 2: Tubulin alpha chain

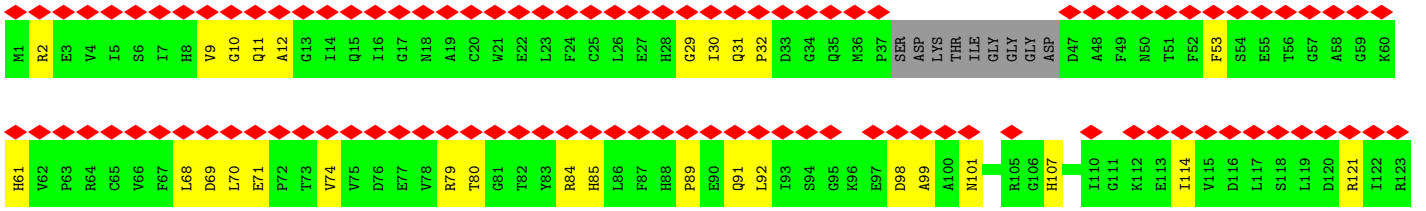
Chain E6:





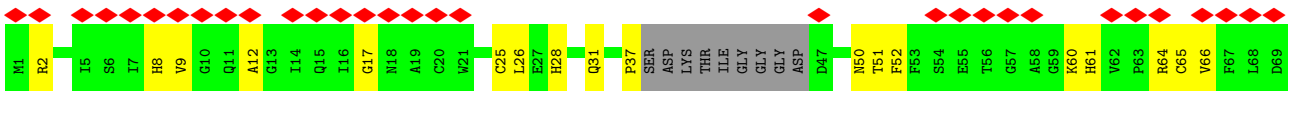
• Molecule 2: Tubulin alpha chain

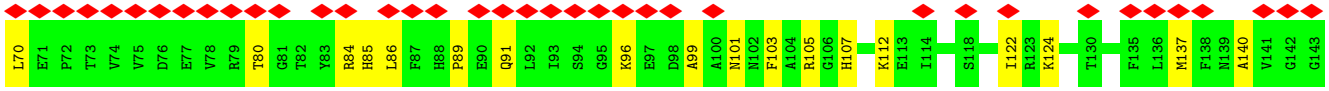
Chain E8:

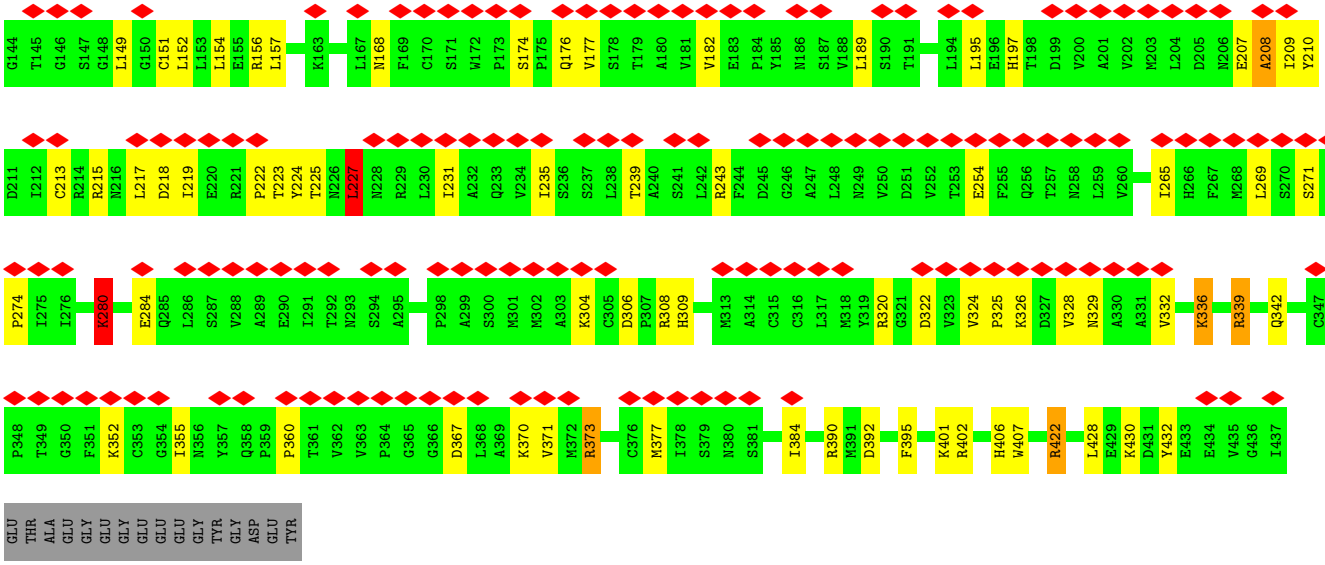


• Molecule 2: Tubulin alpha chain

Chain F0:

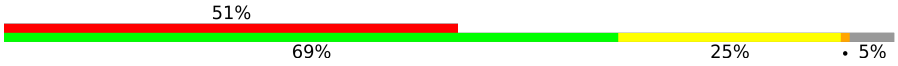


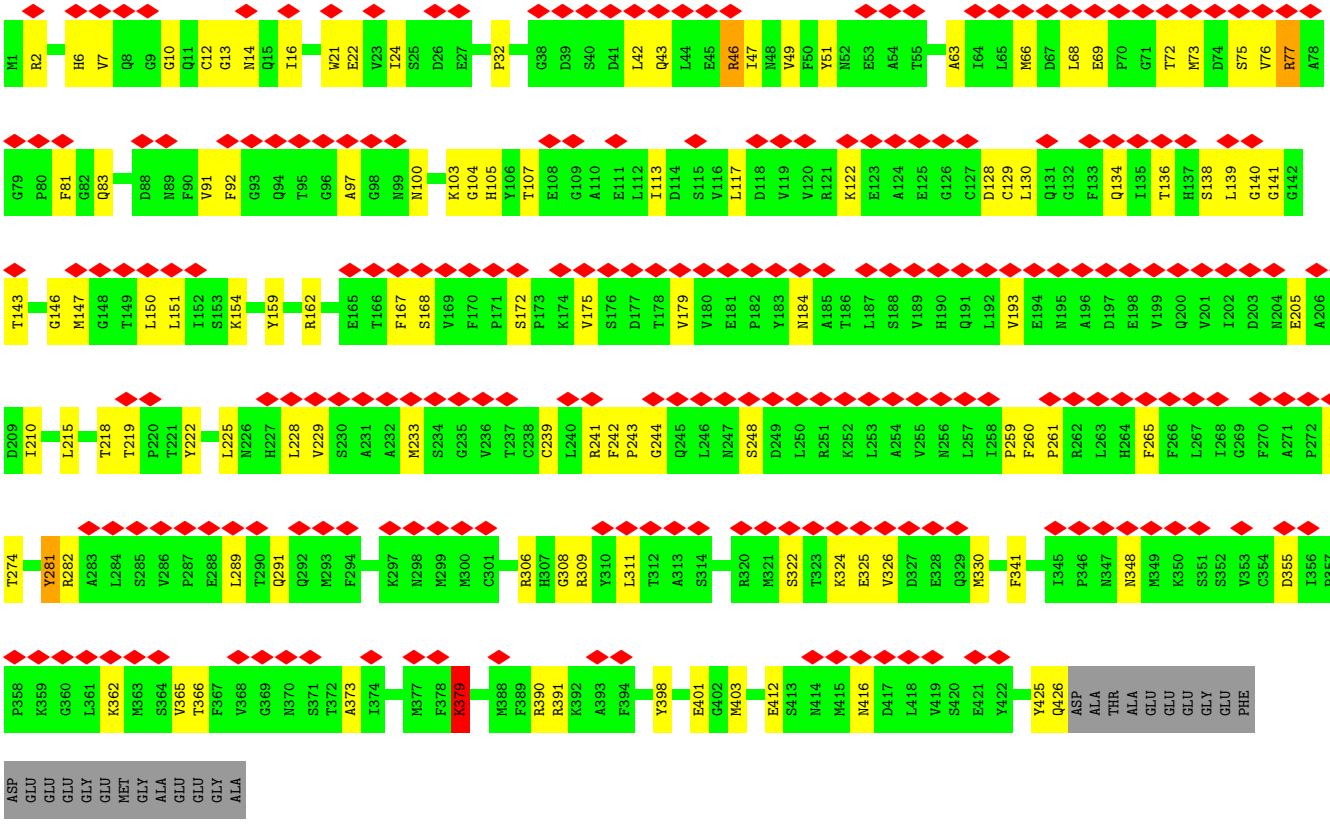




• Molecule 3: Tubulin beta chain

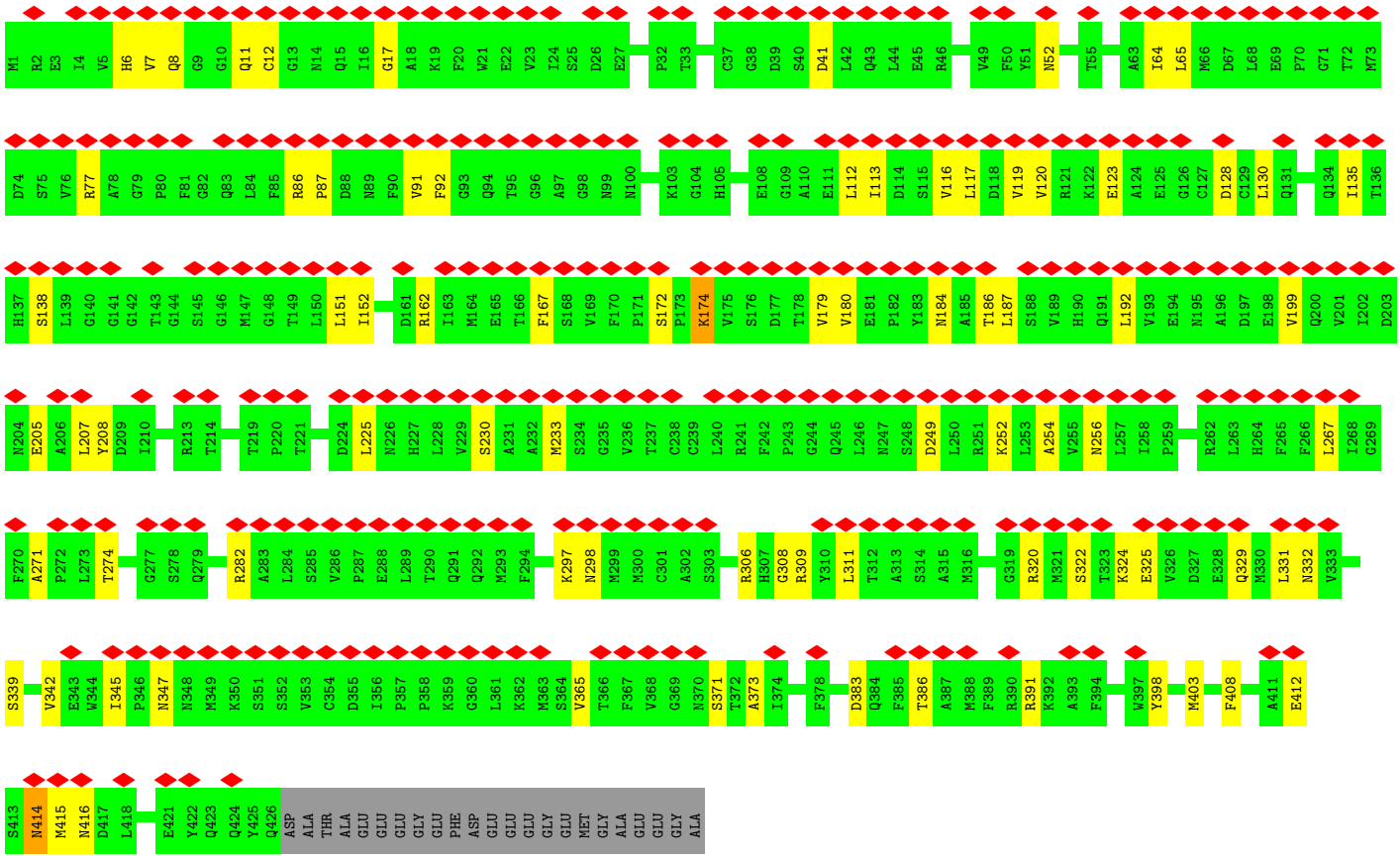
Chain A1:





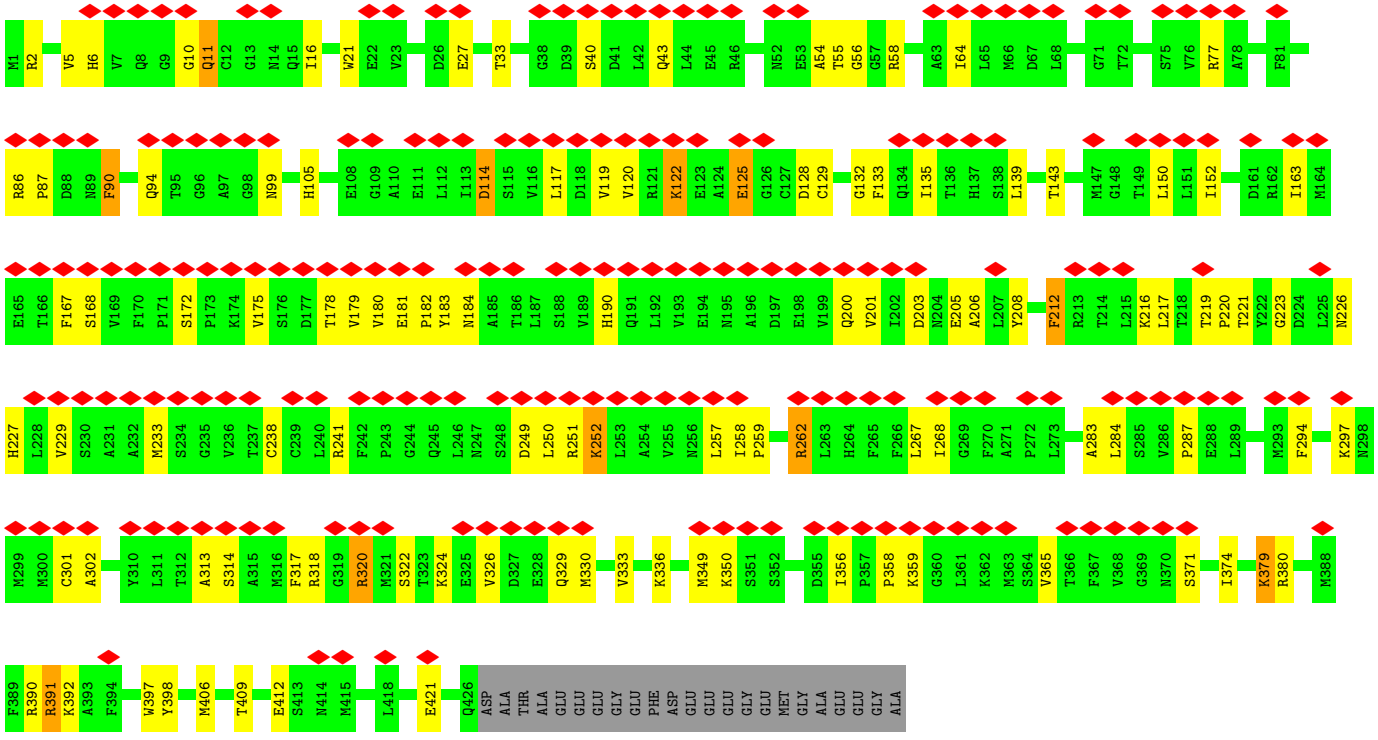
• Molecule 3: Tubulin beta chain

Chain A3:



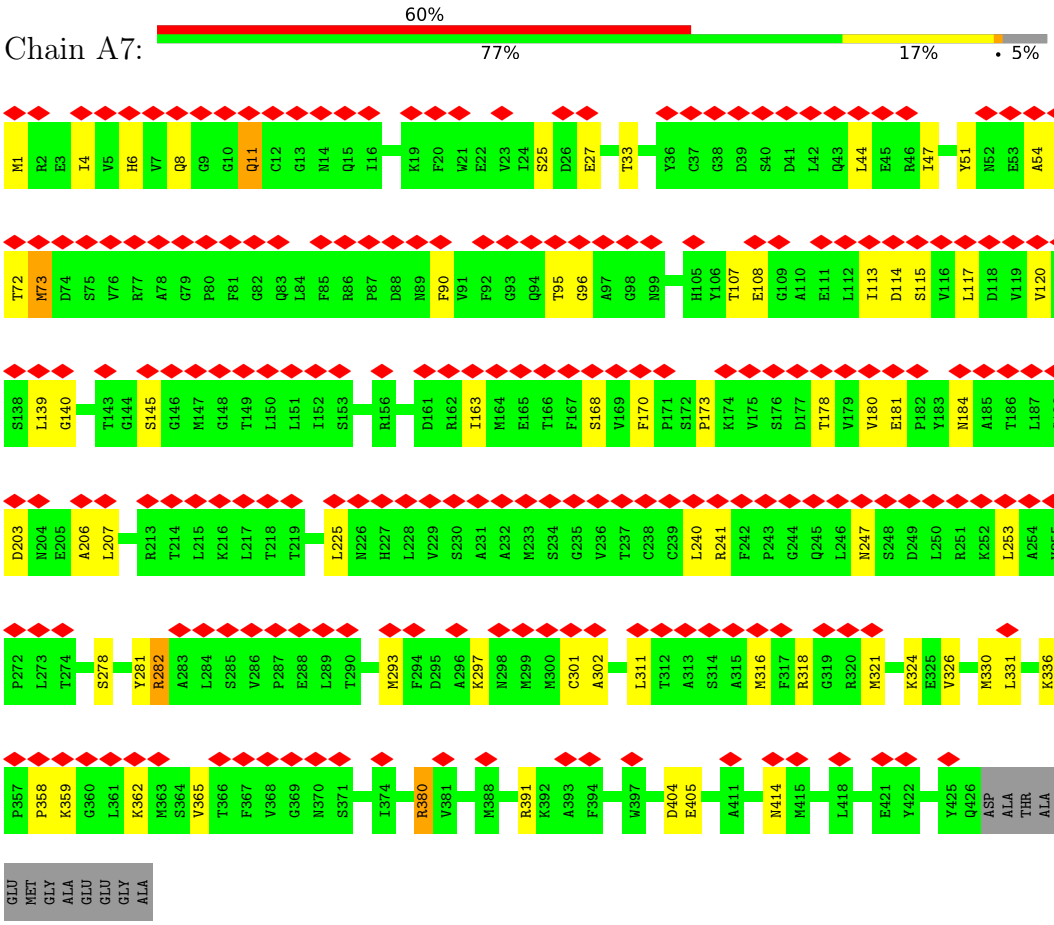
• Molecule 3: Tubulin beta chain

Chain A5:



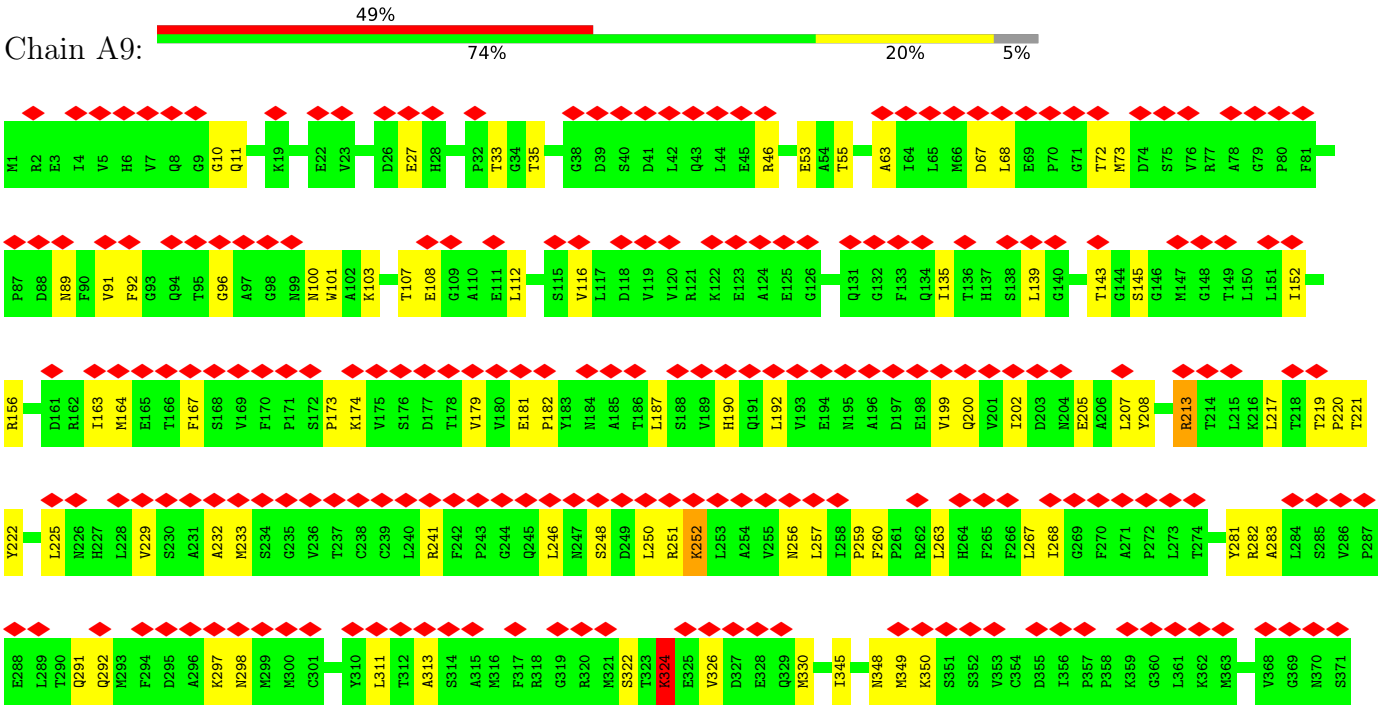
• Molecule 3: Tubulin beta chain

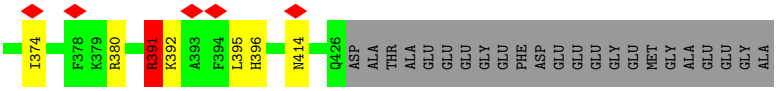
Chain A7:



• Molecule 3: Tubulin beta chain

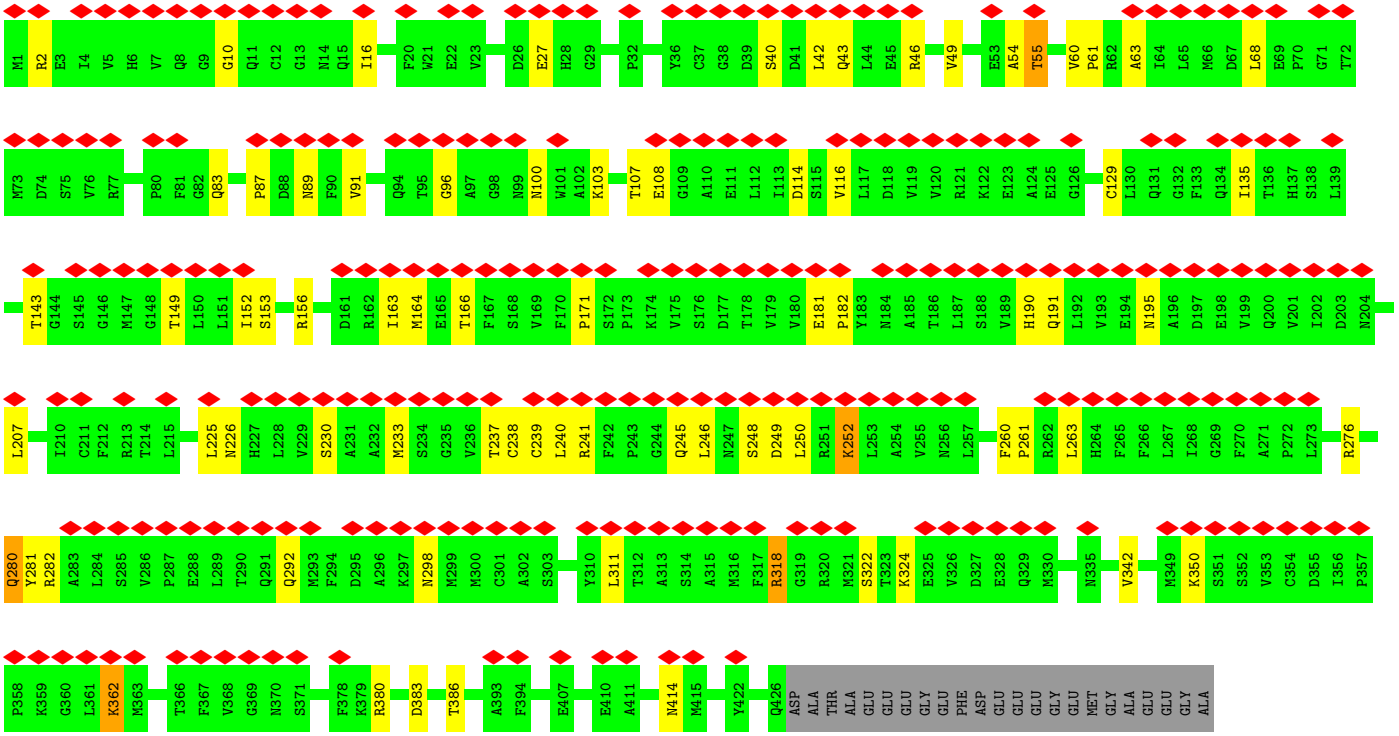
Chain A9:





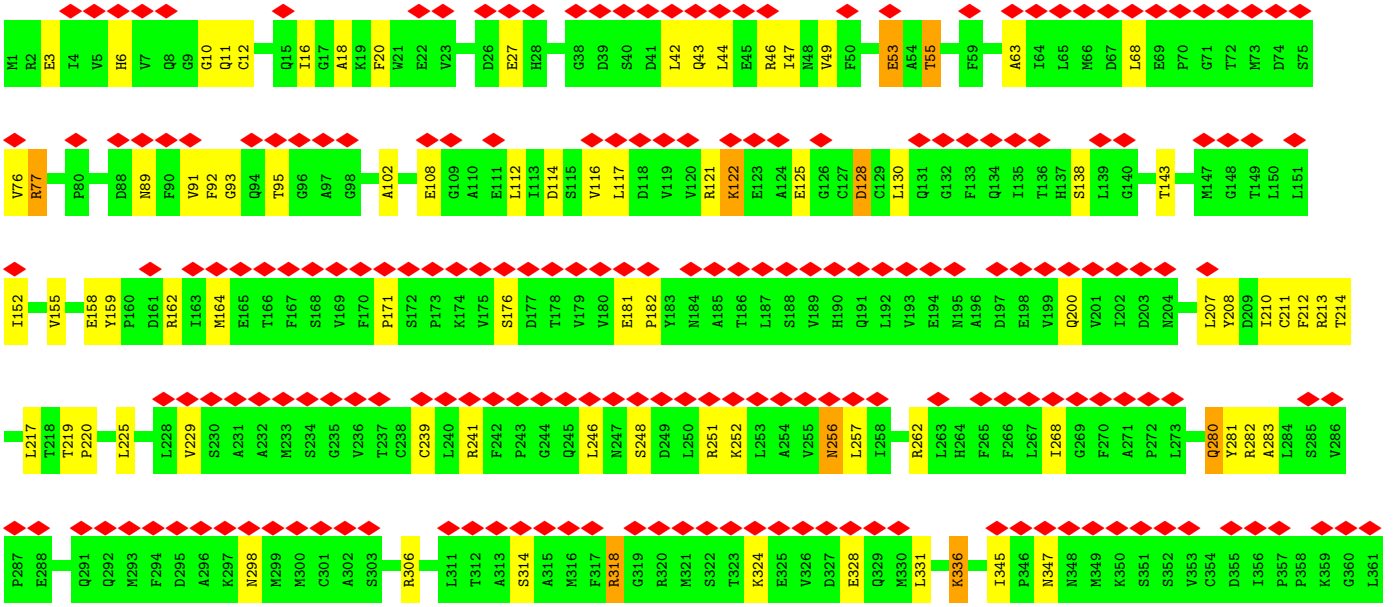
• Molecule 3: Tubulin beta chain

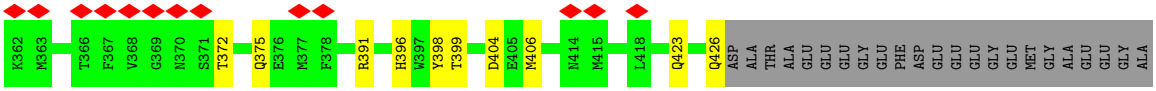
Chain B1:



• Molecule 3: Tubulin beta chain

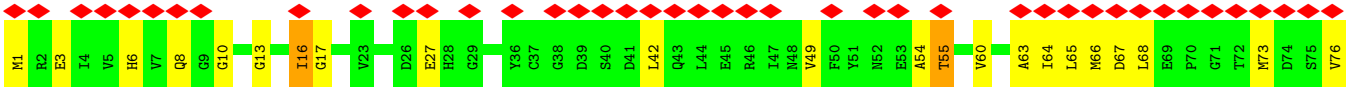
Chain B3:

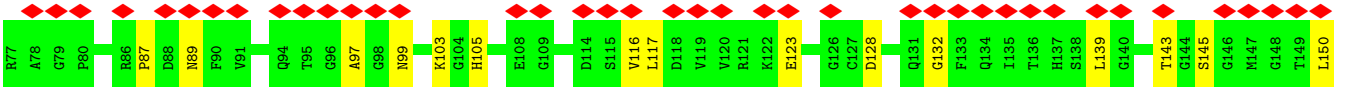


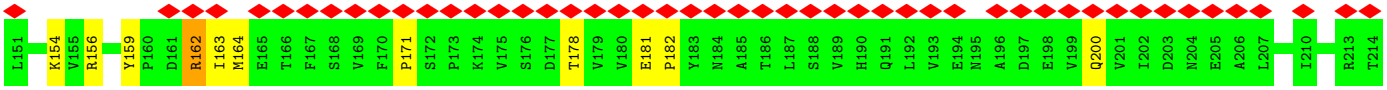


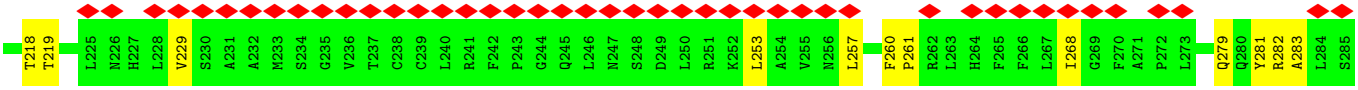
• Molecule 3: Tubulin beta chain

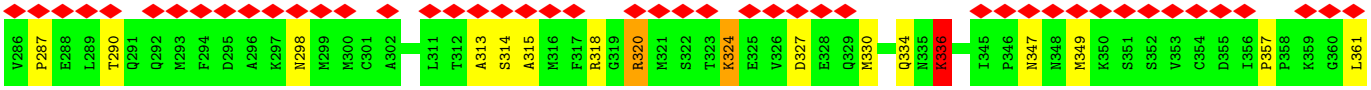
Chain B5:

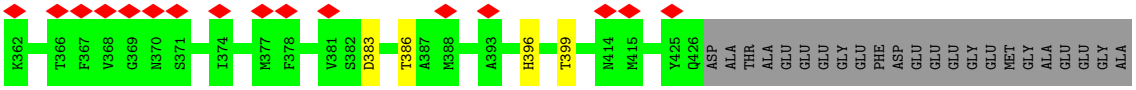






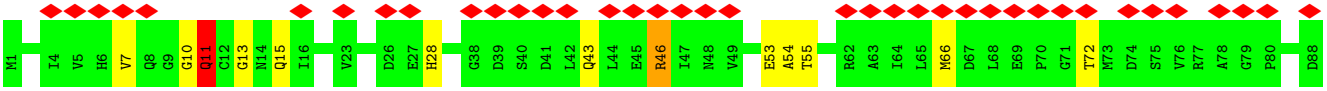


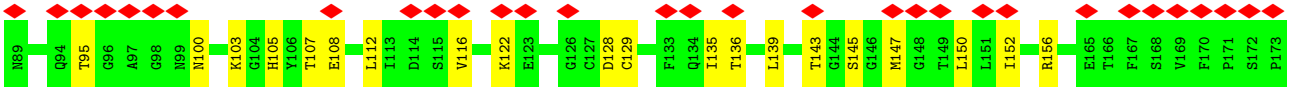


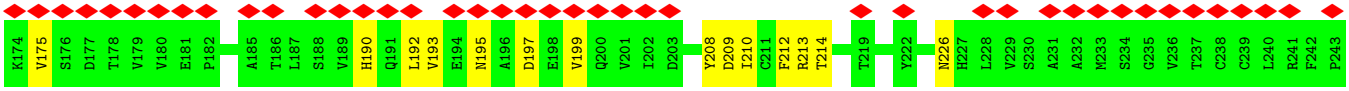


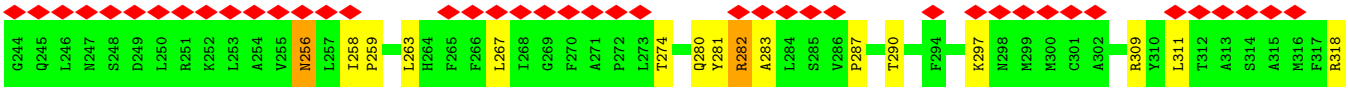
• Molecule 3: Tubulin beta chain

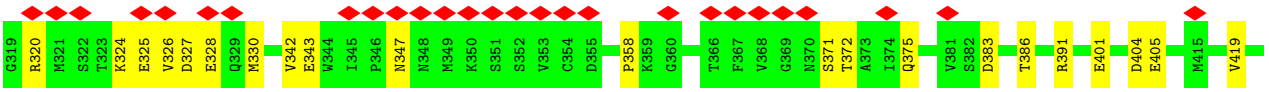
Chain B7:





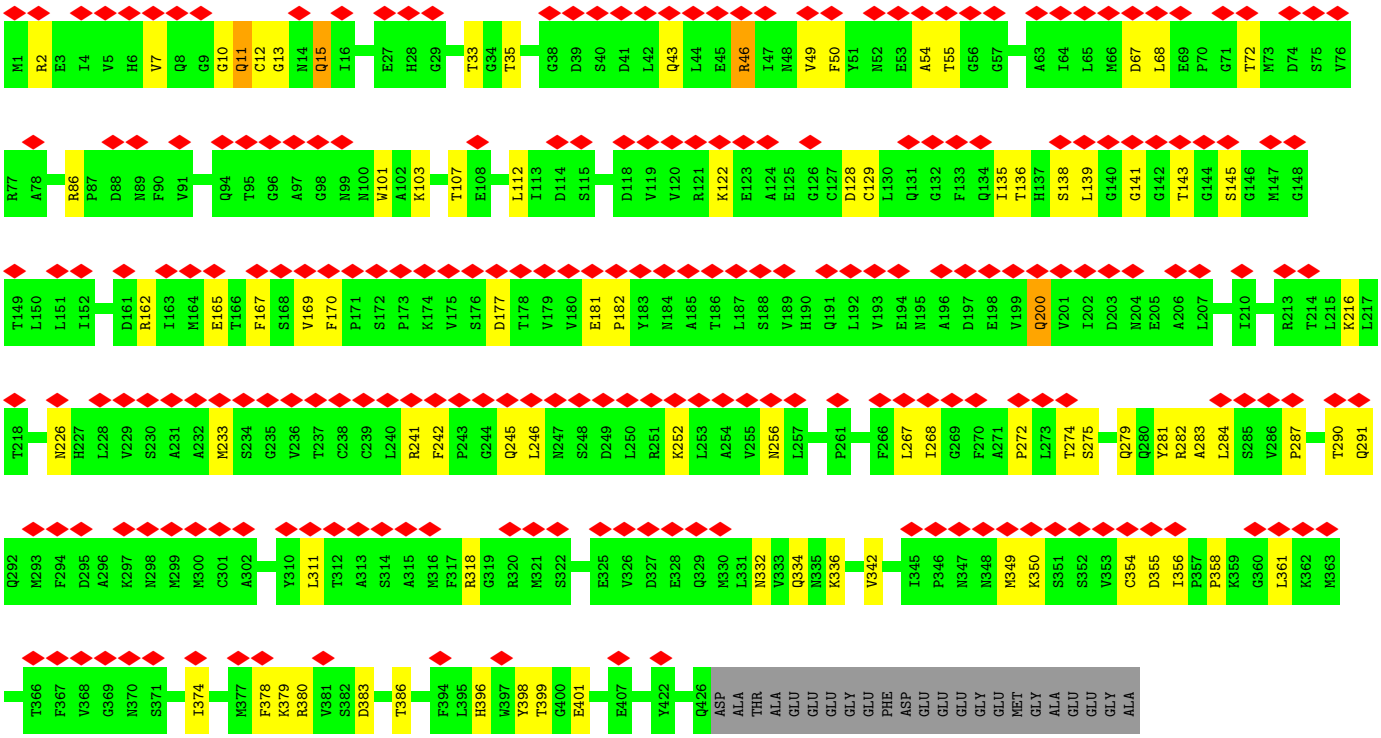






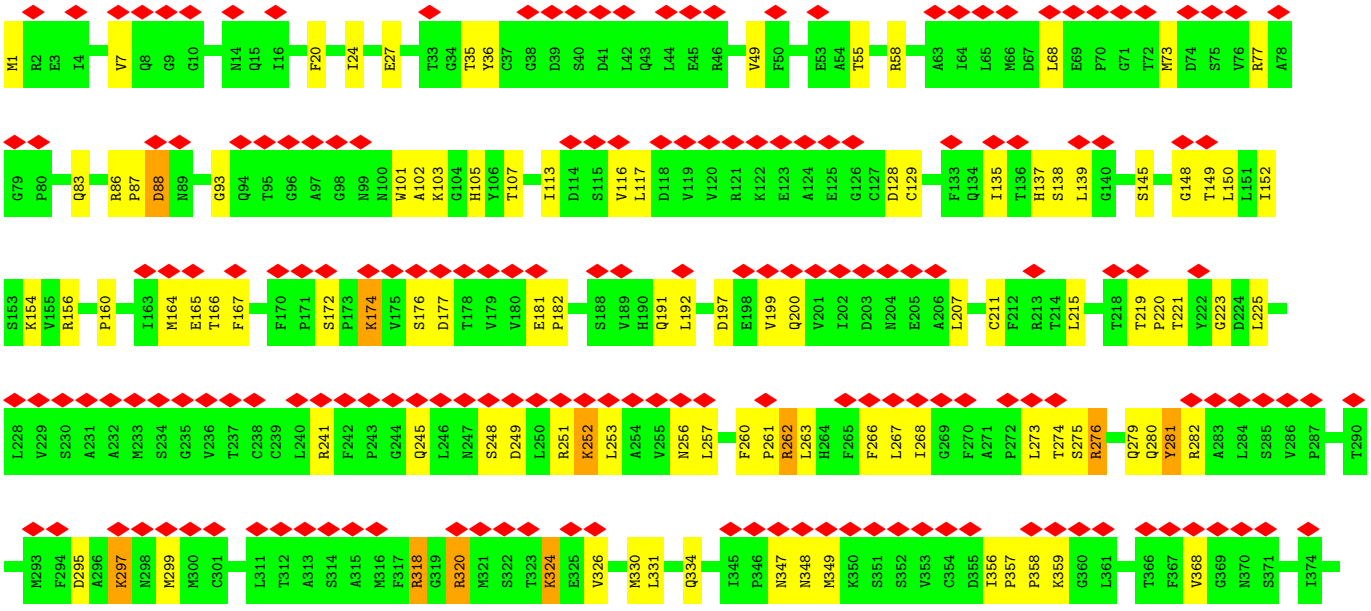
• Molecule 3: Tubulin beta chain

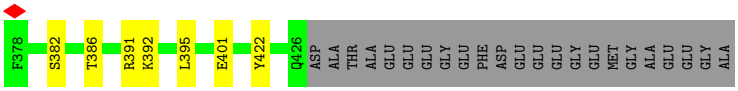
Chain B9:



• Molecule 3: Tubulin beta chain

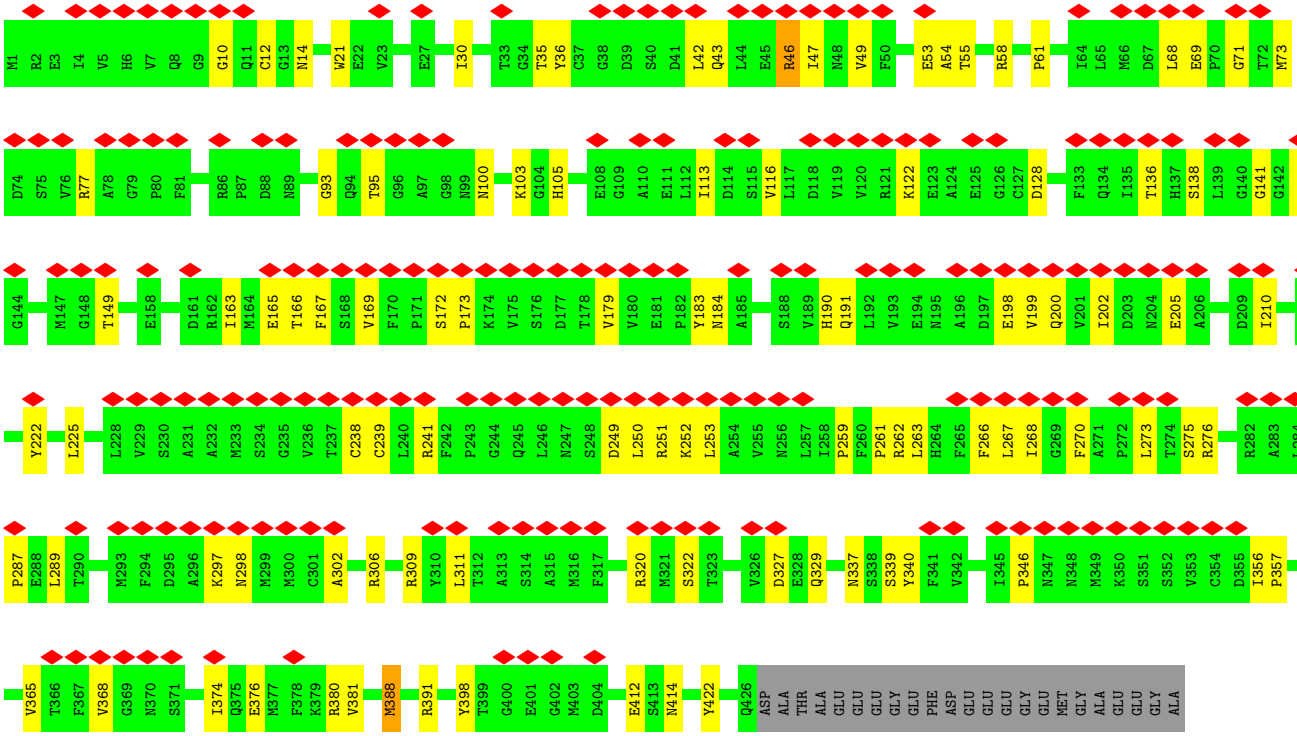
Chain C1:





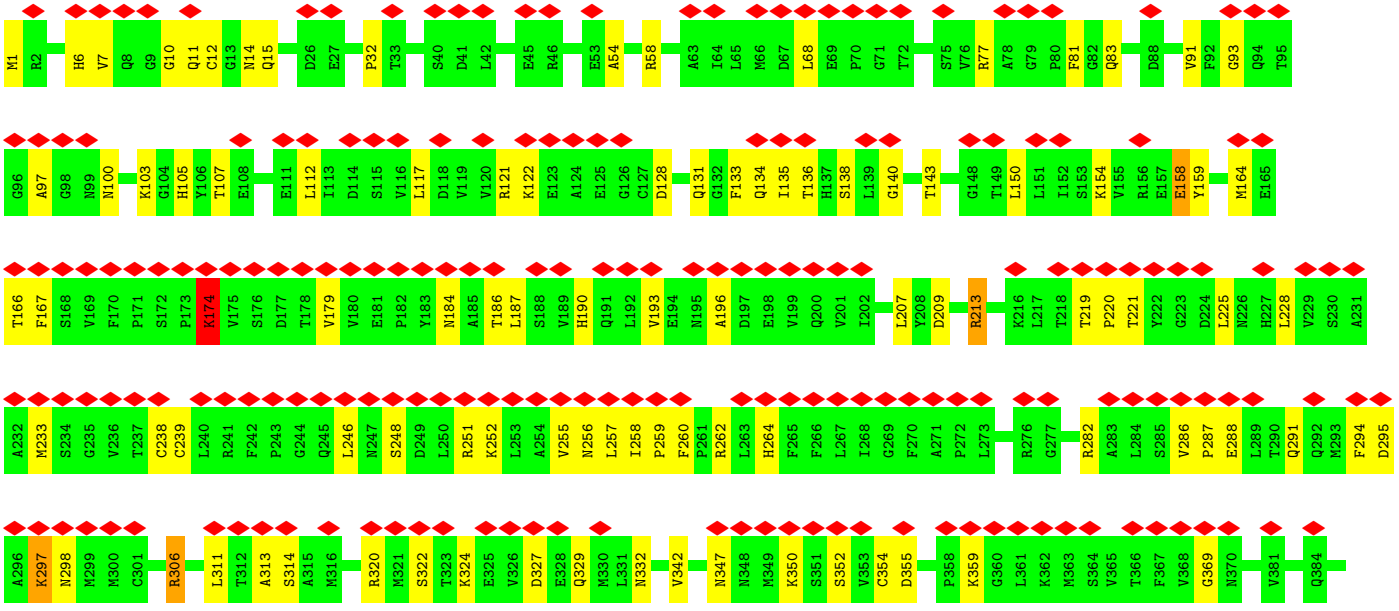
• Molecule 3: Tubulin beta chain

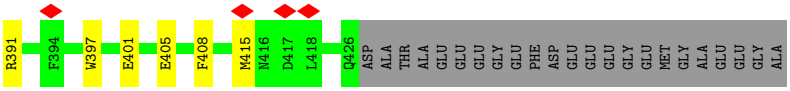
Chain C3:



• Molecule 3: Tubulin beta chain

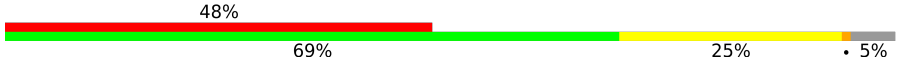
Chain C5:

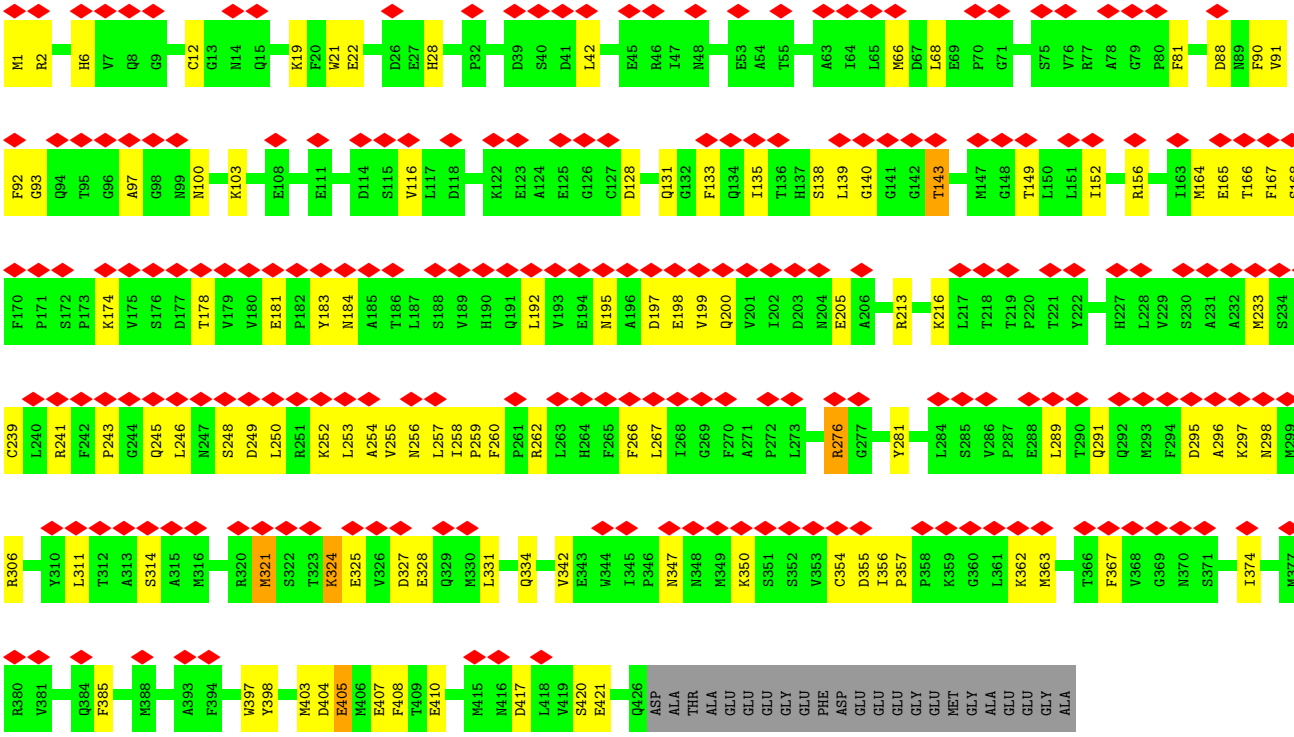




• Molecule 3: Tubulin beta chain

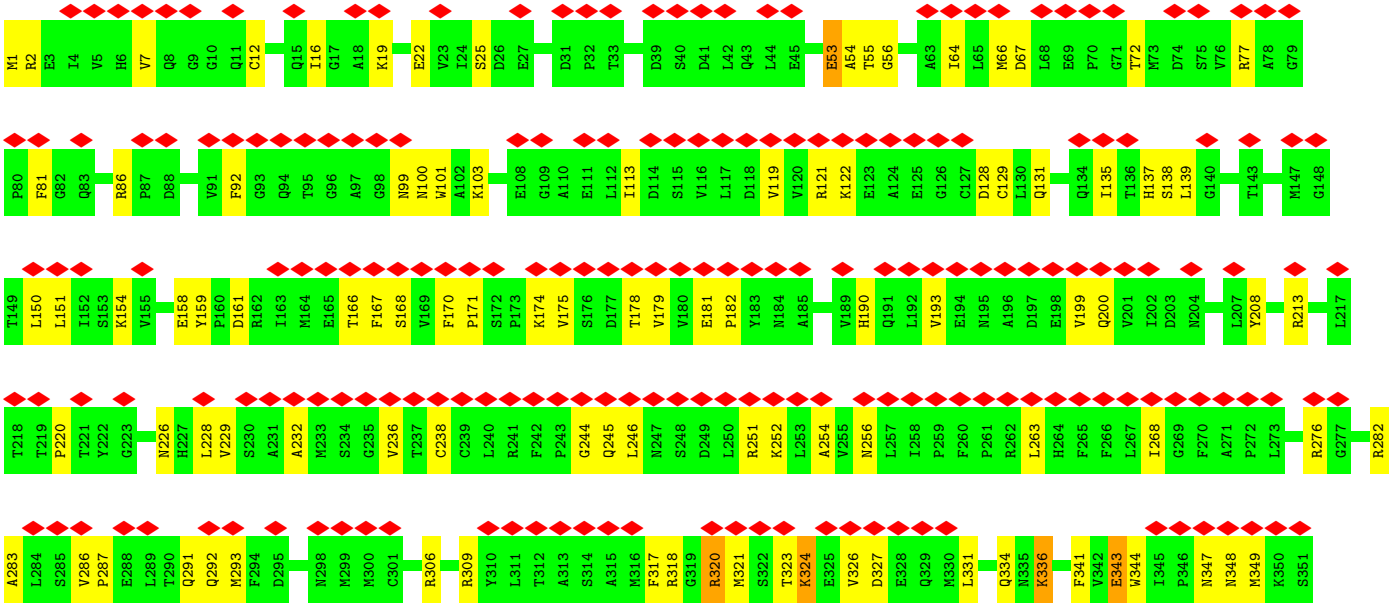
Chain C7:

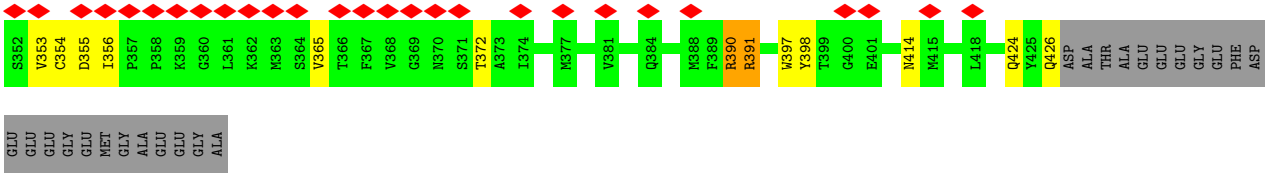




• Molecule 3: Tubulin beta chain

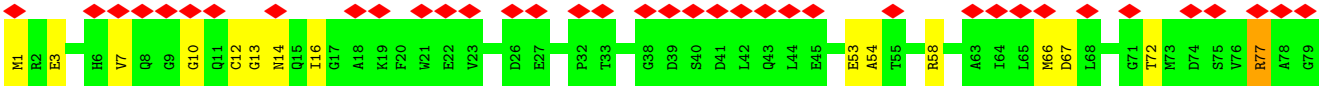
Chain C9:

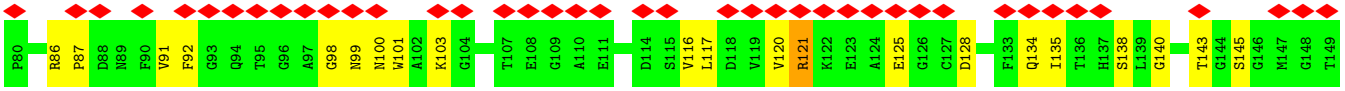


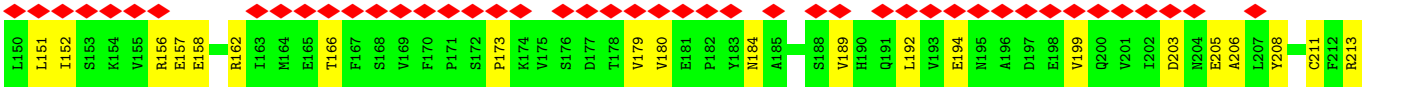


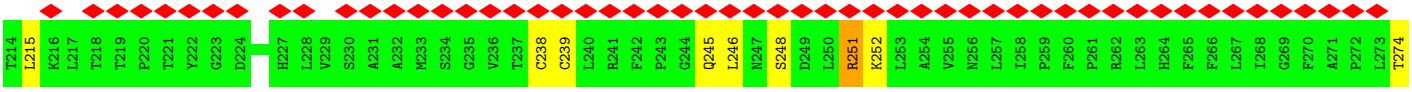
• Molecule 3: Tubulin beta chain

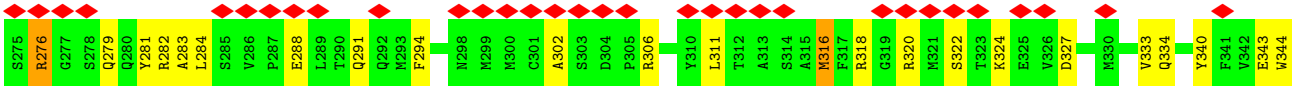
Chain D1:

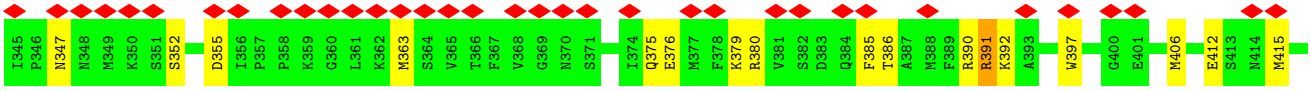


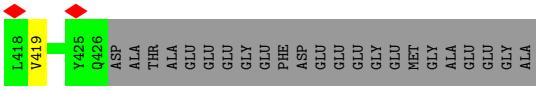






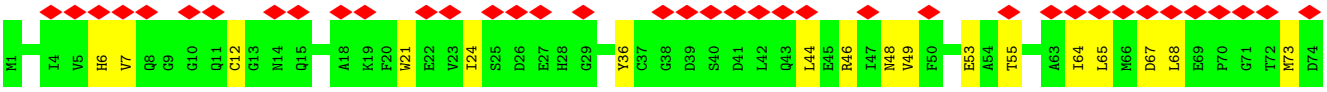


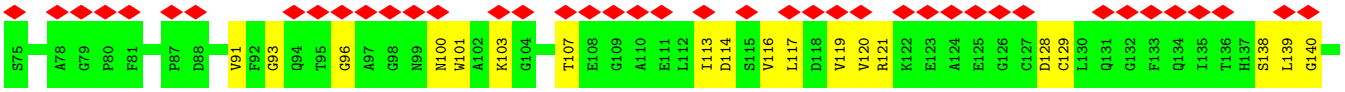


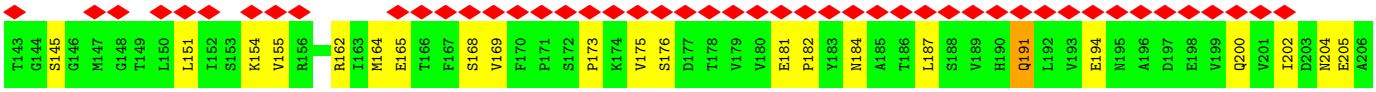


• Molecule 3: Tubulin beta chain

Chain D3:

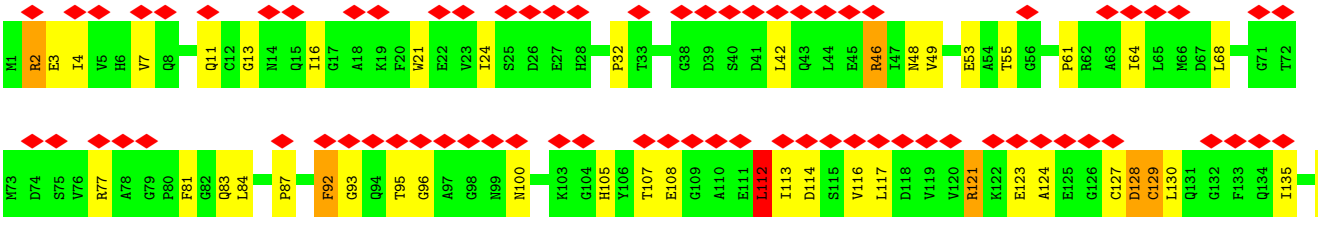






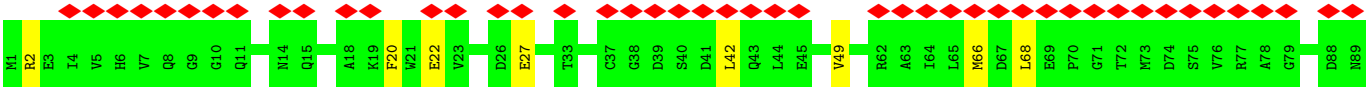
• Molecule 3: Tubulin beta chain

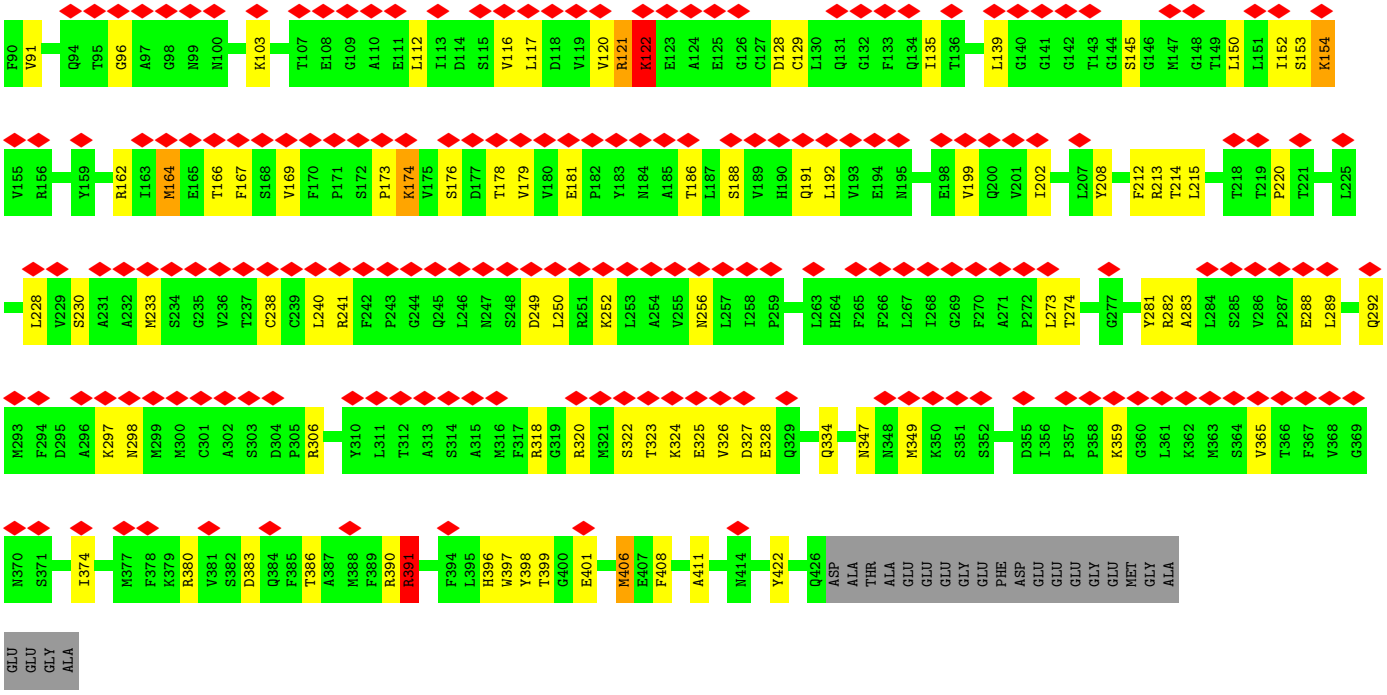
Chain D5:



• Molecule 3: Tubulin beta chain

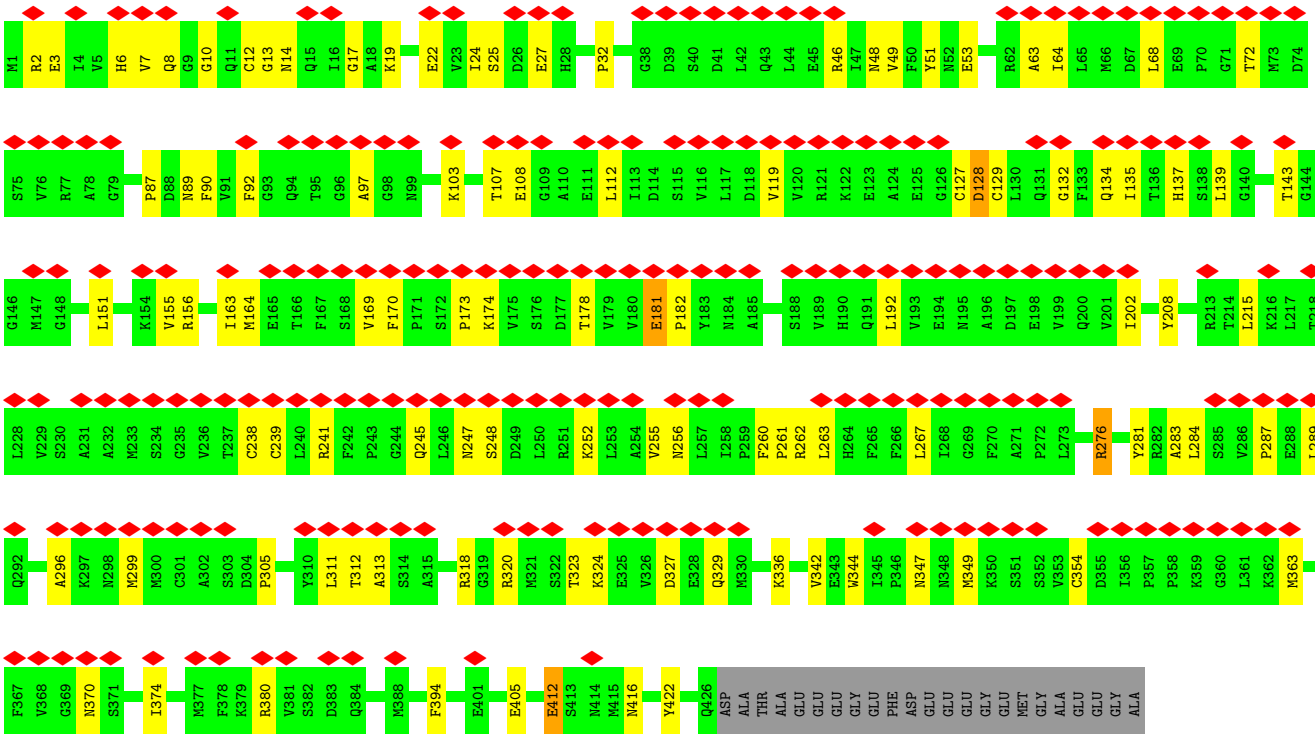
Chain D7:





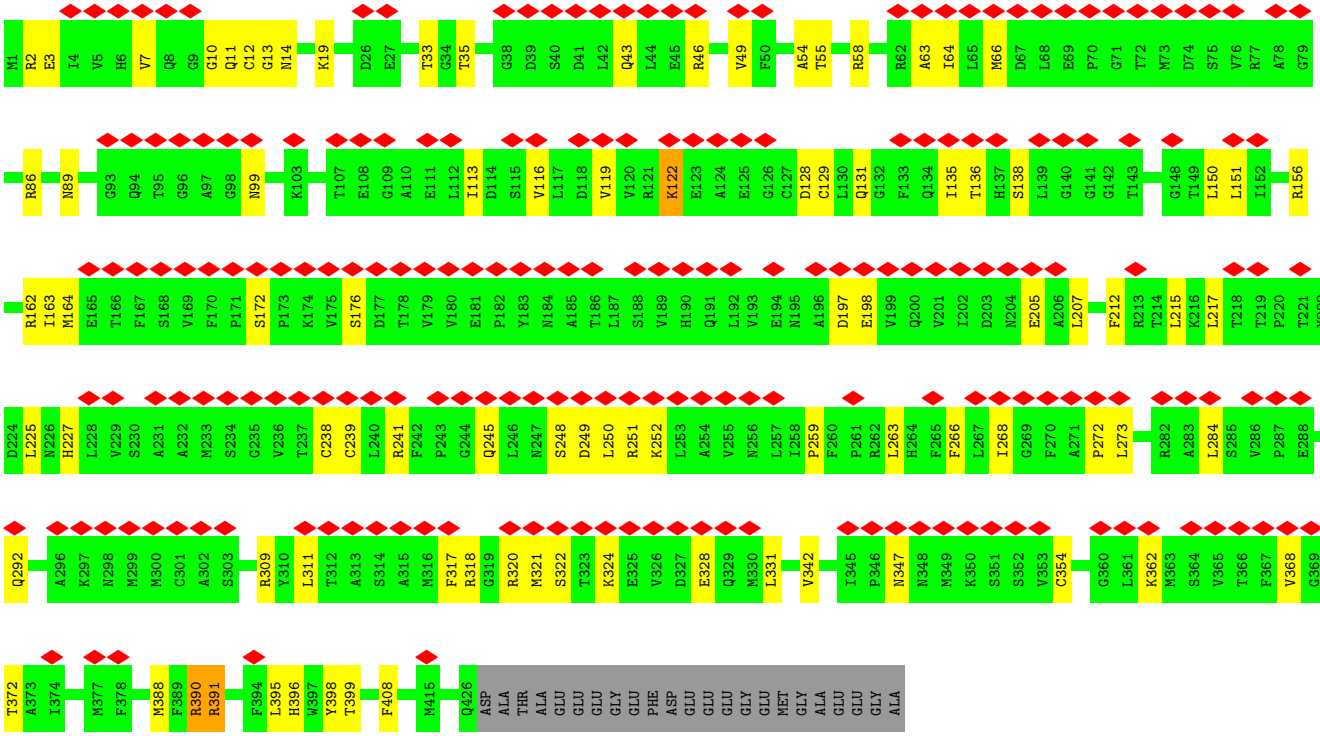
• Molecule 3: Tubulin beta chain

Chain D9:



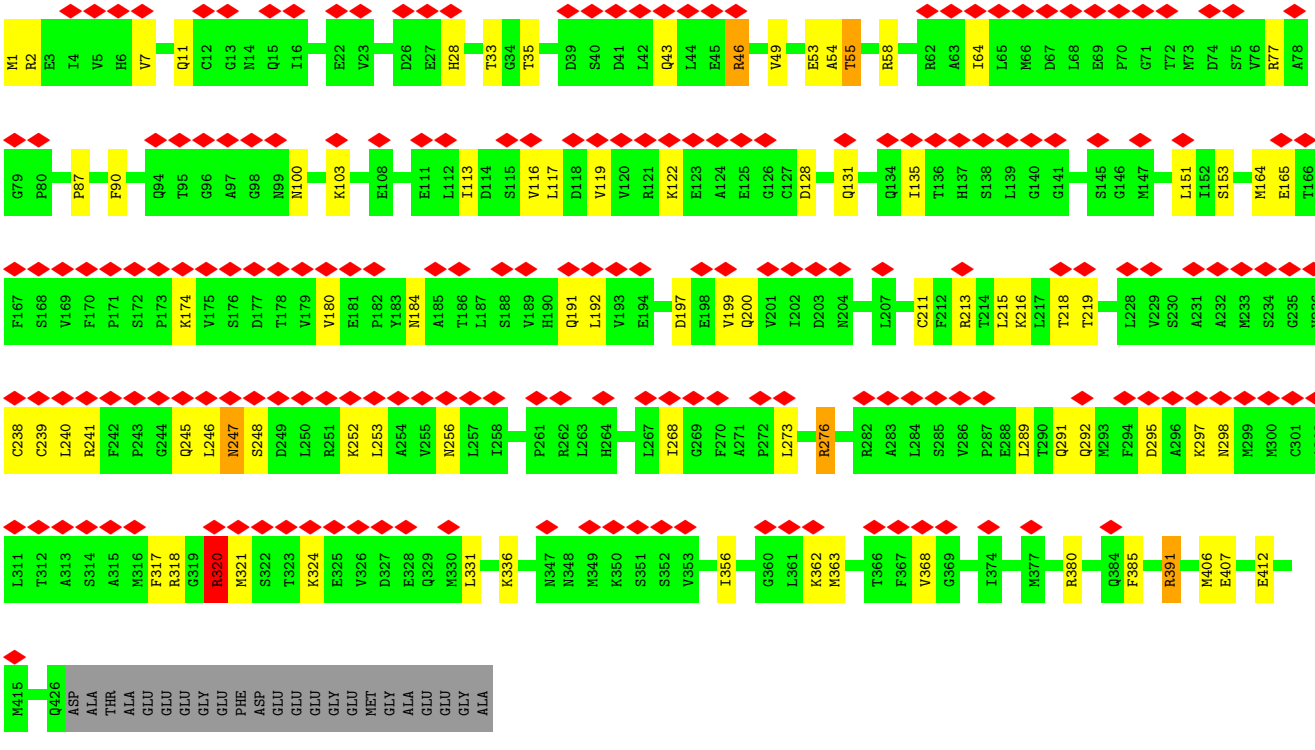
• Molecule 3: Tubulin beta chain

Chain E1:



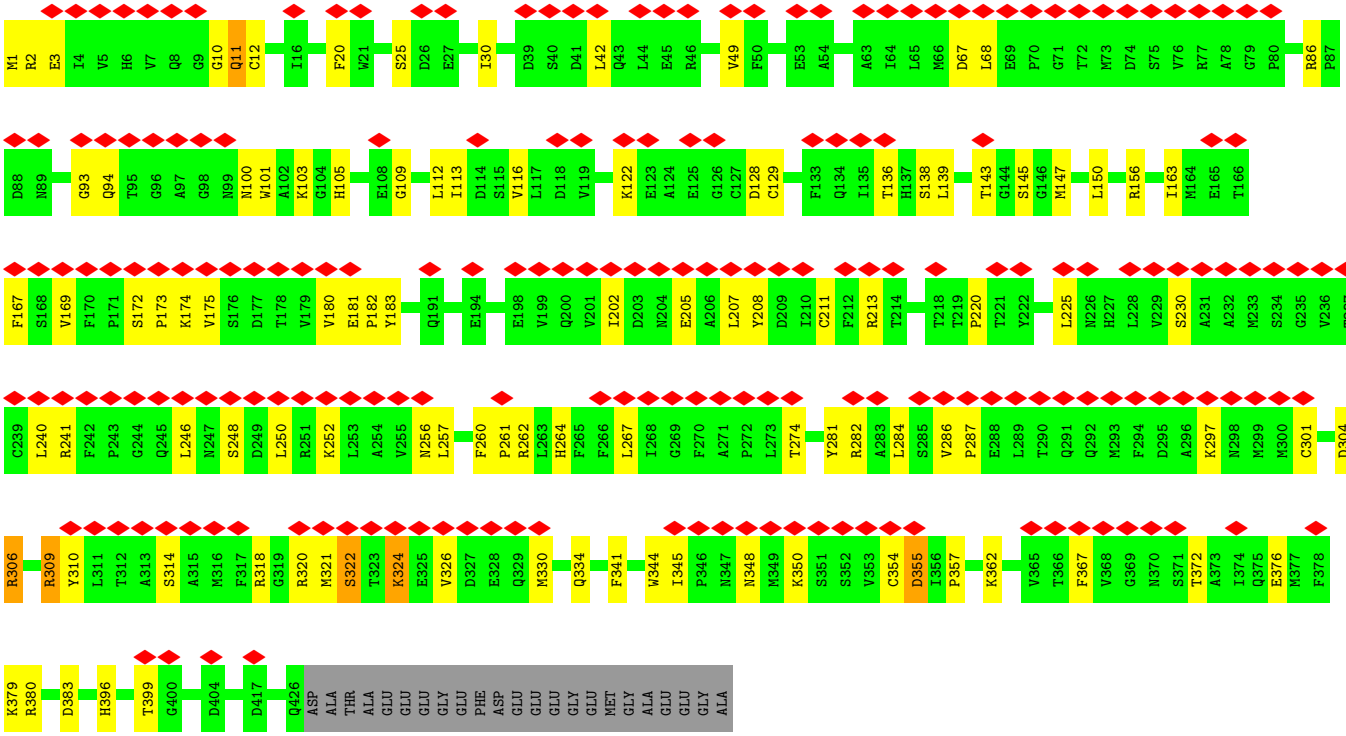
• Molecule 3: Tubulin beta chain

Chain E3:



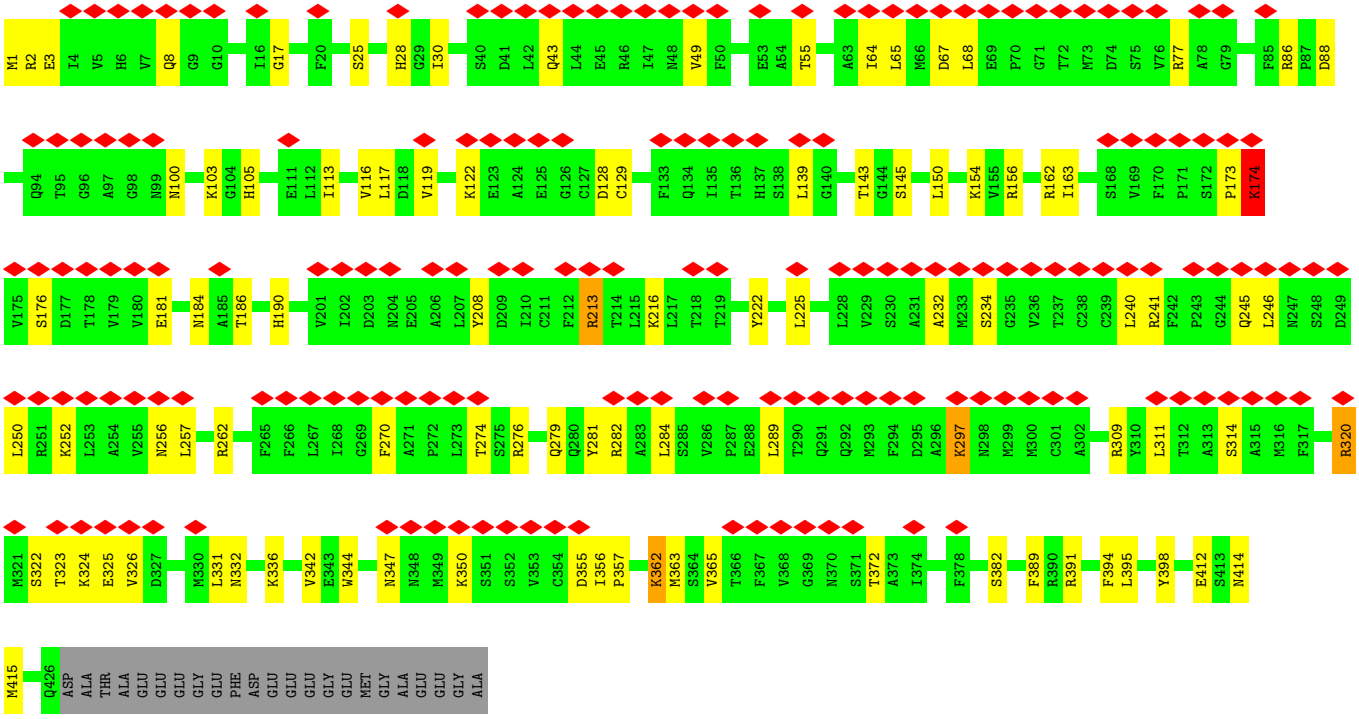
• Molecule 3: Tubulin beta chain

Chain E5:



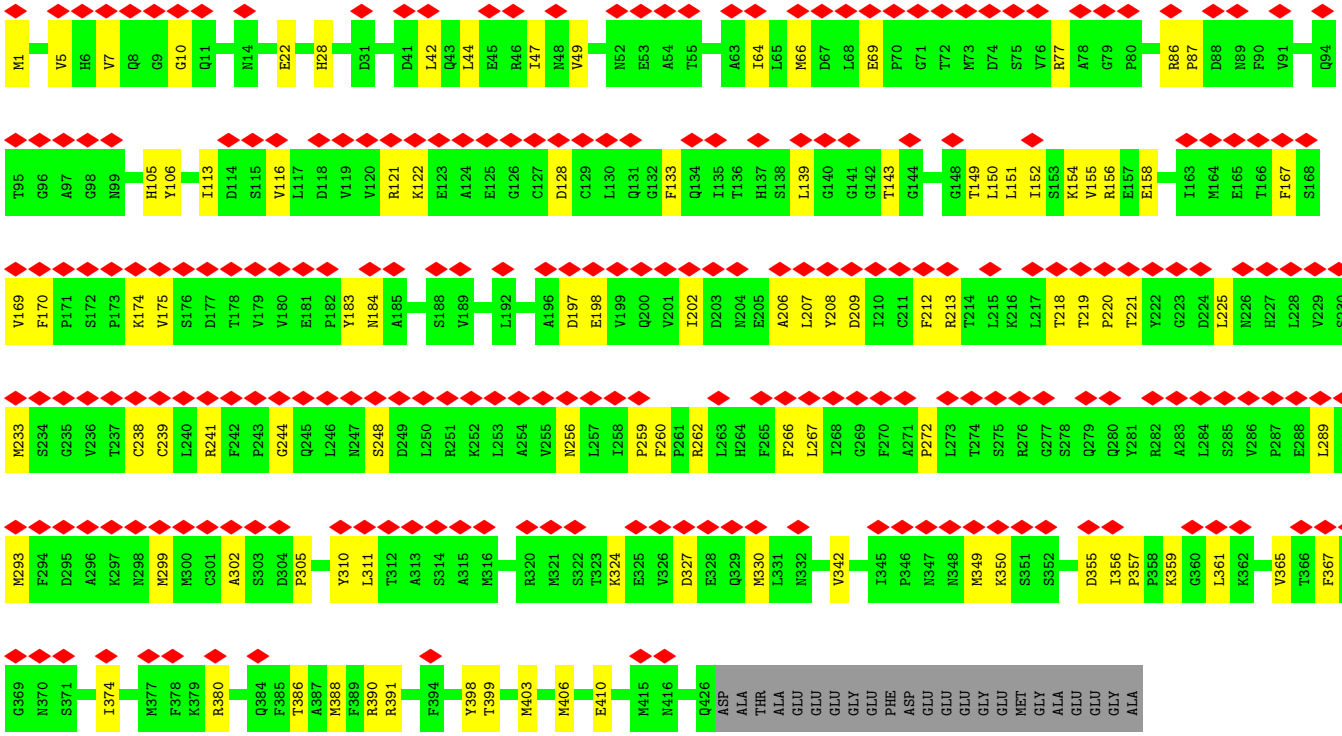
• Molecule 3: Tubulin beta chain

Chain E7:



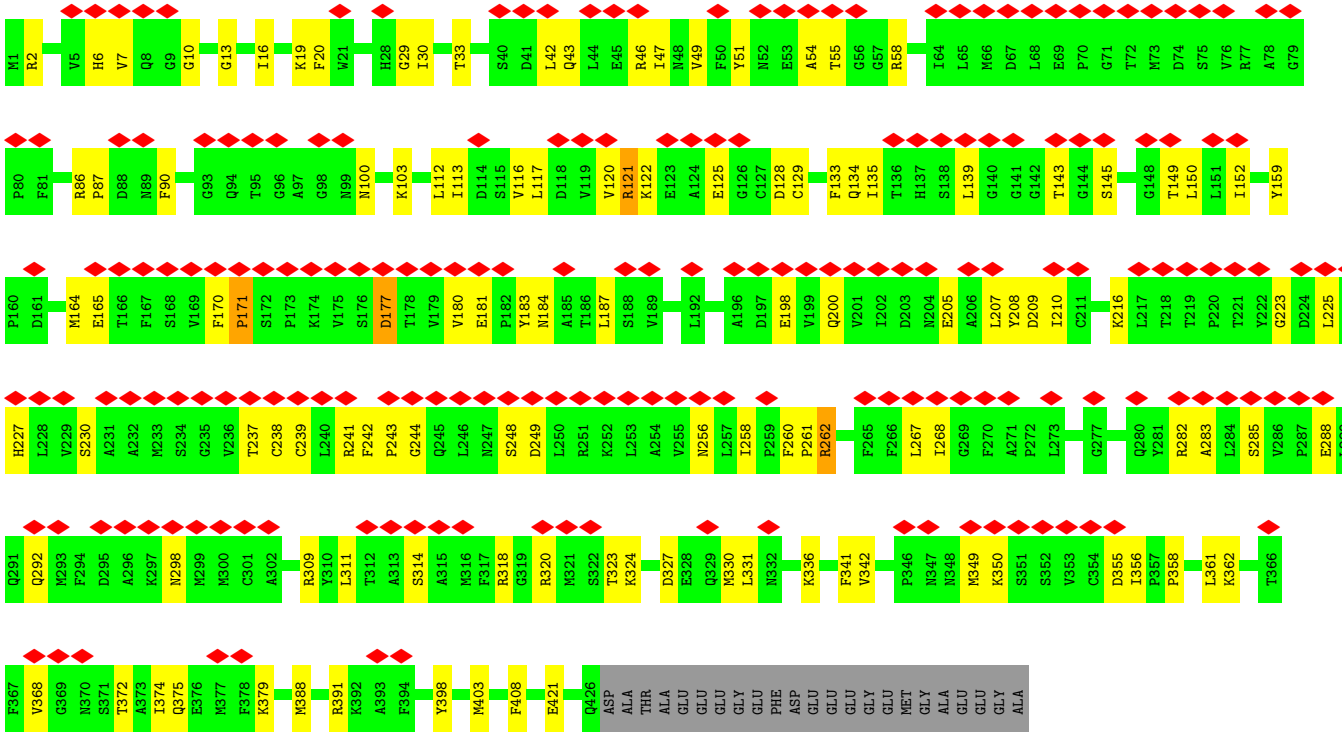
• Molecule 3: Tubulin beta chain

Chain E9:



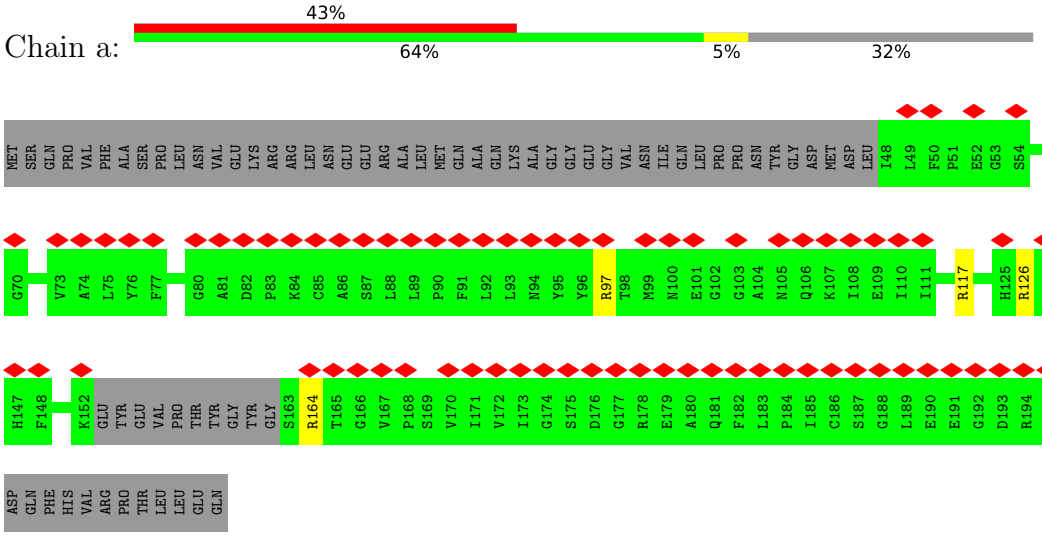
• Molecule 3: Tubulin beta chain

Chain F1:



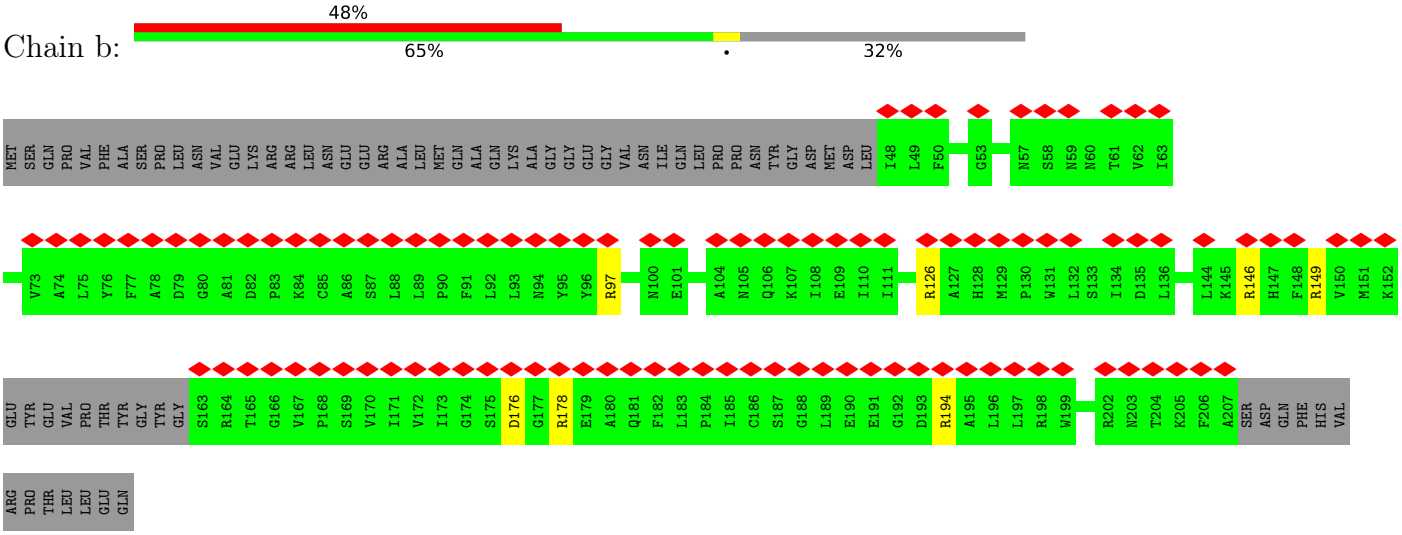
• Molecule 4: PDI family protein

Chain a:



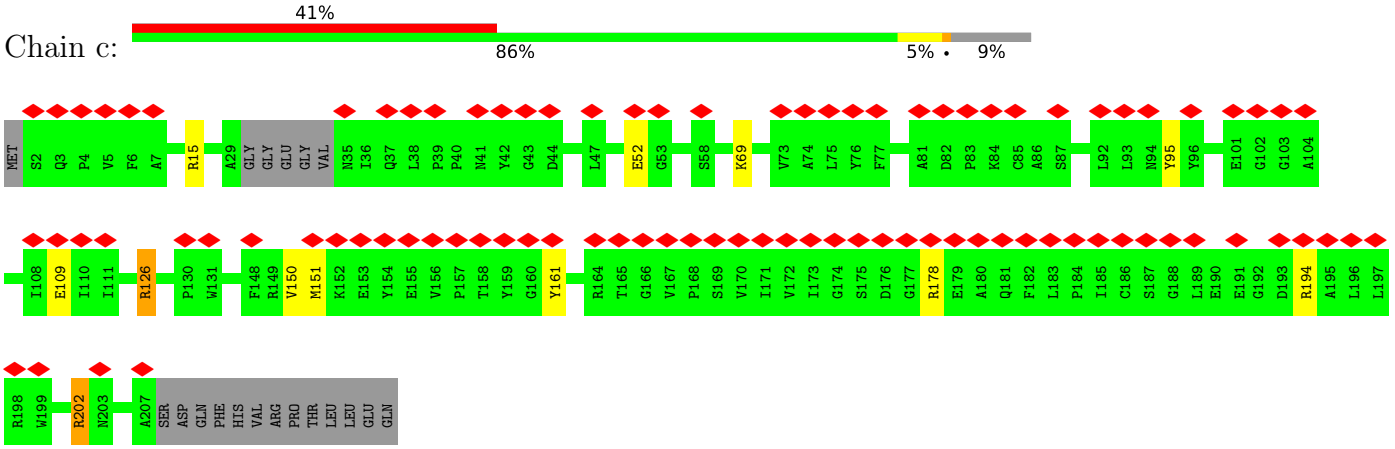
• Molecule 4: PDI family protein

Chain b:



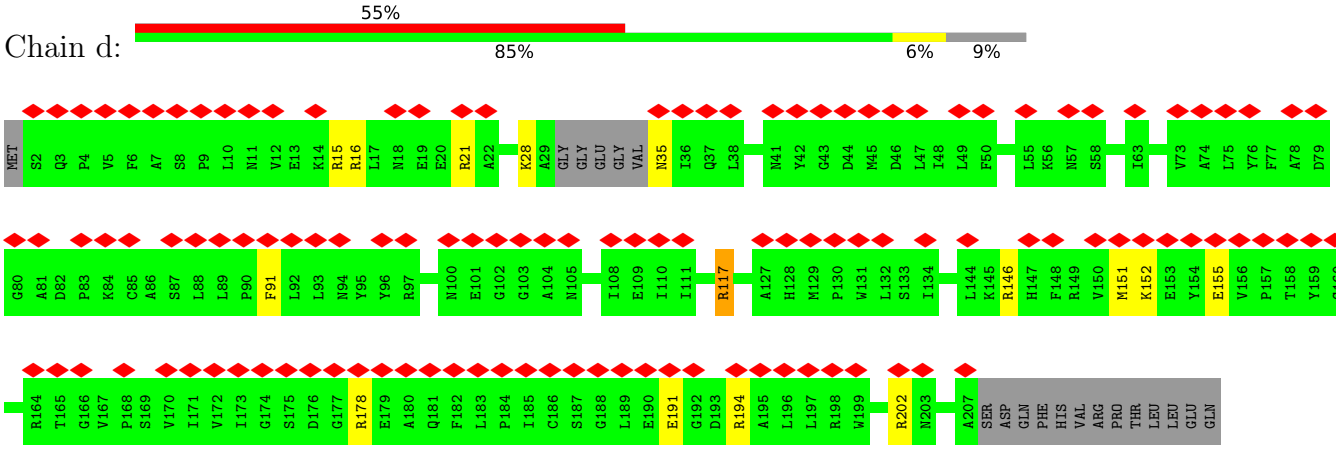
• Molecule 4: PDI family protein

Chain c:



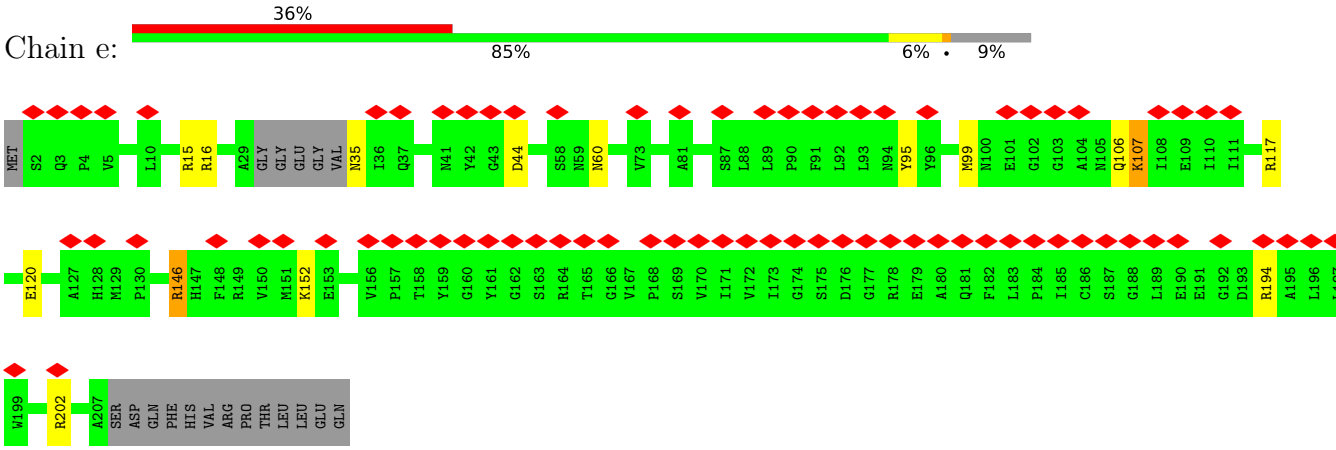
• Molecule 4: PDI family protein

Chain d:



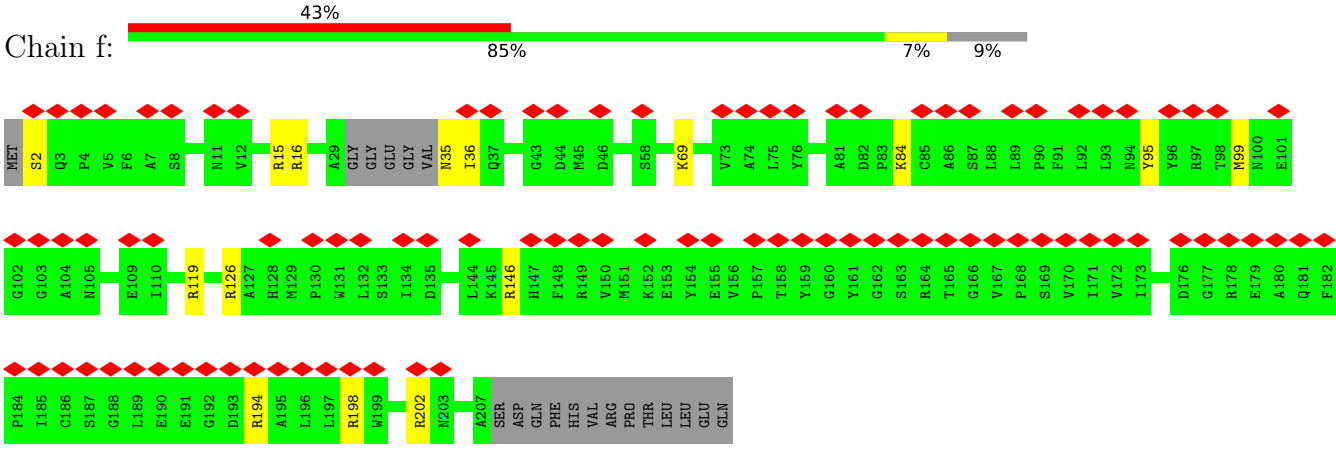
• Molecule 4: PDI family protein

Chain e:



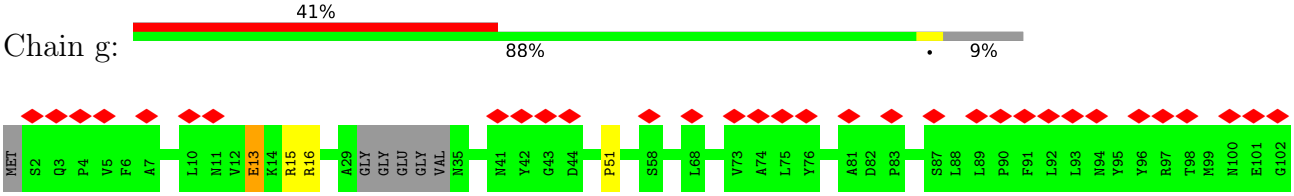
• Molecule 4: PDI family protein

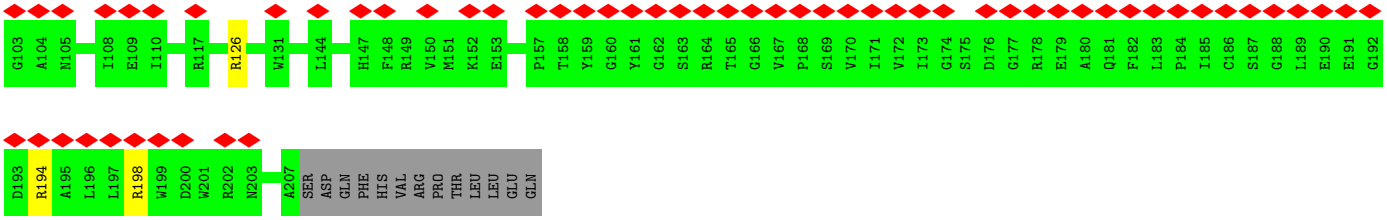
Chain f:



• Molecule 4: PDI family protein

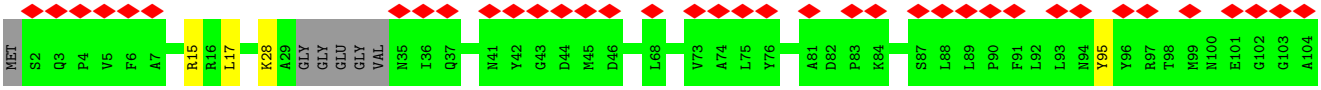
Chain g:





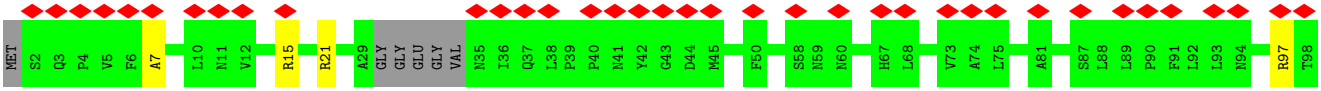
• Molecule 4: PDI family protein

Chain h:



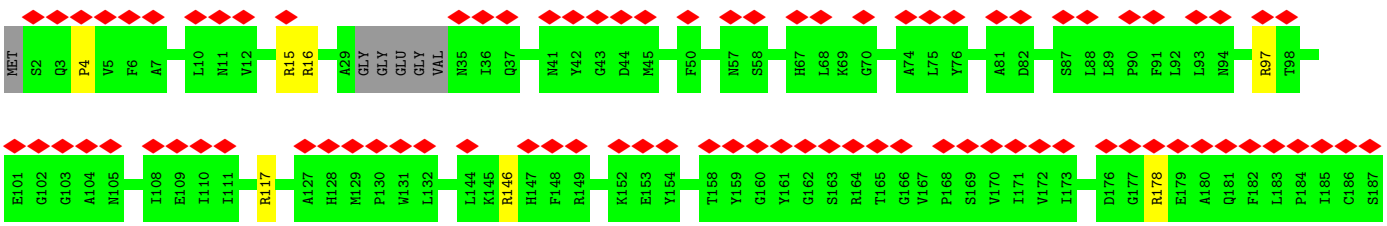
• Molecule 4: PDI family protein

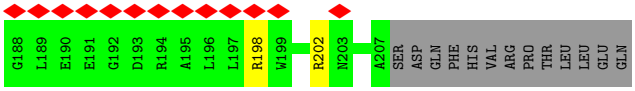
Chain i:



• Molecule 4: PDI family protein

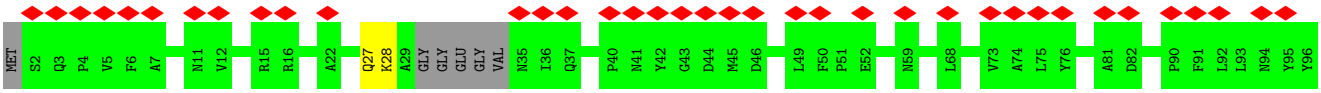
Chain j:

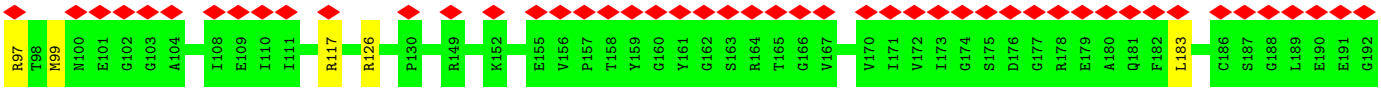


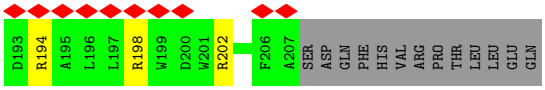


• Molecule 4: PDI family protein

Chain m:

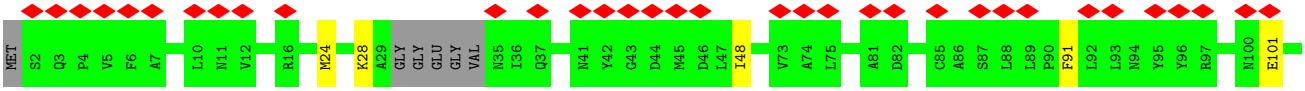


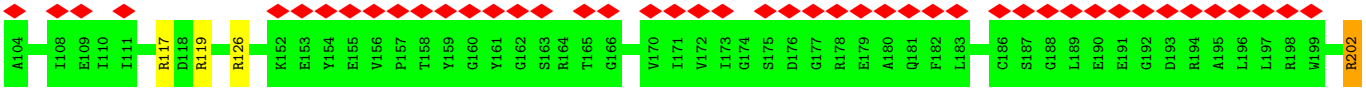


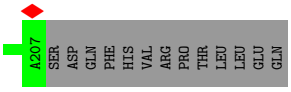


• Molecule 4: PDI family protein

Chain n:

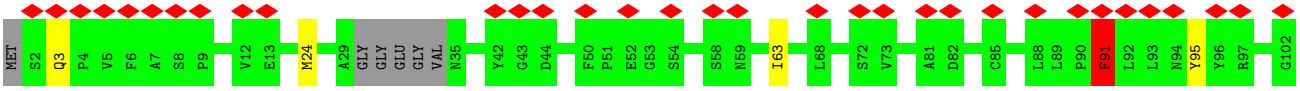


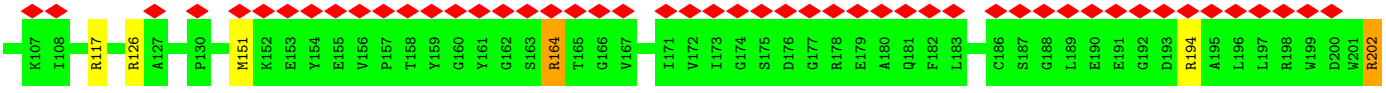


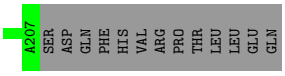


• Molecule 4: PDI family protein

Chain o:

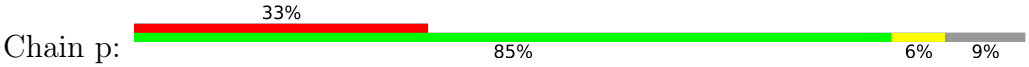


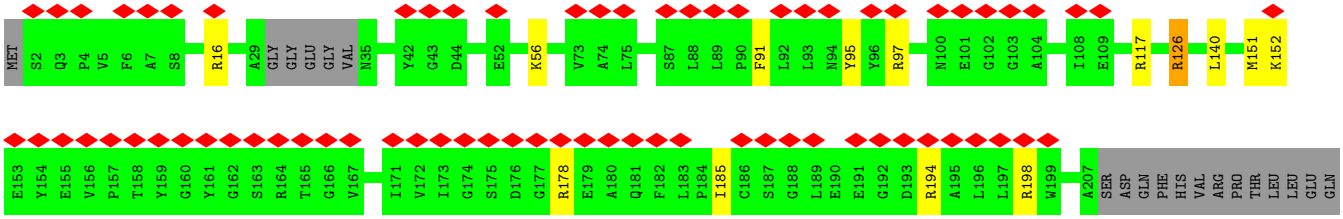




• Molecule 4: PDI family protein

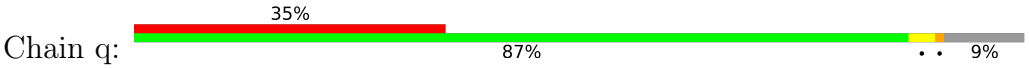
Chain p:

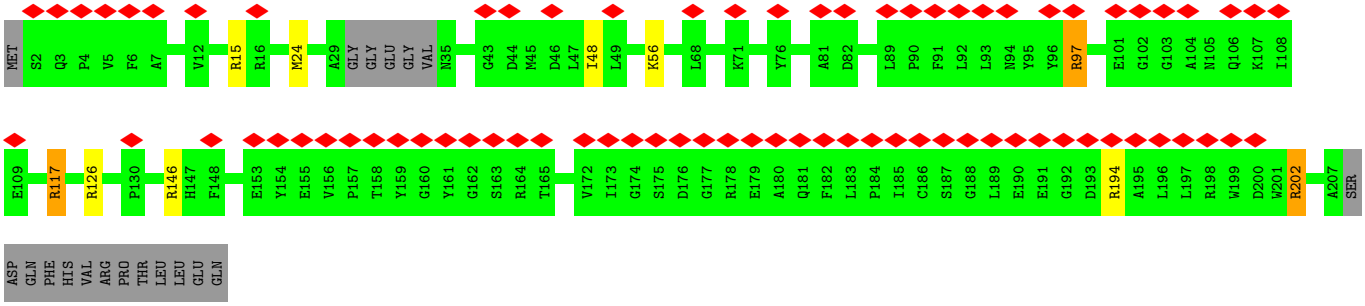




• Molecule 4: PDI family protein

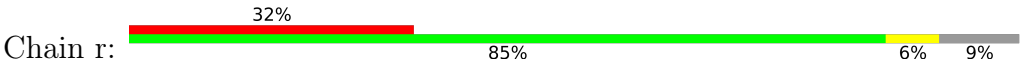
Chain q:

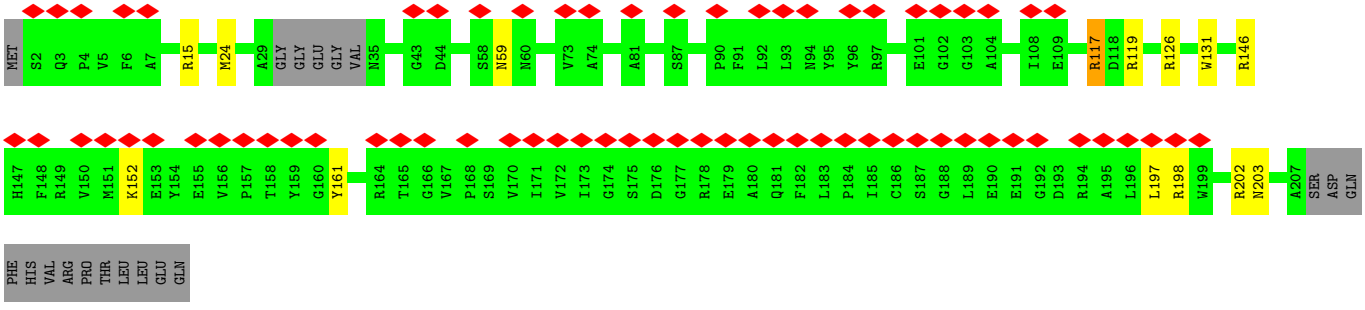




• Molecule 4: PDI family protein

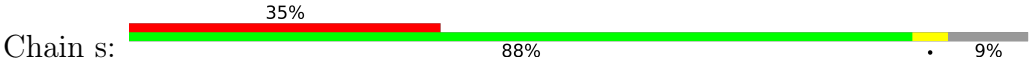
Chain r:

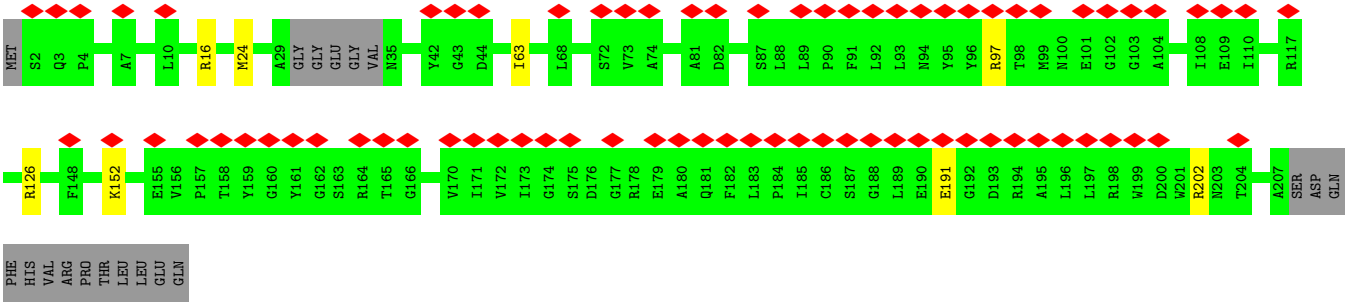




• Molecule 4: PDI family protein

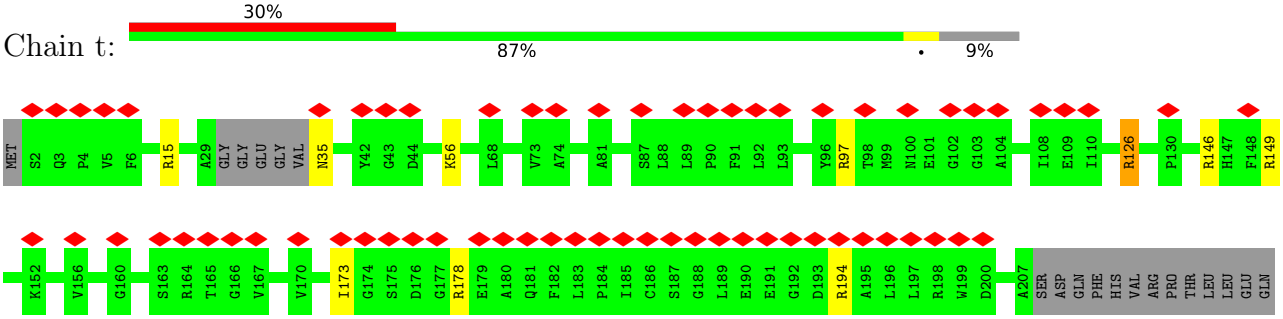
Chain s:





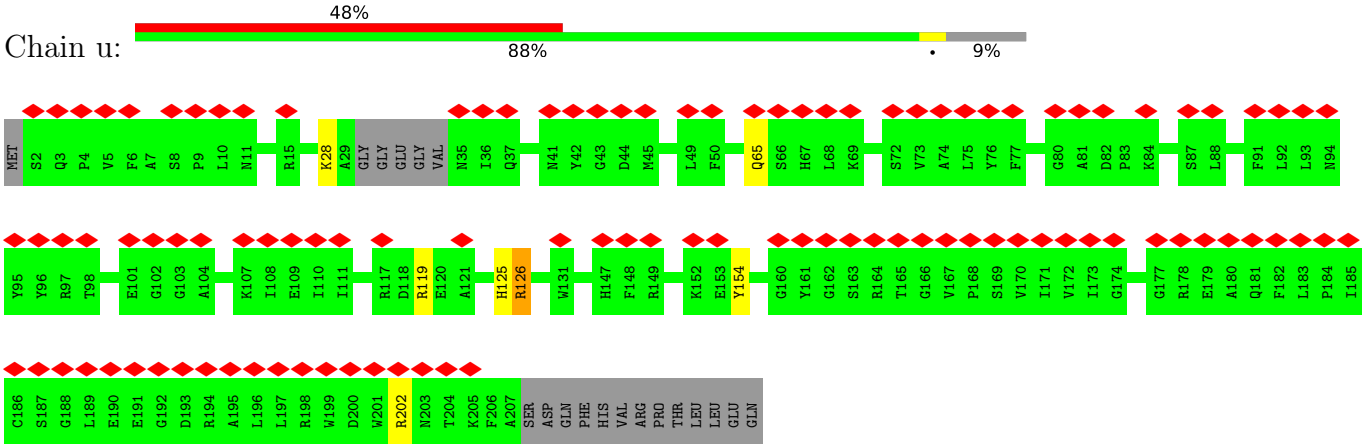
• Molecule 4: PDI family protein

Chain t:



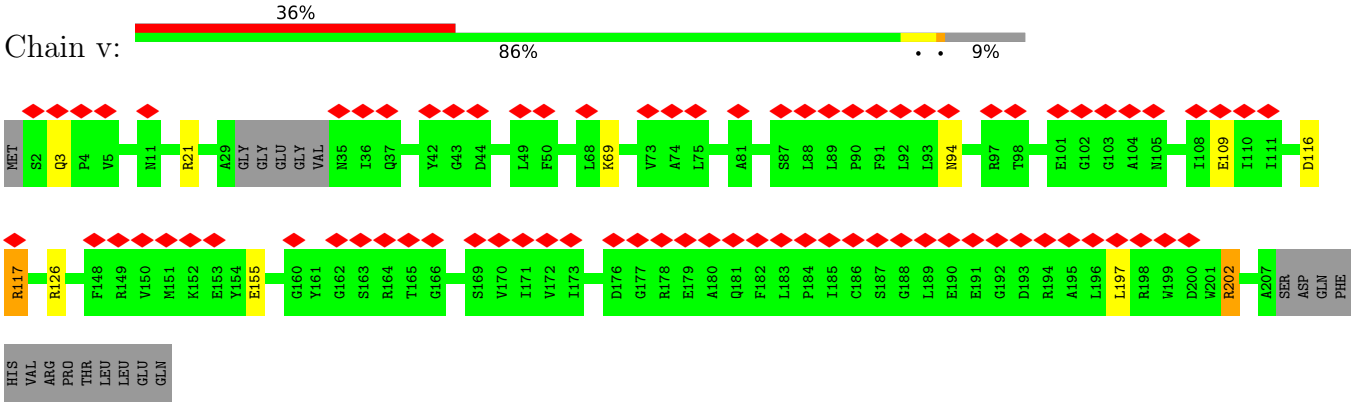
• Molecule 4: PDI family protein

Chain u:



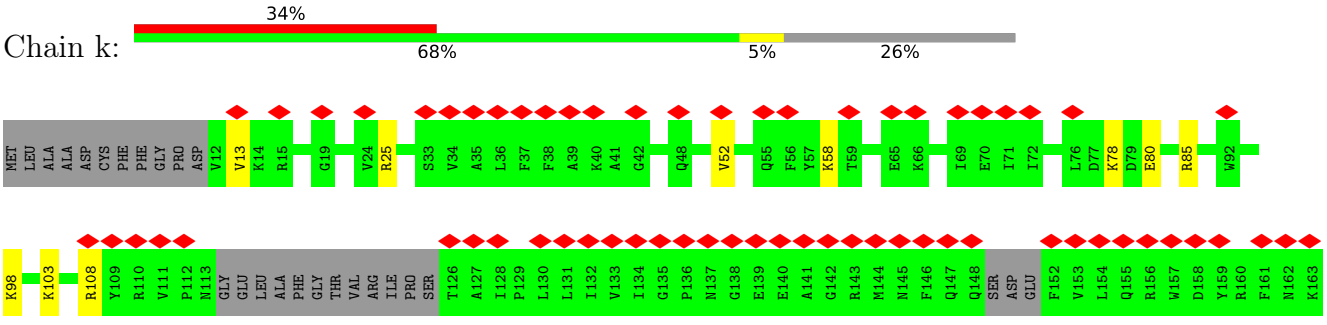
• Molecule 4: PDI family protein

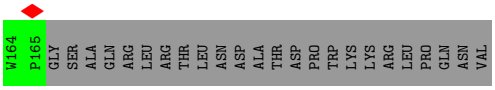
Chain v:



• Molecule 5: PDI family protein

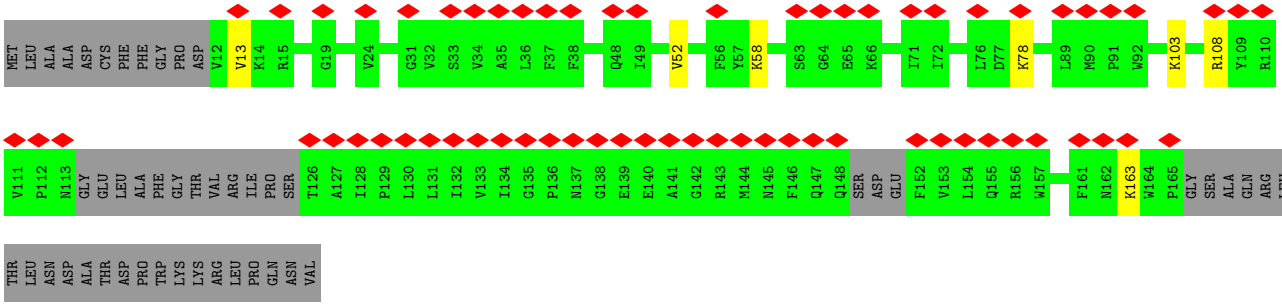
Chain k:





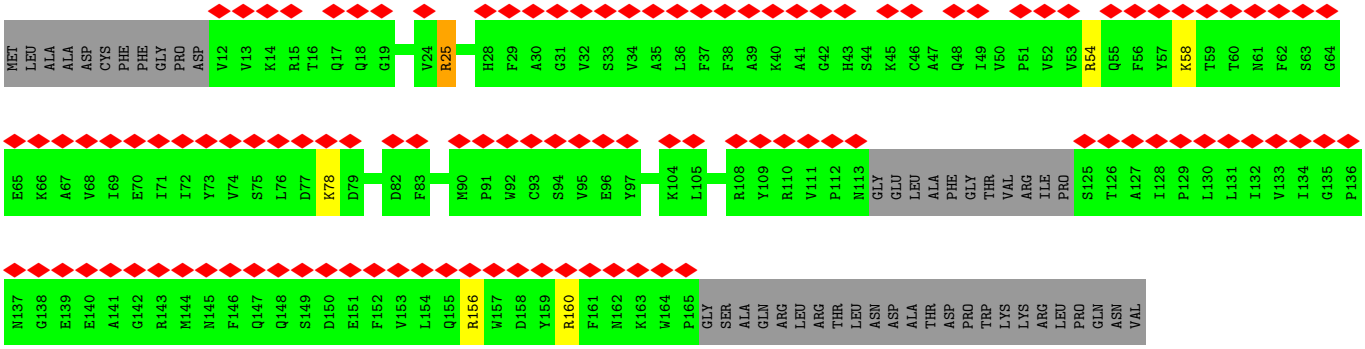
• Molecule 5: PDI family protein

Chain l:



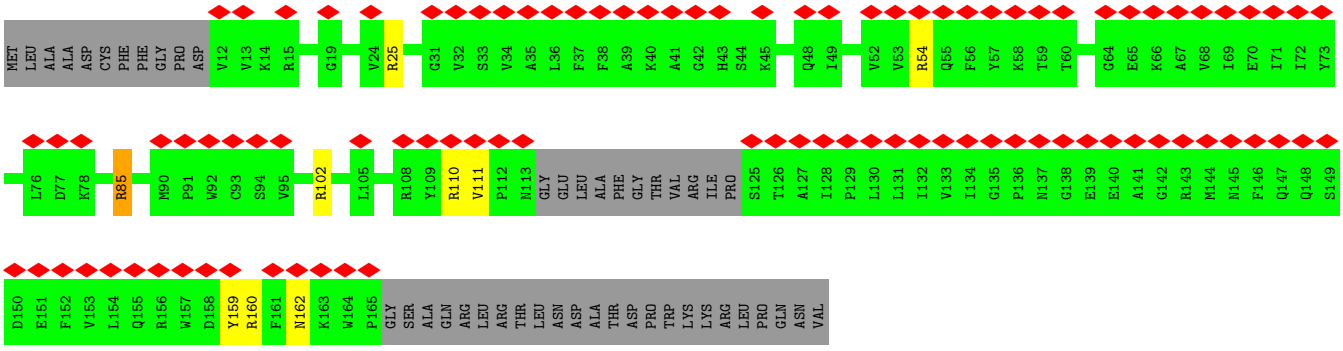
• Molecule 5: PDI family protein

Chain w:



• Molecule 5: PDI family protein

Chain x:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	39122	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	132	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	10.004	Depositor
Minimum map value	-8.373	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.892	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	447.444, 447.444, 447.444	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.0715, 2.0715, 2.0715	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	0.50	0/181	0.96	0/248
1	1	0.52	0/181	0.99	1/248 (0.4%)
1	10	0.41	0/181	0.99	0/248
1	11	0.53	0/181	1.39	3/248 (1.2%)
1	12	0.60	0/181	1.43	2/248 (0.8%)
1	13	0.52	0/181	1.13	0/248
1	14	0.45	0/181	0.88	0/248
1	15	0.60	0/181	1.32	1/248 (0.4%)
1	16	0.53	0/181	0.94	1/248 (0.4%)
1	17	0.60	0/181	1.20	1/248 (0.4%)
1	18	0.46	0/181	0.99	0/248
1	19	0.86	2/181 (1.1%)	1.13	2/248 (0.8%)
1	2	0.57	0/181	1.28	1/248 (0.4%)
1	20	0.45	0/181	0.76	0/248
1	21	0.57	0/181	1.11	1/248 (0.4%)
1	22	0.61	0/166	1.19	1/227 (0.4%)
1	23	0.46	0/166	0.89	0/227
1	3	0.50	0/181	0.94	0/248
1	4	0.45	0/181	1.12	1/248 (0.4%)
1	5	0.44	0/181	1.06	1/248 (0.4%)
1	6	0.45	0/181	1.11	1/248 (0.4%)
1	7	0.44	0/181	0.91	0/248
1	8	0.48	0/181	1.12	1/248 (0.4%)
1	9	0.52	0/181	0.96	0/248
2	A0	0.57	1/3398 (0.0%)	1.11	22/4606 (0.5%)
2	A2	0.51	1/3398 (0.0%)	0.99	15/4606 (0.3%)
2	A4	0.77	4/3398 (0.1%)	1.14	15/4606 (0.3%)
2	A6	0.54	2/3398 (0.1%)	1.01	13/4606 (0.3%)
2	A8	0.68	5/3398 (0.1%)	1.15	21/4606 (0.5%)
2	B0	0.53	0/3398	0.97	11/4606 (0.2%)
2	B2	0.59	2/3398 (0.1%)	1.02	8/4606 (0.2%)
2	B4	0.51	2/3398 (0.1%)	0.92	5/4606 (0.1%)
2	B6	0.51	2/3398 (0.1%)	0.88	5/4606 (0.1%)
2	B8	0.46	0/3398	0.88	9/4606 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	C0	0.47	2/3398 (0.1%)	0.87	4/4606 (0.1%)
2	C2	0.47	0/3398	0.91	7/4606 (0.2%)
2	C4	0.63	6/3398 (0.2%)	0.97	12/4606 (0.3%)
2	C6	0.53	1/3398 (0.0%)	1.00	8/4606 (0.2%)
2	C8	0.58	2/3398 (0.1%)	0.99	11/4606 (0.2%)
2	D0	0.57	2/3398 (0.1%)	1.06	21/4606 (0.5%)
2	D2	0.51	1/3398 (0.0%)	0.96	13/4606 (0.3%)
2	D4	0.64	3/3398 (0.1%)	1.20	25/4606 (0.5%)
2	D6	0.51	0/3398	0.91	12/4606 (0.3%)
2	D8	0.59	1/3398 (0.0%)	1.07	16/4606 (0.3%)
2	E0	0.40	0/3398	0.76	5/4606 (0.1%)
2	E2	0.51	2/3398 (0.1%)	0.93	10/4606 (0.2%)
2	E4	0.39	0/3398	0.73	4/4606 (0.1%)
2	E6	0.47	0/3398	0.87	4/4606 (0.1%)
2	E8	0.35	0/3398	0.70	0/4606
2	F0	0.54	2/3398 (0.1%)	0.90	13/4606 (0.3%)
3	A1	0.58	3/3404 (0.1%)	0.99	10/4606 (0.2%)
3	A3	0.45	0/3404	0.85	2/4606 (0.0%)
3	A5	0.66	3/3404 (0.1%)	1.07	18/4606 (0.4%)
3	A7	0.48	1/3404 (0.0%)	0.86	5/4606 (0.1%)
3	A9	0.59	2/3404 (0.1%)	0.99	9/4606 (0.2%)
3	B1	0.50	0/3404	0.90	3/4606 (0.1%)
3	B3	0.55	3/3404 (0.1%)	1.01	11/4606 (0.2%)
3	B5	0.52	1/3404 (0.0%)	0.95	5/4606 (0.1%)
3	B7	0.49	1/3404 (0.0%)	0.92	7/4606 (0.2%)
3	B9	0.46	0/3404	0.87	6/4606 (0.1%)
3	C1	0.48	1/3404 (0.0%)	0.92	7/4606 (0.2%)
3	C3	0.50	3/3404 (0.1%)	0.90	5/4606 (0.1%)
3	C5	0.54	2/3404 (0.1%)	0.93	10/4606 (0.2%)
3	C7	0.59	4/3404 (0.1%)	1.00	10/4606 (0.2%)
3	C9	0.56	3/3404 (0.1%)	1.02	17/4606 (0.4%)
3	D1	0.75	10/3404 (0.3%)	1.23	29/4606 (0.6%)
3	D3	0.59	1/3404 (0.0%)	1.10	19/4606 (0.4%)
3	D5	0.74	4/3404 (0.1%)	1.23	26/4606 (0.6%)
3	D7	0.55	2/3404 (0.1%)	0.96	7/4606 (0.2%)
3	D9	0.61	3/3404 (0.1%)	1.06	14/4606 (0.3%)
3	E1	0.45	0/3404	0.83	4/4606 (0.1%)
3	E3	0.52	0/3404	0.95	11/4606 (0.2%)
3	E5	0.45	1/3404 (0.0%)	0.88	10/4606 (0.2%)
3	E7	0.52	1/3404 (0.0%)	0.97	11/4606 (0.2%)
3	E9	0.48	2/3404 (0.1%)	0.85	5/4606 (0.1%)
3	F1	0.52	0/3404	1.02	14/4606 (0.3%)
4	a	0.67	4/1225 (0.3%)	1.07	4/1654 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	b	0.60	3/1225 (0.2%)	1.02	9/1654 (0.5%)
4	c	0.97	4/1645 (0.2%)	1.66	12/2225 (0.5%)
4	d	0.64	2/1645 (0.1%)	1.12	15/2225 (0.7%)
4	e	0.55	0/1645	1.06	12/2225 (0.5%)
4	f	0.54	0/1645	1.03	11/2225 (0.5%)
4	g	0.58	1/1645 (0.1%)	1.06	6/2225 (0.3%)
4	h	0.57	1/1645 (0.1%)	1.09	9/2225 (0.4%)
4	i	0.63	2/1645 (0.1%)	1.03	7/2225 (0.3%)
4	j	0.67	2/1645 (0.1%)	1.02	10/2225 (0.4%)
4	m	0.50	0/1645	0.96	9/2225 (0.4%)
4	n	0.65	4/1645 (0.2%)	1.11	9/2225 (0.4%)
4	o	0.55	0/1645	1.01	8/2225 (0.4%)
4	p	0.82	2/1645 (0.1%)	1.20	16/2225 (0.7%)
4	q	0.67	2/1645 (0.1%)	1.03	9/2225 (0.4%)
4	r	0.57	0/1645	1.07	10/2225 (0.4%)
4	s	0.51	1/1645 (0.1%)	0.97	2/2225 (0.1%)
4	t	0.68	2/1645 (0.1%)	1.13	9/2225 (0.4%)
4	u	0.49	0/1645	0.92	3/2225 (0.1%)
4	v	0.68	4/1645 (0.2%)	1.14	9/2225 (0.4%)
5	k	0.54	1/1168 (0.1%)	1.10	5/1578 (0.3%)
5	l	0.55	2/1168 (0.2%)	0.99	2/1578 (0.1%)
5	w	0.48	1/1201 (0.1%)	0.89	2/1623 (0.1%)
5	x	0.60	0/1201	1.15	7/1623 (0.4%)
All	All	0.56	132/217964 (0.1%)	0.99	777/295182 (0.3%)

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	13	0	1
1	15	0	2
1	18	0	1
1	23	0	2
1	4	0	1
1	7	0	1
2	A0	0	1
2	A2	0	2
2	A4	0	2
2	A8	0	3
2	B0	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B4	0	1
2	B6	0	1
2	C4	0	1
2	C8	0	1
2	D0	0	2
2	D2	0	1
2	E2	0	1
3	B3	0	1
3	B9	0	1
3	E5	0	2
4	c	0	1
4	e	0	1
4	o	0	1
4	t	0	1
5	k	0	1
5	l	0	1
All	All	0	35

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c	178	ARG	NE-CZ	24.25	1.64	1.33
4	p	97	ARG	NE-CZ	22.41	1.62	1.33
4	c	178	ARG	CZ-NH1	17.44	1.55	1.33
2	A4	254	GLU	CG-CD	16.52	1.76	1.51
3	D5	3	GLU	CD-OE1	16.43	1.43	1.25
4	j	97	ARG	NE-CZ	15.78	1.53	1.33
4	t	97	ARG	NE-CZ	15.18	1.52	1.33
2	A4	254	GLU	CD-OE2	14.39	1.41	1.25
2	F0	284	GLU	CD-OE1	14.20	1.41	1.25
4	i	202	ARG	NE-CZ	14.06	1.51	1.33
2	C4	2	ARG	CD-NE	13.93	1.70	1.46
4	q	97	ARG	NE-CZ	13.91	1.51	1.33
4	v	202	ARG	CD-NE	12.50	1.67	1.46
4	d	202	ARG	NE-CZ	12.40	1.49	1.33
2	D8	155	GLU	CD-OE1	11.99	1.38	1.25
2	C4	2	ARG	CZ-NH2	11.62	1.48	1.33
2	A4	254	GLU	CD-OE1	10.95	1.37	1.25
3	A5	252	LYS	CD-CE	10.80	1.78	1.51
3	D5	343	GLU	CD-OE1	9.97	1.36	1.25
2	C4	2	ARG	CG-CD	9.81	1.76	1.51
3	D1	343	GLU	CG-CD	9.55	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	g	13	GLU	CD-OE2	-9.54	1.15	1.25
4	n	202	ARG	CZ-NH2	9.32	1.45	1.33
3	A9	252	LYS	CG-CD	9.32	1.84	1.52
3	D1	3	GLU	CD-OE1	9.12	1.35	1.25
3	A5	252	LYS	CE-NZ	8.99	1.71	1.49
2	B6	285	GLN	CD-NE2	8.95	1.55	1.32
3	D1	397	TRP	NE1-CE2	8.56	1.48	1.37
3	C5	158	GLU	CD-OE2	-8.49	1.16	1.25
4	v	155	GLU	CG-CD	8.23	1.64	1.51
3	D9	181	GLU	CD-OE1	8.22	1.34	1.25
4	n	202	ARG	CD-NE	8.21	1.60	1.46
3	A1	69	GLU	CD-OE1	-8.19	1.16	1.25
2	C4	2	ARG	CZ-NH1	8.08	1.43	1.33
4	t	97	ARG	CD-NE	8.05	1.60	1.46
3	C5	158	GLU	CD-OE1	-7.95	1.17	1.25
3	D5	157	GLU	CD-OE2	7.84	1.34	1.25
3	D1	397	TRP	CG-CD2	7.84	1.56	1.43
3	E9	22	GLU	CD-OE1	7.83	1.34	1.25
4	a	142	GLU	CD-OE1	7.72	1.34	1.25
2	A2	55	GLU	CD-OE1	7.68	1.34	1.25
2	D2	196	GLU	CD-OE2	-7.63	1.17	1.25
3	C3	412	GLU	CD-OE2	7.60	1.34	1.25
2	C8	254	GLU	CD-OE2	7.57	1.33	1.25
3	C7	405	GLU	CD-OE1	7.48	1.33	1.25
3	D3	288	GLU	CD-OE1	7.38	1.33	1.25
3	D9	412	GLU	CD-OE1	-7.26	1.17	1.25
2	A8	207	GLU	CD-OE1	7.25	1.33	1.25
2	C8	155	GLU	CD-OE2	7.15	1.33	1.25
3	A1	122	LYS	CD-CE	7.12	1.69	1.51
2	C4	2	ARG	NE-CZ	7.10	1.42	1.33
3	D1	343	GLU	CD-OE1	7.05	1.33	1.25
4	c	109	GLU	CD-OE1	7.03	1.33	1.25
4	n	202	ARG	NE-CZ	6.94	1.42	1.33
4	c	178	ARG	CD-NE	6.80	1.58	1.46
4	q	97	ARG	CD-NE	6.71	1.57	1.46
1	19	248	ARG	CD-NE	6.70	1.57	1.46
4	p	97	ARG	CD-NE	6.60	1.57	1.46
3	C7	205	GLU	CD-OE1	-6.59	1.18	1.25
2	A0	155	GLU	CD-OE1	6.57	1.32	1.25
3	C7	405	GLU	CG-CD	6.54	1.61	1.51
4	s	191	GLU	CD-OE2	-6.53	1.18	1.25
5	w	25	ARG	NE-CZ	6.49	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A1	122	LYS	CE-NZ	6.48	1.65	1.49
2	E2	207	GLU	CD-OE1	6.44	1.32	1.25
2	A6	326	LYS	CG-CD	6.33	1.74	1.52
3	B5	336	LYS	CE-NZ	6.33	1.64	1.49
4	n	101	GLU	CD-OE2	6.32	1.32	1.25
3	A7	194	GLU	CD-OE2	6.30	1.32	1.25
4	b	178	ARG	NE-CZ	6.30	1.41	1.33
4	v	109	GLU	CD-OE2	-6.28	1.18	1.25
2	A8	155	GLU	CD-OE2	6.27	1.32	1.25
2	A8	424	ASP	CG-OD1	6.27	1.39	1.25
3	D5	230	SER	CB-OG	6.23	1.50	1.42
3	D1	157	GLU	CD-OE1	6.18	1.32	1.25
2	D0	221	ARG	CZ-NH1	6.11	1.41	1.33
2	D4	123	ARG	NE-CZ	6.10	1.41	1.33
2	B4	220	GLU	CD-OE2	6.07	1.32	1.25
2	D4	123	ARG	CD-NE	6.05	1.56	1.46
3	D9	22	GLU	CD-OE1	6.04	1.32	1.25
2	A4	2	ARG	NE-CZ	6.02	1.40	1.33
4	b	178	ARG	CD-NE	6.00	1.56	1.46
3	B3	53	GLU	CD-OE1	5.97	1.32	1.25
3	D1	397	TRP	CD2-CE3	5.97	1.49	1.40
4	a	164	ARG	NE-CZ	5.88	1.40	1.33
4	a	146	ARG	NE-CZ	5.88	1.40	1.33
2	A8	254	GLU	CD-OE2	5.88	1.32	1.25
5	k	80	GLU	CD-OE2	5.87	1.32	1.25
2	B4	220	GLU	CD-OE1	5.87	1.32	1.25
2	A8	264	ARG	NE-CZ	5.86	1.40	1.33
2	F0	280	LYS	CG-CD	5.81	1.72	1.52
1	19	248	ARG	NE-CZ	5.78	1.40	1.33
3	C9	276	ARG	NE-CZ	5.68	1.40	1.33
3	B3	158	GLU	CD-OE2	5.65	1.31	1.25
3	C9	53	GLU	CD-OE1	-5.64	1.19	1.25
3	E5	376	GLU	CD-OE2	5.59	1.31	1.25
4	v	202	ARG	NE-CZ	5.56	1.40	1.33
3	D7	122	LYS	CG-CD	5.55	1.71	1.52
3	D1	343	GLU	CD-OE2	5.54	1.31	1.25
3	C3	376	GLU	CD-OE1	5.53	1.31	1.25
5	l	78	LYS	CD-CE	5.53	1.65	1.51
4	a	164	ARG	CD-NE	5.52	1.55	1.46
3	D7	22	GLU	CD-OE1	5.52	1.31	1.25
4	b	178	ARG	CG-CD	5.51	1.65	1.51
3	D1	194	GLU	CD-OE1	-5.49	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E9	410	GLU	CD-OE1	5.49	1.31	1.25
3	C7	22	GLU	CD-OE1	-5.44	1.19	1.25
3	A5	379	LYS	CG-CD	5.44	1.71	1.52
2	D4	183	GLU	CD-OE2	5.43	1.31	1.25
3	C1	27	GLU	CD-OE2	5.41	1.31	1.25
4	i	97	ARG	NE-CZ	5.40	1.40	1.33
2	B6	285	GLN	CD-OE1	5.31	1.35	1.24
3	D1	158	GLU	CD-OE1	5.31	1.31	1.25
3	A9	222	TYR	CG-CD2	5.31	1.46	1.39
4	h	202	ARG	NE-CZ	5.31	1.40	1.33
4	j	97	ARG	CD-NE	5.30	1.55	1.46
3	C3	198	GLU	CD-OE1	5.25	1.31	1.25
3	B3	336	LYS	CE-NZ	5.24	1.62	1.49
2	D0	284	GLU	CD-OE2	-5.24	1.19	1.25
2	B2	386	GLU	CD-OE1	-5.22	1.20	1.25
3	E7	3	GLU	CD-OE2	-5.21	1.20	1.25
3	C9	276	ARG	CD-NE	5.20	1.55	1.46
2	C4	96	LYS	CE-NZ	5.19	1.62	1.49
2	E2	221	ARG	NE-CZ	5.12	1.39	1.33
2	C0	326	LYS	CE-NZ	5.11	1.61	1.49
4	d	202	ARG	CD-NE	5.10	1.55	1.46
2	A6	90	GLU	CD-OE2	-5.09	1.20	1.25
2	C0	430	LYS	CE-NZ	5.07	1.61	1.49
3	B7	343	GLU	CD-OE2	-5.07	1.20	1.25
2	B2	429	GLU	CD-OE2	-5.05	1.20	1.25
5	l	78	LYS	CG-CD	5.02	1.69	1.52
2	C6	207	GLU	CD-OE1	5.01	1.31	1.25

All (777) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	c	178	ARG	NE-CZ-NH1	43.97	142.28	120.30
4	c	178	ARG	NE-CZ-NH2	-27.43	106.59	120.30
2	C4	2	ARG	CG-CD-NE	18.40	150.43	111.80
4	t	97	ARG	NE-CZ-NH1	17.48	129.04	120.30
3	D1	213	ARG	CG-CD-NE	-15.65	78.93	111.80
3	E7	77	ARG	NE-CZ-NH1	-15.64	112.48	120.30
4	t	97	ARG	CD-NE-CZ	15.44	145.22	123.60
3	D1	77	ARG	NE-CZ-NH1	14.65	127.62	120.30
4	c	178	ARG	CD-NE-CZ	14.64	144.10	123.60
4	n	202	ARG	NE-CZ-NH2	14.62	127.61	120.30
2	D4	123	ARG	NE-CZ-NH1	14.57	127.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D5	121	ARG	NE-CZ-NH1	-14.51	113.04	120.30
4	v	202	ARG	NE-CZ-NH1	-14.50	113.05	120.30
4	h	202	ARG	NE-CZ-NH2	14.32	127.46	120.30
3	D5	121	ARG	NE-CZ-NH2	14.05	127.33	120.30
2	D4	123	ARG	CD-NE-CZ	13.42	142.39	123.60
4	v	202	ARG	CG-CD-NE	13.20	139.51	111.80
3	D1	213	ARG	NE-CZ-NH2	12.68	126.64	120.30
2	D8	123	ARG	NE-CZ-NH1	12.64	126.62	120.30
4	o	202	ARG	CB-CG-CD	12.49	144.08	111.60
4	h	198	ARG	CG-CD-NE	12.45	137.95	111.80
3	D1	121	ARG	CG-CD-NE	12.25	137.53	111.80
2	A0	262	TYR	CB-CG-CD2	-11.54	114.08	121.00
2	D4	79	ARG	NE-CZ-NH2	-11.45	114.57	120.30
2	A4	214	ARG	NE-CZ-NH1	-11.26	114.67	120.30
2	D8	214	ARG	NE-CZ-NH1	11.12	125.86	120.30
3	D5	343	GLU	N-CA-CB	11.10	130.58	110.60
2	D0	156	ARG	NE-CZ-NH2	10.80	125.70	120.30
2	D8	123	ARG	NE-CZ-NH2	-10.67	114.97	120.30
4	g	15	ARG	NE-CZ-NH2	10.58	125.59	120.30
3	D5	391	ARG	CB-CG-CD	10.58	139.10	111.60
2	B0	401	LYS	N-CA-CB	10.57	129.63	110.60
3	D5	309	ARG	NE-CZ-NH1	-10.55	115.03	120.30
4	f	16	ARG	NE-CZ-NH2	-10.50	115.05	120.30
4	n	202	ARG	NE-CZ-NH1	-10.48	115.06	120.30
2	A8	64	ARG	NE-CZ-NH1	-10.42	115.09	120.30
3	D7	121	ARG	CG-CD-NE	10.39	133.61	111.80
2	D4	161	TYR	CB-CG-CD2	-10.33	114.80	121.00
2	A2	214	ARG	NE-CZ-NH1	-10.32	115.14	120.30
3	A3	391	ARG	CB-CG-CD	10.30	138.39	111.60
3	D3	213	ARG	NE-CZ-NH1	10.27	125.44	120.30
2	E2	156	ARG	CB-CG-CD	10.23	138.21	111.60
2	A0	264	ARG	NE-CZ-NH1	10.20	125.40	120.30
3	C1	174	LYS	CB-CG-CD	10.18	138.07	111.60
2	A0	224	TYR	CB-CG-CD1	10.12	127.07	121.00
2	A6	214	ARG	CG-CD-NE	9.97	132.73	111.80
3	D9	394	PHE	CG-CD1-CE1	9.94	131.74	120.80
3	A5	380	ARG	NE-CZ-NH2	-9.90	115.35	120.30
4	n	119	ARG	NE-CZ-NH1	-9.82	115.39	120.30
3	C9	291	GLN	CB-CG-CD	9.79	137.06	111.60
4	p	95	TYR	CB-CG-CD2	-9.72	115.17	121.00
2	A4	64	ARG	NE-CZ-NH2	9.71	125.16	120.30
3	D9	394	PHE	CB-CG-CD2	9.68	127.58	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E2	123	ARG	NE-CZ-NH1	-9.68	115.46	120.30
3	D7	391	ARG	CB-CG-CD	9.67	136.75	111.60
4	p	97	ARG	NE-CZ-NH1	-9.61	115.49	120.30
4	t	146	ARG	NE-CZ-NH1	9.59	125.10	120.30
4	g	15	ARG	NE-CZ-NH1	-9.58	115.51	120.30
2	A6	214	ARG	NE-CZ-NH1	-9.57	115.52	120.30
4	i	202	ARG	CG-CD-NE	9.56	131.87	111.80
4	j	97	ARG	NE-CZ-NH1	9.55	125.07	120.30
2	C6	432	TYR	CB-CG-CD2	-9.52	115.29	121.00
2	D8	79	ARG	NE-CZ-NH1	9.48	125.04	120.30
2	D0	221	ARG	NE-CZ-NH1	-9.47	115.56	120.30
3	B9	380	ARG	NE-CZ-NH2	9.44	125.02	120.30
3	D5	340	TYR	CB-CG-CD2	-9.43	115.34	121.00
4	p	97	ARG	NE-CZ-NH2	9.37	124.98	120.30
3	E3	77	ARG	NE-CZ-NH1	-9.30	115.65	120.30
3	A5	251	ARG	NE-CZ-NH1	9.29	124.94	120.30
3	B3	391	ARG	CG-CD-NE	-9.26	92.35	111.80
4	a	164	ARG	NE-CZ-NH2	9.25	124.92	120.30
3	C9	213	ARG	NE-CZ-NH1	9.24	124.92	120.30
3	B3	213	ARG	NE-CZ-NH1	9.23	124.91	120.30
3	B3	213	ARG	CG-CD-NE	9.18	131.09	111.80
4	p	126	ARG	NE-CZ-NH1	-9.18	115.71	120.30
1	15	248	ARG	CG-CD-NE	9.16	131.04	111.80
3	C9	276	ARG	NE-CZ-NH2	9.15	124.87	120.30
3	D3	424	GLN	CB-CG-CD	9.14	135.36	111.60
3	E3	391	ARG	CG-CD-NE	9.13	130.98	111.80
3	C9	390	ARG	CG-CD-NE	9.13	130.98	111.80
4	n	202	ARG	CB-CG-CD	9.10	135.27	111.60
2	C2	2	ARG	NE-CZ-NH1	9.07	124.83	120.30
2	A0	264	ARG	NE-CZ-NH2	-9.06	115.77	120.30
2	A8	79	ARG	NE-CZ-NH2	-9.05	115.77	120.30
3	D1	213	ARG	NE-CZ-NH1	-8.94	115.83	120.30
2	A0	2	ARG	CG-CD-NE	8.91	130.51	111.80
2	A6	229	ARG	NE-CZ-NH1	8.91	124.75	120.30
3	E5	320	ARG	NE-CZ-NH1	8.86	124.73	120.30
2	D4	123	ARG	CG-CD-NE	-8.85	93.21	111.80
2	A4	121	ARG	NE-CZ-NH2	-8.81	115.90	120.30
5	x	54	ARG	CG-CD-NE	8.80	130.27	111.80
3	D1	77	ARG	NE-CZ-NH2	-8.79	115.90	120.30
3	F1	391	ARG	NE-CZ-NH1	8.78	124.69	120.30
4	d	117	ARG	CB-CG-CD	8.76	134.39	111.60
3	A1	122	LYS	CB-CG-CD	8.74	134.34	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C9	320	ARG	NE-CZ-NH1	8.73	124.67	120.30
2	A6	229	ARG	NE-CZ-NH2	-8.73	115.94	120.30
2	D6	123	ARG	NE-CZ-NH2	-8.72	115.94	120.30
4	t	178	ARG	CG-CD-NE	8.69	130.05	111.80
3	D5	46	ARG	CG-CD-NE	8.69	130.04	111.80
3	D5	162	ARG	NE-CZ-NH2	-8.69	115.96	120.30
2	A4	339	ARG	NE-CZ-NH1	8.68	124.64	120.30
3	C9	391	ARG	CG-CD-NE	-8.68	93.57	111.80
2	B6	339	ARG	CG-CD-NE	8.66	129.98	111.80
2	F0	215	ARG	CG-CD-NE	8.65	129.96	111.80
2	D6	221	ARG	NE-CZ-NH2	8.64	124.62	120.30
2	A2	221	ARG	CG-CD-NE	8.64	129.94	111.80
2	C4	401	LYS	CB-CA-C	8.64	127.67	110.40
5	x	102	ARG	NE-CZ-NH2	-8.62	115.99	120.30
2	C4	343	PHE	CB-CG-CD1	-8.61	114.78	120.80
2	B0	64	ARG	NE-CZ-NH1	-8.60	116.00	120.30
2	A6	214	ARG	CB-CG-CD	-8.59	89.27	111.60
4	b	146	ARG	CG-CD-NE	8.57	129.79	111.80
4	e	146	ARG	NE-CZ-NH1	8.53	124.57	120.30
2	A8	214	ARG	NE-CZ-NH2	-8.51	116.04	120.30
2	C8	215	ARG	NE-CZ-NH2	-8.49	116.05	120.30
3	E5	320	ARG	CB-CG-CD	8.49	133.69	111.60
3	D1	391	ARG	CG-CD-NE	-8.49	93.96	111.80
3	E3	276	ARG	NE-CZ-NH1	-8.49	116.05	120.30
4	d	194	ARG	CG-CD-NE	8.49	129.62	111.80
3	E7	391	ARG	CG-CD-NE	-8.48	93.98	111.80
3	E7	394	PHE	CB-CA-C	8.48	127.37	110.40
4	c	202	ARG	CG-CD-NE	8.46	129.56	111.80
2	A8	214	ARG	CG-CD-NE	8.46	129.56	111.80
2	D4	87	PHE	CB-CG-CD2	-8.43	114.90	120.80
3	D3	391	ARG	CB-CG-CD	8.41	133.47	111.60
4	b	194	ARG	CG-CD-NE	8.40	129.44	111.80
2	A0	123	ARG	NE-CZ-NH1	-8.37	116.11	120.30
3	C3	391	ARG	CB-CG-CD	-8.35	89.90	111.60
3	D5	390	ARG	NE-CZ-NH2	8.34	124.47	120.30
4	h	146	ARG	CG-CD-NE	8.34	129.31	111.80
4	d	202	ARG	CD-NE-CZ	8.33	135.26	123.60
2	B2	156	ARG	NE-CZ-NH1	-8.32	116.14	120.30
3	E5	320	ARG	CG-CD-NE	-8.31	94.35	111.80
4	b	149	ARG	NE-CZ-NH1	8.29	124.44	120.30
4	q	117	ARG	CG-CD-NE	8.29	129.21	111.80
2	F0	308	ARG	NE-CZ-NH2	-8.29	116.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B0	339	ARG	NE-CZ-NH2	8.27	124.44	120.30
3	F1	336	LYS	CA-CB-CG	8.27	131.59	113.40
2	F0	215	ARG	NE-CZ-NH2	-8.26	116.17	120.30
3	D9	2	ARG	NE-CZ-NH1	8.26	124.43	120.30
3	D7	121	ARG	NE-CZ-NH2	8.22	124.41	120.30
2	D8	214	ARG	CD-NE-CZ	8.21	135.10	123.60
2	B2	156	ARG	NE-CZ-NH2	8.21	124.41	120.30
4	p	97	ARG	CD-NE-CZ	8.21	135.09	123.60
1	12	248	ARG	CB-CA-C	-8.20	94.00	110.40
3	C7	276	ARG	NE-CZ-NH2	-8.16	116.22	120.30
2	F0	308	ARG	NE-CZ-NH1	8.12	124.36	120.30
2	C0	308	ARG	NE-CZ-NH1	-8.11	116.25	120.30
3	D5	262	ARG	NE-CZ-NH1	-8.10	116.25	120.30
2	A8	105	ARG	NE-CZ-NH2	-8.10	116.25	120.30
2	E0	156	ARG	CB-CG-CD	8.07	132.59	111.60
4	h	17	LEU	CB-CG-CD2	8.00	124.60	111.00
2	B8	156	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	11	246	CYS	CA-CB-SG	7.99	128.39	114.00
4	p	194	ARG	NE-CZ-NH1	7.97	124.29	120.30
3	D3	46	ARG	CG-CD-NE	-7.87	95.28	111.80
4	s	97	ARG	CG-CD-NE	-7.86	95.29	111.80
2	A2	214	ARG	CG-CD-NE	-7.84	95.33	111.80
2	A6	326	LYS	CG-CD-CE	7.83	135.39	111.90
2	A4	123	ARG	NE-CZ-NH1	-7.82	116.39	120.30
2	D2	339	ARG	N-CA-CB	7.81	124.66	110.60
3	E1	390	ARG	CB-CG-CD	7.80	131.87	111.60
3	D1	121	ARG	NE-CZ-NH1	7.77	124.18	120.30
2	D4	123	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	11	251	TYR	CG-CD2-CE2	7.74	127.49	121.30
4	j	15	ARG	NE-CZ-NH2	7.74	124.17	120.30
2	E2	156	ARG	CG-CD-NE	-7.73	95.57	111.80
3	B7	320	ARG	CG-CD-NE	-7.71	95.61	111.80
4	t	97	ARG	NH1-CZ-NH2	-7.69	110.94	119.40
1	16	248	ARG	CG-CD-NE	-7.67	95.70	111.80
2	A8	285	GLN	N-CA-CB	7.66	124.39	110.60
3	A5	320	ARG	NE-CZ-NH2	7.66	124.13	120.30
3	D5	212	PHE	CB-CG-CD2	-7.66	115.44	120.80
3	B9	11	GLN	CB-CG-CD	7.64	131.47	111.60
2	C4	84	ARG	NE-CZ-NH2	-7.62	116.49	120.30
2	A2	372	MET	CG-SD-CE	-7.60	88.05	100.20
3	D1	276	ARG	NE-CZ-NH2	7.59	124.10	120.30
3	D3	213	ARG	NE-CZ-NH2	-7.56	116.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C4	84	ARG	NE-CZ-NH1	7.56	124.08	120.30
2	E4	79	ARG	NE-CZ-NH2	7.56	124.08	120.30
3	D3	46	ARG	CB-CG-CD	7.54	131.20	111.60
4	r	15	ARG	NE-CZ-NH2	7.53	124.07	120.30
4	c	178	ARG	NH1-CZ-NH2	-7.53	111.12	119.40
3	D3	320	ARG	NE-CZ-NH2	7.52	124.06	120.30
3	C1	262	ARG	NE-CZ-NH1	7.50	124.05	120.30
2	D8	79	ARG	NE-CZ-NH2	-7.48	116.56	120.30
4	j	97	ARG	CD-NE-CZ	7.47	134.06	123.60
2	D4	64	ARG	NE-CZ-NH1	-7.47	116.56	120.30
3	A7	380	ARG	NE-CZ-NH2	7.47	124.03	120.30
4	p	194	ARG	CD-NE-CZ	7.46	134.05	123.60
3	C1	320	ARG	CG-CD-NE	7.46	127.47	111.80
3	E5	262	ARG	NE-CZ-NH1	7.43	124.02	120.30
3	A1	379	LYS	CB-CG-CD	-7.41	92.33	111.60
3	B3	280	GLN	CB-CG-CD	7.41	130.87	111.60
2	A8	64	ARG	NE-CZ-NH2	7.41	124.00	120.30
2	D2	123	ARG	CB-CG-CD	-7.40	92.36	111.60
2	A0	262	TYR	CB-CG-CD1	7.37	125.42	121.00
2	B2	156	ARG	CB-CG-CD	7.36	130.74	111.60
2	A2	402	ARG	NE-CZ-NH2	7.36	123.98	120.30
2	D4	84	ARG	NE-CZ-NH1	7.36	123.98	120.30
3	D1	162	ARG	NE-CZ-NH1	-7.35	116.63	120.30
2	B4	221	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	17	248	ARG	CG-CD-NE	7.32	127.17	111.80
2	F0	336	LYS	CB-CG-CD	7.30	130.58	111.60
3	A5	125	GLU	CB-CG-CD	7.30	133.91	114.20
4	c	95	TYR	CB-CG-CD2	-7.29	116.63	121.00
4	c	15	ARG	NE-CZ-NH2	-7.28	116.66	120.30
4	r	117	ARG	CG-CD-NE	7.28	127.09	111.80
4	r	146	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	22	248	ARG	CB-CG-CD	7.25	130.44	111.60
3	C5	11	GLN	N-CA-CB	-7.23	97.58	110.60
2	C6	123	ARG	CG-CD-NE	-7.21	96.66	111.80
3	C3	46	ARG	CB-CG-CD	7.21	130.34	111.60
3	F1	121	ARG	NE-CZ-NH1	7.19	123.89	120.30
3	D7	162	ARG	CG-CD-NE	7.19	126.89	111.80
4	c	69	LYS	CG-CD-CE	7.18	133.45	111.90
3	B7	426	GLN	CB-CA-C	7.18	124.76	110.40
2	E4	79	ARG	NE-CZ-NH1	-7.18	116.71	120.30
2	D6	123	ARG	NE-CZ-NH1	7.17	123.88	120.30
4	h	155	GLU	CB-CG-CD	7.16	133.53	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B7	46	ARG	CG-CD-NE	7.16	126.83	111.80
2	D8	264	ARG	CB-CG-CD	7.15	130.19	111.60
3	C5	77	ARG	CG-CD-NE	7.14	126.80	111.80
4	h	178	ARG	CG-CD-NE	7.14	126.80	111.80
2	E2	221	ARG	CG-CD-NE	-7.14	96.81	111.80
4	e	15	ARG	NE-CZ-NH2	7.14	123.87	120.30
2	A8	79	ARG	NE-CZ-NH1	7.12	123.86	120.30
2	D2	123	ARG	CD-NE-CZ	7.12	133.57	123.60
3	B5	320	ARG	CG-CD-NE	7.12	126.75	111.80
2	D4	401	LYS	CB-CA-C	7.12	124.64	110.40
2	A2	79	ARG	NE-CZ-NH1	-7.10	116.75	120.30
3	B3	77	ARG	NE-CZ-NH1	7.10	123.85	120.30
4	g	16	ARG	NE-CZ-NH2	7.09	123.84	120.30
3	A5	262	ARG	NE-CZ-NH1	7.08	123.84	120.30
3	C9	213	ARG	CG-CD-NE	7.07	126.64	111.80
3	D3	121	ARG	NE-CZ-NH1	-7.06	116.77	120.30
4	j	117	ARG	CG-CD-NE	7.04	126.58	111.80
2	B0	156	ARG	CG-CD-NE	7.04	126.58	111.80
2	C4	2	ARG	CD-NE-CZ	7.00	133.40	123.60
4	c	126	ARG	NE-CZ-NH1	-7.00	116.80	120.30
3	E5	320	ARG	CD-NE-CZ	6.99	133.39	123.60
3	A5	320	ARG	CB-CG-CD	6.98	129.75	111.60
1	5	248	ARG	CG-CD-NE	6.97	126.43	111.80
4	v	202	ARG	CD-NE-CZ	6.96	133.34	123.60
3	D1	291	GLN	CB-CG-CD	6.94	129.64	111.60
3	C3	388	MET	CB-CG-SD	6.92	133.17	112.40
3	B5	162	ARG	NE-CZ-NH1	6.92	123.76	120.30
3	C5	174	LYS	CB-CG-CD	6.91	129.57	111.60
3	E9	406	MET	CG-SD-CE	6.91	111.26	100.20
4	f	15	ARG	NE-CZ-NH2	-6.91	116.84	120.30
3	D1	391	ARG	CB-CG-CD	6.91	129.55	111.60
3	E5	86	ARG	NE-CZ-NH1	-6.90	116.85	120.30
2	D0	156	ARG	NE-CZ-NH1	-6.90	116.85	120.30
4	i	202	ARG	CB-CG-CD	-6.90	93.67	111.60
2	C8	420	GLU	CB-CG-CD	6.89	132.80	114.20
2	D8	401	LYS	CG-CD-CE	6.89	132.57	111.90
4	d	15	ARG	NE-CZ-NH2	6.88	123.74	120.30
4	a	202	ARG	CG-CD-NE	6.88	126.24	111.80
2	A2	373	ARG	CG-CD-NE	6.88	126.24	111.80
3	D3	213	ARG	CD-NE-CZ	6.87	133.22	123.60
3	F1	403	MET	CG-SD-CE	6.87	111.20	100.20
3	D3	318	ARG	NE-CZ-NH1	6.87	123.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C5	320	ARG	CG-CD-NE	6.86	126.21	111.80
4	d	91	PHE	CB-CG-CD1	-6.86	116.00	120.80
3	D1	276	ARG	NE-CZ-NH1	-6.86	116.87	120.30
4	q	97	ARG	CD-NE-CZ	6.86	133.20	123.60
2	D8	214	ARG	CB-CG-CD	-6.85	93.80	111.60
4	b	178	ARG	CD-NE-CZ	6.84	133.18	123.60
2	E6	83	TYR	CB-CG-CD2	-6.83	116.90	121.00
3	D1	406	MET	CB-CG-SD	6.82	132.85	112.40
2	D6	264	ARG	NE-CZ-NH1	-6.82	116.89	120.30
3	E3	128	ASP	CB-CA-C	6.82	124.03	110.40
2	D8	229	ARG	NE-CZ-NH1	6.80	123.70	120.30
4	m	202	ARG	CG-CD-NE	6.78	126.04	111.80
2	D0	210	TYR	CB-CG-CD2	-6.76	116.94	121.00
3	B5	159	TYR	CB-CG-CD2	-6.76	116.94	121.00
2	D0	401	LYS	N-CA-CB	6.76	122.76	110.60
3	F1	164	MET	CG-SD-CE	6.75	111.00	100.20
3	D1	156	ARG	NE-CZ-NH2	-6.75	116.92	120.30
2	A6	326	LYS	CB-CA-C	6.73	123.86	110.40
3	B5	162	ARG	NE-CZ-NH2	-6.73	116.94	120.30
4	q	146	ARG	NE-CZ-NH1	-6.73	116.94	120.30
2	A0	326	LYS	CA-CB-CG	6.73	128.20	113.40
3	D3	425	TYR	CB-CG-CD2	-6.72	116.97	121.00
2	D2	123	ARG	CG-CD-NE	-6.70	97.72	111.80
4	v	117	ARG	NE-CZ-NH1	-6.70	116.95	120.30
4	e	117	ARG	NE-CZ-NH2	-6.70	116.95	120.30
4	d	146	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	21	237	PRO	N-CD-CG	6.68	113.22	103.20
3	B3	280	GLN	CB-CA-C	6.68	123.76	110.40
2	D4	2	ARG	NE-CZ-NH2	-6.68	116.96	120.30
3	E5	262	ARG	NE-CZ-NH2	-6.67	116.96	120.30
4	s	16	ARG	CB-CG-CD	6.67	128.95	111.60
3	D1	306	ARG	NE-CZ-NH1	-6.67	116.97	120.30
4	j	97	ARG	NH1-CZ-NH2	-6.67	112.07	119.40
2	A0	224	TYR	CG-CD2-CE2	6.66	126.63	121.30
3	E3	276	ARG	CB-CG-CD	6.66	128.92	111.60
3	A1	309	ARG	CG-CD-NE	-6.66	97.83	111.80
4	r	198	ARG	CG-CD-NE	6.65	125.76	111.80
2	C2	432	TYR	CB-CG-CD1	-6.64	117.01	121.00
3	D1	343	GLU	N-CA-CB	6.63	122.54	110.60
2	B8	113	GLU	CB-CG-CD	6.62	132.07	114.20
2	B6	121	ARG	NE-CZ-NH2	-6.61	116.99	120.30
2	A4	36	MET	CG-SD-CE	-6.59	89.66	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A0	64	ARG	NE-CZ-NH1	-6.58	117.01	120.30
2	D2	120	ASP	CB-CG-OD1	6.58	124.22	118.30
4	h	202	ARG	NH1-CZ-NH2	-6.57	112.17	119.40
3	E9	77	ARG	NE-CZ-NH1	6.57	123.58	120.30
4	d	117	ARG	CG-CD-NE	6.56	125.58	111.80
2	A6	279	GLU	CB-CG-CD	6.56	131.91	114.20
2	A0	121	ARG	NE-CZ-NH1	-6.56	117.02	120.30
2	D6	120	ASP	CB-CG-OD1	6.56	124.20	118.30
3	D3	425	TYR	CB-CG-CD1	6.55	124.93	121.00
3	B1	280	GLN	CB-CG-CD	6.54	128.59	111.60
4	f	126	ARG	NE-CZ-NH2	-6.53	117.04	120.30
2	B0	83	TYR	CB-CG-CD2	-6.53	117.08	121.00
2	B0	285	GLN	CB-CG-CD	6.52	128.56	111.60
4	p	16	ARG	CG-CD-NE	6.52	125.49	111.80
5	x	111	VAL	CG1-CB-CG2	-6.50	100.50	110.90
2	B6	247	ALA	N-CA-CB	6.49	119.19	110.10
2	A4	210	TYR	CB-CG-CD2	-6.49	117.11	121.00
2	D4	163	LYS	CB-CG-CD	6.49	128.46	111.60
2	C6	372	MET	CB-CG-SD	6.48	131.85	112.40
2	D6	79	ARG	NE-CZ-NH2	-6.48	117.06	120.30
4	m	202	ARG	NE-CZ-NH2	6.47	123.54	120.30
4	q	97	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	11	251	TYR	CB-CG-CD1	6.46	124.88	121.00
2	D0	210	TYR	CB-CG-CD1	6.45	124.87	121.00
2	A0	156	ARG	NE-CZ-NH2	-6.45	117.08	120.30
3	D3	213	ARG	CG-CD-NE	6.45	125.33	111.80
3	C9	159	TYR	CB-CG-CD1	6.44	124.86	121.00
2	A4	210	TYR	CB-CG-CD1	6.43	124.86	121.00
4	e	44	ASP	CB-CG-OD1	6.43	124.09	118.30
4	i	7	ALA	N-CA-CB	6.43	119.10	110.10
2	A2	214	ARG	NE-CZ-NH2	6.42	123.51	120.30
2	D0	390	ARG	NE-CZ-NH2	6.42	123.51	120.30
3	D1	392	LYS	CG-CD-CE	6.42	131.17	111.90
4	n	202	ARG	CD-NE-CZ	6.41	132.58	123.60
2	D4	64	ARG	NE-CZ-NH2	6.41	123.51	120.30
2	D4	163	LYS	CG-CD-CE	6.41	131.13	111.90
3	D9	320	ARG	CG-CD-NE	6.41	125.26	111.80
2	A6	84	ARG	NE-CZ-NH2	6.41	123.50	120.30
4	b	97	ARG	CG-CD-NE	6.41	125.25	111.80
2	A0	124	LYS	CB-CG-CD	6.40	128.24	111.60
2	B0	64	ARG	NE-CZ-NH2	6.40	123.50	120.30
4	d	178	ARG	NE-CZ-NH1	6.40	123.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B8	156	ARG	NE-CZ-NH1	6.39	123.50	120.30
4	e	15	ARG	NE-CZ-NH1	-6.39	117.11	120.30
2	A0	84	ARG	NE-CZ-NH2	-6.38	117.11	120.30
2	D8	373	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	1	248	ARG	CG-CD-NE	6.37	125.18	111.80
4	r	197	LEU	CB-CG-CD2	6.36	121.81	111.00
3	D1	251	ARG	NE-CZ-NH1	-6.36	117.12	120.30
2	F0	422	ARG	NE-CZ-NH1	-6.35	117.12	120.30
3	D1	340	TYR	CB-CG-CD2	-6.35	117.19	121.00
2	D2	215	ARG	NE-CZ-NH2	-6.35	117.12	120.30
2	A8	399	TYR	CB-CG-CD1	6.34	124.81	121.00
3	C9	276	ARG	CD-NE-CZ	6.34	132.47	123.60
4	j	198	ARG	CG-CD-NE	6.34	125.11	111.80
2	D2	221	ARG	CG-CD-NE	-6.34	98.50	111.80
3	B7	11	GLN	CB-CG-CD	6.33	128.06	111.60
2	D0	264	ARG	NE-CZ-NH1	6.33	123.46	120.30
3	E7	391	ARG	CD-NE-CZ	6.31	132.44	123.60
4	f	16	ARG	NE-CZ-NH1	6.31	123.46	120.30
3	D9	156	ARG	NE-CZ-NH1	-6.31	117.14	120.30
3	D1	121	ARG	NE-CZ-NH2	-6.30	117.15	120.30
4	v	21	ARG	NE-CZ-NH2	6.30	123.45	120.30
5	k	85	ARG	NE-CZ-NH1	6.29	123.45	120.30
2	E0	156	ARG	CG-CD-NE	-6.29	98.59	111.80
4	o	164	ARG	NE-CZ-NH2	-6.26	117.17	120.30
3	D5	340	TYR	CG-CD1-CE1	-6.25	116.30	121.30
2	D4	373	ARG	CG-CD-NE	6.24	124.90	111.80
4	u	202	ARG	CG-CD-NE	6.22	124.87	111.80
4	p	95	TYR	CB-CA-C	6.21	122.83	110.40
3	F1	46	ARG	NE-CZ-NH2	6.21	123.41	120.30
3	D1	363	MET	CG-SD-CE	6.21	110.14	100.20
3	D9	208	TYR	CB-CG-CD1	6.20	124.72	121.00
4	a	198	ARG	CB-CG-CD	6.19	127.70	111.60
3	D9	276	ARG	NE-CZ-NH1	6.19	123.39	120.30
4	m	198	ARG	NE-CZ-NH1	6.19	123.39	120.30
2	D0	123	ARG	CG-CD-NE	6.18	124.78	111.80
2	D8	264	ARG	CG-CD-NE	-6.17	98.83	111.80
4	g	16	ARG	CB-CG-CD	6.17	127.65	111.60
2	A8	264	ARG	CD-NE-CZ	6.17	132.24	123.60
2	A0	214	ARG	NE-CZ-NH2	6.16	123.38	120.30
3	C3	391	ARG	CG-CD-NE	6.16	124.73	111.80
2	D4	262	TYR	CB-CG-CD2	-6.16	117.31	121.00
4	i	15	ARG	NE-CZ-NH2	6.15	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D6	264	ARG	NE-CZ-NH2	6.15	123.38	120.30
5	k	25	ARG	CB-CG-CD	6.15	127.59	111.60
3	D5	368	VAL	CG1-CB-CG2	6.13	120.71	110.90
2	D2	64	ARG	NE-CZ-NH2	6.12	123.36	120.30
2	C2	262	TYR	CB-CG-CD1	-6.12	117.33	121.00
1	2	247	TYR	CB-CG-CD1	-6.11	117.33	121.00
2	A0	339	ARG	CG-CD-NE	6.11	124.63	111.80
3	D5	112	LEU	CB-CG-CD2	-6.10	100.64	111.00
4	o	194	ARG	CD-NE-CZ	6.10	132.14	123.60
3	C7	363	MET	CG-SD-CE	6.09	109.95	100.20
5	x	25	ARG	NE-CZ-NH2	6.09	123.35	120.30
2	A8	224	TYR	N-CA-CB	6.09	121.56	110.60
2	B0	214	ARG	NE-CZ-NH1	6.09	123.34	120.30
4	j	97	ARG	CG-CD-NE	6.09	124.59	111.80
4	a	164	ARG	CD-NE-CZ	6.09	132.12	123.60
4	n	91	PHE	CB-CG-CD2	-6.08	116.55	120.80
3	E5	309	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	A2	430	LYS	CB-CG-CD	6.06	127.36	111.60
2	C8	210	TYR	CB-CG-CD1	6.06	124.64	121.00
2	A8	224	TYR	CB-CA-C	-6.05	98.29	110.40
2	D8	229	ARG	NE-CZ-NH2	-6.04	117.28	120.30
3	E3	391	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	4	248	ARG	NE-CZ-NH1	6.02	123.31	120.30
3	B3	391	ARG	CB-CG-CD	6.01	127.22	111.60
3	C7	397	TRP	CD1-CG-CD2	-6.01	101.49	106.30
3	C9	291	GLN	CB-CA-C	6.01	122.42	110.40
3	A3	128	ASP	CB-CA-C	5.99	122.38	110.40
2	D4	203	MET	CB-CG-SD	-5.99	94.43	112.40
2	A8	402	ARG	NE-CZ-NH1	-5.99	117.31	120.30
4	g	198	ARG	NE-CZ-NH2	-5.99	117.31	120.30
2	C8	423	GLU	CB-CG-CD	-5.98	98.06	114.20
3	B3	262	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	D2	64	ARG	NE-CZ-NH1	-5.95	117.32	120.30
4	f	84	LYS	CB-CG-CD	5.95	127.07	111.60
3	A5	262	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	D4	214	ARG	NE-CZ-NH2	-5.94	117.33	120.30
3	A5	227	HIS	CA-CB-CG	5.93	123.67	113.60
3	C7	276	ARG	CB-CG-CD	5.93	127.01	111.60
2	E6	84	ARG	NE-CZ-NH1	-5.92	117.34	120.30
4	q	202	ARG	CB-CG-CD	5.92	127.00	111.60
4	d	117	ARG	NE-CZ-NH2	5.92	123.26	120.30
2	C4	84	ARG	CD-NE-CZ	5.91	131.88	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C9	159	TYR	CB-CG-CD2	-5.91	117.46	121.00
2	A6	214	ARG	CA-CB-CG	5.91	126.39	113.40
2	C6	320	ARG	NE-CZ-NH2	-5.91	117.35	120.30
2	C4	343	PHE	CB-CG-CD2	5.90	124.93	120.80
2	C4	336	LYS	CD-CE-NZ	5.90	125.27	111.70
2	A0	156	ARG	CG-CD-NE	-5.90	99.42	111.80
2	D2	339	ARG	NE-CZ-NH2	-5.90	117.35	120.30
4	p	198	ARG	CG-CD-NE	-5.89	99.44	111.80
3	A9	324	LYS	CD-CE-NZ	5.88	125.24	111.70
3	B3	121	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	A2	402	ARG	NE-CZ-NH1	-5.87	117.36	120.30
3	C7	367	PHE	CB-CG-CD1	-5.87	116.69	120.80
4	r	146	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	B2	84	ARG	NE-CZ-NH1	5.86	123.23	120.30
3	A9	222	TYR	CB-CG-CD2	5.86	124.52	121.00
3	E3	407	GLU	CB-CA-C	-5.86	98.69	110.40
2	C6	156	ARG	CG-CD-NE	-5.85	99.52	111.80
3	D7	162	ARG	NE-CZ-NH1	5.84	123.22	120.30
4	t	149	ARG	NE-CZ-NH1	-5.84	117.38	120.30
3	D1	92	PHE	CB-CG-CD1	5.82	124.88	120.80
3	C7	81	PHE	CB-CG-CD1	5.82	124.87	120.80
2	B8	64	ARG	NE-CZ-NH1	-5.82	117.39	120.30
3	C9	276	ARG	CG-CD-NE	5.80	123.99	111.80
2	C4	326	LYS	CG-CD-CE	5.80	129.30	111.90
2	D4	418	PHE	CB-CG-CD2	-5.80	116.74	120.80
4	e	16	ARG	NE-CZ-NH2	-5.80	117.40	120.30
4	b	97	ARG	NE-CZ-NH1	5.79	123.19	120.30
3	A5	336	LYS	CD-CE-NZ	5.78	125.00	111.70
2	C8	84	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	12	247	TYR	CB-CA-C	5.76	121.92	110.40
2	A4	123	ARG	CG-CD-NE	-5.75	99.72	111.80
2	F0	227	LEU	CB-CG-CD1	5.75	120.78	111.00
3	A1	281	TYR	CB-CG-CD1	5.75	124.45	121.00
3	A5	391	ARG	NE-CZ-NH1	5.75	123.17	120.30
4	q	15	ARG	NE-CZ-NH2	5.75	123.17	120.30
3	E3	320	ARG	CB-CA-C	5.75	121.89	110.40
2	C8	161	TYR	CB-CG-CD2	-5.75	117.55	121.00
2	A2	221	ARG	CD-NE-CZ	5.74	131.63	123.60
2	A2	357	TYR	N-CA-CB	5.73	120.91	110.60
2	B8	221	ARG	NE-CZ-NH1	5.73	123.16	120.30
4	p	140	LEU	CB-CG-CD1	5.73	120.73	111.00
3	D5	164	MET	CB-CG-SD	-5.72	95.22	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B1	129	CYS	CB-CA-C	5.72	121.84	110.40
2	D6	221	ARG	NE-CZ-NH1	-5.71	117.44	120.30
3	D5	128	ASP	O-C-N	5.71	131.84	122.70
3	A7	282	ARG	CD-NE-CZ	5.71	131.59	123.60
5	x	85	ARG	CB-CG-CD	5.71	126.44	111.60
3	A5	380	ARG	NE-CZ-NH1	5.70	123.15	120.30
4	m	183	LEU	CB-CG-CD1	5.70	120.69	111.00
3	C5	159	TYR	CB-CG-CD1	-5.70	117.58	121.00
2	A6	60	LYS	CG-CD-CE	5.70	129.00	111.90
3	D9	276	ARG	CD-NE-CZ	5.70	131.58	123.60
2	C8	2	ARG	NE-CZ-NH1	5.70	123.15	120.30
2	D6	297	GLU	CB-CG-CD	5.70	129.58	114.20
4	p	95	TYR	N-CA-CB	-5.70	100.35	110.60
3	A9	213	ARG	NE-CZ-NH1	-5.69	117.45	120.30
4	h	95	TYR	CB-CG-CD1	-5.69	117.59	121.00
4	m	27	GLN	CB-CG-CD	5.69	126.39	111.60
3	B3	318	ARG	NE-CZ-NH2	5.68	123.14	120.30
2	E2	116	ASP	CB-CG-OD1	-5.68	113.19	118.30
2	A6	156	ARG	CB-CG-CD	5.67	126.35	111.60
4	t	126	ARG	NE-CZ-NH1	-5.67	117.47	120.30
4	f	95	TYR	CB-CG-CD1	-5.66	117.61	121.00
2	D0	161	TYR	CB-CG-CD2	-5.66	117.61	121.00
2	E0	221	ARG	CG-CD-NE	-5.65	99.93	111.80
3	C5	251	ARG	CG-CD-NE	5.65	123.66	111.80
2	D0	279	GLU	CB-CG-CD	-5.65	98.95	114.20
2	A4	64	ARG	NE-CZ-NH1	-5.64	117.48	120.30
3	A5	114	ASP	CB-CA-C	5.64	121.68	110.40
3	D3	48	ASN	CB-CA-C	-5.64	99.12	110.40
3	B7	372	THR	CA-CB-CG2	5.63	120.29	112.40
2	D0	264	ARG	NE-CZ-NH2	-5.63	117.48	120.30
2	E4	221	ARG	CG-CD-NE	5.63	123.63	111.80
4	d	117	ARG	CD-NE-CZ	5.62	131.47	123.60
4	e	44	ASP	CB-CG-OD2	-5.62	113.24	118.30
3	F1	362	LYS	N-CA-CB	5.62	120.72	110.60
3	D9	262	ARG	NE-CZ-NH1	5.62	123.11	120.30
3	A1	159	TYR	CB-CG-CD2	-5.62	117.63	121.00
4	m	194	ARG	NE-CZ-NH1	5.62	123.11	120.30
4	p	151	MET	CG-SD-CE	5.62	109.19	100.20
2	A2	214	ARG	CD-NE-CZ	-5.61	115.74	123.60
2	A4	182	VAL	CG1-CB-CG2	5.61	119.88	110.90
4	n	91	PHE	CB-CA-C	-5.61	99.19	110.40
2	B2	408	TYR	CB-CG-CD2	5.58	124.35	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	e	107	LYS	CD-CE-NZ	-5.58	98.87	111.70
3	C9	343	GLU	N-CA-CB	5.58	120.64	110.60
2	E0	206	ASN	CB-CA-C	5.58	121.55	110.40
4	r	117	ARG	CD-NE-CZ	5.58	131.41	123.60
2	A4	2	ARG	NE-CZ-NH2	5.57	123.09	120.30
3	A9	252	LYS	CG-CD-CE	5.57	128.62	111.90
5	l	58	LYS	CB-CG-CD	5.57	126.09	111.60
3	D5	251	ARG	CG-CD-NE	5.57	123.50	111.80
1	8	248	ARG	CB-CA-C	-5.57	99.26	110.40
1	19	248	ARG	CD-NE-CZ	5.57	131.39	123.60
3	C3	251	ARG	CG-CD-NE	-5.56	100.12	111.80
2	D2	123	ARG	NE-CZ-NH2	-5.56	117.52	120.30
3	D9	394	PHE	CZ-CE2-CD2	5.56	126.78	120.10
2	C8	214	ARG	CG-CD-NE	5.55	123.46	111.80
4	p	178	ARG	NE-CZ-NH1	5.55	123.08	120.30
3	A5	90	PHE	CB-CG-CD1	5.55	124.69	120.80
1	6	237	PRO	N-CD-CG	5.54	111.51	103.20
4	o	91	PHE	CB-CG-CD1	-5.54	116.92	120.80
3	B7	422	TYR	CB-CG-CD1	5.54	124.33	121.00
3	E7	77	ARG	CB-CG-CD	5.54	126.01	111.60
3	A7	282	ARG	NE-CZ-NH2	5.54	123.07	120.30
3	C9	213	ARG	NH1-CZ-NH2	-5.54	113.31	119.40
3	C7	143	THR	OG1-CB-CG2	-5.54	97.26	110.00
4	t	56	LYS	CB-CG-CD	5.53	125.97	111.60
2	A8	85	HIS	CA-CB-CG	5.53	122.99	113.60
2	D0	339	ARG	CB-CA-C	-5.53	99.35	110.40
3	A7	391	ARG	CD-NE-CZ	5.52	131.33	123.60
2	E2	308	ARG	NE-CZ-NH1	5.52	123.06	120.30
4	d	151	MET	CG-SD-CE	5.52	109.03	100.20
3	E7	262	ARG	CG-CD-NE	5.51	123.37	111.80
2	E6	36	MET	CG-SD-CE	5.51	109.01	100.20
2	C8	373	ARG	NE-CZ-NH1	-5.50	117.55	120.30
3	E5	11	GLN	CA-CB-CG	5.50	125.50	113.40
2	E6	280	LYS	CB-CG-CD	5.50	125.91	111.60
2	B0	83	TYR	CB-CG-CD1	5.49	124.30	121.00
4	b	97	ARG	CB-CG-CD	5.49	125.88	111.60
4	i	21	ARG	CG-CD-NE	5.49	123.33	111.80
4	j	16	ARG	NE-CZ-NH1	-5.49	117.55	120.30
2	C0	161	TYR	CB-CG-CD2	-5.49	117.71	121.00
5	x	159	TYR	CB-CG-CD1	-5.49	117.71	121.00
3	C9	86	ARG	CG-CD-NE	-5.48	100.28	111.80
3	E7	320	ARG	CB-CG-CD	5.48	125.84	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A0	401	LYS	CB-CA-C	5.48	121.35	110.40
3	C7	213	ARG	CG-CD-NE	-5.47	100.31	111.80
4	c	194	ARG	NE-CZ-NH1	5.47	123.03	120.30
4	i	97	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	E2	221	ARG	NE-CZ-NH1	5.46	123.03	120.30
3	B7	309	ARG	CG-CD-NE	5.45	123.25	111.80
3	D9	127	CYS	CA-CB-SG	5.44	123.80	114.00
4	j	15	ARG	NE-CZ-NH1	-5.44	117.58	120.30
2	C6	221	ARG	NE-CZ-NH2	5.43	123.02	120.30
2	D8	224	TYR	CB-CG-CD2	-5.43	117.74	121.00
3	B1	318	ARG	NE-CZ-NH1	5.43	123.02	120.30
3	A5	212	PHE	CB-CG-CD2	-5.43	117.00	120.80
3	D1	77	ARG	CD-NE-CZ	5.43	131.20	123.60
4	b	97	ARG	CD-NE-CZ	5.43	131.20	123.60
2	B2	408	TYR	CB-CG-CD1	-5.42	117.75	121.00
2	B6	221	ARG	NE-CZ-NH1	5.42	123.01	120.30
3	D1	291	GLN	CB-CA-C	5.42	121.25	110.40
2	D6	79	ARG	CB-CG-CD	-5.42	97.50	111.60
4	c	150	VAL	CA-CB-CG1	5.42	119.03	110.90
2	D0	402	ARG	NE-CZ-NH1	-5.42	117.59	120.30
3	D5	340	TYR	CB-CG-CD1	5.42	124.25	121.00
2	C2	2	ARG	NE-CZ-NH2	-5.41	117.59	120.30
2	A4	262	TYR	CB-CG-CD2	-5.41	117.75	121.00
2	B0	336	LYS	CB-CG-CD	5.41	125.67	111.60
3	F1	177	ASP	CA-CB-CG	5.41	125.30	113.40
2	C2	96	LYS	CD-CE-NZ	5.41	124.14	111.70
4	u	126	ARG	NE-CZ-NH1	5.41	123.00	120.30
4	h	198	ARG	CD-NE-CZ	5.40	131.16	123.60
3	C1	88	ASP	CB-CA-C	-5.40	99.60	110.40
2	D0	116	ASP	CB-CA-C	5.39	121.18	110.40
4	o	202	ARG	CA-CB-CG	5.39	125.26	113.40
3	A1	390	ARG	CG-CD-NE	5.39	123.12	111.80
3	D9	405	GLU	CB-CG-CD	5.39	128.75	114.20
2	B8	64	ARG	NE-CZ-NH2	5.39	122.99	120.30
3	D7	122	LYS	CG-CD-CE	5.38	128.05	111.90
2	A0	254	GLU	CB-CG-CD	5.38	128.73	114.20
3	D3	114	ASP	CB-CG-OD1	5.38	123.14	118.30
3	A5	122	LYS	CG-CD-CE	5.38	128.03	111.90
2	B0	163	LYS	CB-CA-C	5.37	121.14	110.40
2	C4	404	PHE	CB-CG-CD1	-5.37	117.04	120.80
3	D9	92	PHE	CB-CG-CD1	5.37	124.56	120.80
3	C5	122	LYS	CB-CG-CD	5.36	125.54	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A1	2	ARG	NE-CZ-NH1	5.35	122.98	120.30
3	D5	48	ASN	CB-CA-C	-5.35	99.70	110.40
4	n	91	PHE	CB-CG-CD1	-5.35	117.06	120.80
3	D5	343	GLU	CB-CA-C	-5.34	99.71	110.40
2	A6	264	ARG	CG-CD-NE	5.34	123.02	111.80
3	B9	86	ARG	CG-CD-NE	5.34	123.01	111.80
3	E9	380	ARG	NE-CZ-NH2	5.34	122.97	120.30
2	F0	208	ALA	CB-CA-C	5.34	118.11	110.10
4	r	161	TYR	CB-CG-CD1	-5.33	117.80	121.00
3	E1	391	ARG	CG-CD-NE	5.33	122.99	111.80
4	o	164	ARG	NE-CZ-NH1	5.33	122.97	120.30
4	r	119	ARG	CG-CD-NE	5.33	122.99	111.80
3	A9	391	ARG	CB-CA-C	5.33	121.05	110.40
3	C1	281	TYR	CB-CG-CD1	5.33	124.19	121.00
3	C7	296	ALA	CB-CA-C	5.32	118.09	110.10
4	d	202	ARG	NE-CZ-NH1	-5.32	117.64	120.30
3	B9	291	GLN	CB-CA-C	-5.32	99.76	110.40
4	r	59	ASN	N-CA-CB	5.32	120.17	110.60
3	F1	282	ARG	NE-CZ-NH1	-5.32	117.64	120.30
5	l	108	ARG	CG-CD-NE	5.32	122.97	111.80
3	A9	252	LYS	CB-CG-CD	5.31	125.42	111.60
2	D4	156	ARG	NE-CZ-NH2	-5.31	117.64	120.30
4	v	155	GLU	CG-CD-OE1	5.31	128.92	118.30
3	E7	394	PHE	CB-CG-CD1	5.30	124.51	120.80
2	D4	423	GLU	CB-CG-CD	-5.30	99.89	114.20
2	E4	221	ARG	CB-CG-CD	-5.30	97.82	111.60
3	D3	366	THR	CA-CB-CG2	5.30	119.82	112.40
3	A1	77	ARG	NE-CZ-NH1	5.29	122.95	120.30
5	k	85	ARG	NE-CZ-NH2	-5.29	117.65	120.30
2	A8	402	ARG	NE-CZ-NH2	5.29	122.94	120.30
3	D7	174	LYS	CB-CG-CD	5.29	125.36	111.60
3	E9	410	GLU	CB-CA-C	-5.29	99.82	110.40
3	A1	46	ARG	CG-CD-NE	5.29	122.91	111.80
4	o	194	ARG	NE-CZ-NH1	5.29	122.94	120.30
4	e	106	GLN	N-CA-CB	5.29	120.11	110.60
3	A5	11	GLN	CA-CB-CG	5.28	125.01	113.40
3	B9	380	ARG	CB-CG-CD	5.28	125.32	111.60
3	C5	320	ARG	NE-CZ-NH2	5.27	122.94	120.30
2	C4	339	ARG	CB-CG-CD	5.27	125.30	111.60
4	b	149	ARG	NE-CZ-NH2	-5.27	117.67	120.30
2	D4	224	TYR	CB-CG-CD2	-5.27	117.84	121.00
5	k	58	LYS	CB-CG-CD	5.27	125.29	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B6	422	ARG	NE-CZ-NH2	-5.26	117.67	120.30
3	A9	391	ARG	NE-CZ-NH1	5.26	122.93	120.30
3	C7	216	LYS	CG-CD-CE	5.26	127.68	111.90
3	C5	306	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	C0	84	ARG	CB-CA-C	-5.26	99.89	110.40
2	E0	229	ARG	NE-CZ-NH1	5.26	122.93	120.30
3	D3	222	TYR	CB-CG-CD2	5.25	124.15	121.00
4	v	202	ARG	NE-CZ-NH2	5.25	122.93	120.30
3	C9	306	ARG	NE-CZ-NH1	5.25	122.92	120.30
4	q	97	ARG	CG-CD-NE	5.25	122.81	111.80
4	g	198	ARG	NE-CZ-NH1	5.24	122.92	120.30
4	n	24	MET	CB-CG-SD	5.24	128.13	112.40
3	D5	367	PHE	CB-CG-CD2	5.24	124.47	120.80
2	C2	407	TRP	CB-CG-CD1	-5.24	120.19	127.00
3	F1	209	ASP	CB-CG-OD2	5.23	123.01	118.30
4	d	91	PHE	CB-CG-CD2	5.23	124.46	120.80
2	A8	264	ARG	CB-CA-C	5.23	120.86	110.40
4	q	194	ARG	CG-CD-NE	-5.23	100.81	111.80
4	v	117	ARG	NE-CZ-NH2	5.23	122.91	120.30
3	A1	391	ARG	CG-CD-NE	-5.23	100.82	111.80
2	F0	284	GLU	OE1-CD-OE2	5.23	129.57	123.30
3	F1	391	ARG	NE-CZ-NH2	-5.23	117.69	120.30
2	D0	390	ARG	CG-CD-NE	5.22	122.77	111.80
2	C6	36	MET	CB-CG-SD	5.22	128.06	112.40
2	B4	79	ARG	NE-CZ-NH2	5.22	122.91	120.30
5	w	25	ARG	CG-CD-NE	5.22	122.76	111.80
2	D4	285	GLN	N-CA-CB	5.21	119.97	110.60
4	u	65	GLN	CB-CG-CD	5.21	125.14	111.60
2	A8	402	ARG	CD-NE-CZ	5.21	130.89	123.60
2	F0	373	ARG	NE-CZ-NH1	-5.21	117.70	120.30
2	F0	370	LYS	CB-CG-CD	5.20	125.12	111.60
3	C1	252	LYS	CB-CG-CD	5.20	125.11	111.60
3	D5	367	PHE	CB-CG-CD1	-5.20	117.16	120.80
2	C2	123	ARG	CG-CD-NE	5.19	122.71	111.80
2	E2	121	ARG	NE-CZ-NH2	-5.19	117.70	120.30
3	D1	391	ARG	NE-CZ-NH2	5.19	122.90	120.30
4	e	95	TYR	CB-CA-C	5.19	120.78	110.40
2	E2	372	MET	CB-CG-SD	5.19	127.96	112.40
4	p	91	PHE	CB-CG-CD2	-5.18	117.17	120.80
4	p	117	ARG	NE-CZ-NH1	-5.18	117.71	120.30
2	B4	221	ARG	NE-CZ-NH2	-5.17	117.71	120.30
4	d	21	ARG	NE-CZ-NH2	5.17	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B8	391	MET	CB-CG-SD	-5.17	96.91	112.40
3	A5	125	GLU	CB-CA-C	5.16	120.73	110.40
3	E7	394	PHE	CD1-CG-CD2	-5.16	111.59	118.30
4	f	202	ARG	NE-CZ-NH2	5.16	122.88	120.30
2	D2	373	ARG	NE-CZ-NH2	-5.15	117.72	120.30
4	i	21	ARG	NE-CZ-NH2	5.15	122.88	120.30
3	B5	162	ARG	CD-NE-CZ	5.15	130.81	123.60
2	B8	121	ARG	NE-CZ-NH1	5.15	122.87	120.30
3	C1	318	ARG	NE-CZ-NH1	5.15	122.87	120.30
3	D5	2	ARG	NE-CZ-NH1	5.15	122.87	120.30
2	A0	96	LYS	CB-CG-CD	5.14	124.97	111.60
2	D0	221	ARG	NH1-CZ-NH2	5.14	125.06	119.40
4	m	194	ARG	NE-CZ-NH2	-5.13	117.73	120.30
3	D5	92	PHE	CD1-CE1-CZ	-5.13	113.94	120.10
3	E5	355	ASP	CB-CG-OD1	5.13	122.92	118.30
5	k	108	ARG	CG-CD-NE	5.13	122.58	111.80
3	A9	213	ARG	NE-CZ-NH2	5.13	122.86	120.30
2	B4	156	ARG	NE-CZ-NH1	-5.12	117.74	120.30
2	C8	336	LYS	CD-CE-NZ	-5.12	99.91	111.70
3	E7	222	TYR	CB-CG-CD2	-5.12	117.93	121.00
3	A7	391	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	A8	214	ARG	CD-NE-CZ	5.12	130.76	123.60
4	j	146	ARG	CD-NE-CZ	5.12	130.76	123.60
4	e	99	MET	CB-CG-SD	-5.11	97.06	112.40
4	t	15	ARG	NE-CZ-NH2	5.11	122.86	120.30
2	D0	264	ARG	CG-CD-NE	5.11	122.53	111.80
2	A0	285	GLN	CB-CA-C	-5.11	100.19	110.40
4	f	2	SER	CB-CA-C	5.11	119.80	110.10
2	B8	121	ARG	NE-CZ-NH2	-5.10	117.75	120.30
4	e	202	ARG	NE-CZ-NH1	5.10	122.85	120.30
3	B9	15	GLN	CB-CG-CD	5.10	124.87	111.60
2	D2	409	VAL	CA-CB-CG2	5.10	118.55	110.90
3	D1	3	GLU	N-CA-CB	5.09	119.77	110.60
3	D5	224	ASP	CB-CG-OD2	-5.09	113.72	118.30
3	E1	390	ARG	CG-CD-NE	5.09	122.50	111.80
4	f	146	ARG	NE-CZ-NH1	5.09	122.84	120.30
2	C8	255	PHE	CB-CG-CD2	-5.09	117.24	120.80
4	f	198	ARG	NE-CZ-NH1	-5.09	117.76	120.30
5	x	160	ARG	CG-CD-NE	5.09	122.48	111.80
2	D8	282	TYR	N-CA-CB	5.08	119.75	110.60
3	E3	276	ARG	NE-CZ-NH2	5.08	122.84	120.30
4	m	202	ARG	CA-CB-CG	5.08	124.58	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C6	339	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	A8	214	ARG	CB-CG-CD	-5.08	98.40	111.60
2	F0	339	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	A4	116	ASP	CB-CA-C	5.07	120.55	110.40
3	E3	380	ARG	CB-CG-CD	5.07	124.79	111.60
3	D3	36	TYR	CB-CG-CD2	-5.07	117.96	121.00
2	A2	2	ARG	NE-CZ-NH1	5.06	122.83	120.30
3	A9	281	TYR	CB-CG-CD1	5.05	124.03	121.00
2	A0	238	LEU	CB-CG-CD1	-5.05	102.41	111.00
3	D9	394	PHE	CD1-CE1-CZ	-5.05	114.04	120.10
3	E7	174	LYS	CD-CE-NZ	-5.05	100.08	111.70
4	d	16	ARG	NE-CZ-NH1	-5.05	117.77	120.30
3	F1	86	ARG	CG-CD-NE	5.05	122.41	111.80
3	C5	15	GLN	CB-CG-CD	5.05	124.73	111.60
2	D6	163	LYS	CB-CG-CD	5.05	124.73	111.60
4	c	95	TYR	CZ-CE2-CD2	-5.05	115.26	119.80
2	D8	264	ARG	CB-CA-C	5.05	120.50	110.40
2	D6	221	ARG	CG-CD-NE	5.05	122.40	111.80
2	F0	280	LYS	CG-CD-CE	5.04	127.03	111.90
2	B4	243	ARG	NE-CZ-NH1	-5.04	117.78	120.30
3	D1	316	MET	CG-SD-CE	5.04	108.27	100.20
3	B3	251	ARG	CG-CD-NE	-5.04	101.22	111.80
4	q	24	MET	CB-CG-SD	-5.04	97.29	112.40
3	D3	320	ARG	CB-CG-CD	-5.04	98.51	111.60
1	19	248	ARG	CB-CG-CD	5.03	124.69	111.60
2	A4	183	GLU	CB-CA-C	-5.03	100.33	110.40
3	C9	324	LYS	CB-CG-CD	5.03	124.69	111.60
5	w	54	ARG	CB-CG-CD	5.03	124.69	111.60
4	v	116	ASP	CB-CG-OD2	-5.03	113.77	118.30
2	D0	140	ALA	CB-CA-C	5.03	117.64	110.10
2	A8	115	VAL	CA-CB-CG1	5.02	118.44	110.90
4	o	95	TYR	CB-CG-CD2	-5.02	117.98	121.00
3	D5	260	PHE	CB-CG-CD2	-5.02	117.28	120.80
3	F1	318	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	D4	248	LEU	CB-CG-CD1	5.02	119.54	111.00
3	A5	390	ARG	CG-CD-NE	-5.02	101.26	111.80
3	D1	208	TYR	CB-CG-CD1	5.02	124.01	121.00
2	B2	123	ARG	NE-CZ-NH2	-5.01	117.79	120.30
2	C0	214	ARG	NE-CZ-NH1	5.01	122.81	120.30
3	E3	391	ARG	CD-NE-CZ	5.01	130.62	123.60
3	F1	262	ARG	CB-CG-CD	5.01	124.64	111.60
2	B2	399	TYR	CB-CG-CD1	-5.01	117.99	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D0	399	TYR	CB-CG-CD1	5.01	124.01	121.00
4	m	194	ARG	CD-NE-CZ	5.01	130.62	123.60
2	E2	357	TYR	CB-CA-C	-5.01	100.38	110.40
3	E9	262	ARG	NE-CZ-NH2	-5.01	117.79	120.30
2	A2	308	ARG	CG-CD-NE	5.01	122.32	111.80
2	A8	285	GLN	CB-CG-CD	5.00	124.61	111.60
2	D4	162	GLY	CA-C-O	-5.00	111.59	120.60
2	D0	84	ARG	CG-CD-NE	5.00	122.30	111.80
3	E1	86	ARG	NE-CZ-NH1	-5.00	117.80	120.30
4	f	99	MET	CB-CG-SD	-5.00	97.40	112.40

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	13	255	PRO	Peptide
1	15	237	PRO	Peptide
1	15	240	PRO	Peptide
1	18	242	ASN	Peptide
1	23	239	LEU	Peptide
1	23	255	PRO	Peptide
1	4	240	PRO	Peptide
1	7	237	PRO	Peptide
2	A0	401	LYS	Peptide
2	A2	284	GLU	Peptide
2	A2	401	LYS	Peptide
2	A4	254	GLU	Peptide
2	A4	401	LYS	Peptide
2	A8	107	HIS	Peptide
2	A8	284	GLU	Peptide
2	A8	401	LYS	Peptide
2	B0	401	LYS	Peptide
3	B3	43	GLN	Peptide
2	B4	284	GLU	Peptide
2	B6	338	LYS	Peptide
3	B9	200	GLN	Peptide
2	C4	401	LYS	Peptide
2	C8	284	GLU	Peptide
2	D0	36	MET	Peptide
2	D0	401	LYS	Peptide
2	D2	284	GLU	Peptide
2	E2	162	GLY	Peptide

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Mol	Chain	Res	Type	Group
3	E5	321	MET	Peptide
3	E5	322	SER	Peptide
4	c	161	TYR	Peptide
4	e	35	ASN	Peptide
5	k	13	VAL	Peptide
5	l	13	VAL	Peptide
4	o	91	PHE	Sidechain
4	t	35	ASN	Peptide

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	174	0	171	18	0
1	1	174	0	171	6	0
1	10	174	0	171	24	0
1	11	174	0	171	20	0
1	12	174	0	171	9	0
1	13	174	0	171	10	0
1	14	174	0	171	6	0
1	15	174	0	171	17	0
1	16	174	0	171	18	0
1	17	174	0	171	8	0
1	18	174	0	171	8	0
1	19	174	0	171	24	0
1	2	174	0	171	13	0
1	20	174	0	171	13	0
1	21	174	0	171	20	0
1	22	160	0	156	8	0
1	23	160	0	156	5	0
1	3	174	0	171	8	0
1	4	174	0	171	10	0
1	5	174	0	171	13	0
1	6	174	0	171	15	0
1	7	174	0	171	18	0
1	8	174	0	171	29	0
1	9	174	0	171	32	0
2	A0	3325	0	3252	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A2	3325	0	3252	74	0
2	A4	3325	0	3252	81	0
2	A6	3325	0	3252	78	0
2	A8	3325	0	3252	90	0
2	B0	3325	0	3252	80	0
2	B2	3325	0	3252	73	0
2	B4	3325	0	3252	83	0
2	B6	3325	0	3252	69	0
2	B8	3325	0	3252	93	0
2	C0	3325	0	3252	73	0
2	C2	3325	0	3252	91	0
2	C4	3325	0	3252	91	0
2	C6	3325	0	3252	107	0
2	C8	3325	0	3252	78	0
2	D0	3325	0	3252	86	0
2	D2	3325	0	3252	76	0
2	D4	3325	0	3252	118	0
2	D6	3325	0	3252	63	0
2	D8	3325	0	3252	97	0
2	E0	3325	0	3252	78	0
2	E2	3325	0	3252	56	0
2	E4	3325	0	3252	64	0
2	E6	3325	0	3252	83	0
2	E8	3325	0	3252	72	0
2	F0	3325	0	3252	97	0
3	A1	3331	0	3207	98	0
3	A3	3331	0	3209	54	0
3	A5	3331	0	3207	99	0
3	A7	3331	0	3207	66	0
3	A9	3331	0	3207	79	0
3	B1	3331	0	3209	70	0
3	B3	3331	0	3207	82	0
3	B5	3331	0	3207	56	0
3	B7	3331	0	3209	62	0
3	B9	3331	0	3209	59	0
3	C1	3331	0	3209	110	0
3	C3	3331	0	3209	91	0
3	C5	3331	0	3209	77	0
3	C7	3331	0	3209	93	0
3	C9	3331	0	3209	101	0
3	D1	3331	0	3209	83	0
3	D3	3331	0	3207	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D5	3331	0	3207	107	0
3	D7	3331	0	3207	86	0
3	D9	3331	0	3207	80	0
3	E1	3331	0	3207	78	0
3	E3	3331	0	3209	61	0
3	E5	3331	0	3207	76	0
3	E7	3331	0	3207	86	0
3	E9	3331	0	3207	76	0
3	F1	3331	0	3207	85	0
4	a	1198	0	1194	0	0
4	b	1198	0	1194	0	0
4	c	1608	0	1590	0	0
4	d	1608	0	1590	0	0
4	e	1608	0	1590	0	0
4	f	1608	0	1590	0	0
4	g	1608	0	1590	0	0
4	h	1608	0	1590	0	0
4	i	1608	0	1590	0	0
4	j	1608	0	1590	0	0
4	m	1608	0	1590	0	0
4	n	1608	0	1590	0	0
4	o	1608	0	1590	0	0
4	p	1608	0	1590	0	0
4	q	1608	0	1590	0	0
4	r	1608	0	1590	0	0
4	s	1608	0	1590	0	0
4	t	1608	0	1590	0	0
4	u	1608	0	1590	0	0
4	v	1608	0	1588	0	0
5	k	1140	0	1143	0	0
5	l	1140	0	1143	0	0
5	w	1172	0	1171	0	0
5	x	1172	0	1171	0	0
All	All	213168	0	207664	3610	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 11.

All (3610) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:19:241:PHE:CZ	3:E7:356:ILE:HG23	1.28	1.68
2:C4:2:ARG:CG	2:C4:2:ARG:CD	1.76	1.56
3:A9:252:LYS:CG	3:A9:252:LYS:CD	1.84	1.55
1:19:241:PHE:HZ	3:E7:356:ILE:CG2	1.03	1.54
2:C4:2:ARG:CD	2:C4:2:ARG:NE	1.70	1.54
3:A5:252:LYS:NZ	3:A5:252:LYS:CE	1.71	1.54
3:A5:252:LYS:CE	3:A5:252:LYS:CD	1.78	1.52
2:A4:254:GLU:CG	2:A4:254:GLU:CD	1.76	1.50
1:19:241:PHE:CZ	3:E7:356:ILE:CG2	1.81	1.48
1:6:256:LEU:HD11	2:B6:31:GLN:CG	1.44	1.44
3:A1:219:THR:HA	2:A2:326:LYS:NZ	1.24	1.43
1:8:243:ALA:HB2	3:C1:357:PRO:CD	1.60	1.31
2:B4:283:HIS:O	2:B8:56:THR:CB	1.78	1.31
2:C6:407:TRP:CZ3	3:C7:255:VAL:HA	1.63	1.30
1:8:243:ALA:CB	3:C1:357:PRO:HD2	1.59	1.29
1:19:243:ALA:CB	3:E7:357:PRO:HD2	1.71	1.21
1:6:256:LEU:CD1	2:B6:31:GLN:HG2	1.70	1.20
1:7:256:LEU:HD21	2:B8:31:GLN:HA	1.21	1.19
1:19:243:ALA:HB2	3:E7:357:PRO:CD	1.72	1.18
1:8:241:PHE:HE1	3:C1:356:ILE:CG2	1.56	1.16
2:C6:407:TRP:CH2	3:C7:254:ALA:O	1.98	1.16
2:E0:71:GLU:OE2	3:E1:2:ARG:NH2	1.77	1.16
1:19:257:PRO:CG	2:E6:26:LEU:O	1.95	1.15
1:19:257:PRO:HG2	2:E6:26:LEU:O	0.99	1.14
1:15:256:LEU:HD11	2:D8:31:GLN:CA	1.77	1.14
1:8:241:PHE:CE1	3:C1:356:ILE:HG23	1.83	1.13
1:19:241:PHE:CZ	3:E7:356:ILE:HG21	1.69	1.12
1:8:241:PHE:CE1	3:C1:356:ILE:CG2	2.32	1.11
2:A4:285:GLN:HB2	2:A8:57:GLY:H	1.00	1.11
1:9:257:PRO:HG3	2:C2:26:LEU:HD12	1.25	1.10
3:A1:219:THR:CA	2:A2:326:LYS:NZ	2.14	1.10
1:6:256:LEU:HD11	2:B6:31:GLN:HG3	1.27	1.10
2:C6:407:TRP:HZ3	3:C7:255:VAL:CA	1.64	1.10
2:A2:282:TYR:O	2:A6:60:LYS:NZ	1.85	1.10
2:C2:73:THR:OG1	3:C3:46:ARG:NH1	1.84	1.09
1:0:243:ALA:HB1	3:A5:320:ARG:HD2	1.31	1.09
1:9:243:ALA:HB2	3:C3:357:PRO:HD2	1.12	1.09
2:A4:285:GLN:HB2	2:A8:57:GLY:N	1.68	1.09
3:C7:281:TYR:CD2	3:D1:87:PRO:HD3	1.86	1.09
1:19:256:LEU:HD22	2:E6:31:GLN:HG2	1.16	1.08
2:D8:285:GLN:HB2	2:E2:56:THR:HA	1.33	1.08
2:E4:96:LYS:HD2	3:E5:1:MET:HA	1.12	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:257:PRO:HG2	2:C0:29:GLY:HA2	1.19	1.08
1:8:241:PHE:HE1	3:C1:356:ILE:HG23	1.06	1.07
1:15:256:LEU:HD11	2:D8:31:GLN:HA	1.23	1.07
1:6:256:LEU:CD1	2:B6:31:GLN:CG	2.29	1.06
3:C7:281:TYR:HD2	3:D1:87:PRO:HD3	1.07	1.05
1:19:241:PHE:CE1	3:E7:356:ILE:CG2	2.39	1.05
1:8:241:PHE:HZ	3:C1:356:ILE:HD12	1.19	1.05
2:D0:285:GLN:HB3	2:D4:56:THR:HA	1.38	1.05
1:9:241:PHE:HE1	3:C3:356:ILE:CG2	1.70	1.05
3:B9:283:ALA:HA	3:C3:55:THR:HG23	1.36	1.05
3:C9:220:PRO:HD2	2:D0:326:LYS:HG3	1.08	1.05
1:4:247:TYR:HB3	2:B2:77:GLU:OE2	1.57	1.04
1:9:257:PRO:HG3	2:C2:26:LEU:CD1	1.86	1.04
3:C9:220:PRO:HD2	2:D0:326:LYS:CG	1.87	1.04
1:6:256:LEU:HD11	2:B6:31:GLN:HG2	1.09	1.04
3:A7:282:ARG:O	3:B1:55:THR:HG22	1.58	1.04
2:B6:73:THR:HG22	3:B7:46:ARG:HE	1.17	1.03
2:E0:176:GLN:OE1	3:E1:331:LEU:HD21	1.59	1.03
2:F0:223:THR:HG23	2:F0:225:THR:HG22	1.39	1.02
1:11:244:GLN:H	3:D1:320:ARG:NH2	1.57	1.01
1:4:247:TYR:CE1	2:B2:81:GLY:HA3	1.93	1.01
1:14:256:LEU:HD11	2:D6:31:GLN:HE21	1.25	1.01
1:6:256:LEU:HD21	2:B6:31:GLN:HA	1.38	1.01
1:9:241:PHE:CE1	3:C3:356:ILE:CG2	2.43	1.01
3:A1:219:THR:CA	2:A2:326:LYS:HZ2	1.69	1.01
2:A2:282:TYR:O	2:A6:60:LYS:CE	2.10	0.99
3:C1:281:TYR:O	3:C5:54:ALA:HB1	1.62	0.99
1:19:243:ALA:CB	3:E7:356:ILE:HA	1.93	0.99
1:9:243:ALA:HB3	3:C3:356:ILE:HG23	1.40	0.98
1:19:241:PHE:CE1	3:E7:356:ILE:HG23	1.98	0.98
2:A4:210:TYR:HB3	3:A5:324:LYS:HE3	1.46	0.98
2:D4:210:TYR:HB3	3:D5:324:LYS:HE2	1.46	0.98
2:D4:97:GLU:HB2	2:D4:110:ILE:HD11	1.45	0.97
1:19:243:ALA:HB1	3:E7:355:ASP:O	1.64	0.97
3:A1:281:TYR:HD2	3:A5:87:PRO:HD3	1.27	0.96
3:C9:220:PRO:CD	2:D0:326:LYS:HG3	1.94	0.96
1:9:241:PHE:CE1	3:C3:356:ILE:HG23	1.99	0.96
2:C6:407:TRP:HH2	3:C7:254:ALA:O	1.34	0.96
1:19:256:LEU:HD22	2:E6:31:GLN:CG	1.95	0.96
1:8:241:PHE:CZ	3:C1:356:ILE:HD12	2.01	0.96
1:21:256:LEU:HD21	2:F0:31:GLN:HG2	1.44	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:10:257:PRO:CG	2:C8:26:LEU:O	2.15	0.95
3:D1:284:LEU:HB3	3:D5:55:THR:HG21	1.46	0.95
3:D3:91:VAL:HG21	3:D3:116:VAL:HG22	1.48	0.95
1:8:257:PRO:CG	2:C0:29:GLY:HA2	1.96	0.94
3:C7:281:TYR:HB3	3:D1:86:ARG:HD3	1.48	0.94
2:C6:407:TRP:CZ3	3:C7:255:VAL:CA	2.45	0.94
3:C9:220:PRO:HG2	2:D0:326:LYS:HZ2	1.30	0.94
3:C9:208:TYR:CD1	2:D0:326:LYS:HE2	2.03	0.94
1:10:241:PHE:CZ	3:C9:356:ILE:HG23	2.03	0.94
3:B5:282:ARG:O	3:B9:55:THR:HG22	1.66	0.93
2:C6:168:ASN:HD21	2:C6:194:LEU:HD11	1.31	0.93
1:9:243:ALA:CB	3:C3:357:PRO:HD2	1.99	0.93
2:D6:96:LYS:HE2	3:D7:129:CYS:SG	2.09	0.93
3:C3:259:PRO:HG2	3:C3:311:LEU:HD21	1.50	0.93
3:F1:267:LEU:HD21	3:F1:374:ILE:HD11	1.49	0.93
1:16:247:TYR:HE2	2:E0:81:GLY:HA3	1.32	0.92
3:D3:396:HIS:HE1	2:D4:261:PRO:O	1.52	0.92
1:13:247:TYR:OH	2:D4:18:ASN:ND2	2.03	0.92
1:9:243:ALA:HB2	3:C3:357:PRO:CD	1.98	0.92
1:0:241:PHE:HZ	3:A5:356:ILE:HD12	1.32	0.92
2:C8:292:THR:HG21	2:C8:331:ALA:HB1	1.51	0.92
2:A4:210:TYR:HB3	3:A5:324:LYS:CE	2.00	0.91
1:8:243:ALA:CB	3:C1:357:PRO:CD	2.34	0.91
3:A1:219:THR:CG2	2:A2:324:VAL:HG21	2.00	0.91
3:A1:218:THR:O	2:A2:326:LYS:HE3	1.68	0.91
2:F0:407:TRP:CZ2	3:F1:258:ILE:HD11	2.06	0.91
1:7:256:LEU:HD21	2:B8:31:GLN:CA	2.01	0.91
2:D4:210:TYR:CE2	3:D5:327:ASP:OD2	2.24	0.91
1:10:254:LYS:NZ	2:C8:22:GLU:HG2	1.86	0.91
2:B0:73:THR:HA	3:B1:46:ARG:HH11	1.35	0.91
2:E4:119:LEU:HD12	2:E4:156:ARG:HD3	1.53	0.91
2:A6:222:PRO:HD2	3:A7:324:LYS:HB2	1.51	0.90
1:9:243:ALA:HB1	3:C3:356:ILE:HA	1.53	0.90
2:A8:285:GLN:HB2	2:B2:56:THR:HA	1.52	0.90
2:B0:285:GLN:CD	2:B4:55:GLU:O	2.10	0.90
1:0:244:GLN:HB3	3:A5:320:ARG:HH21	1.37	0.90
2:E6:280:LYS:NZ	2:F0:89:PRO:HB2	1.87	0.90
2:C6:176:GLN:OE1	3:C7:331:LEU:HD11	1.72	0.89
3:C9:220:PRO:HG2	2:D0:326:LYS:NZ	1.86	0.89
2:A4:79:ARG:HB3	2:A4:92:LEU:HD13	1.55	0.89
3:C9:208:TYR:HD1	2:D0:326:LYS:HE2	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A1:219:THR:HA	2:A2:326:LYS:HZ1	1.31	0.89
3:C1:117:LEU:HD13	3:C1:154:LYS:HG2	1.54	0.89
2:C8:178:SER:HB2	3:C9:347:ASN:ND2	1.88	0.89
2:C6:407:TRP:HZ3	3:C7:255:VAL:HA	1.09	0.89
3:A1:219:THR:CB	2:A2:326:LYS:HZ1	1.85	0.89
2:E0:163:LYS:HE2	2:E0:163:LYS:HA	1.53	0.89
3:E9:212:PHE:HE1	2:F0:326:LYS:HZ2	1.21	0.88
1:20:256:LEU:HD11	2:E8:31:GLN:HG3	1.55	0.88
1:8:241:PHE:CE1	3:C1:356:ILE:HG21	2.09	0.88
2:D4:285:GLN:HG2	2:D8:55:GLU:O	1.71	0.88
3:C7:281:TYR:HD2	3:D1:87:PRO:CD	1.86	0.88
2:A2:221:ARG:NE	3:A3:325:GLU:OE1	2.07	0.88
2:E6:280:LYS:HZ3	2:F0:89:PRO:HB2	1.34	0.87
3:A9:220:PRO:HG2	2:B0:326:LYS:HE2	1.54	0.87
1:0:244:GLN:HB3	3:A5:320:ARG:NH2	1.89	0.87
1:18:243:ALA:HB2	3:E5:357:PRO:HD2	1.57	0.87
1:4:245:SER:HB2	3:B3:42:LEU:HD11	1.56	0.87
3:B7:281:TYR:CE2	3:C1:87:PRO:HD3	2.09	0.87
3:E9:219:THR:HB	2:F0:324:VAL:HG21	1.54	0.87
1:2:257:PRO:HD3	2:A8:26:LEU:CD1	2.04	0.86
2:C4:12:ALA:HB3	2:C4:140:ALA:HB2	1.56	0.86
2:C8:178:SER:HB2	3:C9:347:ASN:HD21	1.38	0.86
3:C7:68:LEU:HD13	3:C7:93:GLY:HA3	1.57	0.86
3:D5:135:ILE:HG13	3:D5:152:ILE:HD11	1.57	0.86
1:7:256:LEU:HD11	2:B8:31:GLN:HB3	1.55	0.86
3:E5:281:TYR:CE2	3:E9:87:PRO:HD3	2.09	0.86
2:D6:210:TYR:HE1	2:D6:227:LEU:HD11	1.41	0.85
1:19:256:LEU:CD2	2:E6:31:GLN:HG2	2.04	0.85
3:B3:16:ILE:HD11	3:B3:229:VAL:HG11	1.57	0.85
2:D4:285:GLN:HB3	2:D8:56:THR:HA	1.56	0.85
1:19:243:ALA:HB3	3:E7:356:ILE:HA	1.56	0.85
3:D9:260:PHE:HB3	3:D9:261:PRO:HD2	1.58	0.85
2:E8:210:TYR:HB3	3:E9:324:LYS:HD3	1.58	0.85
2:B0:210:TYR:HB3	3:B1:324:LYS:HD2	1.58	0.85
2:B6:73:THR:CG2	3:B7:46:ARG:HE	1.89	0.85
2:C4:404:PHE:HE1	3:C5:255:VAL:O	1.58	0.84
3:D3:220:PRO:HD2	2:D4:326:LYS:HD3	1.58	0.84
3:B5:99:ASN:HD22	3:B5:178:THR:HG23	1.42	0.84
1:10:257:PRO:HG2	2:C8:26:LEU:O	1.77	0.84
2:A2:282:TYR:O	2:A6:60:LYS:HE2	1.77	0.84
2:D2:292:THR:HG21	2:D2:331:ALA:HB1	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D4:274:PRO:HG3	2:D4:286:LEU:HD23	1.59	0.84
2:E6:221:ARG:HB3	3:E7:322:SER:CB	2.08	0.84
3:D3:175:VAL:HG11	2:D4:333:ALA:HA	1.58	0.84
3:C7:291:GLN:NE2	3:D1:125:GLU:OE1	2.09	0.84
3:E9:218:THR:O	2:F0:326:LYS:NZ	2.11	0.84
2:B0:100:ALA:HA	3:B1:252:LYS:NZ	1.94	0.83
2:A6:210:TYR:HB3	3:A7:324:LYS:HZ3	1.41	0.83
2:E6:221:ARG:HG2	3:E7:322:SER:OG	1.77	0.83
1:15:257:PRO:HG2	2:D8:26:LEU:HD23	1.59	0.83
1:16:247:TYR:CE2	2:E0:81:GLY:HA3	2.13	0.83
2:C6:222:PRO:HD2	3:C7:324:LYS:HG2	1.60	0.83
2:B4:285:GLN:CD	2:B8:55:GLU:O	2.17	0.83
1:5:253:ALA:HB1	2:B4:32:PRO:HG2	1.57	0.83
1:15:256:LEU:HD11	2:D8:31:GLN:N	1.91	0.83
2:A2:210:TYR:HB3	3:A3:324:LYS:HE3	1.61	0.83
2:F0:70:LEU:HD12	2:F0:99:ALA:HB2	1.59	0.83
1:0:251:TYR:OH	2:A4:18:ASN:HB3	1.79	0.82
1:9:243:ALA:CB	3:C3:356:ILE:HA	2.08	0.82
2:E4:96:LYS:HD2	3:E5:1:MET:CA	2.03	0.82
1:16:246:CYS:HA	3:E1:320:ARG:HH22	1.42	0.82
1:21:241:PHE:HZ	3:F1:356:ILE:HG23	1.43	0.82
1:9:241:PHE:HE1	3:C3:356:ILE:HG23	1.34	0.82
2:A6:214:ARG:NH2	3:A7:324:LYS:HZ2	1.77	0.82
2:B2:241:SER:HB2	2:B2:249:ASN:HB2	1.61	0.82
1:4:248:ARG:HH22	2:B2:81:GLY:HA2	1.44	0.82
2:C2:362:VAL:HG11	2:C2:370:LYS:HB3	1.60	0.82
2:B6:73:THR:HG22	3:B7:46:ARG:NE	1.95	0.82
2:C4:181:VAL:HG12	3:C5:256:ASN:HB2	1.58	0.82
3:D5:7:VAL:HG11	3:D5:151:LEU:HD21	1.60	0.82
2:B6:238:LEU:HD11	2:B6:378:ILE:HD11	1.62	0.82
1:10:241:PHE:CE1	3:C9:356:ILE:HG23	2.15	0.81
2:B2:179:THR:N	3:B3:347:ASN:HD21	1.76	0.81
1:16:246:CYS:CA	3:E1:320:ARG:HH22	1.93	0.81
3:C5:397:TRP:CH2	2:C6:260:VAL:HB	2.16	0.81
3:A1:219:THR:HG23	2:A2:324:VAL:HG21	1.59	0.81
2:F0:66:VAL:HG12	2:F0:91:GLN:HB2	1.62	0.81
1:16:256:LEU:HD23	2:E0:31:GLN:HG2	1.63	0.81
2:A6:214:ARG:HH21	3:A7:324:LYS:HZ2	1.28	0.81
3:B3:282:ARG:O	3:B7:55:THR:CG2	2.28	0.81
1:19:257:PRO:HD2	2:E6:29:GLY:HA2	1.61	0.81
1:20:241:PHE:HE1	3:E9:356:ILE:HG21	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D4:177:VAL:CG2	3:D5:331:LEU:HD22	2.12	0.80
1:4:247:TYR:CB	2:B2:77:GLU:OE2	2.29	0.80
3:A1:281:TYR:CD2	3:A5:87:PRO:HD3	2.16	0.80
2:C0:176:GLN:O	3:C1:347:ASN:ND2	2.14	0.80
2:C6:210:TYR:HB3	3:C7:324:LYS:HD2	1.62	0.80
1:14:256:LEU:CD1	2:D6:31:GLN:HE21	1.95	0.80
2:A8:136:LEU:HD13	2:A8:235:ILE:HD11	1.63	0.80
3:E7:213:ARG:HH22	3:E7:297:LYS:HB2	1.45	0.80
1:22:243:ALA:HB2	3:C7:357:PRO:HD2	1.64	0.80
2:A6:214:ARG:HE	3:A7:324:LYS:NZ	1.80	0.80
2:D4:105:ARG:HH12	3:D5:251:ARG:HD3	1.47	0.80
2:F0:406:HIS:CD2	3:F1:261:PRO:HD3	2.16	0.80
2:B0:285:GLN:HB3	2:B4:56:THR:HA	1.64	0.80
2:C6:181:VAL:HB	3:C7:256:ASN:OD1	1.80	0.80
2:E0:292:THR:HG21	2:E0:331:ALA:HB1	1.62	0.80
1:0:241:PHE:CZ	3:A5:356:ILE:HD12	2.16	0.79
2:D8:407:TRP:CE2	3:D9:255:VAL:HA	2.16	0.79
2:E6:221:ARG:HB3	3:E7:322:SER:HB2	1.65	0.79
2:B8:11:GLN:HE22	3:B9:246:LEU:HD12	1.48	0.79
2:F0:407:TRP:HZ2	3:F1:258:ILE:HD11	1.45	0.79
1:11:244:GLN:N	3:D1:320:ARG:NH2	2.31	0.79
1:15:256:LEU:CD1	2:D8:31:GLN:HA	2.09	0.79
1:7:256:LEU:HD11	2:B8:31:GLN:CB	2.12	0.79
2:D2:12:ALA:HB3	2:D2:140:ALA:HB2	1.63	0.79
2:D8:163:LYS:H	2:D8:163:LYS:HD2	1.48	0.79
2:B2:11:GLN:HE22	3:B3:246:LEU:HD13	1.48	0.79
1:8:243:ALA:HB3	3:C1:356:ILE:HG23	1.64	0.78
3:A1:10:GLY:HA2	3:A1:143:THR:HG23	1.64	0.78
2:C8:176:GLN:HB3	3:C9:331:LEU:HD22	1.65	0.78
3:C9:391:ARG:O	2:D0:262:TYR:OH	2.00	0.78
2:C0:217:LEU:HD21	2:C0:275:ILE:HG13	1.64	0.78
2:D0:285:GLN:HG2	2:D4:55:GLU:O	1.83	0.78
3:D1:91:VAL:HG11	3:D1:116:VAL:HG22	1.65	0.78
1:22:243:ALA:CB	3:C7:357:PRO:HD2	2.13	0.78
3:E9:208:TYR:CE1	2:F0:326:LYS:HB3	2.19	0.78
1:21:238:THR:HG21	3:F1:29:GLY:HA2	1.66	0.78
2:A8:210:TYR:CG	3:A9:324:LYS:HG3	2.18	0.77
3:A1:379:LYS:HB2	3:A1:379:LYS:NZ	1.98	0.77
3:D3:291:GLN:HG2	3:D7:122:LYS:NZ	2.00	0.77
1:3:257:PRO:HG2	2:B0:26:LEU:O	1.83	0.77
3:B5:282:ARG:O	3:B9:55:THR:CG2	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B7:391:ARG:O	2:B8:262:TYR:OH	2.01	0.77
2:C6:407:TRP:CZ3	3:C7:254:ALA:O	2.38	0.77
1:5:248:ARG:HH12	3:B5:42:LEU:HD21	1.48	0.77
3:B5:283:ALA:HA	3:B9:55:THR:HB	1.66	0.77
3:D9:169:VAL:HG12	3:D9:202:ILE:HB	1.67	0.77
2:C6:6:SER:HA	2:C6:136:LEU:HB2	1.66	0.76
3:C7:2:ARG:NH1	3:C7:249:ASP:OD2	2.17	0.76
1:11:250:GLU:OE1	2:D0:225:THR:HG21	1.84	0.76
2:D0:285:GLN:HB3	2:D4:56:THR:CA	2.15	0.76
1:4:247:TYR:HE1	2:B2:81:GLY:HA3	1.46	0.76
2:D2:210:TYR:CG	3:D3:324:LYS:HD3	2.21	0.76
1:10:244:GLN:HB2	3:C9:320:ARG:NH1	2.01	0.76
1:6:247:TYR:HE2	2:B6:81:GLY:HA3	1.51	0.76
3:B1:207:LEU:HB3	3:B1:225:LEU:HD22	1.68	0.76
2:C6:176:GLN:OE1	3:C7:331:LEU:CD1	2.34	0.76
1:1:254:LYS:HB3	2:A6:364:PRO:HB2	1.68	0.76
2:A4:110:ILE:O	2:A4:110:ILE:HG13	1.85	0.76
2:A4:222:PRO:HD2	3:A5:324:LYS:HB3	1.68	0.76
1:10:241:PHE:HZ	3:C9:356:ILE:HG23	1.52	0.75
2:D4:210:TYR:HB3	3:D5:324:LYS:CE	2.15	0.75
1:8:243:ALA:HB2	3:C1:357:PRO:HD2	0.80	0.75
1:2:251:TYR:OH	2:A8:18:ASN:HB3	1.86	0.75
3:A5:212:PHE:CG	2:A6:326:LYS:HE2	2.22	0.75
2:D6:222:PRO:O	3:D7:324:LYS:NZ	2.19	0.75
1:9:257:PRO:CG	2:C2:26:LEU:CD1	2.64	0.75
3:B5:260:PHE:HB3	3:B5:261:PRO:HD2	1.68	0.75
2:A4:285:GLN:CB	2:A8:57:GLY:H	1.91	0.75
3:D5:129:CYS:SG	3:D5:162:ARG:NH2	2.60	0.75
3:A3:267:LEU:HD21	3:A3:371:SER:HB3	1.69	0.74
2:C4:241:SER:HB2	2:C4:249:ASN:HB2	1.69	0.74
2:A4:93:ILE:HD11	2:A4:118:SER:HB2	1.69	0.74
3:B7:281:TYR:HE2	3:C1:87:PRO:HD3	1.51	0.74
1:20:256:LEU:CD1	2:E8:31:GLN:HG3	2.17	0.74
3:C9:139:LEU:HD13	3:C9:168:SER:HB2	1.69	0.74
2:D4:210:TYR:HE2	3:D5:327:ASP:OD2	1.69	0.74
2:D4:292:THR:HG21	2:D4:331:ALA:HB1	1.68	0.74
3:D5:260:PHE:HB3	3:D5:261:PRO:HD2	1.68	0.74
2:D8:79:ARG:CG	2:D8:92:LEU:HD12	2.18	0.74
1:9:241:PHE:CE1	3:C3:356:ILE:HG21	2.20	0.74
2:A0:312:TYR:HE1	2:A0:379:SER:HB3	1.52	0.74
3:B3:176:SER:CB	2:B4:349:THR:HG23	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D7:212:PHE:HE1	2:D8:326:LYS:HD3	1.53	0.74
2:E0:96:LYS:HE2	3:E1:128:ASP:HB2	1.69	0.74
1:5:256:LEU:HD13	2:B4:26:LEU:HD12	1.70	0.74
1:9:254:LYS:HB3	1:9:255:PRO:HD2	1.68	0.74
2:A8:210:TYR:HB3	3:A9:324:LYS:HE3	1.67	0.74
3:A9:100:ASN:HB2	3:A9:103:LYS:HG2	1.70	0.74
1:10:257:PRO:HG3	2:C8:26:LEU:O	1.85	0.74
1:7:256:LEU:CD1	2:B8:31:GLN:HB3	2.17	0.74
3:B1:49:VAL:HG21	3:B1:241:ARG:HG2	1.67	0.74
3:D9:7:VAL:HG11	3:D9:151:LEU:CD2	2.17	0.74
2:E4:151:CYS:SG	2:E4:193:SER:OG	2.44	0.74
1:10:244:GLN:HB2	3:C9:320:ARG:HH12	1.51	0.74
3:A9:10:GLY:HA2	3:A9:143:THR:HG23	1.69	0.74
3:D3:176:SER:HB3	2:D4:349:THR:HB	1.68	0.74
3:D3:175:VAL:HG11	2:D4:333:ALA:CA	2.17	0.74
3:D7:391:ARG:O	2:D8:262:TYR:OH	2.05	0.74
3:F1:311:LEU:HD12	3:F1:342:VAL:HG21	1.70	0.73
1:2:247:TYR:HB3	2:A8:77:GLU:OE2	1.88	0.73
2:A4:93:ILE:HG21	2:A4:117:LEU:HD22	1.69	0.73
2:A4:241:SER:HB2	2:A4:249:ASN:HB2	1.69	0.73
2:B0:174:SER:OG	2:B0:177:VAL:O	2.05	0.73
3:C7:281:TYR:CB	3:D1:86:ARG:HD3	2.18	0.73
2:A6:214:ARG:NE	3:A7:324:LYS:HZ2	1.87	0.73
2:D4:66:VAL:HG21	2:D4:122:ILE:HD11	1.70	0.73
2:E4:119:LEU:CD1	2:E4:156:ARG:HD3	2.18	0.73
3:E5:281:TYR:CD2	3:E9:87:PRO:HD3	2.23	0.73
2:A8:183:GLU:HB2	2:A8:184:PRO:HD3	1.70	0.73
2:B6:178:SER:HB3	3:B7:347:ASN:ND2	2.04	0.73
2:D6:210:TYR:CE1	2:D6:227:LEU:HD11	2.23	0.73
2:D6:221:ARG:HA	3:D7:324:LYS:HE3	1.70	0.73
3:D7:406:MET:HA	3:D7:406:MET:CE	2.18	0.73
2:F0:223:THR:CG2	2:F0:225:THR:HG22	2.17	0.73
1:2:257:PRO:HD3	2:A8:26:LEU:HD12	1.69	0.73
2:B8:282:TYR:HE2	2:C2:85:HIS:CG	2.06	0.73
2:C2:73:THR:HG1	3:C3:46:ARG:NH1	1.85	0.73
2:D4:215:ARG:HH12	2:D4:299:ALA:HB1	1.53	0.73
1:18:243:ALA:CB	3:E5:357:PRO:HD2	2.17	0.73
2:B0:221:ARG:HB2	3:B1:322:SER:OG	1.88	0.73
2:C4:7:ILE:HG21	2:C4:153:LEU:HD23	1.70	0.73
2:E4:274:PRO:HD3	2:E4:291:ILE:HD11	1.70	0.73
1:11:244:GLN:H	3:D1:320:ARG:HH21	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C5:397:TRP:HH2	2:C6:260:VAL:HB	1.53	0.72
2:D8:262:TYR:HB3	2:D8:263:PRO:HD2	1.71	0.72
2:A6:214:ARG:CZ	3:A7:324:LYS:HZ2	2.02	0.72
2:A8:210:TYR:HB3	3:A9:324:LYS:CE	2.20	0.72
3:D5:117:LEU:HD22	3:D5:154:LYS:HD2	1.71	0.72
3:F1:113:ILE:HG13	3:F1:150:LEU:HD22	1.71	0.72
2:C6:407:TRP:HZ3	3:C7:255:VAL:C	1.91	0.72
2:D4:96:LYS:NZ	3:D5:128:ASP:HB2	2.04	0.72
2:A6:283:HIS:O	2:B0:56:THR:CB	2.37	0.72
3:B9:181:GLU:HB2	3:B9:182:PRO:HD3	1.71	0.72
2:E0:229:ARG:HH11	2:E0:229:ARG:HG3	1.55	0.72
1:15:257:PRO:HD3	2:D8:26:LEU:HG	1.69	0.72
3:A9:219:THR:HB	2:B0:324:VAL:HG21	1.72	0.72
3:B3:176:SER:OG	2:B4:349:THR:HG23	1.89	0.72
2:B4:282:TYR:HE2	2:B8:85:HIS:HB3	1.54	0.72
1:8:243:ALA:CB	3:C1:356:ILE:HA	2.20	0.72
3:B9:283:ALA:HA	3:C3:55:THR:CG2	2.17	0.72
3:C1:117:LEU:CD1	3:C1:154:LYS:HG2	2.19	0.72
2:E4:223:THR:HG23	2:E4:225:THR:HG22	1.70	0.72
1:2:251:TYR:CZ	2:A8:18:ASN:HB3	2.25	0.72
1:5:256:LEU:HD21	2:B4:31:GLN:HA	1.72	0.72
2:C4:2:ARG:CG	2:C4:2:ARG:HD3	2.13	0.72
2:C4:222:PRO:HD2	3:C5:324:LYS:CB	2.19	0.71
2:D2:215:ARG:HH12	2:D2:299:ALA:HB1	1.54	0.71
2:E6:181:VAL:HG13	3:E7:350:LYS:NZ	2.05	0.71
1:12:257:PRO:HD3	2:D2:26:LEU:HD22	1.72	0.71
1:9:255:PRO:HG2	2:C2:364:PRO:CG	2.20	0.71
2:C0:10:GLY:HA2	2:C0:145:THR:HG23	1.70	0.71
2:D4:151:CYS:HG	2:D4:193:SER:HG	1.36	0.71
2:E6:222:PRO:HD2	3:E7:324:LYS:HB2	1.71	0.71
2:A8:181:VAL:HG21	3:A9:256:ASN:OD1	1.90	0.71
3:A5:284:LEU:CB	3:A9:55:THR:HG21	2.20	0.71
3:B3:93:GLY:HA2	3:B3:112:LEU:HD21	1.72	0.71
2:B8:250:VAL:HG23	2:B8:254:GLU:HG2	1.72	0.71
3:D3:220:PRO:CD	2:D4:326:LYS:HD3	2.20	0.71
1:0:244:GLN:H	3:A5:320:ARG:NE	1.88	0.71
2:C0:223:THR:OG1	3:C1:245:GLN:OE1	2.08	0.71
3:B3:152:ILE:HG23	3:B3:164:MET:HE1	1.72	0.71
2:D6:12:ALA:HB3	2:D6:140:ALA:HB2	1.71	0.71
3:C5:219:THR:HB	2:C6:324:VAL:HG11	1.71	0.71
1:16:246:CYS:HA	3:E1:320:ARG:NH2	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:250:GLU:HG3	2:B2:225:THR:HG21	1.72	0.71
3:C3:190:HIS:HB2	3:C3:414:ASN:HD21	1.56	0.71
3:B1:311:LEU:HD12	3:B1:342:VAL:HG11	1.72	0.71
2:B4:269:LEU:HD21	2:B4:384:ILE:HD11	1.73	0.71
2:C2:406:HIS:CD2	3:C3:261:PRO:HD3	2.26	0.71
2:C4:2:ARG:HB3	2:C4:133:GLN:HE21	1.54	0.71
2:A6:214:ARG:HE	3:A7:324:LYS:HZ2	1.35	0.70
2:C6:168:ASN:ND2	2:C6:194:LEU:HD11	2.06	0.70
2:C6:407:TRP:CE3	3:C7:255:VAL:HA	2.25	0.70
2:C4:404:PHE:CE1	3:C5:255:VAL:O	2.43	0.70
2:E0:223:THR:HG23	2:E0:225:THR:HG22	1.73	0.70
2:E2:96:LYS:HE3	3:E3:1:MET:N	2.07	0.70
3:A1:219:THR:CA	2:A2:326:LYS:HZ1	1.89	0.70
3:B3:49:VAL:HG21	3:B3:241:ARG:HG2	1.74	0.70
3:C3:259:PRO:HG2	3:C3:311:LEU:CD2	2.20	0.70
1:20:243:ALA:HB2	3:E9:357:PRO:HD2	1.72	0.70
2:A4:93:ILE:CD1	2:A4:118:SER:HB2	2.22	0.70
3:A9:220:PRO:HG2	2:B0:326:LYS:CE	2.21	0.70
3:A9:259:PRO:HG2	3:A9:311:LEU:HD21	1.74	0.70
2:A0:221:ARG:HG3	3:A1:325:GLU:HB3	1.74	0.70
3:B1:163:ILE:HD13	3:B1:250:LEU:HB3	1.74	0.70
2:C6:276:ILE:HD12	2:C6:281:ALA:HA	1.74	0.70
3:D7:91:VAL:HG11	3:D7:116:VAL:HB	1.72	0.70
1:10:241:PHE:HZ	3:C9:356:ILE:HD12	1.57	0.70
1:13:253:ALA:CB	2:D4:32:PRO:HG3	2.22	0.70
1:15:257:PRO:CD	2:D8:26:LEU:HG	2.21	0.70
3:A3:135:ILE:HG21	3:A3:152:ILE:HD11	1.73	0.70
3:B3:282:ARG:O	3:B7:55:THR:HG22	1.89	0.70
2:C4:222:PRO:HD2	3:C5:324:LYS:HB3	1.74	0.70
1:8:239:LEU:O	3:C1:359:LYS:HE3	1.90	0.70
2:E8:80:THR:HA	2:E8:84:ARG:HE	1.57	0.69
1:15:257:PRO:HG2	2:D8:26:LEU:CD2	2.22	0.69
1:6:256:LEU:CD1	2:B6:31:GLN:HG3	2.08	0.69
2:A0:79:ARG:HG3	2:A0:92:LEU:HD22	1.74	0.69
2:D6:223:THR:OG1	3:D7:323:THR:HG23	1.92	0.69
1:4:248:ARG:NH2	2:B2:81:GLY:HA2	2.06	0.69
3:C5:12:CYS:HB3	3:C5:138:SER:HB3	1.73	0.69
2:E0:298:PRO:HG3	2:E0:308:ARG:HH22	1.57	0.69
3:C7:97:ALA:HB3	3:C7:143:THR:HG22	1.75	0.69
3:D3:397:TRP:CZ2	2:D4:256:GLN:O	2.46	0.69
2:C8:323:VAL:HG13	2:C8:355:ILE:HG23	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D7:406:MET:HA	3:D7:406:MET:HE2	1.72	0.69
1:2:257:PRO:HG2	2:A8:26:LEU:O	1.91	0.69
1:10:254:LYS:HZ2	2:C8:22:GLU:HG2	1.58	0.69
3:A1:222:TYR:HB2	2:A2:325:PRO:HG2	1.75	0.69
3:B9:282:ARG:O	3:C3:55:THR:OG1	2.11	0.69
3:C9:354:CYS:SG	3:C9:355:ASP:N	2.65	0.69
3:D3:391:ARG:O	2:D4:262:TYR:OH	2.11	0.69
2:D6:176:GLN:O	3:D7:347:ASN:ND2	2.26	0.69
2:F0:176:GLN:CG	3:F1:331:LEU:HD21	2.23	0.69
3:D5:107:THR:HG21	3:D5:401:GLU:HB2	1.74	0.69
2:D6:220:GLU:O	3:D7:324:LYS:HE3	1.93	0.69
3:F1:2:ARG:NH2	3:F1:249:ASP:OD2	2.25	0.69
1:10:241:PHE:CE1	3:C9:356:ILE:CG2	2.76	0.69
3:C1:113:ILE:HG21	3:C1:154:LYS:HD2	1.74	0.69
1:6:256:LEU:CG	2:B6:31:GLN:HG2	2.22	0.68
2:D0:283:HIS:HA	2:D4:60:LYS:HZ3	1.58	0.68
3:E7:163:ILE:HD13	3:E7:250:LEU:HB3	1.74	0.68
3:B5:99:ASN:ND2	3:B5:178:THR:HG23	2.08	0.68
2:C4:209:ILE:HG23	2:C4:227:LEU:HD22	1.75	0.68
2:D4:262:TYR:HB2	2:D4:265:ILE:HD12	1.74	0.68
2:D0:204:LEU:HD13	2:D0:231:ILE:HD12	1.76	0.68
1:15:256:LEU:HD11	2:D8:30:ILE:C	2.13	0.68
2:A2:398:MET:CE	3:A3:345:ILE:HG23	2.24	0.68
2:A6:222:PRO:HD2	3:A7:324:LYS:CB	2.21	0.68
2:B2:53:PHE:HB3	2:B2:61:HIS:HB3	1.75	0.68
3:B3:176:SER:HB2	2:B4:349:THR:HG23	1.74	0.68
2:C8:276:ILE:HG23	2:C8:280:LYS:HB2	1.75	0.68
1:11:244:GLN:H	3:D1:320:ARG:HH22	1.37	0.68
1:16:256:LEU:CD2	2:E0:31:GLN:HG2	2.24	0.68
3:B3:219:THR:HB	2:B4:324:VAL:HG21	1.74	0.68
2:E6:221:ARG:CB	3:E7:322:SER:HB2	2.23	0.68
1:3:257:PRO:CG	2:B0:26:LEU:O	2.42	0.68
2:D4:12:ALA:HB3	2:D4:140:ALA:HB2	1.76	0.68
1:9:244:GLN:H	3:C3:320:ARG:HD2	1.57	0.68
1:11:244:GLN:N	3:D1:320:ARG:HH22	1.92	0.68
3:A9:248:SER:HA	3:A9:252:LYS:HG2	1.76	0.68
3:B3:375:GLN:NE2	3:B3:423:GLN:OE1	2.27	0.68
3:B9:200:GLN:HB2	3:B9:268:ILE:HD11	1.76	0.68
2:D4:210:TYR:HB3	3:D5:324:LYS:HD3	1.75	0.68
3:F1:10:GLY:HA2	3:F1:143:THR:HG23	1.75	0.68
3:A5:287:PRO:HA	3:A5:329:GLN:HE22	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B3:396:HIS:HA	3:B3:399:THR:HG22	1.74	0.68
2:A8:288:VAL:HG21	2:A8:323:VAL:HG13	1.76	0.67
2:D0:8:HIS:CD2	2:D0:17:GLY:HA3	2.29	0.67
3:B3:91:VAL:HG21	3:B3:116:VAL:HG22	1.77	0.67
2:E6:174:SER:OG	2:E6:177:VAL:O	2.09	0.67
1:8:243:ALA:HB1	3:C1:356:ILE:HA	1.76	0.67
3:A7:207:LEU:HB3	3:A7:225:LEU:HD12	1.76	0.67
3:A1:42:LEU:HD21	3:A1:243:PRO:HD2	1.76	0.67
1:17:246:CYS:HB2	3:E3:320:ARG:HH21	1.60	0.67
3:D1:98:GLY:H	3:D1:103:LYS:HD3	1.59	0.67
1:14:256:LEU:HD11	2:D6:31:GLN:NE2	2.04	0.67
2:A0:222:PRO:HD2	3:A1:324:LYS:CB	2.25	0.67
2:A6:177:VAL:HG23	3:A7:331:LEU:HD22	1.75	0.67
3:C9:66:MET:HE3	3:C9:151:LEU:HD22	1.77	0.67
2:D0:174:SER:OG	2:D0:177:VAL:O	2.13	0.67
3:D3:220:PRO:HG2	2:D4:326:LYS:HD3	1.76	0.67
1:15:257:PRO:HD2	2:D8:26:LEU:O	1.95	0.67
3:A1:412:GLU:OE2	3:A1:416:ASN:ND2	2.27	0.67
2:B0:285:GLN:OE1	2:B4:55:GLU:O	2.12	0.67
2:C8:105:ARG:HH12	3:C9:251:ARG:HG2	1.60	0.67
3:D9:14:ASN:HD22	3:D9:72:THR:HG23	1.60	0.67
3:B3:130:LEU:HD23	3:B3:130:LEU:H	1.59	0.67
3:B3:95:THR:OG1	3:B3:108:GLU:OE2	2.10	0.67
3:B5:324:LYS:HA	3:B5:327:ASP:HB2	1.77	0.67
3:D1:67:ASP:OD2	3:D1:72:THR:OG1	2.13	0.67
2:E2:96:LYS:HE3	3:E3:1:MET:H1	1.58	0.67
2:E6:223:THR:HG23	2:E6:225:THR:HG22	1.77	0.67
2:B4:285:GLN:NE2	2:B8:55:GLU:O	2.28	0.67
3:B9:318:ARG:HD2	3:B9:358:PRO:HD3	1.76	0.67
3:D3:293:MET:SD	3:D3:365:VAL:HG11	2.35	0.67
2:E6:221:ARG:HG2	3:E7:322:SER:CB	2.25	0.67
3:E5:274:THR:HG21	3:E5:282:ARG:HD2	1.76	0.66
2:E6:283:HIS:NE2	2:F0:85:HIS:HB3	2.10	0.66
1:11:250:GLU:CD	2:D0:225:THR:HG21	2.14	0.66
2:A8:282:TYR:OH	2:B2:33:ASP:OD1	2.12	0.66
3:B3:336:LYS:HE2	3:B3:336:LYS:HA	1.77	0.66
3:E1:248:SER:HA	3:E1:252:LYS:HG3	1.77	0.66
3:E9:267:LEU:HD21	3:E9:374:ILE:HD11	1.77	0.66
1:9:241:PHE:CZ	3:C3:356:ILE:CG2	2.78	0.66
2:B0:2:ARG:HB2	2:B0:133:GLN:HE22	1.59	0.66
2:B4:178:SER:OG	3:B5:347:ASN:ND2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C2:221:ARG:HB3	3:C3:322:SER:CB	2.25	0.66
3:C5:207:LEU:HB3	3:C5:225:LEU:HD12	1.77	0.66
2:D4:177:VAL:HG23	3:D5:331:LEU:HD22	1.78	0.66
2:D8:407:TRP:CZ2	3:D9:255:VAL:HA	2.31	0.66
3:E5:172:SER:HB2	3:E5:205:GLU:HG2	1.77	0.66
1:8:255:PRO:HG2	2:C0:364:PRO:HG2	1.77	0.66
3:B3:10:GLY:HA2	3:B3:143:THR:HG23	1.76	0.66
3:C3:267:LEU:HD11	3:C3:374:ILE:HD13	1.78	0.66
3:D3:175:VAL:CG1	2:D4:333:ALA:HA	2.25	0.66
2:E6:221:ARG:HB3	3:E7:322:SER:HB3	1.76	0.66
2:E6:339:ARG:NH2	2:E6:342:GLN:OE1	2.29	0.66
1:0:243:ALA:CB	3:A5:320:ARG:HD2	2.19	0.66
3:B7:274:THR:HG21	3:B7:282:ARG:HD2	1.76	0.66
2:B0:100:ALA:HA	3:B1:252:LYS:HZ3	1.61	0.66
3:C1:166:THR:HB	3:C1:199:VAL:HG12	1.78	0.66
3:E5:12:CYS:HB3	3:E5:138:SER:HB2	1.76	0.66
3:A5:172:SER:HB3	3:A5:205:GLU:HG2	1.77	0.66
3:D3:44:LEU:O	3:D3:44:LEU:HD23	1.95	0.66
2:E8:180:ALA:HB3	2:E8:183:GLU:HG2	1.78	0.66
1:10:257:PRO:HD3	2:C8:26:LEU:HD22	1.78	0.66
1:2:257:PRO:HD3	2:A8:26:LEU:HD11	1.76	0.66
2:B0:100:ALA:HA	3:B1:252:LYS:HZ2	1.58	0.66
3:D9:10:GLY:HA2	3:D9:143:THR:HG23	1.78	0.66
2:E6:221:ARG:CG	3:E7:322:SER:CB	2.74	0.66
1:1:239:LEU:HD22	3:A7:359:LYS:HB3	1.76	0.66
3:A1:130:LEU:H	3:A1:162:ARG:HH12	1.42	0.66
2:B0:285:GLN:NE2	2:B4:55:GLU:O	2.28	0.66
2:B8:224:TYR:HB2	3:B9:245:GLN:NE2	2.11	0.66
1:19:250:GLU:HG3	2:E6:225:THR:HG21	1.78	0.65
2:A0:73:THR:HA	3:A1:46:ARG:HH11	1.60	0.65
2:B6:285:GLN:HB3	2:C0:56:THR:HA	1.77	0.65
3:C1:249:ASP:H	3:C1:252:LYS:HB2	1.61	0.65
2:D0:142:GLY:HA3	2:D0:183:GLU:HG2	1.78	0.65
3:A1:205:GLU:HA	3:A1:208:TYR:HD2	1.61	0.65
2:B2:177:VAL:CG1	3:B3:331:LEU:HD22	2.26	0.65
3:B5:257:LEU:HD21	3:B5:314:SER:HB2	1.79	0.65
2:B8:195:LEU:HD21	2:B8:264:ARG:HE	1.61	0.65
3:C9:220:PRO:O	2:D0:326:LYS:HE3	1.96	0.65
2:D0:107:HIS:NE2	2:D0:151:CYS:SG	2.66	0.65
1:13:251:TYR:CE2	2:D4:18:ASN:HB3	2.32	0.65
1:9:241:PHE:CZ	3:C3:356:ILE:HG21	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A5:27:GLU:HA	3:A5:359:LYS:HD2	1.77	0.65
2:C0:220:GLU:HG3	2:C0:220:GLU:O	1.94	0.65
2:C0:274:PRO:HG3	2:C0:286:LEU:HD13	1.77	0.65
2:C4:6:SER:HA	2:C4:136:LEU:HB2	1.78	0.65
2:D8:259:LEU:HD11	2:D8:316:CYS:HB2	1.77	0.65
2:A0:142:GLY:O	2:A0:186:ASN:ND2	2.29	0.65
3:A9:283:ALA:HB2	3:B3:53:GLU:O	1.97	0.65
3:A7:132:GLY:HA3	3:A7:163:ILE:HG22	1.78	0.65
2:B8:241:SER:OG	2:B8:250:VAL:O	2.14	0.65
2:C4:175:PRO:HG3	2:C4:304:LYS:HG2	1.78	0.65
3:D7:68:LEU:HB3	3:D7:96:GLY:HA2	1.78	0.65
2:C4:310:GLY:HA3	2:C4:383:ALA:HB2	1.78	0.65
2:D0:229:ARG:HH11	2:D0:229:ARG:HG3	1.60	0.65
3:E9:208:TYR:CD1	2:F0:326:LYS:HB3	2.31	0.65
1:8:239:LEU:O	3:C1:359:LYS:CE	2.45	0.65
2:B4:223:THR:HG23	2:B4:225:THR:HG22	1.77	0.65
3:C5:354:CYS:SG	3:C5:355:ASP:N	2.68	0.65
2:E6:133:GLN:HG3	2:E6:252:VAL:HG22	1.79	0.65
3:A3:7:VAL:HB	3:A3:135:ILE:HG22	1.79	0.65
3:A3:308:GLY:HA3	3:A3:373:ALA:HB2	1.78	0.65
2:B0:11:GLN:NE2	3:B1:245:GLN:O	2.30	0.65
2:B8:269:LEU:HD12	2:B8:303:ALA:HB3	1.78	0.65
2:D6:33:ASP:O	2:D6:60:LYS:NZ	2.30	0.65
1:11:239:LEU:HG	1:11:240:PRO:HD2	1.78	0.65
3:D5:239:CYS:SG	3:D5:247:ASN:HB3	2.36	0.65
3:A9:256:ASN:HB2	3:A9:350:LYS:HE3	1.79	0.65
3:B3:404:ASP:OD2	3:B3:406:MET:HG2	1.96	0.65
2:D4:176:GLN:CD	3:D5:331:LEU:HD21	2.17	0.65
3:E9:256:ASN:HD21	3:E9:350:LYS:HG2	1.60	0.65
3:A1:117:LEU:HD13	3:A1:154:LYS:NZ	2.12	0.64
2:D6:27:GLU:OE1	2:D6:243:ARG:NH1	2.30	0.64
3:C5:1:MET:N	3:C5:128:ASP:OD2	2.29	0.64
1:10:241:PHE:CZ	3:C9:356:ILE:CG2	2.81	0.64
1:5:253:ALA:CB	2:B4:32:PRO:HG2	2.28	0.64
2:E4:107:HIS:HE2	2:E4:151:CYS:HG	1.37	0.64
3:E9:221:THR:HA	2:F0:325:PRO:CD	2.27	0.64
3:A9:68:LEU:HB3	3:A9:96:GLY:HA2	1.80	0.64
2:B0:73:THR:HA	3:B1:46:ARG:NH1	2.10	0.64
2:D8:79:ARG:HG3	2:D8:92:LEU:HD12	1.78	0.64
1:19:243:ALA:HB2	3:E7:357:PRO:HD2	0.81	0.64
3:A5:284:LEU:HB2	3:A9:55:THR:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:282:TYR:OH	2:B6:33:ASP:OD1	2.13	0.64
3:C3:30:ILE:HD11	3:C3:47:ILE:HD11	1.80	0.64
3:D1:66:MET:CE	3:D1:116:VAL:HG11	2.27	0.64
3:D3:396:HIS:CE1	2:D4:261:PRO:O	2.43	0.64
2:D4:96:LYS:CE	3:D5:128:ASP:HB2	2.27	0.64
3:B3:212:PHE:CZ	2:B4:326:LYS:HG2	2.33	0.64
3:C1:164:MET:HB2	3:C1:197:ASP:H	1.60	0.64
2:C2:406:HIS:CE1	3:C3:261:PRO:HB3	2.32	0.64
2:D0:230:LEU:HD23	2:D0:368:LEU:HD21	1.80	0.64
2:C2:202:VAL:HG22	2:C2:268:MET:HG3	1.78	0.64
3:C5:294:PHE:O	3:C5:306:ARG:NH2	2.27	0.64
2:D0:285:GLN:CB	2:D4:56:THR:HA	2.22	0.64
2:D4:221:ARG:HG2	3:D5:322:SER:HB2	1.79	0.64
2:E6:221:ARG:CG	3:E7:322:SER:HB2	2.28	0.64
3:E9:150:LEU:HD21	3:E9:154:LYS:HZ2	1.63	0.64
1:13:247:TYR:CE2	2:D4:77:GLU:HB3	2.31	0.64
2:A6:168:ASN:HD22	2:A6:194:LEU:HD11	1.63	0.64
3:C5:97:ALA:HB3	3:C5:143:THR:HB	1.80	0.64
2:E4:68:LEU:HD11	2:E4:118:SER:HB2	1.79	0.64
2:A8:22:GLU:OE2	2:A8:229:ARG:NH1	2.30	0.64
3:C3:166:THR:HB	3:C3:199:VAL:HG22	1.79	0.64
2:E0:96:LYS:HZ1	3:E1:129:CYS:N	1.96	0.64
3:A3:186:THR:HG23	3:A3:415:MET:HG3	1.79	0.64
2:D4:210:TYR:HB3	3:D5:324:LYS:CD	2.28	0.64
3:D5:192:LEU:HD21	3:D5:199:VAL:HG11	1.80	0.64
3:E3:2:ARG:HD2	3:E3:240:LEU:HD23	1.79	0.64
1:15:256:LEU:CD1	2:D8:30:ILE:C	2.66	0.63
3:A7:27:GLU:OE2	3:A7:241:ARG:NH2	2.31	0.63
3:B9:267:LEU:HD23	3:B9:374:ILE:HD11	1.80	0.63
3:C5:257:LEU:HD11	3:C5:314:SER:HB3	1.80	0.63
3:E1:176:SER:HB3	2:E2:351:PHE:HB2	1.79	0.63
3:B3:336:LYS:HA	3:B3:336:LYS:CE	2.29	0.63
3:B7:256:ASN:O	3:B7:256:ASN:ND2	2.32	0.63
2:C0:285:GLN:HB2	2:C4:56:THR:HA	1.80	0.63
2:E2:259:LEU:HD21	2:E2:316:CYS:HB2	1.80	0.63
3:E9:221:THR:HA	2:F0:325:PRO:HD2	1.80	0.63
1:12:246:CYS:HB2	3:D3:355:ASP:OD2	1.97	0.63
1:20:253:ALA:HB1	2:E8:32:PRO:HG2	1.79	0.63
2:A6:137:MET:HB3	2:A6:168:ASN:HA	1.80	0.63
2:C2:399:TYR:O	2:C2:402:ARG:NH2	2.30	0.63
2:C4:204:LEU:HD22	2:C4:302:MET:SD	2.38	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C6:136:LEU:HD22	2:C6:167:LEU:HD23	1.79	0.63
2:D0:230:LEU:CD2	2:D0:368:LEU:HD21	2.28	0.63
2:B2:179:THR:N	3:B3:347:ASN:ND2	2.46	0.63
1:16:256:LEU:HD23	2:E0:31:GLN:CG	2.28	0.63
2:A6:22:GLU:OE2	2:A6:229:ARG:NH1	2.32	0.63
2:B0:241:SER:HB2	2:B0:249:ASN:HB2	1.80	0.63
3:B9:332:ASN:OD1	3:B9:336:LYS:NZ	2.32	0.63
2:C6:135:PHE:HD2	2:C6:166:LYS:HG2	1.64	0.63
2:D8:79:ARG:HG2	2:D8:92:LEU:HD12	1.81	0.63
3:A5:132:GLY:HA3	3:A5:163:ILE:HG22	1.79	0.63
2:C4:7:ILE:HG21	2:C4:153:LEU:CD2	2.27	0.63
2:C4:151:CYS:SG	2:C4:193:SER:OG	2.53	0.63
3:F1:239:CYS:SG	3:F1:248:SER:N	2.69	0.63
2:A0:222:PRO:HD2	3:A1:324:LYS:HB3	1.80	0.63
3:A1:207:LEU:HB3	3:A1:225:LEU:HD22	1.81	0.63
3:A3:7:VAL:HG11	3:A3:151:LEU:HD21	1.81	0.63
2:C6:244:PHE:HB2	2:C6:356:ASN:HD21	1.64	0.63
2:D0:90:GLU:HG3	2:D0:121:ARG:HD3	1.81	0.63
2:B4:285:GLN:HB3	2:B8:57:GLY:H	1.63	0.63
2:C6:339:ARG:O	2:C6:342:GLN:NE2	2.32	0.63
3:D1:390:ARG:HG2	3:D1:390:ARG:HH21	1.63	0.63
3:D3:49:VAL:HG21	3:D3:241:ARG:HG2	1.81	0.63
3:D7:153:SER:HB2	3:D7:191:GLN:HE22	1.63	0.63
2:C2:10:GLY:HA2	2:C2:145:THR:HG23	1.81	0.63
2:D2:210:TYR:CD1	3:D3:324:LYS:HD3	2.34	0.63
2:E6:221:ARG:CB	3:E7:322:SER:CB	2.77	0.63
2:E8:292:THR:HG21	2:E8:331:ALA:HB1	1.80	0.63
3:A3:174:LYS:NZ	3:A3:205:GLU:OE1	2.32	0.62
2:B4:254:GLU:OE1	2:B4:352:LYS:NZ	2.32	0.62
3:C1:221:THR:HG22	3:C1:223:GLY:H	1.64	0.62
3:C3:306:ARG:HA	3:C3:340:TYR:HE1	1.64	0.62
2:E4:238:LEU:HD11	2:E4:378:ILE:HG13	1.80	0.62
2:B2:174:SER:OG	2:B2:177:VAL:O	2.17	0.62
3:C3:337:ASN:HB3	3:C3:340:TYR:HB2	1.79	0.62
3:C5:248:SER:HA	3:C5:252:LYS:HE3	1.80	0.62
2:C6:36:MET:HG2	2:C6:36:MET:O	2.00	0.62
2:D0:221:ARG:HB3	3:D1:322:SER:HB2	1.80	0.62
2:D4:177:VAL:HG22	3:D5:331:LEU:HD22	1.81	0.62
3:A3:329:GLN:HA	3:A3:332:ASN:HB2	1.80	0.62
3:A5:313:ALA:HB3	3:A5:349:MET:HG2	1.80	0.62
2:A8:262:TYR:HB3	2:A8:263:PRO:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B8:76:ASP:HA	2:B8:79:ARG:HD2	1.80	0.62
2:C2:221:ARG:HB3	3:C3:322:SER:HB3	1.81	0.62
1:5:256:LEU:HD23	2:B4:31:GLN:CG	2.30	0.62
3:B3:219:THR:HB	2:B4:324:VAL:HG11	1.81	0.62
2:B4:174:SER:OG	2:B4:177:VAL:O	2.17	0.62
3:B5:64:ILE:HD11	3:B5:123:GLU:HG3	1.80	0.62
2:D2:177:VAL:HG11	3:D3:327:ASP:HB3	1.82	0.62
2:F0:407:TRP:HE1	3:F1:258:ILE:HG13	1.64	0.62
1:9:242:ASN:O	3:C3:362:LYS:NZ	2.33	0.62
3:A3:6:HIS:NE2	3:A3:8:GLN:OE1	2.32	0.62
2:B2:11:GLN:HE22	3:B3:246:LEU:CD1	2.13	0.62
3:B9:11:GLN:HA	3:B9:72:THR:HG21	1.81	0.62
3:C3:165:GLU:OE2	3:C3:200:GLN:NE2	2.33	0.62
2:A8:106:GLY:HA3	2:A8:148:GLY:HA3	1.81	0.62
2:C2:76:ASP:OD2	3:C3:46:ARG:NH2	2.30	0.62
3:C9:323:THR:HA	3:C9:326:VAL:HG12	1.81	0.62
3:A5:212:PHE:CB	2:A6:326:LYS:HE2	2.29	0.62
2:B6:50:ASN:O	2:B6:64:ARG:NH2	2.32	0.62
3:D5:7:VAL:HG11	3:D5:151:LEU:CD2	2.28	0.62
2:D6:221:ARG:HA	3:D7:324:LYS:CE	2.29	0.62
3:D7:281:TYR:CE1	3:E1:58:ARG:CZ	2.82	0.62
2:D8:30:ILE:HG22	2:D8:36:MET:HB3	1.82	0.62
3:A1:113:ILE:HG13	3:A1:117:LEU:HD12	1.82	0.62
2:A2:221:ARG:HB2	3:A3:322:SER:OG	2.00	0.62
3:A5:179:VAL:HB	2:A6:351:PHE:O	2.00	0.62
2:B0:11:GLN:HE22	3:B1:246:LEU:HA	1.64	0.62
2:B6:282:TYR:HE2	2:C0:85:HIS:HB3	1.65	0.62
3:C9:16:ILE:HD11	3:C9:229:VAL:HG21	1.82	0.62
2:F0:176:GLN:HG3	3:F1:331:LEU:HD21	1.82	0.62
1:10:244:GLN:H	3:C9:320:ARG:NH1	1.98	0.62
2:A0:3:GLU:OE2	2:A0:64:ARG:NH1	2.33	0.62
2:B8:11:GLN:NE2	3:B9:246:LEU:HD12	2.14	0.62
2:D0:221:ARG:HB3	3:D1:322:SER:CB	2.30	0.62
2:D0:292:THR:HG21	2:D0:331:ALA:HB1	1.80	0.62
3:D7:169:VAL:HG12	3:D7:202:ILE:HB	1.81	0.62
2:B2:177:VAL:HG13	3:B3:331:LEU:HD22	1.81	0.62
3:B7:281:TYR:HD2	3:C1:87:PRO:HD2	1.64	0.62
2:C0:399:TYR:O	2:C0:402:ARG:NH2	2.32	0.62
3:C1:280:GLN:O	3:C5:58:ARG:HD3	1.99	0.62
3:C7:135:ILE:HB	3:C7:166:THR:HG22	1.81	0.62
2:C8:181:VAL:HG12	3:C9:256:ASN:OD1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D6:30:ILE:HG22	2:D6:36:MET:HB3	1.82	0.62
2:E8:274:PRO:HB2	2:E8:276:ILE:HG12	1.82	0.62
2:F0:218:ASP:OD2	2:F0:280:LYS:NZ	2.31	0.62
1:11:255:PRO:HD2	2:D0:364:PRO:CB	2.29	0.61
2:A0:290:GLU:HB2	2:A4:124:LYS:HE2	1.82	0.61
2:B2:286:LEU:O	2:B2:373:ARG:NH1	2.29	0.61
2:C6:31:GLN:NE2	2:C6:33:ASP:OD2	2.33	0.61
3:C9:245:GLN:HB2	3:C9:353:VAL:HG13	1.82	0.61
3:D9:6:HIS:HE1	3:D9:8:GLN:HE21	1.47	0.61
1:8:241:PHE:CZ	3:C1:356:ILE:CG2	2.81	0.61
2:A6:80:THR:HA	2:A6:84:ARG:HH21	1.63	0.61
3:C3:249:ASP:H	3:C3:252:LYS:HB2	1.65	0.61
2:D2:178:SER:OG	3:D3:347:ASN:ND2	2.27	0.61
3:D3:219:THR:HA	2:D4:326:LYS:HE2	1.80	0.61
2:A2:259:LEU:HD21	2:A2:316:CYS:HB2	1.83	0.61
2:A6:214:ARG:NE	3:A7:324:LYS:NZ	2.45	0.61
3:B7:281:TYR:CD2	3:C1:87:PRO:CD	2.83	0.61
2:D2:136:LEU:HD23	2:D2:235:ILE:HD11	1.81	0.61
3:F1:244:GLY:HA2	3:F1:355:ASP:HB2	1.82	0.61
2:A2:91:GLN:HA	2:A2:121:ARG:HH12	1.65	0.61
3:C7:1:MET:N	3:C7:128:ASP:OD2	2.33	0.61
3:C7:165:GLU:OE2	3:C7:200:GLN:NE2	2.33	0.61
2:C8:50:ASN:O	2:C8:64:ARG:NH2	2.32	0.61
2:D0:206:ASN:HD22	2:D0:227:LEU:HD23	1.65	0.61
2:E0:96:LYS:HE2	3:E1:128:ASP:CB	2.29	0.61
3:A5:284:LEU:HB3	3:A9:55:THR:HG21	1.81	0.61
2:A8:209:ILE:HA	2:A8:212:ILE:HG22	1.81	0.61
3:C9:397:TRP:CZ2	2:D0:256:GLN:O	2.53	0.61
3:D3:291:GLN:CG	3:D7:122:LYS:NZ	2.63	0.61
2:E8:301:MET:HE3	2:E8:307:PRO:HG3	1.82	0.61
3:A7:107:THR:OG1	3:A7:108:GLU:OE1	2.18	0.61
2:C2:73:THR:OG1	3:C3:46:ARG:CZ	2.48	0.61
2:D0:223:THR:HG23	2:D0:225:THR:HG22	1.82	0.61
3:D3:248:SER:HA	3:D3:252:LYS:HD3	1.81	0.61
3:D3:397:TRP:CE2	2:D4:256:GLN:O	2.54	0.61
3:D7:49:VAL:HG21	3:D7:241:ARG:HG2	1.83	0.61
2:D8:238:LEU:HD11	2:D8:255:PHE:HE2	1.65	0.61
1:16:256:LEU:HD11	2:E0:30:ILE:O	2.00	0.61
3:D7:139:LEU:HA	3:D7:145:SER:HB2	1.83	0.61
3:A1:130:LEU:O	3:A1:162:ARG:NH1	2.34	0.61
2:A6:214:ARG:HH21	3:A7:324:LYS:NZ	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A7:27:GLU:HA	3:A7:359:LYS:HD2	1.82	0.61
3:C5:133:PHE:HB2	3:C5:164:MET:HB3	1.83	0.61
2:D2:407:TRP:CE2	3:D3:255:VAL:HA	2.35	0.61
2:D8:36:MET:HG2	2:D8:61:HIS:NE2	2.16	0.61
1:11:244:GLN:O	3:D1:355:ASP:OD2	2.19	0.61
1:9:257:PRO:CG	2:C2:26:LEU:HD13	2.29	0.61
2:A0:222:PRO:HD2	3:A1:324:LYS:HG2	1.83	0.61
2:C4:271:SER:HB3	2:C4:377:MET:HB3	1.82	0.61
3:D3:220:PRO:HD2	2:D4:326:LYS:CD	2.30	0.61
2:A2:204:LEU:CD2	2:A2:231:ILE:HD12	2.31	0.60
2:A2:204:LEU:HD23	2:A2:231:ILE:HD12	1.82	0.60
3:B7:281:TYR:CD2	3:C1:87:PRO:HD3	2.35	0.60
3:B7:325:GLU:HA	3:B7:328:GLU:HG3	1.83	0.60
3:C9:232:ALA:HB1	3:C9:268:ILE:HG12	1.83	0.60
3:E5:248:SER:HA	3:E5:252:LYS:HG2	1.83	0.60
2:E6:26:LEU:HD13	2:E6:363:VAL:HG12	1.82	0.60
3:E9:175:VAL:HG23	2:F0:332:VAL:HG11	1.82	0.60
1:13:253:ALA:HB2	2:D4:32:PRO:HG3	1.83	0.60
2:A8:285:GLN:OE1	2:B2:57:GLY:HA2	2.00	0.60
3:C9:7:VAL:HB	3:C9:135:ILE:HG12	1.83	0.60
3:D1:390:ARG:HG2	3:D1:390:ARG:NH2	2.16	0.60
3:D3:238:CYS:SG	3:D3:318:ARG:NE	2.73	0.60
2:E4:119:LEU:HD12	2:E4:156:ARG:CD	2.28	0.60
1:8:243:ALA:CB	3:C1:357:PRO:HD3	2.31	0.60
3:A5:221:THR:HG23	3:A5:223:GLY:H	1.66	0.60
2:B6:213:CYS:HA	2:B6:217:LEU:HD13	1.82	0.60
2:C2:394:LYS:HG2	3:C3:346:PRO:HG3	1.83	0.60
3:D3:220:PRO:CG	2:D4:326:LYS:HD3	2.31	0.60
3:E1:198:GLU:HB2	3:E1:266:PHE:HE2	1.66	0.60
3:E9:10:GLY:HA2	3:E9:143:THR:HG23	1.82	0.60
3:B1:135:ILE:HB	3:B1:166:THR:HG22	1.82	0.60
2:C0:223:THR:HG23	2:C0:225:THR:HG22	1.83	0.60
2:D0:50:ASN:O	2:D0:64:ARG:NH2	2.32	0.60
2:D4:221:ARG:CG	3:D5:322:SER:HB2	2.32	0.60
3:D9:12:CYS:SG	3:D9:13:GLY:N	2.74	0.60
2:E4:283:HIS:NE2	2:E8:85:HIS:O	2.35	0.60
1:5:256:LEU:CD1	2:B4:26:LEU:HD12	2.31	0.60
2:A8:285:GLN:CB	2:B2:56:THR:HA	2.30	0.60
2:B6:230:LEU:HD21	2:B6:368:LEU:HD11	1.84	0.60
3:D3:68:LEU:HB3	3:D3:96:GLY:HA2	1.83	0.60
3:D9:291:GLN:NE2	3:E3:122:LYS:HD2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E6:280:LYS:HE2	2:F0:89:PRO:HD2	1.84	0.60
1:5:248:ARG:NH2	2:B4:77:GLU:HB2	2.17	0.60
3:A9:167:PHE:CE2	3:A9:233:MET:HG2	2.36	0.60
2:B4:223:THR:CG2	2:B4:225:THR:HG22	2.31	0.60
2:C4:387:VAL:HA	2:C4:390:ARG:HH21	1.65	0.60
3:C5:179:VAL:HG22	2:C6:258:ASN:OD1	2.01	0.60
2:D2:328:VAL:HG21	2:D2:355:ILE:HD11	1.83	0.60
3:E7:332:ASN:OD1	3:E7:336:LYS:NZ	2.32	0.60
3:E9:212:PHE:HE1	2:F0:326:LYS:NZ	1.98	0.60
2:A2:207:GLU:HG3	2:A2:304:LYS:HE3	1.84	0.60
3:C9:67:ASP:OD2	3:C9:72:THR:OG1	2.20	0.60
2:D4:97:GLU:HB2	2:D4:110:ILE:CD1	2.26	0.60
3:E5:113:ILE:HD11	3:E5:147:MET:HG3	1.83	0.60
3:A7:117:LEU:HA	3:A7:120:VAL:HG12	1.84	0.60
3:B1:135:ILE:HG13	3:B1:152:ILE:HG12	1.84	0.60
2:C2:250:VAL:HG23	2:C2:352:LYS:HZ3	1.65	0.60
3:D3:202:ILE:HD11	3:D3:268:ILE:HD12	1.84	0.60
3:D7:281:TYR:HE1	3:E1:58:ARG:NH2	2.00	0.60
3:E7:100:ASN:HB3	3:E7:103:LYS:HG2	1.84	0.60
1:17:253:ALA:CB	2:E2:32:PRO:HG2	2.32	0.60
1:5:248:ARG:HH21	2:B4:77:GLU:HB2	1.67	0.60
2:A8:208:ALA:HB2	2:A8:304:LYS:HB2	1.84	0.60
2:B0:73:THR:CB	3:B1:46:ARG:HE	2.14	0.60
3:B5:281:TYR:O	3:B9:54:ALA:HB1	2.01	0.60
2:B6:396:ASP:OD2	2:B6:422:ARG:NH2	2.35	0.60
2:C6:319:TYR:CD1	2:C6:375:VAL:HG22	2.37	0.60
3:D3:175:VAL:HG12	2:D4:336:LYS:HG3	1.83	0.60
3:D5:209:ASP:OD1	3:D5:213:ARG:NH1	2.35	0.60
2:E6:101:ASN:HB3	2:E6:182:VAL:HG11	1.84	0.60
1:21:238:THR:CG2	3:F1:29:GLY:HA2	2.30	0.59
2:A6:241:SER:OG	2:A6:250:VAL:O	2.19	0.59
2:C2:283:HIS:NE2	2:C6:85:HIS:HB3	2.17	0.59
2:A0:88:HIS:HB3	2:A0:91:GLN:HB2	1.84	0.59
2:A0:309:HIS:NE2	2:A0:386:GLU:OE2	2.32	0.59
2:A2:26:LEU:HD22	2:A2:364:PRO:HD3	1.83	0.59
3:C7:354:CYS:SG	3:C7:355:ASP:N	2.75	0.59
3:E3:248:SER:HA	3:E3:252:LYS:HG2	1.84	0.59
2:E4:229:ARG:HD2	2:E4:363:VAL:HG21	1.82	0.59
3:A9:107:THR:OG1	3:A9:108:GLU:OE1	2.20	0.59
2:C4:70:LEU:HD13	2:C4:95:GLY:HA3	1.84	0.59
3:C7:139:LEU:HD13	3:C7:168:SER:HB2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E5:105:HIS:HD2	3:E5:150:LEU:HD22	1.67	0.59
3:A1:140:GLY:O	3:A1:184:ASN:ND2	2.33	0.59
2:A4:191:THR:HA	2:A4:194:LEU:HG	1.84	0.59
2:B6:282:TYR:CE2	2:C0:85:HIS:ND1	2.71	0.59
3:E3:215:LEU:HD21	3:E3:273:LEU:HD22	1.84	0.59
2:E6:71:GLU:HB2	2:E6:98:ASP:HB3	1.84	0.59
2:E8:269:LEU:HD21	2:E8:384:ILE:HD11	1.83	0.59
3:A7:33:THR:O	3:A7:58:ARG:NH2	2.35	0.59
2:C4:2:ARG:CG	2:C4:2:ARG:HD2	2.14	0.59
2:D0:335:ILE:HG23	2:D0:341:ILE:HD13	1.84	0.59
2:F0:269:LEU:HD11	2:F0:384:ILE:HD11	1.84	0.59
3:A3:249:ASP:H	3:A3:252:LYS:HB2	1.65	0.59
3:A7:321:MET:HE1	3:A7:326:VAL:HG22	1.84	0.59
3:B1:238:CYS:SG	3:B1:241:ARG:NH2	2.76	0.59
2:C6:304:LYS:O	2:C6:304:LYS:HD3	2.03	0.59
3:D9:311:LEU:HD12	3:D9:342:VAL:HG11	1.83	0.59
2:E8:311:LYS:HE2	2:E8:344:VAL:HA	1.85	0.59
1:22:247:TYR:OH	2:C6:18:ASN:HB2	2.03	0.59
2:A0:290:GLU:HB3	2:A4:124:LYS:NZ	2.17	0.59
2:A2:195:LEU:HD21	2:A2:264:ARG:HE	1.66	0.59
3:A9:27:GLU:OE2	3:A9:241:ARG:NH1	2.35	0.59
2:B8:109:THR:HG22	2:B8:110:ILE:HG23	1.84	0.59
2:C2:51:THR:HG23	2:C2:52:PHE:HD1	1.66	0.59
3:C5:117:LEU:HD11	3:C5:154:LYS:HB3	1.85	0.59
3:C7:178:THR:OG1	3:C7:181:GLU:OE2	2.21	0.59
3:A1:282:ARG:HA	3:A5:86:ARG:NH1	2.18	0.59
3:A5:397:TRP:CH2	2:A6:256:GLN:HB3	2.38	0.59
2:A6:254:GLU:O	2:A6:258:ASN:ND2	2.36	0.59
2:C0:280:LYS:HA	2:C4:89:PRO:HG2	1.84	0.59
3:D1:283:ALA:HB2	3:D5:53:GLU:O	2.03	0.59
2:D4:210:TYR:CG	3:D5:324:LYS:HD3	2.38	0.59
3:D9:139:LEU:HD12	3:D9:170:PHE:HE1	1.66	0.59
2:E0:163:LYS:HE2	2:E0:163:LYS:CA	2.31	0.59
2:E2:88:HIS:HB3	2:E2:91:GLN:HG2	1.84	0.59
3:E5:256:ASN:HD21	3:E5:350:LYS:HG2	1.67	0.59
3:E9:113:ILE:HA	3:E9:116:VAL:HG12	1.85	0.59
2:B0:53:PHE:HB3	2:B0:61:HIS:HB3	1.83	0.59
3:B5:334:GLN:HE21	3:B5:349:MET:HG2	1.67	0.59
3:C3:68:LEU:HD12	3:C3:143:THR:HG22	1.85	0.59
3:D1:281:TYR:HD2	3:D5:87:PRO:HD3	1.67	0.59
2:D2:182:VAL:HG11	3:D3:255:VAL:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D4:221:ARG:HG3	3:D5:322:SER:CB	2.32	0.59
3:D5:248:SER:HA	3:D5:252:LYS:HG2	1.84	0.59
2:E2:76:ASP:OD1	2:E2:79:ARG:NH2	2.35	0.59
1:23:257:PRO:CG	2:C4:26:LEU:HD12	2.32	0.59
2:A0:132:LEU:HG	2:A0:164:LYS:HE2	1.85	0.59
2:B0:222:PRO:HD2	3:B1:324:LYS:HB3	1.85	0.59
2:E0:229:ARG:HG3	2:E0:229:ARG:NH1	2.18	0.59
2:A6:214:ARG:HE	3:A7:324:LYS:CE	2.16	0.58
2:A8:285:GLN:OE1	2:B2:57:GLY:CA	2.51	0.58
2:B2:177:VAL:HG12	3:B3:331:LEU:HB2	1.83	0.58
3:B9:272:PRO:HG3	3:B9:284:LEU:HD11	1.84	0.58
3:C1:248:SER:HA	3:C1:252:LYS:HG3	1.85	0.58
3:C5:135:ILE:HG12	3:C5:166:THR:HG22	1.85	0.58
2:C8:168:ASN:ND2	2:C8:170:CYS:SG	2.76	0.58
2:D2:217:LEU:HD11	2:D2:275:ILE:HG22	1.85	0.58
2:D4:90:GLU:HB3	2:D4:121:ARG:HD3	1.85	0.58
2:A0:229:ARG:HD3	2:A0:363:VAL:HG21	1.85	0.58
3:A9:263:LEU:H	3:A9:263:LEU:HD23	1.67	0.58
3:B1:237:THR:HG22	3:B1:250:LEU:HD11	1.84	0.58
3:C1:253:LEU:HD11	3:C1:368:VAL:HG21	1.85	0.58
1:15:253:ALA:HB2	2:D8:82:THR:CG2	2.33	0.58
3:B1:171:PRO:O	3:B1:380:ARG:NH1	2.34	0.58
2:B6:329:ASN:HA	2:B6:332:VAL:HG12	1.83	0.58
2:C8:392:ASP:OD1	2:C8:422:ARG:NE	2.35	0.58
3:D3:107:THR:HG21	3:D3:401:GLU:HB2	1.85	0.58
2:D6:286:LEU:O	2:D6:373:ARG:NH1	2.32	0.58
1:21:256:LEU:HD21	2:F0:31:GLN:CG	2.27	0.58
3:A9:73:MET:HG2	3:A9:92:PHE:CE1	2.37	0.58
2:B2:406:HIS:HA	2:B2:409:VAL:HG12	1.85	0.58
2:C2:259:LEU:HD21	2:C2:316:CYS:HB2	1.84	0.58
3:C9:12:CYS:HB3	3:C9:138:SER:HB2	1.85	0.58
3:D9:284:LEU:H	3:E3:55:THR:HB	1.66	0.58
3:E9:305:PRO:HB2	3:E9:310:TYR:HE1	1.68	0.58
1:10:254:LYS:NZ	2:C8:22:GLU:CG	2.65	0.58
1:22:241:PHE:CZ	3:C7:356:ILE:HG23	2.39	0.58
2:A6:119:LEU:HD13	2:A6:122:ILE:HD11	1.85	0.58
3:A9:282:ARG:O	3:B3:55:THR:HG22	2.03	0.58
2:B2:107:HIS:HE2	2:B2:151:CYS:HG	1.49	0.58
2:D2:69:ASP:OD1	2:D2:70:LEU:N	2.36	0.58
2:E4:338:LYS:HZ3	2:E4:340:THR:HG22	1.68	0.58
3:F1:248:SER:OG	3:F1:350:LYS:NZ	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A3:207:LEU:HB3	3:A3:225:LEU:HD22	1.85	0.58
3:A9:220:PRO:HD2	2:B0:326:LYS:HB2	1.85	0.58
2:B2:240:ALA:HB1	2:B2:356:ASN:HD22	1.68	0.58
2:D2:407:TRP:CE3	3:D3:255:VAL:HG22	2.38	0.58
3:A3:117:LEU:HA	3:A3:120:VAL:HG12	1.86	0.58
3:A5:212:PHE:HB2	2:A6:326:LYS:HE2	1.85	0.58
2:C8:386:GLU:OE1	2:C8:390:ARG:NH1	2.37	0.58
2:D2:262:TYR:HB3	2:D2:263:PRO:HD2	1.85	0.58
2:D6:138:PHE:HZ	2:D6:235:ILE:HD12	1.68	0.58
2:D8:276:ILE:HD12	2:D8:281:ALA:HA	1.86	0.58
3:E9:398:TYR:HB3	3:E9:403:MET:HG3	1.84	0.58
1:2:245:SER:OG	2:A8:77:GLU:OE2	2.20	0.58
3:A1:49:VAL:HG11	3:A1:241:ARG:HG2	1.86	0.58
3:A3:7:VAL:HG11	3:A3:151:LEU:CD2	2.34	0.58
2:C0:202:VAL:HA	2:C0:268:MET:HB2	1.86	0.58
3:D7:334:GLN:HE21	3:D7:349:MET:HG2	1.68	0.58
2:E4:71:GLU:HB3	2:E4:98:ASP:HB2	1.85	0.58
3:A9:207:LEU:HB3	3:A9:225:LEU:HD22	1.86	0.58
2:B4:262:TYR:HB3	2:B4:263:PRO:HD2	1.86	0.58
2:B8:175:PRO:HB3	2:B8:390:ARG:HH21	1.69	0.58
2:E2:223:THR:HG23	2:E2:225:THR:HG22	1.84	0.58
1:0:247:TYR:OH	2:A4:81:GLY:HA3	2.04	0.58
1:7:253:ALA:HB2	2:B8:82:THR:HG21	1.86	0.58
3:A1:219:THR:HA	2:A2:326:LYS:HZ2	0.75	0.58
2:A8:151:CYS:SG	2:A8:193:SER:OG	2.57	0.58
3:C3:163:ILE:HD13	3:C3:250:LEU:HB3	1.86	0.58
3:D9:296:ALA:HB2	3:D9:305:PRO:HD2	1.86	0.58
2:E4:422:ARG:HH12	2:E4:426:ALA:HB2	1.68	0.58
3:F1:238:CYS:SG	3:F1:239:CYS:N	2.77	0.58
1:3:248:ARG:NH2	2:B0:82:THR:OG1	2.37	0.57
2:A0:382:THR:HG22	2:A0:382:THR:O	2.04	0.57
2:A2:253:THR:O	2:A2:256:GLN:NE2	2.37	0.57
2:C0:33:ASP:O	2:C0:60:LYS:NZ	2.35	0.57
2:C6:204:LEU:HD13	2:C6:231:ILE:HD12	1.84	0.57
2:D8:222:PRO:HD2	3:D9:324:LYS:HD3	1.86	0.57
2:E8:178:SER:HB3	2:E8:183:GLU:HG3	1.86	0.57
2:E8:191:THR:HG23	2:E8:425:LEU:HD21	1.86	0.57
1:11:244:GLN:HB2	3:D1:320:ARG:NH2	2.19	0.57
2:B8:240:ALA:HB1	2:B8:356:ASN:HD22	1.69	0.57
2:D4:66:VAL:CG2	2:D4:122:ILE:HD11	2.33	0.57
2:E0:259:LEU:HD21	2:E0:316:CYS:HB2	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:15:253:ALA:HB2	2:D8:82:THR:HG21	1.86	0.57
2:B6:53:PHE:HB3	2:B6:61:HIS:HB3	1.86	0.57
2:C4:221:ARG:HB3	3:C5:322:SER:CB	2.35	0.57
2:C6:176:GLN:HB3	3:C7:331:LEU:HD22	1.85	0.57
3:D5:274:THR:OG1	3:D5:279:GLN:OE1	2.23	0.57
2:E0:96:LYS:HE2	3:E1:128:ASP:CG	2.25	0.57
3:E3:180:VAL:O	3:E3:184:ASN:ND2	2.38	0.57
2:E4:107:HIS:NE2	2:E4:151:CYS:SG	2.66	0.57
2:E6:65:CYS:SG	2:E6:66:VAL:N	2.77	0.57
2:A0:174:SER:OG	2:A0:177:VAL:O	2.21	0.57
3:A5:180:VAL:O	3:A5:184:ASN:ND2	2.38	0.57
2:C0:176:GLN:HB3	3:C1:331:LEU:HD21	1.86	0.57
2:D0:241:SER:HB2	2:D0:249:ASN:HB2	1.86	0.57
1:10:241:PHE:HE1	3:C9:356:ILE:CG2	2.18	0.57
3:A5:252:LYS:CE	3:A5:252:LYS:CG	2.79	0.57
2:A8:285:GLN:HB2	2:B2:56:THR:CA	2.30	0.57
2:A8:285:GLN:HG3	2:A8:286:LEU:H	1.69	0.57
3:C3:105:HIS:HE1	3:C3:191:GLN:HE22	1.51	0.57
3:C3:200:GLN:HB3	3:C3:266:PHE:HB2	1.86	0.57
2:C6:407:TRP:CH2	3:C7:258:ILE:HB	2.39	0.57
1:21:250:GLU:OE1	2:F0:225:THR:HG21	2.05	0.57
3:A7:190:HIS:HB2	3:A7:414:ASN:HD22	1.70	0.57
2:A8:102:ASN:HB2	2:A8:105:ARG:HB2	1.86	0.57
2:B6:230:LEU:CD2	2:B6:368:LEU:HD11	2.35	0.57
2:C4:288:VAL:HA	2:C4:291:ILE:HG12	1.86	0.57
2:C6:236:SER:O	2:C6:243:ARG:NH2	2.37	0.57
3:D5:64:ILE:HD11	3:D5:123:GLU:HG3	1.85	0.57
3:E7:389:PHE:HE1	3:E7:395:LEU:HD11	1.69	0.57
1:21:241:PHE:HZ	3:F1:356:ILE:CG2	2.14	0.57
3:B5:396:HIS:HA	3:B5:399:THR:HG22	1.87	0.57
2:D4:96:LYS:HE2	3:D5:128:ASP:HB2	1.86	0.57
3:B5:218:THR:HG23	3:B5:219:THR:HG23	1.87	0.57
2:C8:262:TYR:HB3	2:C8:263:PRO:HD2	1.87	0.57
3:C9:208:TYR:HD1	2:D0:326:LYS:CE	2.14	0.57
3:D5:155:VAL:HG13	3:D5:164:MET:CE	2.35	0.57
3:D5:274:THR:HG21	3:D5:282:ARG:HD3	1.86	0.57
3:D7:213:ARG:HB3	3:D7:297:LYS:HD2	1.87	0.57
3:D9:97:ALA:HA	3:D9:103:LYS:HE2	1.85	0.57
3:E5:113:ILE:HA	3:E5:116:VAL:HG12	1.86	0.57
3:E7:284:LEU:HB3	3:E7:362:LYS:HE3	1.87	0.57
2:A6:296:PHE:CE2	2:A6:335:ILE:HG21	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A7:281:TYR:OH	3:B1:83:GLN:O	2.18	0.57
3:B7:212:PHE:HD1	2:B8:326:LYS:HD3	1.69	0.57
2:C2:168:ASN:HD22	2:C2:198:THR:HG21	1.70	0.57
3:C5:207:LEU:HG	3:C5:228:LEU:HD11	1.86	0.57
3:D9:6:HIS:CE1	3:D9:8:GLN:HE21	2.22	0.57
3:D9:139:LEU:HD11	3:D9:192:LEU:HD13	1.87	0.57
3:E5:169:VAL:HG12	3:E5:202:ILE:HB	1.86	0.57
3:E5:172:SER:OG	3:E5:175:VAL:O	2.22	0.57
2:B6:213:CYS:SG	2:B6:222:PRO:HG3	2.45	0.57
2:B6:262:TYR:HB2	2:B6:265:ILE:HD12	1.87	0.57
2:C2:210:TYR:HE2	3:C3:327:ASP:OD2	1.88	0.57
2:C8:397:LEU:HB3	3:C9:344:TRP:O	2.04	0.57
3:D1:66:MET:HE1	3:D1:116:VAL:HG11	1.87	0.57
2:D8:69:ASP:OD1	2:D8:70:LEU:N	2.37	0.57
2:E8:210:TYR:CB	3:E9:324:LYS:HD3	2.31	0.57
3:F1:210:ILE:HD11	3:F1:298:ASN:HA	1.87	0.57
2:B0:108:TYR:HE2	2:B0:413:MET:HB3	1.70	0.56
3:B5:132:GLY:HA3	3:B5:163:ILE:HG22	1.87	0.56
3:B9:267:LEU:CD2	3:B9:374:ILE:HD11	2.35	0.56
2:C8:176:GLN:HB3	3:C9:331:LEU:CD2	2.33	0.56
3:E3:385:PHE:HE2	3:E3:412:GLU:HB3	1.69	0.56
2:E8:2:ARG:HE	2:E8:133:GLN:HE21	1.53	0.56
3:E9:139:LEU:HD12	3:E9:170:PHE:HE1	1.70	0.56
2:A0:56:THR:HA	3:F1:283:ALA:HB2	1.87	0.56
2:A2:66:VAL:HG21	2:A2:122:ILE:HD11	1.85	0.56
3:A5:318:ARG:HD3	3:A5:358:PRO:HD3	1.87	0.56
3:B5:27:GLU:OE1	3:B5:318:ARG:NH2	2.34	0.56
2:B8:175:PRO:HB3	2:B8:390:ARG:NH2	2.20	0.56
2:B8:406:HIS:HA	2:B8:409:VAL:HG12	1.87	0.56
2:C4:71:GLU:HG2	2:C4:73:THR:HG22	1.88	0.56
2:C6:12:ALA:HB3	2:C6:140:ALA:HB2	1.86	0.56
3:C7:281:TYR:CD2	3:D1:87:PRO:CD	2.71	0.56
2:D0:309:HIS:NE2	2:D0:386:GLU:OE1	2.31	0.56
2:D8:12:ALA:HB3	2:D8:140:ALA:HB2	1.87	0.56
1:8:241:PHE:CZ	3:C1:356:ILE:HG21	2.38	0.56
1:9:257:PRO:HG2	2:C2:26:LEU:O	2.06	0.56
3:A5:27:GLU:OE1	3:A5:241:ARG:NH2	2.38	0.56
2:A6:323:VAL:HG13	2:A6:355:ILE:HG23	1.87	0.56
2:B2:262:TYR:HB3	2:B2:263:PRO:HD2	1.86	0.56
2:B4:56:THR:O	2:B4:60:LYS:HB3	2.05	0.56
2:B4:66:VAL:HG21	2:B4:122:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B9:358:PRO:HG2	3:B9:361:LEU:HD12	1.86	0.56
2:C2:255:PHE:HB3	2:C2:259:LEU:HD12	1.87	0.56
2:C6:121:ARG:HH12	2:C6:124:LYS:HE3	1.71	0.56
3:C7:12:CYS:HB3	3:C7:138:SER:HB3	1.87	0.56
3:D3:129:CYS:SG	3:D3:162:ARG:NH2	2.78	0.56
2:D4:262:TYR:HB3	2:D4:263:PRO:HD2	1.87	0.56
3:D9:283:ALA:HB2	3:E3:54:ALA:HA	1.85	0.56
3:D9:313:ALA:HB3	3:D9:349:MET:HG2	1.88	0.56
3:E3:238:CYS:SG	3:E3:318:ARG:NE	2.78	0.56
2:E6:76:ASP:OD1	2:E6:79:ARG:NH2	2.38	0.56
1:0:244:GLN:H	3:A5:320:ARG:CZ	2.17	0.56
1:9:257:PRO:HG2	2:C2:26:LEU:HA	1.87	0.56
2:A2:285:GLN:OE1	2:A6:57:GLY:O	2.23	0.56
2:C2:76:ASP:HA	2:C2:79:ARG:HD2	1.87	0.56
2:C6:309:HIS:NE2	2:C6:386:GLU:OE1	2.38	0.56
3:C9:309:ARG:H	3:C9:372:THR:HG22	1.71	0.56
3:D1:386:THR:O	3:D1:390:ARG:HG3	2.05	0.56
2:D4:178:SER:H	3:D5:347:ASN:ND2	2.03	0.56
2:D4:274:PRO:HG3	2:D4:286:LEU:CD2	2.32	0.56
3:E1:311:LEU:HD12	3:E1:342:VAL:HG11	1.87	0.56
3:E5:267:LEU:HD12	3:E5:301:CYS:HB3	1.87	0.56
2:E8:181:VAL:HG11	2:E8:404:PHE:CE1	2.40	0.56
1:0:251:TYR:HE2	2:A4:18:ASN:O	1.87	0.56
3:B3:3:GLU:HA	3:B3:49:VAL:HA	1.88	0.56
2:C2:215:ARG:NH2	2:C2:297:GLU:OE2	2.39	0.56
2:C2:267:PHE:O	2:C2:380:ASN:ND2	2.39	0.56
2:D8:210:TYR:HH	3:D9:323:THR:HG1	1.49	0.56
2:E0:221:ARG:HG3	3:E1:322:SER:OG	2.06	0.56
3:E3:100:ASN:HB3	3:E3:103:LYS:HG2	1.88	0.56
2:E6:277:SER:OG	2:E6:278:ALA:N	2.38	0.56
2:F0:80:THR:HA	2:F0:84:ARG:HE	1.69	0.56
2:A4:164:LYS:NZ	2:A4:165:SER:O	2.38	0.56
3:B7:7:VAL:HB	3:B7:135:ILE:HG12	1.87	0.56
3:B7:95:THR:OG1	3:B7:108:GLU:OE2	2.16	0.56
3:D3:176:SER:CB	2:D4:349:THR:HB	2.36	0.56
2:B0:212:ILE:HG12	2:B0:275:ILE:HD11	1.87	0.56
2:C4:277:SER:OG	2:C4:278:ALA:N	2.37	0.56
3:D5:95:THR:OG1	3:D5:108:GLU:OE2	2.22	0.56
2:E4:272:TYR:HB3	2:E4:275:ILE:HD11	1.88	0.56
2:E6:283:HIS:HA	2:F0:60:LYS:HE2	1.87	0.56
2:F0:271:SER:HB2	2:F0:377:MET:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:243:ALA:HA	3:A5:320:ARG:NH1	2.21	0.56
1:13:247:TYR:CD2	2:D4:77:GLU:HB3	2.40	0.56
1:13:248:ARG:NH2	3:D5:42:LEU:HD21	2.20	0.56
2:A2:324:VAL:HG11	2:A2:326:LYS:HZ3	1.71	0.56
3:A5:33:THR:O	3:A5:58:ARG:NH2	2.39	0.56
3:A7:139:LEU:HD12	3:A7:170:PHE:HE1	1.71	0.56
2:A8:221:ARG:HB3	3:A9:322:SER:HB2	1.87	0.56
3:C9:244:GLY:HA2	3:C9:355:ASP:HB2	1.87	0.56
2:D0:397:LEU:HB3	3:D1:344:TRP:O	2.05	0.56
2:E6:100:ALA:HA	3:E7:252:LYS:HD2	1.87	0.56
3:C7:291:GLN:HE22	3:D1:125:GLU:CD	2.08	0.56
3:D7:249:ASP:OD1	3:D7:250:LEU:N	2.38	0.56
2:E0:176:GLN:HB3	3:E1:331:LEU:HD22	1.88	0.56
3:E1:12:CYS:HB3	3:E1:138:SER:HB2	1.88	0.56
2:E4:319:TYR:HB3	2:E4:323:VAL:HG21	1.87	0.56
3:E9:239:CYS:SG	3:E9:248:SER:N	2.76	0.56
2:B2:107:HIS:NE2	2:B2:151:CYS:SG	2.77	0.56
2:B2:269:LEU:HD11	2:B2:384:ILE:HD11	1.87	0.56
3:C3:73:MET:HB3	3:C3:77:ARG:HH22	1.70	0.56
2:C4:309:HIS:NE2	2:C4:386:GLU:OE1	2.39	0.56
2:C4:339:ARG:O	2:C4:342:GLN:NE2	2.39	0.56
3:D1:192:LEU:HD21	3:D1:199:VAL:HG11	1.87	0.56
3:D5:274:THR:CG2	3:D5:282:ARG:HD3	2.36	0.56
3:E1:99:ASN:HD21	2:E2:258:ASN:HD21	1.53	0.56
1:9:255:PRO:HG2	2:C2:364:PRO:HG2	1.88	0.55
3:A5:208:TYR:HB3	2:A6:326:LYS:HD2	1.87	0.55
2:C2:202:VAL:HA	2:C2:268:MET:HB2	1.87	0.55
2:C8:12:ALA:HB3	2:C8:140:ALA:HB2	1.87	0.55
3:D5:49:VAL:HG21	3:D5:241:ARG:HG2	1.87	0.55
3:D7:274:THR:HG21	3:D7:282:ARG:HD2	1.88	0.55
3:A1:12:CYS:HB3	3:A1:138:SER:HB2	1.87	0.55
3:A1:289:LEU:HD21	3:A1:365:VAL:HG11	1.87	0.55
2:A6:109:THR:HG21	2:A6:411:GLU:HB2	1.87	0.55
3:B3:208:TYR:CE1	3:B3:225:LEU:HD11	2.41	0.55
2:B4:285:GLN:HB3	2:B8:57:GLY:N	2.22	0.55
2:B6:274:PRO:HG3	2:B6:286:LEU:HD12	1.87	0.55
3:D3:101:TRP:NE1	3:D3:145:SER:O	2.39	0.55
3:D5:276:ARG:NH2	3:D5:279:GLN:HG3	2.20	0.55
2:E0:244:PHE:HB2	2:E0:356:ASN:HD21	1.70	0.55
1:16:256:LEU:HD21	2:E0:31:GLN:HA	1.89	0.55
2:A2:356:ASN:OD1	2:A2:358:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B5:16:ILE:HD11	3:B5:229:VAL:HG11	1.89	0.55
2:B8:73:THR:HG23	3:B9:46:ARG:NH1	2.22	0.55
2:C6:34:GLY:O	2:C6:61:HIS:N	2.39	0.55
3:D3:117:LEU:HA	3:D3:120:VAL:HG12	1.89	0.55
3:D7:324:LYS:O	3:D7:327:ASP:N	2.39	0.55
2:E0:73:THR:HB	3:E1:46:ARG:HH22	1.71	0.55
3:E5:10:GLY:HA2	3:E5:143:THR:HG23	1.86	0.55
3:E5:334:GLN:OE1	3:E5:348:ASN:ND2	2.38	0.55
3:A5:179:VAL:HG23	2:A6:349:THR:O	2.06	0.55
3:A7:128:ASP:OD1	3:A7:128:ASP:N	2.39	0.55
2:B0:221:ARG:HB2	3:B1:322:SER:CB	2.36	0.55
3:B3:200:GLN:HB3	3:B3:268:ILE:HD11	1.88	0.55
2:C0:207:GLU:HA	2:C0:210:TYR:HB2	1.88	0.55
2:C0:210:TYR:HB3	3:C1:324:LYS:HE3	1.86	0.55
2:C2:404:PHE:CD1	3:C3:259:PRO:HA	2.41	0.55
3:C5:167:PHE:CD2	3:C5:233:MET:HG2	2.41	0.55
2:C6:10:GLY:HA2	2:C6:145:THR:HG23	1.88	0.55
2:D0:34:GLY:O	2:D0:61:HIS:N	2.39	0.55
3:D1:152:ILE:HD13	3:D1:166:THR:HG21	1.89	0.55
2:D4:221:ARG:HG3	3:D5:322:SER:HB3	1.88	0.55
2:E6:283:HIS:CG	2:F0:60:LYS:HE2	2.41	0.55
1:2:257:PRO:CD	2:A8:26:LEU:HD12	2.36	0.55
2:A0:115:VAL:HG21	2:A0:152:LEU:HD22	1.89	0.55
2:B2:120:ASP:OD1	2:B2:123:ARG:NH2	2.39	0.55
2:B8:53:PHE:HB3	2:B8:61:HIS:HB3	1.88	0.55
3:C3:68:LEU:HA	3:C3:93:GLY:HA3	1.88	0.55
3:C5:107:THR:OG1	3:C5:401:GLU:OE2	2.23	0.55
2:D2:30:ILE:HG22	2:D2:36:MET:HB3	1.89	0.55
3:D9:68:LEU:HD23	3:D9:112:LEU:HD13	1.89	0.55
2:E0:276:ILE:HG23	2:E0:280:LYS:HB2	1.89	0.55
3:F1:100:ASN:HB3	3:F1:103:LYS:HG2	1.89	0.55
1:20:241:PHE:CE1	3:E9:356:ILE:HG21	2.34	0.55
1:8:239:LEU:O	3:C1:359:LYS:NZ	2.39	0.55
3:A1:193:VAL:HG12	3:A1:265:PHE:HE2	1.72	0.55
3:A5:94:GLN:O	2:A6:2:ARG:NH2	2.40	0.55
3:A7:200:GLN:HB3	3:A7:268:ILE:HD11	1.89	0.55
3:B9:11:GLN:HG3	3:B9:12:CYS:N	2.22	0.55
2:D4:52:PHE:HD2	2:D4:243:ARG:HD3	1.71	0.55
3:A7:253:LEU:HD21	3:A7:316:MET:SD	2.47	0.55
3:A7:259:PRO:HG2	3:A7:311:LEU:HD21	1.88	0.55
3:A7:282:ARG:O	3:B1:55:THR:CG2	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B3:372:THR:HG21	3:B3:426:GLN:HB3	1.88	0.55
2:B4:282:TYR:OH	2:B8:33:ASP:OD1	2.19	0.55
2:C2:254:GLU:HG2	2:C2:352:LYS:HZ3	1.72	0.55
2:C6:271:SER:HB3	2:C6:377:MET:HB3	1.89	0.55
3:C9:2:ARG:HB3	3:C9:131:GLN:HB2	1.88	0.55
3:D7:282:ARG:O	3:E1:55:THR:HG22	2.06	0.55
3:E1:10:GLY:O	3:E1:14:ASN:ND2	2.39	0.55
3:F1:49:VAL:HG11	3:F1:241:ARG:HG2	1.89	0.55
2:A4:79:ARG:HB3	2:A4:92:LEU:CD1	2.32	0.55
3:A5:257:LEU:HD21	3:A5:314:SER:HB2	1.87	0.55
3:C5:329:GLN:OE1	3:C5:332:ASN:ND2	2.33	0.55
2:D8:2:ARG:HG3	2:D8:51:THR:HG22	1.88	0.55
3:F1:183:TYR:OH	3:F1:388:MET:O	2.22	0.55
3:A9:292:GLN:O	3:A9:298:ASN:ND2	2.40	0.55
2:C4:206:ASN:HA	2:C4:209:ILE:HG22	1.87	0.55
3:D5:321:MET:CE	3:D5:353:VAL:HG22	2.37	0.55
3:D7:322:SER:OG	3:D7:325:GLU:OE2	2.24	0.55
2:E8:101:ASN:HB3	2:E8:182:VAL:HG21	1.87	0.55
2:A2:126:ALA:HB1	2:A2:132:LEU:HD22	1.89	0.55
3:A9:11:GLN:HB2	3:A9:72:THR:HG21	1.89	0.55
3:B9:33:THR:HG23	3:B9:35:THR:HG23	1.88	0.55
3:C1:220:PRO:HG2	2:C2:326:LYS:HB2	1.89	0.55
3:C5:68:LEU:HD12	3:C5:97:ALA:HB2	1.87	0.55
3:C5:350:LYS:NZ	3:C5:352:SER:OG	2.40	0.55
3:D3:21:TRP:HA	3:D3:24:ILE:HG22	1.88	0.55
3:D7:212:PHE:HE1	2:D8:326:LYS:CD	2.18	0.55
3:F1:7:VAL:HB	3:F1:135:ILE:HG12	1.89	0.55
3:F1:117:LEU:HA	3:F1:120:VAL:HG12	1.88	0.55
1:7:253:ALA:HB2	2:B8:82:THR:CG2	2.37	0.54
2:A0:356:ASN:OD1	2:A0:358:GLN:NE2	2.40	0.54
3:A7:73:MET:HG3	3:A7:90:PHE:HD2	1.72	0.54
2:D6:11:GLN:NE2	2:D6:15:GLN:OE1	2.39	0.54
3:F1:358:PRO:HG2	3:F1:361:LEU:HB3	1.88	0.54
2:A8:33:ASP:O	2:A8:60:LYS:NZ	2.40	0.54
3:B1:68:LEU:HB3	3:B1:96:GLY:HA2	1.89	0.54
2:B6:241:SER:HB2	2:B6:249:ASN:HB2	1.89	0.54
2:B8:262:TYR:HB3	2:B8:263:PRO:HD2	1.90	0.54
3:B9:274:THR:HG21	3:B9:279:GLN:HA	1.88	0.54
3:C1:165:GLU:OE2	3:C1:200:GLN:NE2	2.40	0.54
3:D9:135:ILE:HG22	3:D9:137:HIS:HD2	1.72	0.54
2:E0:102:ASN:HB3	2:E0:105:ARG:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E2:319:TYR:HB3	2:E2:323:VAL:HG21	1.90	0.54
3:E7:309:ARG:H	3:E7:372:THR:HG22	1.72	0.54
2:A6:7:ILE:HD11	2:A6:137:MET:HE1	1.89	0.54
2:A6:204:LEU:HD13	2:A6:231:ILE:HD12	1.90	0.54
2:B6:76:ASP:HA	2:B6:79:ARG:HD2	1.89	0.54
2:C6:177:VAL:HG13	3:C7:327:ASP:HB3	1.89	0.54
2:D2:180:ALA:HB1	3:D3:256:ASN:HD21	1.72	0.54
2:D2:210:TYR:HB3	3:D3:324:LYS:HE3	1.88	0.54
2:D4:107:HIS:NE2	2:D4:151:CYS:SG	2.74	0.54
3:F1:139:LEU:HA	3:F1:145:SER:HB2	1.89	0.54
3:F1:200:GLN:HG3	3:F1:268:ILE:HD11	1.90	0.54
2:A6:298:PRO:HG3	2:A6:308:ARG:HH22	1.72	0.54
2:B2:180:ALA:H	3:B3:347:ASN:ND2	2.05	0.54
3:B7:100:ASN:HB3	3:B7:103:LYS:HD3	1.89	0.54
3:C9:179:VAL:HG11	2:D0:258:ASN:O	2.07	0.54
2:D2:98:ASP:O	2:D2:105:ARG:NH2	2.31	0.54
3:D3:291:GLN:HG2	3:D7:122:LYS:HZ1	1.69	0.54
1:11:254:LYS:HD3	2:D0:364:PRO:HD2	1.89	0.54
1:23:257:PRO:HG3	2:C4:26:LEU:HD12	1.89	0.54
1:8:251:TYR:HE1	2:C0:22:GLU:HG2	1.72	0.54
2:A4:291:ILE:HD12	2:A4:375:VAL:HG23	1.89	0.54
2:A8:241:SER:HB2	2:A8:249:ASN:HB2	1.90	0.54
2:C6:26:LEU:HD21	2:C6:363:VAL:HG12	1.88	0.54
3:C7:156:ARG:HG2	3:C7:195:ASN:HB2	1.90	0.54
2:D2:207:GLU:HA	2:D2:210:TYR:HB2	1.89	0.54
2:E0:223:THR:CG2	2:E0:225:THR:HG22	2.38	0.54
2:E6:107:HIS:NE2	2:E6:151:CYS:SG	2.75	0.54
3:E7:190:HIS:HB2	3:E7:414:ASN:HD22	1.73	0.54
1:2:251:TYR:OH	2:A8:18:ASN:CB	2.56	0.54
3:A3:311:LEU:HD12	3:A3:342:VAL:HG11	1.89	0.54
2:B0:283:HIS:O	2:B4:56:THR:CB	2.55	0.54
3:B1:292:GLN:NE2	3:B1:298:ASN:OD1	2.39	0.54
2:B2:174:SER:HB2	2:B2:207:GLU:HG2	1.88	0.54
2:B4:406:HIS:HA	2:B4:409:VAL:HG12	1.90	0.54
2:C0:11:GLN:NE2	2:C0:15:GLN:OE1	2.41	0.54
2:C0:278:ALA:HA	2:C0:369:ALA:HB2	1.88	0.54
2:C6:97:GLU:OE2	2:C6:105:ARG:NH2	2.31	0.54
3:C7:183:TYR:HB3	3:C7:398:TYR:HE2	1.73	0.54
3:C7:262:ARG:NH1	3:C7:421:GLU:OE2	2.40	0.54
2:C8:177:VAL:HG13	3:C9:327:ASP:OD2	2.07	0.54
2:D0:119:LEU:HA	2:D0:122:ILE:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D0:179:THR:OG1	3:D1:246:LEU:CD2	2.55	0.54
2:D0:288:VAL:HA	2:D0:291:ILE:HG12	1.90	0.54
2:D4:210:TYR:CB	3:D5:324:LYS:HD3	2.37	0.54
2:D6:181:VAL:H	3:D7:256:ASN:ND2	2.05	0.54
2:D6:285:GLN:HB2	2:E0:55:GLU:O	2.07	0.54
3:D7:282:ARG:NH1	3:D7:288:GLU:OE2	2.41	0.54
2:E8:236:SER:O	2:E8:243:ARG:NH2	2.38	0.54
3:A1:193:VAL:HG12	3:A1:265:PHE:CE2	2.42	0.54
3:A3:91:VAL:HG21	3:A3:116:VAL:HG12	1.89	0.54
3:B9:311:LEU:HD12	3:B9:342:VAL:HG11	1.89	0.54
2:C8:206:ASN:HD22	2:C8:227:LEU:HD23	1.73	0.54
3:E1:49:VAL:HG21	3:E1:241:ARG:HG2	1.90	0.54
2:E6:181:VAL:HG13	3:E7:350:LYS:HZ1	1.73	0.54
3:E9:220:PRO:HD2	2:F0:326:LYS:CE	2.38	0.54
1:5:256:LEU:HD23	2:B4:31:GLN:HG2	1.88	0.54
2:A0:168:ASN:ND2	2:A0:170:CYS:SG	2.81	0.54
3:A9:345:ILE:O	3:A9:348:ASN:ND2	2.41	0.54
2:B8:283:HIS:HB2	2:C2:88:HIS:CD2	2.43	0.54
2:C2:306:ASP:OD1	2:C2:308:ARG:NH1	2.40	0.54
2:C8:407:TRP:CZ2	3:C9:254:ALA:O	2.60	0.54
3:D1:100:ASN:HB3	3:D1:103:LYS:HG2	1.90	0.54
3:D3:392:LYS:O	2:D4:262:TYR:OH	2.26	0.54
2:D4:96:LYS:HZ3	3:D5:128:ASP:HB2	1.70	0.54
3:D9:412:GLU:O	3:D9:416:ASN:ND2	2.40	0.54
3:E1:2:ARG:HB2	3:E1:131:GLN:HB2	1.90	0.54
3:E3:64:ILE:HD12	3:E3:119:VAL:HG12	1.90	0.54
3:E7:68:LEU:HD12	3:E7:143:THR:HG22	1.90	0.54
3:F1:43:GLN:HA	3:F1:242:PHE:HE1	1.73	0.54
1:0:241:PHE:CZ	3:A5:356:ILE:HG23	2.43	0.54
2:A0:268:MET:N	2:A0:268:MET:SD	2.81	0.54
2:A2:102:ASN:HB2	2:A2:105:ARG:HB2	1.90	0.54
2:A8:71:GLU:HB2	2:A8:98:ASP:OD1	2.08	0.54
3:A9:208:TYR:HE1	3:A9:225:LEU:HD11	1.73	0.54
2:C4:121:ARG:HH22	2:C4:124:LYS:HE3	1.72	0.54
2:C4:236:SER:O	2:C4:243:ARG:NH2	2.39	0.54
2:C6:240:ALA:HB1	2:C6:356:ASN:HD22	1.72	0.54
2:C8:282:TYR:CE2	2:D2:60:LYS:NZ	2.70	0.54
3:D5:13:GLY:HA2	3:D5:16:ILE:HG22	1.89	0.54
2:E0:406:HIS:HA	2:E0:409:VAL:HG12	1.88	0.54
2:E6:217:LEU:HD21	2:E6:367:ASP:HB3	1.89	0.54
1:21:257:PRO:HD3	2:F0:26:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:256:LEU:HD23	2:B4:31:GLN:HG3	1.90	0.54
1:7:256:LEU:HD11	2:B8:31:GLN:N	2.22	0.54
2:A2:174:SER:HB3	2:A2:177:VAL:O	2.07	0.54
2:A4:269:LEU:HB3	2:A4:301:MET:CE	2.38	0.54
2:B0:283:HIS:CD2	2:B4:60:LYS:HE2	2.43	0.54
2:D6:100:ALA:HA	3:D7:252:LYS:HG3	1.89	0.54
2:E6:258:ASN:HB3	2:E6:352:LYS:HE3	1.89	0.54
3:F1:180:VAL:O	3:F1:184:ASN:ND2	2.41	0.54
1:10:246:CYS:N	3:C9:355:ASP:OD2	2.41	0.53
3:A7:180:VAL:O	3:A7:184:ASN:ND2	2.40	0.53
3:B1:260:PHE:HB3	3:B1:261:PRO:HD2	1.90	0.53
3:B9:167:PHE:CZ	3:B9:233:MET:HG2	2.43	0.53
3:C7:237:THR:HG22	3:C7:250:LEU:HD11	1.89	0.53
3:D3:139:LEU:HG	3:D3:168:SER:HB2	1.90	0.53
3:D3:311:LEU:HD23	3:D3:342:VAL:HG11	1.90	0.53
3:D5:238:CYS:SG	3:D5:318:ARG:NE	2.81	0.53
2:D8:407:TRP:CD2	3:D9:255:VAL:HG23	2.43	0.53
2:E4:338:LYS:HZ1	2:E4:341:ILE:HG12	1.73	0.53
3:A1:341:PHE:HB3	3:A1:348:ASN:HD22	1.72	0.53
2:A8:309:HIS:NE2	2:A8:386:GLU:OE1	2.39	0.53
2:B8:306:ASP:OD2	2:B8:308:ARG:NH2	2.39	0.53
3:C1:7:VAL:HB	3:C1:135:ILE:HD13	1.89	0.53
3:D1:385:PHE:CE2	3:D1:412:GLU:HB3	2.43	0.53
2:D2:403:ALA:HB2	3:D3:344:TRP:CZ3	2.43	0.53
2:E0:223:THR:OG1	3:E1:245:GLN:NE2	2.40	0.53
2:E4:279:GLU:OE2	2:E8:89:PRO:HG2	2.08	0.53
2:E6:4:VAL:HG12	2:E6:133:GLN:HB3	1.91	0.53
2:F0:407:TRP:HZ2	3:F1:258:ILE:CD1	2.17	0.53
2:A0:406:HIS:HE1	3:A1:259:PRO:O	1.91	0.53
3:B7:139:LEU:HA	3:B7:145:SER:HB3	1.91	0.53
2:B8:123:ARG:NH1	2:B8:123:ARG:HB3	2.23	0.53
2:C4:274:PRO:HG2	2:C4:371:VAL:HG11	1.90	0.53
2:C6:186:ASN:OD1	2:C6:408:TYR:OH	2.26	0.53
3:D5:213:ARG:HH12	3:D5:297:LYS:HB2	1.72	0.53
2:D8:238:LEU:HD11	2:D8:255:PHE:CE2	2.42	0.53
3:E1:172:SER:HB3	3:E1:205:GLU:HG2	1.90	0.53
3:E5:181:GLU:HB2	3:E5:182:PRO:HD3	1.89	0.53
2:E6:280:LYS:NZ	2:F0:89:PRO:CB	2.68	0.53
3:E7:105:HIS:CD2	3:E7:150:LEU:HB2	2.43	0.53
1:17:253:ALA:HB2	2:E2:32:PRO:HG2	1.91	0.53
2:A4:221:ARG:HB3	3:A5:322:SER:CB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:240:ALA:HB1	2:B4:356:ASN:HD22	1.73	0.53
3:C1:263:LEU:HB2	3:C1:422:TYR:CZ	2.43	0.53
2:D0:168:ASN:ND2	2:D0:170:CYS:SG	2.81	0.53
2:D4:11:GLN:HG3	2:D4:74:VAL:HG21	1.90	0.53
3:E1:318:ARG:HG2	3:E1:354:CYS:HB3	1.91	0.53
2:E4:11:GLN:HE22	3:E5:246:LEU:HA	1.74	0.53
2:E8:12:ALA:HB3	2:E8:140:ALA:HB2	1.90	0.53
2:E8:252:VAL:HA	2:E8:255:PHE:HD2	1.72	0.53
2:F0:209:ILE:HB	2:F0:227:LEU:HD13	1.90	0.53
1:7:256:LEU:CG	2:B8:31:GLN:HB3	2.37	0.53
3:A1:218:THR:O	2:A2:326:LYS:CE	2.50	0.53
2:B4:282:TYR:HD2	2:B4:283:HIS:CE1	2.27	0.53
3:B5:171:PRO:HB3	3:B5:181:GLU:OE1	2.09	0.53
2:C0:286:LEU:O	2:C0:373:ARG:NH1	2.42	0.53
2:C4:287:SER:OG	2:C4:290:GLU:OE1	2.21	0.53
3:C5:6:HIS:CD2	3:C5:134:GLN:HG3	2.43	0.53
2:C6:352:LYS:NZ	2:C6:353:CYS:O	2.40	0.53
2:D4:215:ARG:HH12	2:D4:299:ALA:CB	2.21	0.53
3:F1:113:ILE:HA	3:F1:116:VAL:HG12	1.89	0.53
1:1:254:LYS:CB	2:A6:364:PRO:HB2	2.38	0.53
1:17:247:TYR:HE2	2:E2:82:THR:H	1.56	0.53
1:9:243:ALA:HB1	3:C3:356:ILE:HD13	1.90	0.53
2:A0:136:LEU:HD23	2:A0:167:LEU:HB3	1.89	0.53
3:A1:32:PRO:O	3:A1:83:GLN:NE2	2.41	0.53
2:B2:221:ARG:HG3	2:B2:221:ARG:NH1	2.24	0.53
3:B7:15:GLN:O	3:B7:226:ASN:ND2	2.40	0.53
3:B7:212:PHE:CD1	2:B8:326:LYS:HD3	2.43	0.53
2:B8:278:ALA:HA	2:B8:369:ALA:HB2	1.89	0.53
2:C0:306:ASP:N	2:C0:386:GLU:OE2	2.41	0.53
3:C9:100:ASN:HB3	3:C9:103:LYS:HG2	1.91	0.53
3:D5:100:ASN:ND2	3:D5:397:TRP:O	2.41	0.53
1:20:245:SER:HB3	1:20:248:ARG:HD3	1.91	0.53
3:B3:16:ILE:HD11	3:B3:229:VAL:CG1	2.36	0.53
3:C3:149:THR:O	3:C3:191:GLN:NE2	2.42	0.53
3:C9:174:LYS:NZ	2:D0:329:ASN:O	2.41	0.53
2:D2:96:LYS:NZ	3:D3:128:ASP:HB2	2.23	0.53
2:D4:230:LEU:HD21	2:D4:368:LEU:HD11	1.90	0.53
3:D7:396:HIS:HA	3:D7:399:THR:HG22	1.90	0.53
2:E6:64:ARG:HB3	2:E6:125:LEU:HD21	1.89	0.53
2:E8:396:ASP:OD1	2:E8:422:ARG:NH1	2.42	0.53
2:F0:224:TYR:CD2	3:F1:323:THR:HG21	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A0:180:ALA:HB3	2:A0:183:GLU:HG2	1.90	0.53
2:A4:208:ALA:HA	2:A4:304:LYS:HD3	1.91	0.53
2:A6:174:SER:HB3	2:A6:207:GLU:HG2	1.91	0.53
2:D2:75:VAL:HG11	2:D2:94:SER:HB3	1.90	0.53
2:D6:69:ASP:OD1	2:D6:70:LEU:N	2.41	0.53
2:D8:319:TYR:CD2	2:D8:375:VAL:HG22	2.43	0.53
3:E3:46:ARG:HH21	3:E3:46:ARG:CG	2.22	0.53
3:E7:234:SER:O	3:E7:241:ARG:NH2	2.42	0.53
2:A2:176:GLN:HB3	3:A3:331:LEU:HD22	1.91	0.53
2:A6:79:ARG:NH1	2:A6:94:SER:OG	2.42	0.53
2:C2:265:ILE:HD12	2:C2:432:TYR:CE1	2.44	0.53
3:C3:183:TYR:HB3	3:C3:398:TYR:HE2	1.74	0.53
2:C4:2:ARG:CD	2:C4:2:ARG:CB	2.78	0.53
3:C7:295:ASP:HB3	3:C7:298:ASN:HB2	1.90	0.53
2:C8:141:VAL:HG23	2:C8:170:CYS:HB3	1.91	0.53
3:D1:248:SER:HA	3:D1:252:LYS:HG3	1.91	0.53
3:D3:100:ASN:HB3	3:D3:103:LYS:HB2	1.91	0.53
2:E2:76:ASP:HA	2:E2:79:ARG:HD2	1.90	0.53
2:E4:221:ARG:NH2	3:E5:322:SER:O	2.41	0.53
3:E9:244:GLY:HA2	3:E9:355:ASP:HB2	1.91	0.53
3:A5:317:PHE:CD1	3:A5:365:VAL:HG22	2.43	0.53
2:B2:8:HIS:CE1	2:B2:17:GLY:HA3	2.44	0.53
2:C2:103:PHE:H	2:C2:408:TYR:HE1	1.57	0.53
2:C4:287:SER:HA	2:C4:373:ARG:HH21	1.73	0.53
3:D7:135:ILE:HB	3:D7:166:THR:HG22	1.89	0.53
2:D8:205:ASP:OD1	2:D8:206:ASN:N	2.42	0.53
2:E4:12:ALA:HB3	2:E4:140:ALA:HB2	1.91	0.53
2:E6:222:PRO:HD2	3:E7:324:LYS:CB	2.39	0.53
1:10:239:LEU:HG	1:10:240:PRO:HD2	1.91	0.52
3:A1:77:ARG:HH22	3:A1:92:PHE:HZ	1.56	0.52
3:A5:10:GLY:HA2	3:A5:143:THR:HG23	1.91	0.52
3:A5:105:HIS:CD2	3:A5:150:LEU:HB2	2.44	0.52
2:A6:7:ILE:HD11	2:A6:137:MET:CE	2.38	0.52
3:B9:283:ALA:HB2	3:C3:53:GLU:O	2.08	0.52
3:C3:10:GLY:O	3:C3:14:ASN:ND2	2.42	0.52
2:C4:179:THR:O	3:C5:350:LYS:HD2	2.08	0.52
3:D9:267:LEU:HB3	3:D9:299:MET:HE2	1.90	0.52
2:E8:306:ASP:HB3	2:E8:309:HIS:CE1	2.45	0.52
2:A8:137:MET:SD	2:A8:154:LEU:HD11	2.49	0.52
3:B5:260:PHE:HB3	3:B5:261:PRO:CD	2.37	0.52
3:C1:334:GLN:OE1	3:C1:348:ASN:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C3:35:THR:OG1	3:C3:36:TYR:N	2.41	0.52
3:C5:174:LYS:NZ	2:C6:336:LYS:HB2	2.23	0.52
2:D8:177:VAL:HG11	3:D9:327:ASP:HB3	1.91	0.52
3:E1:164:MET:HB3	3:E1:197:ASP:H	1.73	0.52
3:E1:215:LEU:HB3	3:E1:217:LEU:HD13	1.92	0.52
2:E4:241:SER:HB2	2:E4:249:ASN:HB2	1.89	0.52
3:E5:318:ARG:HG2	3:E5:354:CYS:HB3	1.90	0.52
2:B0:65:CYS:O	2:B0:91:GLN:NE2	2.42	0.52
3:B5:3:GLU:HA	3:B5:49:VAL:HA	1.91	0.52
3:B7:287:PRO:HA	3:B7:290:THR:HG22	1.91	0.52
2:C4:269:LEU:HD11	2:C4:384:ILE:HD11	1.90	0.52
2:C6:277:SER:OG	2:C6:278:ALA:N	2.41	0.52
2:D0:175:PRO:HB3	2:D0:390:ARG:HD3	1.91	0.52
2:D2:11:GLN:NE2	3:D3:245:GLN:O	2.42	0.52
3:D9:7:VAL:HG11	3:D9:151:LEU:HD23	1.90	0.52
3:E5:304:ASP:OD2	3:E5:306:ARG:NH1	2.43	0.52
3:E7:128:ASP:OD1	3:E7:129:CYS:N	2.41	0.52
2:F0:65:CYS:SG	2:F0:66:VAL:N	2.82	0.52
2:A0:18:ASN:HD21	2:A0:78:VAL:HG22	1.74	0.52
2:B2:180:ALA:H	3:B3:347:ASN:HD21	1.58	0.52
3:D7:406:MET:CE	3:D7:406:MET:CA	2.86	0.52
2:D8:204:LEU:HD13	2:D8:231:ILE:HD12	1.90	0.52
2:F0:103:PHE:CD2	2:F0:189:LEU:HB3	2.45	0.52
3:F1:184:ASN:OD1	3:F1:398:TYR:OH	2.24	0.52
1:7:251:TYR:CE2	2:B8:18:ASN:HB3	2.45	0.52
1:9:241:PHE:CZ	3:C3:356:ILE:HG23	2.40	0.52
2:A6:276:ILE:HB	2:A6:280:LYS:HB2	1.91	0.52
2:B0:210:TYR:CB	3:B1:324:LYS:HD2	2.35	0.52
3:B3:18:ALA:HB2	3:B3:76:VAL:HG23	1.90	0.52
2:B6:258:ASN:HB3	2:B6:352:LYS:HG3	1.91	0.52
3:C3:100:ASN:HB3	3:C3:103:LYS:HG2	1.90	0.52
3:C3:113:ILE:HA	3:C3:116:VAL:HG12	1.92	0.52
3:D9:128:ASP:OD1	3:D9:128:ASP:N	2.42	0.52
3:D9:173:PRO:HB3	3:D9:380:ARG:CZ	2.39	0.52
3:D9:238:CYS:SG	3:D9:318:ARG:NE	2.82	0.52
2:E2:79:ARG:NH1	2:E2:92:LEU:O	2.43	0.52
1:11:246:CYS:SG	3:D1:245:GLN:HG2	2.50	0.52
1:18:245:SER:HA	3:E5:355:ASP:OD2	2.09	0.52
3:A9:291:GLN:OE1	3:B3:122:LYS:NZ	2.35	0.52
3:B3:27:GLU:OE2	3:B3:318:ARG:NH2	2.29	0.52
3:B3:283:ALA:HA	3:B7:55:THR:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:282:TYR:CE2	2:B8:85:HIS:HB3	2.40	0.52
2:B6:33:ASP:O	2:B6:60:LYS:NZ	2.42	0.52
3:B9:12:CYS:HB3	3:B9:138:SER:HB2	1.92	0.52
3:C5:311:LEU:HD23	3:C5:342:VAL:HG11	1.90	0.52
2:C8:174:SER:OG	2:C8:177:VAL:O	2.22	0.52
3:C9:7:VAL:HG11	3:C9:66:MET:HE3	1.92	0.52
3:C9:220:PRO:HG2	2:D0:326:LYS:CE	2.39	0.52
3:D1:284:LEU:HB3	3:D5:55:THR:CG2	2.29	0.52
2:E0:96:LYS:HE2	3:E1:128:ASP:OD2	2.09	0.52
2:F0:208:ALA:HB2	2:F0:304:LYS:HB2	1.91	0.52
2:F0:322:ASP:O	2:F0:373:ARG:NH2	2.42	0.52
2:A0:119:LEU:HD11	2:A0:156:ARG:HG2	1.92	0.52
2:A0:339:ARG:O	2:A0:342:GLN:NE2	2.43	0.52
2:B4:188:VAL:HG23	2:B4:425:LEU:HD22	1.92	0.52
2:B6:282:TYR:CE2	2:C0:85:HIS:CG	2.97	0.52
2:B8:50:ASN:O	2:B8:64:ARG:NH2	2.43	0.52
3:D5:330:MET:HG2	3:D5:349:MET:HE2	1.92	0.52
2:E0:221:ARG:CG	3:E1:322:SER:OG	2.58	0.52
3:E3:213:ARG:HH21	3:E3:216:LYS:HE3	1.74	0.52
2:E4:10:GLY:HA2	2:E4:145:THR:HG23	1.92	0.52
2:E8:214:ARG:HH22	2:E8:220:GLU:HG2	1.75	0.52
3:F1:285:SER:N	3:F1:288:GLU:OE2	2.38	0.52
2:A4:28:HIS:CE1	2:A4:243:ARG:HD2	2.45	0.52
2:A6:208:ALA:HB2	2:A6:304:LYS:HG2	1.92	0.52
3:B1:282:ARG:O	3:B5:55:THR:HG22	2.09	0.52
2:B6:179:THR:HG21	3:B7:327:ASP:OD1	2.09	0.52
2:C2:362:VAL:CG1	2:C2:370:LYS:HB3	2.34	0.52
3:C3:69:GLU:HG2	3:C3:71:GLY:H	1.75	0.52
3:C3:380:ARG:HH11	3:C3:381:VAL:HG23	1.75	0.52
3:D1:101:TRP:HD1	3:D1:145:SER:HG	1.56	0.52
2:D4:326:LYS:NZ	2:D4:327:ASP:OD1	2.38	0.52
2:E8:296:PHE:CE2	2:E8:335:ILE:HG21	2.45	0.52
2:F0:176:GLN:HG3	3:F1:331:LEU:CD2	2.40	0.52
2:A0:137:MET:HG3	2:A0:154:LEU:HD12	1.90	0.52
2:A2:324:VAL:HG12	2:A2:326:LYS:H	1.74	0.52
3:A5:6:HIS:HD1	3:A5:21:TRP:HE1	1.57	0.52
3:A7:203:ASP:HB2	3:A7:301:CYS:HA	1.92	0.52
2:A8:285:GLN:N	2:B2:56:THR:CB	2.73	0.52
3:B1:10:GLY:HA2	3:B1:143:THR:HG23	1.91	0.52
3:B5:128:ASP:N	3:B5:128:ASP:OD1	2.42	0.52
2:B6:88:HIS:HB3	2:B6:91:GLN:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B6:306:ASP:OD2	2:B6:308:ARG:NH2	2.40	0.52
2:C4:290:GLU:HA	2:C4:293:ASN:HB2	1.92	0.52
3:D3:239:CYS:SG	3:D3:248:SER:N	2.82	0.52
3:D5:324:LYS:HA	3:D5:327:ASP:HB2	1.91	0.52
2:D8:298:PRO:HB3	2:D8:307:PRO:HD2	1.91	0.52
3:D9:6:HIS:CE1	3:D9:8:GLN:HG2	2.45	0.52
3:E5:309:ARG:H	3:E5:372:THR:HG22	1.75	0.52
3:E7:64:ILE:HD13	3:E7:119:VAL:HG13	1.91	0.52
3:A5:201:VAL:HG13	3:A5:301:CYS:SG	2.50	0.52
2:A8:180:ALA:HA	3:A9:350:LYS:HB3	1.92	0.52
2:A8:241:SER:OG	2:A8:250:VAL:O	2.22	0.52
3:A9:187:LEU:HA	3:A9:190:HIS:CE1	2.45	0.52
3:C1:200:GLN:HG3	3:C1:268:ILE:HD11	1.92	0.52
2:C2:151:CYS:SG	2:C2:193:SER:OG	2.49	0.52
3:C5:68:LEU:HA	3:C5:93:GLY:HA3	1.91	0.52
2:C6:101:ASN:HA	2:C6:144:GLY:CA	2.40	0.52
2:C8:259:LEU:HD21	2:C8:316:CYS:HB2	1.92	0.52
3:D3:7:VAL:HG11	3:D3:151:LEU:HD23	1.90	0.52
2:D8:1:MET:N	2:D8:3:GLU:OE2	2.39	0.52
2:E6:304:LYS:HG3	2:E6:304:LYS:O	2.09	0.52
3:E7:257:LEU:HD21	3:E7:314:SER:HB3	1.91	0.52
2:E8:395:PHE:HZ	2:E8:418:PHE:HB3	1.75	0.52
3:E9:184:ASN:OD1	3:E9:398:TYR:OH	2.26	0.52
3:A1:128:ASP:OD1	3:A1:129:CYS:N	2.43	0.51
3:A5:40:SER:HB3	3:A5:43:GLN:HG3	1.92	0.51
3:B3:210:ILE:O	3:B3:214:THR:OG1	2.27	0.51
2:D2:403:ALA:HB2	3:D3:344:TRP:CH2	2.44	0.51
2:E0:76:ASP:HA	2:E0:79:ARG:HD2	1.92	0.51
3:E9:267:LEU:HB3	3:E9:299:MET:SD	2.50	0.51
1:20:240:PRO:O	3:E9:359:LYS:HG3	2.11	0.51
1:9:243:ALA:HB3	3:C3:356:ILE:CG2	2.28	0.51
3:A3:77:ARG:HH22	3:A3:92:PHE:HZ	1.58	0.51
3:A3:398:TYR:HB3	3:A3:403:MET:HG3	1.92	0.51
2:A8:212:ILE:HG12	2:A8:275:ILE:HD11	1.91	0.51
3:A9:219:THR:C	2:B0:324:VAL:HG11	2.31	0.51
2:B0:115:VAL:HG21	2:B0:152:LEU:HD22	1.92	0.51
3:D3:128:ASP:N	3:D3:128:ASP:OD1	2.41	0.51
3:D3:294:PHE:CD2	3:D3:333:VAL:HG21	2.45	0.51
2:D4:309:HIS:NE2	2:D4:386:GLU:OE1	2.43	0.51
2:D8:395:PHE:HD2	2:D8:422:ARG:HD3	1.75	0.51
3:D9:283:ALA:HB2	3:E3:53:GLU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E5:128:ASP:OD1	3:E5:129:CYS:N	2.43	0.51
3:E5:284:LEU:HD23	3:E5:362:LYS:HG2	1.92	0.51
2:E6:250:VAL:HG21	2:E6:318:MET:SD	2.50	0.51
3:E7:311:LEU:HD12	3:E7:342:VAL:HG11	1.92	0.51
3:E9:121:ARG:NH2	3:E9:158:GLU:OE2	2.43	0.51
1:4:247:TYR:CZ	2:B2:81:GLY:HA3	2.43	0.51
2:A0:315:CYS:HB2	2:A0:351:PHE:CD1	2.46	0.51
3:A1:139:LEU:HD13	3:A1:168:SER:HB2	1.92	0.51
3:A1:205:GLU:HA	3:A1:208:TYR:CD2	2.45	0.51
3:B1:281:TYR:HA	3:B5:54:ALA:HB1	1.91	0.51
3:B3:181:GLU:HB2	3:B3:182:PRO:HD3	1.92	0.51
2:C2:155:GLU:HG2	2:C2:197:HIS:CD2	2.46	0.51
2:D0:191:THR:HG21	2:D0:425:LEU:HD13	1.90	0.51
2:D4:259:LEU:HD21	2:D4:316:CYS:HB2	1.92	0.51
2:D6:298:PRO:HB3	2:D6:307:PRO:HD2	1.92	0.51
3:D7:283:ALA:HB2	3:E1:54:ALA:HA	1.93	0.51
3:D9:107:THR:OG1	3:D9:108:GLU:OE1	2.28	0.51
2:E4:239:THR:OG1	2:E4:243:ARG:NH1	2.43	0.51
3:E5:100:ASN:HB3	3:E5:103:LYS:HG2	1.92	0.51
3:E5:213:ARG:HH12	3:E5:297:LYS:HB3	1.75	0.51
3:F1:375:GLN:HE21	3:F1:379:LYS:HD3	1.74	0.51
1:18:248:ARG:NH1	3:E5:42:LEU:HD21	2.25	0.51
3:A1:210:ILE:HD11	3:A1:228:LEU:HD21	1.91	0.51
2:A8:336:LYS:O	2:A8:339:ARG:NH2	2.43	0.51
3:C1:35:THR:OG1	3:C1:36:TYR:N	2.41	0.51
2:C2:33:ASP:O	2:C2:60:LYS:NZ	2.33	0.51
2:C2:186:ASN:OD1	2:C2:408:TYR:OH	2.27	0.51
3:D1:294:PHE:CD2	3:D1:333:VAL:HG21	2.44	0.51
3:D3:165:GLU:OE2	3:D3:200:GLN:NE2	2.43	0.51
3:D9:139:LEU:HA	3:D9:145:SER:HB2	1.92	0.51
3:E3:213:ARG:NH2	3:E3:216:LYS:HE3	2.25	0.51
3:E7:156:ARG:NH1	3:E7:162:ARG:O	2.42	0.51
1:13:251:TYR:HE2	2:D4:18:ASN:HB3	1.76	0.51
1:16:246:CYS:N	3:E1:320:ARG:HH22	2.08	0.51
1:20:256:LEU:HD21	2:E8:30:ILE:O	2.10	0.51
2:A6:155:GLU:OE1	2:A6:197:HIS:NE2	2.33	0.51
2:B0:79:ARG:HB3	2:B0:92:LEU:HD13	1.91	0.51
3:B7:318:ARG:HD3	3:B7:358:PRO:HD3	1.92	0.51
2:C0:106:GLY:HA3	2:C0:148:GLY:HA3	1.91	0.51
2:C2:217:LEU:HB3	2:C2:219:ILE:HG13	1.92	0.51
3:C3:172:SER:OG	3:C3:205:GLU:OE2	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C4:222:PRO:HD2	3:C5:324:LYS:HB2	1.92	0.51
3:C7:239:CYS:HB3	3:C7:248:SER:O	2.11	0.51
3:C9:137:HIS:HE1	3:C9:166:THR:HB	1.75	0.51
3:C9:347:ASN:OD1	3:C9:349:MET:HB3	2.11	0.51
3:D1:203:ASP:OD2	3:D1:302:ALA:N	2.38	0.51
2:D8:100:ALA:HA	3:D9:252:LYS:HG3	1.92	0.51
2:A4:210:TYR:CE1	2:A4:227:LEU:HD11	2.46	0.51
3:A5:117:LEU:HA	3:A5:120:VAL:HG12	1.92	0.51
3:A5:262:ARG:HD3	3:A5:421:GLU:OE2	2.11	0.51
3:A7:321:MET:CE	3:A7:326:VAL:HG22	2.41	0.51
3:A9:259:PRO:HG2	3:A9:311:LEU:CD2	2.39	0.51
3:C7:100:ASN:HB3	3:C7:103:LYS:HG2	1.93	0.51
3:D3:12:CYS:HB3	3:D3:138:SER:HB2	1.91	0.51
2:D4:221:ARG:CG	3:D5:322:SER:CB	2.89	0.51
2:D6:283:HIS:CD2	2:E0:60:LYS:NZ	2.79	0.51
3:D9:7:VAL:HG11	3:D9:151:LEU:HD21	1.91	0.51
2:E0:176:GLN:HB3	3:E1:331:LEU:CD2	2.41	0.51
2:A0:91:GLN:HA	2:A0:121:ARG:HH12	1.75	0.51
3:A7:139:LEU:HA	3:A7:145:SER:HB2	1.92	0.51
3:B1:16:ILE:HG22	3:B1:226:ASN:OD1	2.10	0.51
2:B4:283:HIS:C	2:B8:56:THR:CB	2.73	0.51
3:B9:49:VAL:HG11	3:B9:241:ARG:HG2	1.92	0.51
2:C4:204:LEU:CD2	2:C4:302:MET:SD	2.98	0.51
2:C6:71:GLU:HB3	2:C6:98:ASP:HB3	1.93	0.51
2:D2:12:ALA:CB	2:D2:140:ALA:HB2	2.37	0.51
2:D2:285:GLN:HB3	2:D6:56:THR:HA	1.92	0.51
3:D7:398:TYR:HB3	3:D7:408:PHE:HZ	1.76	0.51
3:E1:64:ILE:HD12	3:E1:119:VAL:HG12	1.92	0.51
2:E4:422:ARG:NH1	2:E4:426:ALA:HB2	2.26	0.51
2:E6:254:GLU:O	2:E6:258:ASN:ND2	2.44	0.51
3:E7:139:LEU:HA	3:E7:145:SER:HB2	1.93	0.51
3:E7:176:SER:OG	3:E7:181:GLU:OE1	2.28	0.51
2:A4:93:ILE:CG2	2:A4:117:LEU:HD22	2.38	0.51
3:A5:284:LEU:H	3:A9:55:THR:HB	1.74	0.51
2:A8:2:ARG:HG3	2:A8:51:THR:HG22	1.93	0.51
3:B1:2:ARG:NH1	3:B1:249:ASP:OD2	2.43	0.51
3:B9:170:PHE:HE2	3:B9:378:PHE:HE1	1.59	0.51
3:C1:207:LEU:HB3	3:C1:225:LEU:HD22	1.93	0.51
3:C7:140:GLY:O	3:C7:184:ASN:ND2	2.41	0.51
3:D1:10:GLY:HA2	3:D1:143:THR:HG23	1.91	0.51
2:D4:250:VAL:HG22	2:D4:352:LYS:NZ	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D7:397:TRP:NE1	2:D8:257:THR:HA	2.26	0.51
3:E5:281:TYR:CD2	3:E9:86:ARG:HA	2.45	0.51
2:E6:250:VAL:HG12	2:E6:254:GLU:HG2	1.92	0.51
2:E8:80:THR:HG22	2:E8:84:ARG:HH21	1.75	0.51
1:17:247:TYR:CE2	2:E2:81:GLY:HA3	2.46	0.51
2:B2:291:ILE:HD12	2:B2:375:VAL:HG23	1.93	0.51
2:C8:101:ASN:HD22	3:C9:256:ASN:HD21	1.58	0.51
3:C9:66:MET:CE	3:C9:151:LEU:HD22	2.39	0.51
2:D2:269:LEU:HD11	2:D2:384:ILE:HD11	1.92	0.51
2:D8:53:PHE:O	2:D8:64:ARG:NH2	2.44	0.51
2:D8:223:THR:HG23	2:D8:225:THR:H	1.76	0.51
3:F1:30:ILE:HD12	3:F1:51:TYR:HE2	1.76	0.51
3:A3:383:ASP:HA	3:A3:386:THR:HG22	1.93	0.51
2:A6:283:HIS:CD2	2:B0:60:LYS:NZ	2.79	0.51
3:A9:267:LEU:HD21	3:A9:374:ILE:HG22	1.93	0.51
3:C5:7:VAL:HB	3:C5:135:ILE:HG22	1.92	0.51
2:D4:298:PRO:HB3	2:D4:307:PRO:HD2	1.92	0.51
3:D5:289:LEU:HD13	3:D5:365:VAL:HG23	1.92	0.51
2:E4:69:ASP:OD1	2:E4:70:LEU:N	2.44	0.51
3:E7:281:TYR:O	3:F1:54:ALA:HB1	2.11	0.51
2:F0:28:HIS:NE2	2:F0:243:ARG:HD2	2.26	0.51
2:A2:384:ILE:HA	2:A2:387:VAL:HG12	1.93	0.50
3:A5:219:THR:HB	2:A6:324:VAL:HG21	1.93	0.50
2:B0:172:TRP:HB3	2:B0:205:ASP:OD1	2.10	0.50
2:B0:210:TYR:HB3	3:B1:324:LYS:NZ	2.26	0.50
2:B4:286:LEU:O	2:B4:373:ARG:NH1	2.40	0.50
2:C4:12:ALA:CB	2:C4:140:ALA:HB2	2.35	0.50
2:C8:119:LEU:HA	2:C8:122:ILE:HG22	1.93	0.50
3:D9:139:LEU:HD12	3:D9:170:PHE:CE1	2.44	0.50
2:E2:283:HIS:HB3	2:E6:62:VAL:HG11	1.93	0.50
2:E6:221:ARG:HG2	3:E7:322:SER:HG	1.76	0.50
2:A4:245:ASP:N	2:A4:245:ASP:OD1	2.40	0.50
2:C2:261:PRO:HB2	2:C2:262:TYR:CD2	2.47	0.50
2:C6:407:TRP:CZ2	3:C7:258:ILE:HB	2.46	0.50
2:D0:189:LEU:HD11	2:D0:418:PHE:CD1	2.47	0.50
2:D0:275:ILE:HG23	2:D0:368:LEU:HD11	1.93	0.50
3:D7:103:LYS:HB3	3:D7:401:GLU:HG2	1.92	0.50
2:E2:319:TYR:CD1	2:E2:375:VAL:HG22	2.46	0.50
3:E5:112:LEU:HD23	3:E5:112:LEU:O	2.11	0.50
2:F0:239:THR:OG1	2:F0:243:ARG:NH1	2.45	0.50
1:15:256:LEU:CD1	2:D8:31:GLN:N	2.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A3:205:GLU:HA	3:A3:208:TYR:HD2	1.76	0.50
3:A5:175:VAL:HG21	2:A6:329:ASN:O	2.11	0.50
3:A7:278:SER:OG	3:B1:87:PRO:HG2	2.11	0.50
2:B4:9:VAL:HG12	2:B4:68:LEU:HB2	1.93	0.50
3:B7:107:THR:HG21	3:B7:401:GLU:OE2	2.10	0.50
3:C1:68:LEU:HA	3:C1:93:GLY:HA3	1.93	0.50
2:C8:217:LEU:HB3	2:C8:219:ILE:HG13	1.94	0.50
3:D1:12:CYS:HB3	3:D1:138:SER:HB2	1.94	0.50
2:D6:50:ASN:O	2:D6:64:ARG:NH2	2.44	0.50
2:D6:265:ILE:HG22	2:D6:380:ASN:HD21	1.75	0.50
2:E0:88:HIS:HB3	2:E0:91:GLN:HB2	1.93	0.50
2:E0:192:HIS:NE2	2:E0:420:GLU:OE2	2.44	0.50
3:E1:259:PRO:HD2	3:E1:263:LEU:HD11	1.93	0.50
2:E4:221:ARG:CZ	3:E5:322:SER:OG	2.60	0.50
2:E8:268:MET:N	2:E8:268:MET:SD	2.85	0.50
2:B2:208:ALA:HB2	2:B2:304:LYS:HB2	1.94	0.50
2:B8:123:ARG:HB3	2:B8:123:ARG:HH11	1.77	0.50
2:C6:79:ARG:NH1	2:C6:92:LEU:O	2.44	0.50
2:C8:189:LEU:HD11	2:C8:418:PHE:CD1	2.46	0.50
2:D2:134:GLY:HA2	2:D2:164:LYS:HE2	1.93	0.50
3:D3:140:GLY:O	3:D3:184:ASN:ND2	2.42	0.50
2:D4:12:ALA:CB	2:D4:140:ALA:HB2	2.42	0.50
3:D5:93:GLY:HA2	3:D5:112:LEU:HD11	1.94	0.50
3:D5:316:MET:HG3	3:D5:352:SER:HB2	1.92	0.50
2:E0:178:SER:HB3	2:E0:183:GLU:HG2	1.93	0.50
3:E3:153:SER:HB2	3:E3:191:GLN:NE2	2.27	0.50
3:E5:68:LEU:HA	3:E5:93:GLY:HA3	1.93	0.50
2:E8:274:PRO:HG3	2:E8:286:LEU:HD13	1.93	0.50
2:F0:122:ILE:HG21	2:F0:157:LEU:HD21	1.93	0.50
1:14:245:SER:HB2	3:D7:42:LEU:HD11	1.93	0.50
2:A0:222:PRO:HD2	3:A1:324:LYS:CG	2.40	0.50
3:A3:230:SER:HA	3:A3:233:MET:HB3	1.94	0.50
3:A5:128:ASP:OD1	3:A5:129:CYS:N	2.40	0.50
2:A8:238:LEU:HD22	2:A8:255:PHE:CE2	2.46	0.50
2:B0:135:PHE:HD2	2:B0:166:LYS:HG2	1.76	0.50
3:B7:105:HIS:CD2	3:B7:150:LEU:HD12	2.46	0.50
3:B7:281:TYR:CD2	3:C1:87:PRO:HD2	2.44	0.50
2:B8:5:ILE:HD12	2:B8:125:LEU:HD23	1.93	0.50
3:C1:113:ILE:HA	3:C1:116:VAL:HG12	1.93	0.50
2:C6:274:PRO:HG2	2:C6:371:VAL:HG11	1.93	0.50
3:C9:220:PRO:HB2	2:D0:326:LYS:HZ1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D7:406:MET:HA	3:D7:406:MET:HE3	1.92	0.50
3:E5:207:LEU:HB3	3:E5:225:LEU:HD22	1.94	0.50
2:F0:402:ARG:O	3:F1:260:PHE:HE1	1.94	0.50
1:10:241:PHE:CZ	3:C9:356:ILE:HD12	2.44	0.50
1:19:243:ALA:O	3:E7:356:ILE:HD12	2.12	0.50
2:A0:172:TRP:N	2:A0:204:LEU:O	2.45	0.50
2:A6:191:THR:HA	2:A6:194:LEU:HB3	1.94	0.50
2:A6:210:TYR:C	3:A7:324:LYS:NZ	2.65	0.50
2:A8:210:TYR:HB3	3:A9:324:LYS:HE2	1.94	0.50
2:B2:151:CYS:SG	2:B2:193:SER:OG	2.53	0.50
3:B9:43:GLN:HA	3:B9:242:PHE:HE1	1.77	0.50
2:C4:188:VAL:HG13	2:C4:425:LEU:HD23	1.94	0.50
3:C5:91:VAL:HB	3:C5:112:LEU:HD11	1.93	0.50
3:C5:238:CYS:SG	3:C5:239:CYS:N	2.84	0.50
2:C6:288:VAL:HA	2:C6:291:ILE:HG12	1.94	0.50
3:D5:334:GLN:HE22	3:D5:347:ASN:HA	1.76	0.50
2:D6:116:ASP:OD1	2:D6:117:LEU:N	2.44	0.50
3:D9:87:PRO:HA	3:D9:90:PHE:CD1	2.47	0.50
2:E8:151:CYS:SG	2:E8:193:SER:OG	2.55	0.50
3:A3:64:ILE:HD12	3:A3:119:VAL:HG12	1.93	0.50
3:B7:208:TYR:HB3	2:B8:326:LYS:CE	2.41	0.50
3:B7:283:ALA:HA	3:C1:55:THR:HG23	1.94	0.50
2:C2:105:ARG:HG2	2:C2:411:GLU:HG2	1.93	0.50
2:C2:399:TYR:OH	2:C2:415:GLU:OE2	2.30	0.50
3:C9:170:PHE:HD1	3:C9:171:PRO:HD2	1.77	0.50
3:D1:140:GLY:O	3:D1:184:ASN:ND2	2.43	0.50
3:D1:173:PRO:HD3	3:D1:380:ARG:CZ	2.41	0.50
3:D3:155:VAL:HG13	3:D3:164:MET:HE1	1.94	0.50
2:E4:4:VAL:HG21	2:E4:136:LEU:HD13	1.94	0.50
3:E5:94:GLN:HA	2:E6:2:ARG:HH22	1.76	0.50
3:E9:105:HIS:HD2	3:E9:150:LEU:HD12	1.77	0.50
1:2:254:LYS:HD3	2:A8:364:PRO:O	2.12	0.50
2:A0:242:LEU:HD21	2:A0:251:ASP:HB2	1.93	0.50
3:A5:139:LEU:HG	3:A5:168:SER:HB3	1.94	0.50
2:A8:280:LYS:O	2:A8:284:GLU:HG2	2.12	0.50
2:B4:50:ASN:O	2:B4:64:ARG:NH2	2.45	0.50
3:B9:10:GLY:HA2	3:B9:143:THR:HG23	1.94	0.50
3:B9:334:GLN:HE21	3:B9:349:MET:HG2	1.75	0.50
2:C8:285:GLN:HB3	2:D2:56:THR:HA	1.94	0.50
3:C9:167:PHE:HZ	3:C9:236:VAL:HG11	1.76	0.50
2:D2:199:ASP:OD2	2:D2:256:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E0:98:ASP:OD1	2:E0:99:ALA:N	2.45	0.50
3:F1:117:LEU:HB3	3:F1:121:ARG:HH22	1.76	0.50
1:12:257:PRO:CD	2:D2:26:LEU:HD22	2.39	0.50
1:19:243:ALA:CB	3:E7:357:PRO:CD	2.55	0.50
2:A0:103:PHE:HD2	2:A0:189:LEU:HD23	1.75	0.50
2:B2:11:GLN:NE2	3:B3:246:LEU:CD1	2.75	0.50
3:B9:216:LYS:HE2	3:B9:275:SER:HB3	1.94	0.50
3:D3:219:THR:HA	2:D4:326:LYS:CE	2.42	0.50
3:F1:128:ASP:OD1	3:F1:129:CYS:N	2.43	0.50
2:A4:76:ASP:HA	2:A4:79:ARG:HG2	1.93	0.49
3:A7:318:ARG:HD3	3:A7:358:PRO:HD3	1.93	0.49
2:A8:30:ILE:HG21	2:A8:61:HIS:HD2	1.77	0.49
2:B0:209:ILE:HA	2:B0:212:ILE:HG22	1.94	0.49
3:B1:153:SER:HA	3:B1:195:ASN:HD22	1.75	0.49
2:B4:274:PRO:HG3	2:B4:286:LEU:HD12	1.93	0.49
3:B7:404:ASP:OD1	3:B7:405:GLU:N	2.43	0.49
3:D5:114:ASP:N	3:D5:114:ASP:OD1	2.45	0.49
3:E5:163:ILE:HD13	3:E5:250:LEU:HB3	1.94	0.49
2:F0:207:GLU:HA	2:F0:210:TYR:HB2	1.93	0.49
1:0:241:PHE:CE1	3:A5:356:ILE:HG23	2.47	0.49
2:A6:306:ASP:HB3	2:A6:309:HIS:CE1	2.46	0.49
2:A8:27:GLU:OE2	2:A8:243:ARG:NH2	2.44	0.49
2:B0:286:LEU:HD13	2:B0:371:VAL:HG23	1.93	0.49
3:B5:10:GLY:HA2	3:B5:143:THR:HG23	1.95	0.49
3:B9:13:GLY:HA2	3:B9:136:THR:HG22	1.94	0.49
3:C1:113:ILE:HG21	3:C1:154:LYS:CD	2.42	0.49
2:C4:407:TRP:CZ3	3:C5:255:VAL:HG22	2.47	0.49
3:D3:313:ALA:HB1	3:D3:367:PHE:HE1	1.76	0.49
1:21:256:LEU:CD2	2:F0:31:GLN:HA	2.43	0.49
3:A3:52:ASN:ND2	3:A3:123:GLU:OE2	2.42	0.49
2:A6:296:PHE:HE2	2:A6:335:ILE:HG21	1.75	0.49
3:C1:192:LEU:HD11	3:C1:199:VAL:HG11	1.93	0.49
2:C6:177:VAL:HB	2:C6:207:GLU:HB3	1.94	0.49
2:D2:96:LYS:HZ1	3:D3:128:ASP:HB2	1.76	0.49
3:D9:87:PRO:HA	3:D9:90:PHE:HD1	1.77	0.49
1:0:244:GLN:CB	3:A5:320:ARG:NH2	2.69	0.49
2:C0:70:LEU:HD21	2:C0:149:LEU:HD22	1.93	0.49
3:C1:267:LEU:HD23	3:C1:299:MET:HE3	1.94	0.49
2:C4:97:GLU:OE2	2:C4:105:ARG:NH2	2.30	0.49
3:C5:262:ARG:O	3:C5:264:HIS:ND1	2.46	0.49
2:C6:399:TYR:OH	2:C6:415:GLU:OE2	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D4:88:HIS:HB3	2:D4:91:GLN:HG2	1.94	0.49
3:D5:107:THR:OG1	3:D5:108:GLU:N	2.44	0.49
3:D7:152:ILE:HA	3:D7:164:MET:HE1	1.94	0.49
3:D9:260:PHE:HB3	3:D9:261:PRO:CD	2.37	0.49
3:E1:396:HIS:HA	3:E1:399:THR:HG22	1.93	0.49
2:E6:22:GLU:OE1	2:E6:229:ARG:NH1	2.45	0.49
2:E8:107:HIS:NE2	2:E8:151:CYS:SG	2.82	0.49
2:E8:271:SER:HB3	2:E8:377:MET:HB3	1.93	0.49
1:10:244:GLN:H	3:C9:320:ARG:HH11	1.60	0.49
1:21:252:VAL:HG22	1:21:253:ALA:H	1.77	0.49
1:9:241:PHE:CG	3:C3:43:GLN:NE2	2.81	0.49
3:A1:341:PHE:HB3	3:A1:348:ASN:ND2	2.27	0.49
2:A4:422:ARG:HH12	2:A4:426:ALA:HB2	1.78	0.49
3:B1:107:THR:OG1	3:B1:108:GLU:OE1	2.30	0.49
3:B3:68:LEU:HD23	3:B3:112:LEU:HD22	1.92	0.49
3:C7:281:TYR:O	3:D1:86:ARG:CD	2.60	0.49
3:D7:117:LEU:HA	3:D7:120:VAL:HG12	1.94	0.49
2:E2:242:LEU:HD11	2:E2:252:VAL:HG23	1.95	0.49
2:E6:175:PRO:HB3	2:E6:390:ARG:HH21	1.77	0.49
2:E8:10:GLY:HA2	2:E8:145:THR:HG23	1.94	0.49
2:F0:137:MET:O	2:F0:168:ASN:ND2	2.42	0.49
3:F1:262:ARG:NH2	3:F1:421:GLU:OE1	2.46	0.49
1:3:245:SER:HB2	3:B1:42:LEU:HD21	1.94	0.49
3:A1:260:PHE:HB3	3:A1:261:PRO:HD2	1.94	0.49
2:A6:112:LYS:HA	2:A6:115:VAL:HG12	1.95	0.49
3:A9:396:HIS:CE1	2:B0:261:PRO:O	2.65	0.49
2:B8:208:ALA:HB2	2:B8:304:LYS:HB2	1.94	0.49
2:B8:282:TYR:HE2	2:C2:85:HIS:ND1	2.11	0.49
3:B9:281:TYR:CD1	3:C3:58:ARG:HD3	2.47	0.49
2:C2:261:PRO:HB2	2:C2:262:TYR:HD2	1.77	0.49
3:C3:289:LEU:HD12	3:C3:365:VAL:HG12	1.93	0.49
2:C6:251:ASP:N	2:C6:254:GLU:OE2	2.41	0.49
3:D1:10:GLY:O	3:D1:14:ASN:ND2	2.41	0.49
3:D3:293:MET:HG3	3:D3:367:PHE:HB2	1.95	0.49
2:D6:209:ILE:HG21	2:D6:227:LEU:HG	1.94	0.49
3:E1:66:MET:HE2	3:E1:116:VAL:HG21	1.95	0.49
3:F1:19:LYS:NZ	3:F1:223:GLY:O	2.45	0.49
3:A1:105:HIS:CD2	3:A1:150:LEU:HB2	2.48	0.49
2:B4:167:LEU:HD22	2:B4:200:VAL:HB	1.94	0.49
3:B5:63:ALA:O	3:B5:89:ASN:ND2	2.45	0.49
3:C9:334:GLN:HE22	3:C9:348:ASN:N	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D2:214:ARG:HG2	2:D2:214:ARG:HH11	1.77	0.49
3:D5:232:ALA:HB1	3:D5:268:ILE:HG21	1.94	0.49
2:E2:311:LYS:NZ	2:E2:342:GLN:OE1	2.45	0.49
1:16:247:TYR:HB3	2:E0:77:GLU:OE2	2.13	0.49
2:A4:204:LEU:HD13	2:A4:231:ILE:HG12	1.94	0.49
2:A8:172:TRP:HB3	2:A8:205:ASP:OD1	2.13	0.49
3:B5:156:ARG:HD3	3:B5:164:MET:HG2	1.94	0.49
3:C3:270:PHE:O	3:C3:298:ASN:ND2	2.34	0.49
3:D1:180:VAL:O	3:D1:184:ASN:ND2	2.45	0.49
3:D1:284:LEU:CB	3:D5:55:THR:HG21	2.32	0.49
2:D2:98:ASP:OD1	2:D2:99:ALA:N	2.45	0.49
2:D2:259:LEU:HD13	2:D2:268:MET:HE2	1.95	0.49
2:D4:316:CYS:SG	2:D4:352:LYS:HG2	2.52	0.49
3:D7:128:ASP:OD1	3:D7:129:CYS:N	2.40	0.49
2:D8:163:LYS:HD2	2:D8:163:LYS:N	2.23	0.49
2:E4:256:GLN:HE21	2:E4:256:GLN:H	1.59	0.49
1:12:246:CYS:SG	3:D3:245:GLN:HG2	2.52	0.49
3:A5:283:ALA:HB2	3:A9:53:GLU:O	2.12	0.49
3:A7:11:GLN:HA	3:A7:72:THR:HG21	1.95	0.49
3:A7:293:MET:SD	3:A7:365:VAL:HG11	2.52	0.49
3:A9:91:VAL:HG21	3:A9:116:VAL:HG22	1.95	0.49
2:B2:163:LYS:H	2:B2:163:LYS:HD3	1.78	0.49
3:B7:259:PRO:HD2	3:B7:263:LEU:HD11	1.94	0.49
3:B9:354:CYS:SG	3:B9:355:ASP:N	2.86	0.49
2:C0:70:LEU:HD12	2:C0:99:ALA:HB2	1.95	0.49
3:C1:275:SER:OG	3:C1:276:ARG:N	2.46	0.49
3:C5:154:LYS:HB3	3:C5:154:LYS:HE2	1.59	0.49
2:C6:198:THR:O	2:C6:266:HIS:NE2	2.46	0.49
2:D0:2:ARG:HH21	2:D0:133:GLN:NE2	2.11	0.49
2:D4:8:HIS:HD2	2:D4:67:PHE:CE1	2.31	0.49
2:D4:23:LEU:HD11	2:D4:361:THR:HG23	1.94	0.49
3:D7:323:THR:HA	3:D7:326:VAL:HG12	1.95	0.49
2:D8:50:ASN:O	2:D8:64:ARG:NH2	2.46	0.49
3:D9:248:SER:HA	3:D9:252:LYS:HD2	1.94	0.49
2:E0:96:LYS:NZ	3:E1:129:CYS:N	2.61	0.49
3:E1:3:GLU:HA	3:E1:49:VAL:HA	1.94	0.49
2:E2:397:LEU:O	2:E2:397:LEU:HD23	2.12	0.49
3:E3:321:MET:HG2	3:E3:363:MET:SD	2.53	0.49
2:E8:70:LEU:HD12	2:E8:99:ALA:HB2	1.93	0.49
1:19:243:ALA:HB1	3:E7:356:ILE:HA	1.89	0.49
1:7:247:TYR:HE2	2:B8:81:GLY:HA3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A9:225:LEU:HD21	2:B0:326:LYS:HZ2	1.78	0.49
3:B3:248:SER:HA	3:B3:252:LYS:HE2	1.95	0.49
2:D8:5:ILE:HD12	2:D8:125:LEU:HG	1.94	0.49
2:E2:204:LEU:CD2	2:E2:231:ILE:HD12	2.43	0.49
3:E9:212:PHE:CE1	2:F0:326:LYS:NZ	2.72	0.49
2:A0:208:ALA:HB2	2:A0:304:LYS:HB2	1.93	0.48
3:A5:16:ILE:HG22	3:A5:226:ASN:CG	2.33	0.48
3:A7:318:ARG:HH11	3:A7:358:PRO:HD3	1.77	0.48
2:B2:183:GLU:OE2	2:B2:187:SER:OG	2.31	0.48
3:B5:181:GLU:HB2	3:B5:182:PRO:HD3	1.95	0.48
3:B5:330:MET:HE3	3:B5:349:MET:HB3	1.95	0.48
2:C0:1:MET:N	2:C0:129:CYS:SG	2.73	0.48
2:C0:356:ASN:OD1	2:C0:357:TYR:N	2.46	0.48
2:C0:406:HIS:CD2	3:C1:261:PRO:HD3	2.48	0.48
3:C1:73:MET:HB3	3:C1:77:ARG:NH2	2.29	0.48
2:C2:7:ILE:HG22	2:C2:9:VAL:HG23	1.94	0.48
2:C4:2:ARG:HB3	2:C4:133:GLN:NE2	2.26	0.48
2:C8:319:TYR:HB3	2:C8:323:VAL:HG11	1.95	0.48
3:C9:1:MET:N	3:C9:128:ASP:OD2	2.38	0.48
3:D1:189:VAL:HG11	3:D1:415:MET:CE	2.43	0.48
3:D7:208:TYR:HB3	2:D8:326:LYS:HE3	1.95	0.48
3:D7:281:TYR:CE1	3:E1:58:ARG:NH2	2.81	0.48
2:E0:73:THR:CB	3:E1:46:ARG:HH22	2.25	0.48
2:F0:9:VAL:HG13	2:F0:149:LEU:HD23	1.95	0.48
1:22:241:PHE:HZ	3:C7:356:ILE:HG23	1.77	0.48
2:A4:265:ILE:HG23	2:A4:432:TYR:CZ	2.48	0.48
2:A4:310:GLY:HA3	2:A4:383:ALA:HB2	1.95	0.48
2:B6:195:LEU:HD21	2:B6:264:ARG:HE	1.78	0.48
2:C0:103:PHE:H	2:C0:408:TYR:HE1	1.61	0.48
2:C4:79:ARG:NH1	2:C4:92:LEU:O	2.46	0.48
3:C7:164:MET:N	3:C7:197:ASP:OD2	2.41	0.48
2:E0:66:VAL:HG21	2:E0:122:ILE:HD11	1.94	0.48
3:E1:249:ASP:OD1	3:E1:252:LYS:HG2	2.13	0.48
3:E3:49:VAL:HG21	3:E3:241:ARG:HG2	1.95	0.48
2:E4:236:SER:OG	2:E4:243:ARG:NH2	2.46	0.48
3:E9:156:ARG:HH22	3:E9:197:ASP:HB2	1.78	0.48
3:E9:169:VAL:HG12	3:E9:202:ILE:HB	1.94	0.48
3:E9:183:TYR:OH	3:E9:388:MET:O	2.21	0.48
2:F0:274:PRO:HG2	2:F0:371:VAL:HG11	1.95	0.48
1:15:256:LEU:HD12	2:D8:31:GLN:CD	2.34	0.48
3:A7:139:LEU:HG	3:A7:168:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:80:THR:HA	2:B2:84:ARG:HE	1.77	0.48
3:B9:252:LYS:HG3	3:B9:350:LYS:HE3	1.95	0.48
3:C1:101:TRP:NE1	3:C1:145:SER:O	2.39	0.48
2:E2:107:HIS:NE2	2:E2:151:CYS:SG	2.83	0.48
3:E7:274:THR:HG21	3:E7:282:ARG:HD2	1.95	0.48
1:12:241:PHE:CZ	3:D3:356:ILE:HG23	2.48	0.48
2:A4:210:TYR:CB	3:A5:324:LYS:CE	2.83	0.48
2:B0:76:ASP:HA	2:B0:79:ARG:HG2	1.96	0.48
3:B5:73:MET:HA	3:B5:76:VAL:HG12	1.96	0.48
3:C7:407:GLU:HA	3:C7:410:GLU:HB3	1.96	0.48
3:D9:174:LYS:HD2	3:D9:174:LYS:HA	1.79	0.48
1:17:241:PHE:HZ	3:E3:356:ILE:HG23	1.77	0.48
2:A2:407:TRP:HH2	3:A3:254:ALA:HB1	1.78	0.48
2:A4:174:SER:HB3	2:A4:175:PRO:HD2	1.95	0.48
2:A4:221:ARG:HB3	3:A5:322:SER:OG	2.14	0.48
3:A5:238:CYS:SG	3:A5:318:ARG:NE	2.85	0.48
3:B3:283:ALA:HB2	3:B7:53:GLU:O	2.14	0.48
3:B5:97:ALA:HA	3:B5:103:LYS:HE2	1.94	0.48
3:C1:73:MET:HB3	3:C1:77:ARG:HH22	1.77	0.48
3:C1:102:ALA:HB1	3:C1:401:GLU:HB2	1.94	0.48
3:C1:326:VAL:O	3:C1:330:MET:HG2	2.14	0.48
2:C6:51:THR:HG23	2:C6:52:PHE:HD1	1.77	0.48
2:C6:215:ARG:HB2	2:C6:215:ARG:NH1	2.28	0.48
2:D2:282:TYR:O	2:D6:60:LYS:HD3	2.14	0.48
2:D8:241:SER:OG	2:D8:250:VAL:O	2.22	0.48
3:D9:178:THR:O	3:D9:181:GLU:HG2	2.13	0.48
2:E2:392:ASP:OD1	2:E2:422:ARG:NH1	2.46	0.48
1:14:256:LEU:CD1	2:D6:31:GLN:NE2	2.72	0.48
1:7:251:TYR:CZ	2:B8:18:ASN:HB3	2.48	0.48
2:A4:269:LEU:HB3	2:A4:301:MET:HE1	1.94	0.48
2:A6:210:TYR:C	3:A7:324:LYS:HZ1	2.17	0.48
3:B7:208:TYR:HB3	2:B8:326:LYS:HE2	1.96	0.48
2:B8:286:LEU:O	2:B8:373:ARG:NH1	2.36	0.48
2:C6:181:VAL:CB	3:C7:256:ASN:OD1	2.56	0.48
2:D8:2:ARG:HD2	2:D8:133:GLN:HE21	1.78	0.48
3:D9:3:GLU:HA	3:D9:49:VAL:HA	1.94	0.48
3:E9:209:ASP:OD1	3:E9:213:ARG:NH1	2.47	0.48
3:A3:309:ARG:NE	3:A3:339:SER:O	2.46	0.48
3:A9:251:ARG:HG2	3:A9:251:ARG:O	2.13	0.48
3:A9:391:ARG:CZ	3:A9:391:ARG:HB2	2.41	0.48
3:B3:239:CYS:SG	3:B3:248:SER:N	2.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:156:ARG:HA	2:B4:159:VAL:HG12	1.96	0.48
3:C1:281:TYR:O	3:C5:54:ALA:CB	2.49	0.48
2:C6:12:ALA:CB	2:C6:140:ALA:HB2	2.44	0.48
3:C7:281:TYR:CE2	3:D1:87:PRO:HD3	2.43	0.48
3:C9:334:GLN:HE22	3:C9:348:ASN:H	1.61	0.48
3:D1:239:CYS:SG	3:D1:248:SER:N	2.76	0.48
3:D1:379:LYS:HE3	3:D1:419:VAL:HG11	1.96	0.48
2:D8:214:ARG:NH1	3:D9:324:LYS:HE2	2.28	0.48
3:D9:25:SER:HG	3:D9:51:TYR:HH	1.59	0.48
3:D9:318:ARG:HG2	3:D9:354:CYS:HB3	1.95	0.48
2:E4:98:ASP:OD1	2:E4:100:ALA:N	2.40	0.48
2:E6:221:ARG:HD2	3:E7:325:GLU:HB2	1.96	0.48
3:E7:173:PRO:HB2	3:E7:174:LYS:HG3	1.95	0.48
3:E9:66:MET:HG3	3:E9:116:VAL:HG21	1.94	0.48
1:22:246:CYS:HB3	3:C7:245:GLN:HE21	1.79	0.48
2:A0:139:ASN:OD1	2:A0:139:ASN:N	2.46	0.48
2:A0:221:ARG:CG	3:A1:322:SER:OG	2.62	0.48
2:A0:245:ASP:O	2:A0:358:GLN:NE2	2.32	0.48
2:A2:3:GLU:OE1	2:A2:64:ARG:NH1	2.47	0.48
3:A3:135:ILE:HD13	3:A3:152:ILE:HD11	1.95	0.48
3:A7:139:LEU:HD12	3:A7:170:PHE:CE1	2.49	0.48
3:B3:77:ARG:HH22	3:B3:92:PHE:HZ	1.62	0.48
3:B5:313:ALA:HB3	3:B5:349:MET:SD	2.54	0.48
2:B6:178:SER:HB3	3:B7:347:ASN:CG	2.34	0.48
3:B7:311:LEU:HD12	3:B7:342:VAL:HG11	1.95	0.48
2:C0:53:PHE:O	2:C0:64:ARG:NH2	2.46	0.48
2:C0:283:HIS:CD2	2:C4:60:LYS:HE2	2.49	0.48
2:C4:30:ILE:HD13	2:C4:53:PHE:CE2	2.49	0.48
2:D0:177:VAL:HB	3:D1:327:ASP:OD1	2.12	0.48
2:D8:79:ARG:HG3	2:D8:92:LEU:CD1	2.41	0.48
3:E1:317:PHE:HB3	3:E1:321:MET:SD	2.54	0.48
2:E2:224:TYR:HD1	2:E2:227:LEU:HD12	1.79	0.48
2:E4:277:SER:OG	2:E4:278:ALA:N	2.46	0.48
2:E6:12:ALA:HB3	2:E6:140:ALA:HB2	1.96	0.48
3:E7:184:ASN:OD1	3:E7:398:TYR:OH	2.32	0.48
3:E7:186:THR:HG22	3:E7:415:MET:SD	2.53	0.48
3:E9:69:GLU:OE1	2:F0:2:ARG:NH1	2.47	0.48
1:15:257:PRO:CG	2:D8:26:LEU:CD2	2.91	0.48
1:6:244:GLN:NE2	1:6:248:ARG:HB3	2.28	0.48
3:A1:398:TYR:HB3	3:A1:403:MET:HG3	1.95	0.48
3:A5:64:ILE:HD12	3:A5:119:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:183:GLU:HG2	2:B4:184:PRO:HD3	1.95	0.48
2:B8:27:GLU:OE2	2:B8:243:ARG:NH1	2.47	0.48
2:B8:256:GLN:O	2:B8:260:VAL:HG22	2.14	0.48
2:C2:191:THR:HG21	2:C2:425:LEU:HD21	1.94	0.48
2:C6:28:HIS:HE1	2:C6:243:ARG:HD2	1.78	0.48
2:C6:241:SER:HB2	2:C6:249:ASN:HB2	1.95	0.48
2:C8:88:HIS:HB3	2:C8:91:GLN:HB2	1.96	0.48
2:D6:219:ILE:HG22	2:D6:222:PRO:HD3	1.94	0.48
3:D9:239:CYS:SG	3:D9:248:SER:N	2.83	0.48
2:E0:5:ILE:CD1	2:E0:132:LEU:HD11	2.43	0.48
1:9:257:PRO:CG	2:C2:26:LEU:HD12	2.18	0.48
2:A0:221:ARG:CG	3:A1:325:GLU:HB3	2.43	0.48
3:A1:68:LEU:HD12	3:A1:97:ALA:HB2	1.96	0.48
2:A4:328:VAL:O	2:A4:332:VAL:HG23	2.14	0.48
3:B1:383:ASP:HA	3:B1:386:THR:HG22	1.95	0.48
3:C5:6:HIS:HE2	3:C5:136:THR:HG23	1.79	0.48
2:C8:217:LEU:HD13	2:C8:277:SER:HB3	1.96	0.48
2:D4:306:ASP:HB3	2:D4:309:HIS:CE1	2.49	0.48
2:E8:137:MET:HE3	2:E8:154:LEU:HD12	1.96	0.48
3:A1:141:GLY:O	3:A1:184:ASN:ND2	2.39	0.47
2:A6:30:ILE:HG22	2:A6:36:MET:HB3	1.95	0.47
2:A6:174:SER:HB2	2:A6:177:VAL:O	2.13	0.47
3:B1:100:ASN:HB3	3:B1:103:LYS:HG2	1.95	0.47
2:C4:174:SER:HB3	2:C4:177:VAL:O	2.13	0.47
3:C9:53:GLU:OE2	3:C9:54:ALA:N	2.47	0.47
3:D5:307:HIS:ND1	3:D5:376:GLU:OE2	2.45	0.47
3:D5:310:TYR:HD1	3:D5:371:SER:HB2	1.78	0.47
2:D8:75:VAL:CG2	2:D8:92:LEU:HB3	2.44	0.47
2:D8:262:TYR:HB2	2:D8:265:ILE:HD12	1.96	0.47
2:E8:9:VAL:HG22	2:E8:68:LEU:HB3	1.96	0.47
2:E8:319:TYR:HB3	2:E8:323:VAL:HG11	1.95	0.47
1:17:253:ALA:HB1	2:E2:32:PRO:HG2	1.95	0.47
3:B3:257:LEU:HD21	3:B3:314:SER:HB2	1.96	0.47
3:B5:66:MET:HG3	3:B5:116:VAL:HG21	1.96	0.47
2:B6:406:HIS:HA	2:B6:409:VAL:HG12	1.95	0.47
2:B8:73:THR:HA	3:B9:46:ARG:HH22	1.79	0.47
2:C0:181:VAL:HG22	3:C1:256:ASN:CG	2.34	0.47
3:C5:133:PHE:HB2	3:C5:164:MET:CB	2.44	0.47
3:C7:192:LEU:HG	3:C7:199:VAL:HG21	1.95	0.47
2:C8:175:PRO:HB3	2:C8:390:ARG:HD3	1.96	0.47
3:D1:14:ASN:ND2	3:D1:67:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D7:383:ASP:HA	3:D7:386:THR:HG22	1.96	0.47
3:E1:13:GLY:HA2	3:E1:136:THR:HG22	1.95	0.47
3:F1:87:PRO:HA	3:F1:90:PHE:HD1	1.79	0.47
1:16:256:LEU:CD2	2:E0:31:GLN:CG	2.90	0.47
3:A1:208:TYR:CE2	2:A2:329:ASN:ND2	2.82	0.47
2:A2:320:ARG:NH1	2:A2:360:PRO:HA	2.30	0.47
2:A4:306:ASP:HB3	2:A4:309:HIS:CE1	2.50	0.47
2:A6:212:ILE:HG12	2:A6:275:ILE:HD11	1.96	0.47
2:B2:277:SER:OG	2:B2:278:ALA:N	2.47	0.47
3:B3:18:ALA:HB2	3:B3:76:VAL:CG2	2.44	0.47
3:B9:383:ASP:HA	3:B9:386:THR:HG22	1.95	0.47
2:C2:168:ASN:OD1	2:C2:169:PHE:N	2.48	0.47
2:C2:219:ILE:HG22	2:C2:222:PRO:HD3	1.96	0.47
3:C3:141:GLY:O	3:C3:184:ASN:ND2	2.44	0.47
3:C7:385:PHE:HZ	3:C7:408:PHE:HD2	1.61	0.47
2:D0:189:LEU:HD11	2:D0:418:PHE:HD1	1.79	0.47
2:D0:306:ASP:HB3	2:D0:309:HIS:CE1	2.49	0.47
2:D6:309:HIS:NE2	2:D6:386:GLU:OE1	2.47	0.47
3:D9:289:LEU:HD11	3:D9:363:MET:HG2	1.95	0.47
3:F1:207:LEU:HD21	3:F1:225:LEU:HB3	1.95	0.47
1:11:244:GLN:HB2	3:D1:320:ARG:HH22	1.79	0.47
1:13:252:VAL:HA	2:D4:82:THR:HG21	1.97	0.47
1:2:247:TYR:CB	2:A8:77:GLU:OE2	2.58	0.47
2:A0:73:THR:CA	3:A1:46:ARG:HH11	2.26	0.47
2:A4:220:GLU:HG2	2:A4:221:ARG:HG3	1.96	0.47
2:A6:430:LYS:HB2	2:A6:430:LYS:HE2	1.50	0.47
2:C0:2:ARG:NH2	2:C0:133:GLN:OE1	2.38	0.47
3:C3:54:ALA:HB3	3:C3:58:ARG:HG2	1.95	0.47
2:C8:282:TYR:CD2	2:D2:60:LYS:NZ	2.72	0.47
2:D4:221:ARG:HG2	2:D4:221:ARG:O	2.13	0.47
3:D5:239:CYS:SG	3:D5:248:SER:N	2.87	0.47
2:D6:283:HIS:CD2	2:E0:60:LYS:HZ1	2.31	0.47
3:D7:292:GLN:O	3:D7:298:ASN:ND2	2.46	0.47
2:E0:181:VAL:HG23	3:E1:347:ASN:O	2.14	0.47
3:E1:19:LYS:HD2	3:E1:227:HIS:ND1	2.28	0.47
2:E6:8:HIS:ND1	2:E6:65:CYS:SG	2.87	0.47
2:E6:111:GLY:O	2:E6:115:VAL:HG23	2.14	0.47
3:E7:389:PHE:CE1	3:E7:395:LEU:HD11	2.48	0.47
1:12:254:LYS:HD3	2:D2:364:PRO:O	2.15	0.47
1:21:239:LEU:HB3	1:21:240:PRO:HD2	1.97	0.47
1:21:256:LEU:CD1	2:F0:37:PRO:HG3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A1:12:CYS:CB	3:A1:138:SER:HB2	2.44	0.47
3:A3:8:GLN:HE22	3:A3:17:GLY:HA3	1.79	0.47
2:A4:119:LEU:HD13	2:A4:122:ILE:HD11	1.96	0.47
3:A7:200:GLN:HG2	3:A7:268:ILE:HD11	1.96	0.47
2:B2:252:VAL:HA	2:B2:255:PHE:HD2	1.78	0.47
2:B6:265:ILE:HG23	2:B6:432:TYR:CZ	2.49	0.47
3:C1:105:HIS:CE1	3:C1:150:LEU:HD13	2.50	0.47
3:C1:274:THR:OG1	3:C1:282:ARG:NE	2.44	0.47
3:C5:196:ALA:O	3:C5:264:HIS:NE2	2.46	0.47
3:C7:321:MET:N	3:C7:321:MET:SD	2.88	0.47
3:C9:64:ILE:HG12	3:C9:119:VAL:HG12	1.96	0.47
2:D2:298:PRO:HB3	2:D2:307:PRO:HD2	1.97	0.47
3:D5:127:CYS:SG	3:D5:128:ASP:N	2.82	0.47
3:D5:323:THR:O	3:D5:327:ASP:N	2.46	0.47
3:D7:179:VAL:HG11	2:D8:258:ASN:O	2.15	0.47
3:D9:27:GLU:OE2	3:D9:241:ARG:NH1	2.44	0.47
2:E2:11:GLN:HE22	3:E3:246:LEU:CD1	2.27	0.47
2:E4:221:ARG:NH2	3:E5:322:SER:OG	2.47	0.47
2:E6:290:GLU:OE1	2:F0:124:LYS:HE3	2.14	0.47
3:E7:382:SER:OG	3:E7:412:GLU:OE1	2.32	0.47
2:E8:329:ASN:HA	2:E8:332:VAL:HG12	1.95	0.47
1:10:247:TYR:CG	2:C8:77:GLU:OE2	2.67	0.47
3:A3:192:LEU:HG	3:A3:199:VAL:HG21	1.97	0.47
3:A5:183:TYR:HB3	3:A5:398:TYR:HE2	1.80	0.47
3:C1:135:ILE:HG22	3:C1:137:HIS:HD2	1.79	0.47
3:C1:219:THR:HB	2:C2:324:VAL:HG11	1.96	0.47
2:C2:251:ASP:OD1	2:C2:254:GLU:N	2.47	0.47
2:C6:304:LYS:HD3	2:C6:304:LYS:C	2.35	0.47
3:C7:66:MET:HB3	3:C7:91:VAL:HG23	1.96	0.47
3:C9:25:SER:HG	3:C9:81:PHE:HE2	1.63	0.47
3:C9:283:ALA:HB2	3:D3:53:GLU:O	2.14	0.47
2:D0:298:PRO:HB3	2:D0:307:PRO:HD2	1.96	0.47
3:D1:238:CYS:SG	3:D1:318:ARG:NE	2.86	0.47
2:E2:251:ASP:OD1	2:E2:254:GLU:HG2	2.14	0.47
3:E3:213:ARG:NE	3:E3:213:ARG:HA	2.29	0.47
2:E8:234:VAL:HG21	2:E8:302:MET:HE1	1.96	0.47
2:E8:265:ILE:HD12	2:E8:432:TYR:CE1	2.50	0.47
1:21:251:TYR:HE1	2:F0:225:THR:HG1	1.62	0.47
2:A0:315:CYS:HB2	2:A0:351:PHE:HD1	1.78	0.47
2:A2:284:GLU:HG2	2:A2:286:LEU:HD22	1.95	0.47
2:A4:135:PHE:CE2	2:A4:157:LEU:HD12	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A5:267:LEU:HD11	3:A5:371:SER:HB3	1.96	0.47
2:A8:277:SER:OG	2:A8:278:ALA:N	2.47	0.47
2:B0:138:PHE:HZ	2:B0:235:ILE:HD12	1.80	0.47
2:B0:223:THR:OG1	2:B0:225:THR:HG22	2.15	0.47
3:B1:16:ILE:HG22	3:B1:226:ASN:CG	2.35	0.47
3:B3:176:SER:HB2	2:B4:349:THR:CG2	2.41	0.47
2:B6:52:PHE:HD2	2:B6:243:ARG:HD3	1.78	0.47
2:B6:72:PRO:HG2	3:B7:46:ARG:NH1	2.29	0.47
3:B7:28:HIS:ND1	3:B7:43:GLN:O	2.45	0.47
2:B8:26:LEU:HD21	2:B8:364:PRO:HD3	1.96	0.47
2:B8:88:HIS:HB3	2:B8:91:GLN:HG3	1.96	0.47
3:C1:215:LEU:HD21	3:C1:273:LEU:HD22	1.95	0.47
3:C1:382:SER:O	3:C1:386:THR:N	2.43	0.47
2:C4:18:ASN:O	2:C4:22:GLU:HG2	2.15	0.47
2:C8:1:MET:N	2:C8:129:CYS:SG	2.80	0.47
2:C8:7:ILE:HG23	2:C8:66:VAL:HG23	1.97	0.47
2:C8:70:LEU:HD12	2:C8:145:THR:HG22	1.96	0.47
2:C8:170:CYS:HB2	2:C8:203:MET:HE1	1.97	0.47
2:C8:370:LYS:HG3	2:C8:370:LYS:O	2.14	0.47
2:D0:245:ASP:OD1	2:D0:245:ASP:N	2.48	0.47
3:D1:189:VAL:HG11	3:D1:415:MET:HE2	1.96	0.47
2:D2:33:ASP:OD1	2:D2:34:GLY:N	2.48	0.47
2:D2:210:TYR:HB3	3:D3:324:LYS:CE	2.45	0.47
2:D6:222:PRO:HD2	3:D7:324:LYS:HZ2	1.80	0.47
3:D7:2:ARG:HH11	3:D7:240:LEU:HD22	1.79	0.47
2:D8:174:SER:HB2	2:D8:177:VAL:O	2.13	0.47
3:D9:155:VAL:HG13	3:D9:164:MET:CE	2.45	0.47
3:E1:7:VAL:HB	3:E1:135:ILE:HG13	1.97	0.47
3:E1:33:THR:HG23	3:E1:35:THR:HG23	1.97	0.47
2:E2:274:PRO:HB2	2:E2:276:ILE:HG12	1.96	0.47
2:E2:277:SER:OG	2:E2:278:ALA:N	2.48	0.47
2:E4:210:TYR:CE1	2:E4:227:LEU:HD21	2.49	0.47
3:E5:344:TRP:CE3	3:E5:345:ILE:HG13	2.50	0.47
2:E6:286:LEU:O	2:E6:373:ARG:NH1	2.44	0.47
2:F0:329:ASN:HA	2:F0:332:VAL:HG12	1.97	0.47
2:F0:367:ASP:OD1	2:F0:367:ASP:N	2.48	0.47
3:F1:20:PHE:HA	3:F1:230:SER:HB2	1.96	0.47
1:11:251:TYR:CE2	2:D0:18:ASN:ND2	2.82	0.47
1:22:243:ALA:HB1	3:C7:357:PRO:HD2	1.94	0.47
2:A0:133:GLN:O	2:A0:165:SER:OG	2.33	0.47
2:A0:323:VAL:HG11	2:A0:328:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:6:SER:OG	2:A2:8:HIS:NE2	2.48	0.47
2:A8:53:PHE:HB3	2:A8:61:HIS:HB3	1.97	0.47
2:B0:241:SER:OG	2:B0:250:VAL:O	2.26	0.47
2:B4:392:ASP:OD1	2:B4:422:ARG:NE	2.47	0.47
2:C4:405:VAL:HG13	2:C4:418:PHE:HE2	1.79	0.47
3:C5:209:ASP:CG	3:C5:213:ARG:HH21	2.17	0.47
3:C7:91:VAL:HG21	3:C7:116:VAL:HG12	1.96	0.47
3:D1:211:CYS:HA	3:D1:215:LEU:HB2	1.96	0.47
2:D6:269:LEU:HD23	2:D6:301:MET:HG2	1.96	0.47
2:E4:27:GLU:HB3	2:E4:361:THR:HG21	1.97	0.47
3:E5:211:CYS:SG	3:E5:220:PRO:HB3	2.55	0.47
1:12:256:LEU:HA	2:D2:26:LEU:HD22	1.97	0.47
1:8:257:PRO:CB	2:C0:29:GLY:HA2	2.45	0.47
1:9:243:ALA:CB	3:C3:357:PRO:CD	2.75	0.47
3:A1:13:GLY:HA2	3:A1:16:ILE:HG22	1.96	0.47
2:B8:282:TYR:CE2	2:C2:85:HIS:HB3	2.50	0.47
3:C1:139:LEU:HA	3:C1:145:SER:HB2	1.96	0.47
2:C6:101:ASN:HA	2:C6:144:GLY:HA3	1.95	0.47
3:C7:403:MET:HB3	3:C7:408:PHE:HE1	1.79	0.47
3:D3:155:VAL:HG13	3:D3:164:MET:CE	2.44	0.47
2:D6:269:LEU:CD1	2:D6:384:ILE:HD11	2.44	0.47
2:E8:210:TYR:CG	3:E9:324:LYS:HD3	2.49	0.47
1:7:244:GLN:HE22	1:7:249:SER:N	2.13	0.47
2:A0:26:LEU:HD22	2:A0:364:PRO:HD3	1.97	0.47
2:A0:290:GLU:HB3	2:A4:124:LYS:HZ1	1.80	0.47
2:A2:103:PHE:H	2:A2:408:TYR:HE1	1.63	0.47
2:A6:367:ASP:OD1	2:A6:367:ASP:N	2.48	0.47
3:A9:163:ILE:HD13	3:A9:250:LEU:HB3	1.97	0.47
3:B3:6:HIS:CE1	3:B3:20:PHE:CD2	3.03	0.47
2:B6:339:ARG:NH1	2:B6:342:GLN:OE1	2.47	0.47
3:B7:280:GLN:O	3:C1:58:ARG:HD3	2.14	0.47
3:B7:326:VAL:O	3:B7:330:MET:HG2	2.15	0.47
2:B8:1:MET:N	2:B8:129:CYS:SG	2.86	0.47
2:C0:286:LEU:HD12	2:C0:371:VAL:HG12	1.97	0.47
3:C1:279:GLN:HG3	3:C1:282:ARG:NH1	2.30	0.47
2:C2:9:VAL:HG22	2:C2:68:LEU:HB2	1.96	0.47
3:C5:220:PRO:HD2	2:C6:326:LYS:HB2	1.97	0.47
2:C8:98:ASP:O	2:C8:105:ARG:NH2	2.48	0.47
3:C9:336:LYS:HB3	3:C9:336:LYS:HE3	1.60	0.47
2:D0:156:ARG:HG2	2:D0:156:ARG:HH21	1.79	0.47
3:D5:152:ILE:HA	3:D5:155:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D5:156:ARG:HH22	3:D5:197:ASP:HB2	1.80	0.47
2:D6:276:ILE:HD12	2:D6:281:ALA:HA	1.97	0.47
2:E0:97:GLU:OE2	3:E1:251:ARG:NH1	2.43	0.47
2:E6:192:HIS:ND1	2:E6:424:ASP:OD2	2.48	0.47
2:E6:236:SER:OG	2:E6:243:ARG:NH2	2.48	0.47
3:E7:67:ASP:OD1	3:E7:68:LEU:N	2.48	0.47
2:F0:265:ILE:HG23	2:F0:432:TYR:HE1	1.80	0.47
1:0:244:GLN:N	3:A5:320:ARG:CZ	2.78	0.46
2:A8:88:HIS:NE2	2:A8:90:GLU:OE1	2.48	0.46
2:B0:90:GLU:HB2	2:B0:121:ARG:NH2	2.30	0.46
3:B3:220:PRO:HD2	2:B4:326:LYS:HB2	1.97	0.46
3:C5:259:PRO:HB2	3:C5:260:PHE:CD1	2.49	0.46
3:C7:281:TYR:HE1	3:D1:58:ARG:CZ	2.28	0.46
2:D2:277:SER:OG	2:D2:278:ALA:N	2.47	0.46
3:D5:21:TRP:HA	3:D5:24:ILE:HG22	1.97	0.46
3:D5:310:TYR:CD1	3:D5:371:SER:HB2	2.49	0.46
2:D8:262:TYR:HB3	2:D8:263:PRO:CD	2.44	0.46
1:16:253:ALA:HB1	2:E0:32:PRO:HG2	1.97	0.46
1:7:256:LEU:HG	2:B8:31:GLN:HB3	1.96	0.46
2:A4:265:ILE:HG23	2:A4:432:TYR:OH	2.14	0.46
3:A5:203:ASP:OD2	3:A5:302:ALA:N	2.37	0.46
2:B0:102:ASN:HB3	2:B0:105:ARG:H	1.80	0.46
3:B3:282:ARG:O	3:B7:55:THR:HG21	2.14	0.46
3:B5:105:HIS:CE1	3:B5:150:LEU:HD12	2.49	0.46
3:B7:209:ASP:O	3:B7:213:ARG:HG2	2.14	0.46
3:B7:267:LEU:HD13	3:B7:371:SER:HB3	1.97	0.46
2:C0:172:TRP:HB2	2:C0:203:MET:HB3	1.96	0.46
3:D1:282:ARG:NH1	3:D1:288:GLU:OE2	2.47	0.46
2:E2:181:VAL:HG12	3:E3:256:ASN:ND2	2.30	0.46
2:E2:220:GLU:HG3	2:E2:220:GLU:O	2.14	0.46
2:E4:217:LEU:HD21	2:E4:367:ASP:OD2	2.16	0.46
2:F0:25:CYS:SG	2:F0:86:LEU:HD11	2.55	0.46
3:F1:171:PRO:HG3	3:F1:181:GLU:HG3	1.97	0.46
2:A0:132:LEU:HD23	2:A0:132:LEU:H	1.80	0.46
2:A0:244:PHE:CD2	2:A0:358:GLN:HG2	2.50	0.46
2:A2:326:LYS:HB2	2:A2:326:LYS:HE2	1.54	0.46
2:A2:345:ASP:OD1	2:A2:346:TRP:N	2.48	0.46
3:A9:135:ILE:HG13	3:A9:152:ILE:HG12	1.97	0.46
3:C1:105:HIS:O	3:C1:105:HIS:ND1	2.48	0.46
2:C4:167:LEU:HA	2:C4:200:VAL:HG13	1.98	0.46
2:C4:417:GLU:HA	2:C4:420:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C8:97:GLU:HB3	2:C8:110:ILE:CD1	2.45	0.46
2:C8:101:ASN:ND2	3:C9:252:LYS:HD3	2.30	0.46
3:C9:309:ARG:NH1	3:C9:341:PHE:O	2.48	0.46
3:D1:66:MET:HE2	3:D1:116:VAL:HG11	1.97	0.46
3:D5:372:THR:HA	3:D5:422:TYR:CD2	2.50	0.46
2:E0:100:ALA:HA	3:E1:252:LYS:HD2	1.96	0.46
2:E2:176:GLN:HB3	3:E3:331:LEU:HD13	1.97	0.46
2:E4:215:ARG:NH1	2:E4:216:ASN:OD1	2.49	0.46
2:E4:309:HIS:NE2	2:E4:386:GLU:OE1	2.40	0.46
2:E6:176:GLN:HB3	3:E7:331:LEU:CD1	2.45	0.46
3:E9:5:VAL:HB	3:E9:133:PHE:HD1	1.80	0.46
3:E9:149:THR:HA	3:E9:152:ILE:HD12	1.97	0.46
2:F0:50:ASN:O	2:F0:64:ARG:NH2	2.42	0.46
1:20:256:LEU:HD13	2:E8:29:GLY:O	2.16	0.46
1:4:247:TYR:HE1	2:B2:81:GLY:CA	2.20	0.46
3:A1:229:VAL:O	3:A1:233:MET:HB2	2.16	0.46
3:A3:274:THR:HG21	3:A3:282:ARG:HD2	1.97	0.46
3:A5:135:ILE:CD1	3:A5:152:ILE:HG12	2.45	0.46
2:A8:309:HIS:HE2	2:A8:386:GLU:CD	2.19	0.46
2:B0:286:LEU:CD1	2:B0:371:VAL:HG23	2.45	0.46
2:B4:240:ALA:O	2:B4:356:ASN:ND2	2.47	0.46
3:B9:396:HIS:HA	3:B9:399:THR:HG22	1.97	0.46
3:C1:1:MET:N	3:C1:128:ASP:OD2	2.45	0.46
2:C4:210:TYR:CE1	2:C4:227:LEU:HD11	2.50	0.46
3:C5:329:GLN:HA	3:C5:332:ASN:HB3	1.97	0.46
2:C6:231:ILE:HD13	2:C6:302:MET:CE	2.45	0.46
3:C9:101:TRP:HB3	3:C9:398:TYR:HE1	1.80	0.46
2:D0:222:PRO:HD2	3:D1:324:LYS:HB3	1.97	0.46
2:D6:119:LEU:HA	2:D6:122:ILE:HG22	1.97	0.46
2:D8:265:ILE:HG22	2:D8:380:ASN:HD21	1.79	0.46
2:D8:324:VAL:HG23	2:D8:327:ASP:H	1.79	0.46
3:E1:309:ARG:H	3:E1:372:THR:HG22	1.80	0.46
2:E2:185:TYR:HE2	2:E2:404:PHE:HB2	1.81	0.46
2:E4:221:ARG:HA	2:E4:221:ARG:HD2	1.56	0.46
2:E6:223:THR:CG2	2:E6:225:THR:HG22	2.43	0.46
3:E7:323:THR:HA	3:E7:326:VAL:HG12	1.97	0.46
3:E9:1:MET:N	3:E9:128:ASP:OD2	2.34	0.46
3:A3:130:LEU:H	3:A3:162:ARG:HH21	1.64	0.46
2:A8:285:GLN:HG3	2:A8:286:LEU:N	2.31	0.46
3:A9:213:ARG:HE	3:A9:297:LYS:HG3	1.81	0.46
3:B1:114:ASP:N	3:B1:114:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:145:THR:O	2:B2:149:LEU:HB2	2.16	0.46
3:B3:281:TYR:O	3:B7:54:ALA:HB1	2.16	0.46
3:C1:200:GLN:HB3	3:C1:266:PHE:HB2	1.96	0.46
2:C6:336:LYS:HB3	2:C6:336:LYS:HE3	1.68	0.46
3:D1:151:LEU:HD12	3:D1:151:LEU:HA	1.79	0.46
3:D3:6:HIS:HD1	3:D3:21:TRP:HE1	1.62	0.46
2:E0:183:GLU:HG3	2:E0:184:PRO:HD3	1.98	0.46
2:E2:406:HIS:HA	2:E2:409:VAL:HG12	1.97	0.46
3:E9:42:LEU:HD21	3:E9:356:ILE:HD11	1.97	0.46
3:A1:117:LEU:HD13	3:A1:154:LYS:HZ1	1.81	0.46
3:A7:281:TYR:C	3:B1:54:ALA:HB1	2.36	0.46
2:B4:298:PRO:HB3	2:B4:307:PRO:HD2	1.96	0.46
2:C0:403:ALA:HA	3:C1:260:PHE:CE1	2.50	0.46
2:C2:306:ASP:N	2:C2:386:GLU:OE2	2.48	0.46
2:C4:178:SER:HB3	3:C5:347:ASN:ND2	2.31	0.46
2:C6:406:HIS:CE1	3:C7:260:PHE:HA	2.51	0.46
3:C7:2:ARG:HG3	3:C7:131:GLN:HB2	1.98	0.46
3:C7:257:LEU:HD21	3:C7:314:SER:HB2	1.98	0.46
3:C9:286:VAL:N	3:C9:287:PRO:CD	2.78	0.46
2:D0:229:ARG:HG3	2:D0:229:ARG:NH1	2.29	0.46
3:D3:181:GLU:HB2	3:D3:182:PRO:HD3	1.97	0.46
2:D4:79:ARG:HH21	2:D4:79:ARG:HD3	1.43	0.46
2:D4:172:TRP:HE1	2:D4:391:MET:HE1	1.81	0.46
3:D7:238:CYS:SG	3:D7:318:ARG:NE	2.88	0.46
2:E0:5:ILE:HD12	2:E0:132:LEU:HD11	1.97	0.46
3:E1:63:ALA:O	3:E1:89:ASN:ND2	2.48	0.46
2:E4:132:LEU:HG	2:E4:164:LYS:NZ	2.31	0.46
2:E6:8:HIS:HE1	2:E6:21:TRP:HE1	1.62	0.46
3:E7:8:GLN:HE21	3:E7:65:LEU:CD2	2.29	0.46
3:E9:207:LEU:HB3	3:E9:225:LEU:HD22	1.98	0.46
2:F0:406:HIS:NE2	3:F1:261:PRO:HD3	2.29	0.46
3:F1:309:ARG:H	3:F1:372:THR:HG22	1.81	0.46
1:19:241:PHE:CE1	3:E7:356:ILE:HG22	2.43	0.46
3:A1:215:LEU:HD11	3:A1:273:LEU:HD22	1.98	0.46
3:A3:8:GLN:HG3	3:A3:65:LEU:HD13	1.98	0.46
2:A8:288:VAL:HG13	2:A8:319:TYR:HE2	1.81	0.46
2:B8:141:VAL:HA	2:B8:147:SER:HB2	1.98	0.46
2:C2:250:VAL:HG23	2:C2:352:LYS:NZ	2.29	0.46
2:C4:137:MET:HB3	2:C4:168:ASN:HA	1.96	0.46
3:C5:174:LYS:HZ1	2:C6:336:LYS:HB2	1.81	0.46
2:C8:98:ASP:OD1	2:C8:99:ALA:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D2:241:SER:HB2	2:D2:249:ASN:HB2	1.98	0.46
3:D3:65:LEU:HB3	3:D3:73:MET:HE2	1.97	0.46
2:D4:285:GLN:CG	2:D8:55:GLU:O	2.53	0.46
3:D7:2:ARG:HH11	3:D7:240:LEU:CD2	2.29	0.46
2:E0:282:TYR:HB2	2:E0:283:HIS:CD2	2.50	0.46
3:E7:289:LEU:HD12	3:E7:365:VAL:HG12	1.98	0.46
2:E8:79:ARG:NH1	2:E8:92:LEU:O	2.48	0.46
1:21:256:LEU:HD21	2:F0:31:GLN:HA	1.98	0.46
1:21:256:LEU:HD11	2:F0:31:GLN:HE21	1.81	0.46
2:A2:336:LYS:HA	2:A2:336:LYS:HD2	1.77	0.46
2:A4:221:ARG:C	3:A5:322:SER:HB2	2.37	0.46
2:A4:222:PRO:HD2	3:A5:324:LYS:CB	2.42	0.46
3:A9:181:GLU:HB2	3:A9:182:PRO:HD3	1.98	0.46
2:B0:210:TYR:HB3	3:B1:324:LYS:CD	2.39	0.46
3:B1:27:GLU:OE1	3:B1:318:ARG:NH2	2.49	0.46
3:B1:27:GLU:OE2	3:B1:241:ARG:NH1	2.38	0.46
3:B1:40:SER:OG	3:B1:43:GLN:OE1	2.30	0.46
3:B1:281:TYR:HB3	3:B5:60:VAL:HG11	1.97	0.46
3:B3:207:LEU:HB3	3:B3:225:LEU:HD22	1.98	0.46
2:B6:27:GLU:OE2	2:B6:320:ARG:NH2	2.49	0.46
3:B7:281:TYR:CE2	3:C1:87:PRO:CD	2.88	0.46
2:C0:188:VAL:HG12	2:C0:425:LEU:HD13	1.98	0.46
3:C1:156:ARG:HD3	3:C1:160:PRO:HA	1.97	0.46
3:C7:149:THR:HG23	3:C7:152:ILE:HD12	1.96	0.46
2:D0:36:MET:SD	2:D0:61:HIS:NE2	2.76	0.46
3:D1:274:THR:OG1	3:D1:279:GLN:OE1	2.34	0.46
3:D3:64:ILE:HD12	3:D3:119:VAL:HG22	1.97	0.46
3:D9:132:GLY:HA3	3:D9:163:ILE:HG22	1.96	0.46
3:D9:374:ILE:HD11	3:D9:422:TYR:CZ	2.51	0.46
3:E1:19:LYS:NZ	3:E1:223:GLY:O	2.49	0.46
3:E1:128:ASP:OD1	3:E1:129:CYS:N	2.46	0.46
3:E5:174:LYS:HA	3:E5:174:LYS:HD2	1.78	0.46
3:E7:256:ASN:HB3	3:E7:350:LYS:HE2	1.98	0.46
2:F0:51:THR:HG23	2:F0:52:PHE:CD2	2.50	0.46
2:F0:101:ASN:HB3	2:F0:182:VAL:HG21	1.98	0.46
2:F0:390:ARG:NH2	2:F0:390:ARG:HB3	2.30	0.46
3:F1:216:LYS:HD3	3:F1:216:LYS:HA	1.78	0.46
1:11:244:GLN:O	3:D1:355:ASP:CG	2.54	0.46
1:21:244:GLN:O	3:F1:320:ARG:NH2	2.49	0.46
1:8:255:PRO:CG	2:C0:364:PRO:HG2	2.46	0.46
2:A0:312:TYR:CE1	2:A0:379:SER:HB3	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:221:ARG:HD3	3:A3:322:SER:OG	2.16	0.46
2:A4:2:ARG:HG3	2:A4:2:ARG:O	2.15	0.46
2:B0:204:LEU:HD12	2:B0:209:ILE:HD11	1.97	0.46
3:B7:112:LEU:O	3:B7:112:LEU:HD23	2.16	0.46
3:C1:324:LYS:HA	3:C1:324:LYS:HD2	1.52	0.46
3:C3:184:ASN:OD1	3:C3:398:TYR:OH	2.31	0.46
3:D3:247:ASN:O	3:D3:252:LYS:HE2	2.15	0.46
2:D4:172:TRP:HB3	2:D4:205:ASP:OD1	2.16	0.46
3:D9:64:ILE:HD12	3:D9:119:VAL:HG12	1.98	0.46
2:E2:244:PHE:HB2	2:E2:356:ASN:HD21	1.80	0.46
2:E4:72:PRO:HD2	3:E5:2:ARG:HH22	1.79	0.46
1:9:257:PRO:HG2	2:C2:26:LEU:CA	2.45	0.46
2:A0:241:SER:HB3	2:A0:249:ASN:HB3	1.98	0.46
3:A1:22:GLU:OE2	3:A1:81:PHE:HB2	2.15	0.46
3:A1:260:PHE:CE2	3:A1:425:TYR:HE2	2.34	0.46
2:A4:163:LYS:HZ3	2:A4:163:LYS:HG3	1.49	0.46
2:A4:340:THR:HG23	2:A4:341:ILE:HG13	1.98	0.46
3:A5:206:ALA:HB2	3:A5:302:ALA:HB2	1.98	0.46
2:A8:174:SER:HB2	2:A8:177:VAL:O	2.15	0.46
3:A9:213:ARG:HH11	3:A9:213:ARG:HD2	1.58	0.46
2:B0:27:GLU:OE1	2:B0:243:ARG:NH2	2.49	0.46
2:D2:156:ARG:HD2	2:D2:156:ARG:HA	1.69	0.46
2:D2:404:PHE:HZ	3:D3:312:THR:HG21	1.81	0.46
2:D4:189:LEU:HD11	2:D4:418:PHE:CD1	2.51	0.46
2:E6:181:VAL:HG13	3:E7:350:LYS:HZ2	1.79	0.46
2:E6:221:ARG:CG	3:E7:325:GLU:HB2	2.45	0.46
2:E8:91:GLN:HB3	2:E8:121:ARG:HG2	1.97	0.46
3:E9:220:PRO:HD2	2:F0:326:LYS:HE2	1.98	0.46
3:A5:105:HIS:CE1	3:A5:150:LEU:HD12	2.51	0.45
3:B3:324:LYS:O	3:B3:328:GLU:N	2.49	0.45
2:B6:339:ARG:HA	2:B6:339:ARG:HD2	1.65	0.45
3:B7:190:HIS:HA	3:B7:193:VAL:HG12	1.98	0.45
2:B8:188:VAL:HG23	2:B8:189:LEU:HD12	1.98	0.45
3:B9:68:LEU:HD23	3:B9:112:LEU:HD13	1.98	0.45
2:C0:181:VAL:H	3:C1:256:ASN:ND2	2.13	0.45
2:C8:28:HIS:CE1	2:C8:243:ARG:HH11	2.35	0.45
3:D5:61:PRO:HD3	3:D5:84:LEU:HG	1.99	0.45
3:E1:212:PHE:HE1	2:E2:326:LYS:HE3	1.82	0.45
3:E1:388:MET:HG2	2:E2:346:TRP:O	2.15	0.45
3:E3:2:ARG:HB2	3:E3:131:GLN:HB2	1.98	0.45
2:E6:401:LYS:HD2	3:E7:344:TRP:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E7:281:TYR:C	3:F1:54:ALA:HB1	2.35	0.45
2:E8:325:PRO:HA	2:E8:328:VAL:HG12	1.97	0.45
1:0:247:TYR:CE2	2:A4:81:GLY:HA3	2.51	0.45
2:A4:28:HIS:NE2	2:A4:243:ARG:HD2	2.32	0.45
3:B1:239:CYS:SG	3:B1:248:SER:N	2.87	0.45
3:C3:253:LEU:HD11	3:C3:368:VAL:HG21	1.97	0.45
3:C5:140:GLY:O	3:C5:184:ASN:ND2	2.41	0.45
2:C6:191:THR:OG1	2:C6:425:LEU:HD21	2.15	0.45
2:C8:372:MET:HA	2:C8:372:MET:CE	2.46	0.45
3:C9:139:LEU:CD1	3:C9:168:SER:HB2	2.43	0.45
2:D0:221:ARG:N	2:D0:222:PRO:HD3	2.31	0.45
3:D5:309:ARG:H	3:D5:372:THR:HG22	1.81	0.45
3:D5:318:ARG:HD3	3:D5:358:PRO:HD3	1.98	0.45
3:D9:135:ILE:HG22	3:D9:137:HIS:CD2	2.52	0.45
3:D9:281:TYR:CE1	3:E3:58:ARG:CZ	3.00	0.45
2:E4:306:ASP:HB3	2:E4:309:HIS:CE1	2.51	0.45
3:E9:330:MET:SD	3:E9:349:MET:HG3	2.56	0.45
3:F1:292:GLN:O	3:F1:298:ASN:ND2	2.39	0.45
1:20:243:ALA:CB	3:E9:357:PRO:HD2	2.42	0.45
2:A6:210:TYR:O	3:A7:324:LYS:NZ	2.47	0.45
2:A8:238:LEU:HD22	2:A8:255:PHE:HE2	1.81	0.45
2:B2:177:VAL:HG12	3:B3:331:LEU:HD22	1.97	0.45
2:C0:133:GLN:HG3	2:C0:252:VAL:HG22	1.97	0.45
3:C9:181:GLU:HB2	3:C9:182:PRO:HD3	1.96	0.45
2:D0:121:ARG:HA	2:D0:121:ARG:HD2	1.68	0.45
3:D5:105:HIS:CE1	3:D5:150:LEU:HB2	2.50	0.45
3:D5:316:MET:HE3	3:D5:316:MET:HB2	1.60	0.45
3:D7:374:ILE:HD11	3:D7:422:TYR:CZ	2.52	0.45
3:D9:63:ALA:O	3:D9:89:ASN:ND2	2.50	0.45
3:E1:238:CYS:SG	3:E1:239:CYS:N	2.90	0.45
2:E8:296:PHE:CZ	2:E8:317:LEU:HD21	2.51	0.45
3:E9:238:CYS:SG	3:E9:239:CYS:N	2.89	0.45
2:F0:174:SER:HB3	2:F0:177:VAL:O	2.15	0.45
2:F0:177:VAL:HG22	3:F1:331:LEU:HD22	1.99	0.45
2:F0:306:ASP:HB3	2:F0:309:HIS:CE1	2.50	0.45
1:11:244:GLN:CA	3:D1:320:ARG:NH2	2.79	0.45
2:A2:210:TYR:HB3	3:A3:324:LYS:HG3	1.98	0.45
3:A3:187:LEU:HD11	3:A3:408:PHE:CE1	2.51	0.45
2:A8:338:LYS:HG2	2:A8:340:THR:HG22	1.98	0.45
3:A9:67:ASP:OD1	3:A9:68:LEU:N	2.48	0.45
2:B2:12:ALA:HB3	2:B2:140:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:404:PHE:HZ	3:B3:345:ILE:HD13	1.82	0.45
3:B3:6:HIS:HE1	3:B3:20:PHE:CD2	2.34	0.45
2:B6:132:LEU:HB3	2:B6:164:LYS:HE2	1.98	0.45
2:C2:209:ILE:HG22	2:C2:227:LEU:HG	1.98	0.45
3:C3:173:PRO:HG3	3:C3:302:ALA:HB1	1.99	0.45
2:C4:88:HIS:O	2:C4:90:GLU:N	2.49	0.45
2:C4:396:ASP:N	2:C4:396:ASP:OD1	2.49	0.45
2:C6:310:GLY:HA3	2:C6:383:ALA:HB2	1.99	0.45
3:C7:183:TYR:HB3	3:C7:398:TYR:CE2	2.51	0.45
2:C8:147:SER:HB2	2:C8:190:SER:HB3	1.97	0.45
3:C9:282:ARG:NH1	3:C9:292:GLN:OE1	2.49	0.45
3:D3:68:LEU:HA	3:D3:93:GLY:HA3	1.99	0.45
3:D3:294:PHE:CE2	3:D3:333:VAL:HG21	2.51	0.45
3:D3:313:ALA:HB1	3:D3:367:PHE:CE1	2.51	0.45
2:D6:64:ARG:HG2	2:D6:125:LEU:HD11	1.97	0.45
2:D6:209:ILE:CG2	2:D6:227:LEU:HG	2.46	0.45
2:D8:178:SER:HB2	3:D9:347:ASN:HD22	1.82	0.45
2:F0:328:VAL:HG21	2:F0:355:ILE:HD11	1.98	0.45
2:F0:390:ARG:HB3	2:F0:390:ARG:HH21	1.81	0.45
1:11:254:LYS:HB3	2:D0:364:PRO:HG2	1.99	0.45
1:20:241:PHE:CE1	3:E9:356:ILE:CG2	3.00	0.45
2:A0:195:LEU:HD21	2:A0:264:ARG:HE	1.82	0.45
2:A4:422:ARG:NH1	2:A4:426:ALA:HB2	2.31	0.45
2:A6:11:GLN:HG3	2:A6:74:VAL:HG21	1.97	0.45
2:A8:356:ASN:OD1	2:A8:357:TYR:N	2.49	0.45
2:B6:70:LEU:HD12	2:B6:99:ALA:HB2	1.98	0.45
2:B8:238:LEU:HD12	2:B8:238:LEU:HA	1.85	0.45
2:B8:288:VAL:HA	2:B8:291:ILE:HG12	1.97	0.45
3:C5:209:ASP:OD1	3:C5:213:ARG:NH2	2.46	0.45
2:C6:180:ALA:O	3:C7:347:ASN:ND2	2.50	0.45
2:D2:11:GLN:HE22	3:D3:246:LEU:HA	1.81	0.45
2:D2:272:TYR:HD2	2:D2:275:ILE:HG12	1.81	0.45
3:D7:213:ARG:CB	3:D7:297:LYS:HD2	2.46	0.45
2:E0:306:ASP:OD1	2:E0:308:ARG:NH1	2.49	0.45
3:E3:239:CYS:SG	3:E3:248:SER:N	2.83	0.45
3:E3:291:GLN:OE1	3:E7:122:LYS:HD3	2.15	0.45
2:E4:195:LEU:HD11	2:E4:428:LEU:HD22	1.98	0.45
2:E8:69:ASP:OD1	2:E8:70:LEU:N	2.49	0.45
2:E8:172:TRP:N	2:E8:204:LEU:O	2.41	0.45
3:E9:289:LEU:HD23	3:E9:365:VAL:HG12	1.98	0.45
1:10:254:LYS:HZ1	2:C8:22:GLU:HG2	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A4:157:LEU:HB3	2:A4:166:LYS:HE2	1.99	0.45
3:B1:362:LYS:HE2	3:B1:362:LYS:HB2	1.50	0.45
2:C4:14:ILE:O	2:C4:18:ASN:N	2.48	0.45
3:C5:291:GLN:HE22	3:C9:122:LYS:HE2	1.81	0.45
3:D1:7:VAL:HB	3:D1:135:ILE:HG12	1.98	0.45
3:D3:67:ASP:OD1	3:D3:68:LEU:N	2.50	0.45
2:D4:222:PRO:HD2	3:D5:324:LYS:HB3	1.99	0.45
3:D5:404:ASP:OD1	3:D5:405:GLU:N	2.49	0.45
3:D7:212:PHE:CE1	2:D8:326:LYS:HD3	2.40	0.45
2:D8:179:THR:HG21	3:D9:327:ASP:OD1	2.16	0.45
3:D9:129:CYS:O	3:D9:129:CYS:SG	2.74	0.45
3:E3:218:THR:HG23	3:E3:219:THR:HG23	1.99	0.45
2:E4:221:ARG:HH12	3:E5:324:LYS:H	1.65	0.45
2:E6:223:THR:OG1	3:E7:245:GLN:NE2	2.48	0.45
2:E6:423:GLU:O	2:E6:427:ALA:N	2.44	0.45
2:E8:137:MET:HB3	2:E8:168:ASN:HA	1.99	0.45
3:E9:49:VAL:HG21	3:E9:241:ARG:HG2	1.98	0.45
2:A0:290:GLU:CB	2:A4:124:LYS:NZ	2.79	0.45
3:A1:326:VAL:O	3:A1:330:MET:HG2	2.16	0.45
2:A2:199:ASP:OD1	2:A2:200:VAL:N	2.49	0.45
2:B2:28:HIS:CE1	2:B2:243:ARG:HD2	2.51	0.45
2:B6:1:MET:N	2:B6:129:CYS:SG	2.90	0.45
2:C6:207:GLU:HA	2:C6:210:TYR:HB2	1.99	0.45
2:C8:420:GLU:O	2:C8:420:GLU:HG3	2.16	0.45
3:C9:99:ASN:ND2	3:C9:178:THR:HG22	2.32	0.45
3:D1:206:ALA:HB2	3:D1:302:ALA:HB2	1.99	0.45
3:D5:96:GLY:N	3:D5:108:GLU:OE2	2.50	0.45
3:E1:198:GLU:HB2	3:E1:266:PHE:CE2	2.47	0.45
2:E4:271:SER:HB2	2:E4:377:MET:HB3	1.98	0.45
3:E5:256:ASN:HD21	3:E5:350:LYS:CG	2.29	0.45
3:E9:28:HIS:CE1	3:E9:241:ARG:HE	2.34	0.45
2:F0:395:PHE:CD2	2:F0:422:ARG:HD2	2.51	0.45
3:F1:170:PHE:HB3	3:F1:171:PRO:HD2	1.99	0.45
1:19:256:LEU:H	1:19:256:LEU:HG	1.64	0.45
3:A1:100:ASN:HB3	3:A1:103:LYS:HB2	1.98	0.45
3:A7:25:SER:HG	3:A7:51:TYR:HH	1.62	0.45
3:B1:91:VAL:HG21	3:B1:116:VAL:HG12	1.97	0.45
2:B8:5:ILE:HG12	2:B8:132:LEU:HD11	1.98	0.45
2:B8:305:CYS:HG	2:B8:309:HIS:HE2	1.63	0.45
2:C0:276:ILE:HG23	2:C0:281:ALA:HB2	1.99	0.45
3:C7:289:LEU:HD23	3:C7:289:LEU:HA	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C9:190:HIS:HB2	3:C9:414:ASN:HD21	1.82	0.45
2:D4:116:ASP:OD1	2:D4:116:ASP:N	2.49	0.45
3:D5:113:ILE:HD12	3:D5:116:VAL:CG1	2.47	0.45
2:D6:3:GLU:HA	2:D6:51:THR:HA	1.98	0.45
2:D8:73:THR:HA	3:D9:46:ARG:HH12	1.82	0.45
2:E0:96:LYS:CE	3:E1:128:ASP:CG	2.84	0.45
2:E0:195:LEU:HD13	2:E0:264:ARG:HH21	1.81	0.45
3:E1:122:LYS:HD3	3:E1:122:LYS:HA	1.57	0.45
3:E1:268:ILE:HD12	3:E1:368:VAL:HG22	1.98	0.45
2:E4:23:LEU:HD11	2:E4:361:THR:HG23	1.97	0.45
3:F1:198:GLU:OE2	3:F1:200:GLN:NE2	2.45	0.45
2:A0:338:LYS:HE3	2:A0:338:LYS:HB3	1.73	0.45
3:A5:135:ILE:HD12	3:A5:152:ILE:HG12	1.98	0.45
2:A8:269:LEU:HD22	2:A8:303:ALA:HB3	1.99	0.45
2:A8:304:LYS:HD2	2:A8:304:LYS:HA	1.75	0.45
3:A9:202:ILE:HD13	3:A9:229:VAL:HG22	1.99	0.45
3:A9:259:PRO:HB2	3:A9:260:PHE:CD1	2.52	0.45
3:A9:313:ALA:HB3	3:A9:349:MET:HG2	1.99	0.45
2:B0:2:ARG:HB2	2:B0:133:GLN:NE2	2.29	0.45
2:B2:1:MET:N	2:B2:129:CYS:SG	2.76	0.45
2:B4:158:SER:OG	2:B4:166:LYS:NZ	2.49	0.45
2:B4:178:SER:OG	2:B4:179:THR:N	2.49	0.45
2:B4:311:LYS:H	2:B4:382:THR:HG22	1.82	0.45
2:B8:168:ASN:HD22	2:B8:198:THR:HG21	1.81	0.45
3:C1:103:LYS:HA	3:C1:107:THR:HB	1.98	0.45
2:C4:181:VAL:HG12	3:C5:256:ASN:CB	2.40	0.45
2:C8:399:TYR:OH	2:C8:415:GLU:OE1	2.30	0.45
3:C9:77:ARG:HH21	3:C9:92:PHE:HZ	1.63	0.45
3:D3:267:LEU:HB3	3:D3:299:MET:HE2	1.99	0.45
3:D3:397:TRP:CH2	2:D4:260:VAL:O	2.69	0.45
3:D5:4:ILE:HD11	3:D5:240:LEU:HD13	1.98	0.45
3:D5:253:LEU:HD12	3:D5:316:MET:HE2	1.97	0.45
3:D7:214:THR:OG1	3:D7:215:LEU:N	2.48	0.45
2:D8:292:THR:HG21	2:D8:331:ALA:HB1	1.99	0.45
2:E6:209:ILE:HG22	2:E6:227:LEU:HD22	1.98	0.45
3:E7:49:VAL:HG11	3:E7:241:ARG:HG2	1.98	0.45
1:0:247:TYR:CZ	2:A4:81:GLY:HA3	2.52	0.45
1:3:257:PRO:HD3	2:B0:26:LEU:HD12	1.97	0.45
2:A0:301:MET:HE1	2:A0:305:CYS:H	1.81	0.45
2:A2:244:PHE:HD2	2:A2:358:GLN:HG2	1.82	0.45
3:A5:200:GLN:HG3	3:A5:268:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A8:116:ASP:N	2:A8:116:ASP:OD1	2.47	0.45
2:B0:262:TYR:HB3	2:B0:263:PRO:HD2	1.98	0.45
3:B5:336:LYS:HA	3:B5:336:LYS:CE	2.47	0.45
2:B6:52:PHE:CD2	2:B6:243:ARG:HD3	2.52	0.45
3:C1:137:HIS:ND1	3:C1:138:SER:O	2.38	0.45
2:C2:346:TRP:HZ2	2:C2:435:VAL:HG13	1.82	0.45
3:D5:138:SER:HA	3:D5:169:VAL:HG22	1.99	0.45
2:E4:132:LEU:HG	2:E4:164:LYS:HZ1	1.82	0.45
3:E5:105:HIS:CD2	3:E5:150:LEU:HB2	2.51	0.45
3:E9:167:PHE:CE1	3:E9:233:MET:HG2	2.52	0.45
2:F0:195:LEU:HD21	2:F0:428:LEU:HD22	1.98	0.45
1:11:247:TYR:CG	2:D0:77:GLU:OE2	2.70	0.44
1:18:255:PRO:HG2	2:E4:364:PRO:CG	2.47	0.44
2:A8:282:TYR:OH	2:B2:33:ASP:CG	2.56	0.44
3:A9:173:PRO:HG2	3:A9:205:GLU:OE2	2.17	0.44
3:B3:11:GLN:HE22	2:B4:248:LEU:HD12	1.82	0.44
3:B3:171:PRO:HB3	3:B3:181:GLU:OE1	2.17	0.44
3:B5:279:GLN:HG2	3:B5:279:GLN:O	2.17	0.44
2:C0:66:VAL:HG21	2:C0:122:ILE:HD11	1.99	0.44
2:C0:320:ARG:NH2	2:C0:358:GLN:OE1	2.51	0.44
2:C2:2:ARG:O	2:C2:2:ARG:HG2	2.16	0.44
2:C2:432:TYR:O	2:C2:436:GLY:N	2.50	0.44
3:C3:215:LEU:HD21	3:C3:273:LEU:HD22	1.98	0.44
2:C4:390:ARG:O	2:C4:394:LYS:N	2.50	0.44
2:C6:135:PHE:HB2	2:C6:166:LYS:HA	1.99	0.44
2:C8:28:HIS:HE1	2:C8:243:ARG:HH11	1.63	0.44
3:C9:226:ASN:HA	3:C9:229:VAL:HG22	1.98	0.44
3:D1:173:PRO:HD2	3:D1:205:GLU:OE2	2.16	0.44
3:D1:311:LEU:HD12	3:D1:311:LEU:HA	1.89	0.44
2:D4:405:VAL:HG12	2:D4:409:VAL:HG23	2.00	0.44
3:E3:7:VAL:HB	3:E3:135:ILE:HG13	1.99	0.44
3:E5:246:LEU:HA	3:E5:246:LEU:HD12	1.88	0.44
2:E8:210:TYR:HE2	3:E9:327:ASP:OD2	2.00	0.44
1:1:246:CYS:SG	1:1:247:TYR:N	2.91	0.44
2:A2:221:ARG:HB2	3:A3:322:SER:HG	1.81	0.44
2:A8:11:GLN:HE22	3:A9:246:LEU:HA	1.82	0.44
3:A9:225:LEU:HD21	2:B0:326:LYS:NZ	2.32	0.44
3:B1:149:THR:OG1	3:B1:191:GLN:OE1	2.22	0.44
3:B1:230:SER:HA	3:B1:233:MET:HG2	1.99	0.44
2:B8:70:LEU:HD12	2:B8:99:ALA:HB2	1.99	0.44
3:C1:262:ARG:HA	3:C1:262:ARG:HD2	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C6:172:TRP:HB3	2:C6:205:ASP:OD1	2.17	0.44
2:C6:188:VAL:HG13	2:C6:425:LEU:HD23	1.98	0.44
2:C6:407:TRP:CZ3	3:C7:255:VAL:C	2.82	0.44
3:D1:53:GLU:OE2	3:D1:54:ALA:N	2.50	0.44
2:D8:319:TYR:CE2	2:D8:375:VAL:HG22	2.52	0.44
2:E0:210:TYR:CD2	3:E1:324:LYS:HG3	2.52	0.44
3:E5:1:MET:N	3:E5:128:ASP:OD2	2.40	0.44
3:E7:246:LEU:HD12	3:E7:246:LEU:HA	1.89	0.44
2:F0:107:HIS:NE2	2:F0:151:CYS:SG	2.84	0.44
1:1:256:LEU:HA	1:1:257:PRO:HD3	1.87	0.44
1:3:254:LYS:HB3	1:3:255:PRO:HD2	1.98	0.44
3:A7:44:LEU:HD12	3:A7:47:ILE:HD12	2.00	0.44
2:B4:6:SER:OG	2:B4:8:HIS:NE2	2.48	0.44
2:B4:141:VAL:O	2:B4:147:SER:OG	2.36	0.44
3:C1:295:ASP:HB3	3:C1:297:LYS:HG2	2.00	0.44
2:C6:1:MET:HA	2:C6:129:CYS:HB3	2.00	0.44
2:C6:158:SER:OG	2:C6:166:LYS:NZ	2.50	0.44
2:C8:34:GLY:O	2:C8:61:HIS:N	2.45	0.44
2:D6:183:GLU:HA	2:D6:186:ASN:HD22	1.82	0.44
3:E5:281:TYR:CD2	3:E9:87:PRO:CD	2.97	0.44
3:F1:237:THR:O	3:F1:241:ARG:NH1	2.50	0.44
1:21:241:PHE:CZ	3:F1:356:ILE:HG23	2.35	0.44
2:A0:228:ASN:HA	2:A0:231:ILE:HG22	1.99	0.44
2:A0:332:VAL:HG13	2:A0:351:PHE:HD2	1.82	0.44
2:A2:292:THR:HG21	2:A2:331:ALA:HB1	1.99	0.44
3:B3:63:ALA:O	3:B3:89:ASN:ND2	2.51	0.44
3:B5:150:LEU:HD23	3:B5:154:LYS:HD2	1.99	0.44
3:C1:149:THR:O	3:C1:191:GLN:NE2	2.50	0.44
2:C2:277:SER:OG	2:C2:278:ALA:N	2.51	0.44
2:C2:288:VAL:HA	2:C2:291:ILE:HG12	2.00	0.44
2:C4:319:TYR:HB3	2:C4:323:VAL:HG21	1.99	0.44
3:C5:100:ASN:HB3	3:C5:103:LYS:HG2	1.99	0.44
2:D4:69:ASP:OD1	2:D4:70:LEU:N	2.51	0.44
2:D6:98:ASP:OD1	2:D6:99:ALA:N	2.50	0.44
3:D9:8:GLN:NE2	3:D9:17:GLY:HA3	2.32	0.44
3:E1:163:ILE:HD12	3:E1:250:LEU:HB2	1.98	0.44
3:E5:173:PRO:HB3	3:E5:380:ARG:CZ	2.47	0.44
3:A1:73:MET:HA	3:A1:76:VAL:HG12	1.99	0.44
3:A7:404:ASP:OD1	3:A7:405:GLU:N	2.51	0.44
2:B2:259:LEU:HB3	2:B2:268:MET:HE2	1.99	0.44
3:B5:67:ASP:OD1	3:B5:68:LEU:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B9:67:ASP:OD1	3:B9:68:LEU:N	2.51	0.44
3:C5:167:PHE:CE2	3:C5:233:MET:HG2	2.53	0.44
3:C5:187:LEU:HD11	3:C5:408:PHE:CZ	2.52	0.44
3:C5:295:ASP:HB3	3:C5:298:ASN:HB2	2.00	0.44
3:D1:281:TYR:OH	3:D5:83:GLN:HB3	2.18	0.44
2:D6:222:PRO:CD	3:D7:324:LYS:HZ2	2.30	0.44
3:D7:112:LEU:HD12	3:D7:112:LEU:HA	1.79	0.44
2:D8:231:ILE:O	2:D8:235:ILE:HG12	2.17	0.44
3:D9:263:LEU:HD12	3:D9:370:ASN:HD21	1.82	0.44
3:E3:336:LYS:HE2	3:E3:336:LYS:HA	1.99	0.44
3:E5:257:LEU:HD21	3:E5:314:SER:HB2	1.99	0.44
2:E6:417:GLU:HA	2:E6:420:GLU:HG3	2.00	0.44
3:E9:198:GLU:HG3	3:E9:266:PHE:CE2	2.53	0.44
2:F0:339:ARG:O	2:F0:342:GLN:NE2	2.50	0.44
2:A0:240:ALA:HA	2:A0:243:ARG:HE	1.82	0.44
2:A0:343:PHE:HZ	2:A0:351:PHE:CE1	2.35	0.44
2:A2:133:GLN:NE2	2:A2:251:ASP:HB3	2.33	0.44
3:A9:208:TYR:CD1	2:B0:326:LYS:HE3	2.53	0.44
2:B4:10:GLY:HA2	2:B4:145:THR:HG23	1.99	0.44
3:B5:383:ASP:HA	3:B5:386:THR:HG22	1.99	0.44
2:C2:404:PHE:CE1	3:C3:259:PRO:HG3	2.52	0.44
3:C3:42:LEU:HD21	3:C3:356:ILE:HG13	2.00	0.44
2:C4:135:PHE:HB2	2:C4:166:LYS:HA	2.00	0.44
2:C8:191:THR:HG21	2:C8:425:LEU:HD13	2.00	0.44
2:D0:285:GLN:HB3	2:D4:56:THR:CB	2.47	0.44
2:D0:319:TYR:N	2:D0:354:GLY:O	2.47	0.44
2:D4:425:LEU:HD12	2:D4:425:LEU:HA	1.85	0.44
3:D5:276:ARG:HH21	3:D5:279:GLN:HG3	1.82	0.44
2:E0:166:LYS:N	2:E0:199:ASP:OD2	2.51	0.44
3:E1:272:PRO:HG3	3:E1:284:LEU:HD11	2.00	0.44
2:E6:195:LEU:HD21	2:E6:428:LEU:HD22	1.99	0.44
2:E8:269:LEU:CD2	2:E8:384:ILE:HD11	2.47	0.44
2:F0:8:HIS:CD2	2:F0:17:GLY:HA3	2.52	0.44
2:F0:213:CYS:HA	2:F0:217:LEU:HB2	1.99	0.44
3:A1:291:GLN:CB	3:A5:122:LYS:HE3	2.48	0.44
2:A4:11:GLN:HG3	2:A4:74:VAL:HG21	1.99	0.44
2:B0:173:PRO:HG3	2:B0:187:SER:OG	2.18	0.44
3:B5:8:GLN:OE1	3:B5:17:GLY:HA3	2.18	0.44
2:C2:23:LEU:HD13	2:C2:363:VAL:HG13	1.99	0.44
3:C3:49:VAL:HG11	3:C3:241:ARG:HG2	2.00	0.44
2:C4:204:LEU:HD13	2:C4:231:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C6:7:ILE:HG21	2:C6:153:LEU:CD2	2.47	0.44
3:C9:397:TRP:NE1	2:D0:257:THR:HA	2.32	0.44
2:D0:132:LEU:HB3	2:D0:164:LYS:NZ	2.32	0.44
3:D1:334:GLN:HE22	3:D1:347:ASN:HA	1.82	0.44
2:D4:172:TRP:HE1	2:D4:391:MET:CE	2.31	0.44
3:D5:117:LEU:O	3:D5:121:ARG:HG2	2.18	0.44
2:D6:20:CYS:SG	2:D6:235:ILE:HG21	2.57	0.44
3:D7:167:PHE:CE1	3:D7:233:MET:HG2	2.53	0.44
2:E4:223:THR:CG2	2:E4:225:THR:HG22	2.43	0.44
3:E5:3:GLU:HA	3:E5:49:VAL:HA	2.00	0.44
3:E5:49:VAL:HG11	3:E5:241:ARG:HG2	1.99	0.44
3:E5:136:THR:HG22	3:E5:167:PHE:HB2	1.99	0.44
3:E5:156:ARG:HA	3:E5:156:ARG:HD2	1.82	0.44
2:E6:27:GLU:OE2	2:E6:320:ARG:NH2	2.51	0.44
3:A1:219:THR:CG2	2:A2:326:LYS:HZ1	2.31	0.44
3:A1:289:LEU:HD21	3:A1:365:VAL:CG1	2.47	0.44
2:A4:107:HIS:HB3	2:A4:108:TYR:HD1	1.82	0.44
3:A5:77:ARG:HG3	3:A5:90:PHE:HE2	1.81	0.44
3:A7:178:THR:O	3:A7:181:GLU:HG2	2.18	0.44
2:B0:306:ASP:HB3	2:B0:309:HIS:CE1	2.53	0.44
3:B1:63:ALA:O	3:B1:89:ASN:ND2	2.51	0.44
2:C0:71:GLU:HB3	2:C0:98:ASP:HB3	2.00	0.44
2:C0:224:TYR:HA	2:C0:227:LEU:HD12	2.00	0.44
3:C3:73:MET:HB3	3:C3:77:ARG:NH2	2.33	0.44
3:C5:327:ASP:OD1	3:C5:327:ASP:N	2.47	0.44
3:D1:152:ILE:CD1	3:D1:166:THR:HG21	2.47	0.44
3:D3:7:VAL:HG11	3:D3:151:LEU:CD2	2.47	0.44
3:D3:257:LEU:O	3:D3:312:THR:OG1	2.36	0.44
2:D4:96:LYS:HZ3	3:D5:129:CYS:HB2	1.83	0.44
3:D7:289:LEU:HD23	3:D7:289:LEU:HA	1.91	0.44
3:D7:324:LYS:HE2	3:D7:324:LYS:HB2	1.60	0.44
2:E0:311:LYS:NZ	2:E0:342:GLN:OE1	2.45	0.44
2:E0:352:LYS:HD3	2:E0:352:LYS:HA	1.74	0.44
3:E1:273:LEU:H	3:E1:292:GLN:HE22	1.65	0.44
3:E1:398:TYR:HB3	3:E1:408:PHE:HZ	1.82	0.44
2:E4:132:LEU:O	2:E4:164:LYS:NZ	2.51	0.44
3:E5:379:LYS:O	3:E5:383:ASP:N	2.48	0.44
2:E8:53:PHE:HB3	2:E8:61:HIS:HB3	1.99	0.44
2:E8:296:PHE:HZ	2:E8:317:LEU:HD21	1.83	0.44
1:2:256:LEU:CD1	2:A8:31:GLN:HG3	2.48	0.44
1:6:256:LEU:CD2	2:B6:31:GLN:HA	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:257:PRO:HG2	2:B6:26:LEU:O	2.18	0.44
2:A2:241:SER:HB3	2:A2:249:ASN:HB3	2.00	0.44
2:A4:98:ASP:O	2:A4:105:ARG:NH1	2.49	0.44
2:A4:124:LYS:HA	2:A4:124:LYS:HD2	1.80	0.44
3:A5:167:PHE:CE2	3:A5:233:MET:HG2	2.53	0.44
3:A5:217:LEU:HD23	3:A5:220:PRO:HG3	2.00	0.44
2:B0:10:GLY:O	2:B0:14:ILE:HG12	2.18	0.44
2:C0:403:ALA:HA	3:C1:260:PHE:HE1	1.83	0.44
3:C1:318:ARG:HD3	3:C1:358:PRO:HD3	2.00	0.44
2:C2:70:LEU:HD12	2:C2:99:ALA:HB2	1.99	0.44
2:C4:277:SER:C	2:C4:369:ALA:HB2	2.39	0.44
3:C7:200:GLN:HB3	3:C7:266:PHE:HB2	1.99	0.44
2:C8:304:LYS:O	2:C8:304:LYS:HD3	2.18	0.44
3:D1:117:LEU:HA	3:D1:120:VAL:HG12	2.00	0.44
3:D5:208:TYR:O	3:D5:212:PHE:HB3	2.17	0.44
2:E0:132:LEU:HB3	2:E0:164:LYS:NZ	2.33	0.44
2:E2:204:LEU:HD21	2:E2:231:ILE:HD12	1.99	0.44
3:E7:208:TYR:CE1	3:E7:225:LEU:HD11	2.52	0.44
3:E9:175:VAL:HG23	2:F0:332:VAL:CG1	2.47	0.44
1:21:245:SER:OG	3:F1:355:ASP:OD2	2.24	0.43
3:A1:107:THR:HG21	3:A1:401:GLU:HG2	1.99	0.43
3:A3:297:LYS:NZ	3:A3:306:ARG:HH22	2.16	0.43
2:A8:262:TYR:CB	2:A8:263:PRO:HD2	2.44	0.43
2:A8:282:TYR:HD2	2:A8:283:HIS:CE1	2.36	0.43
3:B5:13:GLY:HA2	3:B5:16:ILE:HG22	2.00	0.43
3:B5:287:PRO:HA	3:B5:290:THR:HG22	2.00	0.43
3:C1:295:ASP:CB	3:C1:297:LYS:HG2	2.48	0.43
3:C1:330:MET:HB3	3:C1:349:MET:HG2	2.00	0.43
3:C3:12:CYS:HB3	3:C3:138:SER:HB2	2.00	0.43
3:C3:136:THR:HG23	3:C3:167:PHE:HB2	1.99	0.43
2:C6:119:LEU:HD21	2:C6:156:ARG:HB3	2.00	0.43
2:C8:241:SER:HB2	2:C8:249:ASN:HB2	1.99	0.43
2:D2:276:ILE:HD11	2:D2:286:LEU:HD11	1.99	0.43
3:D5:200:GLN:HB3	3:D5:268:ILE:HD11	2.00	0.43
2:D6:126:ALA:HB1	2:D6:132:LEU:HD22	1.99	0.43
3:D9:6:HIS:HD2	3:D9:134:GLN:NE2	2.16	0.43
2:E2:262:TYR:HD2	2:E2:265:ILE:HD12	1.83	0.43
3:E7:113:ILE:HA	3:E7:116:VAL:HG12	2.00	0.43
3:E7:282:ARG:O	3:F1:55:THR:HG23	2.18	0.43
3:F1:30:ILE:HD12	3:F1:51:TYR:CE2	2.53	0.43
3:F1:33:THR:O	3:F1:58:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A0:306:ASP:HB3	2:A0:309:HIS:CE1	2.53	0.43
2:A8:298:PRO:HB3	2:A8:307:PRO:HD2	2.00	0.43
3:B1:190:HIS:HB2	3:B1:414:ASN:HD22	1.83	0.43
3:B3:93:GLY:CA	3:B3:112:LEU:HD21	2.45	0.43
2:B4:208:ALA:HB2	2:B4:304:LYS:HB2	1.99	0.43
2:B8:262:TYR:HB2	2:B8:265:ILE:HD12	1.99	0.43
2:C0:256:GLN:O	2:C0:260:VAL:HG22	2.18	0.43
2:C0:336:LYS:HG3	2:C0:351:PHE:HE1	1.83	0.43
3:C7:68:LEU:HA	3:C7:93:GLY:HA3	1.99	0.43
2:E0:329:ASN:HA	2:E0:332:VAL:HG12	1.99	0.43
2:E4:277:SER:HB3	2:E4:280:LYS:HB2	2.00	0.43
2:E6:290:GLU:CD	2:F0:124:LYS:HE3	2.38	0.43
2:F0:65:CYS:O	2:F0:91:GLN:HG3	2.18	0.43
1:21:241:PHE:CZ	3:F1:356:ILE:CG2	2.97	0.43
1:8:241:PHE:HZ	3:C1:356:ILE:CD1	2.09	0.43
3:A1:311:LEU:HD12	3:A1:311:LEU:HA	1.93	0.43
3:A1:379:LYS:HB2	3:A1:379:LYS:HZ3	1.76	0.43
2:A2:205:ASP:OD1	2:A2:206:ASN:N	2.51	0.43
3:A3:252:LYS:O	3:A3:256:ASN:ND2	2.52	0.43
2:A6:313:MET:HE3	2:A6:435:VAL:HG11	2.00	0.43
3:B1:156:ARG:HH21	3:B1:164:MET:HB2	1.84	0.43
2:B6:326:LYS:HD2	2:B6:326:LYS:HA	1.56	0.43
3:B7:10:GLY:HA2	3:B7:143:THR:HG23	2.00	0.43
2:B8:391:MET:O	2:B8:395:PHE:N	2.50	0.43
2:C0:121:ARG:HD2	2:C0:121:ARG:HA	1.67	0.43
3:C1:172:SER:HB3	3:C1:176:SER:HB3	1.98	0.43
3:C1:392:LYS:HA	3:C1:395:LEU:HD23	2.00	0.43
2:C2:283:HIS:HA	2:C6:60:LYS:HZ2	1.83	0.43
3:C5:220:PRO:HB2	3:C5:225:LEU:CD2	2.49	0.43
2:C8:28:HIS:NE2	2:C8:243:ARG:HD2	2.33	0.43
3:C9:263:LEU:O	3:C9:263:LEU:HD12	2.17	0.43
2:D2:407:TRP:CD2	3:D3:255:VAL:HG22	2.54	0.43
3:D7:289:LEU:HD22	3:D7:365:VAL:HG12	2.01	0.43
3:D9:25:SER:OG	3:D9:51:TYR:OH	2.32	0.43
2:E0:96:LYS:CE	3:E1:128:ASP:HB2	2.44	0.43
3:E3:33:THR:HG23	3:E3:35:THR:HG23	1.98	0.43
3:E5:20:PHE:HA	3:E5:230:SER:OG	2.19	0.43
2:E6:115:VAL:HG12	2:E6:156:ARG:HE	1.82	0.43
3:E9:105:HIS:HB3	3:E9:106:TYR:CD1	2.53	0.43
2:F0:254:GLU:OE1	2:F0:352:LYS:NZ	2.40	0.43
1:20:256:LEU:HD11	2:E8:31:GLN:CG	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:21:256:LEU:HD21	2:F0:31:GLN:CA	2.49	0.43
1:6:239:LEU:HD13	1:6:240:PRO:HD2	1.99	0.43
2:A0:71:GLU:HB3	2:A0:98:ASP:HB2	2.00	0.43
3:A1:72:THR:HG23	3:A1:73:MET:SD	2.58	0.43
3:B1:103:LYS:HB2	3:B1:108:GLU:OE1	2.18	0.43
2:B8:282:TYR:CE2	2:C2:85:HIS:CG	2.96	0.43
3:B9:256:ASN:HD22	3:B9:350:LYS:HD2	1.84	0.43
2:C0:265:ILE:HG13	2:C0:432:TYR:CZ	2.54	0.43
3:C5:186:THR:HG23	3:C5:415:MET:HE2	1.99	0.43
2:C6:212:ILE:HD13	2:C6:215:ARG:HH22	1.83	0.43
2:D0:174:SER:HB3	2:D0:205:ASP:OD1	2.19	0.43
2:D2:180:ALA:HB1	3:D3:256:ASN:ND2	2.33	0.43
2:D2:425:LEU:HD12	2:D2:425:LEU:HA	1.92	0.43
3:D9:283:ALA:HA	3:E3:55:THR:HB	2.00	0.43
2:E0:64:ARG:HB3	2:E0:125:LEU:HD21	1.99	0.43
2:E2:265:ILE:HG23	2:E2:432:TYR:HE1	1.83	0.43
2:E8:2:ARG:NE	2:E8:133:GLN:HE21	2.15	0.43
2:E8:306:ASP:N	2:E8:386:GLU:OE2	2.51	0.43
1:1:254:LYS:HB3	2:A6:364:PRO:CB	2.41	0.43
2:A0:222:PRO:CD	3:A1:324:LYS:HB3	2.48	0.43
2:A0:290:GLU:CB	2:A4:124:LYS:CE	2.97	0.43
2:A0:356:ASN:OD1	2:A0:357:TYR:N	2.52	0.43
2:A4:407:TRP:HH2	3:A5:258:ILE:HB	1.83	0.43
3:A5:317:PHE:CE1	3:A5:365:VAL:HG22	2.53	0.43
3:A9:208:TYR:HD1	2:B0:326:LYS:HE3	1.83	0.43
3:A9:220:PRO:HD2	2:B0:326:LYS:CG	2.49	0.43
3:C3:222:TYR:HA	3:C3:225:LEU:HB2	1.99	0.43
2:C6:66:VAL:HG12	2:C6:91:GLN:HB2	2.00	0.43
2:C6:210:TYR:CD1	2:C6:222:PRO:HG2	2.53	0.43
2:C6:334:THR:O	2:C6:337:THR:OG1	2.35	0.43
2:D2:184:PRO:HG2	2:D2:398:MET:HE3	1.99	0.43
3:D7:139:LEU:HD22	3:D7:188:SER:HB2	2.01	0.43
3:E1:284:LEU:HD23	3:E1:362:LYS:HG2	2.01	0.43
2:E4:64:ARG:HB3	2:E4:125:LEU:HD21	2.00	0.43
3:E9:151:LEU:O	3:E9:155:VAL:HG12	2.19	0.43
3:F1:13:GLY:HA2	3:F1:16:ILE:HG22	2.00	0.43
1:7:253:ALA:HA	2:B8:32:PRO:HG2	2.00	0.43
2:A0:182:VAL:HG22	2:A0:185:TYR:HB2	2.00	0.43
2:A0:290:GLU:CB	2:A4:124:LYS:HE2	2.48	0.43
3:A1:172:SER:OG	3:A1:175:VAL:O	2.34	0.43
2:A2:282:TYR:CD2	2:A6:60:LYS:HE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B3:125:GLU:HG2	3:B3:159:TYR:OH	2.18	0.43
2:B4:338:LYS:HG2	2:B4:340:THR:HG22	2.00	0.43
2:C0:416:GLY:O	2:C0:420:GLU:N	2.45	0.43
2:C2:414:GLU:HG2	2:C2:417:GLU:OE2	2.19	0.43
3:C3:309:ARG:NH1	3:C3:339:SER:O	2.52	0.43
2:D0:265:ILE:HG23	2:D0:432:TYR:CZ	2.54	0.43
3:D3:175:VAL:HG12	2:D4:336:LYS:CG	2.49	0.43
3:D5:117:LEU:HA	3:D5:117:LEU:HD12	1.73	0.43
3:D5:215:LEU:O	3:D5:216:LYS:HB2	2.18	0.43
2:E2:265:ILE:HG23	2:E2:432:TYR:CE1	2.53	0.43
2:A0:172:TRP:HB3	2:A0:205:ASP:OD1	2.18	0.43
2:A0:224:TYR:O	2:A0:228:ASN:ND2	2.50	0.43
3:A1:308:GLY:HA3	3:A1:373:ALA:HB2	2.01	0.43
2:A2:277:SER:OG	2:A2:278:ALA:N	2.51	0.43
3:A7:4:ILE:HD11	3:A7:240:LEU:HD22	2.01	0.43
2:A8:250:VAL:HG21	2:A8:352:LYS:HE3	2.00	0.43
2:B0:30:ILE:HG21	2:B0:61:HIS:HD2	1.83	0.43
3:B3:122:LYS:HD3	3:B3:122:LYS:HA	1.83	0.43
2:B4:356:ASN:OD1	2:B4:357:TYR:N	2.52	0.43
2:B8:285:GLN:HG3	2:B8:285:GLN:O	2.18	0.43
3:C1:49:VAL:HG11	3:C1:241:ARG:HG2	2.01	0.43
2:C2:417:GLU:OE2	2:C2:417:GLU:N	2.51	0.43
2:C4:189:LEU:HD21	2:C4:418:PHE:HE1	1.83	0.43
2:C6:135:PHE:CD2	2:C6:166:LYS:HG2	2.48	0.43
3:C7:404:ASP:OD1	3:C7:405:GLU:N	2.49	0.43
2:D0:98:ASP:OD1	2:D0:99:ALA:N	2.52	0.43
3:D1:13:GLY:HA2	3:D1:16:ILE:HG22	2.00	0.43
2:D2:283:HIS:NE2	2:D6:85:HIS:O	2.40	0.43
3:D3:291:GLN:CG	3:D7:122:LYS:HZ3	2.31	0.43
2:D8:214:ARG:HH11	2:D8:214:ARG:HG3	1.83	0.43
2:E0:18:ASN:HD21	2:E0:78:VAL:HG22	1.83	0.43
3:E9:44:LEU:HB2	3:E9:47:ILE:HB	2.01	0.43
1:3:257:PRO:HG3	2:B0:26:LEU:O	2.18	0.43
3:A1:244:GLY:HA2	3:A1:355:ASP:HB2	2.01	0.43
3:A1:259:PRO:HB2	3:A1:260:PHE:CD2	2.54	0.43
3:A1:291:GLN:HB3	3:A5:122:LYS:HE3	2.01	0.43
2:A2:191:THR:HA	2:A2:194:LEU:HB3	2.01	0.43
2:A2:208:ALA:HB2	2:A2:304:LYS:HB2	2.00	0.43
2:A4:27:GLU:HG3	2:A4:361:THR:HG21	2.01	0.43
2:A6:264:ARG:HG3	2:A6:264:ARG:HH11	1.84	0.43
3:A7:113:ILE:HG13	3:A7:117:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A8:73:THR:OG1	3:A9:46:ARG:CZ	2.67	0.43
2:B2:10:GLY:HA2	2:B2:145:THR:HG23	2.00	0.43
2:B4:207:GLU:HA	2:B4:210:TYR:HB2	2.00	0.43
3:B5:8:GLN:HE21	3:B5:65:LEU:HD11	1.84	0.43
2:B8:280:LYS:HA	2:B8:280:LYS:HD3	1.66	0.43
2:C0:338:LYS:HA	2:C0:338:LYS:HD2	1.93	0.43
2:C4:76:ASP:OD1	2:C4:77:GLU:N	2.52	0.43
2:C6:209:ILE:HB	2:C6:227:LEU:HD12	2.00	0.43
2:C6:406:HIS:CE1	3:C7:259:PRO:O	2.72	0.43
2:D2:91:GLN:OE1	2:D2:121:ARG:NH2	2.49	0.43
2:E2:224:TYR:HD2	3:E3:245:GLN:HB3	1.84	0.43
3:E3:211:CYS:HA	3:E3:215:LEU:HB2	2.00	0.43
2:E6:180:ALA:HB3	2:E6:183:GLU:HB3	2.01	0.43
3:E7:282:ARG:O	3:F1:55:THR:CG2	2.67	0.43
2:F0:12:ALA:HB3	2:F0:140:ALA:HB2	2.00	0.43
2:F0:154:LEU:HG	2:F0:197:HIS:HB3	2.00	0.43
3:F1:149:THR:HA	3:F1:152:ILE:HD12	2.01	0.43
2:A0:274:PRO:HG2	2:A0:371:VAL:HG11	2.01	0.43
3:A1:68:LEU:HD21	3:A1:147:MET:SD	2.59	0.43
3:A5:294:PHE:CD2	3:A5:333:VAL:HG21	2.54	0.43
2:A6:36:MET:HA	2:A6:37:PRO:HD3	1.86	0.43
3:B1:281:TYR:CD2	3:B5:87:PRO:HD3	2.53	0.43
2:B4:264:ARG:H	2:B4:264:ARG:HG2	1.71	0.43
2:B6:163:LYS:HD3	2:B6:163:LYS:HA	1.80	0.43
2:B8:274:PRO:HG3	2:B8:286:LEU:HD12	1.99	0.43
2:C0:54:SER:OG	2:C0:55:GLU:N	2.52	0.43
2:C0:166:LYS:HE3	2:C0:166:LYS:HB2	1.88	0.43
2:C6:132:LEU:HD13	2:C6:132:LEU:HA	1.89	0.43
3:C7:28:HIS:NE2	3:C7:241:ARG:HD2	2.34	0.43
3:C7:42:LEU:HD12	3:C7:243:PRO:CD	2.49	0.43
2:D4:93:ILE:HG23	2:D4:117:LEU:HD23	2.01	0.43
2:D4:250:VAL:HG22	2:D4:352:LYS:HZ1	1.83	0.43
2:E2:216:ASN:O	2:E2:280:LYS:HE2	2.19	0.43
3:E3:122:LYS:HD3	3:E3:122:LYS:HA	1.85	0.43
2:F0:223:THR:OG1	2:F0:224:TYR:N	2.52	0.43
3:F1:309:ARG:NH1	3:F1:341:PHE:O	2.49	0.43
3:A1:7:VAL:HG11	3:A1:151:LEU:HD23	2.00	0.43
3:A1:66:MET:HA	3:A1:91:VAL:HG23	2.01	0.43
2:A2:143:GLY:O	2:A2:186:ASN:ND2	2.52	0.43
2:A6:265:ILE:HG23	2:A6:432:TYR:CZ	2.54	0.43
2:B0:71:GLU:HG2	2:B0:73:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:397:LEU:HD23	2:B4:397:LEU:HA	1.85	0.43
2:B8:274:PRO:HB2	2:B8:276:ILE:HG12	2.01	0.43
3:C1:257:LEU:HB3	3:C1:266:PHE:CE1	2.53	0.43
2:C4:276:ILE:HD12	2:C4:281:ALA:HA	2.00	0.43
3:C5:207:LEU:HB3	3:C5:225:LEU:CD1	2.46	0.43
3:C7:19:LYS:HA	3:C7:19:LYS:HD3	1.82	0.43
3:C7:311:LEU:HD12	3:C7:342:VAL:HG11	2.01	0.43
2:C8:154:LEU:HB3	2:C8:197:HIS:HB3	2.01	0.43
2:C8:337:THR:O	2:C8:339:ARG:NH1	2.52	0.43
3:C9:161:ASP:OD1	3:C9:161:ASP:N	2.47	0.43
3:D3:113:ILE:HD12	3:D3:113:ILE:HA	1.91	0.43
3:D7:27:GLU:OE1	3:D7:318:ARG:NH2	2.49	0.43
3:D7:324:LYS:O	3:D7:328:GLU:N	2.32	0.43
2:E0:96:LYS:CE	3:E1:128:ASP:OD2	2.67	0.43
2:E0:179:THR:O	2:E0:180:ALA:HB2	2.19	0.43
2:E2:392:ASP:O	2:E2:422:ARG:NH1	2.41	0.43
3:E3:253:LEU:HD11	3:E3:368:VAL:HG21	2.00	0.43
3:E5:310:TYR:HH	3:E5:367:PHE:HE2	1.67	0.43
3:E7:276:ARG:NH2	3:E7:279:GLN:OE1	2.40	0.43
2:A0:11:GLN:HG3	2:A0:74:VAL:HG11	2.01	0.42
2:A0:232:ALA:HA	2:A0:235:ILE:HG22	2.00	0.42
2:A2:306:ASP:HB3	2:A2:309:HIS:CE1	2.54	0.42
2:A4:3:GLU:OE1	2:A4:132:LEU:HD13	2.19	0.42
3:A5:54:ALA:C	3:A5:56:GLY:H	2.22	0.42
3:A7:206:ALA:HB2	3:A7:302:ALA:HB2	2.00	0.42
2:A8:259:LEU:HD11	2:A8:316:CYS:HB2	2.01	0.42
2:B0:73:THR:HB	3:B1:46:ARG:HE	1.81	0.42
2:B0:339:ARG:HG3	2:B0:339:ARG:O	2.19	0.42
3:C3:262:ARG:HA	3:C3:262:ARG:HD2	1.76	0.42
2:C4:25:CYS:HA	2:C4:30:ILE:HG12	2.00	0.42
3:C5:10:GLY:O	3:C5:14:ASN:ND2	2.52	0.42
2:D4:298:PRO:HG2	2:D4:308:ARG:NH1	2.34	0.42
3:E1:113:ILE:HG12	3:E1:150:LEU:HD22	2.00	0.42
3:E3:289:LEU:HD23	3:E3:289:LEU:HA	1.86	0.42
3:E3:317:PHE:HB3	3:E3:321:MET:SD	2.59	0.42
3:E7:86:ARG:HG2	3:E7:88:ASP:H	1.84	0.42
1:16:241:PHE:CD2	3:E1:43:GLN:HG2	2.54	0.42
1:16:256:LEU:HD13	2:E0:26:LEU:HD13	2.01	0.42
1:17:241:PHE:CD2	3:E3:43:GLN:OE1	2.72	0.42
1:23:257:PRO:HG2	2:C4:26:LEU:O	2.19	0.42
2:A0:79:ARG:CG	2:A0:92:LEU:HD22	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A1:6:HIS:CD2	3:A1:134:GLN:HG3	2.53	0.42
3:A3:180:VAL:O	3:A3:184:ASN:ND2	2.52	0.42
2:A4:48:ALA:HB1	2:A4:243:ARG:O	2.19	0.42
2:A4:103:PHE:H	2:A4:408:TYR:HE1	1.67	0.42
3:A5:257:LEU:HD21	3:A5:314:SER:CB	2.49	0.42
2:A8:10:GLY:O	2:A8:14:ILE:HG12	2.18	0.42
3:A9:139:LEU:HA	3:A9:145:SER:HB2	2.01	0.42
3:B5:6:HIS:HE2	3:B5:8:GLN:HB3	1.84	0.42
3:B5:357:PRO:HB2	3:B5:361:LEU:O	2.19	0.42
2:B8:164:LYS:HD3	2:B8:164:LYS:HA	1.71	0.42
2:C0:168:ASN:HD22	2:C0:198:THR:HG21	1.83	0.42
3:C3:263:LEU:HB3	3:C3:422:TYR:HE1	1.83	0.42
3:C3:287:PRO:HB3	3:C3:329:GLN:HE21	1.84	0.42
2:C4:2:ARG:NE	2:C4:2:ARG:HD2	2.08	0.42
2:C4:268:MET:SD	2:C4:380:ASN:ND2	2.92	0.42
3:C5:220:PRO:CD	2:C6:326:LYS:HD3	2.49	0.42
3:C7:6:HIS:HD1	3:C7:21:TRP:HE1	1.67	0.42
2:D0:231:ILE:O	2:D0:235:ILE:HG12	2.19	0.42
2:D2:194:LEU:O	2:D2:198:THR:HG22	2.20	0.42
2:D2:259:LEU:HD21	2:D2:316:CYS:HB2	2.00	0.42
2:D8:262:TYR:CB	2:D8:263:PRO:HD2	2.45	0.42
3:D9:181:GLU:HB2	3:D9:182:PRO:HD3	2.01	0.42
2:E2:70:LEU:HD12	2:E2:99:ALA:HB2	2.00	0.42
3:E3:200:GLN:HB3	3:E3:268:ILE:HD11	2.01	0.42
3:E5:208:TYR:CE1	3:E5:225:LEU:HD11	2.54	0.42
3:E5:309:ARG:NH1	3:E5:341:PHE:O	2.49	0.42
3:E9:7:VAL:HG22	3:E9:64:ILE:HB	2.01	0.42
2:A0:242:LEU:HD21	2:A0:251:ASP:CB	2.49	0.42
3:A1:47:ILE:HG12	3:A1:51:TYR:HB2	2.01	0.42
3:A1:104:GLY:HA3	3:A1:146:GLY:HA3	2.02	0.42
3:A3:41:ASP:OD1	3:A3:41:ASP:N	2.53	0.42
2:A4:250:VAL:HG23	2:A4:250:VAL:O	2.19	0.42
3:A9:190:HIS:HB2	3:A9:414:ASN:HB3	2.00	0.42
2:B2:69:ASP:OD1	2:B2:70:LEU:N	2.51	0.42
3:B3:102:ALA:HB2	3:B3:398:TYR:HD1	1.84	0.42
3:B5:117:LEU:HD12	3:B5:117:LEU:HA	1.84	0.42
3:B9:7:VAL:HB	3:B9:135:ILE:HG13	2.01	0.42
2:C0:411:GLU:OE1	2:C0:411:GLU:N	2.52	0.42
3:C1:167:PHE:HE1	3:C1:200:GLN:NE2	2.17	0.42
3:C1:177:ASP:HB3	2:C2:353:CYS:SG	2.58	0.42
3:C3:200:GLN:HG3	3:C3:268:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C4:287:SER:N	2:C4:290:GLU:OE2	2.46	0.42
2:C8:283:HIS:NE2	2:D2:85:HIS:O	2.48	0.42
3:D5:155:VAL:HG13	3:D5:164:MET:SD	2.59	0.42
3:D5:392:LYS:HG2	3:D5:395:LEU:HD22	2.01	0.42
2:D8:251:ASP:H	2:D8:254:GLU:HG3	1.85	0.42
3:D9:256:ASN:O	3:D9:312:THR:HG21	2.18	0.42
2:E0:189:LEU:HD11	2:E0:418:PHE:HE1	1.84	0.42
2:E0:208:ALA:O	2:E0:212:ILE:HG12	2.19	0.42
3:E3:113:ILE:HA	3:E3:116:VAL:HG12	2.01	0.42
2:E8:238:LEU:HD12	2:E8:238:LEU:HA	1.82	0.42
3:F1:42:LEU:HD11	3:F1:243:PRO:HG3	2.00	0.42
1:12:250:GLU:HG3	1:12:251:TYR:CD1	2.54	0.42
1:7:256:LEU:HD11	2:B8:31:GLN:CA	2.49	0.42
3:A5:250:LEU:HD23	3:A5:250:LEU:HA	1.88	0.42
3:A7:1:MET:N	3:A7:128:ASP:OD2	2.36	0.42
3:A7:95:THR:OG1	3:A7:96:GLY:N	2.52	0.42
2:B2:230:LEU:HD21	2:B2:368:LEU:HD11	2.00	0.42
2:B6:286:LEU:O	2:B6:373:ARG:HD2	2.19	0.42
2:B6:286:LEU:O	2:B6:373:ARG:NH1	2.37	0.42
3:B7:213:ARG:HD3	3:B7:297:LYS:NZ	2.33	0.42
3:B9:103:LYS:HA	3:B9:107:THR:HG22	2.01	0.42
3:C7:267:LEU:HD21	3:C7:374:ILE:CG2	2.48	0.42
2:C8:306:ASP:HB3	2:C8:309:HIS:CE1	2.55	0.42
3:C9:293:MET:SD	3:C9:365:VAL:HG11	2.58	0.42
3:D5:68:LEU:HB3	3:D5:96:GLY:HA2	2.00	0.42
2:D8:407:TRP:CG	3:D9:255:VAL:HG23	2.53	0.42
2:D8:422:ARG:HA	2:D8:422:ARG:HD2	1.65	0.42
3:D9:290:THR:HG21	3:D9:329:GLN:HB3	2.01	0.42
3:E3:164:MET:H	3:E3:197:ASP:HB2	1.84	0.42
3:E3:247:ASN:HD22	3:E3:247:ASN:C	2.22	0.42
3:E9:386:THR:O	3:E9:390:ARG:HG3	2.19	0.42
2:F0:219:ILE:HG13	2:F0:222:PRO:HD3	2.00	0.42
1:10:254:LYS:H	1:10:254:LYS:HG2	1.65	0.42
1:6:247:TYR:CE2	2:B6:81:GLY:HA3	2.41	0.42
2:A0:164:LYS:HD2	2:A0:164:LYS:HA	1.81	0.42
3:A1:308:GLY:HA2	3:A1:426:GLN:NE2	2.35	0.42
2:A2:306:ASP:HB3	2:A2:309:HIS:HE1	1.83	0.42
2:A4:134:GLY:CA	2:A4:164:LYS:HZ1	2.33	0.42
2:A4:154:LEU:HD23	2:A4:154:LEU:HA	1.94	0.42
2:A6:291:ILE:HD12	2:A6:375:VAL:HG23	2.01	0.42
3:A9:220:PRO:HG2	2:B0:326:LYS:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B1:60:VAL:HA	3:B1:61:PRO:HD3	1.94	0.42
3:B3:44:LEU:HG	3:B3:44:LEU:O	2.20	0.42
3:B9:128:ASP:OD1	3:B9:129:CYS:N	2.41	0.42
2:C2:173:PRO:O	2:C2:390:ARG:NH1	2.53	0.42
3:C3:169:VAL:HG12	3:C3:202:ILE:HB	2.00	0.42
3:C3:238:CYS:SG	3:C3:239:CYS:N	2.92	0.42
2:C4:132:LEU:HB3	2:C4:164:LYS:NZ	2.33	0.42
2:C4:139:ASN:N	2:C4:139:ASN:OD1	2.53	0.42
2:C4:209:ILE:CG2	2:C4:227:LEU:HD22	2.47	0.42
2:C4:377:MET:SD	2:C4:379:SER:HB3	2.60	0.42
3:C9:121:ARG:NH2	3:C9:158:GLU:OE2	2.51	0.42
3:D3:291:GLN:HB3	3:D7:122:LYS:NZ	2.35	0.42
2:D8:388:PHE:HB2	2:D8:429:GLU:OE2	2.19	0.42
3:D9:287:PRO:HA	3:D9:290:THR:HG22	2.01	0.42
2:E2:316:CYS:HA	2:E2:352:LYS:HB2	2.02	0.42
3:E3:113:ILE:HD11	3:E3:151:LEU:HB2	2.01	0.42
2:E6:280:LYS:HZ1	2:F0:89:PRO:HB2	1.74	0.42
3:E7:1:MET:N	3:E7:128:ASP:OD2	2.46	0.42
3:E7:25:SER:HB3	3:E7:30:ILE:HB	2.00	0.42
3:E9:206:ALA:HB2	3:E9:302:ALA:HB2	2.01	0.42
1:11:250:GLU:OE2	2:D0:225:THR:HG21	2.20	0.42
1:14:256:LEU:HD21	2:D6:31:GLN:HG3	2.02	0.42
1:6:256:LEU:HD11	2:B6:31:GLN:CA	2.48	0.42
2:A0:9:VAL:HG22	2:A0:68:LEU:HD22	2.00	0.42
3:A9:92:PHE:O	3:A9:112:LEU:HD11	2.20	0.42
2:B0:138:PHE:CZ	2:B0:235:ILE:HD12	2.54	0.42
3:B3:12:CYS:HB3	3:B3:138:SER:OG	2.19	0.42
2:B4:285:GLN:HB3	2:B8:56:THR:HA	2.02	0.42
2:B6:5:ILE:HD12	2:B6:125:LEU:HD23	2.02	0.42
3:B7:66:MET:HE3	3:B7:116:VAL:HG21	2.02	0.42
2:B8:73:THR:OG1	3:B9:2:ARG:NH2	2.52	0.42
2:C0:370:LYS:HE2	2:C0:370:LYS:HB2	1.87	0.42
2:C2:105:ARG:HH21	2:C2:110:ILE:HG21	1.84	0.42
2:C6:130:THR:HG22	2:C6:131:GLY:N	2.35	0.42
3:D1:1:MET:N	3:D1:128:ASP:OD2	2.38	0.42
2:D4:409:VAL:HG22	2:D4:415:GLU:HB2	2.00	0.42
3:D5:139:LEU:HD22	3:D5:188:SER:HB2	2.01	0.42
2:D6:187:SER:O	2:D6:191:THR:OG1	2.36	0.42
3:D7:186:THR:HG22	3:D7:411:ALA:HB1	2.02	0.42
3:D9:6:HIS:HD2	3:D9:134:GLN:HE21	1.66	0.42
3:E1:156:ARG:NH1	3:E1:162:ARG:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E4:194:LEU:O	2:E4:198:THR:HG22	2.20	0.42
3:E5:67:ASP:OD1	3:E5:68:LEU:N	2.53	0.42
3:E5:109:GLY:O	3:E5:113:ILE:HG12	2.19	0.42
3:E7:216:LYS:HD3	3:E7:216:LYS:HA	1.82	0.42
2:F0:99:ALA:O	2:F0:105:ARG:HD3	2.20	0.42
3:F1:43:GLN:HA	3:F1:242:PHE:CE1	2.54	0.42
1:8:241:PHE:CZ	3:C1:356:ILE:HG23	2.41	0.42
2:A2:370:LYS:HE3	2:A2:370:LYS:HB3	1.89	0.42
3:A3:12:CYS:HB3	3:A3:138:SER:HB2	2.01	0.42
2:A4:309:HIS:NE2	2:A4:386:GLU:OE1	2.53	0.42
2:A8:68:LEU:HD23	2:A8:93:ILE:HB	2.01	0.42
2:B2:319:TYR:N	2:B2:354:GLY:O	2.53	0.42
3:B3:117:LEU:HD23	3:B3:117:LEU:HA	1.82	0.42
2:B4:36:MET:HA	2:B4:37:PRO:HD3	1.90	0.42
3:B5:314:SER:OG	3:B5:315:ALA:N	2.51	0.42
2:B6:269:LEU:HD21	2:B6:384:ILE:HD11	2.01	0.42
2:C0:262:TYR:HB2	2:C0:265:ILE:HG22	2.01	0.42
3:C5:239:CYS:SG	3:C5:248:SER:N	2.84	0.42
2:C6:179:THR:OG1	3:C7:246:LEU:HD21	2.19	0.42
3:C7:90:PHE:HB3	3:C7:92:PHE:CE1	2.54	0.42
3:C7:281:TYR:O	3:D1:86:ARG:HD3	2.19	0.42
3:C9:317:PHE:HB3	3:C9:321:MET:HE1	2.01	0.42
2:D4:283:HIS:CD2	2:D8:60:LYS:HE2	2.55	0.42
2:D4:283:HIS:NE2	2:D8:85:HIS:O	2.48	0.42
3:D7:212:PHE:HE1	2:D8:326:LYS:CE	2.33	0.42
2:D8:163:LYS:H	2:D8:163:LYS:CD	2.26	0.42
2:D8:210:TYR:OH	3:D9:323:THR:OG1	2.24	0.42
2:E2:2:ARG:HD3	2:E2:2:ARG:HA	1.90	0.42
3:F1:256:ASN:ND2	3:F1:350:LYS:HG3	2.35	0.42
2:A0:136:LEU:HD23	2:A0:136:LEU:HA	1.89	0.42
2:A0:428:LEU:HD12	2:A0:428:LEU:HA	1.91	0.42
3:A1:21:TRP:CZ2	3:A1:63:ALA:HB2	2.54	0.42
2:A4:36:MET:HA	2:A4:37:PRO:HD3	1.74	0.42
3:A5:178:THR:O	3:A5:181:GLU:HG2	2.19	0.42
2:A8:306:ASP:HB3	2:A8:309:HIS:CE1	2.55	0.42
3:B1:281:TYR:CE2	3:B5:87:PRO:HD3	2.55	0.42
3:B3:152:ILE:HA	3:B3:155:VAL:HG12	2.00	0.42
3:B5:139:LEU:HA	3:B5:145:SER:HB3	2.01	0.42
2:B8:254:GLU:HG2	2:B8:352:LYS:HE2	2.00	0.42
3:B9:15:GLN:O	3:B9:226:ASN:ND2	2.52	0.42
3:B9:101:TRP:H	3:B9:398:TYR:HE1	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B9:287:PRO:HA	3:B9:290:THR:HG22	2.02	0.42
3:C3:275:SER:OG	3:C3:276:ARG:N	2.52	0.42
2:C6:53:PHE:HB3	2:C6:61:HIS:HB3	2.01	0.42
3:C7:167:PHE:CD2	3:C7:233:MET:HG2	2.55	0.42
2:C8:311:LYS:HB3	2:C8:311:LYS:HE3	1.68	0.42
2:D0:119:LEU:HD11	2:D0:157:LEU:HD22	2.01	0.42
2:D0:205:ASP:O	2:D0:209:ILE:HG13	2.20	0.42
3:D3:313:ALA:HB3	3:D3:349:MET:SD	2.60	0.42
2:D6:138:PHE:CZ	2:D6:235:ILE:HD12	2.53	0.42
3:D7:150:LEU:HD21	3:D7:154:LYS:HE2	2.01	0.42
3:D7:173:PRO:HB3	3:D7:380:ARG:HH21	1.84	0.42
3:E3:113:ILE:O	3:E3:117:LEU:HB2	2.20	0.42
2:E4:398:MET:HA	2:E4:398:MET:HE3	2.02	0.42
2:E8:345:ASP:OD1	2:E8:346:TRP:N	2.53	0.42
3:F1:205:GLU:OE1	3:F1:205:GLU:N	2.53	0.42
1:18:241:PHE:HE2	3:E5:42:LEU:HB2	1.85	0.42
1:22:246:CYS:SG	1:22:247:TYR:N	2.93	0.42
2:A8:90:GLU:HB2	2:A8:121:ARG:NH2	2.34	0.42
2:B0:5:ILE:HD12	2:B0:125:LEU:HD23	2.02	0.42
2:B0:250:VAL:HG22	2:B0:352:LYS:NZ	2.35	0.42
3:B1:237:THR:HA	3:B1:240:LEU:HD13	2.02	0.42
2:B2:156:ARG:HA	2:B2:159:VAL:HG12	2.02	0.42
2:B2:163:LYS:HD3	2:B2:163:LYS:N	2.35	0.42
2:B2:422:ARG:HD2	2:B2:422:ARG:HA	1.93	0.42
2:B4:185:TYR:CD2	2:B4:395:PHE:HE1	2.37	0.42
3:B5:150:LEU:CD2	3:B5:154:LYS:HD2	2.50	0.42
2:C2:259:LEU:HD23	2:C2:259:LEU:HA	1.92	0.42
3:C7:133:PHE:HB2	3:C7:164:MET:HB3	2.01	0.42
3:C9:167:PHE:CE1	3:C9:200:GLN:HG3	2.54	0.42
3:C9:174:LYS:HG3	3:C9:175:VAL:N	2.34	0.42
2:D0:221:ARG:HH11	2:D0:221:ARG:HD3	1.72	0.42
2:D0:311:LYS:O	2:D0:382:THR:HG23	2.20	0.42
3:D5:68:LEU:HD12	3:D5:143:THR:HG22	2.02	0.42
3:D5:77:ARG:HH22	3:D5:92:PHE:HZ	1.68	0.42
3:D5:117:LEU:CD2	3:D5:154:LYS:HD2	2.47	0.42
3:D7:273:LEU:HD23	3:D7:273:LEU:HA	1.88	0.42
2:E6:316:CYS:CB	2:E6:352:LYS:HG3	2.50	0.42
2:E6:345:ASP:OD1	2:E6:346:TRP:N	2.52	0.42
3:E9:293:MET:SD	3:E9:367:PHE:HB2	2.60	0.42
3:E9:399:THR:HA	3:E9:403:MET:HB2	2.01	0.42
3:F1:47:ILE:HD12	3:F1:47:ILE:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A1:10:GLY:O	3:A1:14:ASN:ND2	2.43	0.42
3:A1:239:CYS:HB3	3:A1:248:SER:O	2.19	0.42
2:A2:141:VAL:HG11	2:A2:172:TRP:CE3	2.54	0.42
2:A4:112:LYS:HA	2:A4:115:VAL:HG12	2.00	0.42
3:A5:201:VAL:HG11	3:A5:374:ILE:HD11	2.02	0.42
2:A6:125:LEU:HD23	2:A6:125:LEU:HA	1.92	0.42
2:A8:163:LYS:HA	2:A8:163:LYS:HE3	2.02	0.42
2:B0:149:LEU:HD23	2:B0:149:LEU:HA	1.92	0.42
2:B0:259:LEU:HD11	2:B0:316:CYS:HB2	2.01	0.42
3:B1:181:GLU:HB2	3:B1:182:PRO:HD3	2.02	0.42
3:B7:210:ILE:O	3:B7:214:THR:OG1	2.28	0.42
2:B8:215:ARG:HH12	2:B8:299:ALA:HB1	1.85	0.42
2:C0:223:THR:OG1	3:C1:245:GLN:CD	2.58	0.42
3:C1:20:PHE:CE1	3:C1:24:ILE:HG13	2.55	0.42
3:C1:181:GLU:HB2	3:C1:182:PRO:HD3	2.00	0.42
3:C3:173:PRO:HA	3:C3:380:ARG:HH21	1.85	0.42
2:C4:93:ILE:HD12	2:C4:114:ILE:HG13	2.02	0.42
2:C6:103:PHE:HB3	2:C6:189:LEU:HD23	2.02	0.42
2:C6:187:SER:O	2:C6:191:THR:HG23	2.20	0.42
3:C9:113:ILE:HG12	3:C9:150:LEU:HD22	2.02	0.42
2:D2:121:ARG:HD2	2:D2:121:ARG:HA	1.77	0.42
2:D2:174:SER:HB2	2:D2:177:VAL:O	2.19	0.42
3:D3:169:VAL:HG12	3:D3:202:ILE:HB	2.01	0.42
3:D3:385:PHE:HE2	3:D3:412:GLU:HB2	1.84	0.42
3:E3:46:ARG:CG	3:E3:46:ARG:NH2	2.82	0.42
3:E5:2:ARG:HD3	3:E5:240:LEU:HD23	2.01	0.42
2:F0:152:LEU:HD11	2:F0:156:ARG:HH11	1.85	0.42
3:A1:117:LEU:HD13	3:A1:154:LYS:HZ2	1.82	0.41
3:A1:274:THR:HG21	3:A1:282:ARG:HD2	2.02	0.41
2:A4:363:VAL:HA	2:A4:364:PRO:HD3	1.95	0.41
3:A5:181:GLU:HB2	3:A5:182:PRO:HD3	2.02	0.41
2:A8:12:ALA:HB3	2:A8:140:ALA:HB2	2.01	0.41
2:A8:221:ARG:HB3	3:A9:322:SER:CB	2.50	0.41
3:A9:232:ALA:HB1	3:A9:268:ILE:HG21	2.02	0.41
2:B4:25:CYS:SG	2:B4:86:LEU:HD11	2.59	0.41
2:B4:154:LEU:HB3	2:B4:197:HIS:HB3	2.02	0.41
2:B4:277:SER:OG	2:B4:278:ALA:N	2.53	0.41
2:B4:284:GLU:OE2	2:B8:88:HIS:CD2	2.73	0.41
2:B6:239:THR:OG1	2:B6:243:ARG:NH1	2.52	0.41
2:B6:397:LEU:HD23	2:B6:397:LEU:HA	1.88	0.41
2:B8:282:TYR:HE2	2:C2:85:HIS:CB	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B9:165:GLU:OE2	3:B9:200:GLN:NE2	2.52	0.41
3:C1:167:PHE:HE1	3:C1:200:GLN:HE21	1.67	0.41
3:C3:210:ILE:O	3:C3:214:THR:OG1	2.26	0.41
2:C4:23:LEU:HD11	2:C4:233:GLN:OE1	2.20	0.41
3:C5:32:PRO:HD3	3:C5:81:PHE:CZ	2.55	0.41
2:C8:60:LYS:NZ	2:C8:61:HIS:O	2.48	0.41
2:D2:136:LEU:CD2	2:D2:235:ILE:HD11	2.48	0.41
3:D3:207:LEU:HB3	3:D3:225:LEU:HG	2.01	0.41
3:E7:232:ALA:HB2	3:E7:270:PHE:HB2	2.02	0.41
1:12:241:PHE:CE1	3:D3:356:ILE:CG2	3.02	0.41
1:3:255:PRO:HG2	2:B0:364:PRO:HG2	2.02	0.41
2:A0:73:THR:O	3:A1:46:ARG:NH1	2.53	0.41
3:A3:172:SER:HB3	3:A3:205:GLU:HG2	2.03	0.41
3:A5:409:THR:HA	3:A5:412:GLU:HG3	2.02	0.41
2:A6:69:ASP:OD1	2:A6:70:LEU:N	2.54	0.41
2:A8:107:HIS:CE1	2:A8:151:CYS:HB3	2.55	0.41
3:B3:241:ARG:HH11	3:B3:241:ARG:HD2	1.73	0.41
2:B6:345:ASP:OD1	2:B6:346:TRP:N	2.53	0.41
3:B7:383:ASP:HA	3:B7:386:THR:HG22	2.00	0.41
2:B8:192:HIS:ND1	2:B8:424:ASP:OD2	2.48	0.41
3:C5:121:ARG:NH1	3:C5:158:GLU:OE1	2.45	0.41
3:C5:286:VAL:N	3:C5:287:PRO:HD2	2.35	0.41
3:C7:248:SER:HA	3:C7:252:LYS:HD3	2.02	0.41
2:C8:121:ARG:HA	2:C8:121:ARG:HD2	1.87	0.41
3:C9:19:LYS:HA	3:C9:19:LYS:HD3	1.83	0.41
3:C9:128:ASP:OD1	3:C9:129:CYS:N	2.47	0.41
3:D3:117:LEU:HD11	3:D3:154:LYS:HD3	2.02	0.41
2:D6:154:LEU:HB3	2:D6:197:HIS:HB3	2.02	0.41
2:E2:11:GLN:HE22	3:E3:246:LEU:HD12	1.84	0.41
2:E4:403:ALA:HA	3:E5:260:PHE:CE1	2.56	0.41
3:E5:180:VAL:HB	3:E5:183:TYR:HB2	2.03	0.41
3:E5:286:VAL:HG23	3:E5:287:PRO:HD3	2.00	0.41
2:E8:71:GLU:HB3	2:E8:98:ASP:HB2	2.01	0.41
3:E9:113:ILE:HG13	3:E9:150:LEU:HD22	2.01	0.41
3:E9:128:ASP:OD1	3:E9:128:ASP:N	2.50	0.41
3:E9:167:PHE:CZ	3:E9:233:MET:HG2	2.55	0.41
3:E9:259:PRO:HB2	3:E9:260:PHE:HD1	1.86	0.41
3:F1:187:LEU:HD11	3:F1:408:PHE:CE1	2.55	0.41
1:9:243:ALA:CB	3:C3:356:ILE:CD1	2.99	0.41
2:A0:27:GLU:OE2	2:A0:236:SER:OG	2.37	0.41
2:A0:172:TRP:CZ2	2:A0:391:MET:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A0:216:ASN:HD22	2:A0:275:ILE:HG13	1.86	0.41
2:A0:259:LEU:HD21	2:A0:316:CYS:HB2	2.02	0.41
3:A1:43:GLN:HA	3:A1:242:PHE:HE1	1.84	0.41
3:A3:271:ALA:HB3	3:A3:365:VAL:HG22	2.01	0.41
2:A4:264:ARG:HD3	2:A4:431:ASP:OD2	2.19	0.41
2:A6:271:SER:OG	2:A6:377:MET:HB3	2.20	0.41
2:B6:5:ILE:HG12	2:B6:132:LEU:HD11	2.02	0.41
3:B7:152:ILE:HG22	3:B7:195:ASN:HB3	2.02	0.41
3:C1:391:ARG:HE	3:C1:391:ARG:HB3	1.78	0.41
2:C2:210:TYR:CE1	2:C2:227:LEU:HD21	2.56	0.41
3:C3:190:HIS:HB2	3:C3:414:ASN:ND2	2.29	0.41
2:C4:208:ALA:O	2:C4:212:ILE:HG12	2.19	0.41
3:C7:291:GLN:NE2	3:D1:125:GLU:CD	2.70	0.41
2:C8:166:LYS:HE3	2:C8:166:LYS:HB3	1.95	0.41
2:C8:210:TYR:HB3	3:C9:324:LYS:NZ	2.36	0.41
2:C8:215:ARG:HH22	2:C8:300:SER:HB2	1.84	0.41
2:C8:288:VAL:HG21	2:C8:323:VAL:HG23	2.03	0.41
2:C8:407:TRP:HH2	3:C9:254:ALA:HB1	1.85	0.41
2:D2:99:ALA:HA	2:D2:110:ILE:HD11	2.02	0.41
2:D4:258:ASN:ND2	2:D4:352:LYS:HD3	2.35	0.41
3:D5:156:ARG:NH2	3:D5:197:ASP:HB2	2.35	0.41
3:D5:283:ALA:HB2	3:D9:53:GLU:O	2.21	0.41
3:D7:178:THR:HG22	2:D8:352:LYS:HZ3	1.85	0.41
2:E0:214:ARG:NH1	2:E0:220:GLU:OE2	2.52	0.41
2:E2:176:GLN:HB3	3:E3:331:LEU:CD1	2.50	0.41
2:E4:109:THR:HG23	2:E4:411:GLU:OE1	2.20	0.41
2:E6:230:LEU:HD21	2:E6:368:LEU:HD11	2.01	0.41
3:E7:8:GLN:OE1	3:E7:17:GLY:HA3	2.20	0.41
3:E7:362:LYS:HD2	3:E7:363:MET:HB2	2.02	0.41
3:F1:112:LEU:HG	3:F1:112:LEU:O	2.21	0.41
2:A8:210:TYR:CD2	3:A9:324:LYS:HG3	2.55	0.41
2:A8:225:THR:O	2:A8:229:ARG:HG2	2.21	0.41
3:A9:33:THR:HG23	3:A9:35:THR:HG23	2.03	0.41
3:B1:238:CYS:HB3	3:B1:318:ARG:NH1	2.35	0.41
2:B2:3:GLU:OE1	2:B2:64:ARG:NE	2.53	0.41
2:B2:298:PRO:HB3	2:B2:307:PRO:HD2	2.02	0.41
3:B7:128:ASP:OD1	3:B7:129:CYS:N	2.41	0.41
3:B7:175:VAL:HG11	2:B8:332:VAL:HG13	2.02	0.41
2:C0:241:SER:OG	2:C0:250:VAL:O	2.25	0.41
2:C0:274:PRO:HD2	2:C0:374:ALA:HA	2.02	0.41
2:C6:154:LEU:HG	2:C6:197:HIS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C6:215:ARG:HB2	2:C6:215:ARG:HH11	1.85	0.41
3:C9:54:ALA:C	3:C9:56:GLY:H	2.24	0.41
3:C9:220:PRO:HG2	2:D0:326:LYS:CD	2.51	0.41
2:D2:163:LYS:HE3	2:D2:163:LYS:HB3	1.79	0.41
3:D3:317:PHE:HB3	3:D3:321:MET:SD	2.60	0.41
2:D4:28:HIS:CE1	2:D4:243:ARG:HD2	2.56	0.41
2:D4:180:ALA:HB3	2:D4:183:GLU:HG3	2.00	0.41
2:D6:221:ARG:HB3	3:D7:322:SER:CB	2.51	0.41
3:E1:395:LEU:O	3:E1:395:LEU:HG	2.21	0.41
3:E3:165:GLU:OE1	3:E3:200:GLN:NE2	2.53	0.41
1:15:256:LEU:HD13	2:D8:30:ILE:C	2.37	0.41
3:A3:113:ILE:HA	3:A3:116:VAL:HG22	2.01	0.41
2:A4:207:GLU:HA	2:A4:210:TYR:CD2	2.55	0.41
3:B1:249:ASP:H	3:B1:252:LYS:CB	2.33	0.41
3:B3:211:CYS:SG	3:B3:217:LEU:HB2	2.61	0.41
2:B4:96:LYS:HE3	3:B5:1:MET:C	2.40	0.41
2:B4:272:TYR:HD2	2:B4:275:ILE:HD11	1.86	0.41
3:B7:375:GLN:HE22	3:B7:419:VAL:HA	1.85	0.41
3:B9:46:ARG:HE	3:B9:46:ARG:HB2	1.39	0.41
2:C0:76:ASP:HA	2:C0:79:ARG:HD2	2.02	0.41
2:C0:254:GLU:HA	2:C0:257:THR:HG22	2.03	0.41
2:C4:141:VAL:HG11	2:C4:172:TRP:CE3	2.56	0.41
3:C5:105:HIS:ND1	3:C5:150:LEU:HB2	2.36	0.41
2:C8:274:PRO:HB2	2:C8:276:ILE:HG12	2.01	0.41
2:D2:69:ASP:O	2:D2:94:SER:HA	2.20	0.41
2:D2:404:PHE:CZ	3:D3:312:THR:HG21	2.55	0.41
2:D6:174:SER:HB2	2:D6:177:VAL:O	2.20	0.41
2:D6:222:PRO:HD2	3:D7:324:LYS:NZ	2.35	0.41
3:E3:192:LEU:HD21	3:E3:199:VAL:HG21	2.03	0.41
3:E5:281:TYR:HD2	3:E9:86:ARG:HA	1.84	0.41
2:E6:203:MET:SD	2:E6:267:PHE:HD2	2.44	0.41
3:F1:258:ILE:HG13	3:F1:258:ILE:O	2.20	0.41
1:23:254:LYS:HB3	2:C4:364:PRO:HD2	2.02	0.41
1:7:242:ASN:OD1	1:7:242:ASN:N	2.53	0.41
3:A1:24:ILE:HD13	3:A1:24:ILE:HA	1.98	0.41
2:A2:119:LEU:HD23	2:A2:119:LEU:HA	1.85	0.41
2:A2:212:ILE:HG23	2:A2:275:ILE:HD12	2.03	0.41
2:A4:288:VAL:HG21	2:A4:323:VAL:HG13	2.02	0.41
3:A5:5:VAL:HB	3:A5:133:PHE:CD1	2.56	0.41
3:A5:216:LYS:HA	3:A5:216:LYS:HD2	1.91	0.41
3:A7:6:HIS:CD2	3:A7:8:GLN:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A7:173:PRO:HB3	3:A7:380:ARG:HD2	2.03	0.41
2:A8:6:SER:OG	2:A8:8:HIS:NE2	2.45	0.41
3:B5:253:LEU:O	3:B5:257:LEU:HB2	2.20	0.41
2:B6:342:GLN:OE1	2:B6:342:GLN:HA	2.20	0.41
3:B7:156:ARG:NH1	3:B7:197:ASP:OD1	2.53	0.41
2:B8:185:TYR:HE1	2:B8:398:MET:HG2	1.85	0.41
3:B9:12:CYS:SG	3:B9:169:VAL:HG21	2.61	0.41
3:B9:141:GLY:O	3:B9:145:SER:OG	2.30	0.41
2:C2:417:GLU:HA	2:C2:420:GLU:HG3	2.01	0.41
2:C4:210:TYR:CD1	2:C4:227:LEU:HD21	2.56	0.41
3:C5:190:HIS:HA	3:C5:193:VAL:HG22	2.03	0.41
2:C6:231:ILE:HD13	2:C6:302:MET:HE1	2.01	0.41
3:C7:165:GLU:HG3	3:C7:198:GLU:HG3	2.02	0.41
3:C9:166:THR:OG1	3:C9:199:VAL:HG22	2.20	0.41
3:D1:117:LEU:HA	3:D1:117:LEU:HD13	1.97	0.41
3:D3:117:LEU:HA	3:D3:117:LEU:HD23	1.84	0.41
3:D7:27:GLU:HA	3:D7:359:LYS:HD2	2.02	0.41
3:D9:24:ILE:HD13	3:D9:24:ILE:HA	1.93	0.41
3:D9:239:CYS:SG	3:D9:247:ASN:HB3	2.61	0.41
2:E0:178:SER:O	2:E0:179:THR:OG1	2.34	0.41
2:E6:209:ILE:HD13	2:E6:231:ILE:HD11	2.01	0.41
2:F0:392:ASP:OD1	2:F0:422:ARG:NE	2.51	0.41
2:A2:91:GLN:HA	2:A2:121:ARG:NH1	2.33	0.41
3:A3:12:CYS:CB	3:A3:138:SER:HB2	2.50	0.41
3:A3:412:GLU:OE1	3:A3:416:ASN:ND2	2.53	0.41
2:A4:28:HIS:HE2	2:A4:243:ARG:HD2	1.84	0.41
2:A4:115:VAL:HG21	2:A4:152:LEU:HG	2.02	0.41
3:A5:2:ARG:NH2	3:A5:249:ASP:OD2	2.53	0.41
2:A6:27:GLU:HG3	2:A6:361:THR:HG21	2.03	0.41
2:A6:340:THR:HG23	2:A6:341:ILE:HG13	2.02	0.41
3:A7:140:GLY:O	3:A7:184:ASN:ND2	2.50	0.41
3:A9:63:ALA:O	3:A9:89:ASN:ND2	2.54	0.41
3:A9:101:TRP:HD1	3:A9:145:SER:HG	1.67	0.41
3:A9:200:GLN:HB3	3:A9:268:ILE:HD11	2.01	0.41
3:B1:263:LEU:HD23	3:B1:263:LEU:H	1.85	0.41
2:B2:221:ARG:HG3	2:B2:221:ARG:HH11	1.86	0.41
2:B2:221:ARG:HH11	2:B2:221:ARG:CG	2.33	0.41
3:B3:114:ASP:OD1	3:B3:114:ASP:N	2.54	0.41
3:B3:128:ASP:OD1	3:B3:128:ASP:N	2.53	0.41
3:B5:200:GLN:HB3	3:B5:268:ILE:HD11	2.02	0.41
3:C1:148:GLY:O	3:C1:152:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C2:425:LEU:HA	2:C2:425:LEU:HD23	1.80	0.41
2:C4:192:HIS:ND1	2:C4:424:ASP:OD2	2.49	0.41
3:C5:221:THR:O	3:C5:225:LEU:HD23	2.19	0.41
3:C7:238:CYS:SG	3:C7:239:CYS:N	2.94	0.41
3:C7:325:GLU:HA	3:C7:328:GLU:HG2	2.02	0.41
3:C9:228:LEU:HA	3:C9:228:LEU:HD23	1.84	0.41
2:D0:425:LEU:HD12	2:D0:425:LEU:HA	1.93	0.41
3:D3:187:LEU:HD21	3:D3:408:PHE:CD1	2.56	0.41
3:D3:383:ASP:HA	3:D3:386:THR:HG22	2.02	0.41
2:D4:36:MET:HE2	2:D4:36:MET:HB3	1.88	0.41
3:D5:309:ARG:HH11	3:D5:309:ARG:HD2	1.53	0.41
3:D7:117:LEU:HD23	3:D7:121:ARG:NH2	2.36	0.41
3:E5:396:HIS:HA	3:E5:399:THR:HG22	2.02	0.41
2:E8:189:LEU:HD21	2:E8:418:PHE:CD1	2.56	0.41
2:E8:213:CYS:HA	2:E8:217:LEU:HB3	2.03	0.41
2:F0:231:ILE:O	2:F0:235:ILE:HG12	2.21	0.41
1:23:256:LEU:HA	1:23:257:PRO:HD3	1.96	0.41
2:A2:137:MET:HB3	2:A2:168:ASN:HA	2.02	0.41
3:A3:112:LEU:HD12	3:A3:112:LEU:HA	1.92	0.41
2:A6:262:TYR:HB3	2:A6:263:PRO:HD2	2.02	0.41
3:A7:114:ASP:OD1	3:A7:115:SER:N	2.54	0.41
2:B2:180:ALA:O	3:B3:347:ASN:ND2	2.54	0.41
2:B4:359:PRO:HA	2:B4:360:PRO:HD3	1.96	0.41
3:B9:107:THR:HG21	3:B9:401:GLU:OE1	2.21	0.41
3:C1:128:ASP:OD1	3:C1:129:CYS:N	2.52	0.41
3:C1:211:CYS:HA	3:C1:215:LEU:HB2	2.03	0.41
3:C7:256:ASN:HD21	3:C7:350:LYS:HD3	1.86	0.41
2:D0:96:LYS:HD2	2:D0:96:LYS:HA	1.88	0.41
3:D1:375:GLN:HG3	3:D1:419:VAL:HG13	2.02	0.41
2:D4:30:ILE:HG22	2:D4:36:MET:HB3	2.03	0.41
3:D5:32:PRO:HD3	3:D5:81:PHE:CZ	2.54	0.41
2:D8:100:ALA:HB1	3:D9:252:LYS:HA	2.02	0.41
2:E4:98:ASP:OD1	2:E4:99:ALA:N	2.52	0.41
2:F0:320:ARG:HG2	2:F0:360:PRO:HG3	2.03	0.41
1:5:256:LEU:CD2	2:B4:31:GLN:HA	2.47	0.41
2:A0:210:TYR:HD1	2:A0:210:TYR:HA	1.76	0.41
2:A0:269:LEU:HD23	2:A0:303:ALA:HB3	2.02	0.41
3:A1:365:VAL:HG22	3:A1:366:THR:N	2.35	0.41
2:A4:269:LEU:HD23	2:A4:301:MET:HE2	2.03	0.41
3:A5:229:VAL:O	3:A5:233:MET:HG3	2.21	0.41
3:A5:326:VAL:O	3:A5:330:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A6:370:LYS:HE3	2:A6:370:LYS:HB3	1.83	0.41
3:A7:190:HIS:HB2	3:A7:414:ASN:ND2	2.34	0.41
3:A7:259:PRO:HG2	3:A7:311:LEU:CD2	2.49	0.41
3:A9:192:LEU:HD21	3:A9:199:VAL:HG21	2.02	0.41
3:A9:217:LEU:HD23	3:A9:217:LEU:HA	1.91	0.41
2:B0:73:THR:CA	3:B1:46:ARG:HH11	2.19	0.41
2:B2:5:ILE:HG12	2:B2:132:LEU:HD11	2.03	0.41
2:B2:181:VAL:HG11	3:B3:256:ASN:O	2.21	0.41
2:B4:311:LYS:H	2:B4:382:THR:CG2	2.34	0.41
2:B6:215:ARG:NH2	2:B6:299:ALA:O	2.53	0.41
2:B6:302:MET:HB2	2:B6:302:MET:HE2	1.90	0.41
2:B6:392:ASP:HA	2:B6:422:ARG:HH12	1.86	0.41
3:B7:13:GLY:HA2	3:B7:136:THR:HG22	2.03	0.41
3:B7:192:LEU:HD21	3:B7:199:VAL:HG21	2.03	0.41
2:B8:69:ASP:OD1	2:B8:70:LEU:N	2.54	0.41
2:B8:283:HIS:CE1	2:C2:89:PRO:HD3	2.56	0.41
2:C0:181:VAL:H	3:C1:256:ASN:HD21	1.69	0.41
2:C0:275:ILE:HD12	2:C0:368:LEU:HD11	2.02	0.41
2:C2:53:PHE:O	2:C2:64:ARG:NH2	2.54	0.41
2:C2:207:GLU:HA	2:C2:210:TYR:HB2	2.03	0.41
2:C4:105:ARG:HG2	2:C4:411:GLU:HG2	2.03	0.41
2:C4:356:ASN:OD1	2:C4:357:TYR:N	2.51	0.41
3:C5:282:ARG:NH1	3:C5:288:GLU:OE2	2.54	0.41
3:C7:417:ASP:O	3:C7:420:SER:OG	2.27	0.41
3:C9:22:GLU:HG3	3:C9:81:PHE:CD2	2.56	0.41
3:C9:190:HIS:HA	3:C9:193:VAL:HG12	2.03	0.41
2:D0:88:HIS:CD2	2:D0:90:GLU:HB3	2.55	0.41
2:D0:207:GLU:HA	2:D0:210:TYR:HB2	2.03	0.41
2:D2:122:ILE:HD13	2:D2:122:ILE:HA	1.95	0.41
2:D2:176:GLN:OE1	3:D3:331:LEU:HD21	2.20	0.41
3:D3:173:PRO:HD2	3:D3:205:GLU:HG3	2.02	0.41
3:D3:191:GLN:HA	3:D3:194:GLU:HG2	2.03	0.41
2:D6:79:ARG:O	2:D6:84:ARG:HG2	2.21	0.41
2:D6:123:ARG:HH11	2:D6:123:ARG:HG3	1.86	0.41
2:D6:270:SER:HB2	2:D6:302:MET:HB2	2.03	0.41
2:D6:272:TYR:HD2	2:D6:275:ILE:HG23	1.86	0.41
3:D7:20:PHE:HA	3:D7:230:SER:HB2	2.03	0.41
3:D7:66:MET:HB2	3:D7:66:MET:HE2	1.82	0.41
3:D7:220:PRO:HG2	2:D8:326:LYS:HD2	2.03	0.41
3:D7:228:LEU:HD23	3:D7:228:LEU:HA	1.97	0.41
2:D8:12:ALA:CB	2:D8:140:ALA:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D8:392:ASP:OD1	2:D8:422:ARG:NH2	2.49	0.41
2:E0:50:ASN:O	2:E0:64:ARG:NH2	2.54	0.41
2:E0:105:ARG:HH12	3:E1:251:ARG:HD3	1.86	0.41
3:E1:113:ILE:HD11	3:E1:151:LEU:HD13	2.02	0.41
3:E1:207:LEU:HB3	3:E1:225:LEU:HD22	2.02	0.41
2:E2:363:VAL:HA	2:E2:364:PRO:HD3	1.94	0.41
2:E4:276:ILE:HD11	2:E4:280:LYS:HG2	2.03	0.41
3:E5:326:VAL:O	3:E5:330:MET:HG2	2.20	0.41
3:E7:2:ARG:HD2	3:E7:240:LEU:HD23	2.03	0.41
3:E7:28:HIS:HA	3:E7:43:GLN:HG2	2.02	0.41
2:E8:141:VAL:HG11	2:E8:172:TRP:CZ3	2.56	0.41
2:E8:212:ILE:HD13	2:E8:212:ILE:HA	1.95	0.41
2:E8:339:ARG:HD2	2:E8:339:ARG:HA	1.82	0.41
3:F1:19:LYS:HZ1	3:F1:227:HIS:HB2	1.85	0.41
3:F1:133:PHE:HZ	3:F1:159:TYR:HD2	1.68	0.41
3:F1:314:SER:HB3	3:F1:368:VAL:HG13	2.03	0.41
3:F1:330:MET:HG2	3:F1:349:MET:HG2	2.02	0.41
3:A1:136:THR:HG22	3:A1:167:PHE:HD2	1.85	0.41
3:A3:113:ILE:HA	3:A3:113:ILE:HD13	1.97	0.41
2:A4:210:TYR:CG	3:A5:324:LYS:HE2	2.56	0.41
2:A6:132:LEU:H	2:A6:132:LEU:HD23	1.86	0.41
3:B1:248:SER:HA	3:B1:252:LYS:HG2	2.02	0.41
2:B4:274:PRO:HG3	2:B4:286:LEU:CD1	2.50	0.41
3:B9:50:PHE:CE2	3:B9:241:ARG:HD3	2.55	0.41
2:C0:387:VAL:HG13	2:C0:388:PHE:CD1	2.56	0.41
3:C3:103:LYS:HB3	3:C3:103:LYS:HE2	1.86	0.41
3:C5:213:ARG:HH22	3:C5:297:LYS:HG3	1.85	0.41
2:C8:340:THR:O	2:C8:340:THR:HG22	2.21	0.41
2:D2:230:LEU:HD21	2:D2:368:LEU:HD11	2.02	0.41
3:D3:403:MET:HE3	3:D3:403:MET:HB2	1.93	0.41
2:D4:8:HIS:CE1	2:D4:138:PHE:CD2	3.08	0.41
2:D6:204:LEU:HD13	2:D6:231:ILE:HD12	2.02	0.41
3:E5:12:CYS:CB	3:E5:138:SER:HB2	2.47	0.41
3:E5:25:SER:HB3	3:E5:30:ILE:HB	2.03	0.41
3:E5:101:TRP:HD1	3:E5:145:SER:HG	1.66	0.41
3:E5:261:PRO:O	3:E5:264:HIS:ND1	2.50	0.41
2:E6:352:LYS:HA	2:E6:352:LYS:HD3	1.87	0.41
2:E8:191:THR:CG2	2:E8:425:LEU:HD21	2.50	0.41
3:F1:205:GLU:HA	3:F1:208:TYR:HB2	2.03	0.41
1:13:256:LEU:HD13	2:D4:29:GLY:C	2.41	0.40
1:16:253:ALA:N	2:E0:82:THR:HG21	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:257:PRO:HA	1:5:258:PRO:HD3	1.99	0.40
1:8:243:ALA:HB1	3:C1:357:PRO:HD3	2.03	0.40
2:A2:15:GLN:HB3	2:A2:228:ASN:HD21	1.85	0.40
2:A8:73:THR:OG1	3:A9:46:ARG:NH2	2.54	0.40
3:A9:257:LEU:O	3:A9:259:PRO:HD3	2.21	0.40
3:A9:392:LYS:HD3	3:A9:395:LEU:HG	2.02	0.40
2:B2:177:VAL:HG12	3:B3:331:LEU:CB	2.51	0.40
2:B4:69:ASP:OD1	2:B4:70:LEU:N	2.53	0.40
2:B8:167:LEU:HD22	2:B8:200:VAL:HB	2.02	0.40
2:C2:306:ASP:OD1	2:C2:308:ARG:HG2	2.21	0.40
2:C6:88:HIS:HA	2:C6:89:PRO:HD3	1.97	0.40
3:C9:220:PRO:CG	2:D0:326:LYS:NZ	2.71	0.40
3:C9:238:CYS:SG	3:C9:318:ARG:NE	2.90	0.40
3:C9:246:LEU:HD12	3:C9:246:LEU:HA	1.93	0.40
2:D2:6:SER:OG	2:D2:8:HIS:NE2	2.54	0.40
2:D2:434:GLU:HA	2:D2:437:ILE:HD12	2.03	0.40
3:D3:289:LEU:CD2	3:D3:365:VAL:HG23	2.50	0.40
2:D4:298:PRO:HG2	2:D4:308:ARG:HH12	1.85	0.40
2:D6:4:VAL:HG12	2:D6:133:GLN:HB3	2.02	0.40
3:E3:153:SER:HB2	3:E3:191:GLN:HE22	1.86	0.40
3:E3:292:GLN:HG2	3:E3:298:ASN:ND2	2.36	0.40
3:E5:139:LEU:HA	3:E5:145:SER:HB2	2.03	0.40
2:E6:324:VAL:HA	2:E6:325:PRO:HD3	1.89	0.40
3:E7:117:LEU:HD11	3:E7:154:LYS:HB3	2.03	0.40
2:E8:157:LEU:HD23	2:E8:157:LEU:HA	1.96	0.40
3:E9:259:PRO:HB2	3:E9:260:PHE:CD1	2.56	0.40
2:A0:88:HIS:CE1	2:A0:90:GLU:HG3	2.57	0.40
2:A2:172:TRP:N	2:A2:204:LEU:O	2.48	0.40
3:A3:167:PHE:CE2	3:A3:233:MET:HG3	2.56	0.40
3:A5:297:LYS:HB3	3:A5:297:LYS:HE3	1.94	0.40
3:A5:392:LYS:HG3	3:A5:392:LYS:O	2.21	0.40
3:A9:326:VAL:O	3:A9:330:MET:HG2	2.21	0.40
2:B8:172:TRP:HE1	2:B8:391:MET:HE2	1.85	0.40
3:C1:164:MET:H	3:C1:197:ASP:HB3	1.85	0.40
3:C3:21:TRP:CH2	3:C3:61:PRO:HB3	2.56	0.40
3:C5:313:ALA:HA	3:C5:369:GLY:HA2	2.02	0.40
2:C6:191:THR:HA	2:C6:194:LEU:HB3	2.03	0.40
2:C8:323:VAL:CG1	2:C8:355:ILE:HG23	2.48	0.40
3:C9:170:PHE:CD1	3:C9:171:PRO:HD2	2.55	0.40
3:D1:66:MET:CE	3:D1:151:LEU:HD22	2.51	0.40
3:D5:124:ALA:HA	3:D5:130:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D5:164:MET:HE3	3:D5:164:MET:HB2	2.01	0.40
2:D6:425:LEU:HD12	2:D6:425:LEU:HA	1.98	0.40
3:D7:192:LEU:HD21	3:D7:199:VAL:HG11	2.04	0.40
2:D8:238:LEU:CD1	2:D8:255:PHE:HE2	2.33	0.40
2:D8:285:GLN:HB2	2:E2:56:THR:CA	2.24	0.40
3:E3:28:HIS:ND1	3:E3:43:GLN:O	2.53	0.40
3:E3:87:PRO:HA	3:E3:90:PHE:HD1	1.86	0.40
2:E8:11:GLN:HG3	2:E8:74:VAL:HG21	2.04	0.40
2:E8:70:LEU:HD21	2:E8:114:ILE:HG21	2.03	0.40
2:E8:322:ASP:O	2:E8:373:ARG:NE	2.54	0.40
1:18:245:SER:HB3	1:18:248:ARG:HD3	2.03	0.40
2:A0:5:ILE:HG23	2:A0:5:ILE:HD12	1.82	0.40
2:A8:107:HIS:HE1	2:A8:151:CYS:SG	2.44	0.40
3:B1:249:ASP:H	3:B1:252:LYS:HB2	1.86	0.40
3:B3:47:ILE:HD12	3:B3:47:ILE:HA	1.98	0.40
3:B5:324:LYS:HB2	3:B5:324:LYS:HE3	1.64	0.40
3:B7:11:GLN:HA	3:B7:72:THR:HG21	2.03	0.40
2:C0:414:GLU:N	2:C0:414:GLU:OE2	2.54	0.40
3:C1:86:ARG:HD2	3:C1:88:ASP:HB2	2.04	0.40
2:C2:119:LEU:HD23	2:C2:119:LEU:HA	1.83	0.40
3:C3:128:ASP:N	3:C3:128:ASP:OD1	2.53	0.40
3:C5:391:ARG:O	2:C6:262:TYR:OH	2.40	0.40
3:D3:176:SER:HB2	2:D4:349:THR:CG2	2.51	0.40
3:D5:318:ARG:HB3	3:D5:357:PRO:HA	2.02	0.40
2:D8:11:GLN:NE2	3:D9:245:GLN:O	2.55	0.40
2:D8:401:LYS:NZ	3:D9:344:TRP:HB3	2.37	0.40
3:E1:291:GLN:OE1	3:E5:122:LYS:HE2	2.20	0.40
2:E2:1:MET:N	2:E2:3:GLU:OE2	2.43	0.40
2:E2:36:MET:HE2	2:E2:36:MET:HB3	1.75	0.40
3:E3:215:LEU:HD23	3:E3:215:LEU:HA	1.96	0.40
3:E9:207:LEU:HD13	3:E9:225:LEU:HB3	2.02	0.40
3:E9:311:LEU:HD12	3:E9:342:VAL:HG11	2.02	0.40
3:F1:6:HIS:CD2	3:F1:134:GLN:HE21	2.40	0.40
3:F1:165:GLU:HG3	3:F1:165:GLU:O	2.22	0.40
3:F1:327:ASP:HA	3:F1:330:MET:HE1	2.02	0.40
2:A0:221:ARG:CB	3:A1:325:GLU:HB3	2.51	0.40
3:A1:72:THR:O	3:A1:75:SER:OG	2.27	0.40
3:A1:282:ARG:HA	3:A5:86:ARG:HH12	1.86	0.40
3:A3:414:ASN:C	3:A3:414:ASN:HD22	2.25	0.40
3:A5:406:MET:HA	3:A5:409:THR:HG22	2.04	0.40
3:A7:54:ALA:C	3:A7:56:GLY:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A7:281:TYR:CZ	3:B1:83:GLN:O	2.74	0.40
3:A7:362:LYS:HA	3:A7:362:LYS:HE2	2.04	0.40
3:A9:156:ARG:HH21	3:A9:164:MET:HB2	1.87	0.40
2:B2:262:TYR:CB	2:B2:263:PRO:HD2	2.49	0.40
3:B3:46:ARG:HE	3:B3:46:ARG:HB2	1.56	0.40
2:B6:407:TRP:HZ2	3:B7:258:ILE:HD11	1.87	0.40
3:B9:139:LEU:HA	3:B9:145:SER:HB3	2.04	0.40
2:C2:209:ILE:HA	2:C2:212:ILE:HG22	2.03	0.40
2:C6:395:PHE:HZ	2:C6:418:PHE:HB3	1.85	0.40
2:C8:164:LYS:O	2:C8:166:LYS:NZ	2.54	0.40
3:D1:316:MET:HG3	3:D1:352:SER:OG	2.21	0.40
3:D7:176:SER:HB3	3:D7:181:GLU:OE1	2.22	0.40
2:E0:155:GLU:HG3	2:E0:197:HIS:NE2	2.36	0.40
2:E0:282:TYR:HB3	2:E4:60:LYS:CE	2.52	0.40
2:E2:96:LYS:HE3	3:E3:1:MET:H2	1.86	0.40
3:E3:46:ARG:HH21	3:E3:46:ARG:HG2	1.87	0.40
3:E3:295:ASP:OD2	3:E3:297:LYS:HG2	2.21	0.40
2:E4:276:ILE:HG23	2:E4:281:ALA:HB2	2.03	0.40
2:E8:211:ASP:OD1	2:E8:211:ASP:N	2.53	0.40
2:F0:60:LYS:O	2:F0:61:HIS:ND1	2.54	0.40
2:F0:112:LYS:HB3	2:F0:112:LYS:HE3	1.85	0.40
1:16:254:LYS:H	1:16:254:LYS:HG2	1.66	0.40
1:18:250:GLU:OE1	2:E4:229:ARG:NH2	2.54	0.40
1:7:243:ALA:HB3	3:B9:356:ILE:HG23	2.03	0.40
2:A2:156:ARG:HD3	2:A2:156:ARG:HA	1.67	0.40
2:A2:356:ASN:OD1	2:A2:357:TYR:N	2.54	0.40
3:A3:86:ARG:HA	3:A3:87:PRO:HD3	1.97	0.40
2:A8:28:HIS:HD2	2:A8:53:PHE:HE2	1.70	0.40
2:B0:9:VAL:HG13	2:B0:139:ASN:HB3	2.04	0.40
2:B0:69:ASP:OD1	2:B0:70:LEU:N	2.55	0.40
2:B6:430:LYS:HB3	2:B6:430:LYS:HE3	1.88	0.40
2:B8:73:THR:HG23	3:B9:46:ARG:HH12	1.85	0.40
2:C2:214:ARG:O	2:C2:214:ARG:NH1	2.54	0.40
3:C5:258:ILE:HA	3:C5:259:PRO:HD3	1.94	0.40
3:C7:253:LEU:HD12	3:C7:253:LEU:HA	1.86	0.40
2:D2:93:ILE:HG23	2:D2:117:LEU:HD23	2.03	0.40
2:D2:138:PHE:HZ	2:D2:235:ILE:HD13	1.86	0.40
2:D2:217:LEU:HD11	2:D2:275:ILE:CG2	2.50	0.40
2:D4:11:GLN:HE22	3:D5:246:LEU:CD1	2.35	0.40
2:D8:207:GLU:HA	2:D8:210:TYR:HB2	2.03	0.40
2:E2:430:LYS:HE2	2:E2:430:LYS:HB3	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E9:272:PRO:HD2	3:E9:361:LEU:HD13	2.04	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	20/351 (6%)	19 (95%)	1 (5%)	0	100 100
1	1	20/351 (6%)	18 (90%)	2 (10%)	0	100 100
1	10	20/351 (6%)	17 (85%)	3 (15%)	0	100 100
1	11	20/351 (6%)	16 (80%)	4 (20%)	0	100 100
1	12	20/351 (6%)	19 (95%)	1 (5%)	0	100 100
1	13	20/351 (6%)	18 (90%)	2 (10%)	0	100 100
1	14	20/351 (6%)	19 (95%)	1 (5%)	0	100 100
1	15	20/351 (6%)	18 (90%)	2 (10%)	0	100 100
1	16	20/351 (6%)	20 (100%)	0	0	100 100
1	17	20/351 (6%)	20 (100%)	0	0	100 100
1	18	20/351 (6%)	18 (90%)	2 (10%)	0	100 100
1	19	20/351 (6%)	19 (95%)	1 (5%)	0	100 100
1	2	20/351 (6%)	18 (90%)	2 (10%)	0	100 100
1	20	20/351 (6%)	17 (85%)	3 (15%)	0	100 100
1	21	20/351 (6%)	18 (90%)	1 (5%)	1 (5%)	2 20
1	22	18/351 (5%)	16 (89%)	2 (11%)	0	100 100
1	23	18/351 (5%)	15 (83%)	3 (17%)	0	100 100
1	3	20/351 (6%)	18 (90%)	1 (5%)	1 (5%)	2 20
1	4	20/351 (6%)	20 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	6	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	7	20/351 (6%)	20 (100%)	0	0	100	100
1	8	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	9	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
2	A0	424/453 (94%)	398 (94%)	26 (6%)	0	100	100
2	A2	424/453 (94%)	405 (96%)	18 (4%)	1 (0%)	47	81
2	A4	424/453 (94%)	393 (93%)	31 (7%)	0	100	100
2	A6	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
2	A8	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
2	B0	424/453 (94%)	400 (94%)	24 (6%)	0	100	100
2	B2	424/453 (94%)	405 (96%)	19 (4%)	0	100	100
2	B4	424/453 (94%)	408 (96%)	16 (4%)	0	100	100
2	B6	424/453 (94%)	405 (96%)	19 (4%)	0	100	100
2	B8	424/453 (94%)	400 (94%)	24 (6%)	0	100	100
2	C0	424/453 (94%)	402 (95%)	21 (5%)	1 (0%)	47	81
2	C2	424/453 (94%)	399 (94%)	24 (6%)	1 (0%)	47	81
2	C4	424/453 (94%)	386 (91%)	37 (9%)	1 (0%)	47	81
2	C6	424/453 (94%)	397 (94%)	27 (6%)	0	100	100
2	C8	424/453 (94%)	396 (93%)	28 (7%)	0	100	100
2	D0	424/453 (94%)	401 (95%)	23 (5%)	0	100	100
2	D2	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
2	D4	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
2	D6	424/453 (94%)	408 (96%)	16 (4%)	0	100	100
2	D8	424/453 (94%)	407 (96%)	17 (4%)	0	100	100
2	E0	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
2	E2	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
2	E4	424/453 (94%)	399 (94%)	25 (6%)	0	100	100
2	E6	424/453 (94%)	399 (94%)	24 (6%)	1 (0%)	47	81
2	E8	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
2	F0	424/453 (94%)	401 (95%)	23 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A1	424/449 (94%)	397 (94%)	27 (6%)	0	100	100
3	A3	424/449 (94%)	399 (94%)	24 (6%)	1 (0%)	47	81
3	A5	424/449 (94%)	388 (92%)	34 (8%)	2 (0%)	29	69
3	A7	424/449 (94%)	397 (94%)	26 (6%)	1 (0%)	47	81
3	A9	424/449 (94%)	400 (94%)	23 (5%)	1 (0%)	47	81
3	B1	424/449 (94%)	401 (95%)	22 (5%)	1 (0%)	47	81
3	B3	424/449 (94%)	400 (94%)	22 (5%)	2 (0%)	29	69
3	B5	424/449 (94%)	394 (93%)	28 (7%)	2 (0%)	29	69
3	B7	424/449 (94%)	396 (93%)	28 (7%)	0	100	100
3	B9	424/449 (94%)	407 (96%)	17 (4%)	0	100	100
3	C1	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	C3	424/449 (94%)	396 (93%)	27 (6%)	1 (0%)	47	81
3	C5	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	C7	424/449 (94%)	396 (93%)	28 (7%)	0	100	100
3	C9	424/449 (94%)	396 (93%)	27 (6%)	1 (0%)	47	81
3	D1	424/449 (94%)	399 (94%)	24 (6%)	1 (0%)	47	81
3	D3	424/449 (94%)	395 (93%)	28 (7%)	1 (0%)	47	81
3	D5	424/449 (94%)	396 (93%)	28 (7%)	0	100	100
3	D7	424/449 (94%)	399 (94%)	24 (6%)	1 (0%)	47	81
3	D9	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	E1	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	E3	424/449 (94%)	402 (95%)	21 (5%)	1 (0%)	47	81
3	E5	424/449 (94%)	392 (92%)	32 (8%)	0	100	100
3	E7	424/449 (94%)	397 (94%)	26 (6%)	1 (0%)	47	81
3	E9	424/449 (94%)	388 (92%)	36 (8%)	0	100	100
3	F1	424/449 (94%)	389 (92%)	34 (8%)	1 (0%)	47	81
4	a	146/220 (66%)	135 (92%)	11 (8%)	0	100	100
4	b	146/220 (66%)	137 (94%)	9 (6%)	0	100	100
4	c	197/220 (90%)	188 (95%)	9 (5%)	0	100	100
4	d	197/220 (90%)	179 (91%)	18 (9%)	0	100	100
4	e	197/220 (90%)	183 (93%)	13 (7%)	1 (0%)	29	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	f	197/220 (90%)	184 (93%)	13 (7%)	0	100 100
4	g	197/220 (90%)	185 (94%)	11 (6%)	1 (0%)	29 69
4	h	197/220 (90%)	183 (93%)	14 (7%)	0	100 100
4	i	197/220 (90%)	186 (94%)	11 (6%)	0	100 100
4	j	197/220 (90%)	184 (93%)	13 (7%)	0	100 100
4	m	197/220 (90%)	180 (91%)	17 (9%)	0	100 100
4	n	197/220 (90%)	186 (94%)	11 (6%)	0	100 100
4	o	197/220 (90%)	179 (91%)	18 (9%)	0	100 100
4	p	197/220 (90%)	182 (92%)	15 (8%)	0	100 100
4	q	197/220 (90%)	187 (95%)	10 (5%)	0	100 100
4	r	197/220 (90%)	185 (94%)	12 (6%)	0	100 100
4	s	197/220 (90%)	179 (91%)	18 (9%)	0	100 100
4	t	197/220 (90%)	184 (93%)	13 (7%)	0	100 100
4	u	197/220 (90%)	189 (96%)	7 (4%)	1 (0%)	29 69
4	v	197/220 (90%)	183 (93%)	14 (7%)	0	100 100
5	k	133/189 (70%)	127 (96%)	6 (4%)	0	100 100
5	l	133/189 (70%)	128 (96%)	5 (4%)	0	100 100
5	w	139/189 (74%)	133 (96%)	6 (4%)	0	100 100
5	x	139/189 (74%)	129 (93%)	10 (7%)	0	100 100
All	All	26906/37032 (73%)	25298 (94%)	1580 (6%)	28 (0%)	54 86

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A3	179	VAL
3	A5	55	THR
3	A7	55	THR
3	B3	55	THR
3	C3	179	VAL
3	D1	179	VAL
3	D3	55	THR
1	3	251	TYR
3	B1	55	THR
3	B5	55	THR
3	A9	179	VAL

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Mol	Chain	Res	Type
2	C4	89	PRO
3	C9	55	THR
3	E3	55	THR
2	E6	81	GLY
4	e	60	ASN
3	B5	336	LYS
2	C2	58	ALA
3	D7	320	ARG
3	E7	55	THR
3	F1	171	PRO
1	21	253	ALA
3	B3	128	ASP
2	C0	83	TYR
4	u	154	TYR
2	A2	32	PRO
4	g	51	PRO
3	A5	259	PRO

5.3.2 Protein sidechains (i)

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	20/304 (7%)	20 (100%)	0	100 100
1	1	20/304 (7%)	19 (95%)	1 (5%)	24 49
1	10	20/304 (7%)	20 (100%)	0	100 100
1	11	20/304 (7%)	19 (95%)	1 (5%)	24 49
1	12	20/304 (7%)	18 (90%)	2 (10%)	7 26
1	13	20/304 (7%)	19 (95%)	1 (5%)	24 49
1	14	20/304 (7%)	19 (95%)	1 (5%)	24 49
1	15	20/304 (7%)	20 (100%)	0	100 100
1	16	20/304 (7%)	20 (100%)	0	100 100
1	17	20/304 (7%)	19 (95%)	1 (5%)	24 49
1	18	20/304 (7%)	18 (90%)	2 (10%)	7 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	19	20/304 (7%)	17 (85%)	3 (15%)	3 15
1	2	20/304 (7%)	20 (100%)	0	100 100
1	20	20/304 (7%)	20 (100%)	0	100 100
1	21	20/304 (7%)	19 (95%)	1 (5%)	24 49
1	22	18/304 (6%)	17 (94%)	1 (6%)	21 46
1	23	18/304 (6%)	18 (100%)	0	100 100
1	3	20/304 (7%)	19 (95%)	1 (5%)	24 49
1	4	20/304 (7%)	18 (90%)	2 (10%)	7 26
1	5	20/304 (7%)	19 (95%)	1 (5%)	24 49
1	6	20/304 (7%)	19 (95%)	1 (5%)	24 49
1	7	20/304 (7%)	20 (100%)	0	100 100
1	8	20/304 (7%)	20 (100%)	0	100 100
1	9	20/304 (7%)	20 (100%)	0	100 100
2	A0	359/379 (95%)	349 (97%)	10 (3%)	43 65
2	A2	359/379 (95%)	354 (99%)	5 (1%)	67 80
2	A4	359/379 (95%)	350 (98%)	9 (2%)	47 68
2	A6	359/379 (95%)	349 (97%)	10 (3%)	43 65
2	A8	359/379 (95%)	356 (99%)	3 (1%)	81 89
2	B0	359/379 (95%)	350 (98%)	9 (2%)	47 68
2	B2	359/379 (95%)	351 (98%)	8 (2%)	52 71
2	B4	359/379 (95%)	354 (99%)	5 (1%)	67 80
2	B6	359/379 (95%)	355 (99%)	4 (1%)	73 84
2	B8	359/379 (95%)	353 (98%)	6 (2%)	60 78
2	C0	359/379 (95%)	355 (99%)	4 (1%)	73 84
2	C2	359/379 (95%)	354 (99%)	5 (1%)	67 80
2	C4	359/379 (95%)	352 (98%)	7 (2%)	57 75
2	C6	359/379 (95%)	351 (98%)	8 (2%)	52 71
2	C8	359/379 (95%)	352 (98%)	7 (2%)	57 75
2	D0	359/379 (95%)	352 (98%)	7 (2%)	57 75
2	D2	359/379 (95%)	351 (98%)	8 (2%)	52 71
2	D4	359/379 (95%)	350 (98%)	9 (2%)	47 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D6	359/379 (95%)	353 (98%)	6 (2%)	60	78
2	D8	359/379 (95%)	351 (98%)	8 (2%)	52	71
2	E0	359/379 (95%)	357 (99%)	2 (1%)	86	92
2	E2	359/379 (95%)	352 (98%)	7 (2%)	57	75
2	E4	359/379 (95%)	354 (99%)	5 (1%)	67	80
2	E6	359/379 (95%)	351 (98%)	8 (2%)	52	71
2	E8	359/379 (95%)	357 (99%)	2 (1%)	86	92
2	F0	359/379 (95%)	353 (98%)	6 (2%)	60	78
3	A1	364/381 (96%)	360 (99%)	4 (1%)	73	84
3	A3	364/381 (96%)	358 (98%)	6 (2%)	62	79
3	A5	364/381 (96%)	356 (98%)	8 (2%)	52	71
3	A7	364/381 (96%)	357 (98%)	7 (2%)	57	75
3	A9	364/381 (96%)	359 (99%)	5 (1%)	67	80
3	B1	364/381 (96%)	359 (99%)	5 (1%)	67	80
3	B3	364/381 (96%)	358 (98%)	6 (2%)	62	79
3	B5	364/381 (96%)	358 (98%)	6 (2%)	62	79
3	B7	364/381 (96%)	358 (98%)	6 (2%)	62	79
3	B9	364/381 (96%)	359 (99%)	5 (1%)	67	80
3	C1	364/381 (96%)	357 (98%)	7 (2%)	57	75
3	C3	364/381 (96%)	360 (99%)	4 (1%)	73	84
3	C5	364/381 (96%)	356 (98%)	8 (2%)	52	71
3	C7	364/381 (96%)	354 (97%)	10 (3%)	44	65
3	C9	364/381 (96%)	358 (98%)	6 (2%)	62	79
3	D1	364/381 (96%)	356 (98%)	8 (2%)	52	71
3	D3	364/381 (96%)	358 (98%)	6 (2%)	62	79
3	D5	364/381 (96%)	351 (96%)	13 (4%)	35	59
3	D7	364/381 (96%)	356 (98%)	8 (2%)	52	71
3	D9	364/381 (96%)	357 (98%)	7 (2%)	57	75
3	E1	364/381 (96%)	359 (99%)	5 (1%)	67	80
3	E3	364/381 (96%)	354 (97%)	10 (3%)	44	65
3	E5	364/381 (96%)	361 (99%)	3 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	E7	364/381 (96%)	358 (98%)	6 (2%)	62 79
3	E9	364/381 (96%)	361 (99%)	3 (1%)	81 89
3	F1	364/381 (96%)	360 (99%)	4 (1%)	73 84
4	a	130/190 (68%)	125 (96%)	5 (4%)	33 57
4	b	130/190 (68%)	128 (98%)	2 (2%)	65 80
4	c	174/190 (92%)	170 (98%)	4 (2%)	50 70
4	d	174/190 (92%)	168 (97%)	6 (3%)	37 60
4	e	174/190 (92%)	169 (97%)	5 (3%)	42 64
4	f	174/190 (92%)	169 (97%)	5 (3%)	42 64
4	g	174/190 (92%)	171 (98%)	3 (2%)	60 78
4	h	174/190 (92%)	168 (97%)	6 (3%)	37 60
4	i	174/190 (92%)	171 (98%)	3 (2%)	60 78
4	j	174/190 (92%)	171 (98%)	3 (2%)	60 78
4	m	174/190 (92%)	169 (97%)	5 (3%)	42 64
4	n	174/190 (92%)	169 (97%)	5 (3%)	42 64
4	o	174/190 (92%)	165 (95%)	9 (5%)	23 48
4	p	174/190 (92%)	170 (98%)	4 (2%)	50 70
4	q	174/190 (92%)	168 (97%)	6 (3%)	37 60
4	r	174/190 (92%)	167 (96%)	7 (4%)	31 55
4	s	174/190 (92%)	169 (97%)	5 (3%)	42 64
4	t	174/190 (92%)	171 (98%)	3 (2%)	60 78
4	u	174/190 (92%)	170 (98%)	4 (2%)	50 70
4	v	174/190 (92%)	167 (96%)	7 (4%)	31 55
5	k	122/164 (74%)	118 (97%)	4 (3%)	38 61
5	l	122/164 (74%)	119 (98%)	3 (2%)	47 68
5	w	127/164 (77%)	122 (96%)	5 (4%)	32 56
5	x	127/164 (77%)	124 (98%)	3 (2%)	49 69
All	All	23164/31512 (74%)	22699 (98%)	465 (2%)	57 74

All (465) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	252	VAL

Continued on next page...

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Mol	Chain	Res	Type
1	11	246	CYS
1	12	248	ARG
1	12	256	LEU
1	13	248	ARG
1	14	256	LEU
1	17	248	ARG
1	18	248	ARG
1	18	256	LEU
1	19	238	THR
1	19	248	ARG
1	19	256	LEU
1	21	256	LEU
1	22	248	ARG
1	3	241	PHE
1	4	248	ARG
1	4	254	LYS
1	5	248	ARG
1	6	254	LYS
2	A0	119	LEU
2	A0	163	LYS
2	A0	221	ARG
2	A0	285	GLN
2	A0	290	GLU
2	A0	336	LYS
2	A0	370	LYS
2	A0	397	LEU
2	A0	401	LYS
2	A0	430	LYS
3	A1	179	VAL
3	A1	306	ARG
3	A1	362	LYS
3	A1	379	LYS
2	A2	163	LYS
2	A2	336	LYS
2	A2	372	MET
2	A2	401	LYS
2	A2	402	ARG
3	A3	11	GLN
3	A3	174	LYS
3	A3	298	ASN
3	A3	320	ARG
3	A3	347	ASN

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Mol	Chain	Res	Type
3	A3	414	ASN
2	A4	15	GLN
2	A4	60	LYS
2	A4	163	LYS
2	A4	251	ASP
2	A4	308	ARG
2	A4	338	LYS
2	A4	370	LYS
2	A4	372	MET
2	A4	401	LYS
3	A5	11	GLN
3	A5	99	ASN
3	A5	114	ASP
3	A5	125	GLU
3	A5	190	HIS
3	A5	350	LYS
3	A5	379	LYS
3	A5	391	ARG
2	A6	2	ARG
2	A6	60	LYS
2	A6	163	LYS
2	A6	254	GLU
2	A6	308	ARG
2	A6	326	LYS
2	A6	370	LYS
2	A6	401	LYS
2	A6	413	MET
2	A6	430	LYS
3	A7	11	GLN
3	A7	73	MET
3	A7	122	LYS
3	A7	247	ASN
3	A7	297	LYS
3	A7	330	MET
3	A7	336	LYS
2	A8	120	ASP
2	A8	401	LYS
2	A8	402	ARG
3	A9	174	LYS
3	A9	221	THR
3	A9	324	LYS
3	A9	380	ARG

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Mol	Chain	Res	Type
3	A9	391	ARG
2	B0	92	LEU
2	B0	96	LYS
2	B0	98	ASP
2	B0	156	ARG
2	B0	163	LYS
2	B0	308	ARG
2	B0	336	LYS
2	B0	372	MET
2	B0	430	LYS
3	B1	252	LYS
3	B1	276	ARG
3	B1	280	GLN
3	B1	350	LYS
3	B1	362	LYS
2	B2	2	ARG
2	B2	156	ARG
2	B2	163	LYS
2	B2	196	GLU
2	B2	297	GLU
2	B2	370	LYS
2	B2	393	HIS
2	B2	430	LYS
3	B3	122	LYS
3	B3	162	ARG
3	B3	256	ASN
3	B3	280	GLN
3	B3	298	ASN
3	B3	306	ARG
2	B4	163	LYS
2	B4	224	TYR
2	B4	253	THR
2	B4	264	ARG
2	B4	336	LYS
3	B5	16	ILE
3	B5	162	ARG
3	B5	298	ASN
3	B5	320	ARG
3	B5	324	LYS
3	B5	336	LYS
2	B6	285	GLN
2	B6	308	ARG

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Mol	Chain	Res	Type
2	B6	326	LYS
2	B6	339	ARG
3	B7	11	GLN
3	B7	122	LYS
3	B7	147	MET
3	B7	256	ASN
3	B7	282	ARG
3	B7	324	LYS
2	B8	11	GLN
2	B8	96	LYS
2	B8	124	LYS
2	B8	308	ARG
2	B8	397	LEU
2	B8	401	LYS
3	B9	46	ARG
3	B9	122	LYS
3	B9	162	ARG
3	B9	177	ASP
3	B9	379	LYS
2	C0	96	LYS
2	C0	112	LYS
2	C0	221	ARG
2	C0	370	LYS
3	C1	83	GLN
3	C1	174	LYS
3	C1	251	ARG
3	C1	276	ARG
3	C1	297	LYS
3	C1	320	ARG
3	C1	324	LYS
2	C2	96	LYS
2	C2	163	LYS
2	C2	256	GLN
2	C2	353	CYS
2	C2	372	MET
3	C3	95	THR
3	C3	122	LYS
3	C3	297	LYS
3	C3	388	MET
2	C4	2	ARG
2	C4	124	LYS
2	C4	280	LYS

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Mol	Chain	Res	Type
2	C4	326	LYS
2	C4	390	ARG
2	C4	401	LYS
2	C4	422	ARG
3	C5	83	GLN
3	C5	131	GLN
3	C5	174	LYS
3	C5	213	ARG
3	C5	246	LEU
3	C5	297	LYS
3	C5	359	LYS
3	C5	405	GLU
2	C6	36	MET
2	C6	85	HIS
2	C6	112	LYS
2	C6	336	LYS
2	C6	339	ARG
2	C6	401	LYS
2	C6	422	ARG
2	C6	430	LYS
3	C7	88	ASP
3	C7	174	LYS
3	C7	276	ARG
3	C7	297	LYS
3	C7	306	ARG
3	C7	321	MET
3	C7	324	LYS
3	C7	334	GLN
3	C7	362	LYS
3	C7	379	LYS
2	C8	96	LYS
2	C8	163	LYS
2	C8	224	TYR
2	C8	311	LYS
2	C8	338	LYS
2	C8	352	LYS
2	C8	401	LYS
3	C9	154	LYS
3	C9	336	LYS
3	C9	343	GLU
3	C9	390	ARG
3	C9	424	GLN

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Mol	Chain	Res	Type
3	C9	426	GLN
2	D0	156	ARG
2	D0	215	ARG
2	D0	264	ARG
2	D0	339	ARG
2	D0	377	MET
2	D0	401	LYS
2	D0	402	ARG
3	D1	77	ARG
3	D1	99	ASN
3	D1	121	ARG
3	D1	134	GLN
3	D1	251	ARG
3	D1	276	ARG
3	D1	376	GLU
3	D1	391	ARG
2	D2	155	GLU
2	D2	163	LYS
2	D2	264	ARG
2	D2	297	GLU
2	D2	311	LYS
2	D2	339	ARG
2	D2	370	LYS
2	D2	401	LYS
3	D3	191	GLN
3	D3	204	ASN
3	D3	213	ARG
3	D3	343	GLU
3	D3	362	LYS
3	D3	391	ARG
2	D4	124	LYS
2	D4	156	ARG
2	D4	163	LYS
2	D4	214	ARG
2	D4	248	LEU
2	D4	285	GLN
2	D4	401	LYS
2	D4	430	LYS
2	D4	437	ILE
3	D5	2	ARG
3	D5	11	GLN
3	D5	46	ARG

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Mol	Chain	Res	Type
3	D5	112	LEU
3	D5	129	CYS
3	D5	209	ASP
3	D5	246	LEU
3	D5	298	ASN
3	D5	316	MET
3	D5	343	GLU
3	D5	391	ARG
3	D5	397	TRP
3	D5	410	GLU
2	D6	96	LYS
2	D6	163	LYS
2	D6	297	GLU
2	D6	338	LYS
2	D6	401	LYS
2	D6	430	LYS
3	D7	122	LYS
3	D7	154	LYS
3	D7	164	MET
3	D7	174	LYS
3	D7	306	ARG
3	D7	390	ARG
3	D7	391	ARG
3	D7	406	MET
2	D8	92	LEU
2	D8	96	LYS
2	D8	163	LYS
2	D8	214	ARG
2	D8	282	TYR
2	D8	297	GLU
2	D8	326	LYS
2	D8	430	LYS
3	D9	19	LYS
3	D9	32	PRO
3	D9	48	ASN
3	D9	128	ASP
3	D9	215	LEU
3	D9	276	ARG
3	D9	336	LYS
2	E0	96	LYS
2	E0	221	ARG
3	E1	11	GLN

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Mol	Chain	Res	Type
3	E1	122	LYS
3	E1	328	GLU
3	E1	390	ARG
3	E1	391	ARG
2	E2	89	PRO
2	E2	160	ASP
2	E2	163	LYS
2	E2	184	PRO
2	E2	338	LYS
2	E2	397	LEU
2	E2	430	LYS
3	E3	11	GLN
3	E3	46	ARG
3	E3	174	LYS
3	E3	247	ASN
3	E3	276	ARG
3	E3	320	ARG
3	E3	324	LYS
3	E3	362	LYS
3	E3	391	ARG
3	E3	406	MET
2	E4	97	GLU
2	E4	256	GLN
2	E4	280	LYS
2	E4	358	GLN
2	E4	401	LYS
3	E5	11	GLN
3	E5	306	ARG
3	E5	324	LYS
2	E6	101	ASN
2	E6	124	LYS
2	E6	163	LYS
2	E6	221	ARG
2	E6	280	LYS
2	E6	285	GLN
2	E6	338	LYS
2	E6	401	LYS
3	E7	174	LYS
3	E7	213	ARG
3	E7	297	LYS
3	E7	320	ARG
3	E7	347	ASN

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Mol	Chain	Res	Type
3	E7	362	LYS
2	E8	401	LYS
2	E8	430	LYS
3	E9	122	LYS
3	E9	174	LYS
3	E9	391	ARG
2	F0	96	LYS
2	F0	227	LEU
2	F0	280	LYS
2	F0	336	LYS
2	F0	401	LYS
2	F0	430	LYS
3	F1	122	LYS
3	F1	125	GLU
3	F1	177	ASP
3	F1	324	LYS
4	a	66	SER
4	a	97	ARG
4	a	117	ARG
4	a	126	ARG
4	a	196	LEU
4	b	126	ARG
4	b	176	ASP
4	c	52	GLU
4	c	126	ARG
4	c	151	MET
4	c	202	ARG
4	d	28	LYS
4	d	35	ASN
4	d	117	ARG
4	d	152	LYS
4	d	155	GLU
4	d	191	GLU
4	e	107	LYS
4	e	120	GLU
4	e	146	ARG
4	e	152	LYS
4	e	194	ARG
4	f	35	ASN
4	f	36	ILE
4	f	69	LYS
4	f	119	ARG

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Mol	Chain	Res	Type
4	f	194	ARG
4	g	13	GLU
4	g	126	ARG
4	g	194	ARG
4	h	15	ARG
4	h	28	LYS
4	h	117	ARG
4	h	126	ARG
4	h	194	ARG
4	h	198	ARG
4	i	117	ARG
4	i	119	ARG
4	i	194	ARG
4	j	4	PRO
4	j	178	ARG
4	j	202	ARG
5	k	52	VAL
5	k	78	LYS
5	k	98	LYS
5	k	103	LYS
5	l	52	VAL
5	l	103	LYS
5	l	163	LYS
4	m	28	LYS
4	m	97	ARG
4	m	99	MET
4	m	117	ARG
4	m	126	ARG
4	n	28	LYS
4	n	48	ILE
4	n	117	ARG
4	n	126	ARG
4	n	202	ARG
4	o	3	GLN
4	o	24	MET
4	o	63	ILE
4	o	91	PHE
4	o	117	ARG
4	o	126	ARG
4	o	151	MET
4	o	164	ARG
4	o	202	ARG

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Mol	Chain	Res	Type
4	p	56	LYS
4	p	126	ARG
4	p	152	LYS
4	p	185	ILE
4	q	48	ILE
4	q	56	LYS
4	q	97	ARG
4	q	117	ARG
4	q	126	ARG
4	q	202	ARG
4	r	24	MET
4	r	117	ARG
4	r	126	ARG
4	r	131	TRP
4	r	152	LYS
4	r	202	ARG
4	r	203	ASN
4	s	24	MET
4	s	63	ILE
4	s	126	ARG
4	s	152	LYS
4	s	202	ARG
4	t	126	ARG
4	t	173	ILE
4	t	194	ARG
4	u	28	LYS
4	u	119	ARG
4	u	125	HIS
4	u	126	ARG
4	v	3	GLN
4	v	69	LYS
4	v	94	ASN
4	v	117	ARG
4	v	126	ARG
4	v	197	LEU
4	v	202	ARG
5	w	25	ARG
5	w	58	LYS
5	w	78	LYS
5	w	156	ARG
5	w	160	ARG
5	x	85	ARG

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Mol	Chain	Res	Type
5	x	110	ARG
5	x	162	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (165) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	244	GLN
1	2	244	GLN
1	3	242	ASN
2	A0	228	ASN
2	A0	285	GLN
2	A0	406	HIS
3	A1	256	ASN
3	A1	426	GLN
2	A2	102	ASN
2	A2	133	GLN
2	A2	206	ASN
2	A2	216	ASN
2	A2	358	GLN
3	A3	347	ASN
3	A3	348	ASN
3	A3	414	ASN
3	A3	426	GLN
2	A4	186	ASN
3	A5	191	GLN
3	A5	329	GLN
2	A6	11	GLN
2	A6	128	ASN
2	A6	256	GLN
2	A6	283	HIS
3	A7	245	GLN
3	A7	247	ASN
3	A7	335	ASN
2	A8	11	GLN
2	A8	101	ASN
2	A8	107	HIS
3	A9	137	HIS
2	B0	11	GLN
2	B0	91	GLN
2	B0	233	GLN
2	B0	283	HIS
2	B2	11	GLN

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Mol	Chain	Res	Type
3	B3	6	HIS
3	B3	11	GLN
3	B3	99	ASN
3	B3	134	GLN
3	B3	347	ASN
2	B4	228	ASN
3	B5	99	ASN
3	B5	334	GLN
3	B5	347	ASN
3	B5	375	GLN
3	B7	105	HIS
2	B8	11	GLN
2	B8	258	ASN
3	B9	245	GLN
2	C0	258	ASN
2	C0	406	HIS
2	C2	11	GLN
2	C2	233	GLN
2	C2	256	GLN
2	C2	380	ASN
3	C3	14	ASN
3	C3	105	HIS
3	C3	191	GLN
2	C4	31	GLN
2	C4	133	GLN
3	C5	291	GLN
2	C6	168	ASN
3	C7	8	GLN
3	C7	245	GLN
2	C8	28	HIS
2	C8	101	ASN
2	C8	168	ASN
2	C8	206	ASN
3	C9	11	GLN
3	C9	99	ASN
3	C9	298	ASN
3	C9	334	GLN
3	C9	423	GLN
2	D0	18	ASN
2	D0	133	GLN
2	D0	139	ASN
2	D0	206	ASN

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Mol	Chain	Res	Type
2	D0	258	ASN
2	D0	283	HIS
2	D2	11	GLN
2	D2	88	HIS
2	D2	101	ASN
2	D2	293	ASN
3	D3	256	ASN
3	D3	347	ASN
3	D3	384	GLN
3	D3	396	HIS
2	D4	11	GLN
2	D4	18	ASN
2	D4	216	ASN
3	D5	256	ASN
3	D5	298	ASN
3	D5	347	ASN
2	D6	31	GLN
2	D6	176	GLN
3	D7	99	ASN
3	D7	191	GLN
3	D7	204	ASN
3	D9	6	HIS
3	D9	14	ASN
3	D9	134	GLN
3	D9	204	ASN
3	D9	291	GLN
3	E1	14	ASN
3	E1	99	ASN
2	E2	11	GLN
2	E4	11	GLN
2	E4	31	GLN
2	E4	256	GLN
2	E4	285	GLN
3	E5	6	HIS
3	E5	11	GLN
3	E5	256	ASN
2	E6	11	GLN
2	E6	101	ASN
3	E7	347	ASN
2	E8	133	GLN
3	E9	14	ASN
3	E9	204	ASN

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Mol	Chain	Res	Type
3	E9	256	ASN
3	E9	396	HIS
2	F0	18	ASN
2	F0	31	GLN
2	F0	258	ASN
3	F1	105	HIS
3	F1	134	GLN
3	F1	375	GLN
4	d	35	ASN
4	d	181	GLN
4	f	18	ASN
4	g	25	GLN
4	g	37	GLN
4	h	37	GLN
4	h	106	GLN
4	i	3	GLN
4	i	94	ASN
4	j	3	GLN
4	j	59	ASN
5	k	17	GLN
5	k	28	HIS
5	l	18	GLN
4	m	11	ASN
4	m	94	ASN
4	m	147	HIS
4	n	94	ASN
4	n	105	ASN
4	o	125	HIS
4	p	3	GLN
4	p	18	ASN
4	p	203	ASN
4	q	37	GLN
4	q	181	GLN
4	s	25	GLN
4	s	59	ASN
4	t	11	ASN
4	t	94	ASN
4	t	181	GLN
4	u	59	ASN
4	u	181	GLN
4	v	18	ASN
4	v	94	ASN

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Mol	Chain	Res	Type
5	w	155	GLN
5	x	55	GLN
5	x	137	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

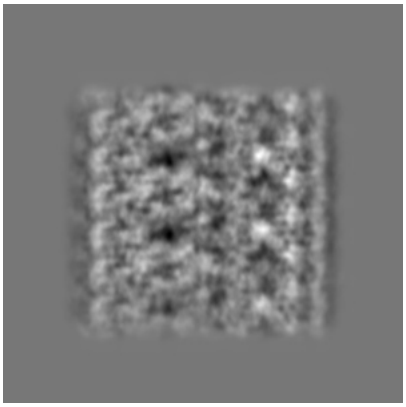
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26018. These allow visual inspection of the internal detail of the map and identification of artifacts.

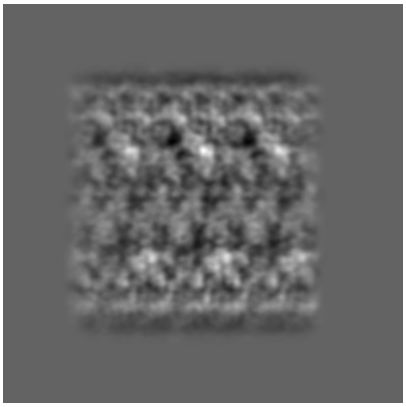
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

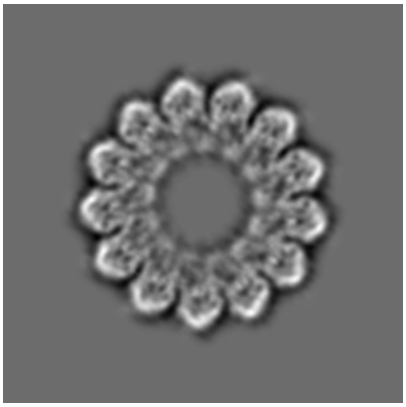
6.1.1 Primary map



X



Y

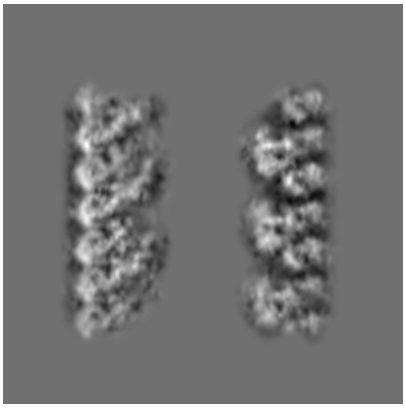


Z

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

6.2 Central slices

6.2.1 Primary map



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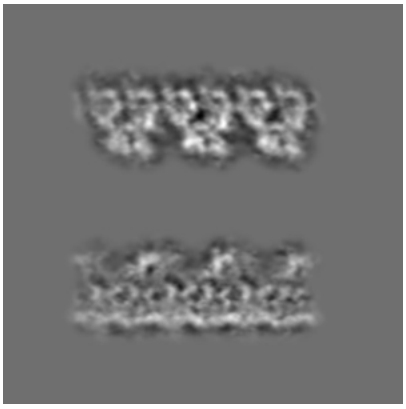
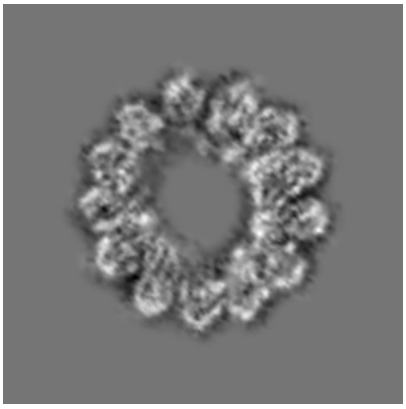


Y Index: 108

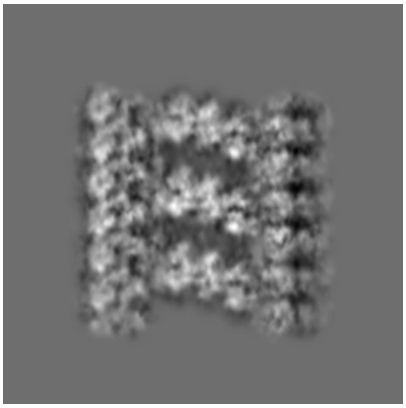


Z Index: 108

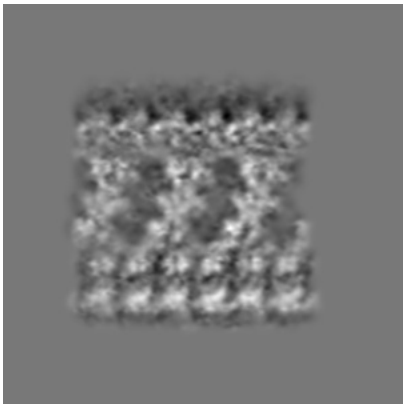
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 137



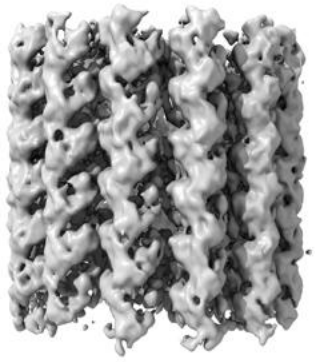
Y Index: 139

Z Index: 114

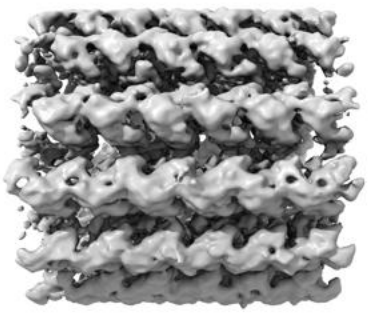
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

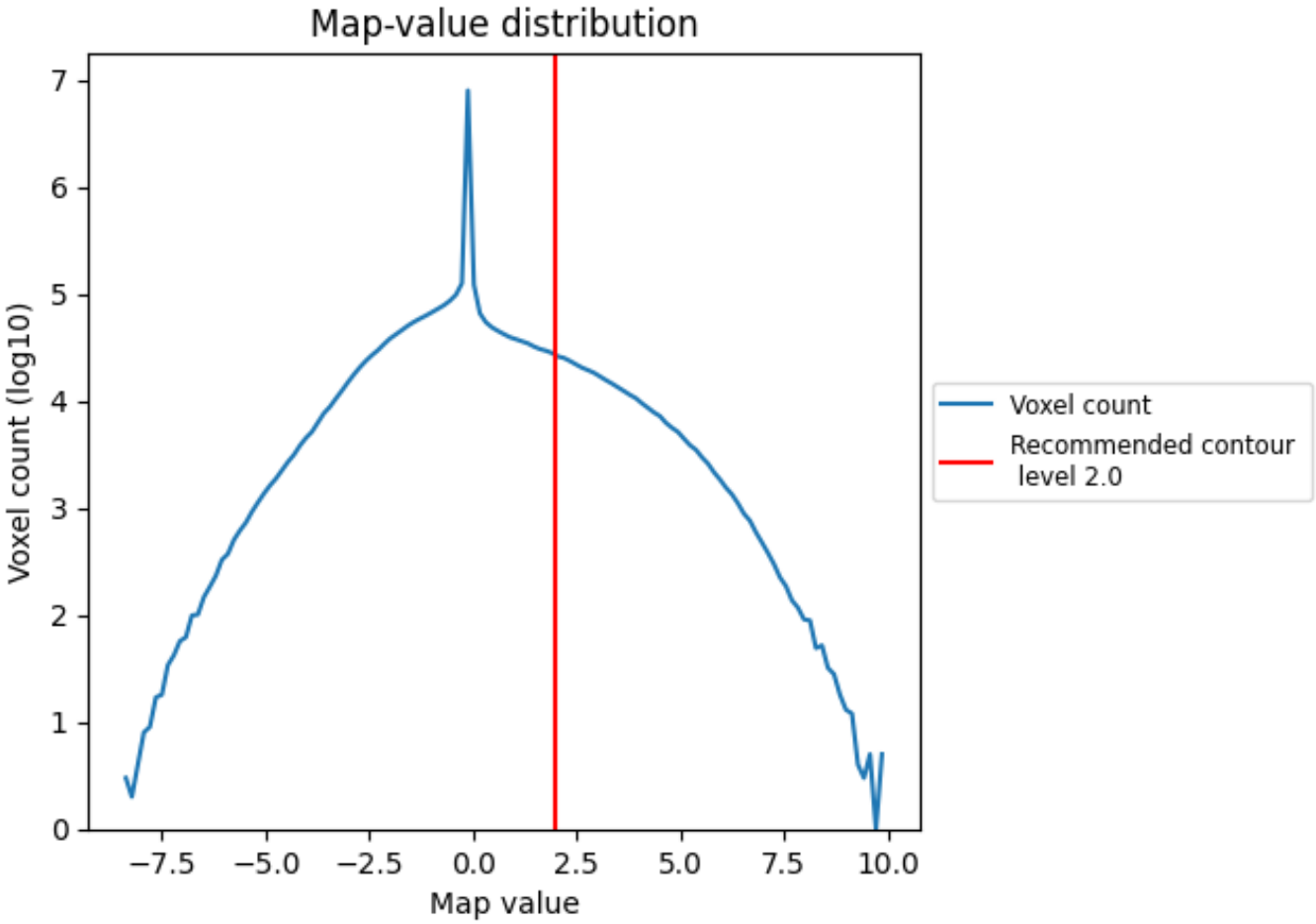
6.5 Mask visualisation (i)

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

7 Map analysis

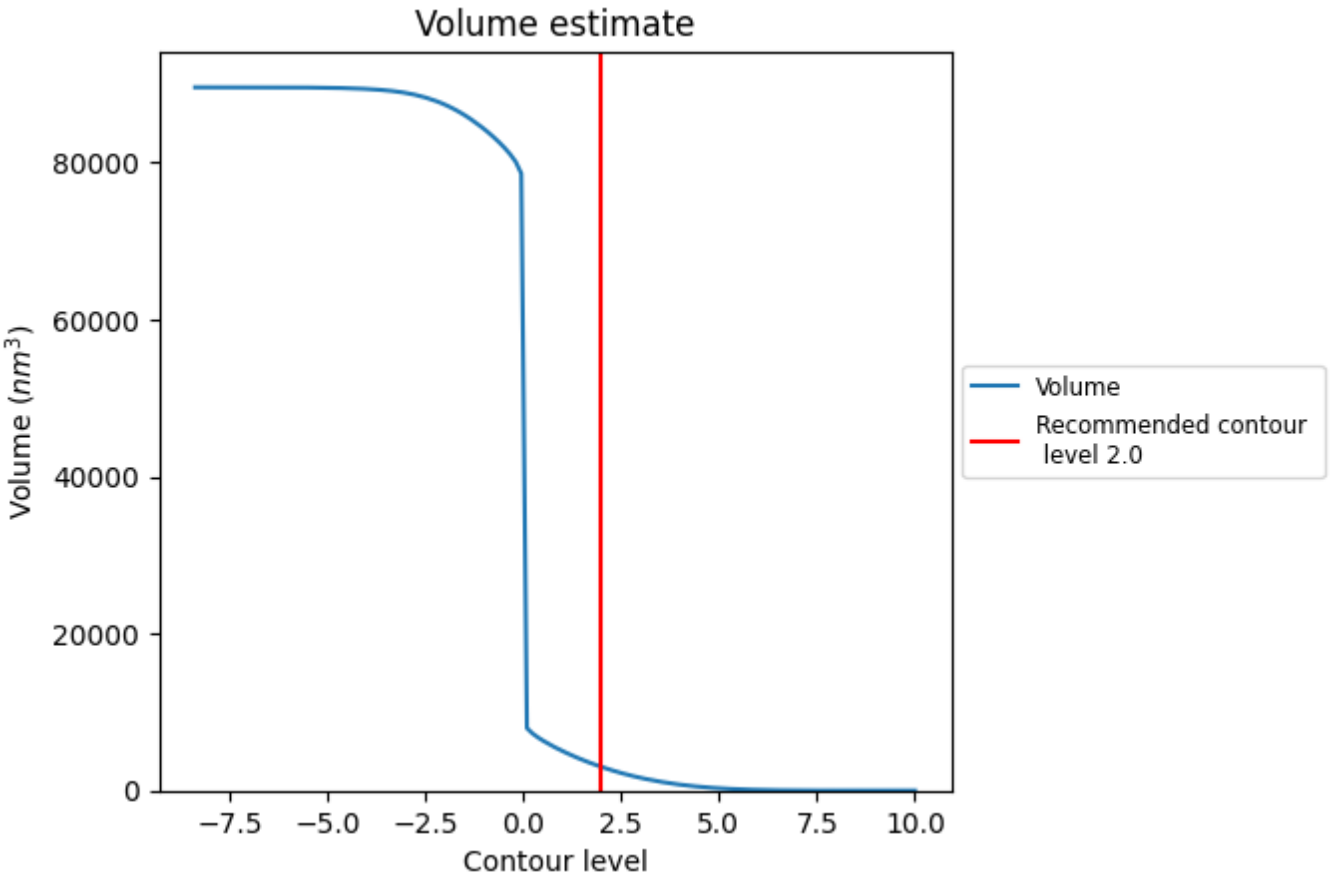
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

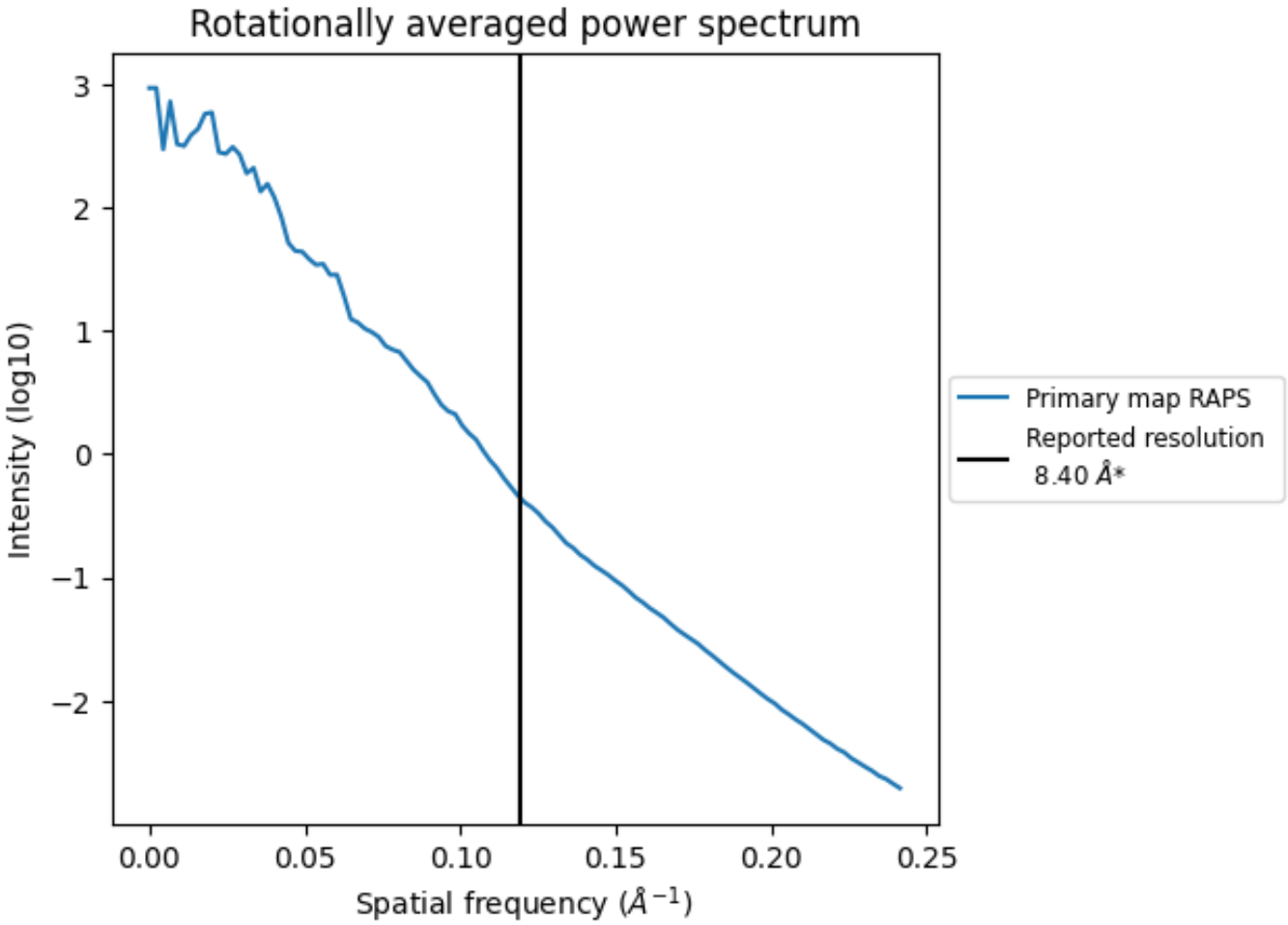
7.2 Volume estimate



The volume at the recommended contour level is 3015 nm^3; this corresponds to an approximate mass of 2724 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 (i)



*Reported resolution corresponds to spatial frequency of 0.119 $Å^{-1}$

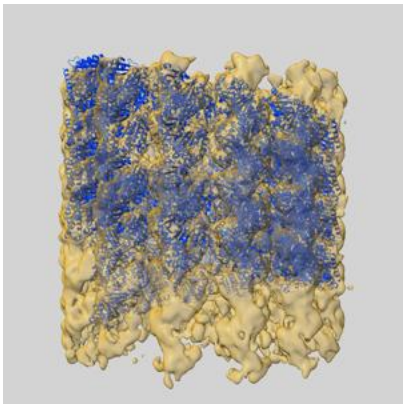
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

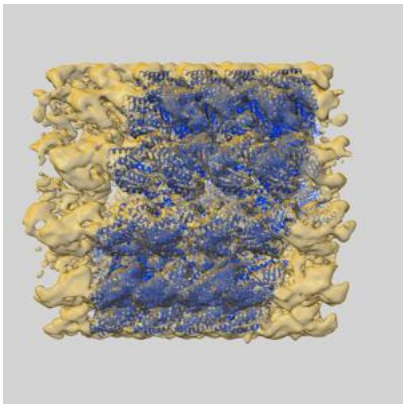
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26018 and PDB model 7TNQ. Per-residue inclusion information can be found in section 3 on page 13.

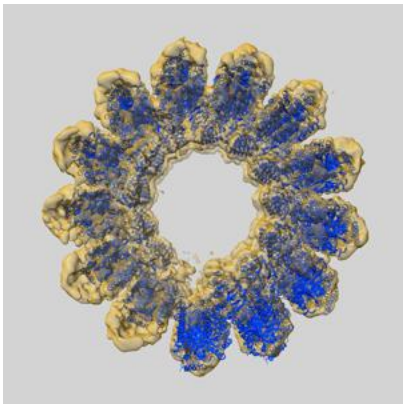
9.1 Map-model overlay



X



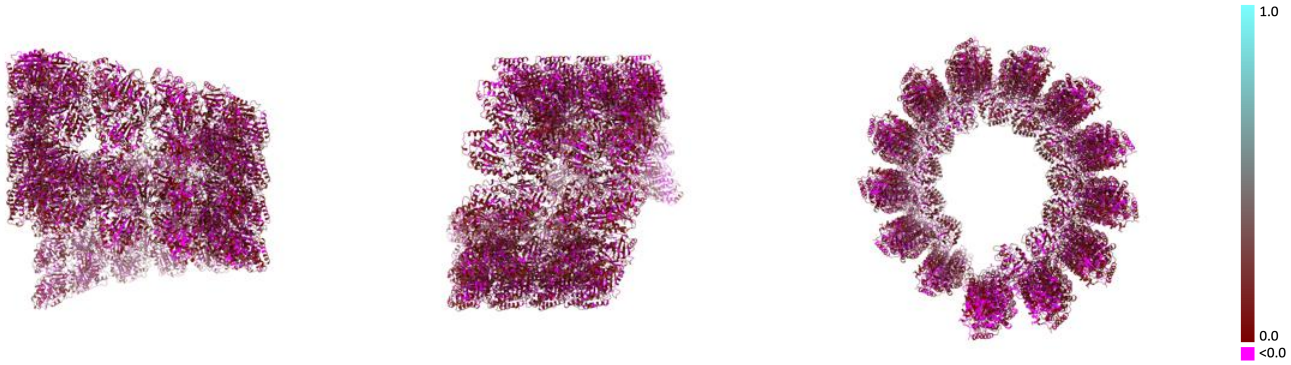
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

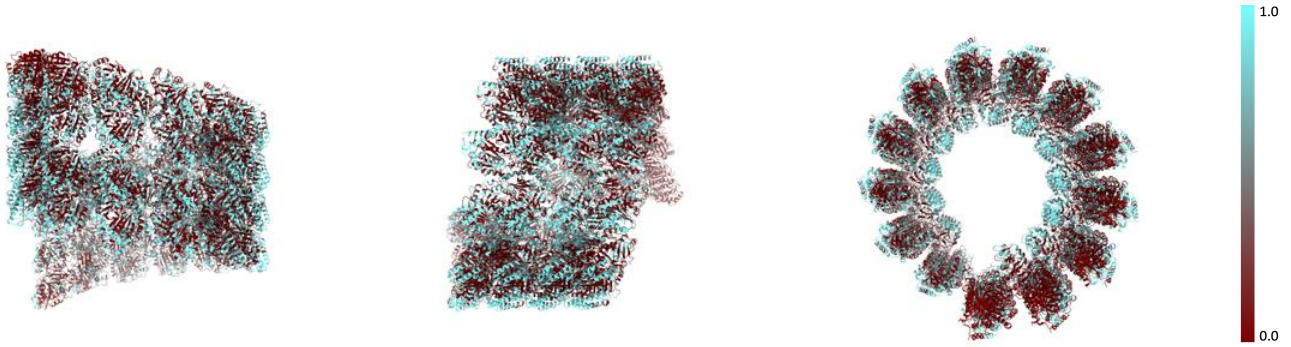
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

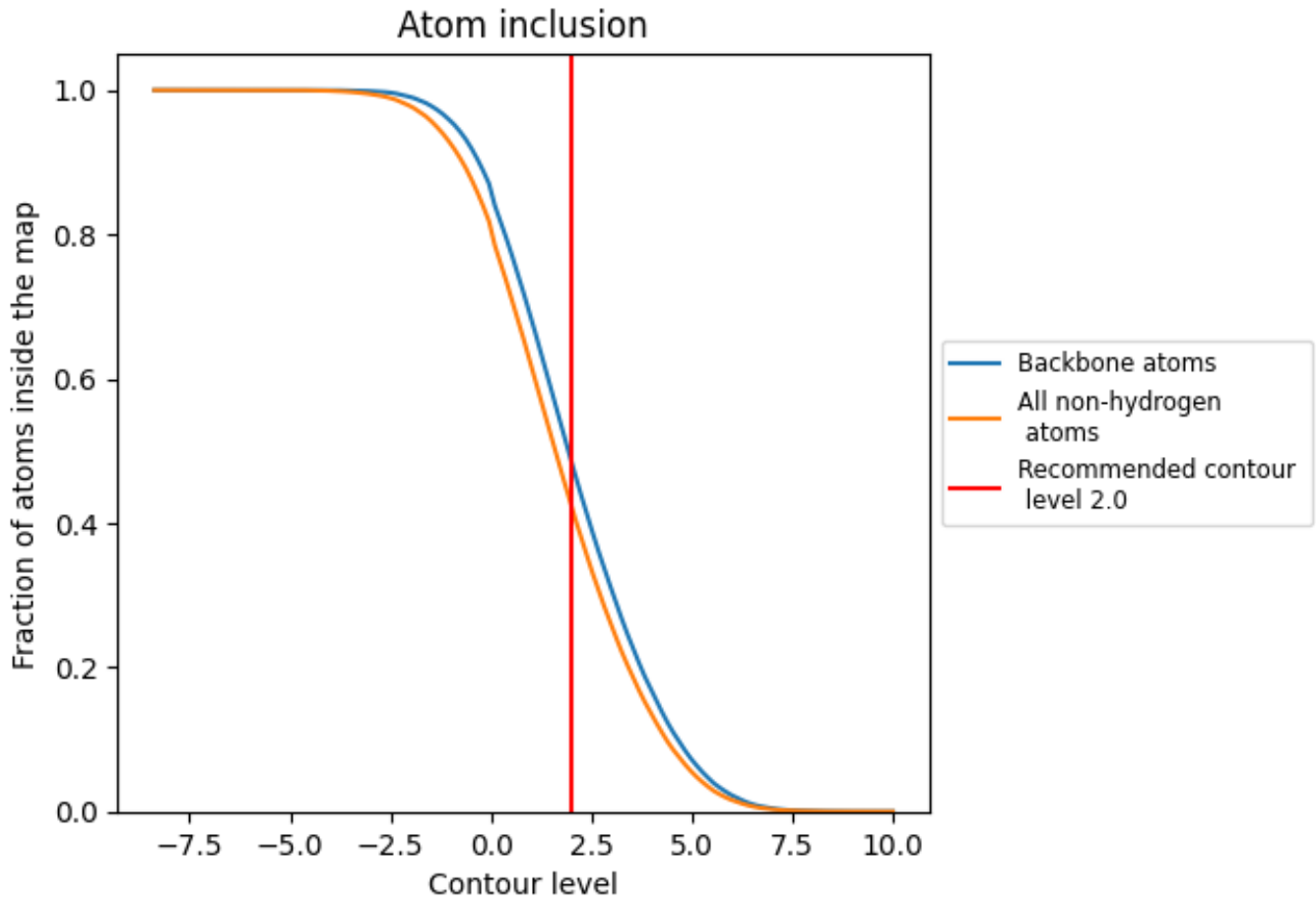
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (2.0).

9.4 Atom inclusion (i)



At the recommended contour level, 49% of all backbone atoms, 42% 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 (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4243	0.0760
0	0.1294	0.1680
1	0.0000	0.0940
10	0.0824	0.0720
11	0.0471	0.1110
12	0.1706	0.1250
13	0.1471	0.1000
14	0.0176	0.0900
15	0.0941	0.1000
16	0.1353	0.1160
17	0.2588	0.1140
18	0.1824	0.0380
19	0.2412	0.0440
2	0.1118	0.1250
20	0.1412	0.0080
21	0.4235	0.0670
22	0.0192	0.0960
23	0.0128	0.1160
3	0.0647	0.1040
4	0.1294	0.1020
5	0.1176	0.1400
6	0.1294	0.0710
7	0.1471	0.1150
8	0.0765	0.0500
9	0.0294	0.0540
A0	0.4571	0.0780
A1	0.4221	0.0750
A2	0.4213	0.0760
A3	0.2961	0.0730
A4	0.4697	0.0730
A5	0.4627	0.0750
A6	0.4378	0.0780
A7	0.3429	0.0670
A8	0.4372	0.0720
A9	0.4450	0.0830

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Chain	Atom inclusion	Q-score
B0	0.4225	0.0810
B1	0.3686	0.0780
B2	0.4203	0.0800
B3	0.4477	0.0790
B4	0.4344	0.0810
B5	0.3970	0.0760
B6	0.4145	0.0790
B7	0.5223	0.0920
B8	0.4770	0.0920
B9	0.4334	0.0850
C0	0.4228	0.0770
C1	0.5342	0.0910
C2	0.4688	0.0920
C3	0.4728	0.0890
C4	0.4007	0.0880
C5	0.4716	0.0910
C6	0.4547	0.0830
C7	0.4462	0.0890
C8	0.3753	0.0630
C9	0.4450	0.0740
D0	0.4292	0.0600
D1	0.3939	0.0560
D2	0.3459	0.0480
D3	0.4022	0.0600
D4	0.4093	0.0630
D5	0.3915	0.0520
D6	0.3358	0.0680
D7	0.4163	0.0710
D8	0.4197	0.0730
D9	0.4306	0.0690
E0	0.2843	0.0700
E1	0.4704	0.0890
E2	0.4412	0.0810
E3	0.4963	0.0820
E4	0.1811	0.0390
E5	0.4743	0.0670
E6	0.4782	0.0800
E7	0.5309	0.0850
E8	0.1176	-0.0050
E9	0.4117	0.0750
F0	0.4418	0.0840
F1	0.5003	0.0860

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Chain	Atom inclusion	Q-score
a	0.3479	0.1010
b	0.2641	0.0810
c	0.4898	0.1010
d	0.3898	0.0780
e	0.5522	0.0950
f	0.4873	0.0930
g	0.5363	0.0850
h	0.5172	0.0850
i	0.4535	0.0550
j	0.4624	0.0640
k	0.4653	0.0850
l	0.4770	0.0960
m	0.4803	0.0800
n	0.5185	0.1010
o	0.5299	0.0910
p	0.5650	0.1010
q	0.5510	0.0870
r	0.5860	0.1040
s	0.5573	0.0850
t	0.6025	0.0800
u	0.4427	0.0570
v	0.5675	0.0740
w	0.1919	0.0270
x	0.2875	0.0190